スクリーニング委員会による化合物評価データ

（2001年1月から2002年12月までに登録された化合物）

凡例

構造式（天然物粗抽出物の場合は、origin および抽出法などを記載）

JCI.No

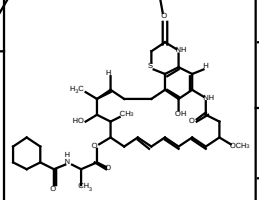
供給者コード（注）

化合物名

評価結果

10055	87
Thiazinotrienomycin E	

1 2 3 4 5 6 7 8 9
☒☐☒☒☒☒☒☒☒



1	2	3	4	5	6	7	8	9
HCC panel	P388	PK	Topo.	Tub.	p-Gp	Inv.	Angio.	Apo.
YES		NO	NO	NO	NO	NO	NO	YES
GI50 -7.04	T/C% (mg/kg)	spec.	I	mode				
Delta 0.69	( )	Y1 M1	—					
			II					
Range 2.29			±					

実施したスクリーニング
1 HCC panel：ヒト培養癌細胞パネル
2 P388：マウスP388白血病
3 PK：プロテインキナーゼ阻害
4 Topo.：トポイソメラーゼ阻害
5 Tub.：チューブリン阻害
6 p-Gp：制がん剤耐性克服
7 Inv.：基底膜浸潤阻害
8 Angio.：血管新生阻害
9 Apo.：アポトーシス誘導

Topoisomerase II

Topoisomerase I

Mode of action
poly.：チューブリンの重合阻害
depoly.：チューブリンの脱重合阻害

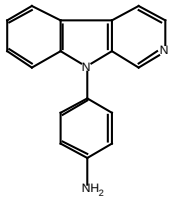
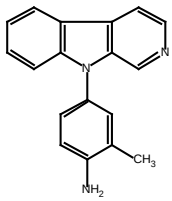
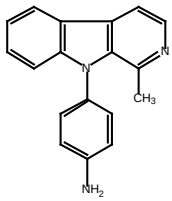
阻害されたキナーゼの種類
C：Cキナーゼ
Y：srcファミリーのチロシンキナーゼ
M：カルモジュリン依存性プロテインキナーゼ III
A：Aキナーゼ
E ：EGFレセプターチロシンキナーゼ
阻害の強さは 1 ～ 4 で表示し、2 以上のときにYES。

GI50：50%増殖阻害するモル濃度のLog値。但し（％）が付記されている場合は、% 濃度のLog値。
Delta、Range は判定基準参照

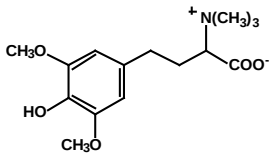
(注) サンプル提供者にご連絡をとりたい場合、スクリーニング委員会へご照会ください。

連絡先：http://www.jfcr.or.jp/cads/contact.html

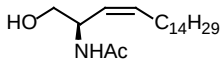
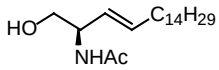
Alkaloid / Carboline

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11780	74		NO	NO	NO	NO		NO	NO	NO	NO	NO
9-(4'-aminophenyl)-9H-pyrido[3,4-b]indole (APNH)			GI50 -4.66	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.25		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒			Range 0.65		II —							
11781	74		NO	NO	NO	NO		NO	NO	NO	YES	NO
9-(4'-amino-3'-methylphenyl)-9H-pyrido[3,4-b]indole (AMPNH)			GI50 -4.71	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.46		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒			Range 0.75		II —							
11782	74		±	NO	NO	NO		NO	NO	NO	NO	NO
9-(4'-aminophenyl)-1-methyl-9H-pyrido[3,4-b]indole (APH)			GI50 -4.65	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.97		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒			Range 1.22		II —							

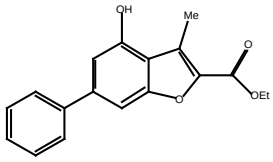
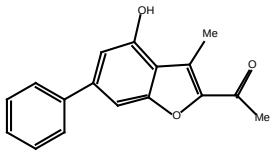
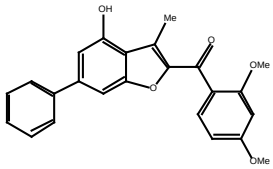
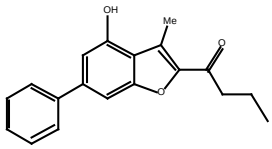
Amino acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11881	39		NO									
Sorolinine			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.12		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.12									

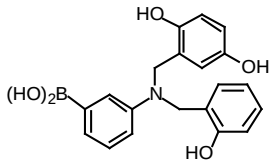
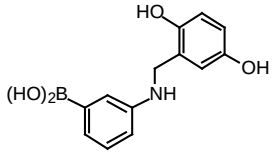
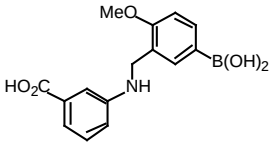
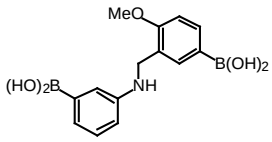
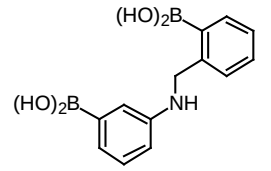
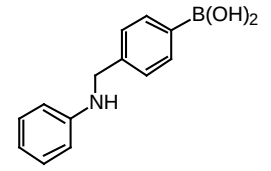
Aminoalcohol

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12243	41		NO									
(2R,3Z)-2-N-acetamino-3-octadecen-1-ol 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.77 Delta 0.22 Range 0.35	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
12244	41		NO									
(2R,3E)-2-N-acetamino-3-octadecen-1-ol 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.67 Delta 0.14 Range 0.81	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )

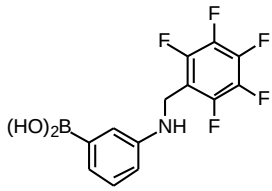
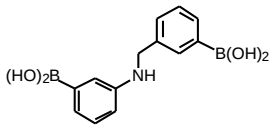
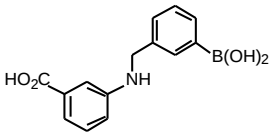
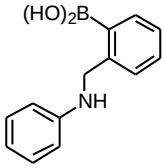
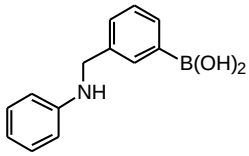
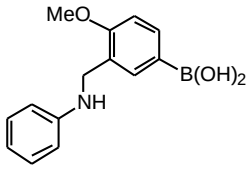
Benzofuran

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
10904	55		YES									
PFA-001			GI50 -6.31	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.09		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 2.4									
11324	55		YES*									
PFA-002			GI50 -5.63	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.09		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 2.72									
11325	55		YES									
PFA-003			GI50 -7.13	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.87		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 3.18									
11326	55		YES									
PFA-004			GI50 -5.15	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.69		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.84									

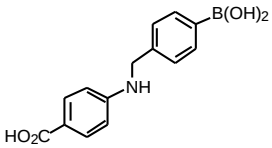
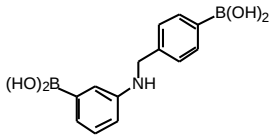
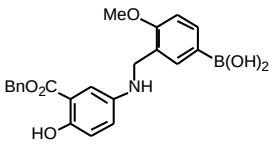
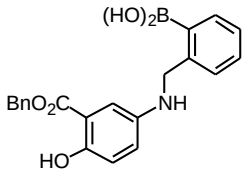
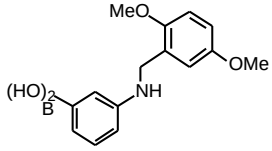
Boronic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11918	51		NO	NO								
TO-N-6-57			GI50 -4.61	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.22	A1 C1 M1 Y1 E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.52									
11919	51		NO	YES								
TO-N-6-55			GI50 -4.66	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.25	E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.71									
11920	51		NO	NO								
TO-N-6-61			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.53	A1 C1 M1 Y1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.56									
11921	51		NO	NO								
TO-N-6-59			GI50 -4.17	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.5		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.67									
11922	51		NO	NO								
TO-N-6-71			GI50 -4.07	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.6		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.67									
11923	51		NO	NO								
TO-N-6-51			GI50 -4.17	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.58		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.75									

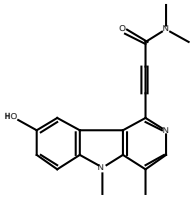
Boronic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11941	51		NO	NO								
TO-N-6-78			GI50 -4.77	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.22		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.34									
11942	51		NO	NO								
TO-N-6-73			GI50 -4.05	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.35		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.4									
11943	51		NO	YES								
TO-N-6-53			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.24	C1 M1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.25	E2								
12124	51			NO								
GN-6-O51			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12125	51			NO								
GN-6-M51			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12126	51			NO								
GN-6-75			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									

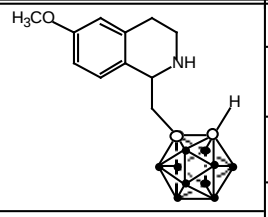
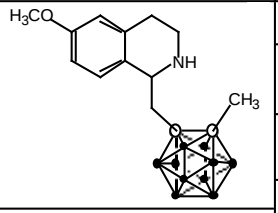
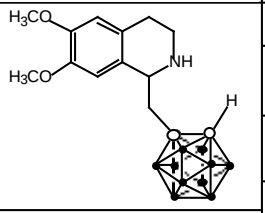
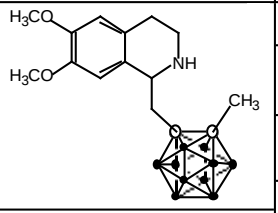
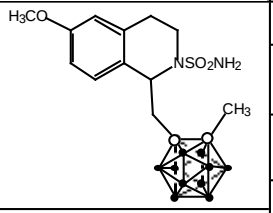
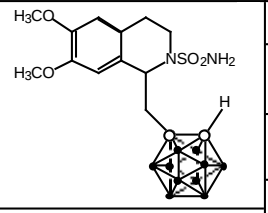
Boronic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12128	51			YES								
GN-6-53para			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	C1 M1 E2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12129	51			NO								
GN-6-73para			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12131	51			NO								
GN-6-83-Bn			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12132	51			NO								
GN-6-86-Bn			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12133	51			NO								
GN-7-47			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									

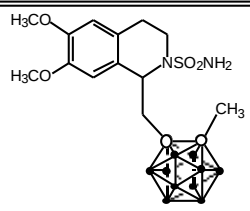
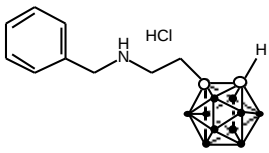
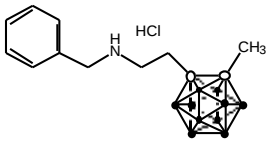
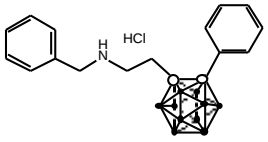
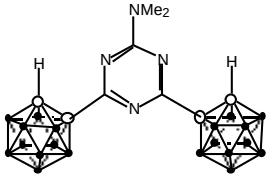
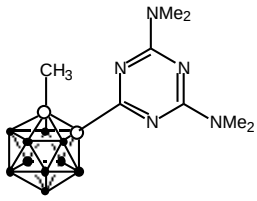
Carboline

JCI.No compound screening	sup. code	screening No.	1	2	3	4	5	6	7	8	9	10
		structure/comments	HCC panel	PK	Topo.	Tub.	HDAC.	p-Gp	Inv.	Angio.	Apo.	P388
11138	15		YES	NO	YES							
T-6403			GI50 -6.36	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.39	M1	—		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ □ □ □ □ □ □ □			Range 1.21		+							

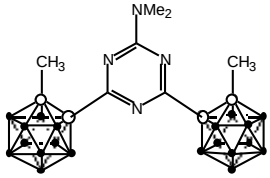
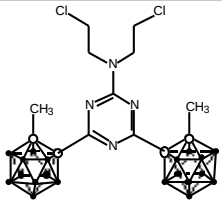
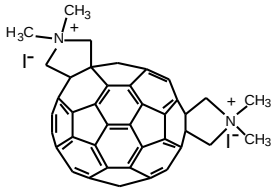
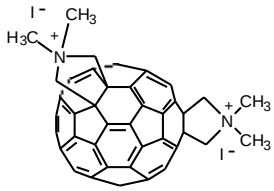
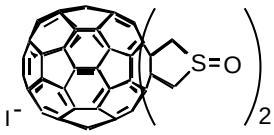
Carbon cluster

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12159	51		NO									
JD-001			GI50 -4.3	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.56		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.85									
12160	51		NO									
JD-002			GI50 -4.62	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.26		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.67									
12161	51		NO		NO	NO		NO	NO	NO	YES	
JD-003			GI50 -4.61	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.33		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 0.59		—							
12162	51		NO									
JD-004			GI50 -4.59	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.2		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.45									
12163	51		NO									
JD-005			GI50 -4.75	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.19		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.37									
12164	51		NO		NO	NO	NO	NO	NO	NO	NO	
JD-006			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0		— II		>1.2 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 0		—							

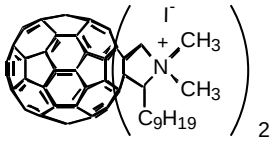
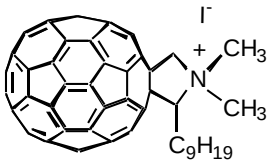
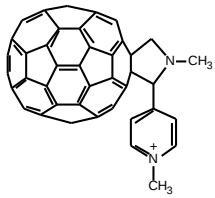
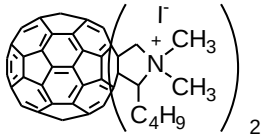
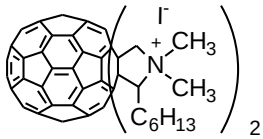
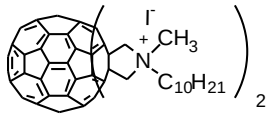
Carbon cluster

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12165	51		YES									
JD-007			GI50 -4.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.66		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.02									
12166	51		YES									
JD-011			GI50 -4.95	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.79		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.01									
12167	51		YES		NO	NO		NO	NO	NO	YES	
JD-012			GI50 -4.96	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.76		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 1.02		—							
12168	51		YES									
JD-013			GI50 -4.91	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.8		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1									
12169	51		±		+ / -	NO	NO	NO	NO	NO	YES	
TAZ-001			GI50 -4.08	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.34		± II		>1.2 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 1.42		—							
12170	51		NO									
TAZ-002			GI50 -4.49	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.24		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.73									

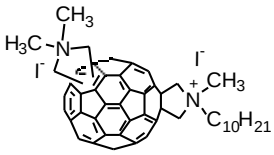
Carbon cluster

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12171	51		YES									
TAZ-006			GI50 -4.91	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.8		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 1									
12172	51		NO									
TAZ-008			GI50 -4.71	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.58		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 0.95									
11820	60		YES	NO	YES	NO						
KTM-1			GI50 -5.44	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.5	A1 C1 M1 Y1 E1	– II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ □			Range 0.87		++							
11821	60		YES	NO	YES	NO						
KTM-2			GI50 -5.18	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.39	A1 C1 M1 Y1 E1	– II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ □			Range 1.52		++							
11822	60		YES	NO	YES	NO						
KTM-3			GI50 -5.18	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.37	A1 C1 M1 Y1 E1	– II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ □			Range 1.55		++							
11823	60		NO									
KTM-4			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 0									

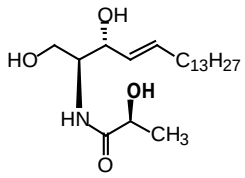
Carbon cluster

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11824	60		YES	NO	YES	NO						
KTM-5			GI50 -5.61	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.12	C1 Y1	+		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ □			Range 1.74	E1	II +							
11825	60		±									
KTM-6			GI50 -4.12	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.63		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 1.75									
11826	60		±									
KTM-7			GI50 -4.13	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.65		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 1.78									
12181	60		±	NO	YES	NO						
KTM-8			GI50 -5.42	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.28	C2 M2 Y2 A1 E2	++ II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ □			Range 0.9		++							
12182	60		YES	NO	YES	NO						
KTM-9			GI50 -5.48	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.29	C2 M2 Y2 A1 E2	+ II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ □			Range 0.92		++							
12183	60		YES	NO	+ / -	NO						
KTM-10			GI50 -4.79	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.78	A1 Y1	+ II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ □			Range 1.28	E2	±							

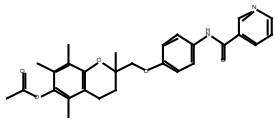
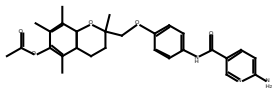
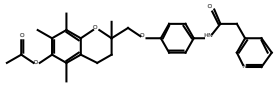
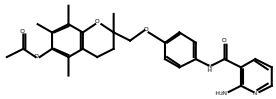
Carbon cluster

JCI.No compound screening	sup. code	screening No.	1	2	3	4	5	6	7	8	9	10
		structure/comments	HCC panel	PK	Topo.	Tub.	HDAC.	p-Gp	Inv.	Angio.	Apo.	P388
12184	60		YES	NO	YES	NO						
KTM-11			GI50 -4.74	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.73	A1 C1 M1 Y1 E2	++		( )					( )
			Range 1.47		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □					++							

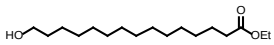
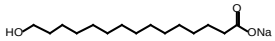
Ceramide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12242	41		YES	NO		NO						
(2S,3R,4E,2R)-2-(2'hydroxypropanoyl)-amino-octadec-4-en-1,3-diol			GI50 -5.43	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.47	C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.27									

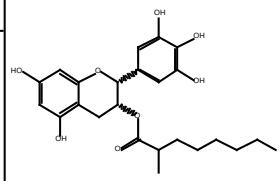
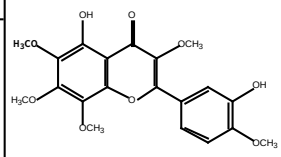
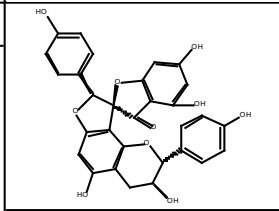
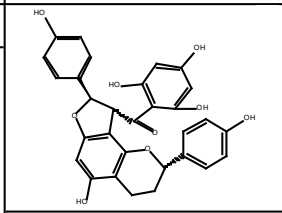
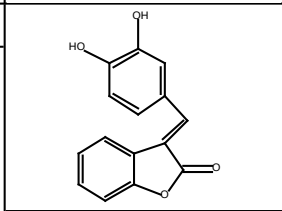
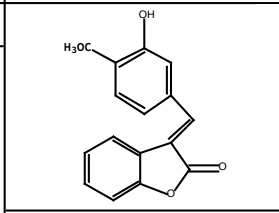
Chroman

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
10699	25		YES									
FT-1			GI50 -5.46	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.85		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.5									
10700	25		YES									
FT-2			GI50 -5.89	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.95		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.9									
10701	25		YES									
FT-3			GI50 -5.43	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.73		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 2.73									
10702	25		YES									
FT-4			GI50 -5.14	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.15		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 2.06									

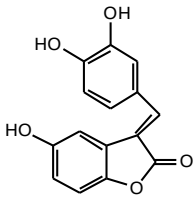
Fatty acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12032	46		NO			NO						
Ethyl 15-hydroxypentacl ecanoate 1 2 3 4 5 6 7 8 9 10 ☒ □ □ ☒ □ □ □ □ □ □			GI50 -4.53 Delta 0.32 Range 0.86	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
12037	46		NO									
Sodium 15-hydroxypentade canoate 1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			GI50 -4.17 Delta 0.73 Range 0.9	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )

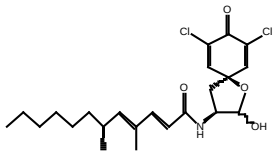
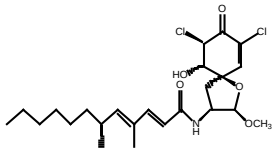
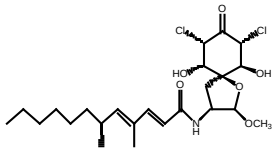
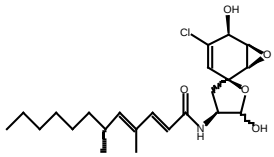
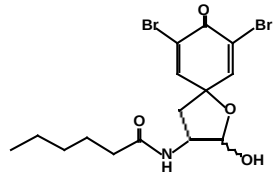
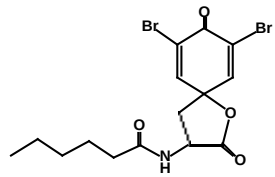
Flavonoid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11851	11		NO									
MO-EGC			GI50 -4.15	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.51		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.66									
10704	15		YES	NO	NO	YES		NO	NO	NO	YES	
T-063			GI50 -7.17	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.83	A1	— II	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 3.42		—							
12137	20		NO									
Dophnodorin I			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.27		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.28									
12139	20		NO									
Dophnodorin A			GI50 -4.24	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.31		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.55									
11953	37		NO	NO			NO				YES	
3',4'-Dihydroxy-Isoaurone			GI50 -4.08	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.6	A1 C1 M1 Y1 E1	II		711 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ ☒ □ □ □ ☒ □			Range 0.68									
11954	37		NO	NO			NO				YES	
3'-Hydroxy-4'-methoxy-Isoaurone			GI50 -4.09	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.64		II		>1 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ ☒ □ □ □ ☒ □			Range 0.72									

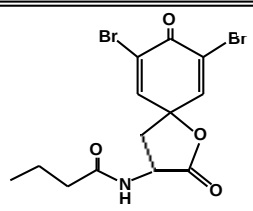
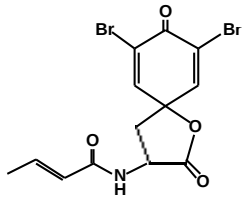
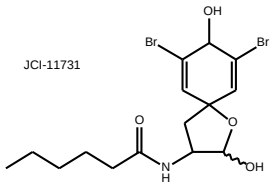
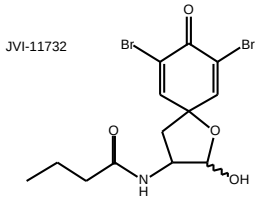
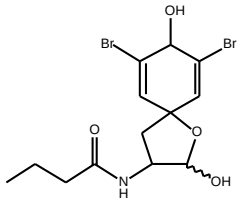
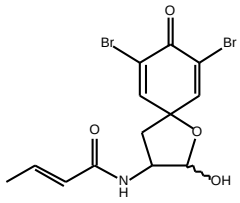
Flavonoid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12057	37		NO									
3',4',5-trihydroxy -isoaurone			GI50 -4.43	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.44		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.86									

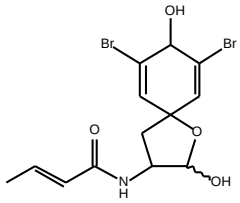
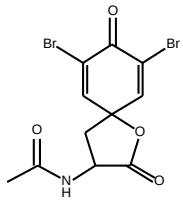
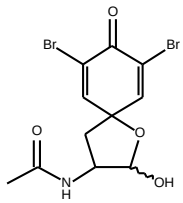
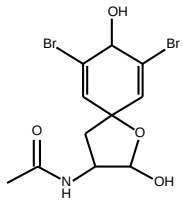
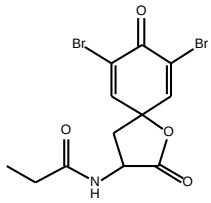
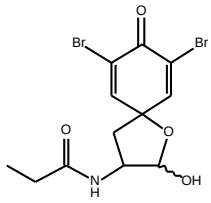
Gymnastatin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11253	52		YES*	YES	YES	YES		NO	YES	NO		NO
Gymnastatin A			GI50 -5.34	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.5	M2 Y2 A1	++	depoly	( )					( )
			Range 1.1		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ □ ☒		ユニークな化学構造			++							
11254	52		YES	NO	YES	YES		NO	+ / -	NO		
Gymnastatin B			GI50 -5.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.37		++	depoly	( )					( )
			Range 1.05		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ □ □		ユニークな化学構造			+							
11255	52		YES*	NO	YES			NO				
Gymnastatin C			GI50 -5.43	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.51		++		( )					( )
			Range 1.14		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ □ □ ☒ □ □ □ □		ユニークな化学構造			+							
11256	52		NO	NO	YES	NO		NO	+ / -	NO		
Gymnastatin D			GI50 -4.85	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.46	Y1	+		( )					( )
			Range 0.59	E1	II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ □ □		ユニークな化学構造			+							
11525	52		YES	YES	NO	YES		NO	NO	NO	YES	
Gym.analog 1			GI50 -5.46	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.41	M2 Y2 A1 C1	±	poly.	( )					( )
			Range 3.27		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □					−							
11526	52		YES	YES	YES	NO		NO	YES	NO	YES	
Gym.analog 2			GI50 -4.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.87	M2 Y2 A1 C1 E3	+		( )					( )
			Range 1.13		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □					−							

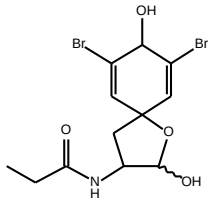
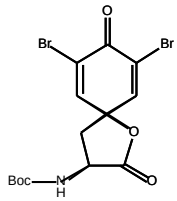
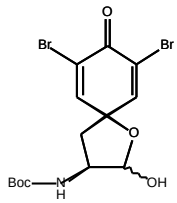
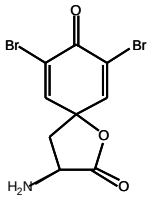
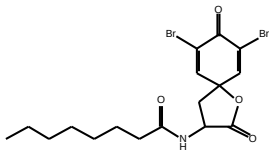
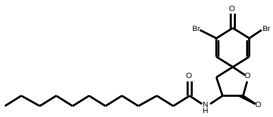
Gymnastatin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11527	52		NO	YES				NO				
Gym.analog 3			GI50 -4.63	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.29	Y2 A1 C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.91	E2								
11528	52		±	YES				NO	NO			
Gym.analog 4			GI50 -4.71	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.92	Y2 A1 C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ ☒ □ □ □			Range 2.32	E1								
11731	52		NO	NO				NO				
Gym.Analog-5			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.26		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.29									
11732	52		YES	YES				NO				
Gym.Analog-6			GI50 -4.67	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.15	Y3 C2 A1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.35									
11733	52		NO	NO				NO				
Gym.Analog-7			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.07		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.08									
11734	52		YES	YES				NO				
Gym.Analog-8			GI50 -4.69	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.12	Y3 C2 A1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.28	E1								

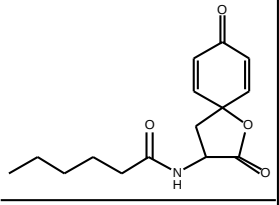
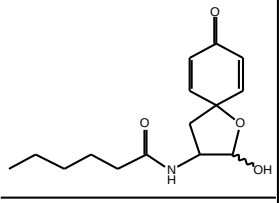
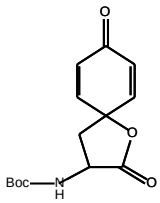
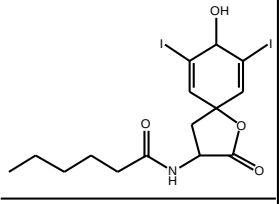
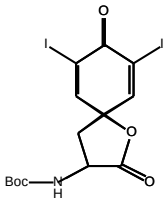
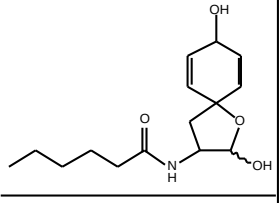
Gymnastatin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11735	52		NO	NO				NO				
Gym.Analog-9			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.14		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.14									
11736	52		NO	YES				NO				
Gym.Analog-10			GI50 -4.3	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.38	Y2 A1 C1 E2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.68									
11737	52		NO	YES				NO				
Gym.Analog-11			GI50 -4.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.13	Y3 C2 A1 E2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.61									
11738	52		NO	NO				NO				
Gym.Analog-12			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.05		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.05									
11739	52		NO	YES				NO				
Gym.Analog-13			GI50 -4.42	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.27	Y3 A2 C2 E2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.69									
11740	52		YES	YES				NO				
Gym.Analog-14			GI50 -4.68	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.13	Y3 C2 A1 E2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 0.33									

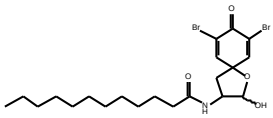
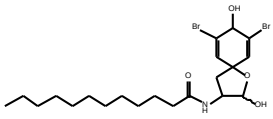
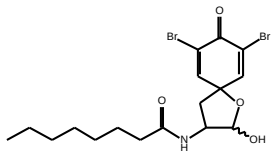
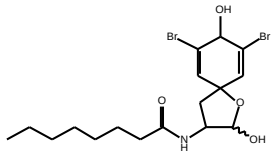
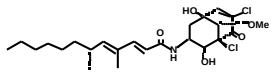
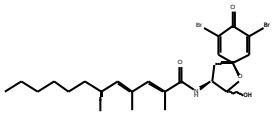
Gymnastatin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11752	52			NO				NO				
Gym.Analog-15			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ ⊠ □ □ □ □			Range									
11753	52			YES				NO				
Gym.Analog-16			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y2 A2 C2 M1 E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ ⊠ □ □ □ □			Range									
11754	52			YES				NO				
Gym.Analog-17			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y2 A1 C1 E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ ⊠ □ □ □ □			Range									
11756	52			NO				NO				
Gym.Analog-20			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ ⊠ □ □ □ □			Range									
11757	52			YES				NO				
Gym.Analog-21			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y2 C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ ⊠ □ □ □ □			Range									
11758	52			YES				NO				
Gym.Analog-22			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y2 A1 C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ ⊠ □ □ □ □			Range									

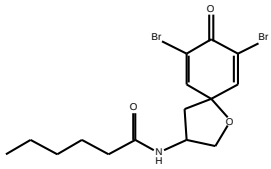
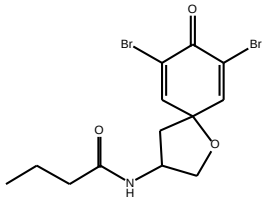
Gymnastatin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11759	52		YES	NO				NO	NO			
Gym.Analog-23			GI50 -4.98	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.57		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ ☒ □ □ □			Range 0.94	E1								
11760	52		YES	NO		NO		NO				
Gym.Analog-24			GI50 -5.08	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.72		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ ☒ □ ☒ □ □ □ □			Range 1.11									
11761	52			NO				NO				
Gym.Analog-26			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ ☒ □ □ □ □			Range	E1								
11762	52		NO	YES				NO	NO			
Gym.Analog-27			GI50 -4.73	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.46	A2 C2 Y2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ ☒ □ □ □			Range 0.74									
11763	52		YES	YES				NO				
Gym.Analog-28			GI50 -4.7	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.75	Y2 A1 C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ ☒ □ □ □ □			Range 1.45									
11785	52			NO				NO				
Gym.Analog-25			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ ☒ □ □ □ □			Range	E1								

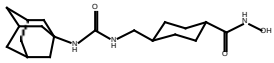
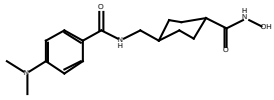
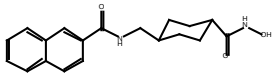
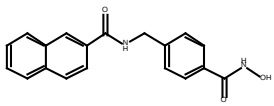
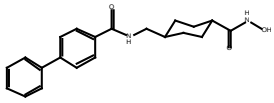
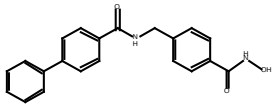
Gymnastatin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11786	52		YES*	YES		YES		NO				
Gym.Analog-29			GI50 -5.71	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.73	Y4 C2	II	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ ☒ □ ☒ □ □ □ □			Range 1.7									
11787	52			NO				NO				
Gym.Analog-30			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ ☒ □ □ □ □			Range									
11788	52		YES*	YES		YES		NO				
Gym.Analog-31			GI50 -5.37	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.59	Y1	II	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ ☒ □ ☒ □ □ □ □			Range 1.97									
11789	52			YES				NO				
Gym.Analog-32			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y2 A1 C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ ☒ □ □ □ □			Range									
11805	52		NO									
Gymnastatin Q			GI50 -4.81	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.66		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.88									
11849	52		YES	YES	YES	YES						
Gymnastatin I			GI50 -5.77	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.8	Y3 C2 M2 A1	+	depoly	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.2		II							
					−							

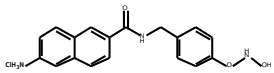
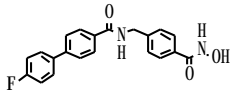
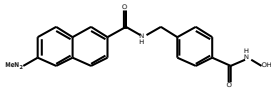
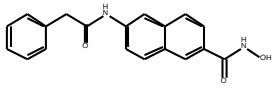
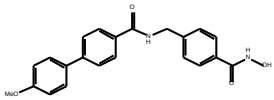
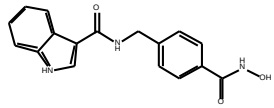
Gymnastatin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11977	52		YES	YES	YES	NO						
Gym-Analog-33			GI50 -5.6	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.35	M2 Y2 A1 C1	+		( )					( )
			Range 1.26		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □					±							
11978	52		YES*	YES	NO	NO						
Gym-Analog-34			GI50 -5.42	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.55	M2 Y2 A1 C1 E1	±		( )					( )
			Range 1.2		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □					–							

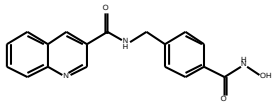
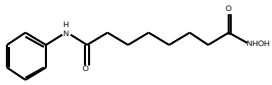
Hydroxamic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11628	11		±									
K-15			GI50 -4.69	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.33		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		HDAC阻害剤のモデル合成化合物	Range 2.83									
11629	11		YES									
K-10			GI50 -4.69	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.51		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		HDAC阻害剤のモデル合成化合物	Range 1.2									
11649	11		YES	NO	YES	NO					YES	
K-23			GI50 -5.19	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.63		+		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ ☒ □		HDAC阻害剤のモデル合成化合物	Range 1		II —							
11726	11		YES									
K-24			GI50 -6.09	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.62		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		HDAC阻害剤のモデル合成化合物	Range 1.8									
11727	11		YES									
K-27			GI50 -5.44	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.2		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		HDAC阻害剤のモデル合成化合物	Range 1.78									
11728	11		YES*									
K-28			GI50 -5.39	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.76		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		HDAC阻害剤のモデル合成化合物	Range 1.41									

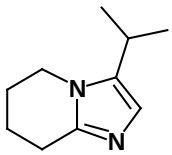
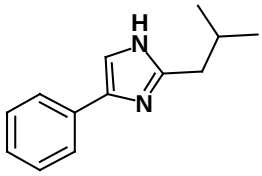
Hydroxamic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11729	11	 HDAC阻害剤のモデル合成化合物	YES									
K-32			GI50 -5.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.21		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 2									
11971	11		YES				YES				YES	
K-40			GI50 -5.5	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.99		II		1.37 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ ☒ □ □ □ ☒ □			Range 2.05									
11972	11	 HDAC阻害剤のモデル合成化合物	NO				N.D					
K-60			GI50 -4.18	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.56		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ ☒ □ □ □ □ □			Range 0.74									
11973	11		YES				+ / -				YES	
K-70			GI50 -4.7	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.08		II		397 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ ☒ □ □ □ ☒ □			Range 1.65									
11974	11	 HDAC阻害剤のモデル合成化合物	NO				NO				NO	
K-80			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.31		II		>1 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ ☒ □ □ □ ☒ □			Range 0.34									
12108	11		±				YES				NO	
k-130			GI50 -4.38	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.38		II		10.6 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ ☒ □ □ □ ☒ □			Range 1.77									

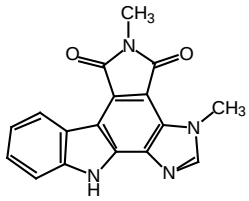
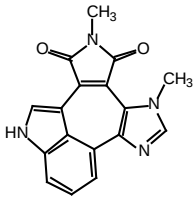
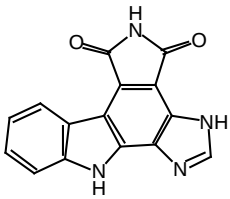
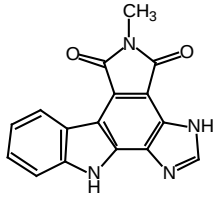
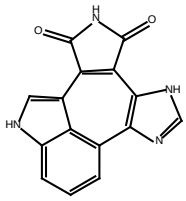
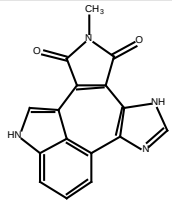
Hydroxamic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12111	11		YES				YES				YES	
k-120			GI50 -5.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.24		II		500 (nM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ ☒ □ □ □ ☒ □			Range 3.31									
12251	67						YES			NO	NO	
SAHA			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		1.06 (μM)					( )
1 2 3 4 5 6 7 8 9 10 □ □ □ □ ☒ □ □ ☒ ☒ □		HDAC阻害剤Trichostatin類似構造	Range									

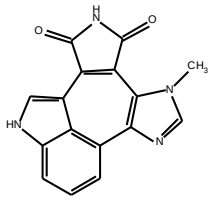
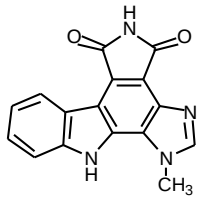
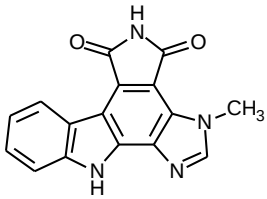
Imidazole

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11767	71		NO	NO	NO	NO		NO	NO	NO	NO	
Catharsitoxin C			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		—		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.48		—							
11768	71		NO	NO	NO	NO		NO	NO	NO	NO	
Catharsitoxin D			GI50 -4.1	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.46		—		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.56		—							

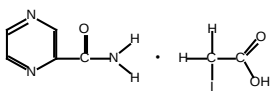
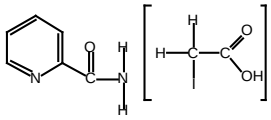
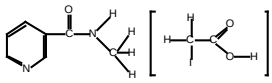
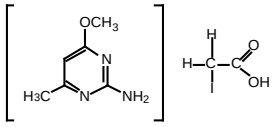
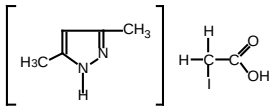
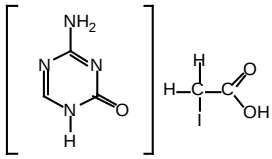
Indolomaleimide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11773	68		YES	NO	NO	NO						
10,17-Dimethylgranulatimide 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.73	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.74		−		( )					( )
			Range 2.47		II							
					−							
11949	68		±	NO	NO							
4,6-dimethyl-imidazo[4",5":4,5]pyrrolo[3,4:6,7]cyclohept[1,2,3-cd]-indole-3,5-dione 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.16	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.04		−		( )					( )
			Range 1.21		II							
					−							
11950	68		YES	NO	YES							
Glanulatimide 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.62	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.77		+		( )					( )
			Range 2.39		II							
					++							
11951	68		NO	NO	YES							
10-Methylgranulatimide 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.49		+		( )					( )
			Range 0.52		II							
					±							
12149	68		YES	YES	YES							
1H-imidazo[4",5":4,5]pyrrolo[3,4':6,7]cyclohept[1,2,3-cd]-indole-3,5-dione 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -5	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.61	Y3 C2 M1			( )					( )
			Range 1.12		II							
					++							
12150	68		YES	NO	NO							
4-methyl-imidazo[4",5":4,5]pyrrolo[3,4':6,7]cyclohept[1,2,3-cd]-indole-3,5-dione 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.6	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.08		−		( )					( )
			Range 1.68		II							
					−							

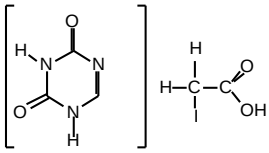
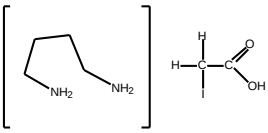
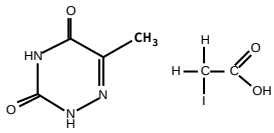
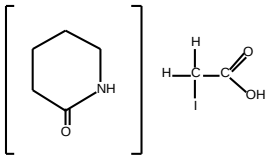
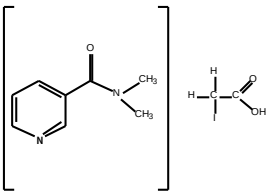
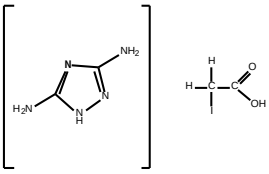
Indolomaleimide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12151	68		YES	YES	NO							
6-methyl-imidazo[4",5":4,5]pyrrolo[3,4':6,7]cyclohept[1,2,3-cd]-indole-3,5-dione			GI50 -5.34	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ □ □ □ □ □ □ □			Delta 0.83	Y2 C2 M1 E1	— II —		( )					( )
			Range 1.47									
12173	68		YES	YES								
15-Methylgranulatimide			GI50 -4.67	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □		Staurosporine類似構造	Delta 0.73	A2 M2 C1 Y1	II		( )					( )
			Range 1.17									
12174	68		NO	NO								
17-Methylgranulatimide			GI50 -4.07	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □		Staurosporine類似構造	Delta 0.73		II		( )					( )
			Range 0.8									

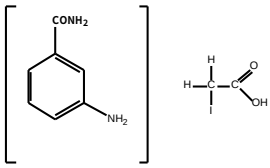
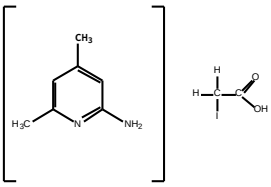
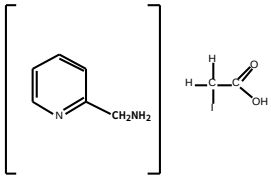
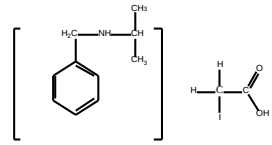
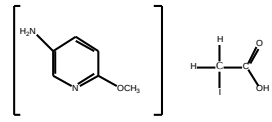
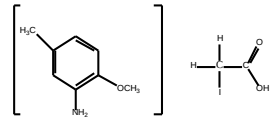
Iodoacetate salt

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
10615	45		YES								YES	NO
Pyrazin amide mono iodo acetate			GI50 -5.26	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.46		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ ☒ ☒			Range 0.91									
11123	45		±								YES	NO
2-Picolinamide Monoiodoacetate			GI50 -5.55	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.45		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ ☒ ☒			Range 3.09									
11453	45		YES			NO					YES	NO
N-methyl nicotinamide Monoiodoacetate			GI50 -5.27	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.47		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ ☒ □ □ □ □ ☒ ☒			Range 1.12									
11691	45		YES									NO
2-Amino-4-methoxy-6-methyl pyrimidine monoiodoacetate			GI50 -5.32	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.61		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 1.93									
11692	45		YES									NO
3,5-Dimethyl pyrazole monoiodoacetate			GI50 -5.4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.4		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 1.01									
11693	45		YES									NO
5-AzaCytosine monoiodoacetate			GI50 -5.26	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 1.06									

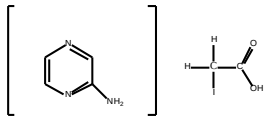
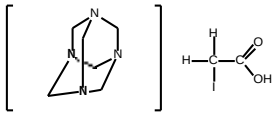
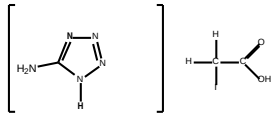
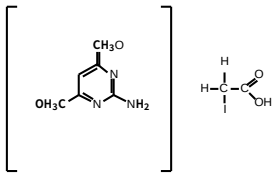
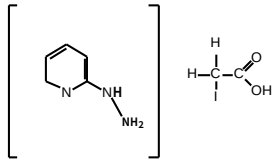
Iodoacetate salt

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11694	45		YES									NO
6-Azauracil monoiodoacetate 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☒			GI50 -5.32	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.43		II		( )					( )
			Range 1.09									
11910	45		±									
Tetramethylenediamine Monoiodoacetate 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.84	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.61		II		( )					( )
			Range 2									
11911	45		YES*									
6-Azathymine Monoiodoacetate 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -5.23	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.63		II		( )					( )
			Range 1.17									
11912	45		YES*									
δ-Valerolactam Monoiodoacetate 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -5.25	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.6		II		( )					( )
			Range 1.2									
11913	45		YES*								YES	NO
N,N-Dimethylnicotinamide Monoiodoacetate 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☒ ☒			GI50 -5.15	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.62		II		( )					( )
			Range 1.21									
11955	45		±									
3,5-Diamino-1,2,4-triazole monoiodoacetate 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -5.28	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		II		( )					( )
			Range 0.99									

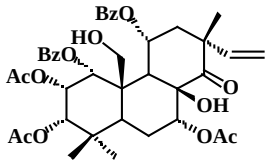
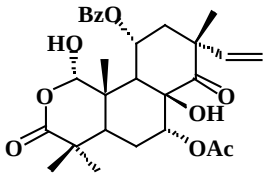
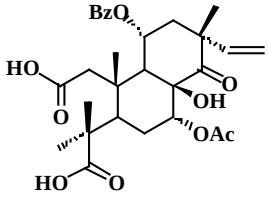
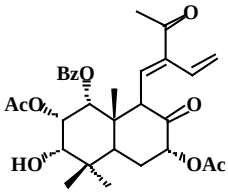
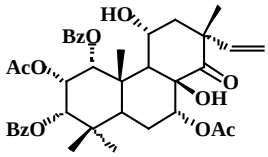
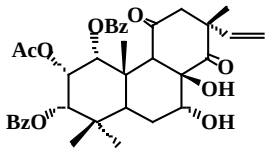
Iodoacetate salt

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11956	45		YES*								YES	
3-Amino benzamide monoiodoacetate			GI50 -5.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.7		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☒ ☐			Range 1.14									
11957	45		±									
2-Amino-4,6-dimethyl pyridine monoiodoacetate			GI50 -5.32	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.47		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.08									
11958	45		YES*									
2-Amino methyl pyridine monoiodoacetate			GI50 -5.21	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.57		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.13									
12044	45		±									
N-Isopropylbenzylamine monoiodoacetate			GI50 -5.33	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.46		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.09									
12045	45		±									
5-Amino-2-methoxy pyridine monoiodoacetate			GI50 -4.84	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.83		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.24									
12046	45		±									
2-Methoxy-5-methylaniline monoiodoacetate			GI50 -5.22	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.66		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.13									

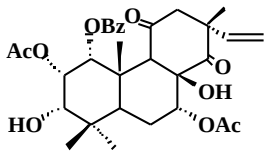
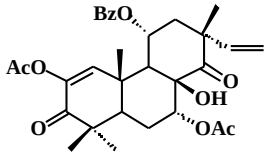
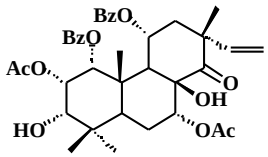
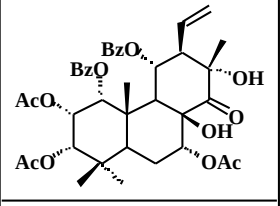
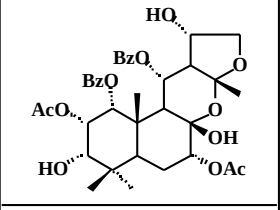
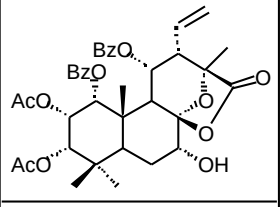
Iodoacetate salt

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12047	45		YES*									
Aminopyazine monoiodoacetate			GI50 -5.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.86		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.3									
12175	45		NO									NO
Hexamethylene tetramine monoiodoacetate			GI50 -4.72	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.69		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 0.99									
12176	45		YES*									NO
5-Aminotetrazole monoiodoacetate			GI50 -5.06	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.71		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 1.37									
12177	45		YES*									NO
2-Amino-4,6-dimethoxy pyrimidine monoiodoacetate			GI50 -5	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.69		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 1.22									
12178	45		±									NO
2-Hydrazino pyridine monoiodoacetate			GI50 -5.07	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.62		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 1.06									

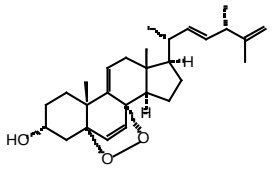
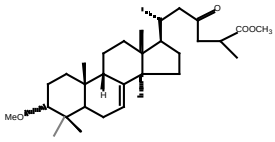
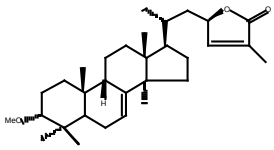
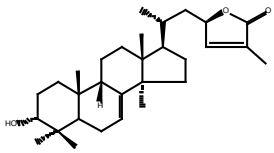
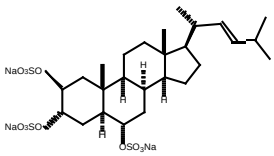
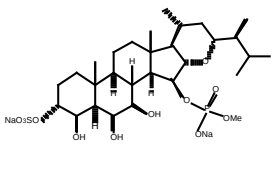
Isoprenoid / Diterpene

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12225	20			NO								
Siphonol A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12226	20			NO								
Nororthosiphonolide A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12227	20			NO								
Secoorthosiphol A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12228	20			NO								
Norstaminine A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12229	20			NO								
Orthosiphol O			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12230	20			NO								
Orthosiphol N			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									

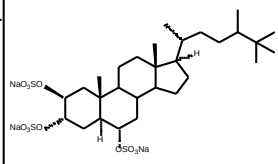
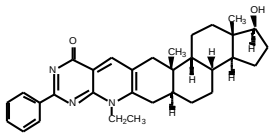
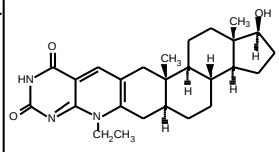
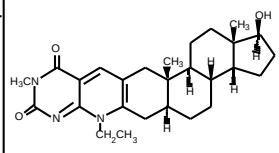
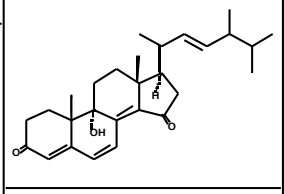
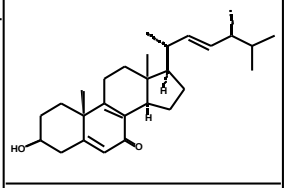
Isoprenoid / Diterpene

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12231	20			NO								
Orthosiphol M			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12232	20			NO								
Orthosiphol D			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12233	20			NO								
Orthosiphol A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12234	20			NO								
Staminol A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12235	20			NO								
Norstaminol B			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									
12236	20			NO								
Staminolacton A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range									

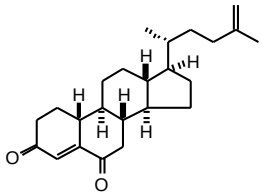
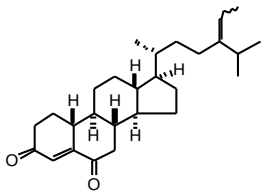
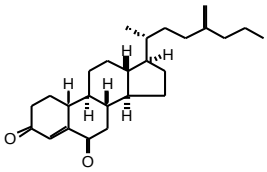
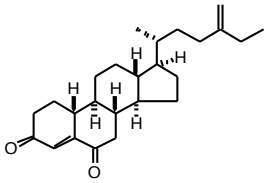
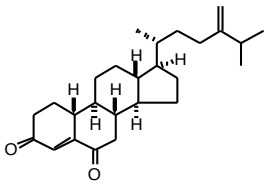
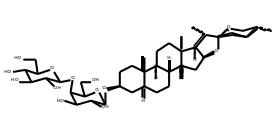
Isoprenoid / Steroid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11583	6		YES									
KKM-02			GI50 -5.69	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.51		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.05									
11751	43		YES	NO	NO	N.D.	NO	NO			NO	
Abiesenonic acid methyl ester			GI50 -4.43	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.82		— II		>1 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ □ □ ☒ □			Range 1.25		±							
12221	43		NO									
AVB-1			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.43		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.44									
12222	43		NO									
AVB-4			GI50 -4.36	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.41		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.77									
11709	48		YES	YES					NO	NO		
Halistanol sulfate D			GI50 -4.35	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.43	A3 C3 M2 Y2 E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ ☒ ☒ □ □			Range 0.78									
11710	48		NO	NO					NO	NO		
Haspolosamate A			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.08		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ ☒ ☒ □ □			Range 0.08	E1								

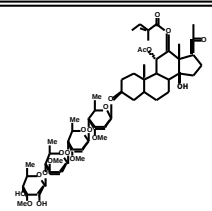
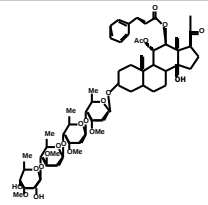
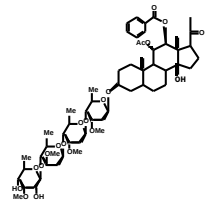
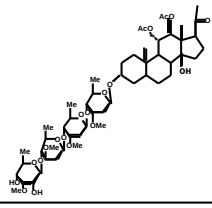
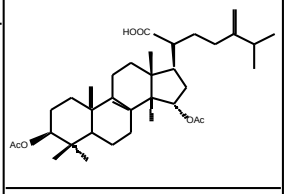
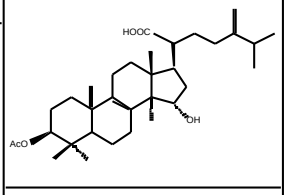
Isoprenoid / Steroid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11798	48		NO									
Halistanol sulfate			GI50 -4.49	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.38		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.87									
11750	50		±	NO	YES	NO		NO	NO	NO	NO	NO
8-Ethyl-17β-hydroxy-2'-phenyl-5α-androst-2-eno[2,3:5',6']pyrido[2',3'-d]pyrimidin-4'(8'H)-one			GI50 -4.82	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.3		+		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒			Range 2.65		II							
					–							
11815	50		NO	NO	NO	NO		NO	NO	NO	NO	
5'-Deaza-8'-ethyl-17β-hydroxy-5α-androst-2-eno[2,3-g]pteridine-2',4'(3'H,8'H)-dion			GI50 -4.24	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.5		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.73		II							
					–							
11816	50		NO	NO	NO	NO		NO	NO	NO	NO	
5'-Deaza-8'-ethyl-17β-hydroxy-3'-methyl-5α-androst-2-eno[2,3-g]pteridine-2',4'(3'H,8'H)-dione			GI50 -4.52	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.42		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.62		II							
					–							
11804	52		±									
Gymnasterone G			GI50 -4.29	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.33		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 2.62									
11806	52		±									
3β-Hydroxy-(22E,24R)-ergosta-5,8,22-trien-7-one			GI50 -4.7	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.16		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.65									

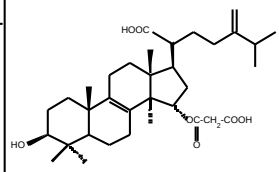
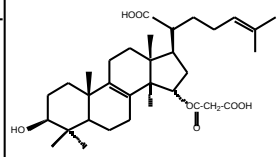
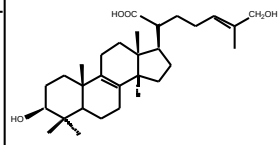
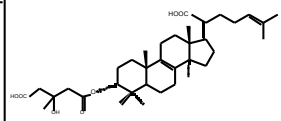
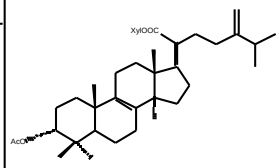
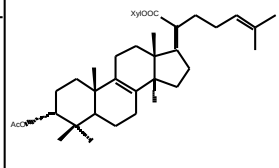
Isoprenoid / Steroid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12008	57		NO									
m-m-sp3			GI50 -4.83	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.47		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.61									
12009	57		NO									
ipr-et-sp3			GI50 -4.19	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.42		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.61									
12010	57		YES									
p-m-sp3			GI50 -4.93	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.8		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.07									
12011	57		YES									
e-m-sp3			GI50 -4.94	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.52		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.75									
12012	57		NO									
ipr-m-sp3			GI50 -4.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.3		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.54									
12043	65	* 	NO								YES	
AU-16			GI50 -4.71	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.13		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☒ ☐			Range 0.22									

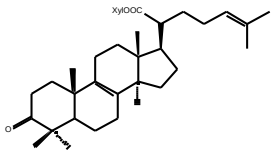
Isoprenoid / Steroid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11682	72		NO									
MJ-7			GI50 -4.19	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.29		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.48									
11683	72		NO									
MJ-12			GI50 -4.55	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.19		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.47									
11684	72		NO									
MJ-14			GI50 -4.63	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.19		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.5									
11685	72		NO									
MJ-19			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.27		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.29									
11799	72		NO									
Laetip-1			GI50 -4.68	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.3		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.6									
11800	72		YES	NO	NO	NO						
Laetip-2			GI50 -4.88	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.06		±		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.55		II							
					−							

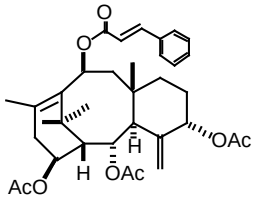
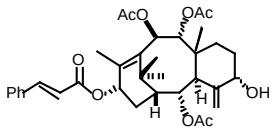
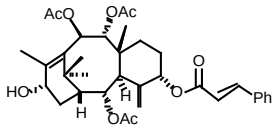
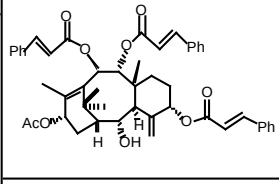
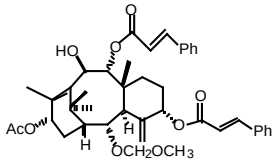
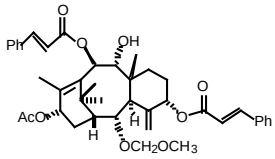
Isoprenoid / Steroid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11801	72		NO									
Laetip-3			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.28		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.29									
11802	72	 *	±									
Laetip-4			GI50 -4.04	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.98		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.02									
11803	72		NO									
Laetip-5			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.28		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.31									
12258	72		NO									
Fp-1			GI50 -4.81	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.43		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.53									
12259	72		NO									
Fp-2			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.03		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.03									
12260	72		NO									
Fp-3			GI50 -4.78	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.21		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.29									

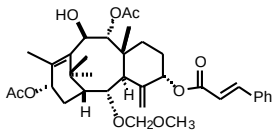
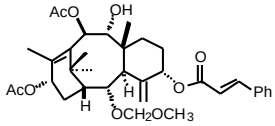
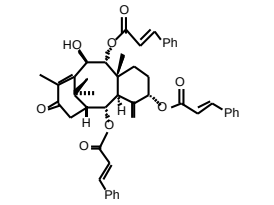
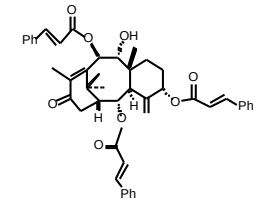
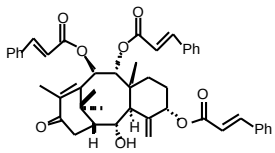
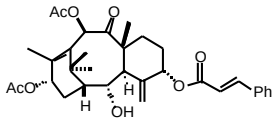
Isoprenoid / Steroid

JCI.No compound screening	sup. code	screening No.	1	2	3	4	5	6	7	8	9	10
		structure/comments	HCC panel	PK	Topo.	Tub.	HDAC.	p-Gp	Inv.	Angio.	Apo.	P388
12261	72		NO									
Fp-4			GI50 -4.78	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.18		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.29									

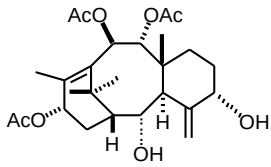
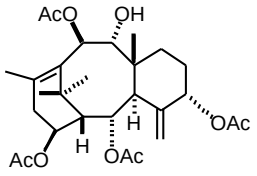
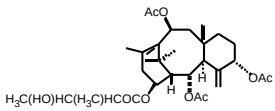
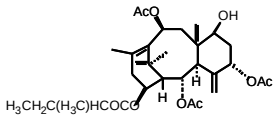
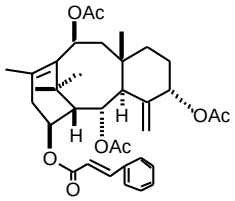
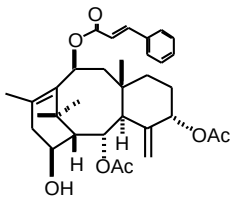
Isoprenoid / Taxoid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11914	4		YES	NO	NO	NO		YES				
10-cinnamoyloxy-taxuyunnanine C 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☐ ☒ ☐ ☐ ☐ ☐			GI50 -4.41	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.23		–		( )					( )
					II							
			Range 1.64		–							
11915	4		NO					YES				
9α,10β,2α-triacetoxy-5α-hydroxy-13α-cinnamoyloxytaxa-4(20),11-dine 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			GI50 -4.08	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.64				( )					( )
					II							
			Range 0.72									
11916	4		YES	NO	NO	NO		YES				
9α,10β,2α-triacetoxy-5α-cinnamoyloxy-13α-hydroxytaxa-4(20),11-dine 1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☐ ☒ ☐ ☐ ☐ ☐			GI50 -4.34	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.07		–		( )					( )
					II							
			Range 1.4		±							
11917	4		NO					NO				
9α,10β,5α-triacinnamoyloxy-13α-acetoxy-2α-hydroxytaxa-4(20),11-dine 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.59				( )					( )
					II							
			Range 0.62									
11979	4							NO				
13α-acetoxy-5α,9α-dicinamoyloxy-10β-hydroxy-2α-methoxymethoxytaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					( )
					II							
			Range									
11980	4							NO				
13α-acetoxy-5α,10β-dicinamoyloxy-9α-hydroxy-2α-methoxymethoxytaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					( )
					II							
			Range									

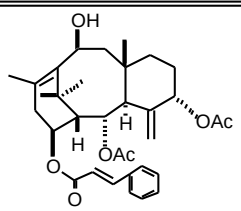
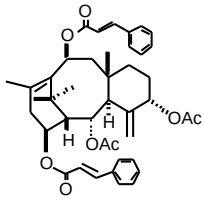
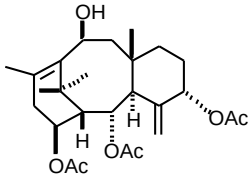
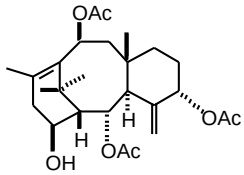
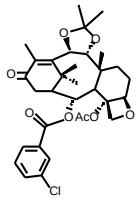
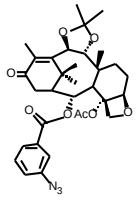
Isoprenoid / Taxoid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11981	4							YES				
9α,13α -diacetoxy-5α -cinamoyloxy-10β -hydroxy-2α -methoxymethoxytaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50 Delta Range	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
11982	4							YES				
10β,13α -diacetoxy-5α -cinamoyloxy-9α -hydroxy-2α -methoxymethoxytaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50 Delta Range	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
11983	4							NO				
2α,5α,9α -tricinamoyloxy-10β -hydroxy-13-oxotaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50 Delta Range	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
11984	4							NO				
2α,5α,10β -tricinamoyloxy-9α -hydroxy-13-oxotaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50 Delta Range	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
11985	4							NO				
5α,9α,10β -tricinamoyloxy-2α -hydroxy-13-oxotaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50 Delta Range	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
11986	4							NO				
10β,13α -diacetoxy-5α -cinamoyloxy-2α -hydroxy-9-oxotaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50 Delta Range	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )

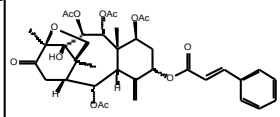
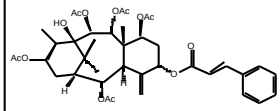
Isoprenoid / Taxoid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11987	4							NO				
9α,10β,13α -triacetoxy-2α,5α -dihydroxy-taxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
			Range									
11988	4							NO				
2α,5α,10β,14β -tetra-acetoxy-9α -hydroxy-taxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
			Range									
11989	4							NO				
2α,5α,10β -triacetoxy-14β (3-hydroxy-2-methylbutyryl)oxy-taxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
			Range									
11990	4							NO				
2α,5α,10β -triacetoxy-7β -hydroxy-14β (2-methylbutyryl)oxy-taxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
			Range									
11991	4							NO				
2α,5α,10β -triacetoxy-14β -cinnamoyloxytaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
			Range									
11992	4							NO				
2α,5α-diacetoxy-10β-cinnamoyloxy-14β -hydroxytaxa-4(20),11-diene 1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
			Range									

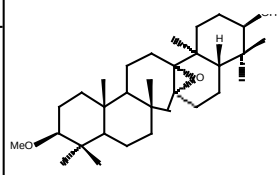
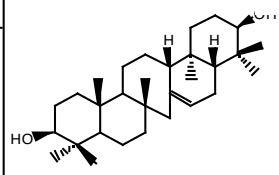
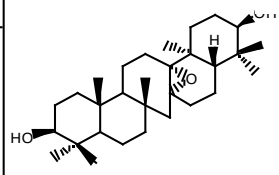
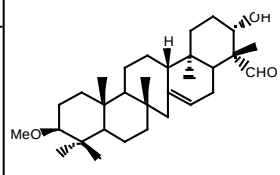
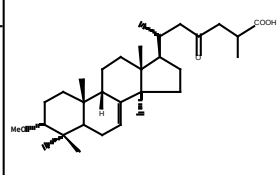
Isoprenoid / Taxoid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11993	4							NO				
2α,5α -diacetoxy-14β -cinnamoyloxy-10β -hydroxytaxa-4(20),11-diene			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			Delta		II		( )					( )
			Range									
11994	4							NO				
2α,5α -diacetoxy-10β,14β -dicinnamoyloxytaxa-4(20),11-diene			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			Delta		II		( )					( )
			Range									
11995	4							NO				
2α,5α,14β -triacetoxy-10β -hydroxytaxa-4(20),11-diene			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			Delta		II		( )					( )
			Range									
11996	4							NO				
2α,5α,10β -triacetoxy-14β -hydroxytaxa-4(20),11-diene			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ⊠ □ □ □ □			Delta		II		( )					( )
			Range									
11672	18		NO	NO	NO	NO		NO				
2-m-chlorobaccatin III			GI50 -4.21	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ ⊠ □ □ □ □			Delta 0.38		– II		( )					( )
			Range 0.59		–							
11673	18		NO	NO	YES	NO		NO				
2-m-azidobaccatin III			GI50 -4.32	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ ⊠ □ □ □ □			Delta 0.34		+ II		( )					( )
			Range 0.66		+							

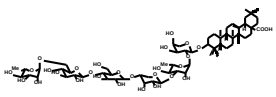
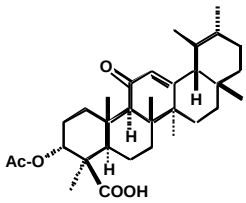
Isoprenoid / Taxoid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11303	28		NO									
Taxagifine 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -5.27 Delta 0.35 Range 0.62	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )
11304	28		NO									
Taxuspine D 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -5.42 Delta 0.39 Range 0.81	spec.	I II	mode	IC50 ( )					T/C% (mg/kg) ( )

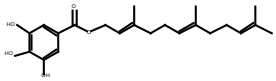
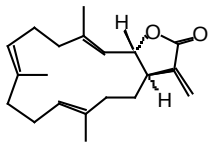
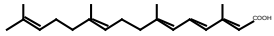
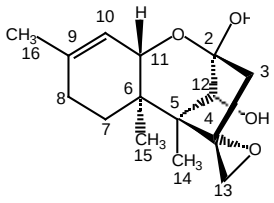
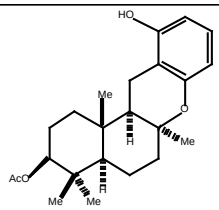
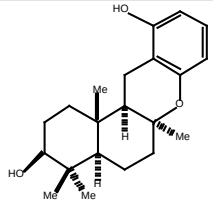
Isoprenoid / Triterpene

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11687	43		YES	NO	NO	N.D.		NO			NO	
PJJ-34			GI50 -4.93	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.7		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ □ □ ☒ □			Range 1.24		II –							
11829	43		NO									
PJJ-5			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.41		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.43									
12083	43		NO	NO	NO	NO						
PJJ-3			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.22		– II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 0.23		–							
12084	43		YES	NO	NO	NO						
PJJ-3-13-enepoxy			GI50 -4.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.75		± II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.06		–							
12085	43		NO									
PJ-20			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.51		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.53									
12219	43		NO									
AVB-1 acid			GI50 -4.6	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.17		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.34									

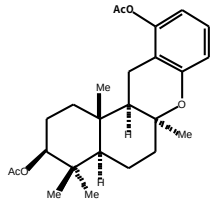
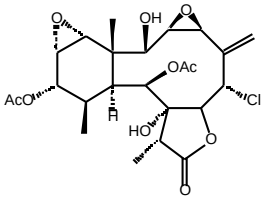
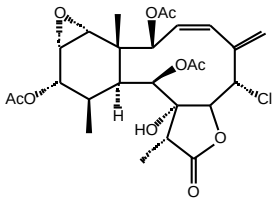
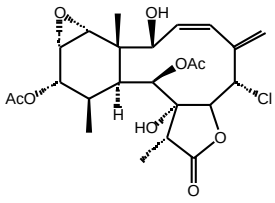
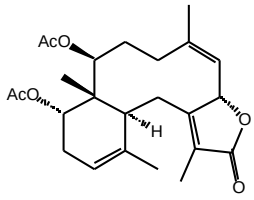
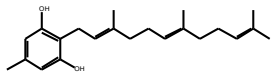
Isoprenoid / Triterpene

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12188	65	* 	±									
Clematisaponin A 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -5.7	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.18		II		( )					( )
			Range 0.31									
12189	65		NO									
3-O-acetyl-11-keto-β-boswellic acid (AKBA) 1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			GI50 -4.74	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.07		II		( )					( )
			Range 0.15									

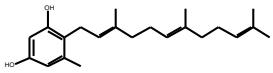
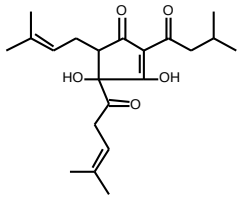
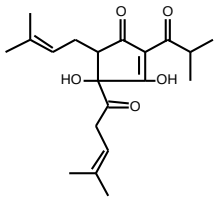
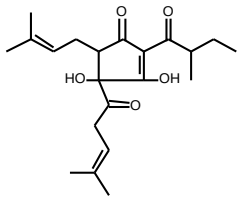
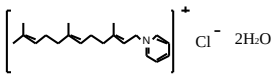
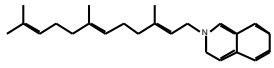
Isoprenoid / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12136	3		YES	NO	YES	NO	NO	YES	NO	NO	YES	
Farnesyl gallate (Gallic acid farnesyl ester)			GI50 -5.09	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.67	A1 C1 M1 Y1	++		>1.3 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 1.01		II							
					±							
11582	6		YES									
KKM-01			GI50 -5.21	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		Michaelアクセプター／SH酵素阻害剤の可能性。	Range 1.01									
11946	7		NO	NO	YES	NO	+ / -	NO	+ / -	NO		
NIK-333			GI50 -4.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.63	C1	+		216 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □ □			Range 0.87		II							
					−							
11678	16		YES									
Curvularol			GI50 -6.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.35		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.48									
12118	19		±	NO	NO	NO	NO	NO	+ / -	NO	YES	
KI-01			GI50 -4.86	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.31		−		>1.3 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 1.61		II							
					−							
12119	19		±	NO	NO	NO	NO	NO	NO	NO	YES	
KI-02			GI50 -4.69	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.79		−		>1.5 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 1.13		II							
					−							

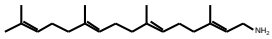
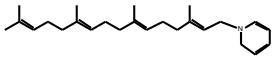
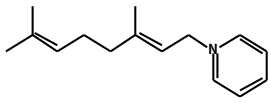
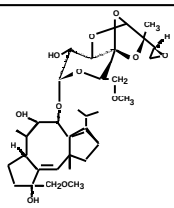
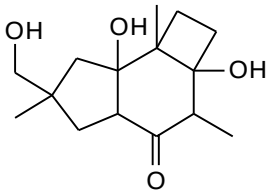
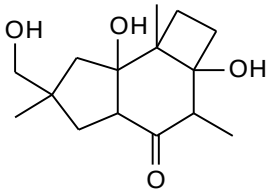
Isoprenoid / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12120	19		NO	NO	NO	NO	NO	NO	NO	NO	YES	
KI-03			GI50 -4.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.41		—		>1.2 (μM)					
					II							( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☐			Range 0.7		—							
11155	28							NO				
SC-CF			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			Range									
11156	28							NO				
BRIANT-Z			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			Range									
11158	28							NO				
BRIANT-X			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			Range									
11159	28							NO				
BRIANT-W			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			Range									
12070	29		NO	NO			NO			NO		
Grifolin			GI50 -4.73	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.08				>1.5 (mM)					
					II							( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☐ ☐ ☒ ☐ ☐ ☒ ☐ ☐			Range 0.34									

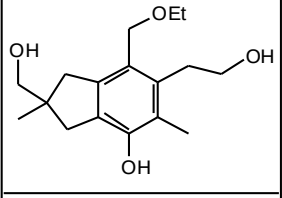
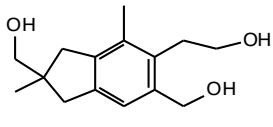
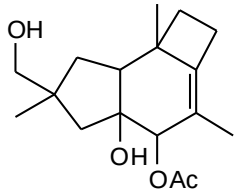
Isoprenoid / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12071	29		NO	NO			NO			NO		
Neogrifolin			GI50 -4.72	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.08	A1 M1 Y1	II		>1.5 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ ☒ □ □ ☒ □ □			Range 0.2									
11795	32		NO					NO				
Isohumulone			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.22		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ ☒ □ □ □ □			Range 0.24									
11796	32		NO					NO				
Isocohumulone			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.75		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ ☒ □ □ □ □			Range 0.78									
11797	32		NO					NO				
Isoadhumulone			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.22		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ ☒ □ □ □ □			Range 0.23									
11367	42		YES	NO	NO	NO		NO			YES	NO
1-Farnesyl-pyridinium chloride・2H2O			GI50 -5.87	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.98		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ □ □ ☒ ☒			Range 2.07		—							
12049	42		YES	NO	NO	NO						
Farnesylisoquinolinium			GI50 -5.84	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.32	C1 M1 Y1	— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 2.3	E1	—							

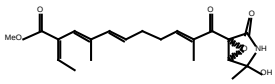
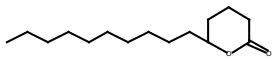
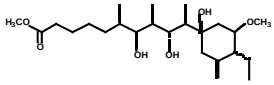
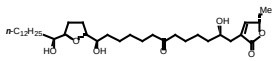
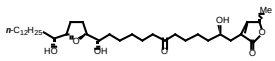
Isoprenoid / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12050	42		YES									
Geranylgeranylamine			GI50 -5.26	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.54		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.41									
12051	42		YES	NO	NO	NO						
Geranylgeranylpyridinium			GI50 -5.87	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.14	M1 Y1	— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.76	E1	±							
12200	42							NO				
Geranylpyridinium			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ ☒ □ □ □ □			Range									
12158	58		NO	NO								
Cotylenin A			GI50 -4.3	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.4		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.7	E1								
12052	72		NO	NO	NO	NO	NO	NO	YES	NO	NO	
Russ-1			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.3		— II		>1.8 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 0.32		—							
12053	72		NO									
Russ-2			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.46		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.49									

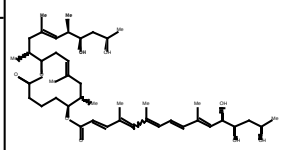
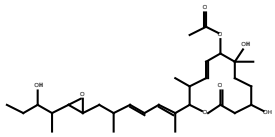
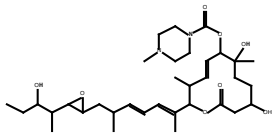
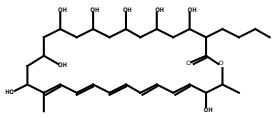
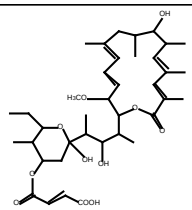
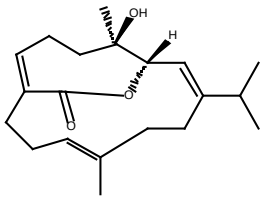
Isoprenoid / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12054	72		NO									
Russ-3			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.52		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.54									
12055	72		NO									
Russ-4			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.26		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.27									
12056	72		NO									
Russ-5			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.65		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.68									

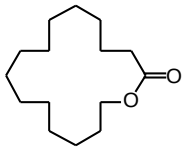
Linear polyketide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11723	16		YES									
Epolactaene			GI50 -5.37	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.36		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DNA polymeraseおよびtopo II阻害剤	Range 1.03									
12033	46		NO			NO						
5-Hexadecanolide			GI50 -4.64	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.32		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ ☒ □ □ □ □ □ □			Range 0.95									
11807	52		NO									
92DRT-I			GI50 -4.29	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.74									
11666	59		YES*	NO	NO	NO		NO			YES	
mosin B			GI50 -5.38	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.62		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ □ □ ☒ □		ミトコンドリア電子伝達阻害剤と考えられる	Range 3.31		—							
11667	59		YES*	NO	NO	NO		NO			YES	
mosin B analog			GI50 -5.9	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.1		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ □ □ ☒ □		ミトコンドリア電子伝達阻害剤と考えられる	Range 2.72		—							

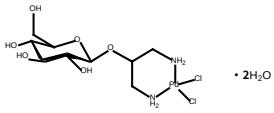
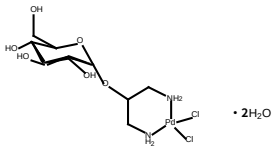
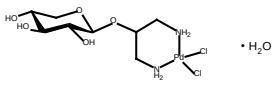
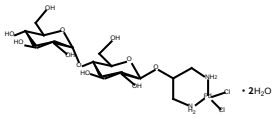
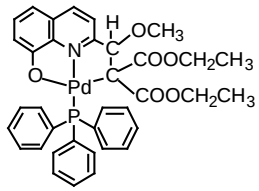
Macrolide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12093	1	* 	YES									
MCL1			GI50 -8.18	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.82		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 3.33									
12094	1		YES									
ME-2			GI50 -8.65	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.76		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.32									
12096	1		YES									
ME-155			GI50 -9.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.72		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 2.17									
11813	5		±	NO	N.D.	NO		NO	+ / -	NO	YES	
Chainin			GI50 -5.68	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.11		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □		コレステロール結合性細胞膜障害物質	Range 0.4									
11668	21		YES*									
Hygrolidin			GI50 -5.86	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.78		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		V-ATPase阻害剤	Range 2.92									
11779	28			NO								
ECHDL-A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ □ □ □ □ □			Range									

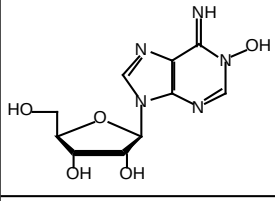
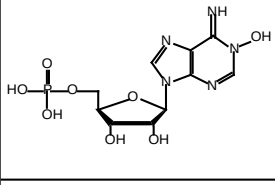
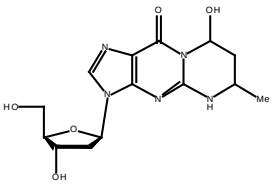
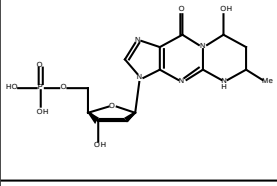
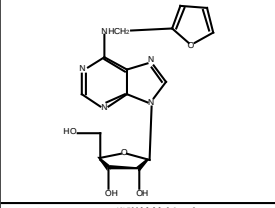
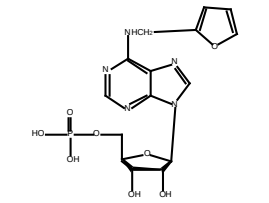
Macrolide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12036	46		NO									
pentadecan-15-olide			GI50 -4.36	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.63		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.99									

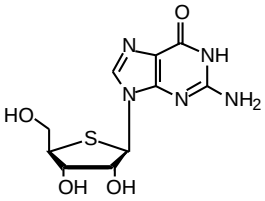
Metal complex

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12206	70		NO									NO
Pd-Glc			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.29		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 0.29									
12207	70		NO									NO
Pd-αGal			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.51		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 0.53									
12208	70		NO									NO
Pd-Xyl			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 0									
12209	70		NO									YES
Pd-Mal			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0		II		( )					120 (400)
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ ☒			Range 0									
11748	73		YES*	NO	NO	N.D.		NO	NO	NO	YES	
{Diethyl2-[methoxy(8-oxy-kO-2-quinolyl-kN)-methyl]malonato-kC}(triphenylphosphine)palladium(II)			GI50 -5.15	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.64	Y1	— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 1.15	E1	—							

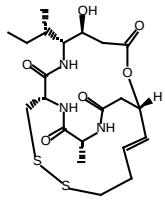
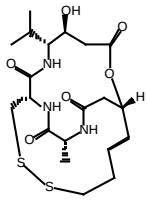
Nucleoside

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12004	33		YES			NO						
Adenosine 1-Oxide			GI50 -4.97	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.56		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ ☒ □ □ □ □ □ □			Range 1.34									
12007	33		YES	NO		N.D.						
Adenosine 5'-Monophosphate 1-Oxide			GI50 -4.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.54		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.11									
12030	33		NO									
1,N^2-cyclic deoxyguanosine			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.37		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.38									
12031	33		NO									
1,N^2-cyclic dGMP			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.75		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.79									
12153	58		YES	NO	NO	NO						
Kinetin riboside			GI50 -5.41	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.12		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □		ATPまたはdATPの代謝拮抗剤と考えられる	Range 2.42		—							
12154	58		YES	NO								
Kinetin riboside-monophosphate			GI50 -5.31	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.99		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □		ATPまたはdATPの代謝拮抗剤と考えられる	Range 2.24									

Nucleoside

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11686	63		NO	NO						NO		
4'-Thioguanosine			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.23		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐			Range 0.24									

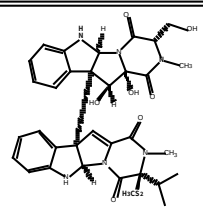
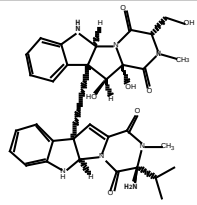
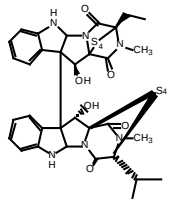
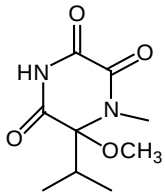
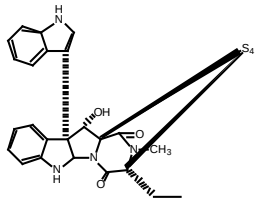
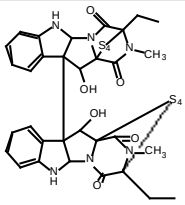
Peptide / Cyclic depsipeptide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11561	34		±	NO	NO	NO						
Spiruchostatin B			GI50 -8.25	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.57	C1 M1 Y1	±		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □		ヒストンデアセチラーゼ阻害剤	Range 2.18		±							
11562	34		±	NO	NO	NO						
Spiruchostatin A			GI50 -8.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.52	M1 Y1	±		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □		ヒストンデアセチラーゼ阻害剤	Range 2.21		±							

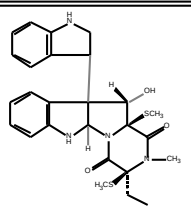
Peptide / Cyclic peptide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11439	54								NO			
Mb 2127-1		Cyclo(Leu-Ala-Ile-Pro-Phe-Gly-Ser)	GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ □ □ □ □ □ ⊠ □ □ □			Range									
11440	54			NO	NO			NO	NO		NO	
Mb 2152-1		Cyclo(Leu-Ala-Ile-Pro-Phe-Asn-Gly)	GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		—		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 □ ⊠ ⊠ □ □ ⊠ ⊠ □ ⊠ □			Range		—							
11441	54		±	NO	NO			NO	NO		NO	
Mb 2152-2		Cyclo(Leu-Ala-Gly-Pro-Phe-Asn-Ser)	GI50 -4.11	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 3		—		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ □ □ ⊠ ⊠ □ ⊠ □			Range 3.11		—							

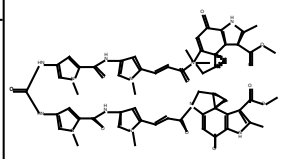
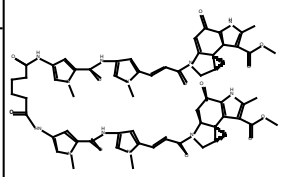
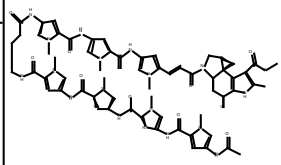
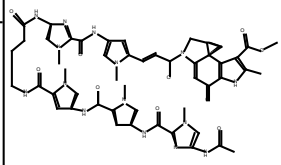
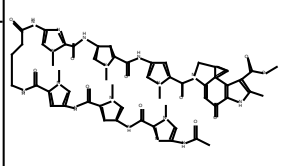
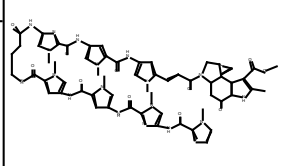
Peptide / Diketopiperazine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11847	52		NO									
Leptosin O			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.38		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.39									
11848	52		NO									
Leptosin S			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.12		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.13									
12059	52		YES									
Leptosin U			GI50 -5.79	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.81		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.13									
12060	52		NO									
Leptoperazin A			GI50 -4.27	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.32		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.59									
12061	52				NO							
Candecin B			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		±		( )					( )
1 2 3 4 5 6 7 8 9 10 □ □ ☒ □ □ □ □ □ □ □			Range		II							
					±							
12062	52				YES							
Candecin G			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		±		( )					( )
1 2 3 4 5 6 7 8 9 10 □ □ ☒ □ □ □ □ □ □ □			Range		II							
					++							

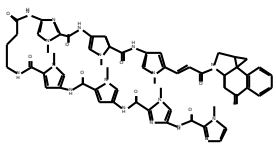
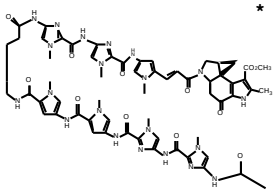
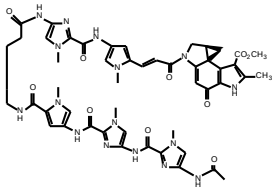
Peptide / Diketopiperazine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12190	52		NO									
Candecin A			GI50 -4.69	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.3		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.57									

Peptide / Duocarmycin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11873	36		±									
CO(PyPyLDu86)2			GI50 -7.99	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.01		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DistamycinのDNA結合部位とDuocarmycinのアルキル化部位のハイブリッド化合物	Range 2.63									
11874	36		±									
4CH2(PyPyLDu86)2			GI50 -7.52	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.48		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DistamycinのDNA結合部位とDuocarmycinのアルキル化部位のハイブリッド化合物	Range 3.17									
11875	36	* 	±									
PylmlmlmγPyPyPyLDu86			GI50 -5.24	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.02		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DistamycinのDNA結合部位とDuocarmycinのアルキル化部位のハイブリッド化合物	Range 1.26									
11876	36		±									
lmPyPyγlmPyLDu86			GI50 -6.14	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.79		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DistamycinのDNA結合部位とDuocarmycinのアルキル化部位のハイブリッド化合物	Range 1.69									
11877	36	* 	±									
lmPyPyγlmPyPyLDu86			GI50 -6.14	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.93		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DistamycinのDNA結合部位とDuocarmycinのアルキル化部位のハイブリッド化合物	Range 2.96									
12024	36	* 	±									
lmlmPyPy-γ-lmPyPyLDu86			GI50 -6.67	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.29		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DistamycinのDNA結合部位とDuocarmycinのアルキル化部位のハイブリッド化合物	Range 2.61									

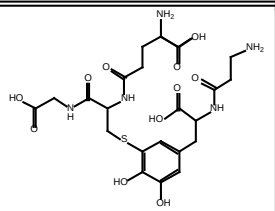
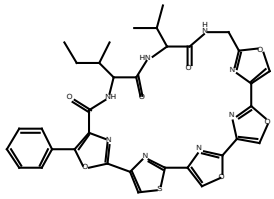
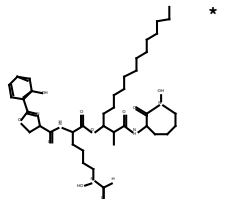
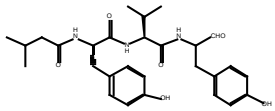
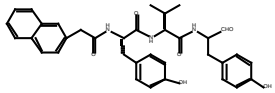
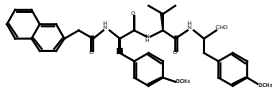
Peptide / Duocarmycin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12028	36	* 	±									
ImImPyPy-γ-ImPyPyLLCB1			GI50 -7.58	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.42		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		DistamycinのDNA結合部位とDuocarmycinのアルキル化部位のハイブリッド化合物	Range 3									
12112	36	* 	±									
AcimimPyPy-γ-ImImPyLDu86			GI50 -5.4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.65		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		Duocarmycinとdistamaycinのハイブリッド化合物	Range 2.05									
12113	36		±									
AcImImPy-γ-ImPyLDu86			GI50 -6.22	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.52		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		Duocarmycinとdistamaycinのハイブリッド化合物	Range 2.61									

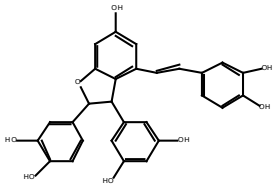
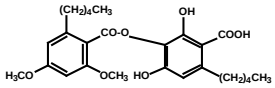
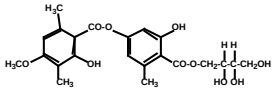
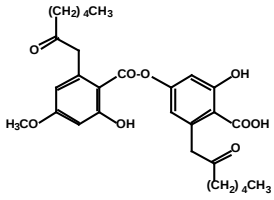
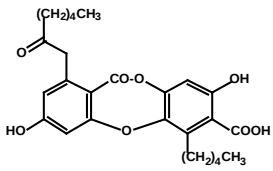
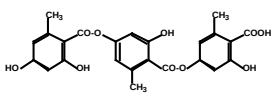
Peptide / Linear oligopeptide

JCI.No compound screening	sup. code	screening No.	1	2	3	4	5	6	7	8	9	10
		structure/comments	HCC panel	PK	Topo.	Tub.	HDAC.	p-Gp	Inv.	Angio.	Apo.	P388
11765	28	*						NO				
DICT-A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta				( )					
					II							( )
			Range									
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐												

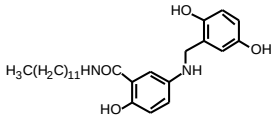
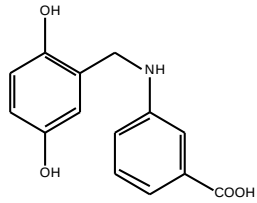
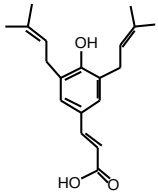
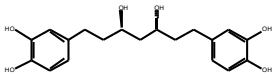
Peptide / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
10425	27		±	YES		NO						
5-S-GAD			GI50 -4.09	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.22	A1 C1 M1 Y1 E2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ ☒ □ □ □ □ □ □			Range 2.31									
12080	44		YES	NO	YES	NO						
YM-216391			GI50 -7.43	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.4	A1 C1 M1 Y1	++		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.77		II / −							
10905	55	 *	YES									
A77543			GI50 -6.29	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.27		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □		金属イオンキレート作用が推測される	Range 0.96									
12248	69		YES	NO		NO						
Tyropeptin A			GI50 -4.85	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.72		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.57									
12249	69		YES	NO		NO						
IMO-1			GI50 -6.4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.91		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 2.03									
12250	69		YES	NO		NO						
IMO-2			GI50 -8.16	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.84	A1 M1 Y1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 2.76									

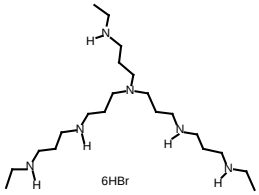
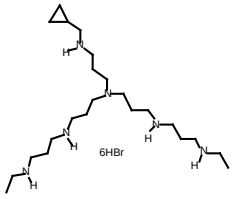
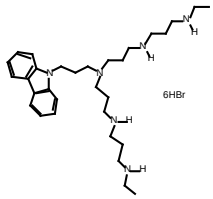
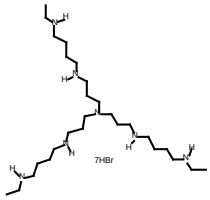
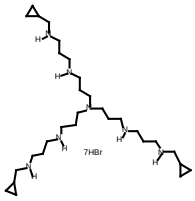
Phenol

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12140	20		NO									
Scirpusin A			GI50 -4.47	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.22		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.69									
11879	39		NO									
4-O-Methylcryptochlorophaeic acid			GI50 -4.69	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.23		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.63									
11880	39		NO									
Erythrin			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0									
11884	39		NO									
Microphyllinic acid			GI50 -4.47	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.29		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.76									
11885	39		NO									
Physodic acid			GI50 -4.64	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.14		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.78									
11887	39		NO									
Gyropholic acid			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.41		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.42									

Phenol

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11944	51		YES	YES								
TO-N-6-50			GI50 -5.79	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.94	A1 C1 M1 E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 1.48									
12130	51			YES								
GN-6-61-NA			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	E2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ □ □ □ □ □			Range									
11764	56			NO								
Artepillin C (synthetic)			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ □ □ □ □ □			Range									
12042	65		NO								NO	
TE-30			GI50 -4.06	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.55		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ ☒ □			Range 0.61									

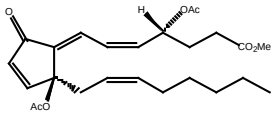
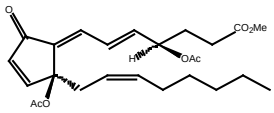
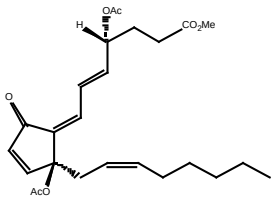
Polyamine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12193	10		NO									
RKH1447			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.14		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.14									
12194	10		NO									
RKH1448			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.24		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.25									
12195	10		YES	NO	YES	NO						
RKH1449			GI50 -5.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.64	M2 C1	++ II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.04	E2	++							
12196	10		NO									
RKH1450			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.23		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.25									
12197	10		NO									
RKH1451			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.25		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.26									

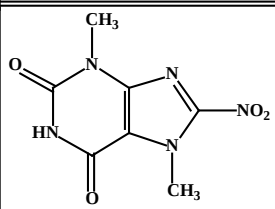
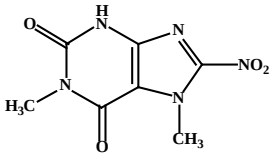
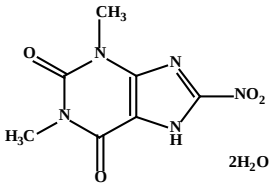
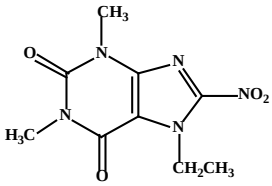
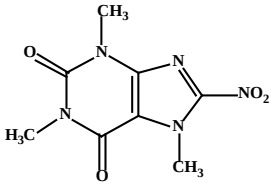
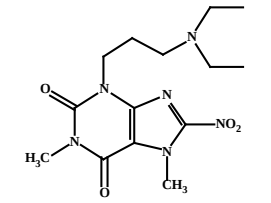
Polyether

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11889	57	*	YES*									
N-12			GI50 -5.15	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.68		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.33									
11890	57		NO									
N-13			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.62		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.64									
11891	57		NO									
N-14			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.25		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.25									
11892	57		NO									
N-15			GI50 -5.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.44		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.46									
11893	57		NO									
N-16			GI50 -5.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.25		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.26									

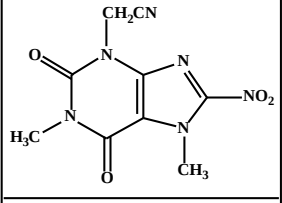
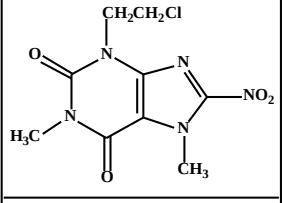
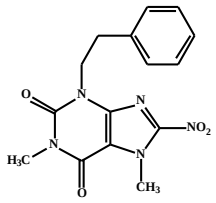
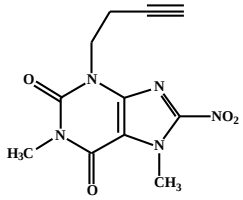
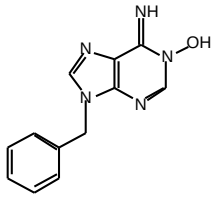
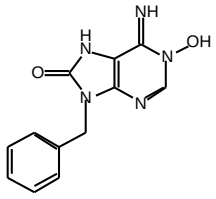
Prostaglandin

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11858	6		YES									
KKM-14			GI50 -5.55	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.3		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.03									
11859	6		YES									
KKM-15			GI50 -5.45	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.3		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.04									
11860	6		YES									
KKM-16			GI50 -5.52	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.39		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.15									

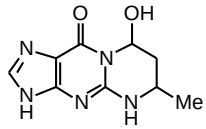
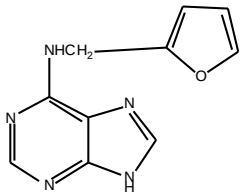
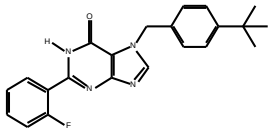
Purine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11703	24		YES*	NO	NO	YES		NO	NO	NO	YES	
PR-3067			GI50 -5.07	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.66		−	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 1.09		II							
					±							
11704	24		NO	NO	NO	NO		NO	NO	NO	YES	
PR-3101			GI50 -4.81	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.73		−		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.9		II							
					±							
11705	24		NO	NO	NO	NO		NO	NO	NO	NO	
PR-3044			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.34		−		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.37		II							
					±							
11706	24		YES	NO	YES	YES		NO	NO	NO	YES	
PR-3144			GI50 -4.96	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.62	M1	−	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.99		II							
					+							
11707	24		YES*	YES	YES	YES		NO	NO	NO	YES	
PR-3064			GI50 -5.06	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.68	M1	−	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 1.09		II							
					+							
11842	24		±									
PR-3367			GI50 -5.74	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.89				( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.03		II							

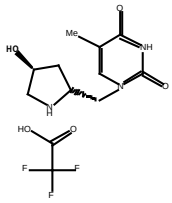
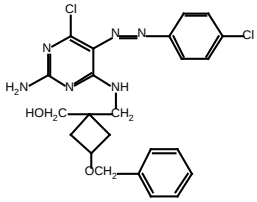
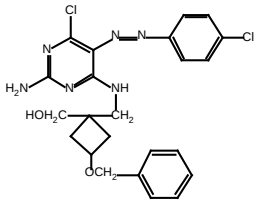
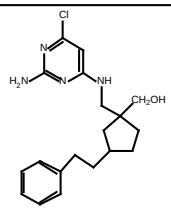
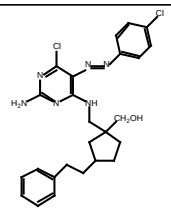
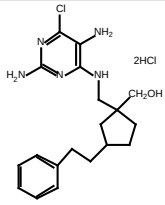
Purine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11843	24		±									
PR-3289			GI50 -5.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.72		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.85									
11844	24		±									
PR-3285			GI50 -5.74	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.14		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.24									
11845	24		±									
PR-3281			GI50 -5.78	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.71		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.87									
11846	24		±									
PR-3309			GI50 -5.72	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.21		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.4									
12005	33		NO			NO						
9-Benzyladenine 1-Oxide			GI50 -4.48	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.4		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ ☒ □ □ □ □ □ □			Range 0.72									
12006	33					NO						
9-Benzyl-8-hydroxyadenine 1-Oxide			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ □ □ ☒ □ □ □ □ □ □			Range									

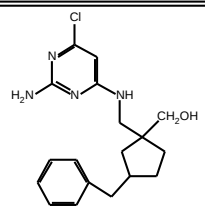
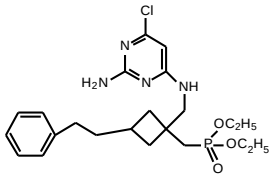
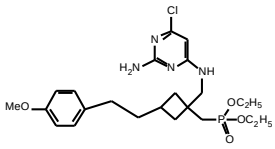
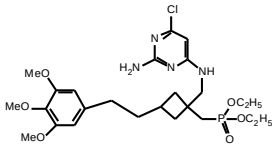
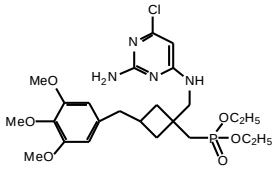
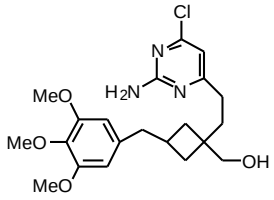
Purine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12029	33		NO									
1,N^2-cyclic guanine			GI50 -4.04	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.87		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.91									
12152	58		NO	NO								
Kinetin			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.47	C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 0.5									
11373	61		YES	NO	NO	YES						
JE-231			GI50 -6.29	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.35		—	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 1.69		II ±							

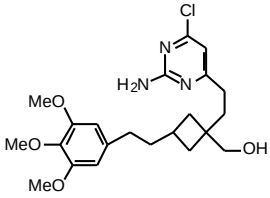
Pyrimidine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12218	14		NO	NO	NO	NO	NO	NO	NO	NO	NO	
TProOH			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.18		—		>1.5 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 0.18		II —							
10634	53		±		NO	NO			YES	NO		
NF-1065-A			GI50 -4.32	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.12		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ ☒ □ □ ☒ ☒ □ □			Range 1.45		II —							
10635	53		±		NO	NO			NO	NO		
NF-1065-B			GI50 -5.09	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.63		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ ☒ □ □ ☒ ☒ □ □			Range 0.95		II —							
11197	53		±	NO	NO	NO			NO			NO
NF-5001			GI50 -4.99	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.7		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ ☒ □ □ ☒			Range 3.11		II —							
11198	53		YES*	NO	NO	NO			NO			NO
NF-5002			GI50 -5.08	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.77		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ ☒ □ □ ☒			Range 2.16		II ±							
11199	53		±	NO	NO	NO			NO			NO
NF-5003			GI50 -4.95	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 3.05		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ ☒ □ □ ☒			Range 3.54		II —							

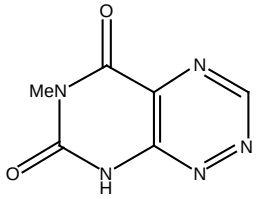
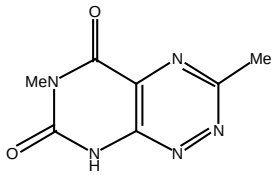
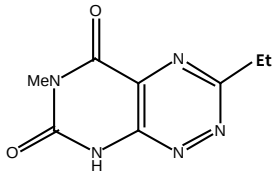
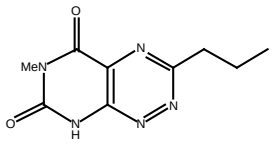
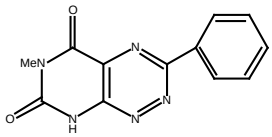
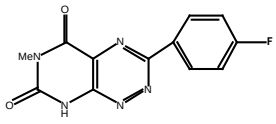
Pyrimidine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11200	53		±	NO	NO	NO			NO			NO
NF-5004			GI50 -4.67	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 2.3		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ ☒ □ □ ☒			Range 2.82		II –							
12065	53		NO	NO	NO	NO		YES	NO	NO	NO	
NF-4001			GI50 -4.67	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.15		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.3		II ±							
12066	53		NO	NO	YES	NO		YES	NO	NO	NO	
NF-4002			GI50 -4.68	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.2	A1 C1 M1 Y1	+		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.45		II –							
12067	53		NO	NO	NO	NO		NO	NO	NO	NO	
NF-4003			GI50 -4.55	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.69		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 0.97		II –							
12068	53		NO	NO	NO	NO		NO	NO		NO	
NF-4004			GI50 -4.33	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ □ ☒ □			Range 0.79		II –							
12179	53		YES	NO	NO	NO		NO	NO	NO	YES	
MN-4101			GI50 -4.29	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.41		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 1.71	E1	II –							

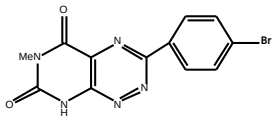
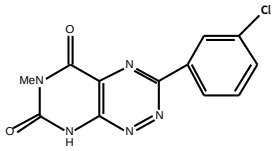
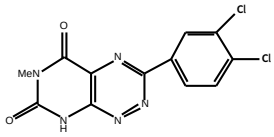
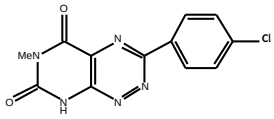
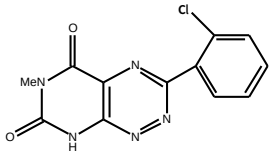
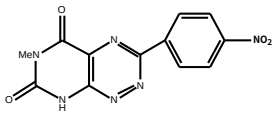
Pyrimidine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12180	53		YES	NO	NO	NO		NO	NO	NO	NO	
MN-4203			GI50 -4.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.51		—		( )					
					II							( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 2.09	E1	—							

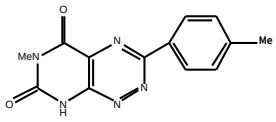
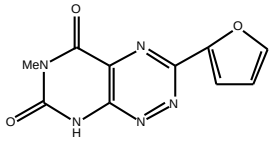
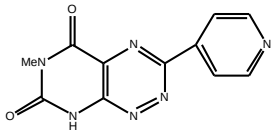
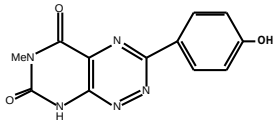
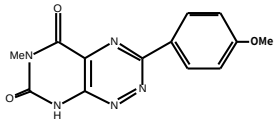
Pyrimidotriazine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11924	50			YES								
6-Methylpyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M2	II		( )					( )
			Range									
11925	50			YES								
3,6-Dimethylpyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M2 C1	II		( )					( )
			Range									
11926	50			NO								
3-Ethyl-6-methylpyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11927	50			NO								
6-Methyl-3-(n-propyl)primido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11928	50			NO								
6-Methyl-3-phenylpyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11929	50			NO								
3-(4-Fluorophenyl)-6-methylpyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									

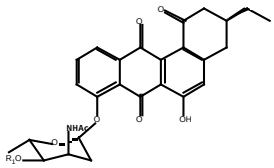
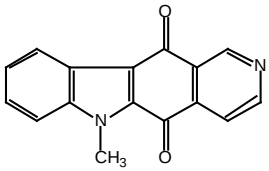
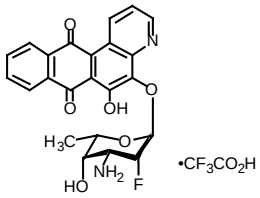
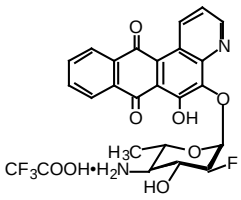
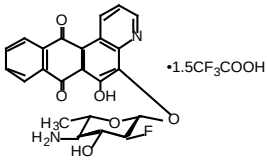
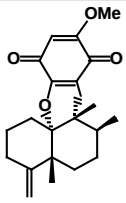
Pyrimidotriazine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11930	50			NO								
3-(4-Bromophenyl)-6-methylpyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11931	50			NO								
3-(3-Chlorophenyl)-6-methylpyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11932	50			NO								
3-(3,4-Dichlorophenyl)-6-methylpyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1 Y1	II		( )					( )
			Range									
11933	50			NO								
3-(4-Chlorophenyl)-6-methylpyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11934	50			NO								
3-(2-Chlorophenyl)-6-methylpyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11935	50			NO								
6-Methyl-3-(4-nitrophenyl)pyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									

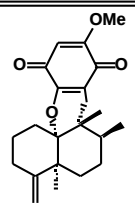
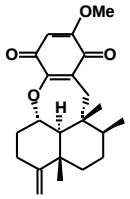
Pyrimidotriazine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11936	50			NO								
6-Methyl-3-(4-methylphenyl)pyromido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									
11937	50			NO								
3-(2-furyl)-6-methylpyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1 Y1 E1	II		( )					( )
			Range									
11938	50			YES								
6-Methyl-3-(4-pyridyl)pyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M2	II		( )					( )
			Range									
11939	50			NO								
3-(4-Hydroxyphenyl)-6-methylpyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta		II		( )					( )
			Range									
11940	50			NO								
3-(4-Methoxyphenyl)-6-methylpyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Delta	M1	II		( )					( )
			Range									

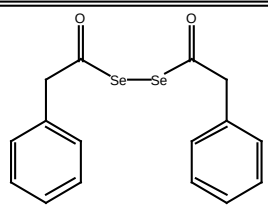
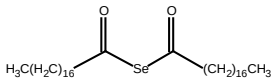
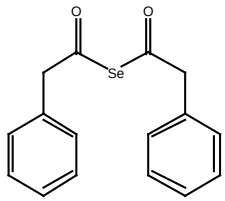
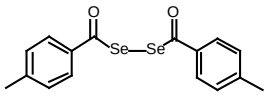
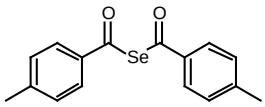
Quinone / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
10506	28							NO				
BRAQ-D			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐			Range									
11623	30		YES									
Q6			GI50 -6.12	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.11		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 2.4									
11688	38		YES	NO	NO	YES		NO			YES	
FAA-301			GI50 -7.25	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.75	A1 C1 M1 Y1	—	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☐ ☒ ☐ ☐ ☒ ☐			Range 1.52		II							
					±							
11689	38		YES	NO	NO	YES		YES			YES	
FAA-401			GI50 -7.11	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.74		—	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☐ ☒ ☐ ☐ ☒ ☐			Range 1.98		II							
					±							
11690	38		YES	NO	NO	NO		NO			YES	
FAA-402			GI50 -7.28	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.72		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☐ ☒ ☐ ☐ ☒ ☐			Range 1.59		II							
					±							
11870	66		NO		NO							
Dactyloquinone A			GI50 -4.71	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.14		±		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.42		II							
					±							

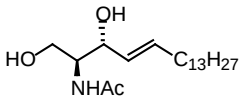
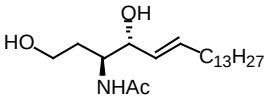
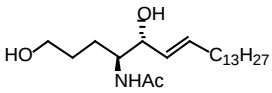
Quinone / Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11871	66		NO		YES							
Dactyloquinone B 1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ □ □ □ □ □ □ □			GI50 -4.72	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.13		+		( )					( )
					II							
			Range 0.41		−							
11872	66		±		NO							
Dactyloquinone C 1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ □ □ □ □ □ □ □			GI50 -4.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.8		±		( )					( )
					II							
			Range 1.15		−							

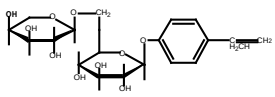
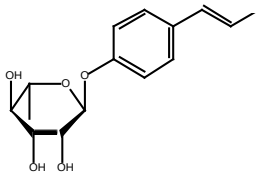
Selenium compound

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11809	26						+ / -					
Diphenylacetyl diselenide			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		49.7 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐ ☐			Range									
11810	26						NO					
Distearoyl selenid			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		>163 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐ ☐			Range									
11811	26						+ / -					
Diphenylacetyl selenide			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		95.9 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☐ ☐ ☐ ☒ ☐ ☐ ☐ ☐ ☐			Range									
11660	26		YES	NO	NO	N.D.	+ / -					
Di-ρ-tolunoyl diselenide			GI50 -5.21	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.91	M1	—		22.9 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☐ ☐ ☐ ☐ ☐			Range 1.61		II / —							
11661	26			NO			+ / -					
Di-ρ-tolunoyl selenide			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	C1 M1	II		29.6 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☐ ☒ ☐ ☐ ☒ ☐ ☐ ☐ ☐ ☐			Range									

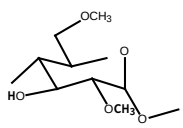
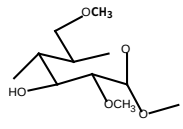
Sphingenine

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12245	41		NO									
(2S,3R,4E)-2-Acetylaminooctadec-4-en-1,3-diol			GI50 -4.77	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.1		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.17									
12246	41		NO									
(3S,4R,5E)-3-Acetylamino-5-nonadecen-1,4-diol			GI50 -4.11	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.66		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.77									
12247	41		NO									
(4S,5R,6E)-4-Acetylamino-eicos-6-en-1,5-diol			GI50 -4.22	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.54		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.77									

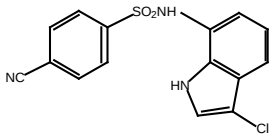
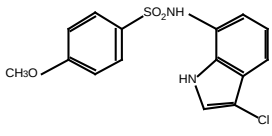
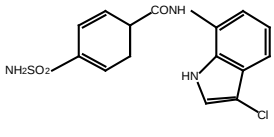
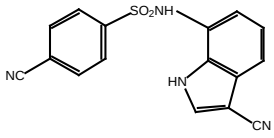
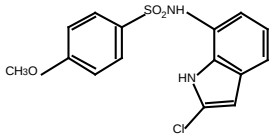
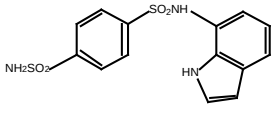
Sugar

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12016	9		NO	NO	NO			NO				
02 [201] T			GI50 -4.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.59		—		( )					( )
					II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ □ □ ☒ □ □ □ □			Range 0.62		—							
11674	49		YES	NO	NO	NO	NO	NO	NO	NO	NO	
B20			GI50 -4.5	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.81		—		>1 (mM)					( )
					II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 1.3		—							

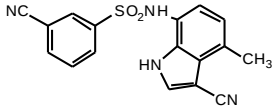
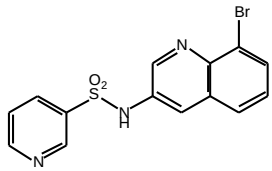
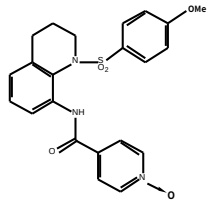
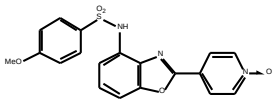
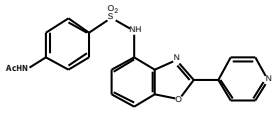
Sugar / Oligosaccharide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12078	47		±									
Dimethyl-α-Cyclodextrin			GI50 -2.79	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.29		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.49									
12079	47		±									
Dimethyl-β-Cyclodextrin			GI50 -3.4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.41		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.96									

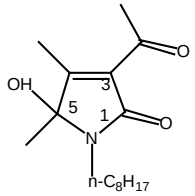
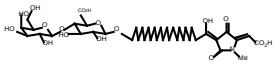
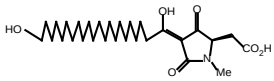
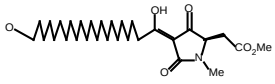
Sulfonamide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11697	1		YES									
ER-35748		G1期阻害剤E7070の類縁体	GI50 -5.04	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Delta 1.34		II		( )					( )
			Range 1.83									
11698	1		YES									
ER-67880		G1期阻害剤E7070の類縁体	GI50 -5.71	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Delta 0.66		II		( )					( )
			Range 1.46									
11699	1		NO									
S455		G1期阻害剤E7070の類縁体	GI50 -4.44	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Delta 0.29		II		( )					( )
			Range 0.63									
11700	1		YES									
ER-68487		G1期阻害剤E7070の類縁体	GI50 -4.62	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Delta 1.65		II		( )					( )
			Range 2.27									
11701	1		±									
ER-68378		G1期阻害剤E7070の類縁体	GI50 -6.49	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Delta 0.93		II		( )					( )
			Range 2.43									
11702	1		NO									
S452		G1期阻害剤E7070の類縁体	GI50 -4.12	spec.	I	mode	IC50					T/C% (mg/kg)
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Delta 0.49		II		( )					( )
			Range 0.61									

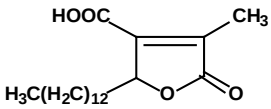
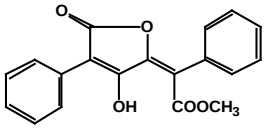
Sulfonamide

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12104	1		±									
LA-820			GI50 -4.81	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.82		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 2.29									
12106	1		±									
LA-1074			GI50 -4.19	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.85		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.05									
11207	8		YES	NO	NO	YES		NO	NO	NO	YES	
FC-4353			GI50 -7.05	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.57		— II	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 3.12		—							
11208	8		YES	NO	NO	YES		NO	NO	NO	YES	
FC-4677			GI50 -5.7	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.75		— II	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 2.35		—							
11209	8		YES	NO	NO	YES		NO	NO	NO	YES	
FC-4711			GI50 -7.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.65		— II	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 3.13		—							

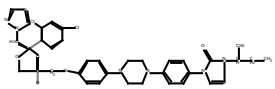
Tetramic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11677	16		NO									
MT-21			GI50 -4.62	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.16		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.4									
11712	48		NO	NO					NO	NO		
Ancorinoside B			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0	A1 C1 Y1 E1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ ☒ ☒ □ □			Range 0									
11713	48		NO	NO					NO	NO		
Ancorinoside aglycon			GI50 -4.04	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.35		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ ☒ ☒ □ □			Range 0.38									
11714	48		NO	NO					NO	NO		
Ancorinoside aglycon methylester			GI50 -4.05	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.41		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ ☒ ☒ □ □			Range 0.47									

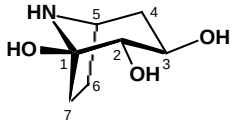
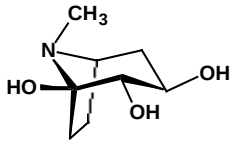
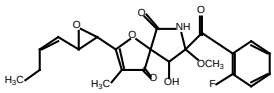
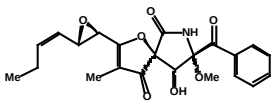
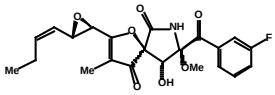
Tetronic acid

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11883	39		NO									
Lichesterinic acid			GI50 -4.55	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.67									
11886	39		NO									
Vulpinic acid			GI50 -4.46	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.31		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 0.77									

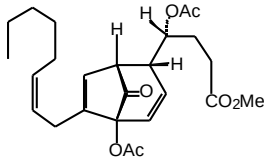
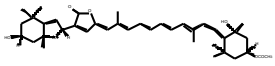
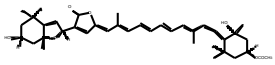
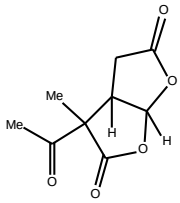
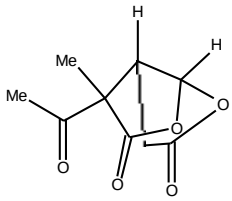
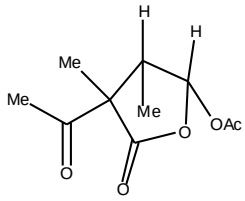
Triazole

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12198	47		±					NO				
Itraconazole			GI50 -7.74	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.26		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ ☒ □ □ □ □		抗真菌剤、免疫抑制活性も報告されている	Range 3.65									

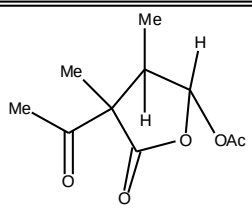
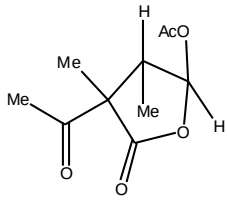
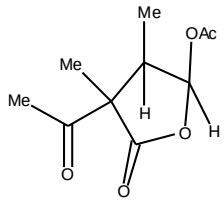
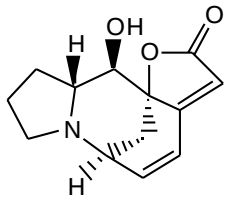
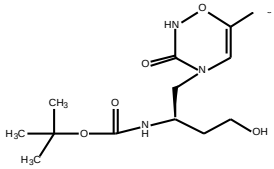
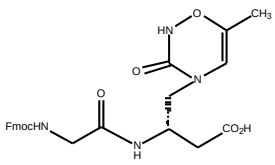
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11969	2		NO	NO	NO	NO			NO			
Calystegine A3			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ ☒ □ □ □			Range 0		II							
					—							
11970	2		NO	NO	NO	NO			NO			
N-Methyl-calystegine A3			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ ☒ □ □ □			Range 0		II							
					—							
11009	5		YES	NO	NO			NO			YES	
2-Fluorosynerazol			GI50 -5.68	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.01		—		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ □ □ ☒ □ □ ☒ □			Range 2.13		II							
					—							
12148	5	*	NO	NO	NO	NO	NO	NO			NO	
Clethramycin			GI50 -4.74	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.12		—		953 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ □ □ ☒ □			Range 0.31		II							
					—							
12210	5		YES	NO								
Synerazol			GI50 -5.48	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.88				( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 1.86		II							
12211	5		YES	NO								
3-Fluorosynerazol			GI50 -4.53	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.15				( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ □ □			Range 1.61		II							

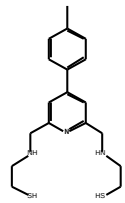
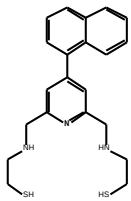
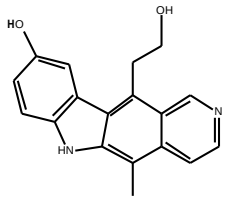
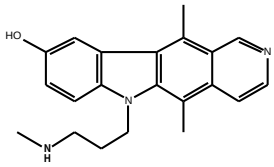
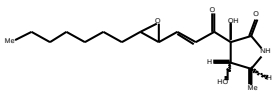
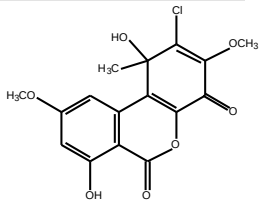
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11584	6		NO									
KKM-03			GI50 -4.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.45		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 0.71									
11861	6	* 	YES									
KKM-17			GI50 -4.66	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.62		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 1.28									
11862	6	* 	YES									
KKM-18			GI50 -4.95	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.55		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ □ □ □ □ □ □ □ □ □			Range 1.33									
12114	12		±	NO	YES	NO	NO	NO	NO		YES	
Bislactone 1			GI50 -4.25	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 3.17	A1 C1 M1 Y1	+ II +		793 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ ⊠ ⊠ ⊠ □ ⊠ □			Range 3.42									
12115	12		NO	YES	YES	NO	NO	NO	NO		YES	
Bislactone 2			GI50 -4.12	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.68	C2 A1 M1 Y1	+ II +		370 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ ⊠ ⊠ ⊠ □ ⊠ □			Range 0.8									
12116	12		YES	NO	YES	NO	NO	NO	YES		YES	
Acetomycin			GI50 -5.45	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.38	A1 C1 M1 Y1	++ II −		>2.3 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ ⊠ ⊠ ⊠ □ ⊠ □			Range 1.06									

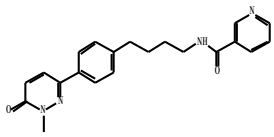
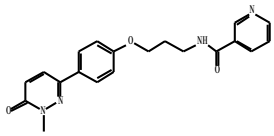
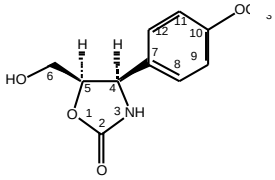
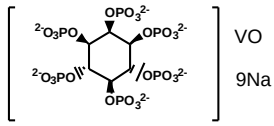
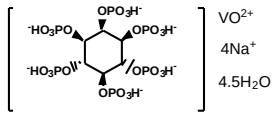
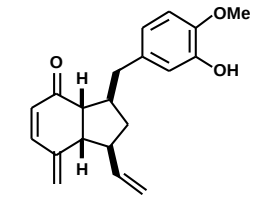
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12121	12		YES	NO	NO	NO	NO	NO	NO		YES	
4-epi-Acetomycin			GI50 -4.81	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.76	A1 C1 M1	±		>2.3 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☐ ☒ ☐			Range 1.01		II ±							
12122	12		YES	YES	NO	NO	NO	NO	NO		NO	
5-epi-Acetomycin			GI50 -5.45	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.43	C2 A1 M1 Y1	—		>2.3 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☐ ☒ ☐			Range 1.27		II ±							
12123	12		YES	NO	NO	NO	NO	NO	NO		YES	
4,5-Diepi-Acetomycin			GI50 -4.82	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.78	A1 C1 M1	—		>3.4 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☐ ☒ ☐			Range 1.15		II ±							
12063	13		NO	NO							NO	
SS-9-3			GI50 -4	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.15		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☒ ☐			Range 0.15									
12214	14		±	NO	NO	NO	NO	NO	NO	NO	NO	
TASpOH			GI50 -4.04	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.28		— II		>1.6 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☐			Range 1.32		—							
12215	14		NO	NO	NO	NO	NO	NO	NO	NO	NO	
TGlyAsp			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.42		— II		11.6 (mM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☐			Range 0.43		—							

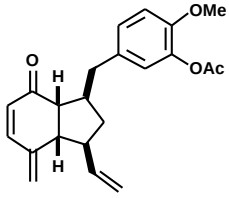
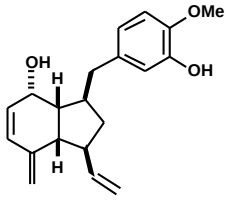
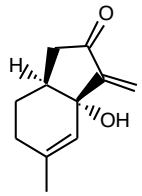
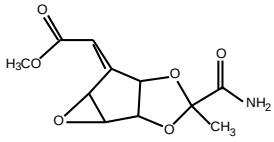
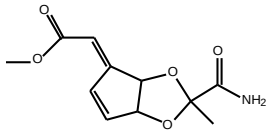
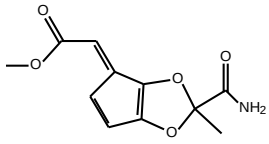
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12216	14		±	YES	NO	NO		NO	NO	NO	YES	
4-Tol-HPH-SH			GI50 -5.74	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.22	A1 C1 M1 E2	–		( )					( )
			Range 0.3		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □					–							
12217	14		±	NO	NO	N.D.		NO	NO	NO	YES	
1-Naph-HPH-SH			GI50 -5.71	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.1	A1 C1 M1 Y1 E1	–		( )					( )
			Range 0.21		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □					–							
11137	15		YES*	NO	YES							
T-722			GI50 -6.2	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.62	A1 C1 Y1	–		( )					( )
			Range 1.26		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ □ □ □ □ □ □ □					++							
11214	15		YES		YES							
T-107			GI50 -7.48	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.52		–		( )					( )
			Range 1.48		II							
1 2 3 4 5 6 7 8 9 10 ☒ □ ☒ □ □ □ □ □ □ □					++							
11552	15		NO	NO	YES	NO		NO	NO	NO	YES	NO
LGZK-060			GI50 -4.72	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.75	A1 C1 Y1 E1	+		( )					( )
			Range 0.99		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒					++							
11553	15		YES*	YES	YES	YES		NO	NO	NO	YES	NO
LGZK-064			GI50 -5.63	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.63	-	+	poly.	( )					( )
			Range 1.27	E3	II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒					++							

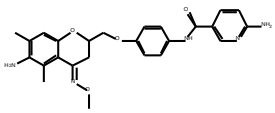
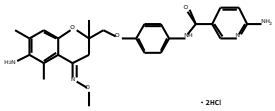
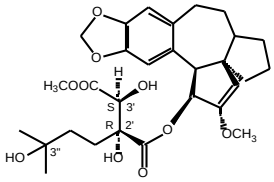
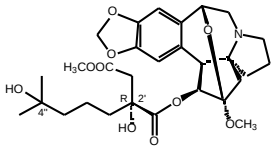
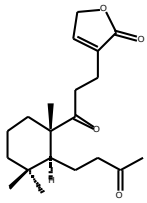
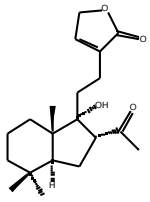
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11612	15		±	NO	NO	NO		NO	NO	NO	NO	
T-3999			GI50 -4.3	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.07		−		( )					( )
			Range 1.37		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □					−							
11613	15		YES	NO	NO	NO		NO	NO	NO	YES	
T-1008			GI50 -4.42	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.11		−		( )					( )
			Range 1.53		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □					−							
11680	16		NO									
Cytoxazone			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.17				( )					( )
			Range 0.18		II							
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □												
11867	17		NO	NO	YES	N.D.		NO	NO	NO	NO	NO
Sodium vanadyl phytate (VP-IP6)			GI50 -4.08	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.69		±		( )					( )
			Range 0.77		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒					++							
11952	17		NO	NO	NO	N.D.		NO	NO	NO	NO	NO
myo-Inositol 1,2,3,4,5,6-hexaphosphate/Sodium vanadyl phytate-IIII			GI50 -5.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.56		−		( )					( )
			Range 0.58		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒					±							
12203	19		YES*	NO	NO	YES		NO	NO	NO	YES	
HA-01			GI50 -8.26	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.31		−	poly.	( )					( )
			Range 3.56		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □					−							

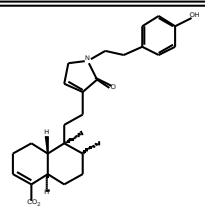
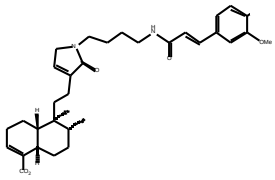
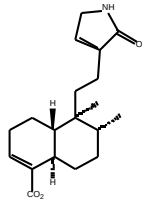
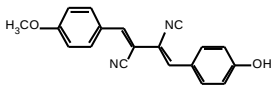
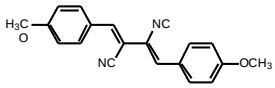
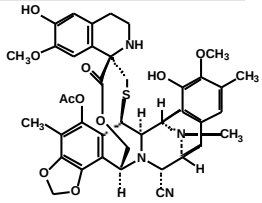
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
12204	19		YES*	YES	+ / -	YES		NO	NO	NO	YES	
HA-02			GI50 -8.22	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.32	Y1	±	poly.	( )					( )
			Range 3.55	E2	II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □					—							
12205	19		YES	NO	+ / -	YES		NO			YES	
HA-03			GI50 -6.73	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.27	C1 M1 Y1	±	poly.	( )					( )
			Range 4	E1	II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ □ □ ☒ □					—							
12077	22		NO	NO	NO	NO	NO	NO	NO	NO	YES	NO
Jolkinolide D pharmacophore			GI50 -4.65	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.1		—		>2.7 (mM)					( )
			Range 0.43		II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒					—							
11419	23		NO									
Stresgenin A			GI50 -4.01	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.31		II		( )					( )
			Range 0.31									
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □												
11420	23		YES*	NO	YES	NO		NO	NO	NO	YES	
Stresgenin B			GI50 -5.03	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.61	M1	+		( )					( )
			Range 1.01	E1	II							
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □					++							
11421	23		NO									
Dehydro-Stresgenin B			GI50 -4.09	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.57		II		( )					( )
			Range 0.66									
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □												

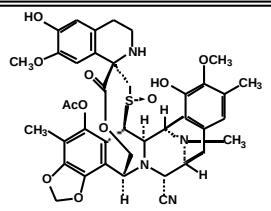
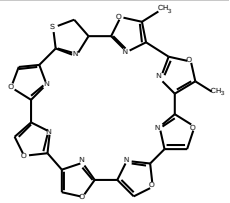
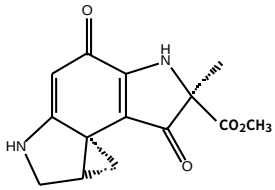
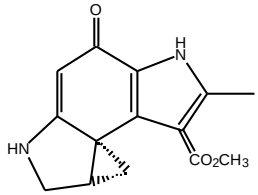
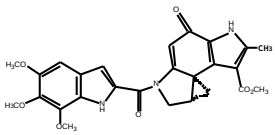
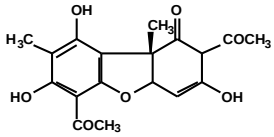
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11330	25		YES									
FT-5			GI50 -7.11	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.89		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 3									
11368	25			NO	NO	YES						
FT-6			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		—	poly.	( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ ☒ ☒ □ □ □ □ □ □			Range		II —							
11498	28		YES	NO	NO							
Cephalezomine C			GI50 -6.76	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.85	-	— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ □ □ □ □ □ □ □			Range 1.96		—							
11499	28		YES									
Cephalezomine A			GI50 -7.29	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.47		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.11									
11774	28			NO								
CHAPEC-A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ □ □ □ □ □			Range									
11775	28			NO								
CHAPEC-B			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ □ □ □ □ □			Range									

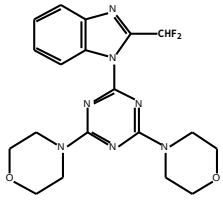
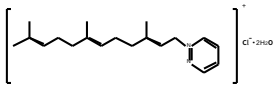
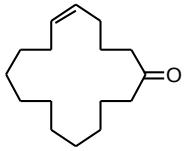
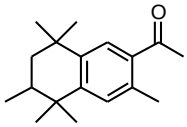
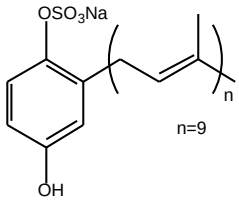
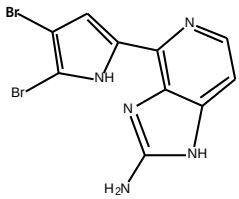
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11776	28			NO								
ECHNP-A			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ □ □ □ □ □			Range									
11777	28			NO								
ECHNP-B			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ □ □ □ □ □			Range									
11778	28			NO								
ECHNP-C			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta		II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ⊠ □ □ □ □ □ □ □ □			Range									
12072	29		±	NO						NO		
Xanthocillin X monomethyl ether			GI50 -5.65	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.27		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ □ □ ⊠ □ □ ⊠ □ □			Range 1.2									
12073	29		YES*	NO	NO	NO				NO		
Xanthocillin X dimethyl ether			GI50 -6.21	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.13		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ ⊠ □ □ ⊠ □ □			Range 3.34		—							
11783	31		YES	NO	NO	NO		NO		NO	YES	
Ecteinascidin (Et 770)			GI50 -8.62	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.39		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ ⊠ □ ⊠ ⊠ □			Range 1.01		±							

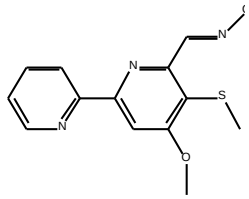
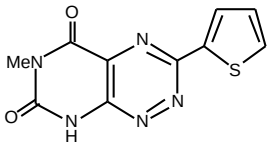
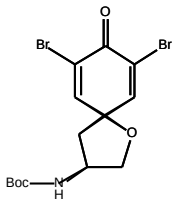
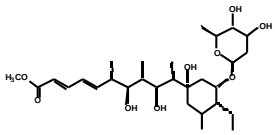
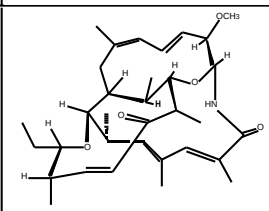
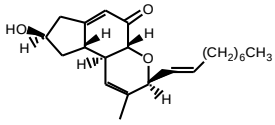
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11784	31		YES	NO	NO	NO		NO		NO	YES	
Ecteinascidin 786 (Et 786)			GI50 -7.61	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.66		±		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ □ ☒ ☒ □			Range 1.53		II							
					–							
11863	35	 テロメラーゼ阻害物質	YES									
Telomestatin (GM95)			GI50 -5.19	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.79				( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.83		II							
12025	36	 DNAアルキル化物質Duocarmycinの部分構造	YES									
Seg A of DuA			GI50 -4.89	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.31				( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.79		II							
12026	36	 DNAアルキル化物質Duocarmycinの部分構造	±									
Seg A of 86			GI50 -5.97	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.87				( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.45		II							
12027	36	 DNAアルキル化物質Duocarmycinの部分構造	YES									
Du86			GI50 10.4!	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.66				( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.56		II							
11882	39		YES	NO	NO	NO		NO	NO			NO
d-Usnic acid			GI50 -4.8	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.57		–		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ □ □ ☒			Range 0.78		II							
					–							

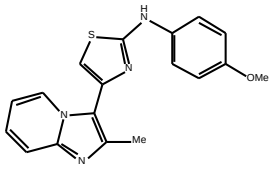
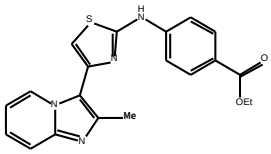
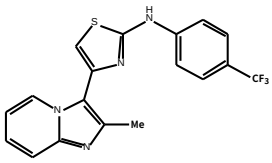
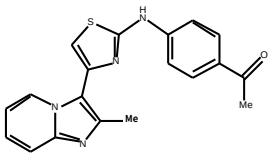
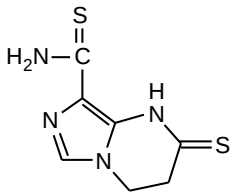
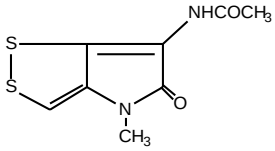
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11596	40		YES									
ZSTK474			GI50 -6.37	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.95		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 1.86									
11830	42		YES	NO	YES	NO						
Farnesyl-pyridazinium chloride・2H2O			GI50 -5.63	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.4		+ II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ □ □ □ □ □			Range 2.15		+							
12034	46		NO									
5-Cyclohexadecen-1-one			GI50 -4.44	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.31		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.74									
12035	46		NO									
1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthalenyl)-ethanone			GI50 -4.64	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.49		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.94									
11708	48		NO	YES						NO		
Nonaprenylhydroquinone sulfate			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.35	A2 C2	II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ □ □ □ □ □ □ ☒ □ □		強い界面活性作用が予測される	Range 0.38									
12048	48		YES	NO	NO	NO		NO	NO	NO	NO	
Ageladiine A			GI50 -4.86	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.97	A1 Y1	− II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ □			Range 1.44		−							

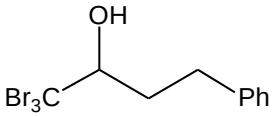
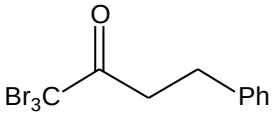
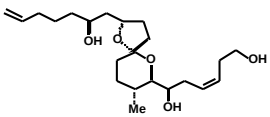
Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11968	49		YES						YES			
MN4004A			GI50 -6.2	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.33		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ ☒ □ □ □			Range 2.02									
11749	50		NO	YES	NO	NO		NO	NO	NO	NO	NO
6-Methyl-3-thienyl pyrimido[5,4-e]-1,2,4-triazine-5,7(6H,8H)-dione			GI50 -4.05	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.76	Y2 C2 A1	— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ ☒			Range 0.81		—							
11755	52			YES				NO				
Gym.Analog-19			GI50	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta	Y2 A1 C1	II		( )					( )
1 2 3 4 5 6 7 8 9 10 □ ☒ □ □ □ ☒ □ □ □ □			Range									
11808	52		YES*									
92DRT-II			GI50 -5.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.97		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 3.01									
11850	52		YES	NO	NO	NO		NO	NO	NO	YES	
Halichomycin			GI50 -5.68	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.96		— II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ □ ☒ ☒ ☒ ☒ □			Range 1.79		—							
12058	52		NO									
Penostatin A			GI50 -4.77	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.2		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ □ □ □ □ □ □ □ □ □			Range 0.34									

Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11023	55		YES									
PFB-001			GI50 -7.95	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.39		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 3.34									
11327	55		YES									
PFB-002			GI50 -7.28	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.72		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 2.2									
11328	55		YES									
PFB-003			GI50 -7.23	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.77		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 3.1									
11329	55		YES									
PFB-004			GI50 -7.35	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.65		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 3.1									
12074	62		±	YES	YES	NO	NO	NO	NO	NO	YES	
8-Thiocarbamoyl-1,2,3,4-tetrahydroimidazo[1,5-a]pyrimidin-2[1H]-thione			GI50 -4.18	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 1.04	M2 Y2 A1 C1 E1	– II		874 (μM)					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☒ ☐			Range 1.22		+							
11770	64		YES									
Thiolutin			GI50 -6.65	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.37		II		( )					( )
1 2 3 4 5 6 7 8 9 10 ☒ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐			Range 1.13									

Miscellaneous

JCI.No compound screening	sup. code	screening No. / structure/comments	1 HCC panel	2 PK	3 Topo.	4 Tub.	5 HDAC.	6 p-Gp	7 Inv.	8 Angio.	9 Apo.	10 P388
11414	71		NO	NO	YES	NO						NO
SCRC99-6			GI50 -4.47	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.32		−		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ ⊠			Range 0.6		II							
					+							
11415	71		NO	YES	YES	NO						NO
SCRC99-7			GI50 -4.57	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.2	M2 Y2 A1 C1 E1	++		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ □ □ □ □ ⊠			Range 0.78		II							
					++							
11769	71		NO	NO	NO	NO		NO	NO	NO	NO	
Attenol A			GI50 -4.02	spec.	I	mode	IC50					T/C% (mg/kg)
			Delta 0.47		−		( )					( )
1 2 3 4 5 6 7 8 9 10 ⊠ ⊠ ⊠ ⊠ □ ⊠ ⊠ ⊠ ⊠ □			Range 0.49		II							
					−							