

Table S5.167 potential bioactive compounds targeting SMAD2-ETV4 interaction.

Number	Name	Molecular weight(g/mol)	Binding energy(kcal/mol)
1	Adenosine 5'-diphosphoribose sodium	581.3	-8.92
2	Parishin B	728.65	-8.618
3	NADP disodium salt	787.37	-8.26
4	NADPH tetracyclohexanamine	1142.12	-8.253
5	NADH disodium salt	709.4	-8.193
6	AICAR monophosphate	338.21	-7.913
7	Rebaudioside A	967.01	-7.779
8	Isolugrandoside	640.59	-7.509
9	Coenzyme A	767.53	-7.498
10	Tubuloside A	828.76	-7.483
11	2'-Deoxycytidine-5'-monophosphoric acid	307.2	-7.458
12	CTP disodium dihydrate	563.15	-7.454
13	Cytidine 5'-monophosphate	323.2	-7.395
14	Asiaticoside	959.12	-7.347
15	Adenosine 5'-monophosphate disodium salt	391.18	-7.328
16	Adenosine 5'-monophosphate monohydrate	365.24	-7.328
17	Adenosine monophosphate	347.22	-7.328
18	INOSINIC ACID	348.21	-7.289
19	Triciribine phosphate	400.28	-6.94
20	Vidarabine phosphate	347.22	-6.937
21	L-Chicoric Acid	474.37	-6.913
22	2'-Deoxyadenosine-5'-monophosphate	331.22	-6.83
23	Ceftibuten dihydrate	446.46	-6.703
24	Carba-NAD TEA	762.64	-6.672
25	Luteolin 7-diglucuronide	638.48	-6.598
26	Parishin C	728.65	-6.583
27	MethADP	425.23	-6.566
28	cangrelor tetrasodium	864.29	-6.553
29	diaminohydroxypropanetetraacetic acid	322.27	-6.487
30	2-({5,5-dimethyl-6-oxa-17-thia-2,12,14-triazatetracyclo[8.7.0.0^{3,8}.0^{11,16}]heptadeca-1(10),2,8,11(16),12,14-hexaen-15-yl}sulfanyl)acetic acid	361.43	-6.423
31	Sennoside C	848.76	-6.418
32	Latanoprost acid	390.51	-6.365
33	dADP disodium	455.17	-6.327
34	Cytidine-5'-triphosphate disodium	527.12	-6.321
35	dFdCTP trisodium	569.08	-6.316
36	3-O-Methylgallic acid	184.15	-6.297
37	Epithalon TFA (307297-39-8 free base)	504.37	-6.265
38	Secologanoside	390.34	-6.245
39	D-Ribose 5-phosphate disodium dihydrate	310.1	-6.235
40	Sodium Glucuronic Acid	216.12	-6.228
41	ATP dimagnesium	551.76	-6.214
42	Fludarabine	285.23	-6.213
43	Pyrroloquinoline quinone	330.21	-6.2
44	NADP sodium salt	765.39	-6.187
45	6-amino-4-(furan-3-yl)-3-methyl-1H,4H-pyrano[2,3-c]pyrazole-5-carbonitrile	242.238	-6.185
46	D-Glucose 6-phosphate sodium	282.12	-6.161
47	Dextrorotation nimorazole phosphate ester TFA	464.29	-6.142
48	Aztreonam	435.43	-6.121
49	SF2312	197.08	-6.108
50	GSK2983559 free acid	538.53	-6.089
51	ATP	507.18	-6.056
52	Tiludronate disodium	362.57	-6.029
53	Rhizoferrin	436.37	-6.027
54	Cytidine 5'-diphosphate trisodium salt	472.15	-6.02
55	Ceftaroline fosamil	744.74	-5.993
56	Cefonicid sodium	586.53	-5.958
57	Cytidine 5'-diphosphate disodium	447.14	-5.946
58	Sulbactam Sodium	403.18	-5.946

59	3'-Adenylic acid	347.22	-5.936
60	2'-Fluoro-2'-Deoxyadenosine	269.23	-5.823
61	Gallic acid	170.12	-5.755
62	(2RS)-FPMPA	305.2	-5.744
63	Tigemonam	437.41	-5.734
64	2'-Deoxyadenosine-5'-triphosphate trisodium	557.13	-5.726
65	Tenofovir	287.21	-5.72
66	Adenosine	267.24	-5.708
67	NAD+	663.43	-5.694
68	Pemetrexed disodium	471.37	-5.688
69	2'-O-Methyladenosine	281.27	-5.687
70	Cefixime	453.45	-5.674
71	ATP disodium salt	551.14	-5.668
72	L-Ascorbic acid 2-phosphate magnesium	289.53	-5.657
73	Diacerein	368.29	-5.653
74	Citicoline sodium	510.31	-5.628
75	Folic acid	441.4	-5.627
76	Adenosine 5'-diphosphate	427.2	-5.619
77	4-({2-[(furan-2-yl)methyl]carbamoyl}methyl)sulfanyl]-4-oxo-3H,4H-thieno[3,2-d]pyrimidin-3-yl}methyl)benzoic acid	455.5	-5.614
78	Thyrotropin-Releasing Hormone (TRH), Free Acid	363.37	-5.598
79	T-1105	139.11	-5.584
80	Sparfosic Acid	255.12	-5.575
81	WAY-297174	268.36	-5.566
82	2-(1,3-benzoxazol-2-ylsulfanyl)butanoic acid	237.27	-5.556
83	5-[2-(1,3-dioxo-2,3-dihydro-1H-isoindol-2-yl)acetamido]benzene-1,3-dicarboxylic acid	368.301	-5.555
84	Cidofovir	279.19	-5.533
85	Cidofovir dihydrate	315.22	-5.533
86	(-)-Hydroxycitric acid	208.12	-5.486
87	Brevifolincarboxylic acid	292.2	-5.462
88	Risedronate Sodium	305.09	-5.459
89	Risedronic Acid	283.11	-5.459
90	H-Gly-Arg-Gly-Asp-Asn-Pro-OH	614.61	-5.452
91	2-Aminopurine	135.13	-5.439
92	2-PMPA	226.12	-5.425
93	NAAD sodium salt	686.4	-5.406
94	FPI-1523 sodium	344.27	-5.404
95	Protocatechuic acid	154.12	-5.374
96	Cordycepin	251.24	-5.358
97	D-Saccharic acid 1,4-lactone hydrate	317.81	-5.34
98	ATP disodium trihydrate	605.19	-5.33
99	Fludarabine Phosphate	365.21	-5.271
100	Besifovir	299.22	-5.262
101	3-(3-carboxypropanamido)benzoic acid	237.211	-5.258
102	2'-Deoxycytidine-5'-diphosphate trisodium	453.12	-5.254
103	Levorotation nimorazole phosphate ester TFA	464.29	-5.222
104	3-({4-[(2-carboxyethyl)amino]-9,10-dioxo-9,10-dihydroanthracen-1-yl}amino)propanoic acid	382.372	-5.193
105	Alendronate sodium hydrate	325.12	-5.193
106	Erdosteine	249.31	-5.18
107	Oxaquin TEA	807.77	-5.123
108	L-Ascorbic acid 2-phosphate trisodium	322.05	-5.11
109	Alendronic Acid	249.1	-5.107
110	Pyrrroloquinoline quinone disodium salt	374.17	-5.071
111	5-Acetylsalicylic acid	180.16	-5.067
112	DL-Isocitric acid trisodium salt	258.07	-5.067
113	Pamidronate Disodium	279.03	-5.059
114	Pamidronate disodium pentahydrate	371.13	-5.059
115	Pamidronic acid	235.07	-5.059
116	Gastrodenol	704.47	-5.028
117	Bismuth Subcitrate Potassium	780.66	-5.023
118	Prednisolone disodium phosphate	484.39	-5.021

119	Citric acid trilithium salt tetrahydrate	281.98	-5.008
120	Hydroxycitric acid tripotassium hydrate	324.41	-5.008
121	Oxaceprol	173.17	-5.005
122	7-Aminocephalosporanic acid	272.28	-4.996
123	Hexa-His	840.85	-4.992
124	Deferitricin	253.27	-4.955
125	Isovanillic acid	168.15	-4.953
126	Pemetrexed	427.41	-4.949
127	Pemetrexed disodium hemipenta hydrate	518.43	-4.949
128	BAPTA	476.43	-4.938
129	Fibrinogen-Binding Peptide fb-acetate	681.8	-4.89
130	Clodronate disodium tetrahydrate	360.92	-4.889
131	Fast Green FCF	808.85	-4.868
132	2',5'-Dideoxyadenosine	235.24	-4.848
133	Tetrahydrofolic acid	445.43	-4.825
134	Pyrocatechuic acid	154.12	-4.807
135	AB-680	580.82	-4.79
136	D-(-)-3-Phosphoglyceric acid disodium	230.02	-4.769
137	Gadopentetate dimeglumine	938	-4.751
138	3,5-Dihydroxybenzoic acid	154.12	-4.743
139	Carboxyatractyloside	770.82	-4.74
140	Aminopterin	440.41	-4.722
141	Pimodivir	399.39	-4.688
142	2-({1-[3-(ethoxycarbonyl)-5-ethylthiophen-2-yl]-2,5-dioxopyrrolidin-3-yl}sulfanyl)benzoic acid	433.49	-4.683
143	3-[(2E)-2-[(pyridin-3-yl)methylidene]hydrazin-1-yl]benzoic acid	241.25	-4.678
144	N-Acetyl-L-aspartic acid	175.14	-4.667
145	5-Aminosalicyclic Acid	153.14	-4.66
146	Stafib-2	644.46	-4.644
147	Semax acetate(80714-61-0 free base)	873.98	-4.635
148	Aspirin	180.16	-4.631
149	Penicillin G benzathine	909.13	-4.619
150	Pentetic Acid	393.35	-4.618
151	Levovirin	244.2	-4.542
152	4-Pyridoxic Acid	183.16	-4.538
153	N2-methylguanine	165.15	-4.538
154	N-[(2-chlorophenyl)methyl]-2- {[4-oxo-3-(2-phenylacetamido)-3,4-dihydroquinazolin-2-yl}sulfanyl}acetamide	492.98	-4.531
155	10-Formylfolic acid	469.41	-4.503
156	2-(7-hydroxy-2-oxo-2H-chromen-4-yl)acetic acid	220.1782	-4.467
157	Cefsulodin sodium	554.52	-4.46
158	Splenopentin diacetate	753.84	-4.456
159	Tricarballic acid	176.12	-4.455
160	Favipiravir	157.1	-4.444
161	LY 345899	471.42	-4.424
162	Sodium etidronate	249.99	-4.423
163	DL-O-Phosphoserine	185.07	-4.421
164	O-Phospho-L-serine	185.07	-4.421
165	Picolinamide	122.12	-4.416
166	Aurintricarboxylic acid	422.34	-4.412
167	Zoledronic Acid	272.09	-4.411