

### Supplementary material

Descriptors	Butyric acid	CBHA	Depudecin	MS-275	Oxamflatin	Phenyl butyrate	PXD-101	Pyroxa-mide	SAHA	SFHA	TSA	Valproic acid
<b>LogP</b>	0.996	0.305	0.202	2.03	2.187	2.151	2.22	1.396	2.47	3.343	2.68	1.68
<b>Solubility</b>	-1	-2.56	-1.98	-4.21	-5.17	-2.13	-3.61	-2.53	-3.33	-5.03	-3.26	-1.43
<b>Molecular weight</b>	88.106	222.2	212.245	376.416	342.376	164.204	318.354	265.313	264.325	286.356	302.374	116.16
<b>TPSA</b>	37.229	98.652	65.512	106.345	95.495	37.299	95.495	91.316	78.424	61.353	69.635	37.299
<b>n Atoms</b>	6	16	15	28	24	12	22	19	19	20	22	8
<b>n ON</b>	2	6	4	7	6	2	6	6	5	4	5	2
<b>n OHNH</b>	1	4	2	4	3	1	3	3	3	3	2	1
<b>n Violations</b>	0	0	0	0	0	0	0	0	0	0	0	0
<b>n Rotatable bonds</b>	2	3	5	7	4	4	5	6	8	5	6	3
<b>Volume</b>	89.801	190.268	197.632	339.353	288.25	161.45	266.106	251.487	255.644	252.803	293.12	123.19
<b>Drug score</b>	0.18	0.41	0.39	0.11	0.28	0.47	0.15	0.37	0.35	0.13	0.37	0.61
<b>Drug Likeness</b>	-3.94	-2.45	-3.52	-14.52	-5.31	-7.06	-7.33	-7.22	-8.87	-3.22	1.24	0.36
<b>Binding Score of HDAC 1,2,3 &amp; 8 respectively in kcal/mol.</b>	-5.73, -6.47, -6.63, -6.96	-7.08, -7.77, -7.75, -7.82	-5.73, -6.64, -5.91, -6.83	-7.89, -10.5, -9.92, -8.84	-7.23, -11.38, -8.88, Nil	-7.55, -8.56, -8.62, -9.0	-7.50, Nil, -9.08, -7.43	-6.44, -8.17, -7.28, -6.55	-6.42, -9.02, -7.45, -9.0	-8.08, -9.87, -9.7, -10.16	-8.99, -8.58, -8.9, -9.34	-7.04, -8.48, -8.82, -9.24

Table 1: Molecular descriptors value for the twelve HDACi'.