

Table 3. AML: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]*.

Name	MW	LogP	LogS	TPSA	Rotb	HBD	HBA	BBB	HIA	HERG	AMES	FHM	HBT	TPT	CYP1A2	CYP2C9	CYP2C19	CYP2D6	CYP3A4
408383	372.3	3.87	-4.67	66.48	4	1	3	0.99	0.98	0.16	0.16	1	0.24	0.98	0.68	0.67	0.66	0.27	0.42
676443	369.38	-0.69	-5.12	112.58	4	3	5	0.99	0.94	0.61	0.61	0.03	0.84	0	0.75	0.22	0.29	0.14	0.33
627757	370.49	2.29	-3.95	38.33	2	1	2	1	0.62	0.01	0.01	0	0.8	0	0.14	0.13	0.27	0.16	0.37
749518	304.35	0.37	-3.84	69.11	4	2	2	0.94	0.99	0.01	0.01	0.35	0.93	0.88	0.87	0.38	0.63	0.06	0.4
641596	314.72	1.33	-4.35	57.53	3	2	5	1	1	0.01	0.01	1	0	0.95	0.4	0.56	0.6	0.03	0.24
116535	327.21	4.79	-5.89	53.49	2	2	2	1	0.98	0.95	0.95	0.41	0.02	0.96	0.76	0.42	0.55	0.12	0.24
722325	374.35	1.96	-5.23	133.11	5	1	4	0.95	0.98	0.1	0.1	0.03	0.14	0.88	0.85	0.19	0.4	0.08	0.31
666597	296.27	2.73	-3.34	97.99	2	4	5	0.89	0.98	0.04	0.04	0.99	0.7	0.87	0.55	0.13	0.36	0.08	0.18
105132	332.35	3.43	-5.2	43.37	1	0	3	0.93	0.99	0.35	0.35	0.36	0.99	0.95	0.83	0.57	0.62	0.28	0.53
673181	290.32	1.59	-5.19	48.78	3	2	4	0.97	0.98	0.09	0.09	0.08	0.22	0.88	0.91	0.2	0.44	0.55	0.28
609964	275.34	4.47	-5.48	29.1	2	1	2	1	0.98	0.13	0.13	0.79	0.93	0.98	0.49	0.22	0.42	0.36	0.25
168470	308.29	2.46	-4.86	112.48	4	2	3	0.73	0.98	0.59	0.59	0.34	0.29	0.89	0.96	0.35	0.49	0.09	0.32
267461	302.28	2.43	-2.04	100.9	2	2	6	0.69	0.96	0.01	0.01	1	0.98	0.94	0.18	0.3	0.4	0.04	0.41
743508	378.4	1.54	-5.51	64.63	6	1	5	0.81	0.9	0.01	0.01	0.92	0.81	0.95	0.93	0.79	0.75	0.07	0.8
695267	350.4	-2.92	-4.37	129.38	2	4	4	1	0.95	0.36	0.36	0.98	0.49	0.93	0.76	0.14	0.5	0.3	0.46
707801	303.33	3.3	-2.68	50.72	1	2	4	1	0.82	0.55	0.55	0.77	0.97	0.94	0.05	0.43	0.2	0.53	0.75
718154	330.34	3.74	-4.53	69.89	3	2	4	0.96	0.96	0.07	0.07	0.9	0.37	0.88	0.86	0.3	0.45	0.1	0.24
59937	262.3	4.73	-5.89	26.3	3	0	2	1	0.98	0.09	0.09	0.8	0.7	0.98	0.77	0.18	0.37	0.26	0.23
684700	360.29	0.13	-4.94	40.13	5	0	3	0.95	0.99	0.57	0.57	0.73	0.15	0.96	0.62	0.24	0.65	0.09	0.75
656591	315.32	4.39	-5.67	47.56	0	1	3	0.83	1	0.09	0.09	0.01	0.77	0.87	0.61	0.34	0.78	0.23	0.61

*Listed are NSC-408383, NSC-676443, NSC-627757, NSC-749518, NSC-641596, NSC-116535, NSC-722325, NSC-666597, NSC-105132, NSC-673181, NSC-609964, NSC-168470, NSC-267461, NSC-743508, NSC-695267, NSC-707801, NSC-718154, NSC-59937, NSC-684700, and NSC-656591. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.

Table 4. Breast cancer: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]*.

Name	MW	LogP	LogS	TPSA	Rotb	HBD	HBA	BBB	HIA	HERG	AMES	FHM	HBT	TPT	CYP1A2	CYP2C9	CYP2C19	CYP2D6	CYP3A4
749518	304.35	0.37	-3.84	69.11	4	2	2	0.94	0.99	0.01	0.01	0.35	0.93	0.88	0.87	0.38	0.63	0.06	0.4
657704	376.32	2.23	-3.57	113.01	2	2	5	0.1	1	0.03	0.03	1	0.98	0.94	0.43	0.59	0.54	0.09	0.53
716825	368.48	-0.59	-5.17	29.1	2	1	3	0.96	1	0.07	0.07	0.01	0.03	0.96	0.66	0.8	0.83	0.09	0.79
669736	297.43	4.81	-4.37	20.31	3	0	2	0.99	0.98	0.09	0.09	1	0.83	0.98	0.1	0.05	0.3	0.5	0.2
726904	308.76	4.19	-5.56	29.1	1	1	1	0.99	0.96	0.47	0.47	1	0.01	0.98	0.64	0.75	0.71	0.22	0.51
362664	251.28	2.62	-4.42	44.7	2	1	2	1	0.98	0.68	0.68	0.41	0.02	0.96	0.76	0.31	0.5	0.12	0.24
668836	390.52	4.05	-4.62	37.38	1	1	2	0.94	0.99	0.08	0.08	0	0.16	0.98	0.3	0.39	0.53	0.29	0.46
649750	334.33	-0.28	-5.7	41.46	3	1	4	0.95	0.27	0.4	0.4	1	0.59	0.95	0.95	0.36	0.94	0.23	0.24
684322	206.24	4.31	-4.95	47.7	0	2	2	1	0.97	0.04	0.04	1	0.7	0.94	0.61	0.09	0.21	0.18	0.09
50648	308.29	3.53	-5.09	117.19	4	2	2	0.97	0.93	0.03	0.03	0.78	0.11	0.95	0.82	0.34	0.43	0.2	0.44
766871	332.32	-3.09	-4.41	49.33	4	2	6	0.26	1	0.05	0.05	0	0.05	0.88	0.68	0.42	0.48	0.07	0.49
382584	299.3	3.71	-4.65	134.62	3	1	2	1	0.99	0.09	0.09	0	0.31	0.96	0.9	0.5	0.71	0.03	0.23
98710	290.32	0.72	-5.19	76.76	3	2	4	1	0.99	0.03	0.03	0.88	0.22	0.89	0.96	0.21	0.38	0.1	0.27
110383	244.31	3.26	-5.9	0	0	0	0	1	0.98	0.08	0.08	0.31	0.36	0.95	0.82	0.1	0.41	0.28	0.21
684969	303.31	1.95	-5.14	50.09	3	1	4	0.06	0.9	0.14	0.14	0.37	0.25	0.96	0.83	0.19	0.5	0.21	0.52
673841	387.2	-3.42	-3.41	102.78	2	4	5	0.99	1	0.07	0.07	0.01	0.7	0.97	0.65	0.46	0.33	0.04	0.1
657996	396.42	0.58	-3.33	138.94	3	5	6	1	0.55	0.48	0.48	1	0.22	0.95	0.42	0.85	0.86	0.18	0.83
652182	396.39	3.39	-3.94	97.66	6	1	7	0.78	0.96	0.03	0.03	1	0.66	0.98	0.28	0.46	0.41	0.07	0.6
699471	343.17	3.4	-5.51	49.33	0	3	2	0.94	1	0.43	0.43	0	0.01	0.98	0.89	0.64	0.85	0.52	0.56
694620	365.36	1.1	-5.33	94.16	4	0	2	0.86	0.94	0.04	0.04	0.6	0.05	1	0.8	0.37	0.58	0.03	0.51

*Listed are NSC-749518, NSC-657704, NSC-716825, NSC-669736, NSC-726904, NSC-362664, NSC-668836, NSC-649750, NSC-684322, NSC-50648, NSC-766871, NSC-382584, NSC-98710, NSC-110383, NSC-684969, NSC-673841, NSC-657996, NSC-652182, NSC-699471, and NSC-694620. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.

Table 5. Lung cancer: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]*.

Name	MW	LogP	LogS	TPSA	Rotb	HBD	HBA	BBB	HIA	HERG	AMES	FHM	HBT	TPT	CYP1A2	CYP2C9	CYP2C19	CYP2D6	CYP3A4
720447	278.31	2.32	-5.3	34.14	2	2	2	0.99	0.94	0.01	0.01	1	0.99	0.98	0.85	0.53	0.36	0.02	0.25
107129	358.51	4.7	-2.77	46.53	1	1	2	0.99	0.94	0.02	0.02	1	0.97	0.69	0.05	0.02	0.12	0.02	0.04
351710	261.34	2.56	-5.83	0	0	1	0	1	0.98	0.6	0.6	0.18	0.27	0.95	0.77	0.16	0.45	0.48	0.21
719502	249.27	1.22	-4.63	17.07	0	1	2	0.83	0.98	0.28	0.28	0.96	0.27	1	0.61	0.18	0.2	0.08	0.18
117917	296.28	3.33	-4.99	121.35	3	2	2	1	0.98	0.51	0.51	0.76	0.02	0.95	0.88	0.34	0.46	0.04	0.34
703104	252.27	-1.7	-4.47	24.39	3	2	4	1	0.69	0.04	0.04	0.99	0.21	0	0.85	0.16	0.45	0.35	0.14
669455	298.21	-5.19	-2.71	90.92	2	0	4	0.99	0.38	0.04	0.04	1	0.35	0.92	0.65	0.15	0.27	0.05	0.21
695333	399.9	3.17	-5.01	85.58	6	2	2	0.16	0.78	0.3	0.3	0	0.05	0	0.41	0.67	0.84	0.05	0.7
732287	329.7	2.53	-5.06	55.12	4	2	2	1	0.98	0.14	0.14	0	0.71	0.88	0.82	0.45	0.68	0.08	0.7
91397	396.91	4.31	-5.77	35.94	6	1	3	0.87	0.95	0.17	0.17	0.34	0.38	0.97	0.45	0.34	0.53	0.62	0.33
680553	311.31	1.64	-5.71	38.33	5	1	3	0.98	1	0.01	0.01	0.16	0.02	0	0.94	0.34	0.39	0.02	0.3
715722	394.23	3.01	-5.16	55.87	2	0	2	0.64	0.89	0.49	0.49	0.88	0.27	0.95	0.79	0.14	0.3	0.3	0.59
653384	400.42	4.02	-4.01	64.61	5	0	7	1	0.99	0.07	0.07	1	0.94	0.94	0.46	0.33	0.39	0.17	0.33
627505	291.37	2.58	-5.85	9.23	1	1	1	0.95	0.98	0.58	0.58	0.4	0.27	0.95	0.75	0.25	0.58	0.47	0.31
20527	371.02	3.44	-4.89	49.33	3	2	2	0.97	0.98	0.03	0.03	0.48	0.11	0.95	0.63	0.39	0.49	0.22	0.35
4290	313.37	2.88	-5.13	84.93	8	0	1	1	0.98	0.38	0.38	0.18	0.27	0.98	0.64	0.37	0.45	0.19	0.33
706989	296.34	2.68	-4.59	27.69	3	0	3	0.97	0.96	0.24	0.24	0.21	0.27	0.98	0.73	0.34	0.6	0.54	0.56
648273	302.37	2.77	-4.94	83.13	6	1	2	0.99	0.98	0.35	0.35	0	0.16	0.98	0.83	0.17	0.48	0.71	0.65
709923	244.29	1.46	-4.69	26.02	1	1	1	1	0.97	0.06	0.06	0.18	0.37	0.89	0.85	0.34	0.69	0.1	0.38
717889	270.39	1.82	-2.31	74.46	0	1	1	0.99	0.94	0.04	0.04	0	0.4	0.5	0.51	0.45	0.52	0.08	0.11

*Listed are NSC-720447, NSC-107129, NSC-351710, NSC-719502, NSC-117917, NSC-703104, NSC-669455, NSC-695333, NSC-732287, NSC-91397, NSC-680553, NSC-715722, NSC-653384, NSC-627505, NSC-20527, NSC-4290, NSC-706989, NSC-648273, NSC-709923, and NSC-717889. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.

Table 6. Colon cancer: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]*.

Name	MW	LogP	LogS	TPSA	Rotb	HBD	HBA	BBB	HIA	HERG	AMES	FHM	HBT	TPT	CYP1A2	CYP2C9	CYP2C19	CYP2D6	CYP3A4
771557	355.39	1.83	-5.31	72.19	3	2	3	1	0.98	0.43	0.43	0	0.02	0.98	0.79	0.72	0.77	0.37	0.93
768051	360.38	2.59	-5.79	35.82	4	1	3	1	0.99	0.07	0.07	0.47	0.45	0.96	0.89	0.12	0.57	0.45	0.76
754670	337.4	1.41	-5.09	72.19	3	2	3	1	0.98	0.26	0.26	0	0.02	0.98	0.81	0.62	0.74	0.38	0.93
722316	315.37	1.37	-5.86	24.39	3	1	3	0.99	0.88	0.49	0.49	0	0.2	0.95	0.82	0.27	0.37	0.39	0.22
684405	345.28	0.75	-3.2	88.59	5	1	5	0.42	0.98	0.04	0.04	0	0.59	0.95	0.47	0.32	0.4	0.08	0.33
676188	250.3	2.64	-5.79	17.07	1	1	2	0.9	0.98	0.29	0.29	0.02	0.06	0.89	0.9	0.13	0.46	0.2	0.4
754664	385.87	2.56	-5.92	72.19	3	2	3	1	0.98	0.27	0.27	0	0	0.98	0.81	0.81	0.87	0.38	0.94
753802	371.84	2.05	-5.59	72.19	3	2	3	1	0.98	0.36	0.36	0	0	0.98	0.81	0.81	0.87	0.38	0.93
382053	359.43	-1.54	-5.77	52.04	5	2	4	0.88	0.98	0.07	0.07	1	0.01	0.95	0.69	0.48	0.56	0.31	0.49
754567	355.39	1.83	-5.31	72.19	3	2	3	1	0.98	0.55	0.55	0	0.02	0.98	0.79	0.62	0.74	0.4	0.93
665497	368.34	4.23	-4.27	72.45	3	0	6	0.93	0.99	0.18	0.18	1	0.98	0.94	0.34	0.45	0.68	0.33	0.41
754666	351.42	1.92	-5.43	72.19	3	2	3	1	0.98	0.19	0.19	0	0.02	0.98	0.81	0.63	0.72	0.38	0.94
656158	283.25	3.7	-5.31	35.53	1	1	3	0.96	0.97	0.46	0.46	0.68	0.18	0.95	0.92	0.23	0.74	0.39	0.69
753211	314.13	0.53	-5.05	23.79	0	0	4	0.96	1	0.02	0.02	0.78	0.66	0.86	0.73	0.35	0.46	0.16	0.3
765699	359.31	-1.11	-5.41	26.02	4	1	3	0.46	0.63	0.26	0.26	0.02	0.16	0.88	0.86	0.39	0.73	0.46	0.63
768313	367.42	1.46	-5.11	81.42	4	2	4	1	0.98	0.39	0.39	0	0.02	0.98	0.81	0.72	0.72	0.42	0.94
778318	351.47	2.19	-5.71	55.12	3	2	2	1	0.98	0.62	0.62	0	0.02	0.98	0.71	0.64	0.73	0.4	0.91
703110	336.33	1.03	-5.5	24.39	4	1	3	1	0.74	0.11	0.11	0	0.08	0.96	0.86	0.33	0.67	0.08	0.32
656155	280.28	2.56	-4.68	61.55	1	2	3	0.81	0.97	0.42	0.42	0.68	0.22	0.95	0.94	0.23	0.76	0.44	0.73
774959	347.37	2.1	-5.97	47.56	4	2	4	0.81	0.99	0.26	0.26	0.04	0.18	0.98	0.72	0.71	0.74	0.13	0.66

*Listed are NSC-771557, NSC-768051, NSC-754670, NSC-722316, NSC-684405, NSC-676188, NSC-754664, NSC-753802, NSC-382053, NSC-754567, NSC-665497, NSC-754666, NSC-656158, NSC-753211, NSC-765699, NSC-768313, NSC-778318, NSC-703110, NSC-656155, and NSC-774959. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.