**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]\*.**



\*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]\*.**



\*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]\*.**



\*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]\*.**



\*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.