

**Table S2. MOE analysis of binding potentials of human ANGPTL8 on differentially small-molecule compounds.**

<b>Compounds</b>	<b>S (kcal/mol)</b>	<b>Compounds</b>	<b>S (kcal/mol)</b>	<b>Compounds</b>	<b>S (kcal/mol)</b>
Crocin I	-8.82489777	Crocin II	-8.0201292	Carthamin	-7.93572044
Pentatriacontane	-7.38030052	Henicosane	-7.18698978	Octacosane	-6.93933153
Crosatoside A	-6.7941823	N-heptanal	-6.73505402	N-hexacosane	-6.45244598
Safflor yellow A	-6.41271162	Oleic acid	-6.23085499	Nonanal	-6.23030519
Kaempferol-3-glucoside	-6.20494461	Zeaxanthin	-6.16738033	Foron	-6.13261795
TWT	-6.1281786	Heriguard	-6.08009052	4,8,12,16-tetramethyl heptadecan-4-olide	-5.98412561
Methyl palmitate	-5.74573565	Oktadekan	-5.74225616	Phytane	-5.71008921

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Picrocrocin	-5.70954657	LFA	-5.70352316	Chlorogenic Acid	-5.69701338
Linoleic acid	-5.61998081	Erucylamide	-5.61367369	Searic acid	-5.58145428
Palmitic acid	-5.53179741	Methyl myristate	-5.52501774	Picrocrocin	-5.43375015
Crocetin	-5.40475988	Irhamnetin	-5.40287876	Kaempferol	-5.316782
Pentadecylic acid	-5.26692772	Helichryoside	-5.24754238	Quercetin	-5.1906414
Methyl laurate	-5.13606262	Methylinolenate	-5.10763025	$\alpha$ -Cadinol	-5.02424431
Lauric acid	-4.98192072	ZINC04661833	-4.85859871	Allyl heptoate	-4.79072237
myristic acid	-4.72815323	3-Buten-2-one	-4.72404194	$\beta$ -Ionone	-4.71634007

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4-Oxo-b-ionone	-4.70850515	Globulol	-4.62366533	(+)-Ledol	-4.59873343
Nonacosane	-4.59612799	Isodecanoic acid	-4.59388494	Linalool	-4.57969236
9-Oxononanoic acid	-4.51769543	trans-2,4-decadienal	-4.4915905	Oxophorone	-4.47103739
(4S)-4-hydroxy-3,5,5-trimethylcyclohex-2-en-1-one	-4.35457468	L-alpha-phellandrene	-4.32484055	Dihydroactinidiolide	-4.32221556
$\beta$ -Phorone	-4.30234051	Benzaldehyde	-4.24006128	Safranal	-4.2399888
Methylheptadi-none	-4.23608589	Myristicin	-4.2360425	Geranylacetone	-4.23517609
Caffeate	-4.21950054	Caprylic acid	-4.1796937	Octenal	-4.12097836
Cis-Hept-2-enal	-4.04651785	4,4-dimethylcyclopent-2-en-1-one	-3.96291542	2,4-Heptdial	-3.87174559

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Catechol

-3.82163954

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