

## Supplementary data-IV- ADME predictions

### Colorectal anti-cancer activity of a novel class of triazolic triarylmethanes derivatives

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## PART 2: ADME predictions

ID	#rot	MW	HBD	HBA	PlogBB	PPMDCK	PPCaco	PlogS	logPo/w	RuleOfFive
8a	13	453.543	2.5	5.5	-1.375	56.703	122.759	-5.637	5.154	1
8b	11	486.572	0.5	4.5	-0.943	1008.17	1932.18	-8.29	7.53	1
8c	12	507.634	0.5	6.5	-0.519	240.166	466.713	-5.263	6.054	2
9a	13	619.724	0	6.5	-1.503	254.166	540.02	-6.952	7.621	2
9b	15	661.848	0	10.5	-0.92	16.321	35.324	-3.942	5.607	3
9c	15	805.975	0	11.5	-2.345	113.103	255.318	-10.126	9.064	3

**#rot:** Number of non-trivial (not CX3), non-hindered (not alkene, amide, small ring) rotatable bonds. **Recommended: 0 – 15**

**MW:** Molecular weight of the molecule. **Recommended: 130.0 – 725.0**

**HBD:** Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer. **Recommended: 0.0 – 6.0**

**HBA:** Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution. Values are averages taken over a number of configurations, so they can be non-integer. **Recommended: 2.0 – 20.0**

**PlogBB:** Predicted brain/blood partition coefficient. Note: QikProp predictions are for orally delivered drugs so, for example, dopamine and serotonin are CNS negative because they are too polar to cross the blood-brain barrier. **Recommended: -3.0 – 1.2**

**PPMDCK:** Predicted apparent MDCK cell permeability in nm/sec. MDCK cells are considered to be a good mimic for the blood-brain barrier. QikProp predictions are for non-active transport. **Recommended: <25 poor, >500 great.**

**PPCaco:** Predicted apparent Caco-2 cell permeability in nm/sec. Caco-2 cells are a model for the gut-blood barrier. QikProp predictions are for non-active transport. **Recommended: <25 poor, >500 great**

**PlogS:** Predicted aqueous solubility, log S. S in mol dm<sup>-3</sup> is the concentration of the solute in a saturated solution that is in equilibrium with the crystalline solid. **Recommended: -6.5 – 0.5**

**logPo/w:** Predicted octanol/water partition coefficient. **Recommended: -2.0 – 6.5**

**RuleOfFive:** Number of violations of Lipinski's rule of five. The rules are:  $\text{mol\_MW} < 500$ ,  $\text{QPlogPo/w} < 5$ ,  $\text{donorHB} \leq 5$ ,  $\text{accptHB} \leq 10$ . Compounds that satisfy these rules are considered drug-like. (The "five" refers to the limits, which are multiples of 5.) **Recommended: maximum is 4**

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