

# Effect of glycoconjugation on cytotoxicity and selectivity of 8-aminoquinoline derivatives compared to 8-hydroxyquinoline

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## 1. Cytotoxicity data of glycoconjugation substrates

**Table S1.** Screening of cytotoxicity of substrates for quinoline glycoconjugates synthesis.

Compound	Activity IC <sub>50</sub> [μM] <sup>a</sup>		
	HCT 116 <sup>b</sup>	MCF-7 <sup>c</sup>	NHDF-Neo <sup>b</sup>
1	> 800	> 400	> 800
2	9.33 ± 0.22	3.01 ± 0.05	9.34 ± 0.25
3	549.81 ± 16.37	295.04 ± 8.49	> 800
4	> 800	95.95 ± 4.29	> 800
5	115.08 ± 13.36	47.10 ± 8.49	415.2 ± 10.6
6	461.39 ± 1.34	244.44 ± 1.34	782.3 ± 8.7
7	> 800	> 800	> 800
8	> 800	> 800	> 800
9	> 800	> 800	> 800
10	> 800	> 800	> 800
11	> 800	> 800	> 800
12	> 800	> 800	> 800

<sup>a</sup> Cytotoxic was evaluated using the MTT assay

<sup>b</sup> Incubation time 24 h

<sup>c</sup> Incubation time 72 h

2. Physicochemical data prediction *in silico* for substrates, 8-HQ glycoconjugates and metabolites

**Table S2.** Molecular physicochemical descriptors analysis of compounds using Molinspiration online software tools.

Structure	LogP	TPSA (Å <sup>2</sup> )	MW (g)	Vol (Å <sup>3</sup> )	nON	nOHNH	nrotb
<b>1</b>	1.38	38.91	144.18	135.17	2	2	0
<b>2</b>	1.68	33.12	145.16	131.90	2	1	0
<b>3</b>	1.91	24.92	182.23	175.34	2	1	2
<b>4</b>	2.11	22.13	183.21	171.92	2	0	2
<b>5</b>	2.72	74.67	227.27	211.58	5	1	5
<b>6</b>	2.92	71.88	228.25	208.16	5	0	5
<b>7</b>	1.07	164.21	373.32	314.73	12	0	10
<b>8</b>	1.07	164.21	373.32	314.73	12	0	10
<b>9</b>	1.06	173.44	417.37	357.31	13	0	13
<b>10</b>	1.06	173.44	417.37	357.31	13	0	13
<b>11</b>	0.51	123.35	386.35	337.88	10	0	11
<b>12</b>	0.51	123.35	386.35	337.88	10	0	11
<b>13a</b>	1.76	167.30	556.53	475.33	14	0	13
<b>14a</b>	1.76	167.30	556.53	475.33	14	0	13
<b>15a</b>	1.74	176.53	600.58	517.92	15	0	16
<b>16a</b>	1.74	176.53	600.58	517.92	15	0	16
<b>17a</b>	2.21	176.53	614.61	534.72	15	0	17
<b>18a</b>	2.21	176.53	614.61	534.72	15	0	17
<b>19a</b>	1.07	73.07	270.29	239.75	6	1	5
<b>20a</b>	1.54	73.54	284.32	256.55	6	1	6

LogP: molinspiration predicted LogP; TPSA: topological polar surface area; MW: molecular weight; Vol: molecular volume, nON: number of hydrogen bond acceptors; nOHNH: number of hydrogen bond donors; nrotb: number of rotatable bonds.