

Supplementary Material:

3-(4-Bromophenyl)-4-[[3-hydroxy-6-(hydroxymethyl)-4-oxo-4*H*-pyran-2-yl](*m*-tolyl)methyl]isoxazol-5(2*H*)-one

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Docking studies

Table S8. The results of docking studies (the optimal modes are highlighted in bold font).

Compound	Mode	<i>dG</i> , [kcal/mol]	VS score	Rank score
W54011	0	-8.68474	-9.69690	-7.48939
	1	-8.17647	-9.35321	-7.28414
	2	-8.03824	-9.19979	-6.86431
	3	-8.42309	-9.36626	-6.76917
	4	-8.29765	-9.16574	-6.25298
	5	-7.76890	-8.90452	-5.58263
Compound 4	0	-8.63288	-10.25378	-7.70940
	1	-7.99954	-9.52038	-7.45379
	2	-8.82071	-9.68365	-7.16583
	3	-9.04198	-10.25908	-7.08559
	4	-7.97529	-8.89952	-6.96472
	5	-8.48109	-9.69929	-6.91912
	6	-7.81728	-8.96362	-6.83275
	7	-7.36376	-8.65361	-6.48038
	8	-7.83456	-8.68553	-6.05203