

Supplementary information

In silico targeting of the long noncoding RNA MALAT1

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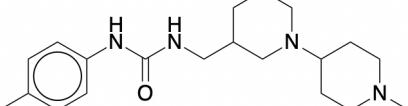
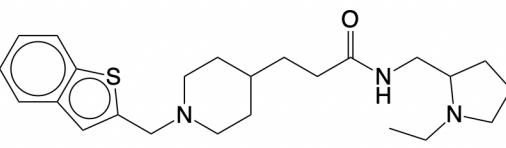
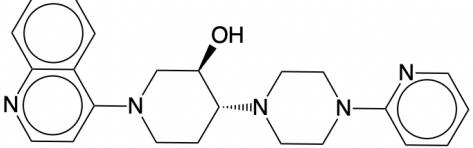
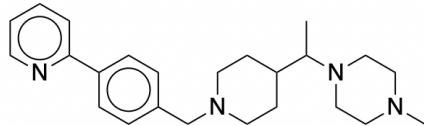
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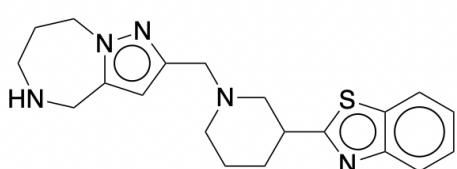
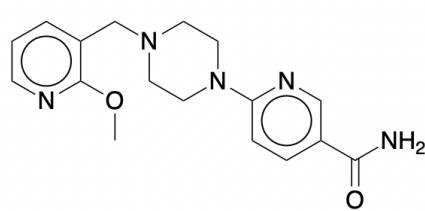
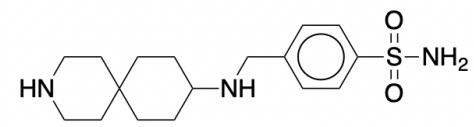
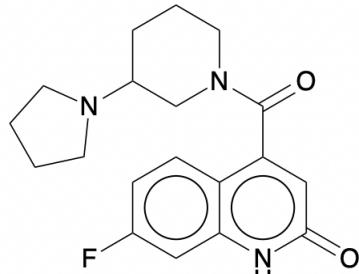
Supplementary information content:

Table S1: Structure, chemical name and docking scores of *in-silico* docking top hits.

Figure S1: Sitemap prediction of pockets on MALAT1 triple helix.

Table S1: Structure, chemical name and docking scores of *in-silico* docking top hits.

Study ID	Structure	Chemical Name	XP Glide Score	Target Site
MTC01		N-[(1'-methyl-1,4'-bipiperidin-3-yl)methyl]-N'-(4-methylphenyl)urea	-7.844	2
MTC02		3-[1-(1-benzothien-2-ylmethyl)-4-piperidinyl]-N-[(1-ethyl-2-pyrrolidinyl)methyl]prop anamide	-6.956	3
MTC03		(3R*,4R*)-4-[4-(2-pyridinyl)-1-piperazinyl]-1-(4-quinolinyl)-3-piperidinol	N/A	Non-specific
MTC04		1-methyl-4-{1-[1-(4-pyridin-2-ylbenzyl)piperidin-4-yl]ethyl}piperazine	-7.557	3

MTC05		2-{[3-(1,3-benzothiazol-2-yl)-1-piperidinyl]methyl}-5,6,7,8-tetrahydro-4H-pyrazolo[1,5-a][1,4]diazepine dihydrochloride	-6.806	3
MTC06		6-{4-[(2-methoxypyridin-3-yl)methyl]piperazin-1-yl}nicotinamide	-7.547	1
MTC07		4-[(3-azaspiro[5.5]undec-9-ylamino)methyl]benzenesulfonamide dihydrochloride	-7.395	2
MTC08		7-fluoro-4-{[3-(1-pyrrolidinyl)-1-piperidinyl]carbonyl}-2(1H)-quinolinone	-6.538	1

MTC09		4-[4-(2-propoxyethyl)piperazin-1-yl]-6-pyrrolidin-1-ylpyrimidin-2-amine	N/A	Non-specific
MTC10		8-(1,3-benzodioxol-5-ylmethyl)-2-[2-(1H-imidazol-4-yl)ethyl]-2,8-diazaspiro[5.5]undecan-3-one	-8.717	3
MTC11		6-[2-(aminomethyl)-2,3-dihydro-1-benzofuran-7-yl]-1,3-benzodioxole-5-carboxamide	-6.795	1
MTC12		6-fluoro-3-[(4-hydroxy-1-methylpiperidin-4-yl)methyl]quinazolin-4(3H)-one	-6.687	1

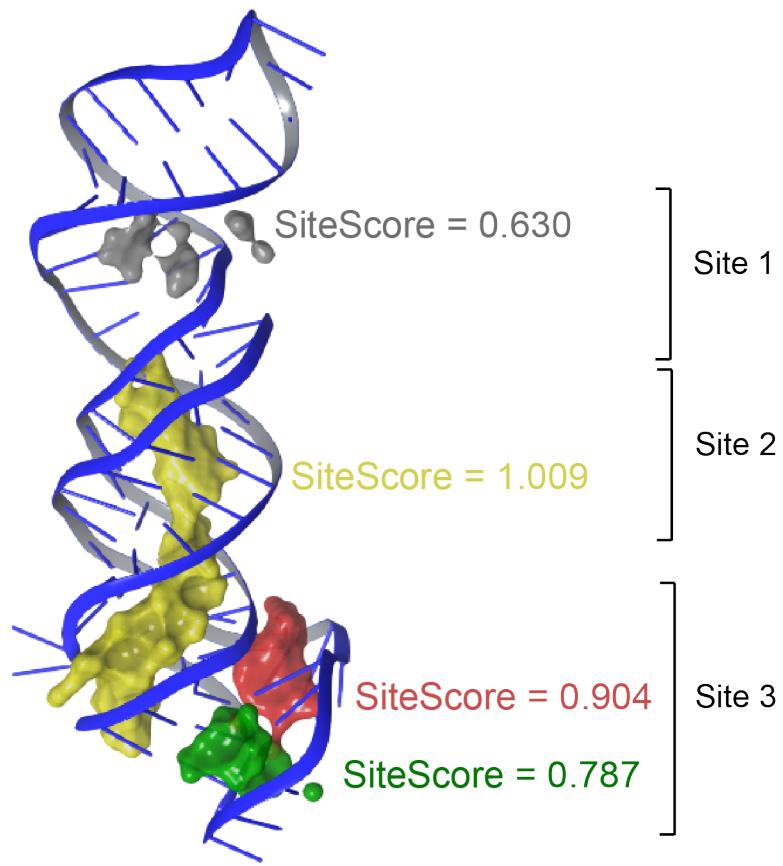


Figure S1: Sitemap prediction of pockets on MALAT1 triple helix. Sitemap was used to identify targetable sites within MALAT1 triple helix (PDB ID: 4plx). Four regions were identified (*yellow, red, green and grey*) and ranked based on their SiteScore, that assesses a site's propensity for ligand binding. Three docking sites were chosen based on the Sitemap results.