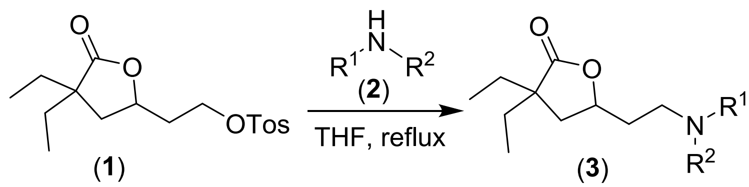
Supporting Information

Selectivity profile comparison for certain γ-butyrolactone and oxazolidinone-based ligands on sigma 2 receptor over sigma 1: A molecular docking approach

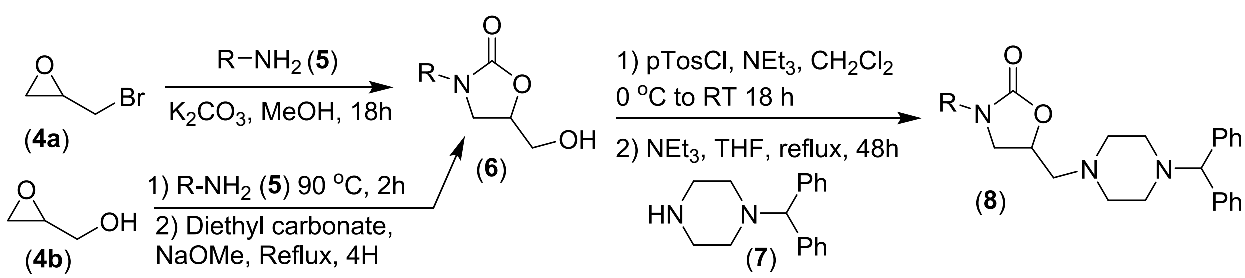
Synthetic procedure

Synthesis of γ-butyrolactones: γ-butyrolactones (**3**) are prepared according to the method described in **Scheme 1**. The known tosylate (**1**) is reacted with a variety of amine (**2**) by refluxing in THF to provide the desired product (**3**).



Scheme 1. General protocol for the synthesis of γ-butyrolactone derivatives.[1]

Synthesis of Oxazolidinones: Oxazolidinones (**8**) were prepared according to the methods described in **Scheme 2**. Epibromohydrin (**4a**) is reacted with an amine (**5**) in the presence of K_2CO_3 in methanol to provide (**6**). Alternatively, Glycidol (**4b**) is reacted with amine (**5**) at 90 °C and the resulting product is reacted with diethyl carbonate in the presence of sodium methoxide and refluxing in methanol to provide (**6**). Conversion of (**6**) to the corresponding tosylate (pTosCl, NEt3, THF), followed by displacement of the leaving group with an amine (**7**) provided the final target compounds (**8**).



Scheme 2. General protocol for the synthesis of oxazolidinones.[2]

References

1. Blass BE, Gao R, Blattner KM, Gordon JC, Pippin DA, Canney DJ. Synthesis and evaluation of novel, selective, functionalized γ-butyrolactones as sigma-2 ligands. Medicinal Chemistry Research. 2022; 31(2):337-349. DOI: 10.1007/s00044-021-02831-5.
2. Blass BE, Bhandare RR, Canney DJ. Discovery of oxazolidinone-based heterocycles as subtype selective sigma-2 ligands. Medicinal Chemistry Research. 2022, 31(3):416-425. DOI: 10.1007/s00044-022-02848-4.

Library of compounds

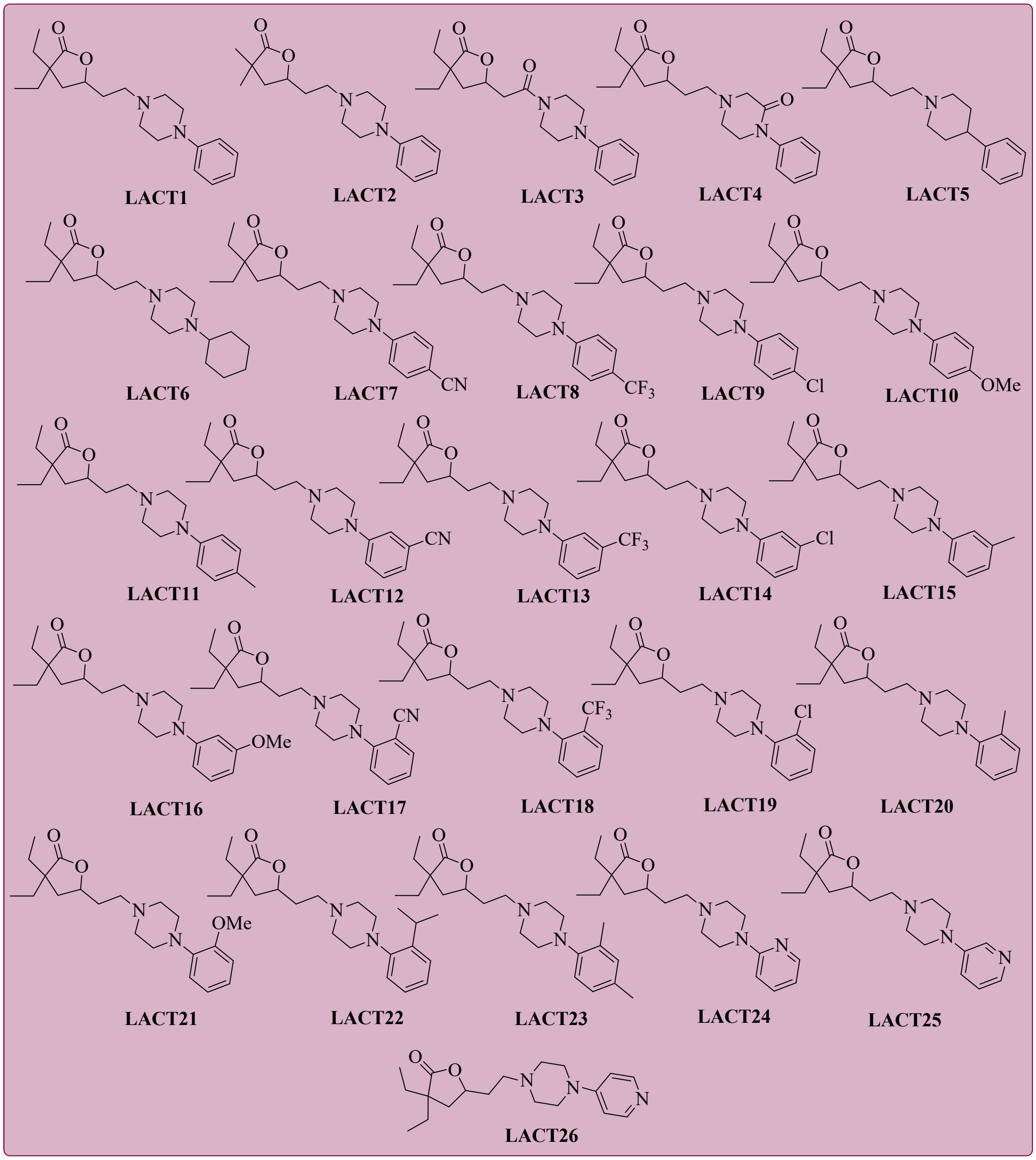


Figure S1A. Library of compounds with γ-butyrolactone scaffold.

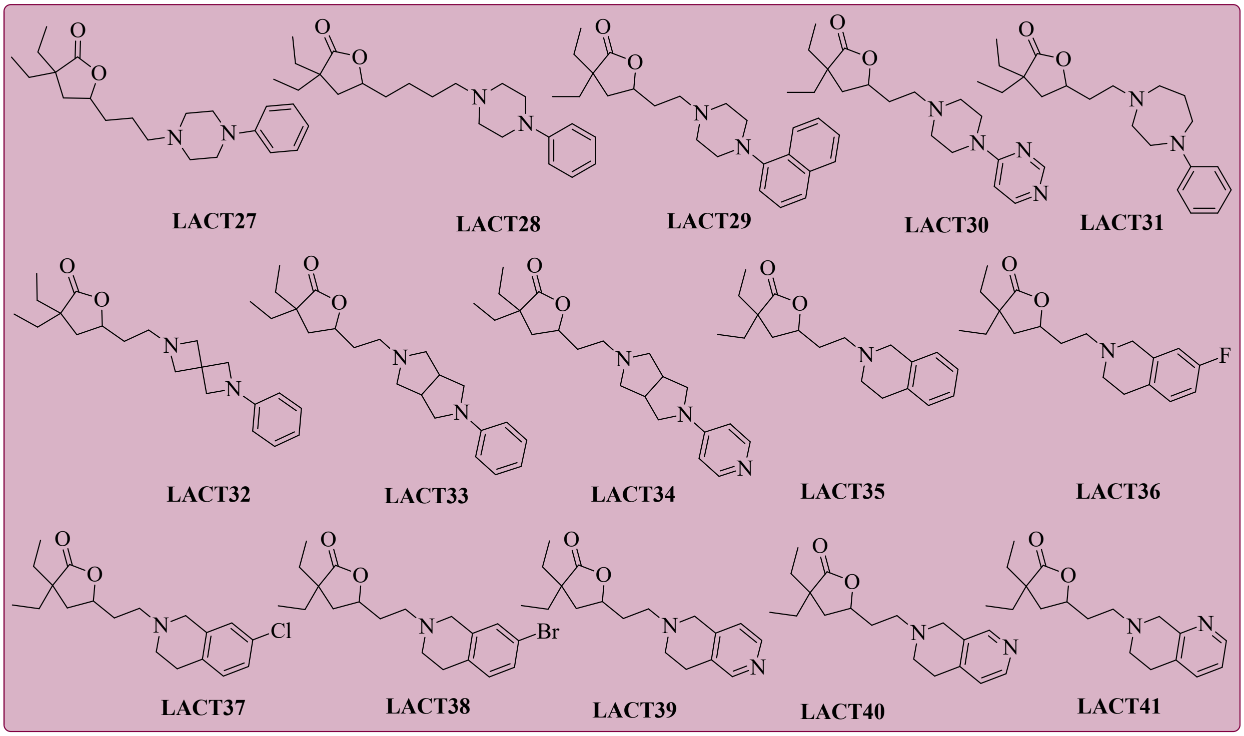


Figure S1B. Library of compounds with γ-butyrolactone scaffold.

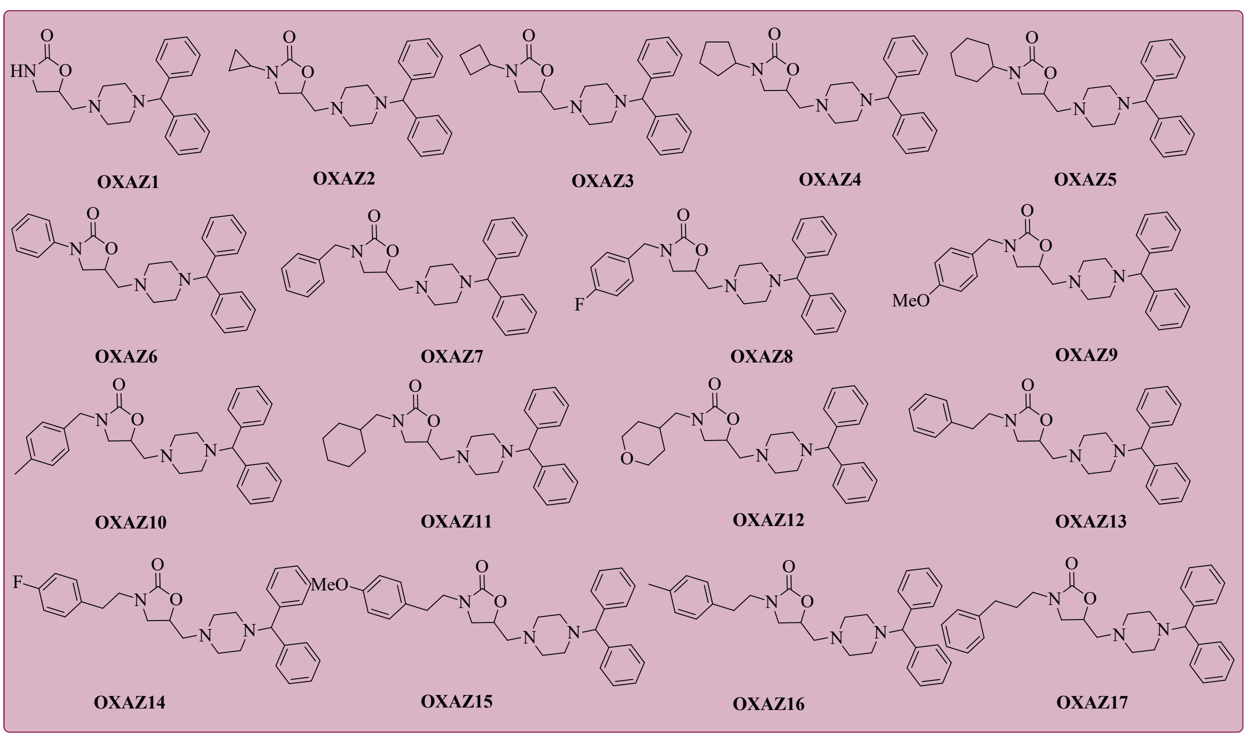


Figure S2. Library of compounds with oxazolidinone scaffold.

Molecular Docking:

Table S1. GLIDE docking score for certain γ-butyrolactone and oxazolidinone-based ligands at the active sites of sigma intracellular receptor 1 and 2 (σ_1 and σ_2).

S.no	Ligand ID	Receptor Name	Ki (nM)	Docking Score	Interactions		
					H-bonds	Pi-Pi stacking	Hydrophobic
1	LACT1	σ_1	138	-5.304	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Ala185, Tyr206
		σ_2	82	-5.295	Asp29, Glu73	Tyr50	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Phe81, Leu111, Ile114, Val146, Tyr147, Tyr150
2	LACT2	σ_1	279	-4.296	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	753	-5.728	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
3	LACT3	σ_1	10000	-4.289	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Ala185, Tyr206
		σ_2	10000	-3.872	-	Tyr50	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
4	LACT4	σ_1	10000	-6.182	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	5289	-5.359	Asp29	-	Ile24, Met28, Tyr50, Leu59, Phe66, Phe69, Leu70, Tyr103, Leu111, Ile114, Val146, Tyr147, Tyr150
5	LACT5	σ_1	2.7	-6.815	-	Tyr103, Tyr206	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	6.4	-8.732	-	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Val146, Tyr147,

							Tyr150
6	LACT6	σ_1	26	-7.841	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	5.4	-7.931	-	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
7	LACT7	σ_1	98	-6.753	-	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	34	-7.877	-	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
8	LACT8	σ_1	14	-8.024	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	7.3	-8.037	-	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
9	LACT9	σ_1	17	-7.180	-	Leu182	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	12	-7.069	Val146	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Val146, Tyr147, Tyr150
10	LACT10	σ_1	79	-7.288	Glu172	His154	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	53	-7.456	Asp29, Glu73	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Phe81, Leu111, Ile114, Val146, Tyr147, Tyr150
11	LACT11	σ_1	10000	-5.705	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Ala185, Tyr206
		σ_2	14	-6.850	-	Tyr50	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Cys72, Leu111, Ile114, Val146, Tyr147, Tyr150
12	LACT12	σ_1	159	-7.956	-	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178,

							Leu182, Ala185, Tyr206
		σ_2	46	-8.157	Glu73	-	Ile24, Met28, Tyr50, Leu59, Phe66, Phe69, Leu70, Tyr103, Leu111, Ile114, Val146, Tyr147, Tyr150
13	LACT13	σ_1	65	-6.752	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Ala185, Tyr206
		σ_2	12	-7.365	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Tyr103, Leu111, Ile114, Val146, Tyr147, Tyr150
14	LACT14	σ_1	84	-7.919	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	9.9	-8.797	Asp29, Glu73	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Phe81, Leu111, Ile114, Val146, Tyr147, Tyr150
15	LACT15	σ_1	59	-6.452	-	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	30	-6.381	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
16	LACT16	σ_1	169	-7.972	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Leu203, Tyr206
		σ_2	62	-7.841	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
17	LACT17	σ_1	351	-8.027	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	61	-8.301	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
18	LACT18	σ_1	67	-6.495	-	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	17	-6.906	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150

19	LACT19	σ_1	35	-6.988	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	7.0	-7.780	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
20	LACT20	σ_1	36	-5.385	-	-	Val84, Ala86, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	9.3	-6.343	-	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
21	LACT21	σ_1	1168	-5.681	-	-	Val84, Ala86, Trp89, Met93, Leu95, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	44	-7.550	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
22	LACT22	σ_1	195	-4.693	-	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Leu186, Tyr206
		σ_2	5.9	-7.891	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Leu70, Leu111, Ile114, Val146, Tyr147, Pro149, Tyr150
23	LACT23	σ_1	10	-8.279	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Met170, Ile178, Leu182, Ala185, Leu186, Tyr206
		σ_2	9.2	-8.254	Asp29, Glu73	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Tyr103, Leu111, Ile114, Val146, Tyr147, Tyr150
24	LACT24	σ_1	1499	-5.811	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	268	-3.480	-	Tyr50	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
25	LACT25	σ_1	10000	-5.096	-	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Met170,

							Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	10000	-5.856	Asp29, Glu73	Tyr50	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
26	LACT26	σ_1	10000	-4.983	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	142	-7.914	Asp29, Glu73	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
27	LACT27	σ_1	31	-6.769	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Ala185, Tyr206
		σ_2	7.7	-7.487	Val146	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Val146, Tyr147, Tyr150
28	LACT28	σ_1	5.5	-7.111	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Ile178, Leu182, Ala185, Tyr206
		σ_2	12	-7.300	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Cys72, Leu111, Ile114, Val146, Tyr147, Tyr150
29	LACT29	σ_1	2167	-6.486	Glu172	Tyr103, Tyr206	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	32	-7.915	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
30	LACT30	σ_1	1017	-5.351	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	10000	-5.404	Asp29, Glu73	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
31	LACT31	σ_1	17	-6.752	-	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Leu203, Tyr206
		σ_2	6.8	-9.046	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150

32	LACT32	σ_1	12	-8.088	Glu172	Phe133	Val84, Trp89, Met93, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val152, Val153, Val162, Trp164, Ile178, Leu182, Phe184, Ala185
		σ_2	53	-8.064	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
33	LACT33	σ_1	31	-7.978	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	3.5	-9.142	Asp29	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
34	LACT34	σ_1	171	-7.461	Glu172	Tyr206	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	29	-8.192	Asp29, Gln77	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Phe81, Tyr103, Leu111, Ile114, Val146, Tyr147, Tyr150
35	LACT35	σ_1	125	-7.416	-	His154	Val84, Trp89, Met93, Leu95, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Leu186
		σ_2	6.1	-10.62	Asp29, Gln77	-	Ile24, Met28, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
36	LACT36	σ_1	68	-7.661	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	7.4	-9.377	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
37	LACT37	σ_1	59	-7.642	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	2.8	-9.880	Asp29	-	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
38	LACT38	σ_1	4.7	-8.107	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Met170, Ile178,

							Leu182, Phe184, Ala185, Tyr206
		σ_2	8.9	-9.323	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
39	LACT39	σ_1	10000	-8.482	Glu172	-	Val84, Trp89, Met93, Leu95, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	10000	-8.121	Asp29	-	Ile24, Met28, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
40	LACT40	σ_1	1156	-7.113	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Ala185, Tyr206
		σ_2	10000	-7.241	Asp29	-	Ile24, Met28, Tyr50, Leu59, Phe66, Phe69, Leu70, Cys72, Leu111, Ile114, Val146, Tyr147, Tyr150
41	LACT41	σ_1	10000	-7.582	Glu172	-	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Tyr206
		σ_2	277	-9.292	Asp29	-	Ile24, Met28, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Tyr150
42	OXAZ1	σ_1	10000	-3.314	Tyr120	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Phe107, Tyr120, Ile124, Phe133, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Leu186, Tyr206
		σ_2	10000	-2.254	Asp29	Tyr50	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Leu70, Leu111, Ile114, Val146, Tyr147, Pro149, Tyr150
43	OXAZ2	σ_1	10000	-5.445	-	Tyr103	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Leu186, Tyr206
		σ_2	119	-7.113	Asp29	Tyr50	Ile24, Met28, Trp49, Tyr50, Leu59, Phe66, Leu70, Leu111, Ile114, Val146, Tyr147, Pro149, Tyr150
44	OXAZ3	σ_1	10000	ND	-	-	-
		σ_2	465	-7.708	Asp29, Glu73	Phe54	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Val146, Tyr147, Pro149, Tyr150
45	OXAZ4	σ_1	10000	ND	-	-	-
		σ_2	206	-7.627	Asp29	Phe54	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Leu70, Phe81, Tyr103, Leu111,

							Ile114, Val146, Tyr147, Pro149, Tyr150
46	OXAZ5	σ_1	10000	-4.569	-	Tyr103, Tyr206	Val84, Trp89, Met93, Leu95, Ala98, Tyr103, Leu105, Tyr120, Ile124, Phe133, Val152, Val162, Trp164, Ile178, Leu182, Phe184, Ala185, Leu186, Tyr206
		σ_2	530	-6.371	-	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Phe81, Tyr103, Leu111, Ile114, Val146, Tyr147, Tyr150
47	OXAZ6	σ_1	10000	ND	-	-	-
		σ_2	192	-7.609	Asp29		Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Vall46, Tyr147, Pro149, Tyr150
48	OXAZ7	σ_1	10000	ND	-	-	-
		σ_2	91	-8.164	Asp29	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Vall46, Tyr147, Tyr150
49	OXAZ8	σ_1	2847	-1.104	-	Trp121	Tyr120, Trp121, Ala183, Phe184, Ala187, Phe191
		σ_2	36	-10.15	-	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Vall46, Tyr147, Tyr150
50	OXAZ9	σ_1	10000	-1.683	Arg119	His116	Tyr120, Trp121, Trp136, Ala159, Ala161, Ala183, Phe184, Ala187
		σ_2	10000	-6.505	Asp29, Gln77	-	Ile24, Met28, Leu46, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Cys72, Tyr103, Leu111, Ile114, Val146, Tyr147, Pro149, Tyr150
51	OXAZ10	σ_1	10000	-1.663	Arg119	His116	Tyr120, Trp121, Trp136, Ala159, Ala161, Ala183, Phe184, Ala187
		σ_2	10000	-6.183	-	-	Ile24, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Vall46, Tyr147, Tyr150
52	OXAZ11	σ_1	10000	ND	-	-	-
		σ_2	1379	-6.229	-	-	Pro23, Ile24, Phe27, Met28, Leu46, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Phe81, Tyr103, Leu111, Ile114, Vall46, Tyr147, Tyr150
53	OXAZ12	σ_1	10000	-1.324	Gly87	Trp121	Ala86, Tyr120, Trp121, Ala183, Phe184, Ala187
		σ_2	2428	-5.336	Asp29	Phe54	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Phe81, Tyr103, Leu111, Ile114, Vall46, Tyr147, Pro149, Tyr150
54	OXAZ13	σ_1	10000	ND	-	-	-
		σ_2	49	-8.832	Asp29	Tyr150	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114,

							Vall46, Tyr147, Pro149, Tyr150
55	OXAZ14	σ_1	10000	-1.068	-	Trp121	Tyr120, Trp121, Ala183, Phe184
		σ_2	2338	-4.268	-	-	Ile24, Met28, Leu46, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Leu111, Ile114, Vall46, Tyr147, Tyr150
56	OXAZ15	σ_1	10000	-1.517	Arg119	-	Tyr120, Trp121, Ala159, Ala183, Phe184, Ala187
		σ_2	10000	-6.248	Asp29	-	Ile24, Met28, Leu46, Trp49, Tyr50, Leu59, Phe66, Phe69, Leu70, Tyr103, Leu111, Ile114, Vall46, Tyr147, Tyr150
57	OXAZ16	σ_1	10000	-0.375	-	-	Trp121, Ala183, Phe184, Ala187
		σ_2	10000	-3.750	-	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Cys72, Leu111, Ile114, Vall46, Tyr147, Pro149, Tyr150
58	OXAZ17	σ_1	10000	-1.135	-	Trp121	Tyr120, Trp121, Ala183, Phe184, Ala187
		σ_2	1245	-6.506	Asp29	-	Ile24, Met28, Trp49, Tyr50, Phe54, Leu59, Phe66, Phe69, Leu70, Phe81, Leu111, Ile114, Vall46, Tyr147, Pro149, Tyr150
ND# Not docked at the active site							