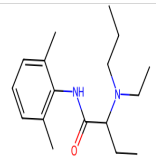
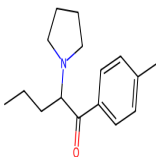
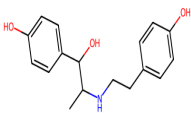
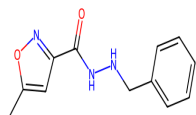


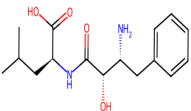
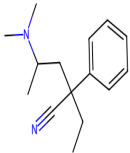
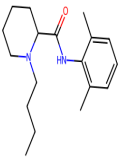
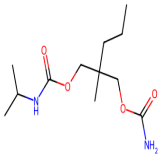
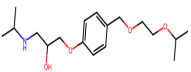
312 Molecules in the StoL25 dataset

Table S8: The basic information of 200 molecules of StoL25 dataset.

No.	ChEMBL ID	Images	Description
1	CHEMBL492		Name: ETIDOCAINE Formula: C₁₇H₂₈N₂O SMILES: <chem>CCCN(CC)C(CC)C(=O)Nc1c(C)cccc1C</chem>
2	CHEMBL201960		Name: PYROVALERONE Formula: C₁₆H₂₃NO SMILES: <chem>CCCC(C(=O)c1ccc(C)cc1)N1CCCC1</chem>
3	CHEMBL83063		Name: RITODRINE Formula: C₁₇H₂₁NO₃ SMILES: <chem>CC(NCCc1ccc(O)cc1)C(O)c1ccc(O)cc1</chem>
4	CHEMBL1201168		Name: ISOCARBOXAZID Formula: C₁₂H₁₃N₃O₂ SMILES: <chem>Cc1cc(C(=O)NNC2CCCC2)no1</chem>

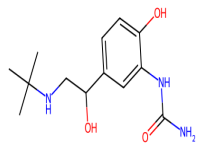
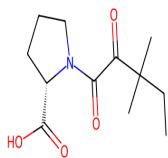
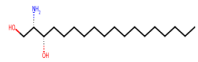
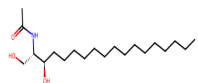
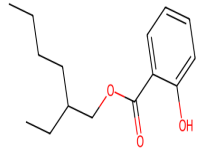
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
5	CHEMBL29292		Name: UBENIMEX Formula: C₁₆H₂₄N₂O₄ SMILES: <chem>CC(C)C[C@H](NC(=O)[C@@H](O)[C@H](N)Cc1ccccc1)C(=O)O</chem>
6	CHEMBL2104277		Name: ETAMINILE Formula: C₁₅H₂₂N₂ SMILES: <chem>CCC(C##N)(CC(C)N(C)C)c1ccccc1</chem>
7	CHEMBL1098		Name: BUPIVACAINE Formula: C₁₈H₂₈N₂O SMILES: <chem>CCCCN1CCCCC1C(=O)Nc1c(C)cccc1C</chem>
8	CHEMBL1233		Name: CARISOPRODOL Formula: C₁₂H₂₄N₂O₄ SMILES: <chem>CCCC(C)(COC(N)=O)COC(=O)NC(C)C</chem>
9	CHEMBL645		Name: BISOPROLOL Formula: C₁₈H₃₁NO₄ SMILES: <chem>CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1</chem>

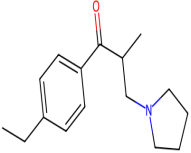
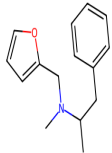
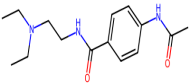
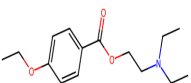
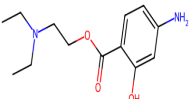
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
10	CHEMBL2110780		Name: CARBUTEROL Formula: C₁₃H₂₁N₃O₃ SMILES: <chem>CC(C)(C)NCC(O)c1ccc(O)c(NC(N)=O)c1</chem>
11	CHEMBL4297382		Name: GPI-1485 Formula: C₁₂H₁₉NO₄ SMILES: <chem>CCC(C)(C)C(=O)C(=O)N1CCC[C@H]1C(=O)O</chem>
12	CHEMBL1442934		Name: SAFINGOL Formula: C₁₈H₃₉NO₂ SMILES: <chem>CCCCCCCCCCCCCCCC[C@H](O)[C@@H](N)CO</chem>
13	CHEMBL155886		Name: CERAMIDE Formula: C₂₀H₄₁NO₃ SMILES: <chem>CCCCCCCCCCCCCCCC[C@@H](O)[C@H](CO)NC(C)=O</chem>
14	CHEMBL1329203		Name: OCTISALATE Formula: C₁₅H₂₂O₃ SMILES: <chem>CCCCC(CC)COC(=O)c1ccccc1O</chem>

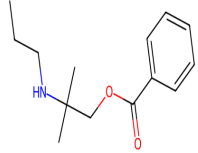
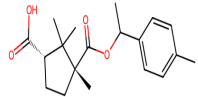
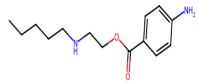
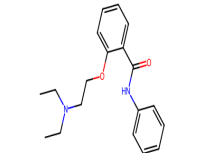
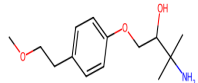
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
15	CHEMBL1797127		Name: INAPERISONE Formula: C₁₆H₂₃NO SMILES: <chem>CCc1ccc(C(=O)C(C)CN2CCCC2)cc1</chem>
16	CHEMBL2107558		Name: FURFENOREX Formula: C₁₅H₁₉NO SMILES: <chem>CC(Cc1ccccc1)N(C)Cc1ccco1</chem>
17	CHEMBL1097		Name: ACECAINIDE Formula: C₁₅H₂₃N₃O₂ SMILES: <chem>CCN(CC)CCNC(=O)c1ccc(NC(C)=O)cc1</chem>
18	CHEMBL421669		Name: PARETHOXYCAINE Formula: C₁₅H₂₃NO₃ SMILES: <chem>CCOc1ccc(C(=O)OCCN(CC)CC)cc1</chem>
19	CHEMBL2106320		Name: HYDROXYPROCAINE Formula: C₁₃H₂₀N₂O₃ SMILES: <chem>CCN(CC)CCOC(=O)c1ccc(N)cc1O</chem>

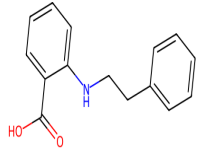
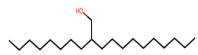
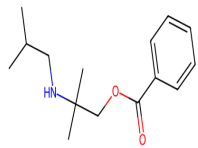
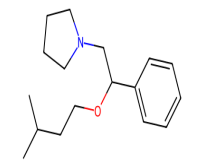
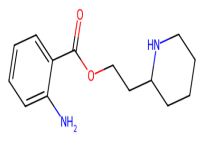
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
20	CHEMBL127810		Name: MEPRYLCAINE Formula: C₁₄H₂₁NO₂ SMILES: <chem>CCCN(C)(C)COC(=O)c1ccccc1</chem>
21	CHEMBL4594620		Name: TOCAMPHYL FREE ACID Formula: C₁₉H₂₆O₄ SMILES: <chem>Cc1ccc(C(C)OC(=O)[C@]2(C)CC[C@H](C(=O)O)C2(C)C)cc1</chem>
22	CHEMBL2110915		Name: NAEPAIN Formula: C₁₄H₂₂N₂O₂ SMILES: <chem>CCCCCNCCOC(=O)c1ccc(N)cc1</chem>
23	CHEMBL2105271		Name: SALVERINE Formula: C₁₉H₂₄N₂O₂ SMILES: <chem>CCN(CC)CCOc1ccccc1C(=O)Nc1ccccc1</chem>
24	CHEMBL1742421		Name: ARNOLOL Formula: C₁₄H₂₃NO₃ SMILES: <chem>COCCc1ccc(OCC(O)C(C)(C)N)cc1</chem>

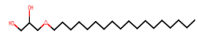
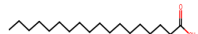
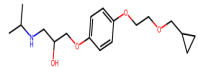
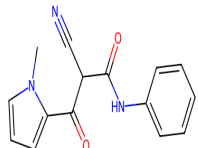
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
25	CHEMBL2106178		Name: ENFENAMIC ACID Formula: C₁₅H₁₅NO₂ SMILES: <chem>O=C(O)c1ccccc1NCCc1ccccc1</chem>
26	CHEMBL1572050		Name: OCTYLDODECANOL Formula: C₂₀H₄₂O SMILES: <chem>CCCCCCCCCCCC(CO)CCCCCCCC</chem>
27	CHEMBL2111069		Name: ISOBUCAINE Formula: C₁₅H₂₃NO₂ SMILES: <chem>CC(C)CNC(C)(C)COC(=O)c1ccccc1</chem>
28	CHEMBL2104080		Name: AMIXETRINE Formula: C₁₇H₂₇NO SMILES: <chem>CC(C)CCOC(CN1CCCC1)c1ccccc1</chem>
29	CHEMBL2110989		Name: PIRIDOCAINE Formula: C₁₄H₂₀N₂O₂ SMILES: <chem>Nc1ccccc1C(=O)OCCN1CCCC1</chem>

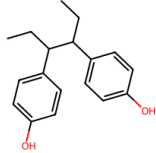
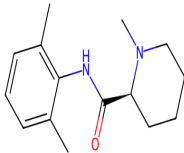
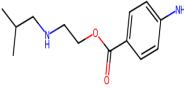
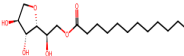
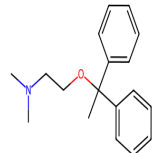
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
30	CHEMBL1482516		Name: BATILOL Formula: C₂₁H₄₄O₃ SMILES: <chem>CCCCCCCCCCCCCCCCCOCC(O)CO</chem>
31	CHEMBL46403		Name: STEARIC ACID Formula: C₁₈H₃₆O₂ SMILES: <chem>CCCCCCCCCCCCCCCC(=O)O</chem>
32	CHEMBL139055		Name: ISOPROPYL PALMITATE Formula: C₁₉H₃₈O₂ SMILES: <chem>CCCCCCCCCCCCCCCC(=O)OC(C)C</chem>
33	CHEMBL2110772		Name: CICLOPROLOL Formula: C₁₈H₂₉NO₄ SMILES: <chem>CC(C)NCC(O)COc1ccc(OCCOCC2CC2)cc1</chem>
34	CHEMBL2111033		Name: PRINOMIDE Formula: C₁₅H₁₃N₃O₂ SMILES: <chem>Cn1cccc1C(=O)C(C#N)C(=O)Nc1ccccc1</chem>

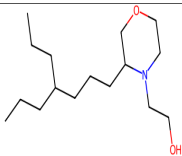
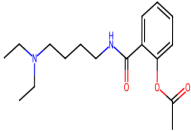
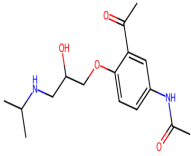
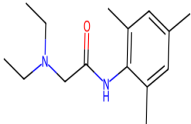
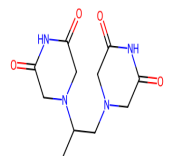
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
35	CHEMBL1795380		Name: Undefined Formula: C₁₉H₂₄N₂O₃ SMILES: <chem>CCC(c1ccc(O)cc1)C(CC)c1ccc(O)cc1</chem>
36	CHEMBL2104634		Name: DEXIVACAINE Formula: C₁₅H₂₂N₂O SMILES: <chem>Cc1cccc(C)c1NC(=O)[C@@H]1CCCCN1C</chem>
37	CHEMBL124211		Name: BUTETHAMINE Formula: C₁₃H₂₀N₂O₂ SMILES: <chem>CC(C)CNCCOC(=O)c1ccc(N)cc1</chem>
38	CHEMBL3706389		Name: SORBITAN MONOLAURATE Formula: C₁₈H₃₄O₆ SMILES: <chem>CCCCCCCCCCCC(=O)OC[C@H](O)[C@H]1OC[C@H](O)[C@H]1O</chem>
39	CHEMBL1742465		Name: MOXASTINE Formula: C₁₈H₂₃NO SMILES: <chem>CN(C)CCOC(C)(c1ccccc1)c1ccccc1</chem>

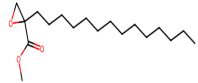
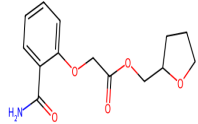
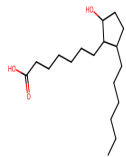
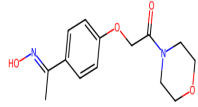
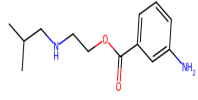
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
40	CHEMBL2104220		Name: DELMOPINOL Formula: C₁₆H₃₃NO₂ SMILES: <chem>CCCC(CCC)CCCC1COCCN1CCO</chem>
41	CHEMBL2106263		Name: DIBUSADOL Formula: C₁₇H₂₆N₂O₃ SMILES: <chem>CCN(CC)CCCCNC(=O)c1ccccc1OC(C)=O</chem>
42	CHEMBL2110821		Name: DIACETOLOL Formula: C₁₆H₂₄N₂O₄ SMILES: <chem>CC(=O)Nc1ccc(OCC(O)CNC(C)C)c(C(C)=O)c1</chem>
43	CHEMBL1618597		Name: TRIMECAINE Formula: C₁₅H₂₄N₂O SMILES: <chem>CCN(CC)CC(=O)Nc1c(C)cc(C)cc1C</chem>
44	CHEMBL444186		Name: RAZOXANE Formula: C₁₁H₁₆N₄O₄ SMILES: <chem>CC(CN1CC(=O)NC(=O)C1)N1CC(=O)NC(=O)C1</chem>

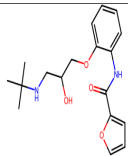
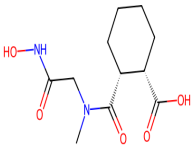
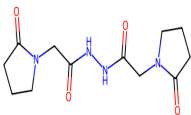
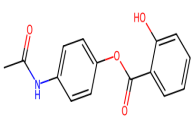
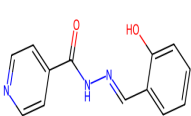
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
45	CHEMBL12261		Name: METHYL PALMOXIRATE Formula: C₁₈H₃₄O₃ SMILES: <chem>CCCCCCCCCCCCCCCC1(C(=O)OC)CO1</chem>
46	CHEMBL2104233		Name: FENAMIFURIL Formula: C₁₄H₁₇NO₅ SMILES: <chem>NC(=O)c1cccc1OCC(=O)OCC1CCCO1</chem>
47	CHEMBL3989708		Name: ROSAPROSTOL Formula: C₁₈H₃₄O₃ SMILES: <chem>CCCCCCC1CCC(O)C1CCCCCCC(=O)O</chem>
48	CHEMBL2105185		Name: MOFOXIME Formula: C₁₄H₁₈N₂O₄ SMILES: <chem>C/C(=N"O)c1ccc(OCC(=O)N2CCOCC2)cc1</chem>
49	CHEMBL2110959		Name: METABUTETHAMINE Formula: C₁₃H₂₀N₂O₂ SMILES: <chem>CC(C)CNCCOC(=O)c1cccc(N)c1</chem>

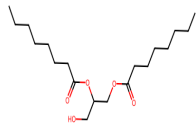
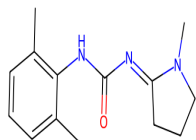
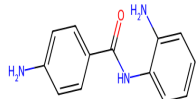
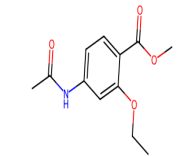
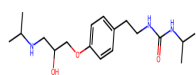
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
50	CHEMBL1742449		Name: ANCAROLOL Formula: C₁₈H₂₄N₂O₄ SMILES: <chem>CC(C)(C)NCC(O)COc1ccccc1NC(=O)c1ccco1</chem>
51	CHEMBL2104330		Name: IDRAPRIL Formula: C₁₁H₁₈N₂O₅ SMILES: <chem>CN(CC(=O)NO)C(=O)[C@@H]1CCCC[C@@H]1C(=O)O</chem>
52	CHEMBL2104359		Name: DUPRACETAM Formula: C₁₂H₁₈N₄O₄ SMILES: <chem>O=C(CN1CCCC1=O)NNC(=O)CN1CCCC1=O</chem>
53	CHEMBL92590		Name: ACETAMINOSALOL Formula: C₁₅H₁₃NO₄ SMILES: <chem>CC(=O)Nc1ccc(OC(=O)c2ccccc2O)cc1</chem>
54	CHEMBL201761		Name: SALINAZID Formula: C₁₃H₁₁N₃O₂ SMILES: <chem>O=C(N/N=C/c1ccccc1O)c1ccncc1</chem>

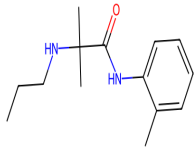
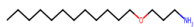
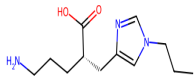
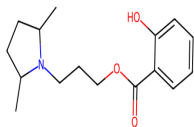
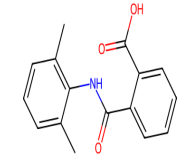
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
55	CHEMBL24609		Name: MONOCTANOIN COMPONENT C Formula: C₁₉H₃₆O₅ SMILES: <chem>CCCCCCCC(=O)OCC(CO)OC(=O)CCCCCCC</chem>
56	CHEMBL382769		Name: XILOBAM Formula: C₁₄H₁₉N₃O SMILES: <chem>Cc1cccc(C)c1NC(=O)/N=C1CCCN1C</chem>
57	CHEMBL1351761		Name: DINALINE Formula: C₁₃H₁₃N₃O SMILES: <chem>Nc1ccc(C(=O)Nc2ccccc2N)cc1</chem>
58	CHEMBL458769		Name: ETHOPABATE Formula: C₁₂H₁₅NO₄ SMILES: <chem>CCOc1cc(NC(C)=O)ccc1C(=O)OC</chem>
59	CHEMBL152371		Name: PAFENOLOL Formula: C₁₈H₃₁N₃O₃ SMILES: <chem>CC(C)NCC(O)COc1ccc(CCNC(=O)NC(C)C)cc1</chem>

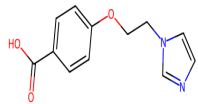
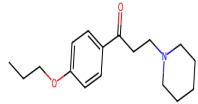
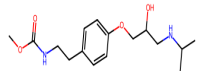
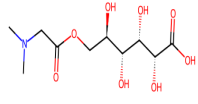
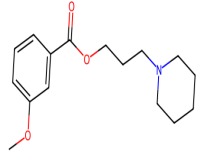
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
60	CHEMBL2105272		Name: QUATACAINE Formula: C₁₄H₂₂N₂O SMILES: <chem>CCCNC(C)(C)C(=O)Nc1ccccc1C</chem>
61	CHEMBL1887483		Name: LAURIXAMINE Formula: C₁₅H₃₃NO SMILES: <chem>CCCCCCCCCCCCCOCCCN</chem>
62	CHEMBL398110		Name: UK-396,082 Formula: C₁₂H₂₁N₃O₂ SMILES: <chem>CCCN1cnc(C[C@H](CCCN)C(=O)O)c1</chem>
63	CHEMBL2105256		Name: PRANOSAL Formula: C₁₆H₂₃NO₃ SMILES: <chem>CC1CCC(C)N1CCCOC(=O)c1ccccc1O</chem>
64	CHEMBL1308252		Name: FTAXILIDE Formula: C₁₆H₁₅NO₃ SMILES: <chem>Cc1cccc(C)c1NC(=O)c1ccccc1C(=O)O</chem>

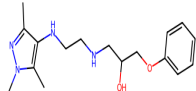
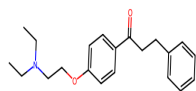
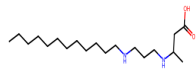
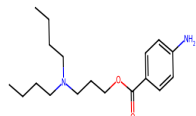
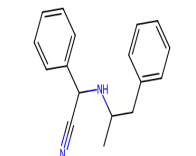
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
65	CHEMBL267473		Name: DAZOXIBEN Formula: C₁₂H₁₂N₂O₃ SMILES: <chem>O=C(O)c1ccc(OCCn2ccnc2)cc1</chem>
66	CHEMBL1625125		Name: PROPIPOCAINE Formula: C₁₇H₂₅NO₂ SMILES: <chem>CCCOc1ccc(C(=O)CCN2CCCCC2)cc1</chem>
67	CHEMBL2110710		Name: PAMATOLOL Formula: C₁₆H₂₆N₂O₄ SMILES: <chem>COC(=O)NCCc1ccc(OCC(O)CNC(C)C)cc1</chem>
68	CHEMBL3707449		Name: PANGAMIC ACID Formula: C₁₀H₁₉NO₈ SMILES: <chem>CN(C)CC(=O)OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C(=O)O</chem>
69	CHEMBL2105314		Name: PRIBECAINE Formula: C₁₆H₂₃NO₃ SMILES: <chem>COc1cccc(C(=O)OCCCN2CCCCC2)c1</chem>

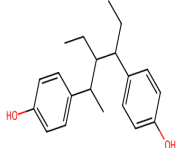
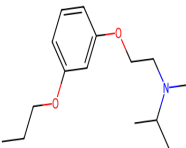
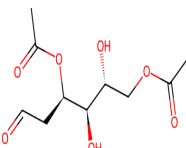
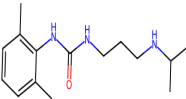
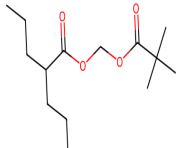
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
70	CHEMBL2106134		Name: DALBRAMINOL Formula: C₁₇H₂₆N₄O₂ SMILES: <chem>Cc1nn(C)c(C)c1NCCNCC(O)COc1ccccc1</chem>
71	CHEMBL2104343		Name: DIETIFEN Formula: C₂₁H₂₇NO₂ SMILES: <chem>CCN(CC)CCOc1ccc(C(=O)CCc2ccccc2)cc1</chem>
72	CHEMBL2104206		Name: DAPABUTAN Formula: C₁₉H₄₀N₂O₂ SMILES: <chem>CCCCCCCCCCCCCNCCNC(C)CC(=O)O</chem>
73	CHEMBL129529		Name: BUTACAINE Formula: C₁₈H₃₀N₂O₂ SMILES: <chem>CCCCN(CCCC)CCOC(=O)c1ccc(N)cc1</chem>
74	CHEMBL2104064		Name: AMFETAMINIL Formula: C₁₇H₁₈N₂ SMILES: <chem>CC(Cc1ccccc1)NC(C#N)c1ccccc1</chem>

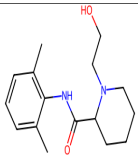
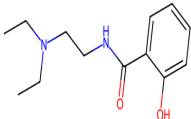
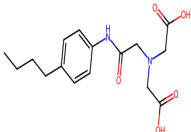
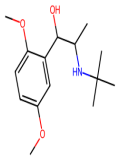
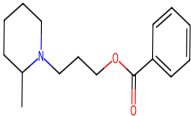
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
75	CHEMBL2104644		Name: BENZESTROL Formula: C₂₀H₂₆O₂ SMILES: <chem>CCC(c1ccc(O)cc1)C(CC)C(C)c1ccc(O)cc1</chem>
76	CHEMBL2106326		Name: EDRONOCAINE Formula: C₁₅H₂₅NO₂ SMILES: <chem>CCCOc1cccc(OCCN(C)C(C)C)c1</chem>
77	CHEMBL5095263		Name: WP-1122 Formula: C₁₀H₁₆O₇ SMILES: <chem>CC(=O)OC[C@H](O)[C@@H](O)[C@H](CC=O)OC(C)=O</chem>
78	CHEMBL551786		Name: RECAINAM Formula: C₁₅H₂₅N₃O SMILES: <chem>Cc1cccc(C)c1NC(=O)NCCCNC(C)C</chem>
79	CHEMBL2107232		Name: VALPROATE PIVOXIL Formula: C₁₄H₂₆O₄ SMILES: <chem>CCCC(CCC)C(=O)OCOC(=O)C(C)(C)C</chem>

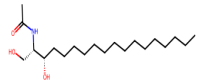
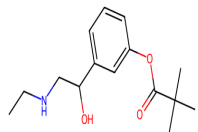
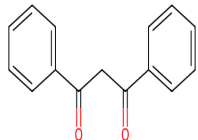
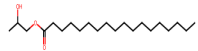
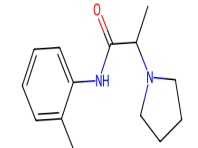
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
80	CHEMBL2106609		Name: DROXICAINIDE Formula: C₁₆H₂₄N₂O₂ SMILES: <chem>Cc1cccc(C)c1NC(=O)C1CCCCN1CCO</chem>
81	CHEMBL2110707		Name: SALETHAMIDE Formula: C₁₃H₂₀N₂O₂ SMILES: <chem>CCN(CC)CCNC(=O)c1ccccc1O</chem>
82	CHEMBL2104651		Name: BUTILFENIN Formula: C₁₆H₂₂N₂O₅ SMILES: <chem>CCCCc1ccc(NC(=O)CN(CC(=O)O)CC(=O)O)cc1</chem>
83	CHEMBL289093		Name: BUTOXAMINE Formula: C₁₅H₂₅NO₃ SMILES: <chem>COc1ccc(OC)c(C(O)C(C)NC(C)(C)C)c1</chem>
84	CHEMBL127865		Name: PIPEROCAINE Formula: C₁₆H₂₃NO₂ SMILES: <chem>CC1CCCCN1CCCOC(=O)c1ccccc1</chem>

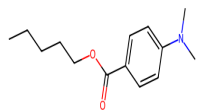
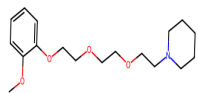
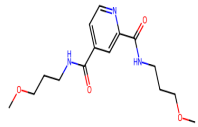
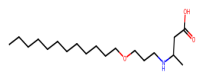
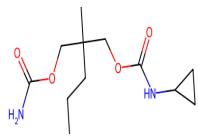
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
85	CHEMBL2104082		Name: CEDEFINGOL Formula: C₂₀H₄₁NO₃ SMILES: <chem>CCCCCCCCCCCCCCCC[C@H](O)[C@H](CO)NC(C)=O</chem>
86	CHEMBL2105571		Name: ETILEFRINE PIVALATE Formula: C₁₅H₂₃NO₃ SMILES: <chem>CCNCC(O)c1cccc(OC(=O)C(C)(C)C)c1</chem>
87	CHEMBL371523		Name: DIBENZOYLMETHANE Formula: C₁₅H₁₂O₂ SMILES: <chem>O=C(CC(=O)c1ccccc1)c1ccccc1</chem>
88	CHEMBL1551666		Name: PROPYLENE GLYCOL MONOSTEARATE Formula: C₂₁H₄₂O₃ SMILES: <chem>CCCCCCCCCCCCCCCCCCCC(=O)OCC(C)O</chem>
89	CHEMBL2104078		Name: APTOCAINE Formula: C₁₄H₂₀N₂O SMILES: <chem>Cc1ccccc1NC(=O)C(C)N1CCCC1</chem>

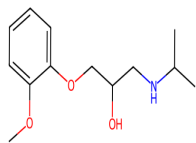
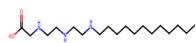
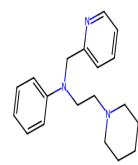
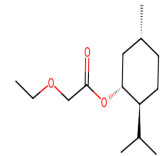
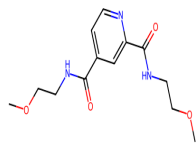
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
90	CHEMBL2107071		Name: PADIMATE A Formula: C₁₄H₂₁NO₂ SMILES: <chem>CCCCCOC(=O)c1ccc(N(C)C)cc1</chem>
91	CHEMBL2106641		Name: GUAIAPATE Formula: C₁₈H₂₉NO₄ SMILES: <chem>COc1ccccc1OCCOCCOCCN1CCCCC1</chem>
92	CHEMBL2105464		Name: SAFIRONIL Formula: C₁₅H₂₃N₃O₄ SMILES: <chem>COCCCN(C(=O)c1ccnc(C(=O)NCCCOc1)C1</chem>
93	CHEMBL2107406		Name: LOPOBUTAN Formula: C₁₉H₃₉NO₃ SMILES: <chem>CCCCCCCCCCCCOCCCN(C)CC(=O)O</chem>
94	CHEMBL2106702		Name: LORBAMATE Formula: C₁₂H₂₂N₂O₄ SMILES: <chem>CCCC(C)(COC(N)=O)COC(=O)NC1CC1</chem>

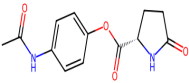
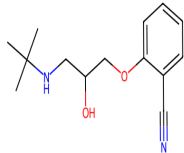
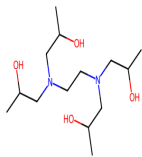
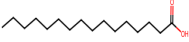
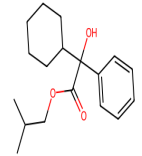
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
95	CHEMBL156901		Name: MOPROLOL Formula: C₁₃H₂₁NO₃ SMILES: <chem>COc1ccccc1OCC(O)CNC(C)C</chem>
96	CHEMBL2105028		Name: DODICIN Formula: C₁₈H₃₉N₃O₂ SMILES: <chem>CCCCCCCCCCCCNCCNCCNCC(=O)O</chem>
97	CHEMBL2105250		Name: PICOPERINE Formula: C₁₉H₂₅N₃ SMILES: <chem>c1ccc(N(CCN2CCCCC2)Cc2cccn2)cc1</chem>
98	CHEMBL3989469		Name: MENGLYTATE Formula: C₁₄H₂₆O₃ SMILES: <chem>CCOCC(=O)O[C@@H]1C[C@H](C)CC[C@H]1C(C)C</chem>
99	CHEMBL2106793		Name: LUFIRONIL Formula: C₁₃H₁₉N₃O₄ SMILES: <chem>COCCNC(=O)c1ccnc(C(=O)NCCOC)c1</chem>

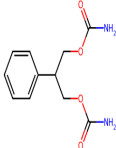
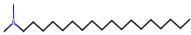
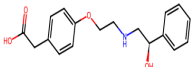
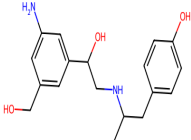
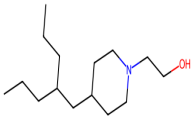
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
100	CHEMBL2105249		Name: PIDOLACETAMOL Formula: C₁₃H₁₄N₂O₄ SMILES: <chem>CC(=O)Nc1ccc(OC(=O)[C@@H]2CCC(=O)N2)cc1</chem>
101	CHEMBL418134		Name: BUNITROLOL Formula: C₁₄H₂₀N₂O₂ SMILES: <chem>CC(C)(C)NCC(O)COc1ccccc1C#N</chem>
102	CHEMBL1573178		Name: EDETOL Formula: C₁₄H₃₂N₂O₄ SMILES: <chem>CC(O)CN(CCN(CC(C)O)CC(C)O)CC(C)O</chem>
103	CHEMBL82293		Name: PALMITIC ACID Formula: C₁₆H₃₂O₂ SMILES: <chem>CCCCCCCCCCCCCCCC(=O)O</chem>
104	CHEMBL2104313		Name: IBUVERINE Formula: C₁₈H₂₆O₃ SMILES: <chem>CC(C)COC(=O)C(O)(c1ccccc1)C1CCCCC1</chem>

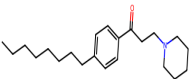
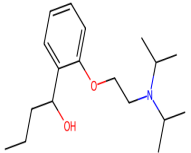
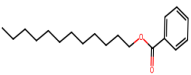
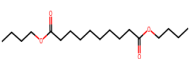
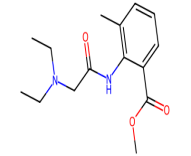
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
105	CHEMBL1094		Name: FELBAMATE Formula: C₁₁H₁₄N₂O₄ SMILES: <chem>NC(=O)OCC(COC(N)=O)c1ccccc1</chem>
106	CHEMBL2110847		Name: DYMANTHINE Formula: C₂₀H₄₃N SMILES: <chem>CCCCCCCCCCCCCCCCCN(C)C</chem>
107	CHEMBL1616411		Name: TALIBEGRON Formula: C₁₈H₂₁NO₄ SMILES: <chem>O=C(O)Cc1ccc(OCCNC[C@H](O)c2ccccc2)cc1</chem>
108	CHEMBL2106256		Name: ETANTEROL Formula: C₁₈H₂₄N₂O₃ SMILES: <chem>CC(Cc1ccc(O)cc1)NCC(O)c1cc(N)cc(CO)c1</chem>
109	CHEMBL2104582		Name: OCTAPINOL Formula: C₁₅H₃₁NO SMILES: <chem>CCCC(CCC)CC1CCN(CCO)CC1</chem>

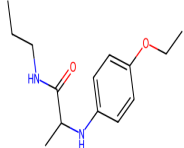
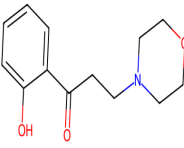
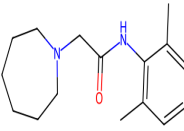
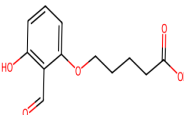
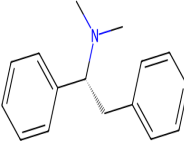
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
110	CHEMBL2106960		Name: PIPOCTANONE Formula: C₂₂H₃₅NO SMILES: <chem>CCCCCCCCc1ccc(C(=O)CCN2CCCCC2)cc1</chem>
111	CHEMBL2104326		Name: KETOCAINOL Formula: C₁₈H₃₁NO₂ SMILES: <chem>CCCC(O)c1ccccc1OCCN(C(C)C)C(C)C</chem>
112	CHEMBL472518		Name: ALKYL (C12-15) BENZOATE Formula: C₁₉H₃₀O₂ SMILES: <chem>CCCCCCCCCCCCCOC(=O)c1ccccc1</chem>
113	CHEMBL2106225		Name: DIBUTYL SEBACATE Formula: C₁₈H₃₄O₄ SMILES: <chem>CCCCOC(=O)CCCCCCCCC(=O)OCCCC</chem>
114	CHEMBL2105549		Name: TOLYCAINE Formula: C₁₅H₂₂N₂O₃ SMILES: <chem>CCN(CC)CC(=O)Nc1c(C)cccc1C(=O)OC</chem>

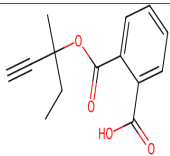
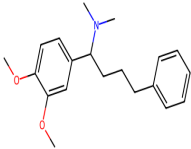
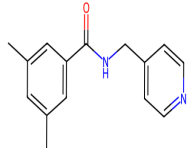
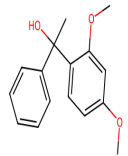
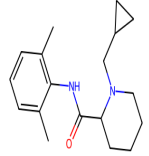
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
115	CHEMBL2106532		Name: PROPETAMIDE Formula: C₁₄H₂₂N₂O₂ SMILES: <chem>CCCNC(=O)C(C)Nc1ccc(OCC)cc1</chem>
116	CHEMBL2105316		Name: ROMIFENONE Formula: C₁₃H₁₇NO₃ SMILES: <chem>O=C(CCN1CCOCC1)c1ccccc1O</chem>
117	CHEMBL1867802		Name: PINCAINIDE Formula: C₁₆H₂₄N₂O SMILES: <chem>Cc1ccc(C)c1NC(=O)CN1CCCCC1</chem>
118	CHEMBL2107643		Name: VELARESOL Formula: C₁₂H₁₄O₅ SMILES: <chem>O=Cc1c(O)cccc1OCCCCC(=O)O</chem>
119	CHEMBL3185938		Name: LEFETAMINE Formula: C₁₆H₁₉N SMILES: <chem>CN(C)[C@H](Cc1ccccc1)c1ccccc1</chem>

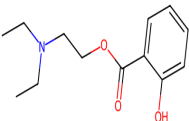
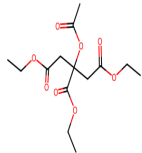
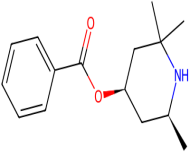
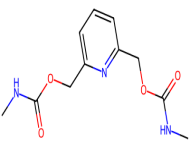
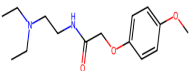
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
120	CHEMBL2107106		Name: PHTHALOFYNE Formula: C₁₄H₁₄O₄ SMILES: <chem>C#CC(C)(CC)OC(=O)c1cccc1C(=O)O</chem>
121	CHEMBL2104458		Name: VETRABUTINE Formula: C₂₀H₂₇NO₂ SMILES: <chem>COc1ccc(C(CCCc2ccccc2)N(C)C)cc1OC</chem>
122	CHEMBL1581974		Name: PICOBENZIDE Formula: C₁₅H₁₆N₂O SMILES: <chem>Cc1cc(C)cc(C(=O)NCc2ccncc2)c1</chem>
123	CHEMBL2107639		Name: FENOCINOL Formula: C₁₆H₁₈O₃ SMILES: <chem>COc1ccc(C(C)(O)c2ccccc2)c(OC)c1</chem>
124	CHEMBL2107683		Name: IPRAVACAINE Formula: C₁₈H₂₆N₂O SMILES: <chem>Cc1ccc(C)c1NC(=O)C1CCCCN1CC1CC1</chem>

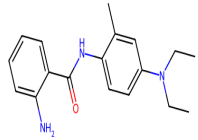
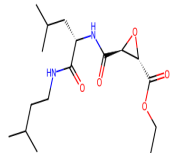
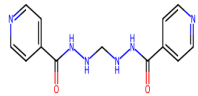
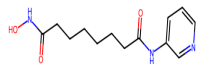
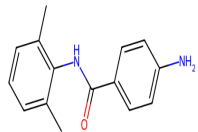
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
125	CHEMBL2106172		Name: DETANOSAL Formula: C₁₃H₁₉NO₃ SMILES: <chem>CCN(CC)CCOC(=O)c1ccccc1O</chem>
126	CHEMBL2105928		Name: ACETYLTRIETHYL CITRATE Formula: C₁₄H₂₂O₈ SMILES: <chem>CCOC(=O)CC(CC(=O)OCC)(OC(C)=O)C(=O)OCC</chem>
127	CHEMBL2110936		Name: EUCAINE Formula: C₁₅H₂₁NO₂ SMILES: <chem>C[C@H]1C[C@@H](OC(=O)c2ccccc2)CC(C)(C)N1</chem>
128	CHEMBL1620144		Name: PYRICARBATE Formula: C₁₁H₁₅N₃O₄ SMILES: <chem>CNC(=O)OCc1cccc(COC(=O)NC)n1</chem>
129	CHEMBL1368380		Name: MEFEXAMIDE Formula: C₁₅H₂₄N₂O₃ SMILES: <chem>CCN(CC)CCNC(=O)COc1ccc(OC)cc1</chem>

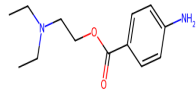
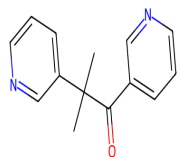
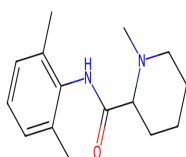
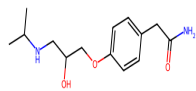
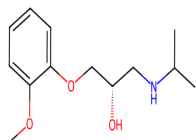
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
130	CHEMBL2106015		Name: ATOLIDE Formula: C₁₈H₂₃N₃O SMILES: <chem>CCN(CC)c1ccc(NC(=O)c2ccccc2N)c(C)c1</chem>
131	CHEMBL63440		Name: ALOXISTATIN Formula: C₁₇H₃₀N₂O₅ SMILES: <chem>CCOC(=O)[C@H]1O[C@@H]1C(=O)N[C@@H](CC(C)C)C(=O)NCCC(C)C</chem>
132	CHEMBL1526558		Name: METAZIDE Formula: C₁₃H₁₄N₆O₂ SMILES: <chem>O=C(NNCNNC(=O)c1ccncc1)c1ccncc1</chem>
133	CHEMBL353581		Name: PYROXAMIDE Formula: C₁₃H₁₉N₃O₃ SMILES: <chem>O=C(CCCCCC(=O)Nc1ccncc1)NO</chem>
134	CHEMBL22916		Name: AMELTOLIDE Formula: C₁₅H₁₆N₂O SMILES: <chem>Cc1cccc(C)c1NC(=O)c1ccc(N)cc1</chem>

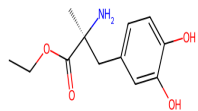
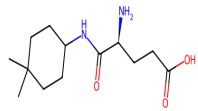
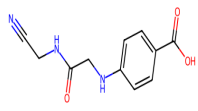
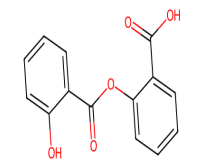
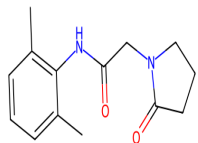
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
135	CHEMBL569		Name: PROCAINE Formula: C₁₃H₂₀N₂O₂ SMILES: <chem>CCN(CC)CCOC(=O)c1ccc(N)cc1</chem>
136	CHEMBL934		Name: METYRAPONE Formula: C₁₄H₁₄N₂O SMILES: <chem>CC(C)(C(=O)c1cccn1)c1cccn1</chem>
137	CHEMBL1087		Name: MEPIVACAINE Formula: C₁₅H₂₂N₂O SMILES: <chem>Cc1ccc(C)c1NC(=O)C1CCCCN1C</chem>
138	CHEMBL24		Name: ATENOLOL Formula: C₁₄H₂₂N₂O₃ SMILES: <chem>CC(C)NCC(O)COc1ccc(CC(N)=O)cc1</chem>
139	CHEMBL2106030		Name: LEVOMOPROLOL Formula: C₁₃H₂₁NO₃ SMILES: <chem>COc1ccccc1OC[C@H](O)CNC(C)C</chem>

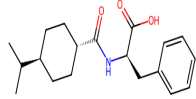
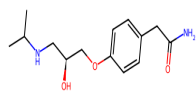
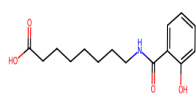
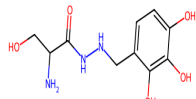
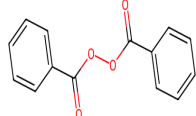
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
140	CHEMBL1201233		Name: METHYLDOPATE Formula: C₁₂H₁₇NO₄ SMILES: <chem>CCOC(=O)[C@@](C)(N)Cc1ccc(O)c(O)c1</chem>
141	CHEMBL1255840		Name: NEBOGLAMINE Formula: C₁₃H₂₄N₂O₃ SMILES: <chem>CC1(C)CCC(NC(=O)[C@@H](N)CCC(=O)O)CC1</chem>
142	CHEMBL4802134		Name: H-100 Formula: C₁₁H₁₁N₃O₃ SMILES: <chem>N#CCNC(=O)CNc1ccc(C(=O)O)cc1</chem>
143	CHEMBL154111		Name: SALSALATE Formula: C₁₄H₁₀O₅ SMILES: <chem>O=C(Oc1ccccc1C(=O)O)c1ccccc1O</chem>
144	CHEMBL260829		Name: NEFIRACETAM Formula: C₁₄H₁₈N₂O₂ SMILES: <chem>Cc1ccc(C)c1NC(=O)CN1CCCC1=O</chem>

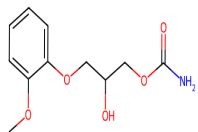
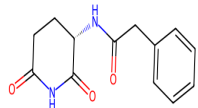
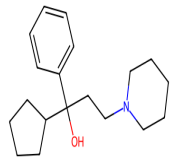
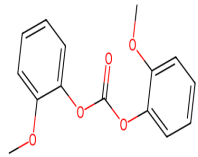
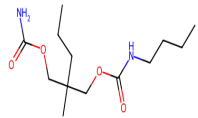
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
145	CHEMBL783		Name: NATEGLINIDE Formula: C₁₉H₂₇NO₃ SMILES: <chem>CC(C)[C@H]1CC[C@H](C(=O)N[C@H](Cc2ccccc2)C(=O)O)CC1</chem>
146	CHEMBL343633		Name: ESATENOLOL Formula: C₁₄H₂₂N₂O₃ SMILES: <chem>CC(C)NC[C@H](O)COc1ccc(CC(N)=O)cc1</chem>
147	CHEMBL16503		Name: SALCAPROZIC ACID Formula: C₁₅H₂₁NO₄ SMILES: <chem>O=C(O)CCCCCCCNC(=O)c1ccccc1O</chem>
148	CHEMBL1096979		Name: BENSERAZIDE Formula: C₁₀H₁₅N₃O₅ SMILES: <chem>NC(CO)C(=O)NNCc1ccc(O)c(O)c1O</chem>
149	CHEMBL1200370		Name: BENZOYL PEROXIDE Formula: C₁₄H₁₀O₄ SMILES: <chem>O=C(OOC(=O)c1ccccc1)c1ccccc1</chem>

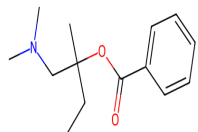
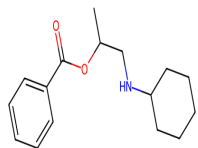
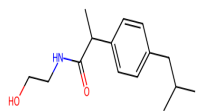
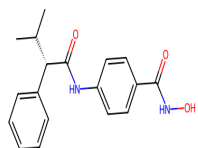
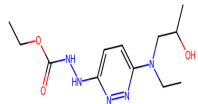
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
150	CHEMBL1201117		Name: METHOCARBAMOL Formula: C₁₁H₁₅NO₅ SMILES: <chem>COc1ccccc1OCC(O)COC(N)=O</chem>
151	CHEMBL1980825		Name: ANTINEOPLASTON A10 Formula: C₁₃H₁₄N₂O₃ SMILES: <chem>O=C1CC[C@H](NC(=O)Cc2ccccc2)C(=O)N1</chem>
152	CHEMBL1201227		Name: CYCRIMINE Formula: C₁₉H₂₉NO SMILES: <chem>OC(CCN1CCCCC1)(c1ccccc1)C1CCCC1</chem>
153	CHEMBL1898058		Name: GUAIACOL CARBONATE Formula: C₁₅H₁₄O₅ SMILES: <chem>COc1ccccc1OC(=O)Oc1ccccc1OC</chem>
154	CHEMBL2104816		Name: TYBAMATE Formula: C₁₃H₂₆N₂O₄ SMILES: <chem>CCCCNC(=O)OCC(C)(CCC)COC(N)=O</chem>

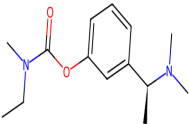
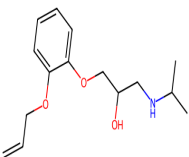
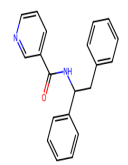
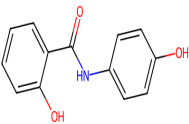
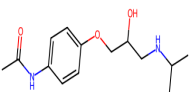
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
155	CHEMBL1740065		Name: AMYLOCAINE Formula: C₁₄H₂₁NO₂ SMILES: <chem>CCC(C)(CN(C)C)OC(=O)c1ccccc1</chem>
156	CHEMBL1197		Name: HEXYLCAINE Formula: C₁₆H₂₃NO₂ SMILES: <chem>CC(CNC1CCCCC1)OC(=O)c1ccccc1</chem>
157	CHEMBL2105154		Name: MABUPROFEN Formula: C₁₅H₂₃NO₂ SMILES: <chem>CC(C)Cc1ccc(C(C)C(=O)NCCO)cc1</chem>
158	CHEMBL191482		Name: AR-42 Formula: C₁₈H₂₀N₂O₃ SMILES: <chem>CC(C)[C@H](C(=O)Nc1ccc(C(=O)NO)cc1)c1ccccc1</chem>
159	CHEMBL2106561		Name: CADRALAZINE Formula: C₁₂H₂₁N₅O₃ SMILES: <chem>CCOC(=O)NNc1ccc(N(CC)CC(C)O)nn1</chem>

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Table S8 – Continued

No.	ChEMBL ID	Images	Description
160	CHEMBL636		Name: RIVASTIGMINE Formula: C₁₄H₂₂N₂O₂ SMILES: <chem>CCN(C)C(=O)Oc1cccc([C@H](C)N(C)C)c1</chem>
161	CHEMBL546		Name: OXPRENOLOL Formula: C₁₅H₂₃NO₃ SMILES: <chem>C=CCOc1cccc1OCC(O)CNC(C)C</chem>
162	CHEMBL3707234		Name: NICOFETAMIDE Formula: C₂₀H₁₈N₂O SMILES: <chem>O=C(NC(Cc1cccc1)c1cccc1)c1ccnc1</chem>
163	CHEMBL389507		Name: OSALMID Formula: C₁₃H₁₁NO₃ SMILES: <chem>O=C(Nc1ccc(O)cc1)c1ccccc1O</chem>
164	CHEMBL6995		Name: PRACTOLOL Formula: C₁₄H₂₂N₂O₃ SMILES: <chem>CC(=O)Nc1ccc(OCC(O)CNC(C)C)cc1</chem>

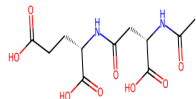
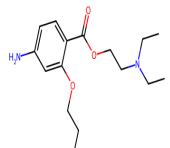
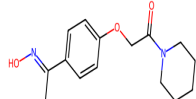
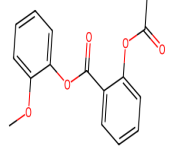
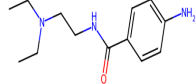
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
165	CHEMBL1651913		Name: OXYFEDRINE Formula: C₁₉H₂₃NO₃ SMILES: <chem>COc1cccc(C(=O)CCN[C@@H](C)[C@H](O)c2ccccc2)c1</chem>
166	CHEMBL118722		Name: TRIBUTYRIN Formula: C₁₅H₂₆O₆ SMILES: <chem>CCCC(=O)OCC(COC(=O)CCC)OC(=O)CCC</chem>
167	CHEMBL1196		Name: PROPARACAINE Formula: C₁₆H₂₆N₂O₃ SMILES: <chem>CCCOc1ccc(C(=O)OCCN(CC)CC)cc1N</chem>
168	CHEMBL1852164		Name: LX-2931 Formula: C₉H₁₅N₃O₅ SMILES: <chem>C/C(=N"O)c1ncc([C@@H](O)[C@H](O)[C@H](O)CO)[nH]1</chem>
169	CHEMBL1451173		Name: DIPYROCETYL Formula: C₁₁H₁₀O₆ SMILES: <chem>CC(=O)Oc1cccc(C(=O)O)c1OC(C)=O</chem>

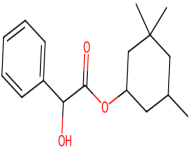
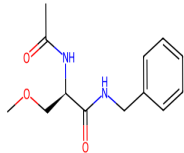
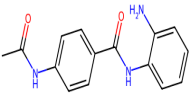
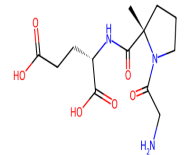
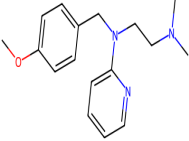
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
170	CHEMBL2105616		Name: SPAGLUMIC ACID Formula: C₁₁H₁₆N₂O₈ SMILES: <chem>CC(=O)N[C@@H](CC(=O)N[C@@H](CCC(=O)O)C(=O)O)C(=O)O</chem>
171	CHEMBL1195		Name: PROPOXYCAINE Formula: C₁₆H₂₆N₂O₃ SMILES: <chem>CCCOc1cc(N)ccc1C(=O)OCCN(CC)CC</chem>
172	CHEMBL1998966		Name: PIFOXIME Formula: C₁₅H₂₀N₂O₃ SMILES: <chem>C/C(=N\O)c1ccc(OCC(=O)N2CCCCC2)cc1</chem>
173	CHEMBL2105097		Name: GUACETISAL Formula: C₁₆H₁₄O₅ SMILES: <chem>COc1cccc1OC(=O)c1cccc1OC(C)=O</chem>
174	CHEMBL640		Name: PROCAINAMIDE Formula: C₁₃H₂₁N₃O SMILES: <chem>CCN(CC)CCNC(=O)c1ccc(N)cc1</chem>

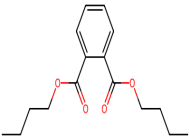
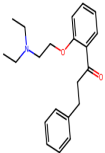
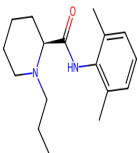
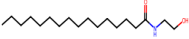
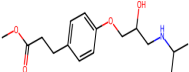
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
175	CHEMBL1480987		Name: CYCLANDELATE Formula: C₁₇H₂₄O₃ SMILES: <chem>CC1CC(OC(=O)C(O)c2ccccc2)CC(C)(C)C1</chem>
176	CHEMBL58323		Name: LACOSAMIDE Formula: C₁₃H₁₈N₂O₃ SMILES: <chem>COC[C@@H](NC(C)=O)C(=O)NCc1ccccc1</chem>
177	CHEMBL235191		Name: TACEDINALINE Formula: C₁₅H₁₅N₃O₂ SMILES: <chem>CC(=O)Nc1ccc(C(=O)Nc2ccccc2N)cc1</chem>
178	CHEMBL197084		Name: TROFINETIDE Formula: C₁₃H₂₁N₃O₆ SMILES: <chem>C[C@@]1(C(=O)N[C@@H](CCC(=O)O)C(=O)O)CCCN1C(=O)CN</chem>
179	CHEMBL511		Name: PYRILAMINE Formula: C₁₇H₂₃N₃O SMILES: <chem>COc1ccc(CN(CCN(C)C)c2ccccc2)cc1</chem>

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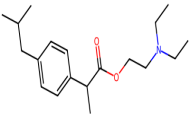
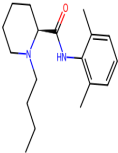
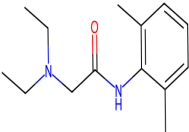
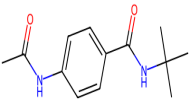
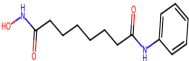
Table S8 – Continued

No.	ChEMBL ID	Images	Description
180	CHEMBL272485		Name: DIBUTYL PHTHALATE Formula: C₁₆H₂₂O₄ SMILES: <chem>CCCCOC(=O)c1ccccc1C(=O)OCCCC</chem>
181	CHEMBL1736151		Name: ETAFENONE Formula: C₂₁H₂₇NO₂ SMILES: <chem>CCN(CC)CCOc1ccccc1C(=O)CCc1ccccc1</chem>
182	CHEMBL1077896		Name: ROPIVACAINE Formula: C₁₇H₂₆N₂O SMILES: <chem>CCCN1CCCC[C@H]1C(=O)Nc1c(C)cccc1C</chem>
183	CHEMBL417675		Name: PALMIDROL Formula: C₁₈H₃₇NO₂ SMILES: <chem>CCCCCCCCCCCCCCCC(=O)NCCO</chem>
184	CHEMBL768		Name: ESMOLOL Formula: C₁₆H₂₅NO₄ SMILES: <chem>COC(=O)CCc1ccc(OCC(O)CNC(C)C)cc1</chem>

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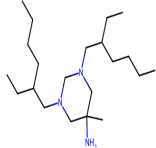
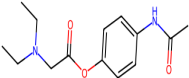
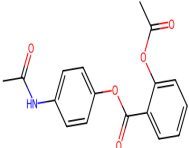
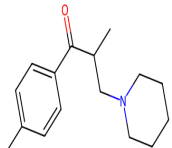
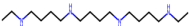
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
190	CHEMBL5314598		Name: IBUPROFEN TRELAMINE Formula: C₁₉H₃₁NO₂ SMILES: <chem>CCN(CC)CCOC(=O)C(C)c1ccc(CC(C)C)cc1</chem>
191	CHEMBL1201193		Name: LEVOBUPIVACAINE Formula: C₁₈H₂₈N₂O SMILES: <chem>CCCCN1CCCC[C@H]1C(=O)Nc1c(C)cccc1C</chem>
192	CHEMBL79		Name: LIDOCAINE Formula: C₁₄H₂₂N₂O SMILES: <chem>CCN(CC)CC(=O)Nc1c(C)cccc1C</chem>
193	CHEMBL4297369		Name: CP1-1189 Formula: C₁₃H₁₈N₂O₂ SMILES: <chem>CC(=O)Nc1ccc(C(=O)NC(C)(C)C)cc1</chem>
194	CHEMBL98		Name: VORINOSTAT Formula: C₁₄H₂₀N₂O₃ SMILES: <chem>O=C(CCCCCC(=O)Nc1cccc1)NO</chem>

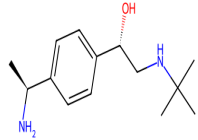
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Table S8 – Continued

No.	ChEMBL ID	Images	Description
195	CHEMBL144673		Name: HEXETIDINE Formula: C₂₁H₄₅N₃ SMILES: <chem>CCCCC(CC)CN1CN(CC(CC)CCCC)CC(C)(N)C1</chem>
196	CHEMBL1851805		Name: PROPACETAMOL Formula: C₁₄H₂₀N₂O₃ SMILES: <chem>CCN(CC)CC(=O)Oc1ccc(NC(C)=O)cc1</chem>
197	CHEMBL162036		Name: BENORILATE Formula: C₁₇H₁₅NO₅ SMILES: <chem>CC(=O)Nc1ccc(OC(=O)c2ccccc2OC(C)=O)cc1</chem>
198	CHEMBL1076211		Name: TOLPERISONE Formula: C₁₆H₂₃NO SMILES: <chem>Cc1ccc(C(=O)C(C)CN2CCCCC2)cc1</chem>
199	CHEMBL77101		Name: DIETHYLHOMOSPERMINE Formula: C₁₆H₃₈N₄ SMILES: <chem>CCNCCCCNCCCCNCCCCNCC</chem>

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Table S8 – Continued

No.	ChEMBL ID	Images	Description
200	CHEMBL5314387	 The chemical structure of MK-1496 is shown. It consists of a central benzene ring. On the left side of the ring, there is a chiral center (indicated by a wedge bond) attached to an amino group (-NH2). On the right side of the ring, there is another chiral center (indicated by a dashed bond) attached to a hydroxyl group (-OH). The hydroxyl group is further connected to a side chain that includes a secondary amine (-NH-) which is bonded to a quaternary carbon atom (C) with three methyl groups.	Name: MK-1496 Formula: C₁₄H₂₄N₂O SMILES: <chem>C[C@H](N)c1ccc([C@H](O)CNC(C)(C)C)cc1</chem>