

Supporting Information

Revisiting automated G-protein coupled receptor modelling:

The benefit of additional template structures for a Neurokinin-1 receptor model

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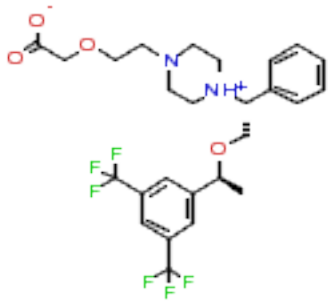
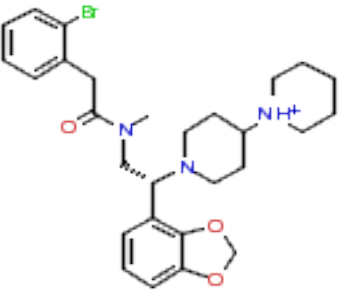
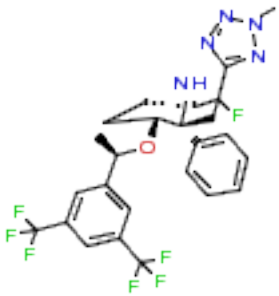
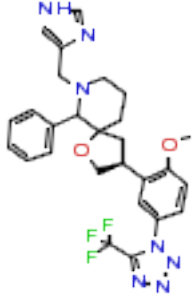
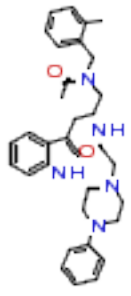
§ These authors contributed equally to this work

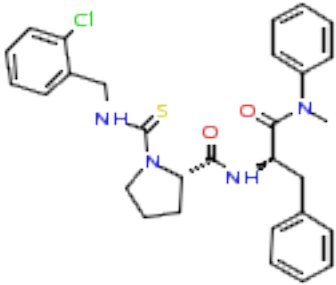
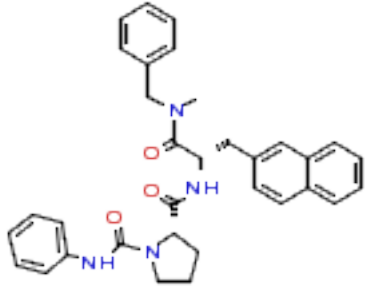
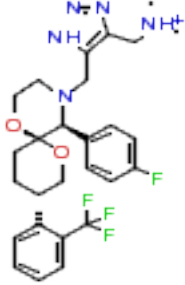
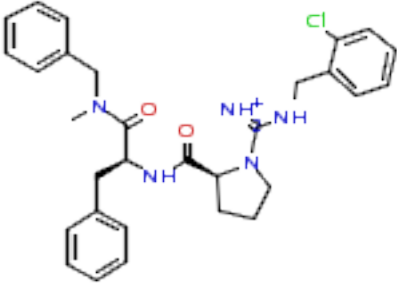
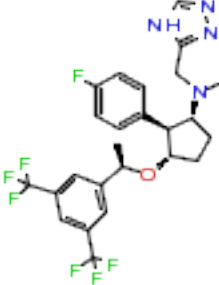
* Corresponding author: phone: +49 (7351) 54-94030, fax: +49 (7531) 83-94030, email:
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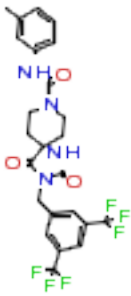
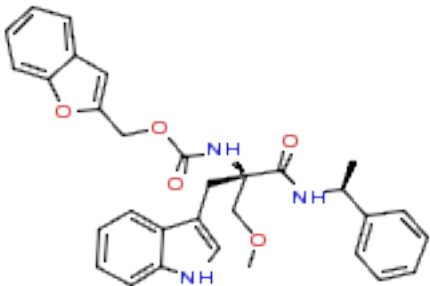
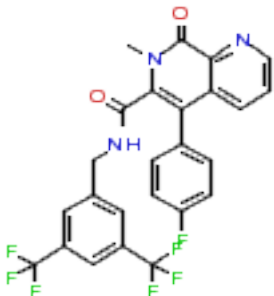
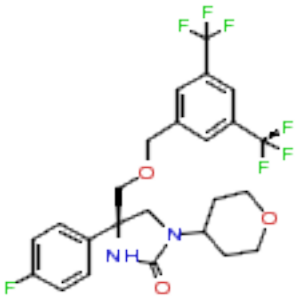
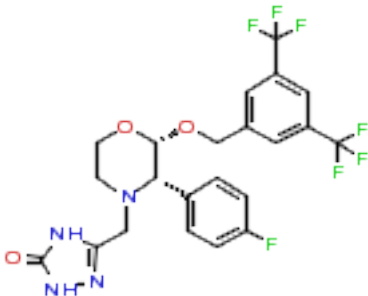
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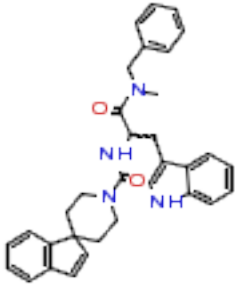
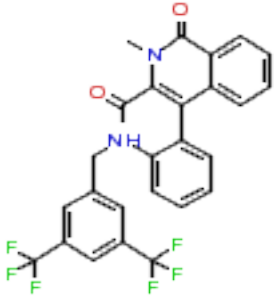
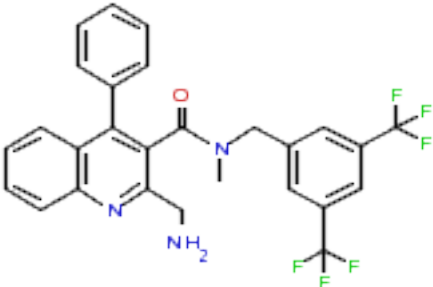
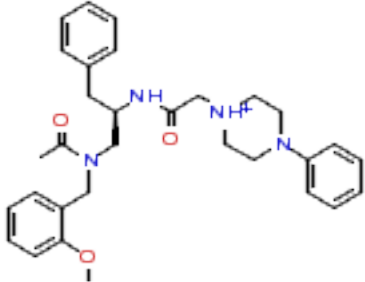
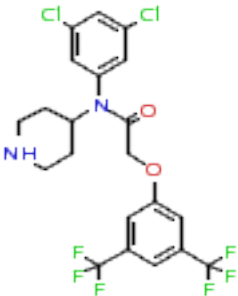
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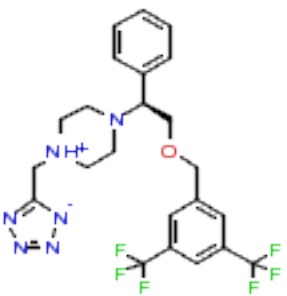
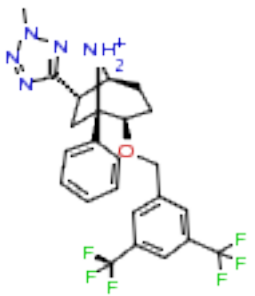
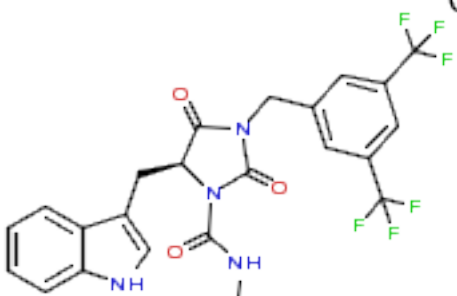
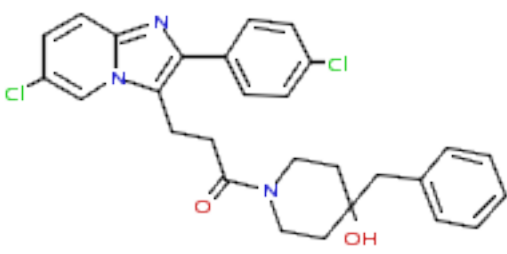
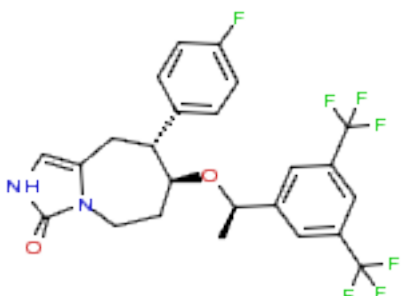
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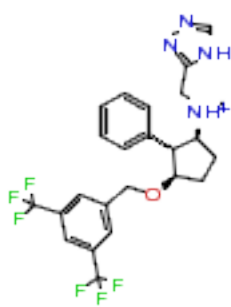
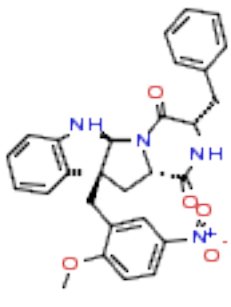
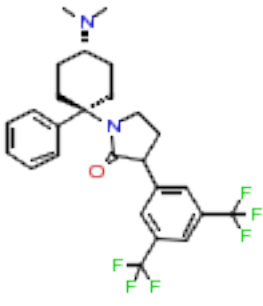
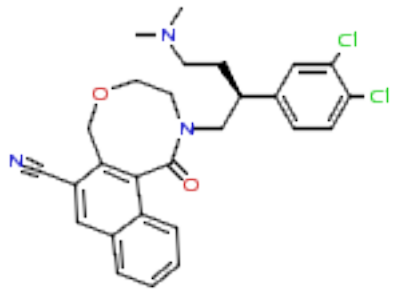
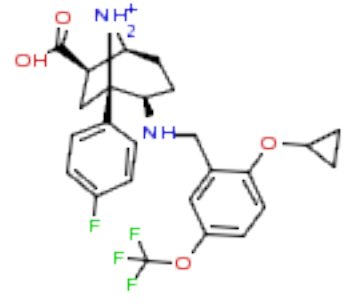
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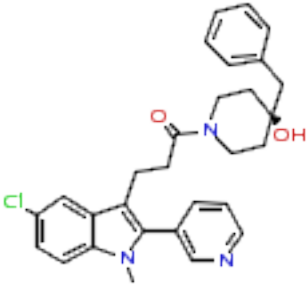
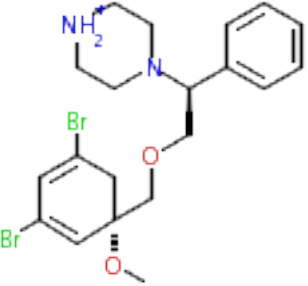
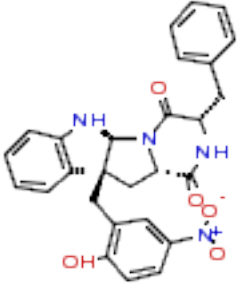
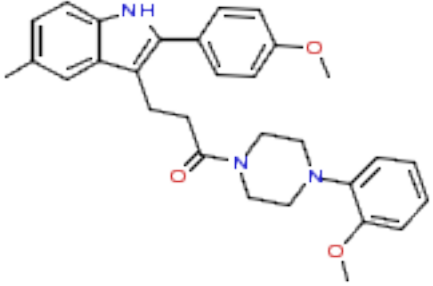
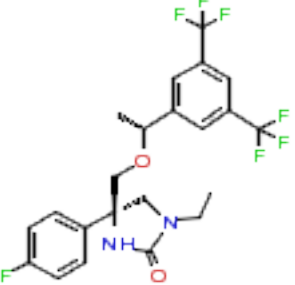
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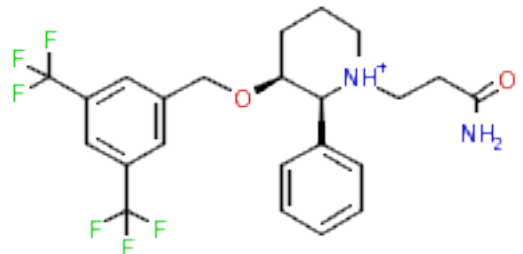
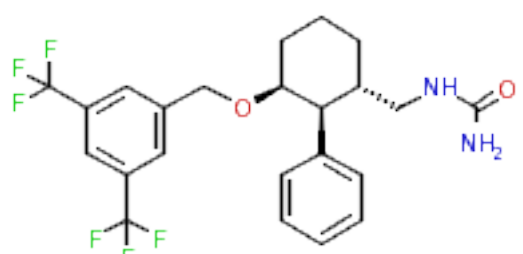
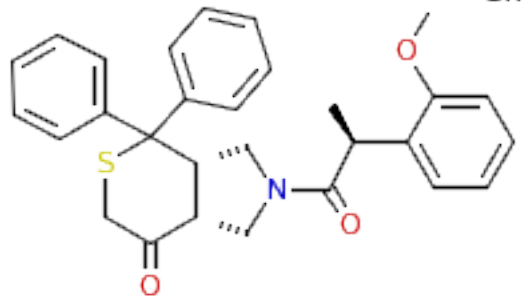
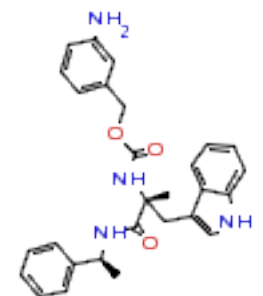
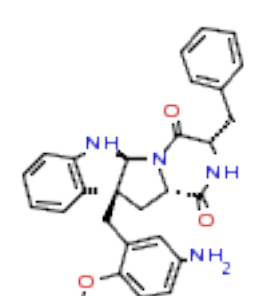
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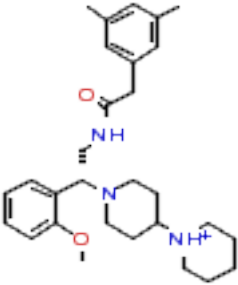
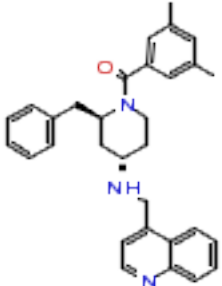
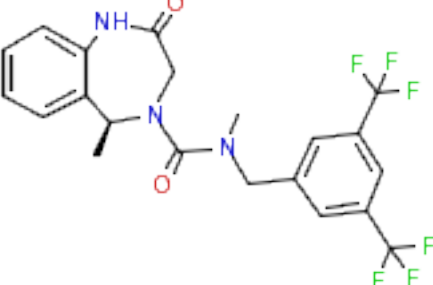
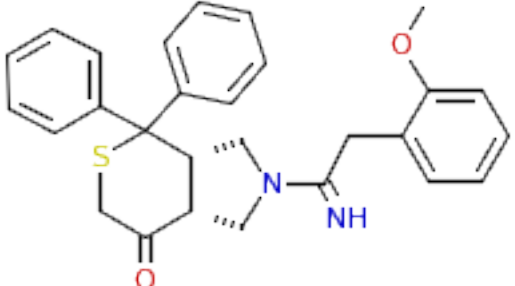
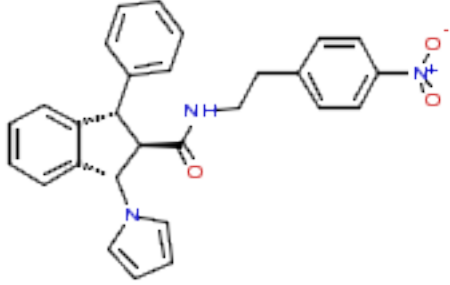
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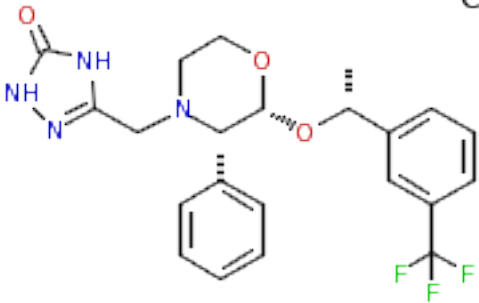
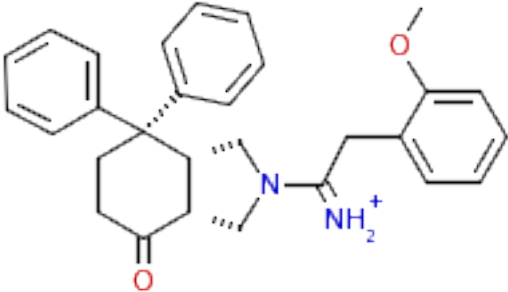
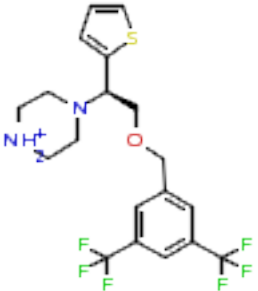
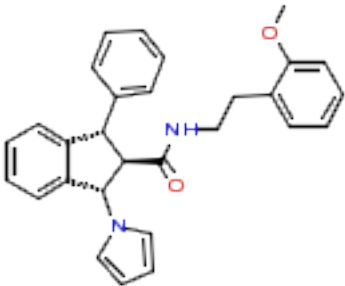
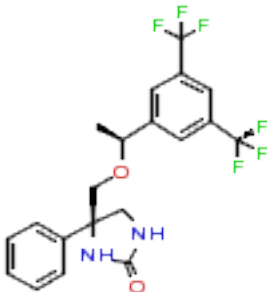
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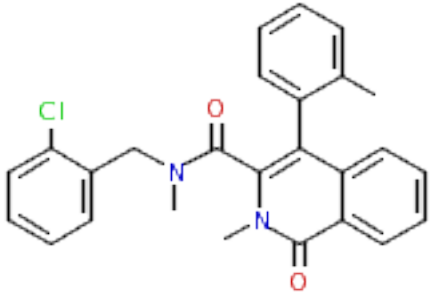
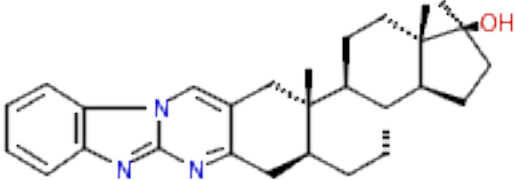
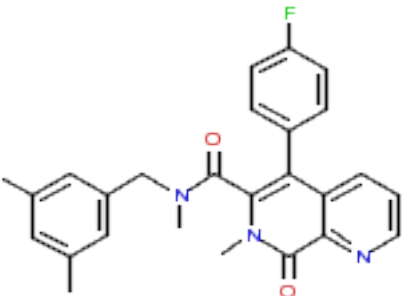
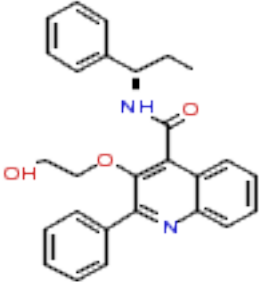
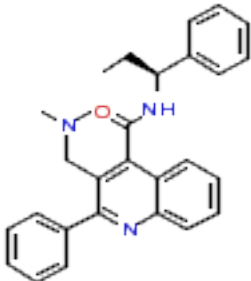
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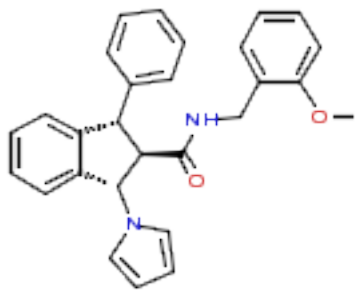
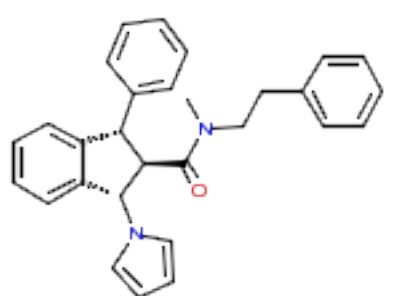
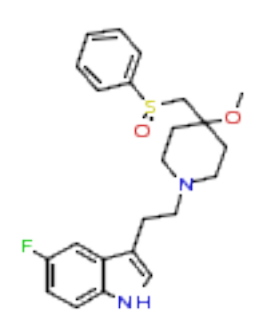
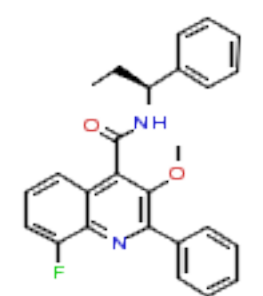
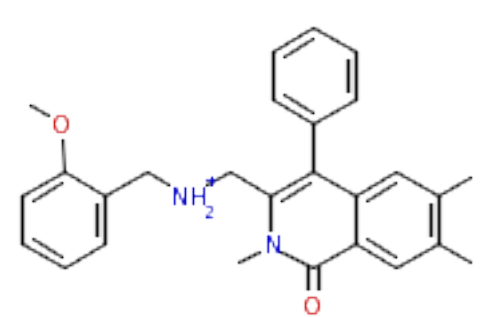
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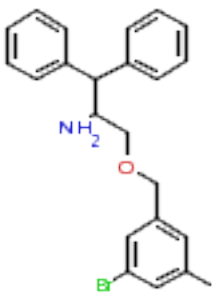
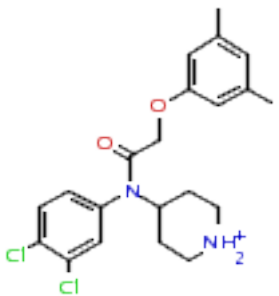
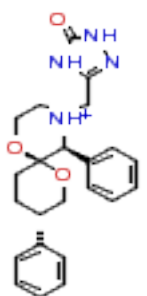
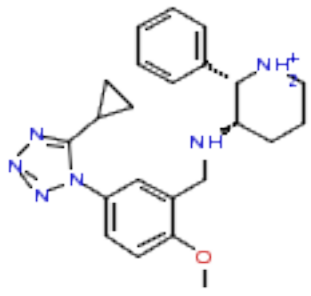
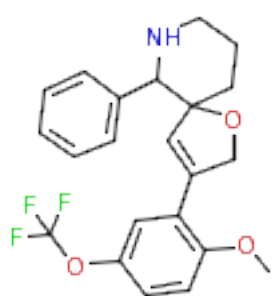
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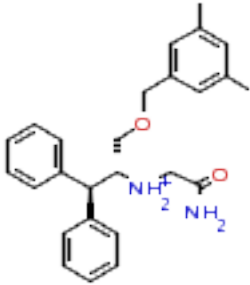
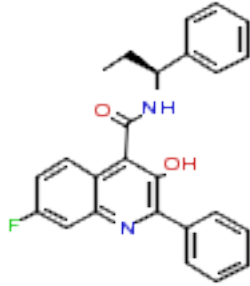
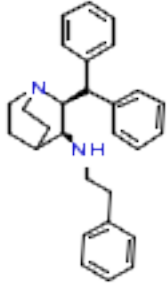
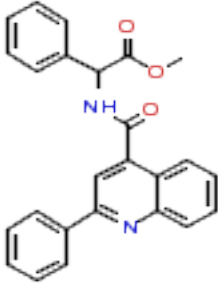
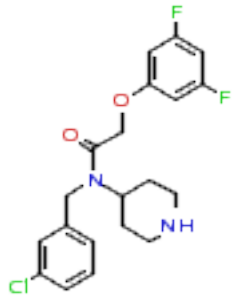
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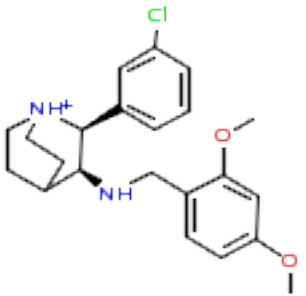
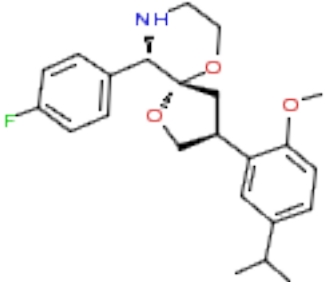
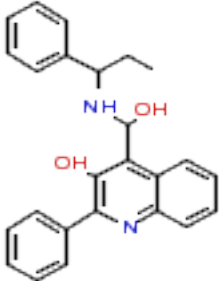
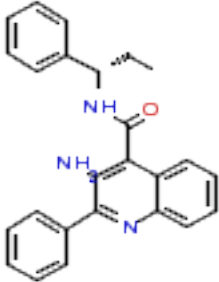
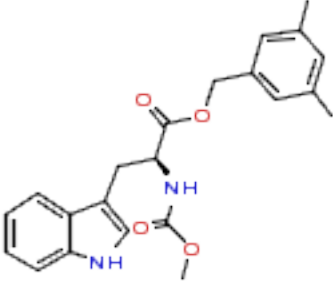
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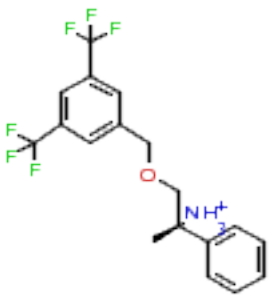
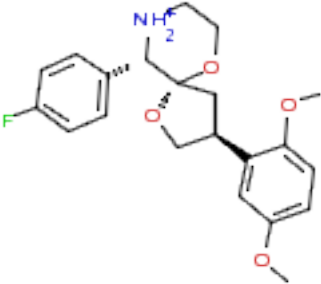
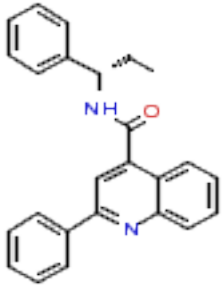
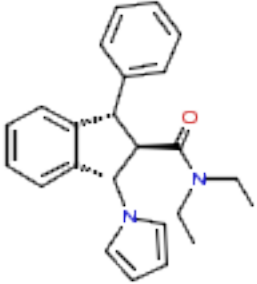
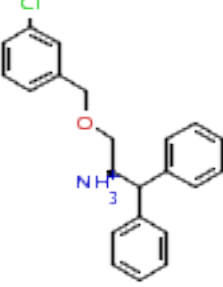
Molecule	Aureus ID	Publication
	77003	J. Med. Chem. VOL. 38 PAG. 3106
Chiral 	100881	Mol. Pharmacol. VOL. 41 PAG. 772
	77025	J. Med. Chem. VOL. 38 PAG. 3106
Chiral 	72705	J. Med. Chem. VOL. 42 PAG. 1053
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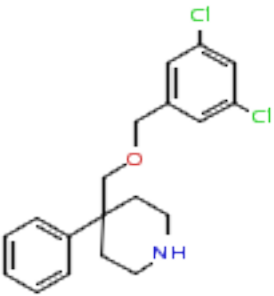
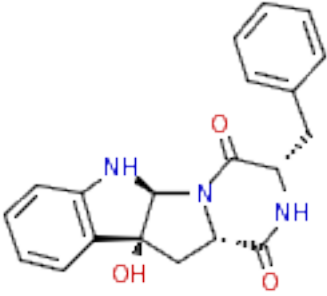
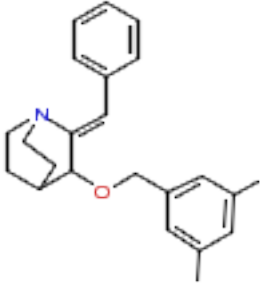
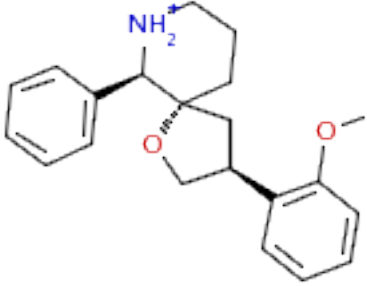
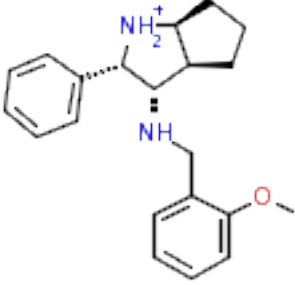
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Chiral 	198651	Bioorg. Med. Chem. VOL. 10 PAG. 1043
Chiral 	76717	Pharmacology. VOL. 65 PAG. 96
Chiral 	292880	Bioorg. Med. Chem. VOL. 12 PAG. 4533
	77013	J. Med. Chem. VOL. 38 PAG. 3106

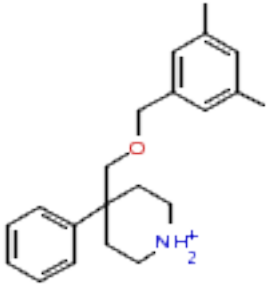
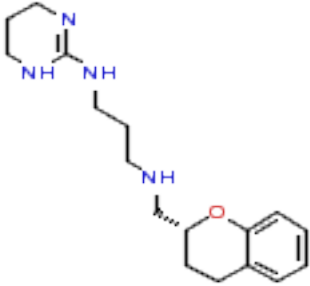
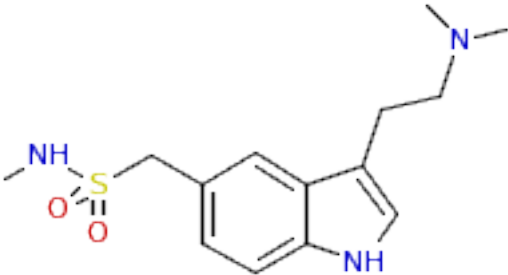
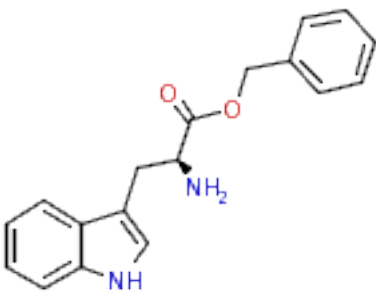
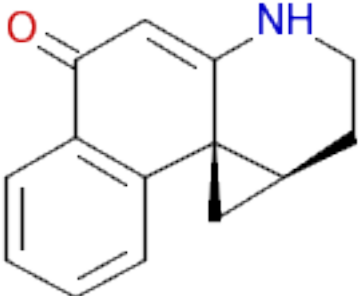
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Chiral 	85781	Bioorg. Med. Chem. Lett. VOL. 4 PAG. 1903
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Chiral 	195451	Bioorg. Med. Chem. Lett. VOL. 12 PAG. 2515
Chiral 	39044	Bioorg. Med. Chem. Lett. VOL. 6 PAG. 1015
Chiral 	182130	Bioorg. Med. Chem. Lett. VOL. 12 PAG. 2719

Molecule	Aureus ID	Publication
Chiral 	86843	Bioorg. Med. Chem. Lett. VOL. 4 PAG. 1903
Chiral 	292879	Bioorg. Med. Chem. VOL. 12 PAG. 4533
Chiral 	93405	Bioorg. Med. Chem. Lett. VOL. 3 PAG. 1361
Chiral 	36241	J. Med. Chem. VOL. 39 PAG. 2281
	181010	Bioorg. Med. Chem. Lett. VOL. 12 PAG. 261

Molecule	Aureus ID	Publication
Chiral 	85168	Bioorg. Med. Chem. Lett. VOL. 4 PAG. 839
Chiral 	195476	Bioorg. Med. Chem. Lett. VOL. 12 PAG. 2515
Chiral 	99389	J. Pharmacol. Exp. Ther. VOL. 281 PAG. 1303
Chiral 	72626	J. Med. Chem. VOL. 42 PAG. 1053
Chiral 	68919	J. Med. Chem. VOL. 37 PAG. 1269

Molecule	Aureus ID	Publication
Chiral 	38942	Bioorg. Med. Chem. Lett. VOL. 5 PAG. 2761
Chiral 	195474	Bioorg. Med. Chem. Lett. VOL. 12 PAG. 2515
Chiral 	36244	J. Med. Chem. VOL. 39 PAG. 2281
Chiral 	198646	Bioorg. Med. Chem. VOL. 10 PAG. 1043
Chiral 	85777	Bioorg. Med. Chem. Lett. VOL. 4 PAG. 1903

Molecule	Aureus ID	Publication
	77137	J. Med. Chem. VOL. 38 PAG. 1264
Chiral 	39006	Bioorg. Med. Chem. Lett. VOL. 5 PAG. 377
Chiral 	124569	Bioorg. Med. Chem. Lett. VOL. 5 PAG. 1261
Chiral 	182134	Bioorg. Med. Chem. Lett. VOL. 12 PAG. 2719
Chiral 	86845	Bioorg. Med. Chem. Lett. VOL. 17 PAG. 6887

Molecule	Aureus ID	Publication
	77139	J. Med. Chem. VOL. 38 PAG. 1264
Chiral 	5897	Mol. Pharmacol. VOL. 50 PAG. 1567
	2885	Mol. Pharmacol. VOL. 50 PAG. 1567
Chiral 	113486	J. Med. Chem. VOL. 37 PAG. 1269
Chiral 	98334	J. Neurochem. VOL. 60 PAG. 868