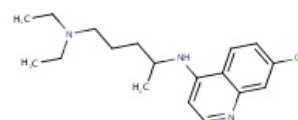


Run parameters

Library screened ZincLeadLike
 Screening method Electroshape
 Date Wed Jan 1 08:38:21 2020

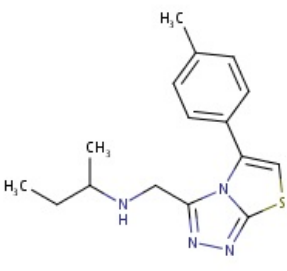
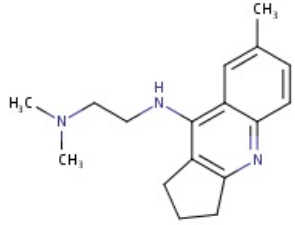
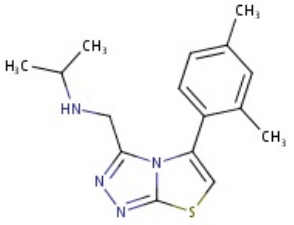
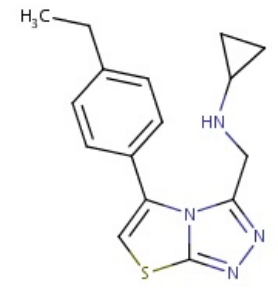
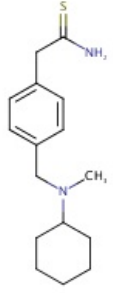
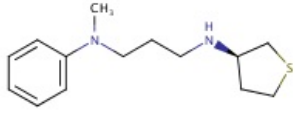
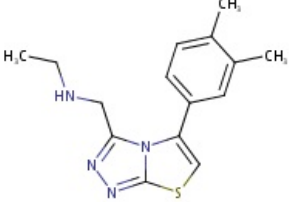
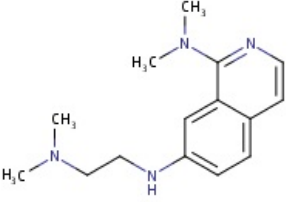
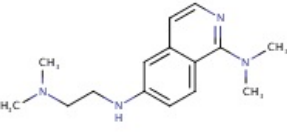
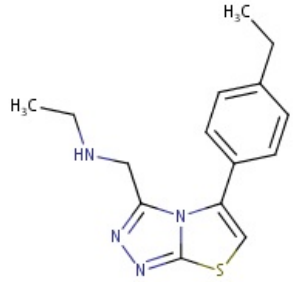
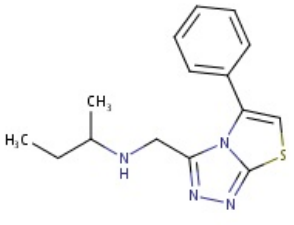
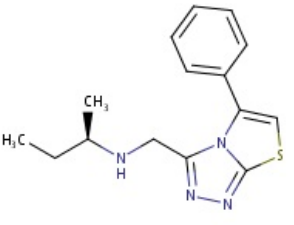
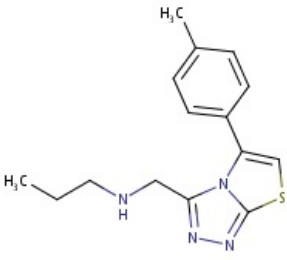
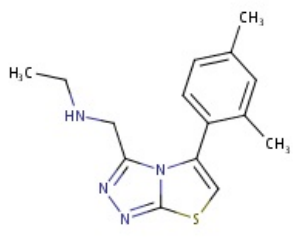
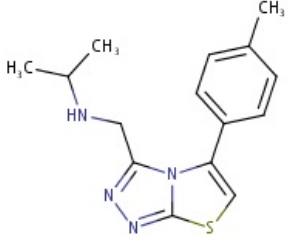
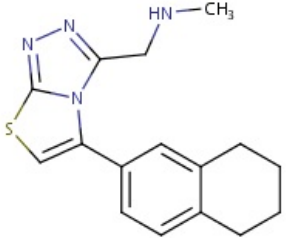
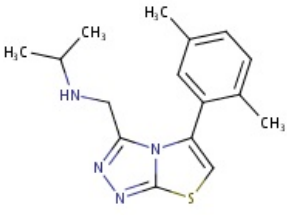
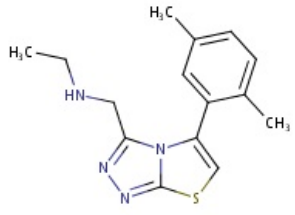
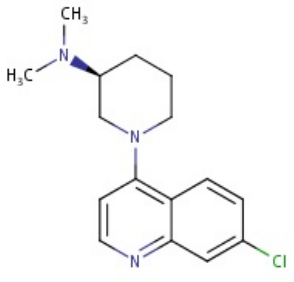
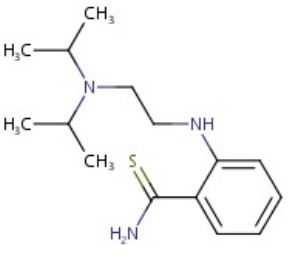
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

Query Molecule

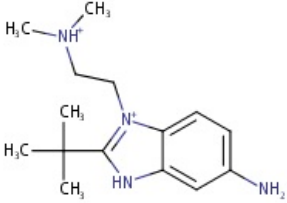
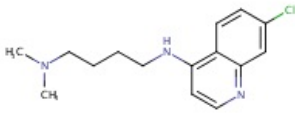
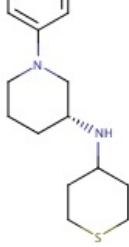
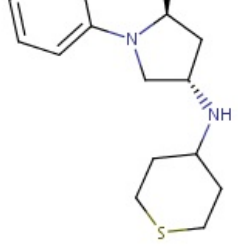
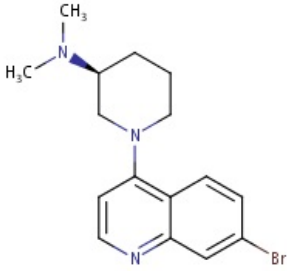
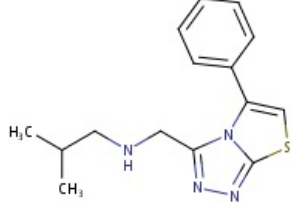
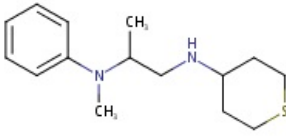
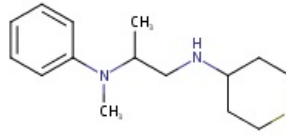
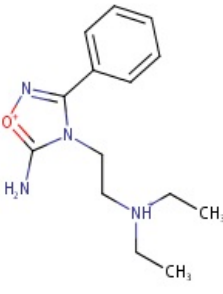
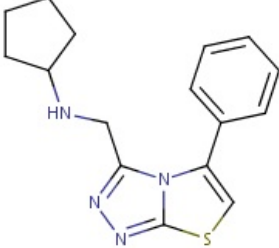
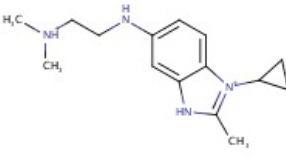
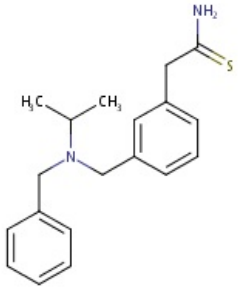
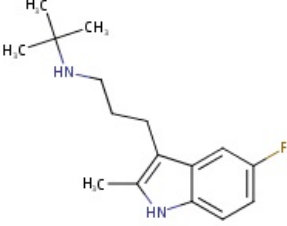
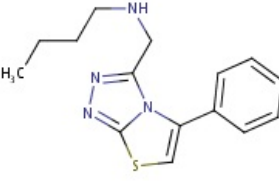
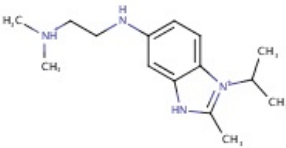
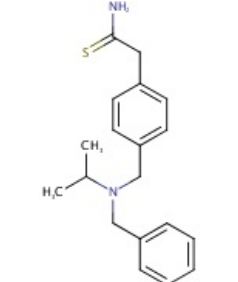
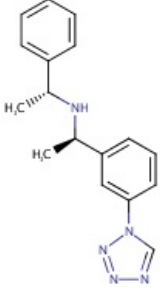
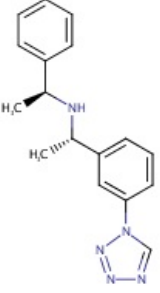
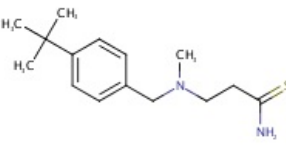
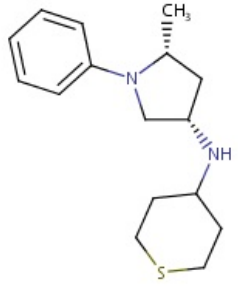




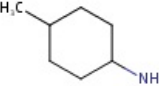
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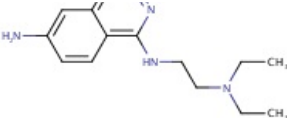
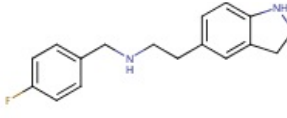
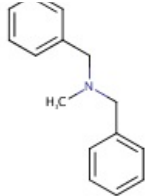
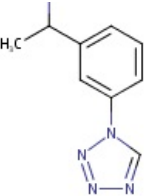
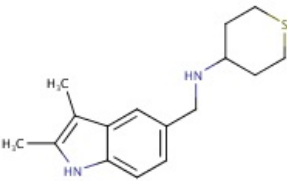
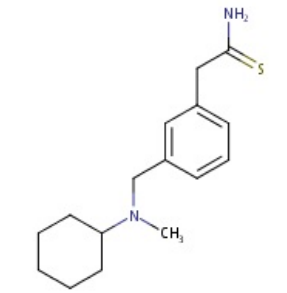
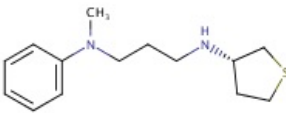
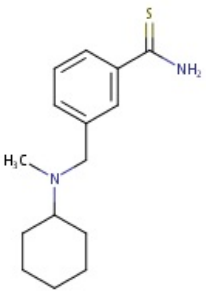
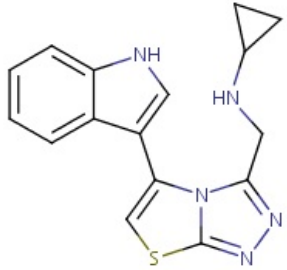
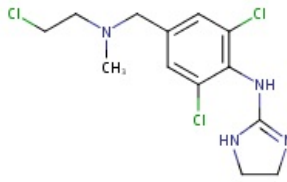
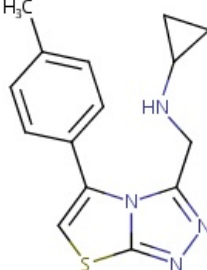
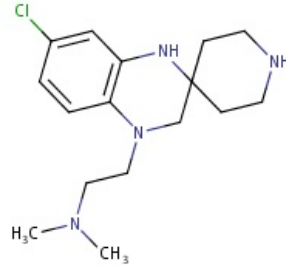
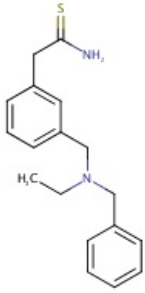
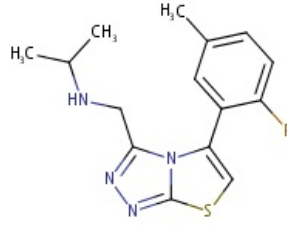
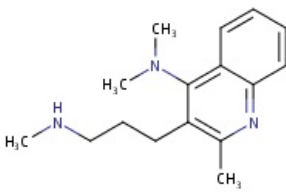
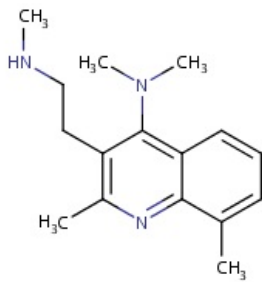
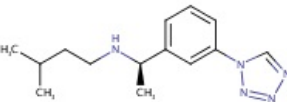
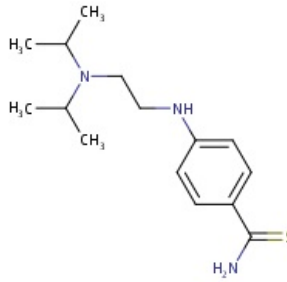
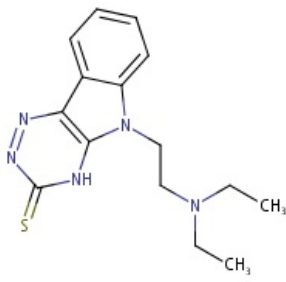
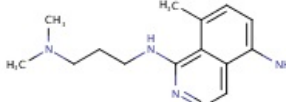
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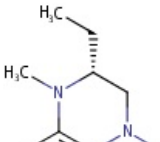
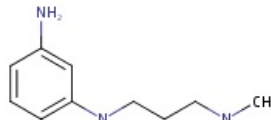


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|  |  |  |  |
| Score : 0.908 | Score : 0.907 | Score : 0.907 | Score : 0.906 |
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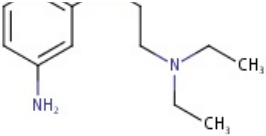
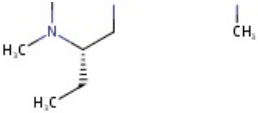
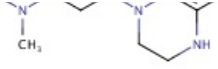
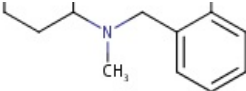
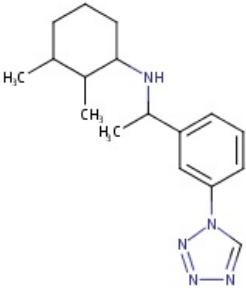
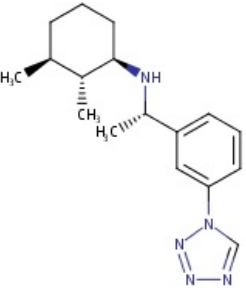
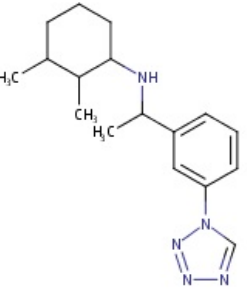
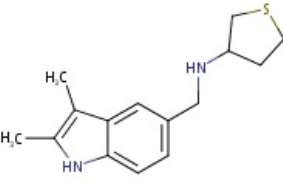
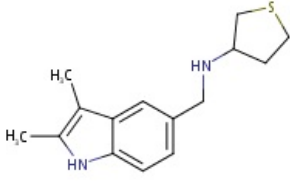
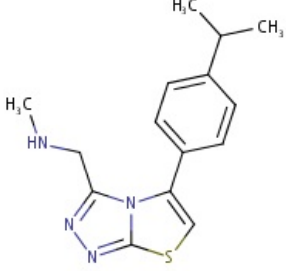
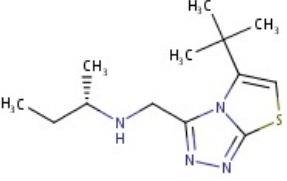
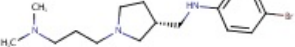
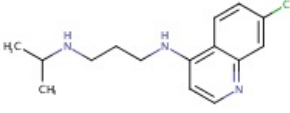
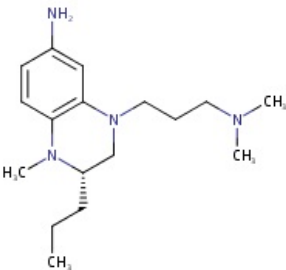
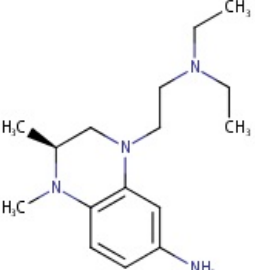
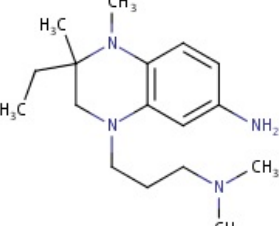
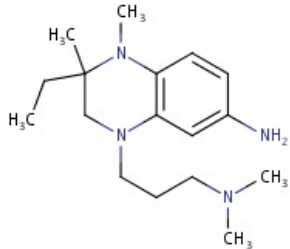
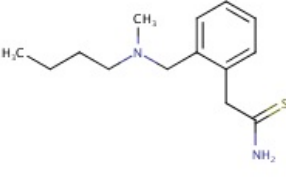
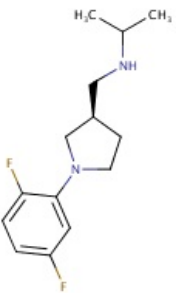
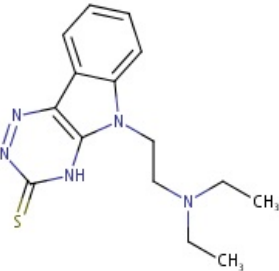
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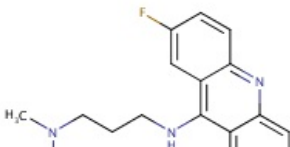
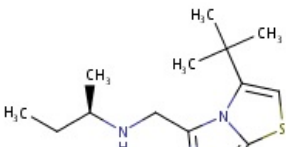
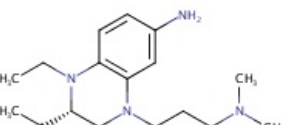
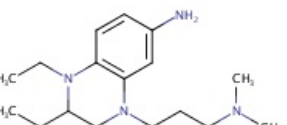
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| Score : 0.898 | Score : 0.898 | Score : 0.898 | Score : 0.898 |
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| Score : 0.898 | Score : 0.898 | Score : 0.898 | Score : 0.897 |
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| Score : 0.897 | Score : 0.897 | Score : 0.896 | Score : 0.896 |
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| Score : 0.896 | Score : 0.895 | Score : 0.895 | Score : 0.895 |
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| Score : 0.894 | Score : 0.894 | Score : 0.893 | Score : 0.893 |
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| Score : 0.893 | Score : 0.892 | Score : 0.892 | Score : 0.892 |
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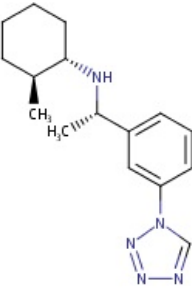
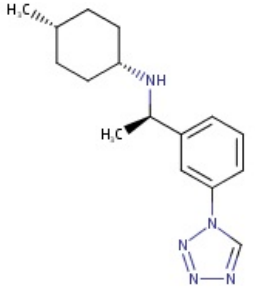
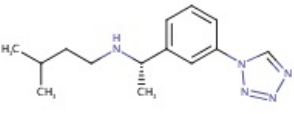
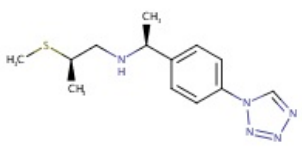
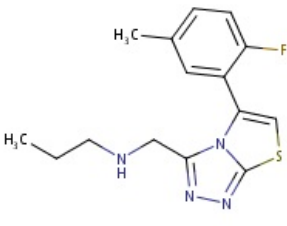
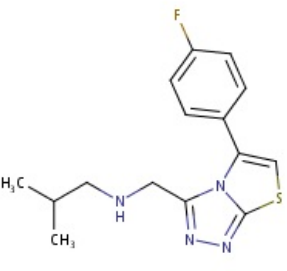
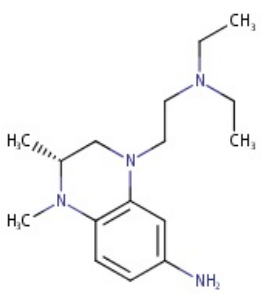
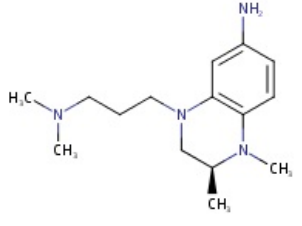
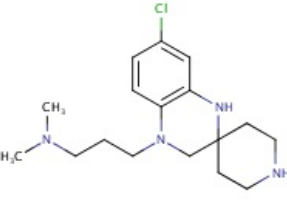
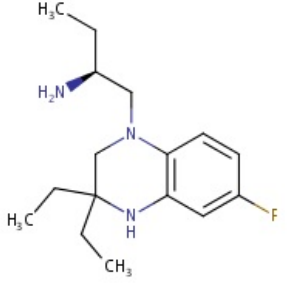
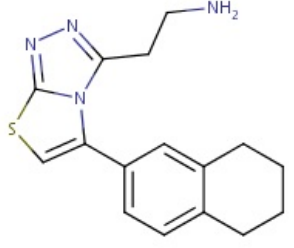
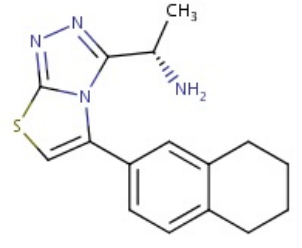
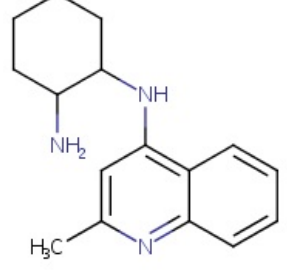
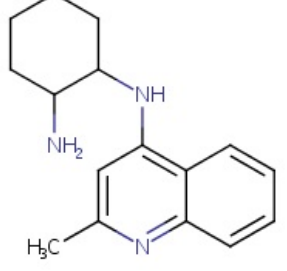
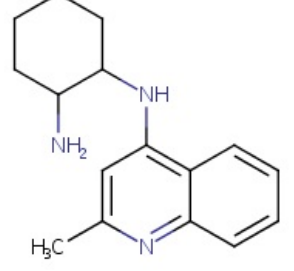
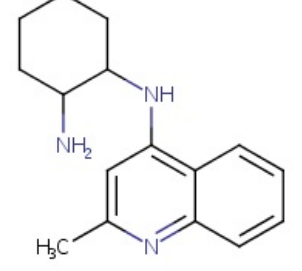
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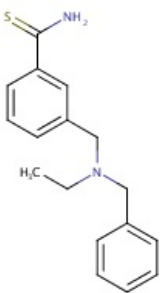
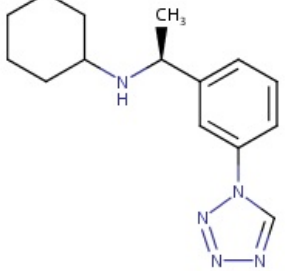
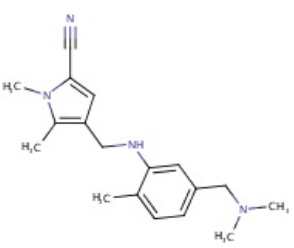
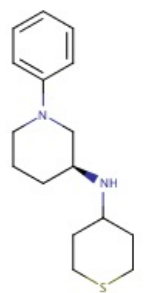
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| Score : 0.891 | Score : 0.890 | Score : 0.890 | Score : 0.890 |
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| Score : 0.890 | Score : 0.889 | Score : 0.889 | Score : 0.889 |
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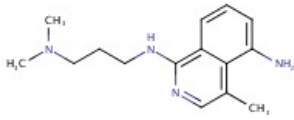
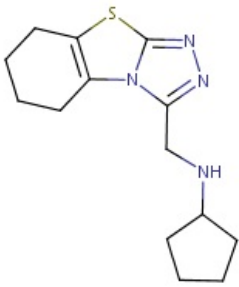
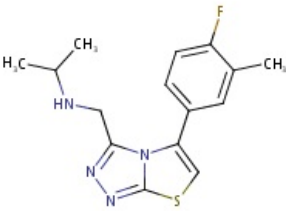
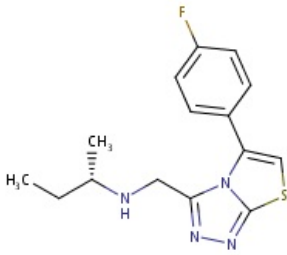
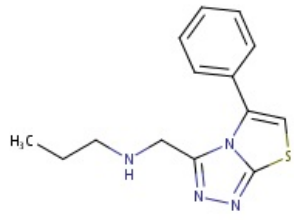
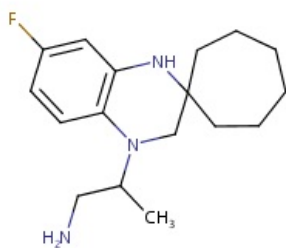
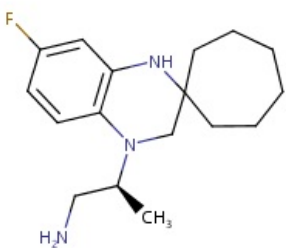
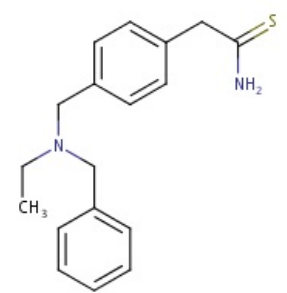
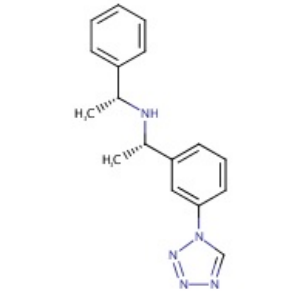
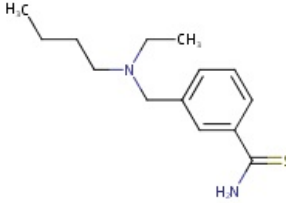
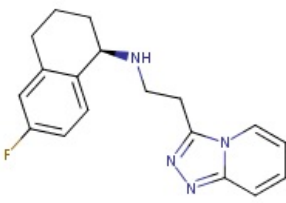
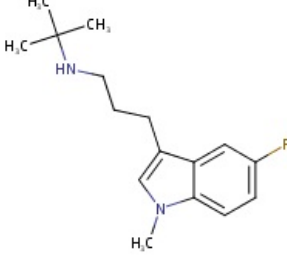
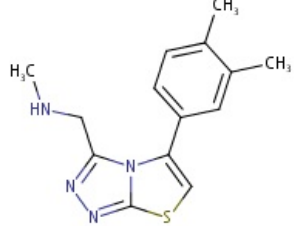
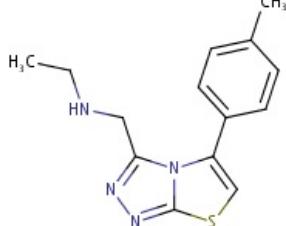
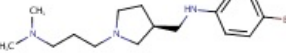
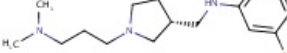
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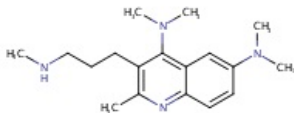
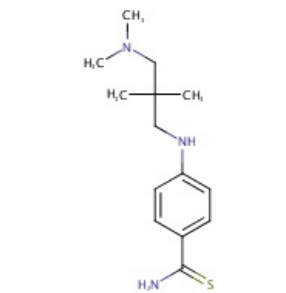
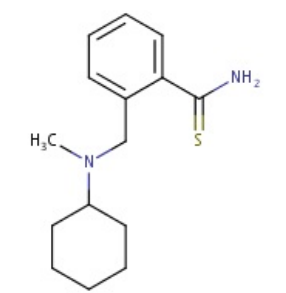
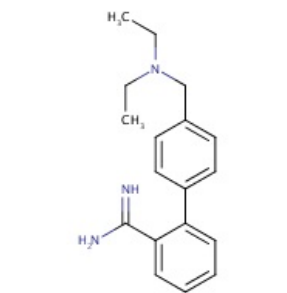




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| <chem>CC</chem> | <chem>C#N</chem> | <chem>CC</chem> | <chem>CC</chem> |
| Score : 0.888 | Score : 0.888 | Score : 0.888 | Score : 0.888 |
| <chem>CCN(C)CCNC1=CC=C2C(=C1)N(C)C2C3CC3</chem> | <chem>CCCCN(C)Cc1ccc(cc1)CC(=S)N</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CN(C)Cc1ccc(cc1)C(=S)N</chem> |
| Score : 0.887 | Score : 0.887 | Score : 0.887 | Score : 0.887 |
| <chem>CC1(CCN1C2=CC=CC=C2)N[C@H]3CCSCC3</chem> | <chem>CCN(C)CCNC1=CC=C2C(=C1)N(C)C2C3CC3</chem> | <chem>CCN(C)CCNC1=CC=C2C(=C1)N(C)C2C3CC3</chem> | <chem>CC1(CCN1C2=CC=CC=C2)N[C@H]3CCSCC3</chem> |
| Score : 0.887 | Score : 0.887 | Score : 0.887 | Score : 0.887 |
| <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> |
| Score : 0.887 | Score : 0.886 | Score : 0.886 | Score : 0.886 |
| <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> |

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|---|---|---|---|
| Score : 0.886 | Score : 0.886 | Score : 0.886 | Score : 0.886 |
| <chem>CC1=CC=C2C(=C1)N(C)C2C3CC3</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> | <chem>CC(C)CNC[C@H]1CC[C@H](N1)c2ccc(F)cc2</chem> |

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| <p>Score : 0.886</p>  | <p>Score : 0.886</p>  | <p>Score : 0.886</p>  | <p>Score : 0.885</p>  |
| <p>Score : 0.885</p>  | <p>Score : 0.885</p>  | <p>Score : 0.885</p>  | <p>Score : 0.885</p>  |
| <p>Score : 0.885</p>  | <p>Score : 0.885</p>  | <p>Score : 0.885</p>  | <p>Score : 0.885</p>  |
| <p>Score : 0.885</p>  | <p>Score : 0.885</p>  | <p>Score : 0.885</p>  | <p>Score : 0.885</p>  |

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| <p>Score : 0.885</p>  | <p>Score : 0.885</p>  | <p>Score : 0.884</p>  | <p>Score : 0.884</p>  |
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| Score : 0.884 | Score : 0.884 | Score : 0.884 | Score : 0.884 |
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| Score : 0.884 | Score : 0.884 | Score : 0.884 | Score : 0.884 |
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| Score : 0.884 | Score : 0.884 | Score : 0.883 | Score : 0.883 |
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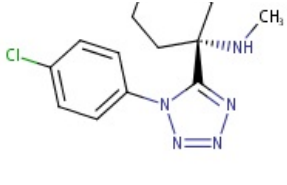
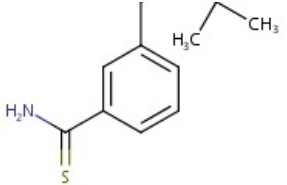
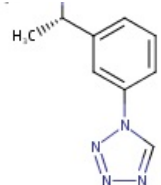
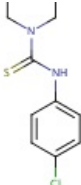
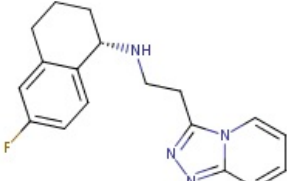
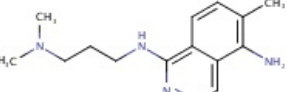
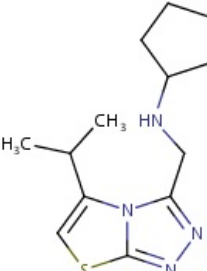
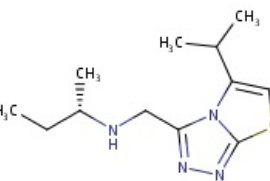
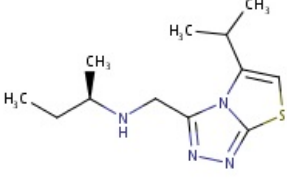
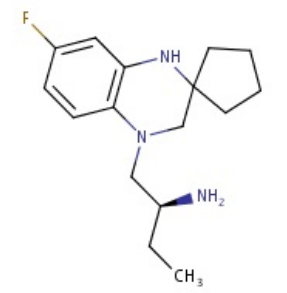
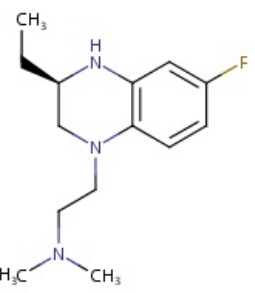
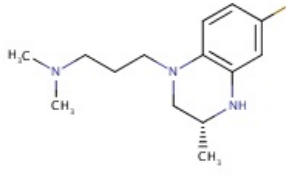
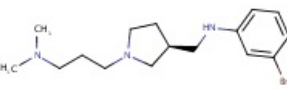
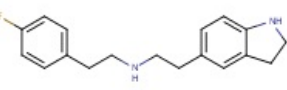
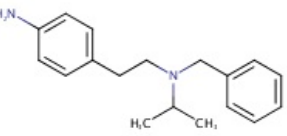
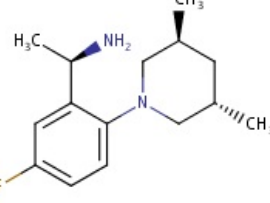
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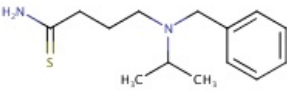
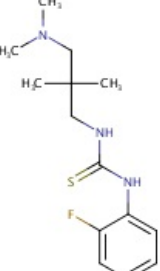
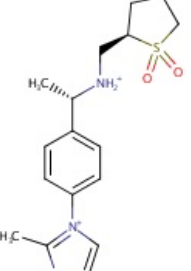
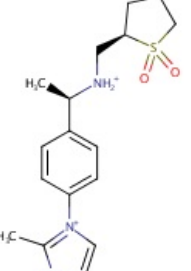
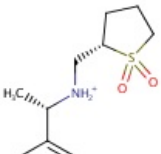
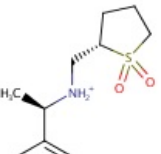
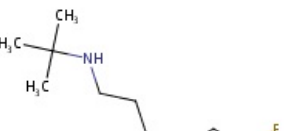
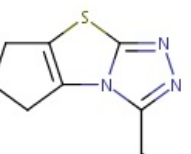
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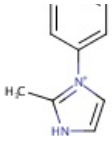
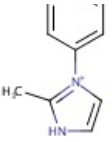
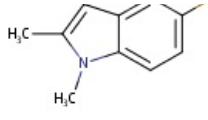

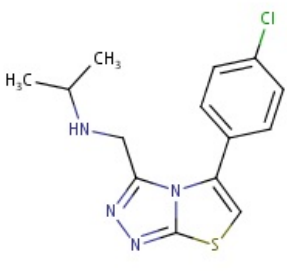
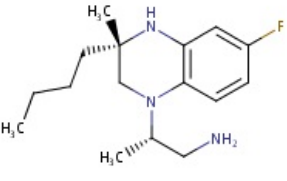
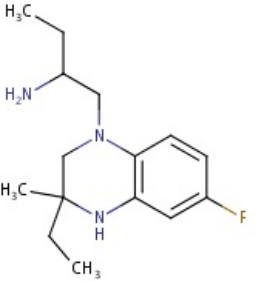
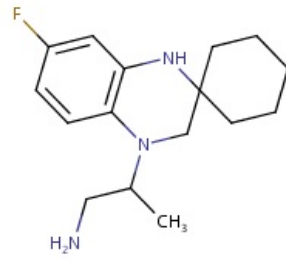
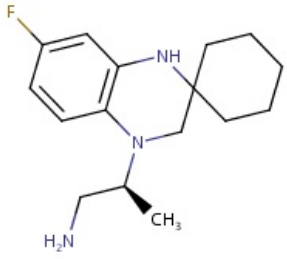
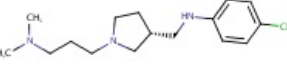
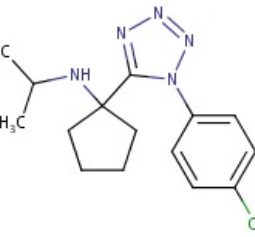
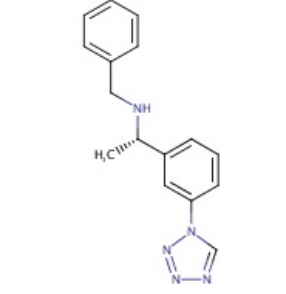
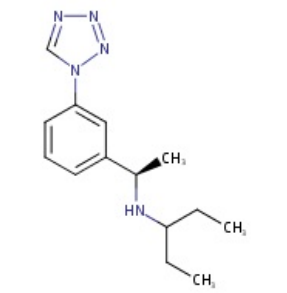
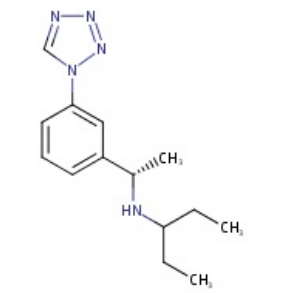
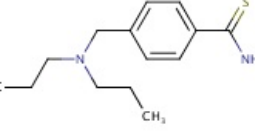
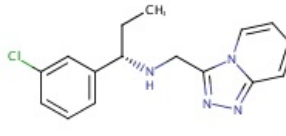
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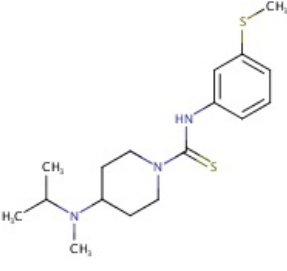
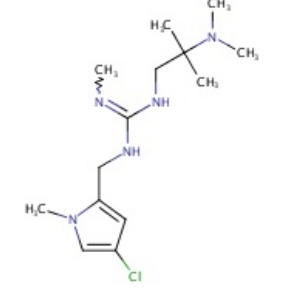
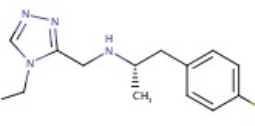
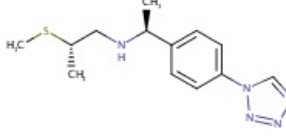
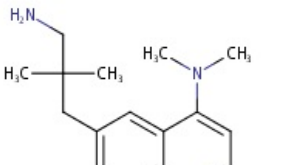
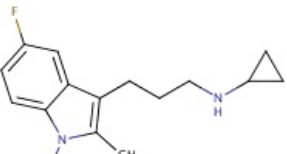
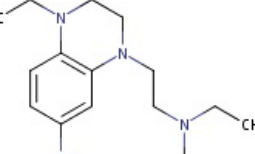
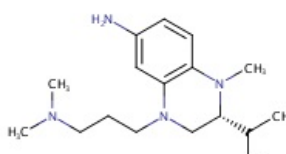
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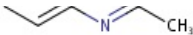



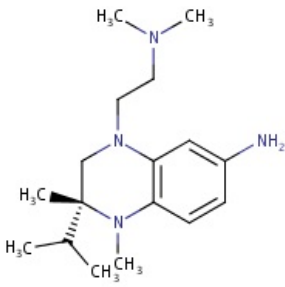
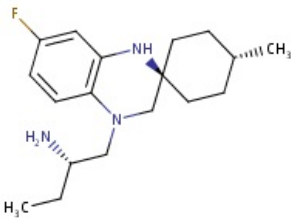
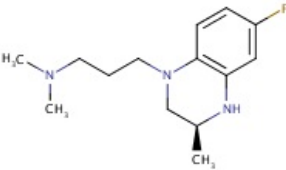
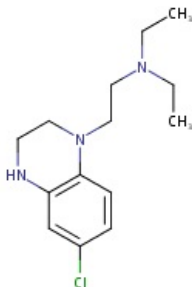
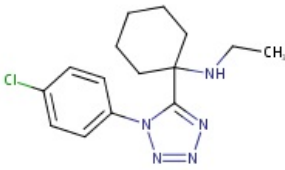
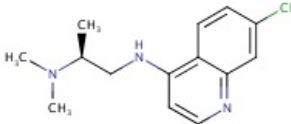
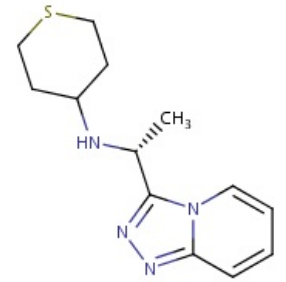
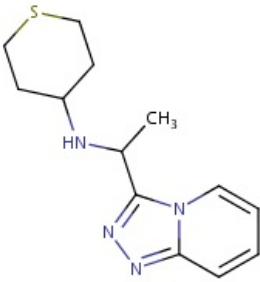
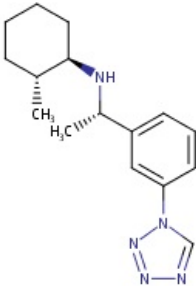
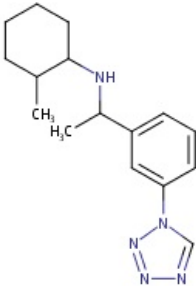
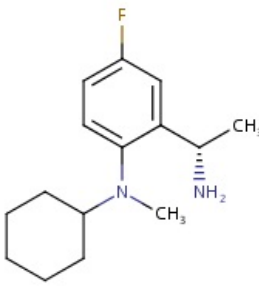
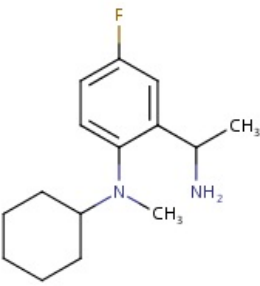
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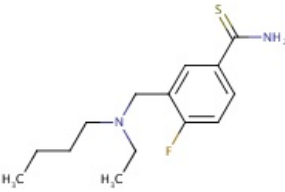
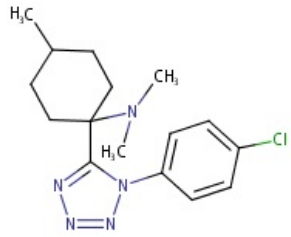
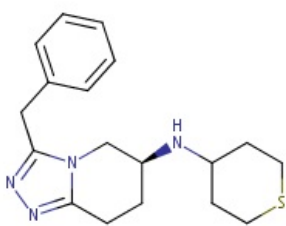
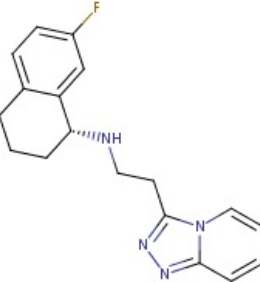
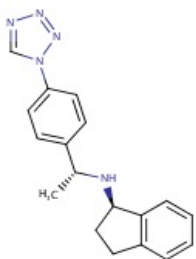
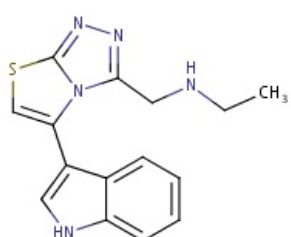
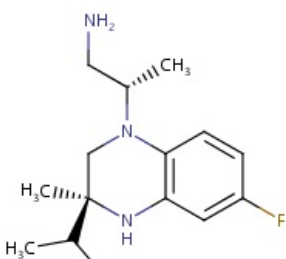
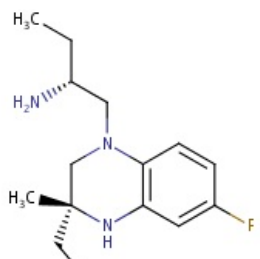
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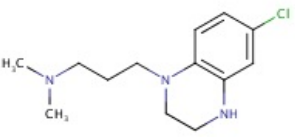
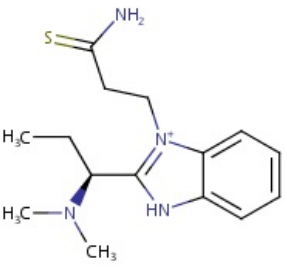
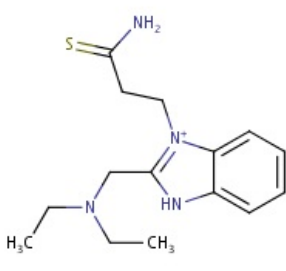
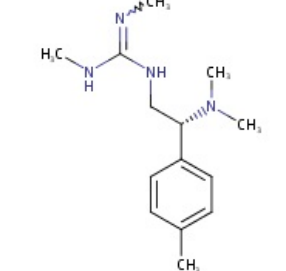
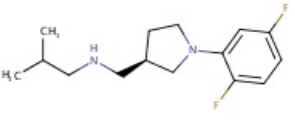
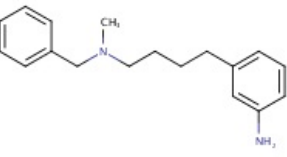
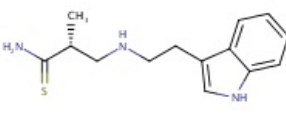
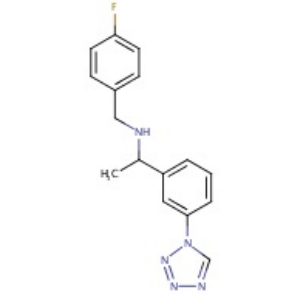
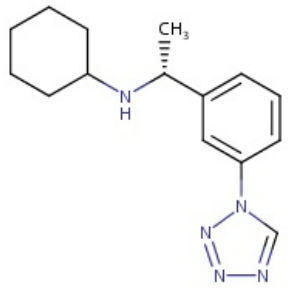
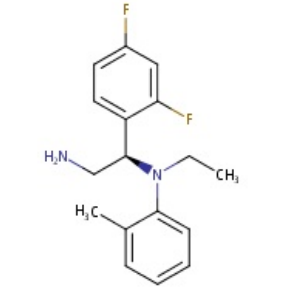
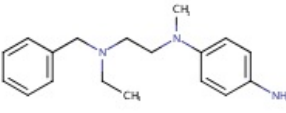
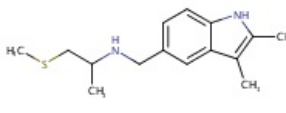
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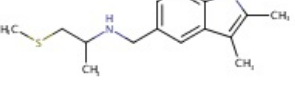
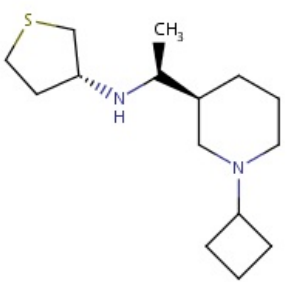
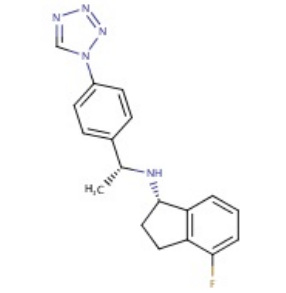
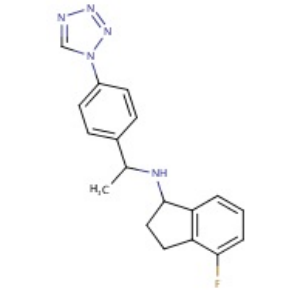
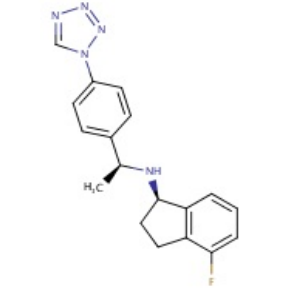
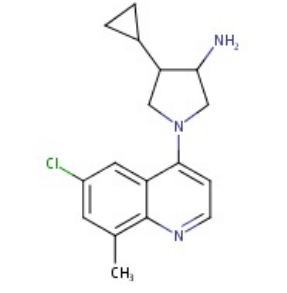
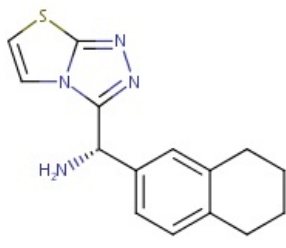
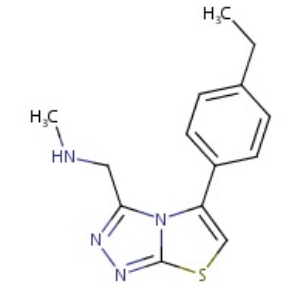
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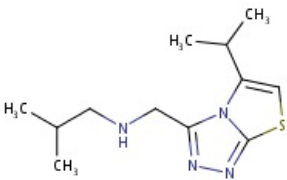
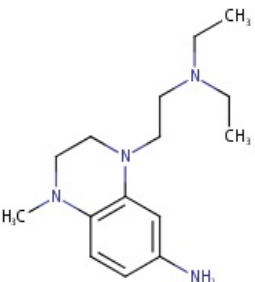
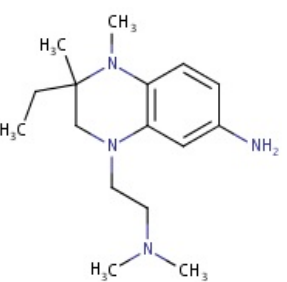
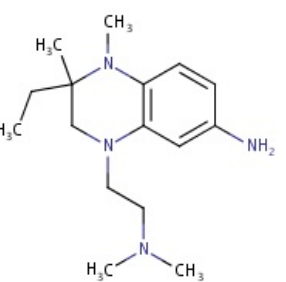
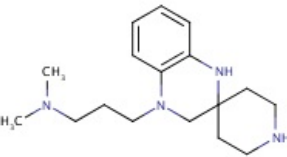
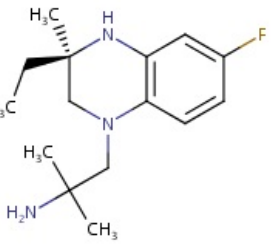
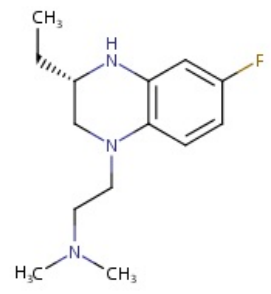
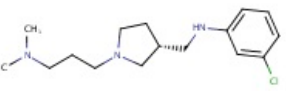
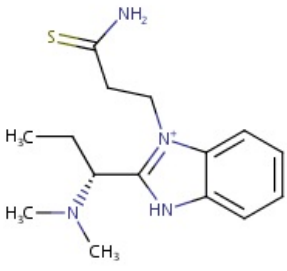
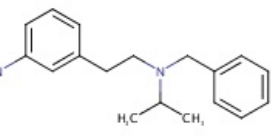
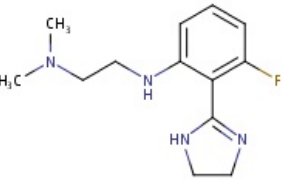
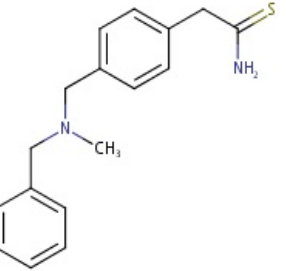
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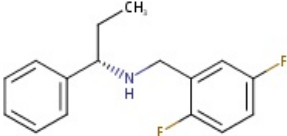
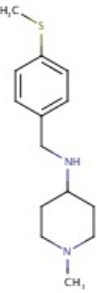
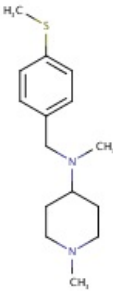
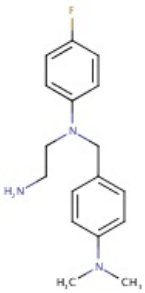
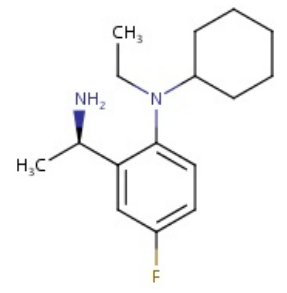
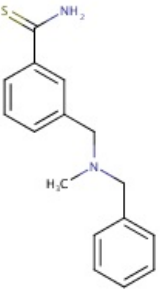
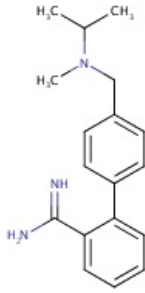
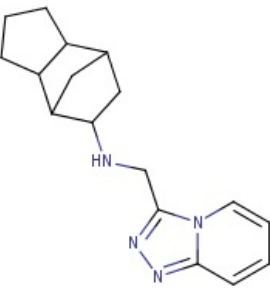
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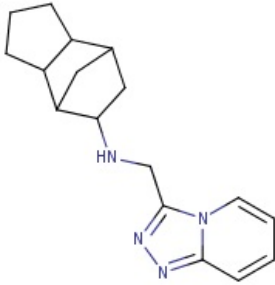
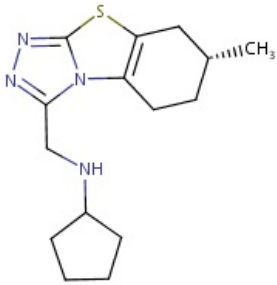
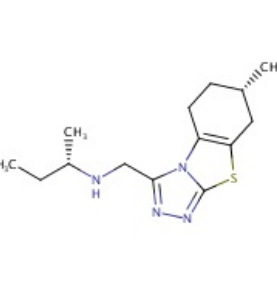
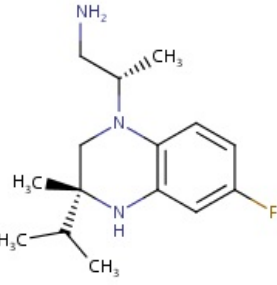
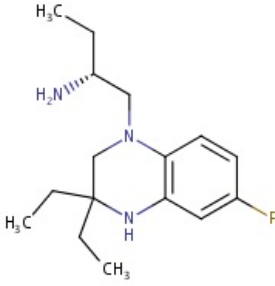
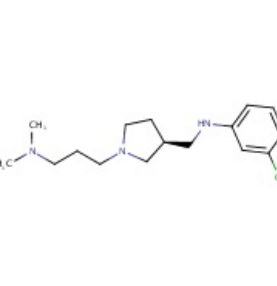
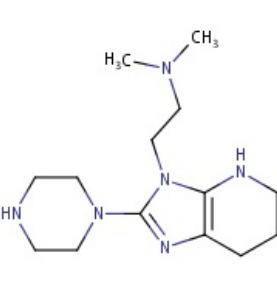
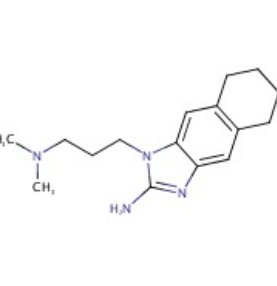
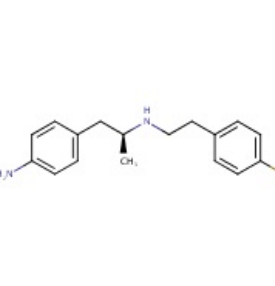
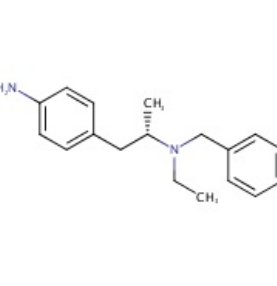
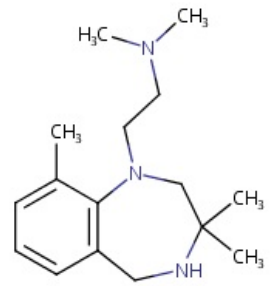
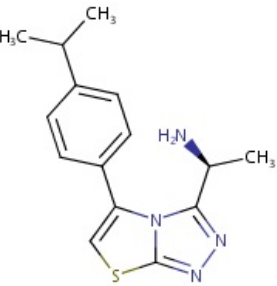
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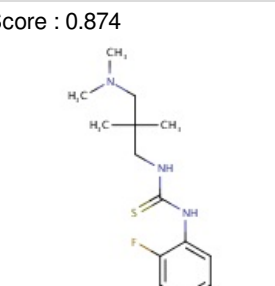
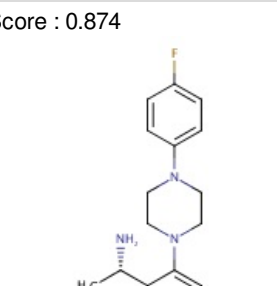
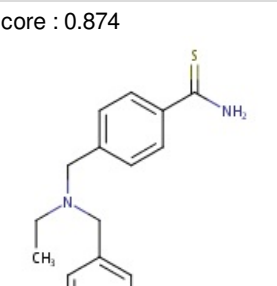
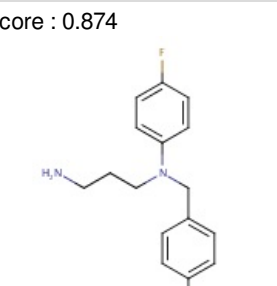
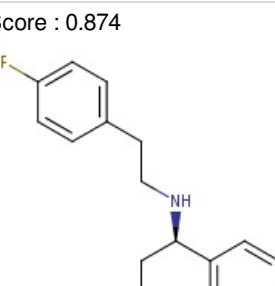
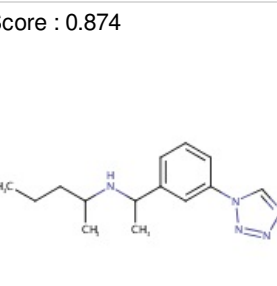
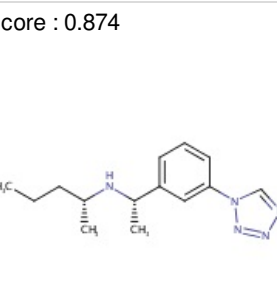
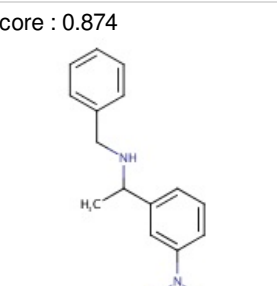
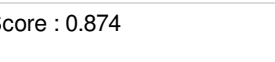



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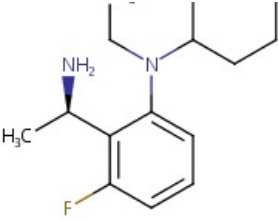
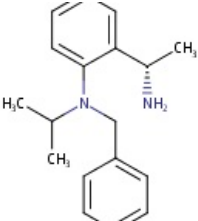
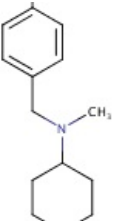
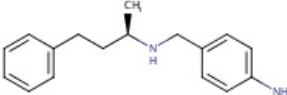
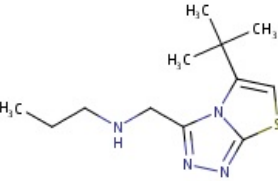
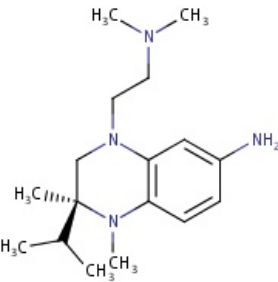
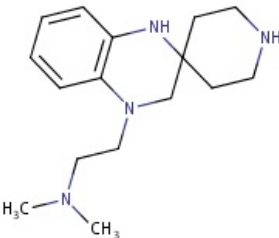
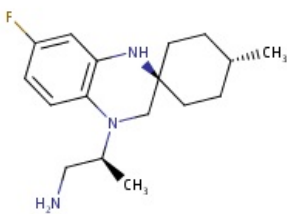
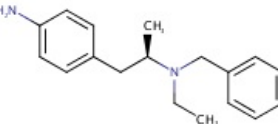
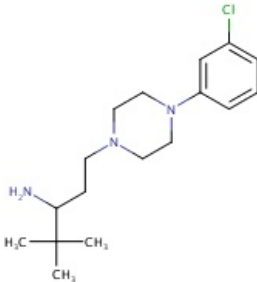
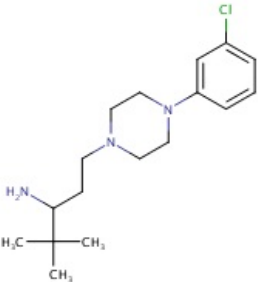
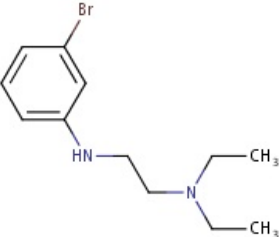
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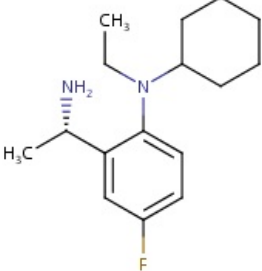
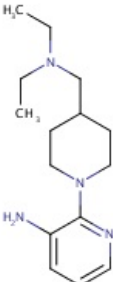
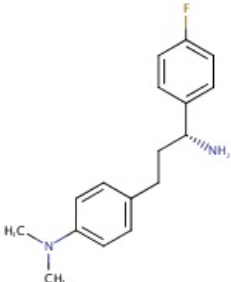
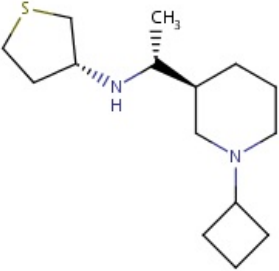
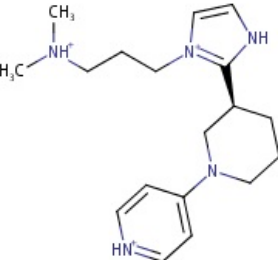
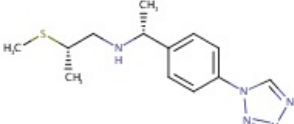
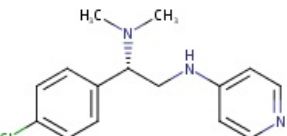
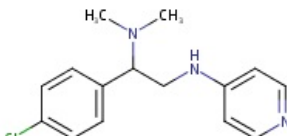

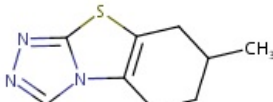

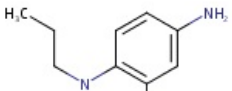
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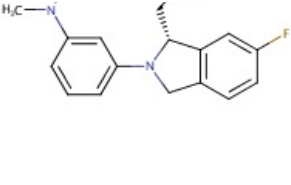
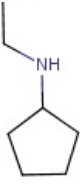
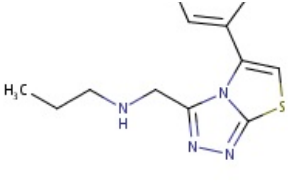
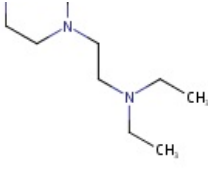
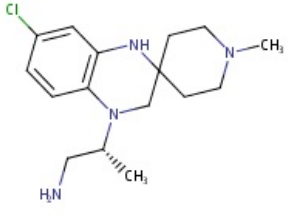
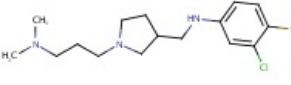
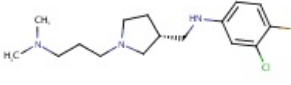
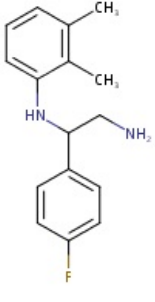
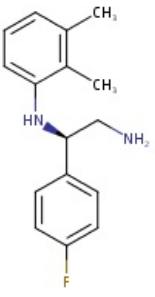
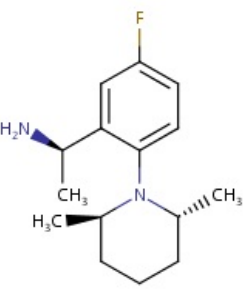
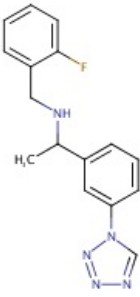
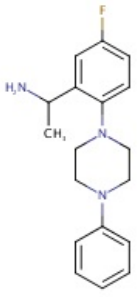
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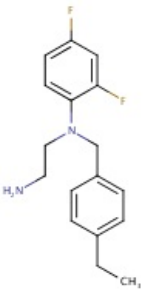
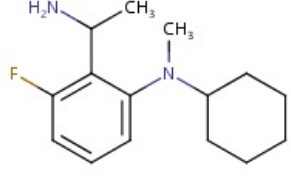
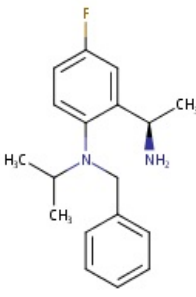
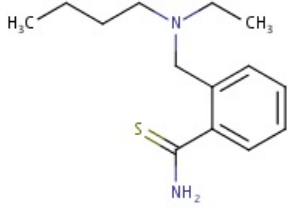
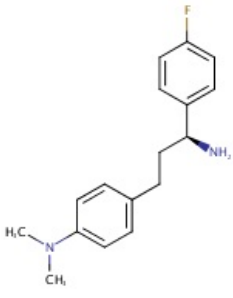
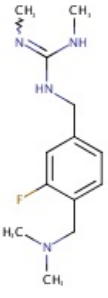
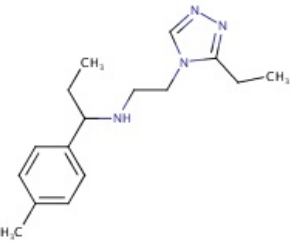
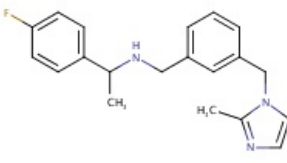
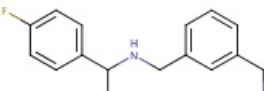
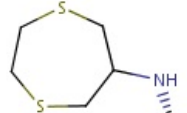

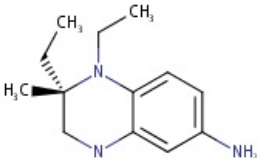
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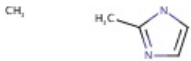
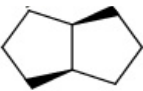
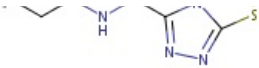
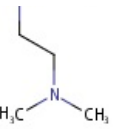
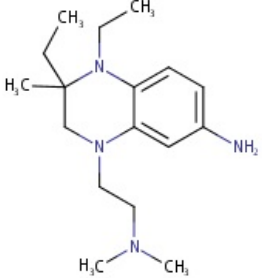
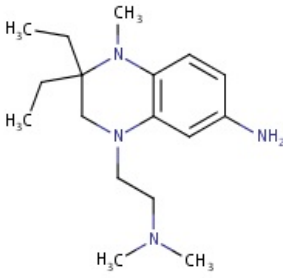
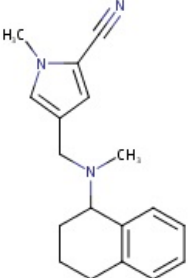
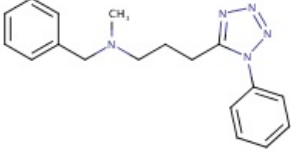
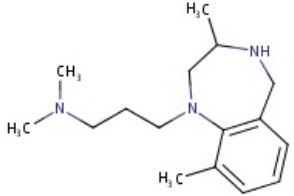
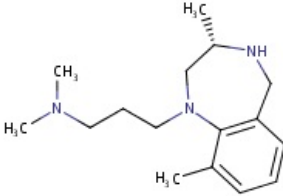
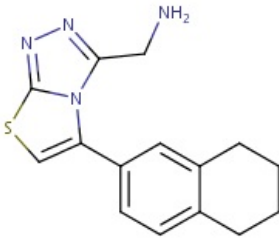
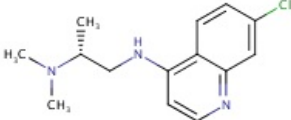
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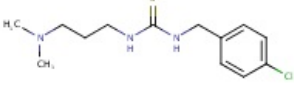
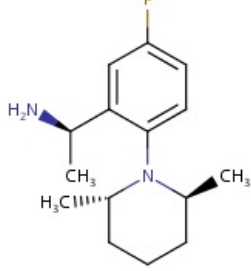
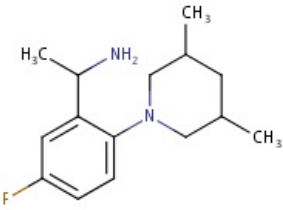
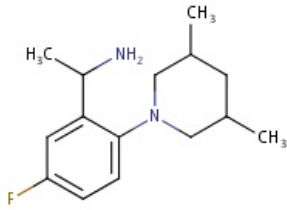
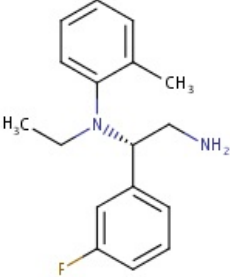
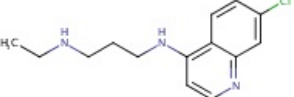
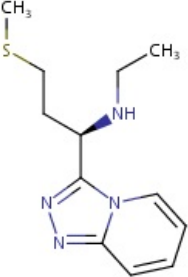
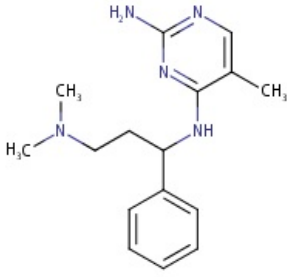
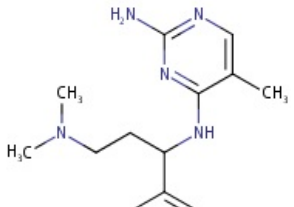
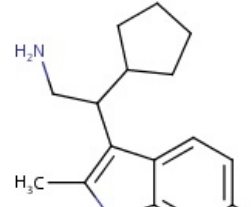
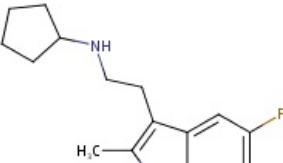
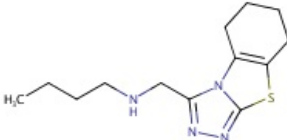
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
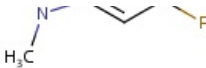

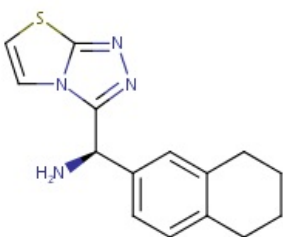
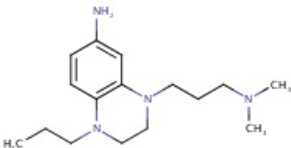
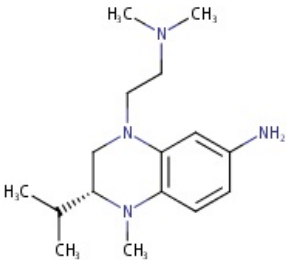
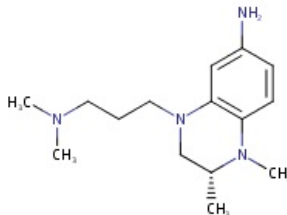
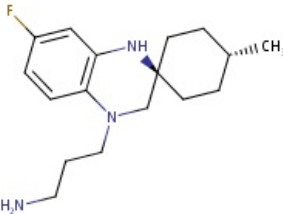
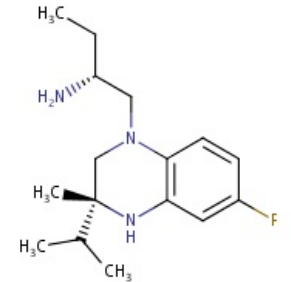
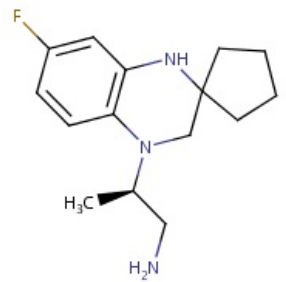
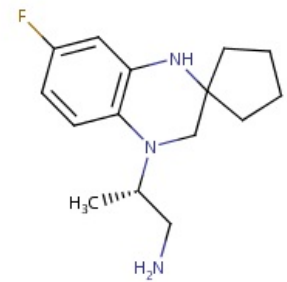
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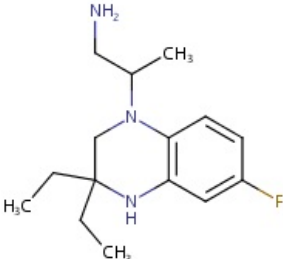
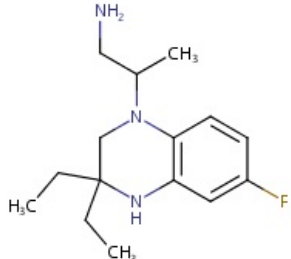
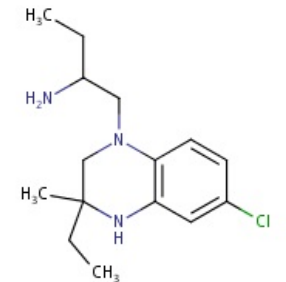
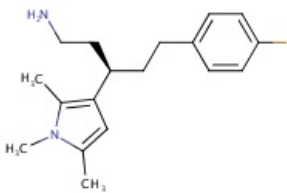
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