

Inhibitor Discovery for TMPRSS2 and Analysis of its Backbone Hydrogen Bonds Using a Simple Descriptor

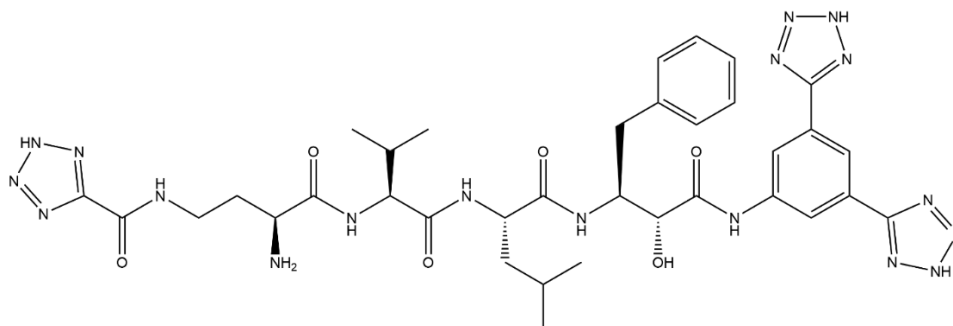
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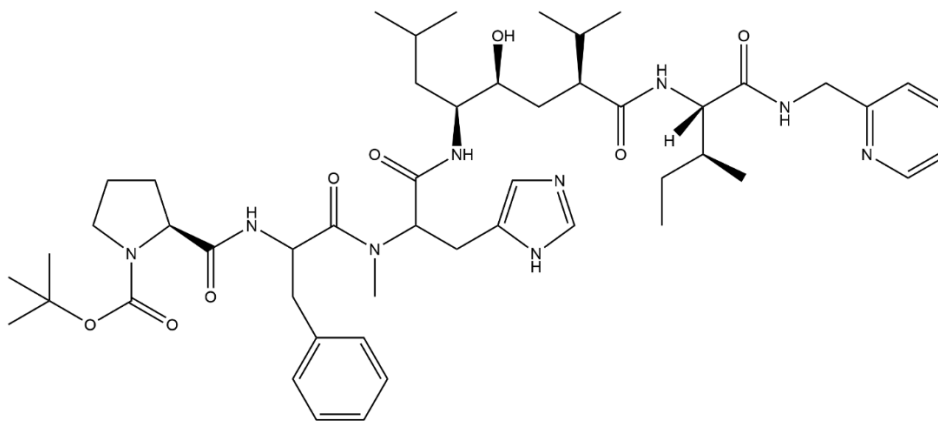
Purdue University, West Lafayette, IN 47907, USA

Online Resource 2 Molecular structures of the ten compounds with the highest Hawkins GB/SA scores

1. PubChem CID: 102148004
Grid-based score = -83.58 kcal/mol
Hawkins GB/SA score = -60.06 kcal/mol

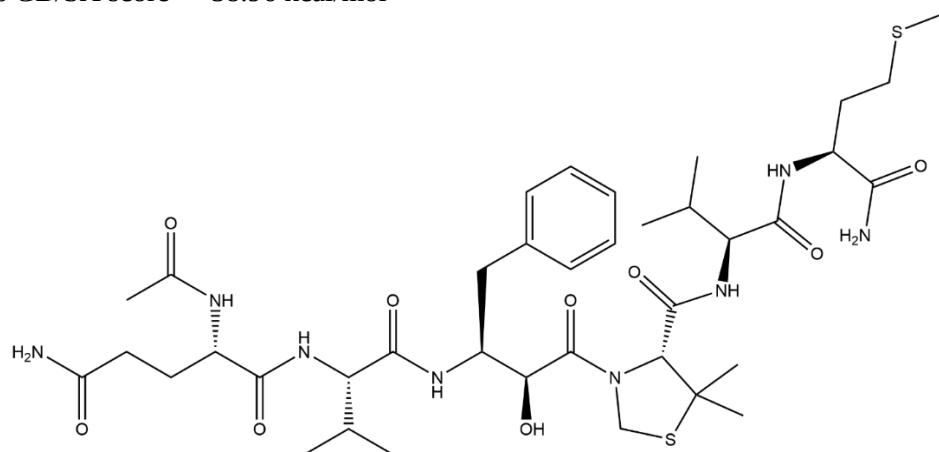


2. PubChem CID: 5464201
Grid-based score = -75.38 kcal/mol
Hawkins GB/SA score = -59.42 kcal/mol

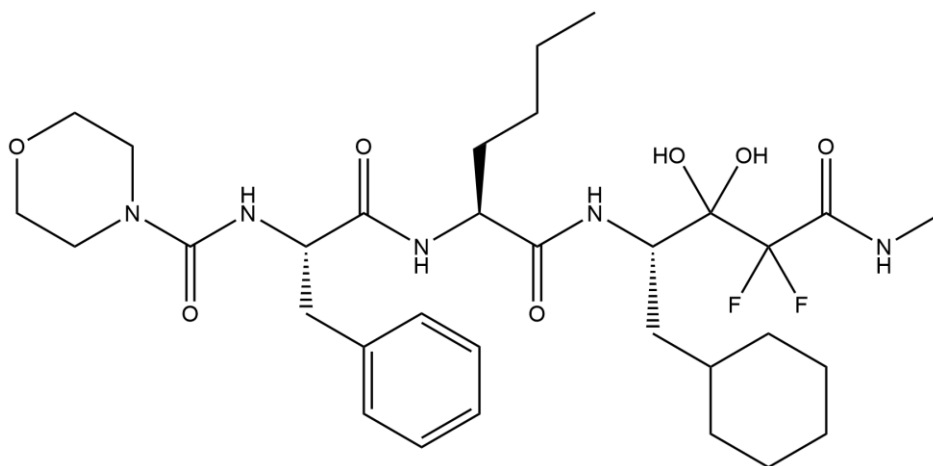


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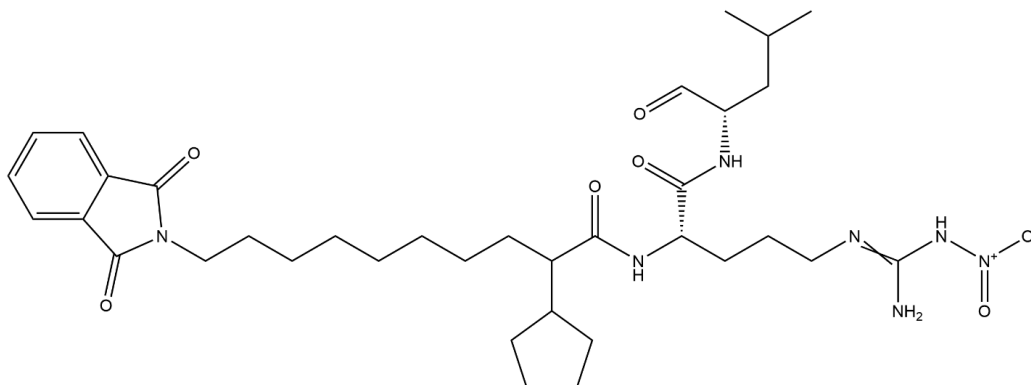
3. PubChem CID: 44430647
Grid-based score = -75.67 kcal/mol
Hawkins GB/SA score = -58.96 kcal/mol



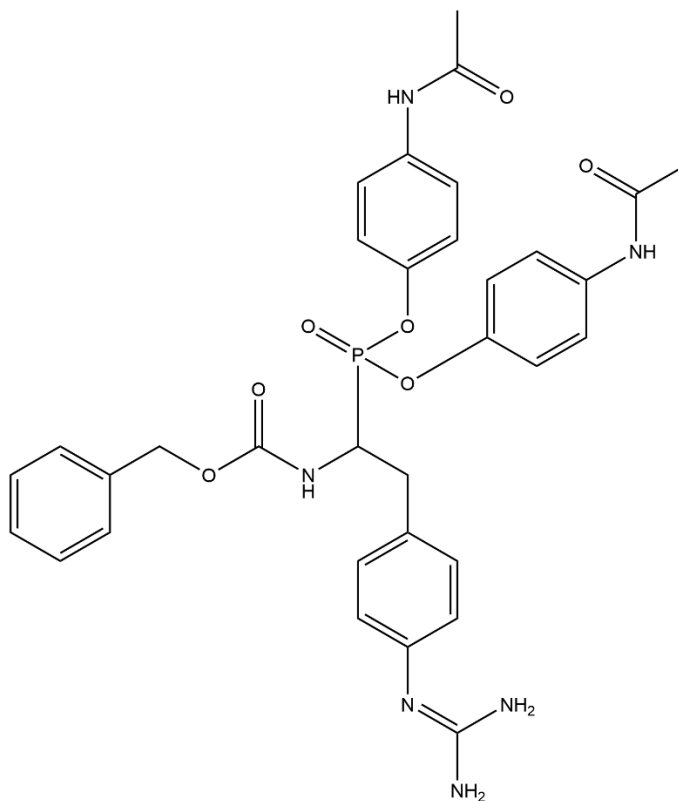
4. PubChem CID: 445400
Grid-based score = -69.61 kcal/mol
Hawkins GB/SA score = -57.61 kcal/mol



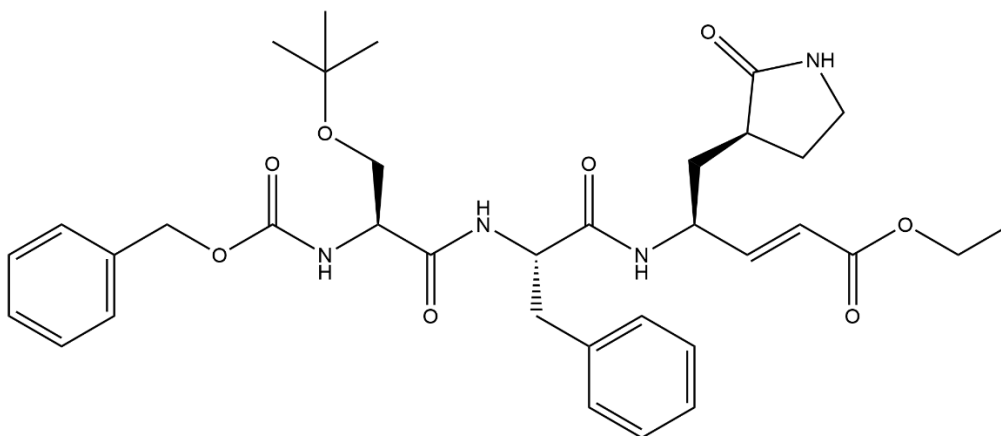
5. PubChem CID: 9939783
Grid-based score = -75.10 kcal/mol
Hawkins GB/SA score = -57.15 kcal/mol



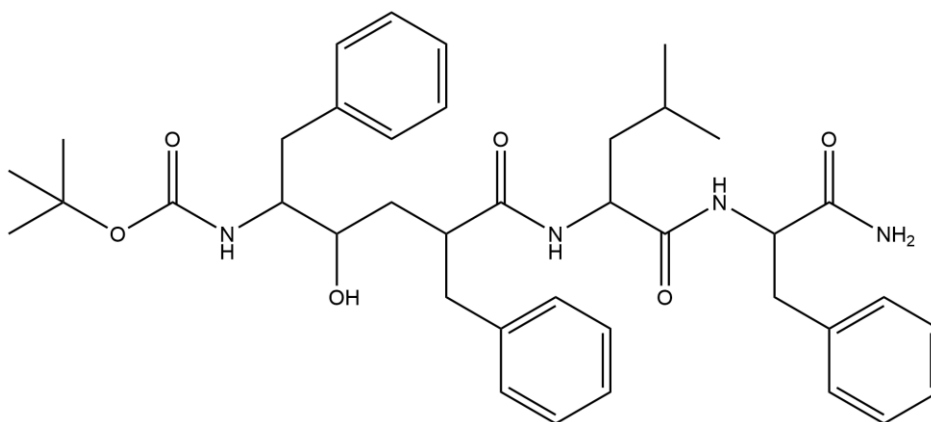
6. PubChem CID: 24749175
Grid-based score = -75.08 kcal/mol
Hawkins GB/SA score = -56.30 kcal/mol



7. PubChem CID: 52914324
Grid-based score = -72.10 kcal/mol
Hawkins GB/SA score = -55.83 kcal/mol



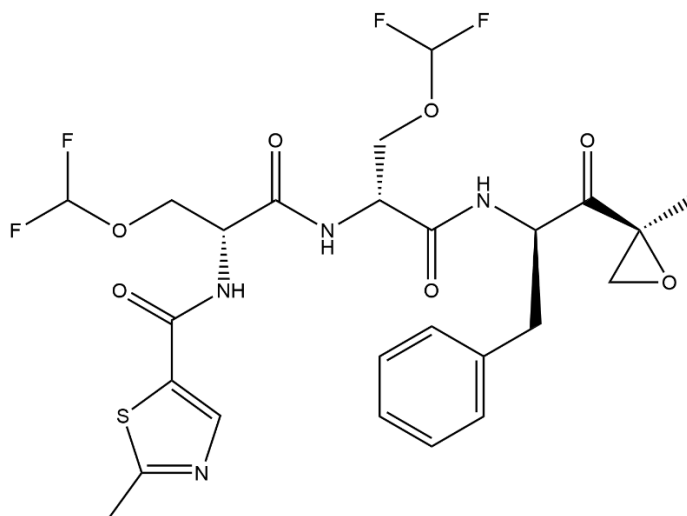
8. PubChem CID: 3849
Grid-based score = -64.94 kcal/mol
Hawkins GB/SA score = -55.54 kcal/mol



9. PubChem CID: 137704649

Grid-based score = -63.44 kcal/mol

Hawkins GB/SA score = -55.23 kcal/mol



10. PubChem CID: 146683669

Grid-based score = -64.91 kcal/mol

Hawkins GB/SA score = -55.13 kcal/mol

