



SwissBioisostere



SwissTargetPrediction





SwissSimilarity



Swiss Institute of Bioinformatics

- Contact
- Citing
- Command-line
- **Tutorials**
- <u>FAQ</u>
- About
- <u>Home</u>

Run parameters

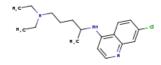
Query Molecule

ZINC_lead Library screened Screening method ECFP4

Date September 30, 2024, 11:32 am UTC

If you publish these results, please, cite the following paper:

Zoete, V., Daina, A., Bovigny, C., & Michielin, O. SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening., *J. Chem. Inf. Model.*, **2016**, *56*(8), 1399-1404.



Results

ZINC000006020572 Score: 0.692

ZINC000006487127 Score: 0.692

ZINC000006036375

Score: 0.692

Retrieve data:

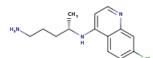






ZINC000001683543

Score: 0.692



ZINC000001843040 Score: 0.632

ZINC000001843038 Score: 0.632

ZINC000001706243 Score: 0.593

ZINC000044136210 Score: 0.581

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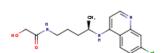
Score: 0.581

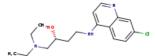
Score: 0.559

 $\underline{ZINC000044136213} \qquad \underline{ZINC000002042605} \qquad \underline{ZINC000001700323} \qquad \underline{ZINC000001687502}$

Score: 0.559

Score: 0.550



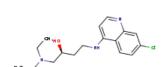


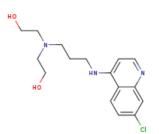
ZINC000005573151 Score: 0.550

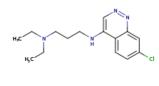
ZINC000001542122 Score: 0.509

ZINC000001687508 Score: 0.508

ZINC000001621246 Score: 0.508







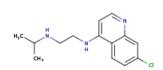
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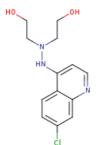
ZINC000001709130 Score: 0.500

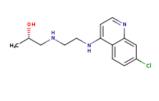
ZINC000001709131 Score: 0.483

ZINC000071771375 Score: 0.474

ZINC000045221330 Score: 0.452







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ZINC000045221334

ZINC000001629357

ZINC000065230431

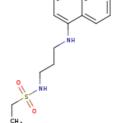
ZINC000001803506

Score: 0.429

Score: 0.452

Score: 0.448

Score: 0.438



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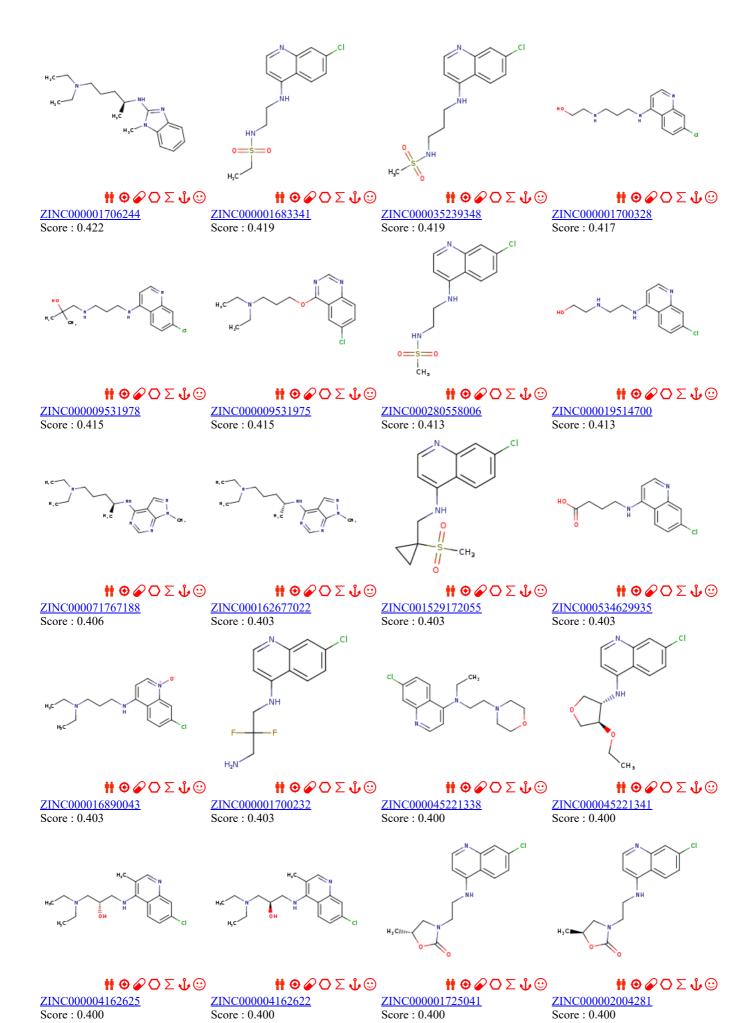
ZINC000001803508

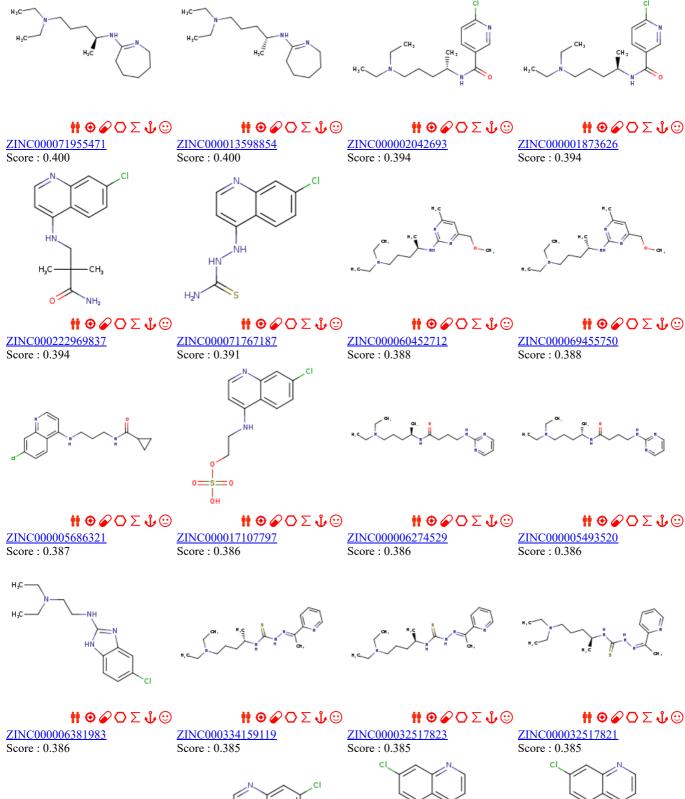
Score: 0.429

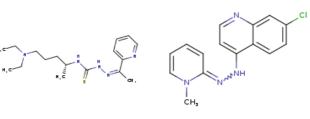
ZINC000223025788 Score: 0.429

ZINC000220646934 Score: 0.429

ZINC000028706440 Score: 0.426







Score: 0.385

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Score: 0.385

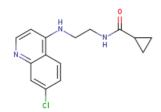
 $\bullet \bullet \bullet \bigcirc \Sigma \bullet \odot$ ZINC000005179682

Score: 0.385

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ZINC000006382019

 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$ ZINC000006567594 Score: 0.385



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ZINC000004777584

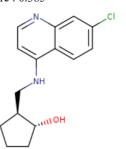
Score: 0.385

ZINC000006567596 Score: 0.385

ZINC000072404802 Score: 0.385

ZINC000001666088 Score: 0.385

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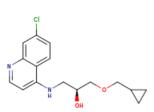
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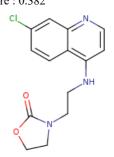
ZINC000225890844 Score: 0.384

ZINC000078649662 Score: 0.382

ZINC000078649658 Score: 0.382

ZINC000045221327 Score: 0.382





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ZINC000225890824

ZINC000012957443 Score: 0.377

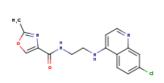
ZINC000003912509

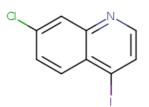
ZINC000003912510

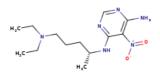
Score: 0.380

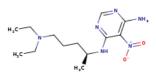
Score: 0.377

Score: 0.377









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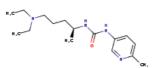
ZINC000096153430 Score: 0.373

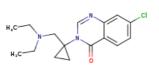
ZINC000096153431 ZINC000584894639 ZINC000057364358

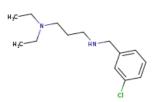
Score: 0.373

Score: 0.373

Score: 0.373







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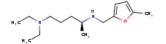
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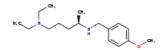
ZINC000007002579 Score: 0.371

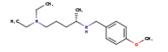
ZINC000007002582 Score: 0.371

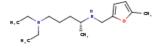
ZINC000007002588 Score: 0.371

ZINC000007002573 Score: 0.371

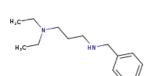








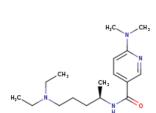
ZINC000002933158 Score: 0.368 ZINC000020816477 Score: 0.368 ZINC000254797937 Score: 0.368 ZINC000001756824 Score: 0.368

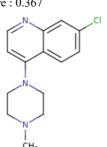


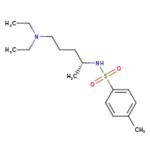
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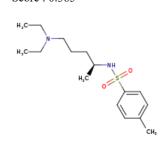
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ZINC000031730029 Score: 0.368 ZINC000020031309 Score: 0.367 ZINC000005453226 Score: 0.365









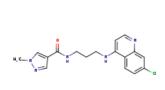
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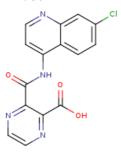
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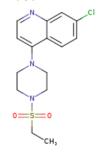
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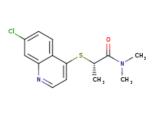
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ZINC000225888523 Score: 0.365 ZINC000072402068 Score: 0.364 ZINC000000171621 Score: 0.364 ZINC000089368719 Score: 0.364









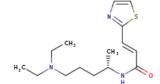
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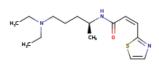
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ZINC000089368720 Score: 0.364 ZINC000096257377 Score: 0.362 ZINC000069451763 Score: 0.362 ZINC000096257378 Score: 0.362

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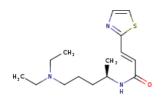


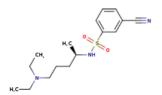


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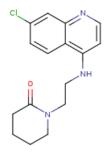
ZINC000069451762 Score: 0.362 ZINC000006933776 Score: 0.362 ZINC000006933782 Score: 0.362

ZINC000405305539 Score: 0.362









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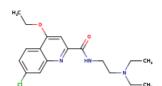
⊕ 6 0 Σ **1 0**

ZINC000001706245 Score: 0.361

ZINC000096403265 Score: 0.361

ZINC000096403266 Score: 0.361

ZINC000005453182 Score: 0.359



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ZINC000003100416

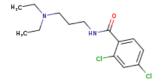
ZINC000002747173

ZINC000019914696

ZINC000019914694

Score: 0.359

Score: 0.359



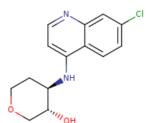
⊕ ⊘ ○ ∑ **↓ ○**

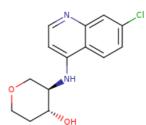
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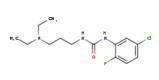
ZINC000220091599 Score: 0.358

ZINC000220527060 Score: 0.358

ZINC000040023799 Score: 0.358







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ZINC000000171642

Score: 0.358

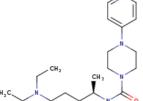
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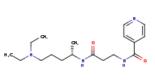
Score: 0.357

ZINC000426549050 Score: 0.357

Score: 0.357

ZINC000071844414 Score: 0.357





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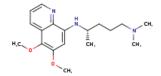
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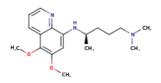
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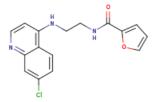
ZINC000001843144 Score: 0.357

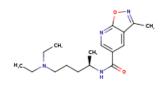
ZINC000006747692

ZINC000061424414 Score: 0.356





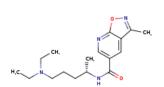




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ZINC000065369709 Score: 0.356 ZINC000225888504 Score: 0.356 ZINC000225992415 Score: 0.356 ZINC000019919230 Score: 0.356

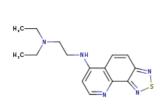


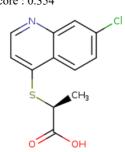
⊕ 6 6 5 3 4 9

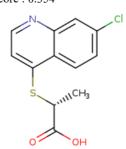
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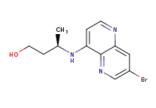
⊕ ⊘ ○ ∑ **↓** ⊙

ZINC000000362659 Score: 0.354 ZINC000019485005 Score: 0.354 ZINC000019485003 Score: 0.354 ZINC000135525857 Score: 0.354









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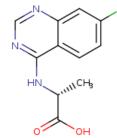
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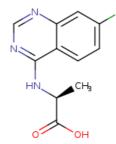
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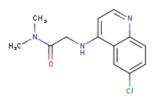
ZINC000004294379

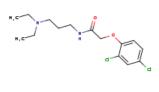
Score : 0.354

ZINC000004294378 Score: 0.354 ZINC000089311982 Score: 0.354 ZINC000004696129 Score: 0.353







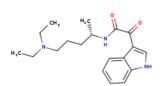


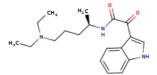
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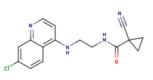
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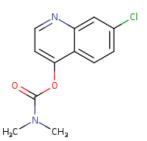
⊕ ⊘ ○ ∑ **↓ ○**

ZINC000004163113 Score: 0.352 ZINC000004163111 Score: 0.352 ZINC000225992398 Score: 0.352 ZINC000000197440 Score: 0.349





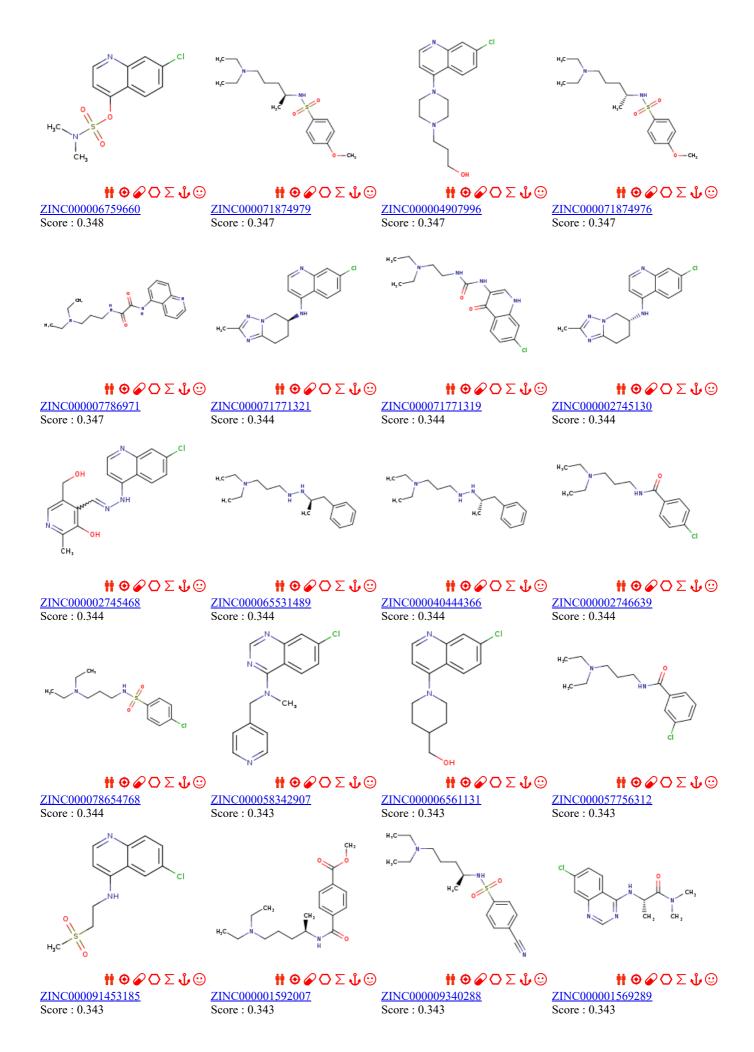


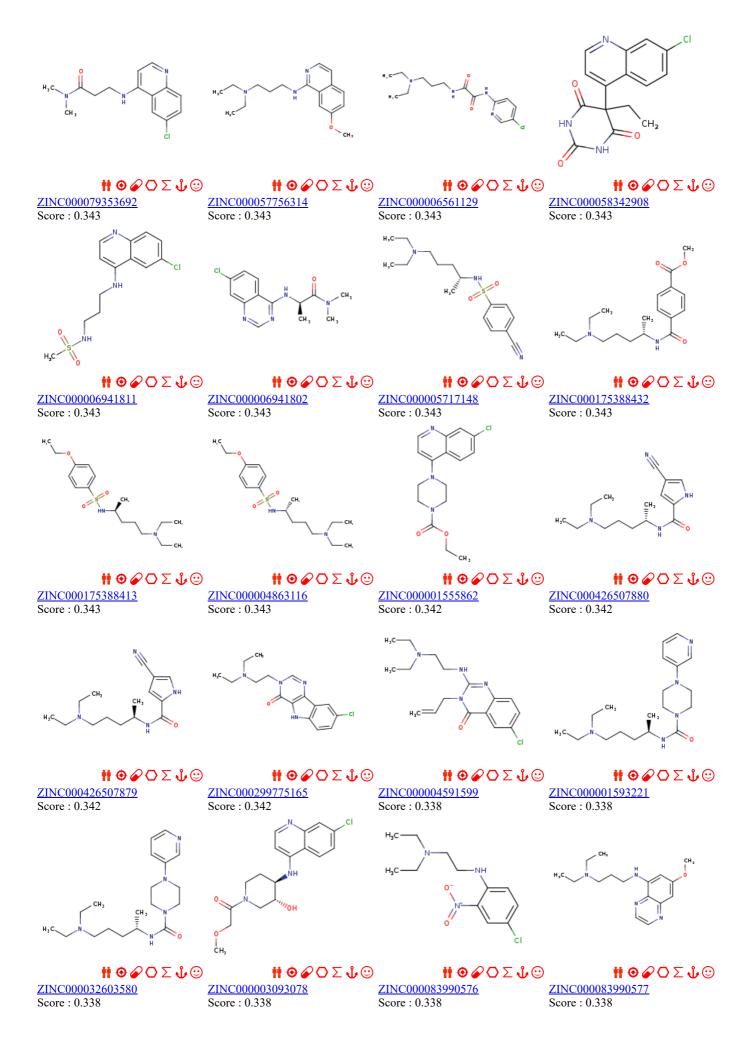


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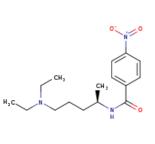
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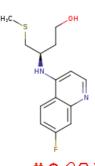
ZINC000027194330 Score: 0.349 ZINC000006509655 Score: 0.348 ZINC000039930838 Score: 0.348 ZINC000006509654 Score: 0.348

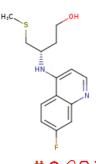












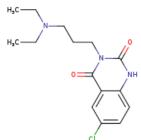
⊕ ⊘ ○ ∑ **↓** ⊙

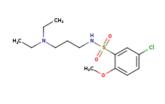
⊕ ⊘ ○ ∑ **↓** ⊙

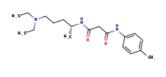
ZINC000033829460 Score: 0.338

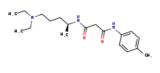
ZINC<u>000055197976</u> Score: 0.338

ZINC000055197984 Score: 0.338









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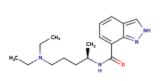
 $\oplus \bullet \bullet \supset \bot \oplus \odot$

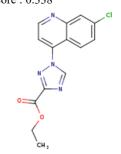
ZINC000003093079 Score: 0.338

<u>ZINC000058326002</u> <u>ZINC000058325998</u> Score: 0.338

Score: 0.338

ZINC000005796505 Score: 0.338





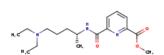
⊕ ⊘ ○ ∑ **↓ ○**

ZINC000069415755 Score: 0.338

Score: 0.338

<u>ZINC000069415757</u> <u>ZINC000225885781</u> Score: 0.338

ZINC000002824999 Score: 0.333



 $\mathsf{H} \bullet \mathscr{D} \circ \Sigma \, \mathsf{J} \odot \qquad \qquad \mathsf{H} \bullet \mathscr{D} \circ \Sigma \, \mathsf{J} \odot \qquad \qquad \mathsf{H} \bullet \mathscr{D} \circ \Sigma \, \mathsf{J} \odot \qquad \qquad \mathsf{H} \bullet \mathscr{D} \circ \Sigma \, \mathsf{J} \odot$

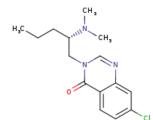
ZINC000584894466

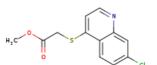
Score: 0.333

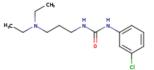
Score: 0.333

Score: 0.333

Score: 0.333







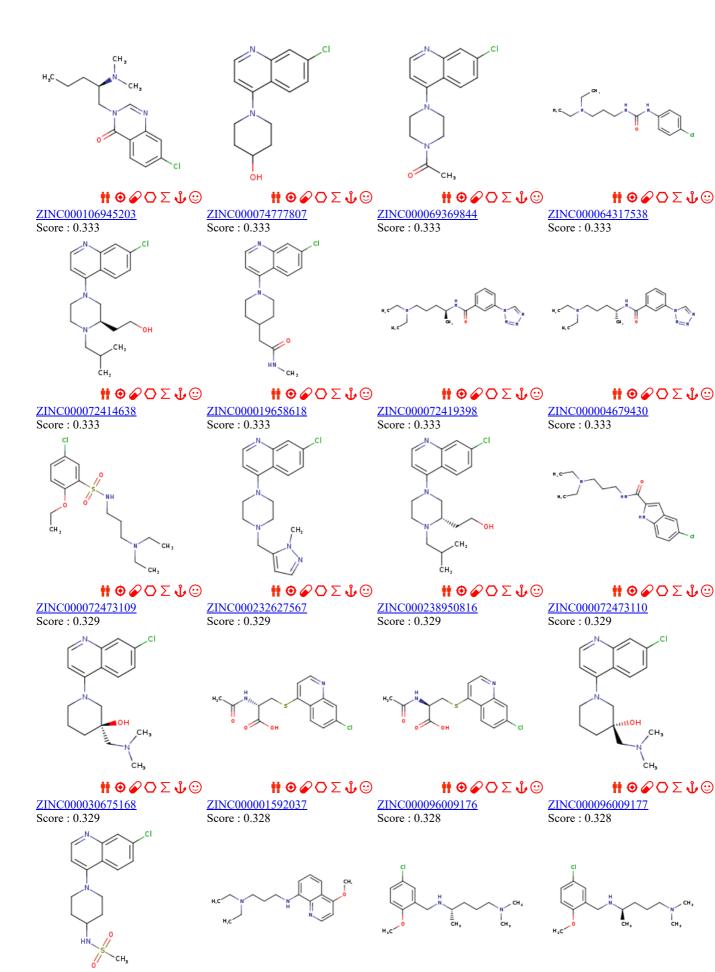
⊕ ⊘ ○ ∑ **↓ ○**

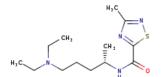
 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$

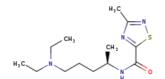
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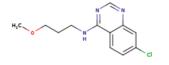
Score: 0.333

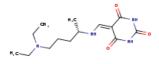
<u>ZINC000040412048</u> <u>ZINC000000171631</u> <u>ZINC000006462730</u> Score: 0.333











⊕ ⊘ ○ ∑ **↓** ⊙

⊕ ⊘ ○ ∑ **↓** ⊙

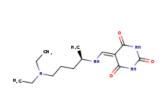
⊕ ∂ ○ Σ ♣ ⊙

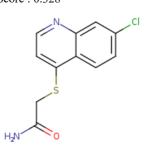
ZINC000019595256 Score: 0.328

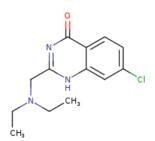
ZINC000263622784 Score: 0.328

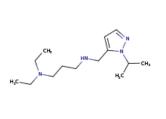
ZINC000017283505 Score: 0.328

ZINC000256051870 Score: 0.328









⊕ 6 6 7 3 4 9

 $\oplus \bullet \bullet \supset \bot \oplus \odot$

ZINC000000161683

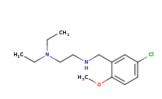
 $\oplus \bullet \bullet \supset \bot \oplus \odot$

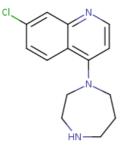
ZINC000022076442 Score: 0.328

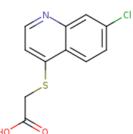
Score: 0.328

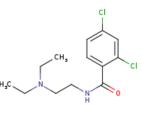
ZINC000003716216 Score: 0.328











ZINC000001603460

⊕ ⊘ ○ ∑ **↓ ○**

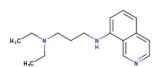
 $\bullet \bullet \bullet \bigcirc \Sigma \bullet \odot$

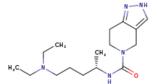
ZINC000001621250 Score: 0.328

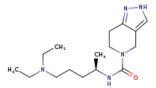
ZINC000058343946 Score: 0.324

ZINC000534644139 Score: 0.324

ZINC000534644138 Score: 0.324







 $\mathbf{H} \oplus \mathscr{O} \bigcirc \Sigma \mathring{\mathbf{J}} \odot \qquad \qquad \mathbf{H} \oplus \mathscr{O} \bigcirc \Sigma \mathring{\mathbf{J}} \odot$

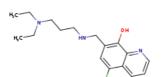
⊕ ⊘ ○ ∑ **↓** ⊙

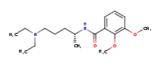
ZINC000058343947 Score: 0.324

ZINC000426701492 ZINC000001571039 Score: 0.324

Score: 0.324

ZINC000003229838 Score: 0.324





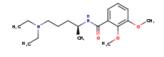
 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$

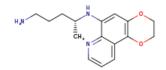
ZINC000003229839 Score: 0.324

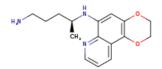
ZINC000005551274 Score: 0.324

ZINC000001568053 Score: 0.324

ZINC000075105354 Score: 0.324







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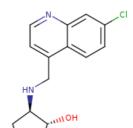
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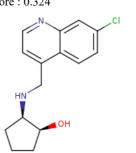
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ZINC000004839447 Score: 0.324

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ZINC000004792281 Score: 0.324

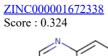




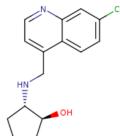
⊕ 6 6 7 3 4 9

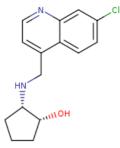
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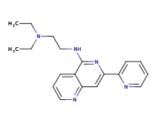
Score: 0.324

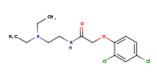


ZINC000019526416 Score: 0.324









⊕ ⊘ ○ ∑ **↓ ○**

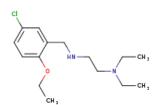
⊕ ⊘ ○ ∑ **↓** ⊙

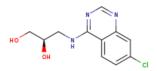
ZINC000022075937 Score: 0.323

ZINC000006567485 Score: 0.323

ZINC000001683323 Score: 0.323

ZINC000019813425 Score: 0.323





 $\mathbf{H} \oplus \mathscr{O} \supset \mathbf{J} \oplus \qquad \qquad \mathbf{H} \oplus \mathscr{O} \supset \mathbf{J} \oplus$

 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$

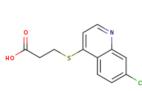
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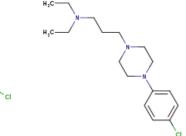
Score: 0.323

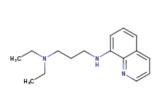
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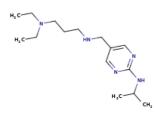
ZINC000001873620 Score: 0.323

ZINC000062718451 Score: 0.323









⊕ 6 0 Σ **↓ 0**

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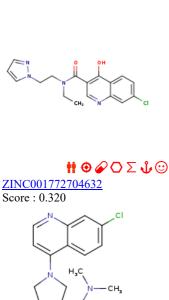
 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$

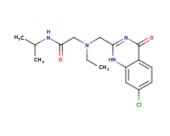
ZINC000215617220 Score: 0.321

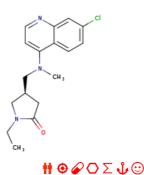
ZINC000013039192 Score: 0.320

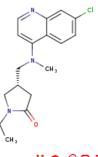
ZINC001506412840 Score: 0.320

ZINC001506412843 Score: 0.320









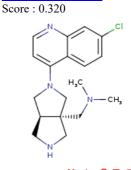
⊕ ∂ ○ Σ ♣ ⊙ ZINC001772704627

ZINC001772704631

⊕ ⊘ ○ ∑ **↓** ⊙ ZINC001772704633

Score: 0.320

Score : 0.320



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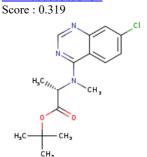
⊕ ∂ ○ Σ ♣ ⊙

⊕ 6 0 Σ **↓ 0** ZINC000075093132

ZINC000005453541 Score: 0.319

ZINC000075093133 Score: 0.319

ZINC000077322891 Score: 0.319



⊕ ⊘ ○ ∑ **↓ ○**

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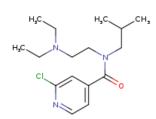
 $\bullet \bullet \bullet \bigcirc \Sigma \bullet \odot$

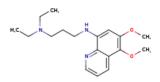
ZINC000037991463 Score: 0.319

ZINC000009418324 Score: 0.319

ZINC000001592009 Score: 0.319

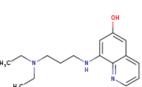
ZINC000006841191 Score: 0.319



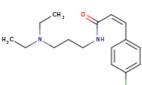


ZINC000003396078 Score: 0.318

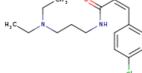
ZINC000001873623 Score: 0.318

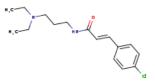


ZINC000033410672 Score: 0.318



ZINC000004696218 Score: 0.318





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⊕ 6 0 Σ **↓ 0**

⊕ ⊘ ○ ∑ **↓ ○**

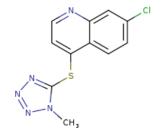
 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$

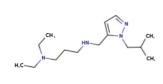
ZINC000008718286 Score: 0.318

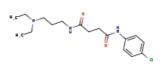
ZINC000256050857 Score: 0.318

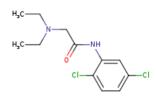
ZINC000013896034 Score: 0.318

ZINC000000152106 Score: 0.317









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ZINC000001771417 Score: 0.317

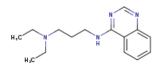
ZINC000001690148 Score: 0.317

ZINC000002044173

ZINC000002044174

Score: 0.317

Score: 0.317



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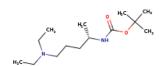
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<u>ZINC000083502173</u> <u>ZINC000001690147</u>

ZINC000019636295

Score: 0.317

Score: 0.317



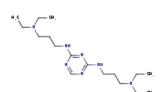
 $\bullet \bullet \bullet \circ \Sigma \bullet \odot$

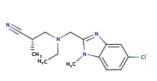
 $\bullet \bullet \bullet \bigcirc \Sigma \bullet \odot$

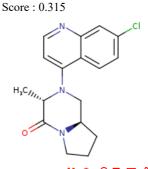
ZINC000004691967 Score: 0.316

ZINC000049236497 Score: 0.315

ZINC000049236499 Score: 0.315







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ZINC000065539602

Score: 0.315

Score: 0.315

Score: 0.315



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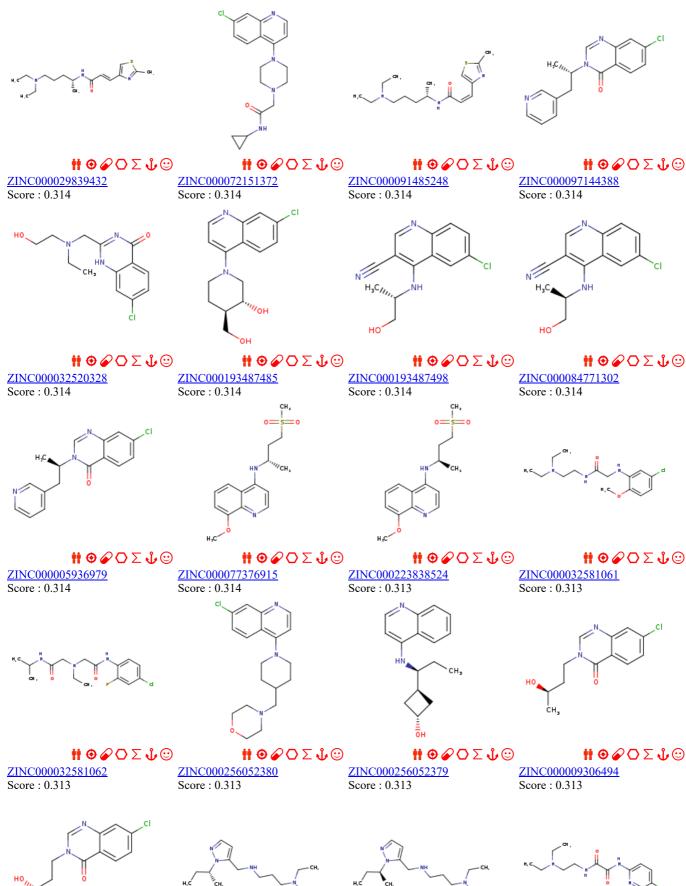
 $\bullet \bullet \bullet \circ \Sigma \bullet \odot$

ZINC000069452438 Score: 0.315

ZINC000032743518 Score: 0.315

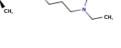
ZINC000103722981 ZINC000032520326 Score: 0.315

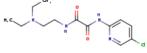
Score: 0.314











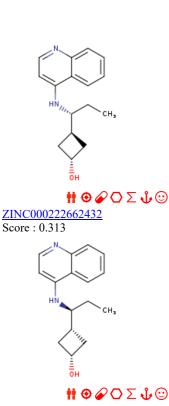
⊕ ⊘ ○ ∑ **↓ ○**

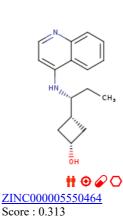
 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$

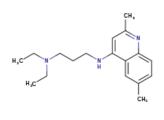
ZINC000223838470 ZINC000222662364 Score: 0.313 Score: 0.313

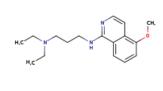
ZINC000005809468 Score: 0.313

ZINC000001873631 Score: 0.313









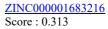
⊕ ∂ ○ Σ ♣ ⊙

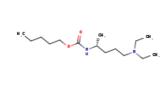
⊕ ⊘ ○ ∑ **↓** ⊙

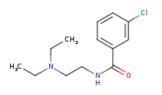
⊕ ⊘ ○ ∑ **↓** ⊙

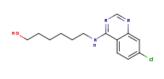
ZINC000002835777

Score: 0.313









⊕ 6 6 7 3 4 9

⊕ 6 0 Σ **↓ 0**

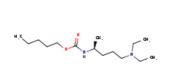
⊕ ∂ ○ Σ ♣ ⊙

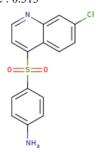
 $\bullet \bullet \bullet \bigcirc \Sigma \bullet \odot$

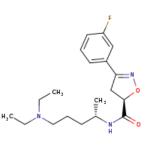
ZINC000004742749 Score: 0.313

ZINC000001671435 Score: 0.313

ZINC000006140601 Score: 0.313







⊕ ⊘ ○ ∑ **↓ ○**

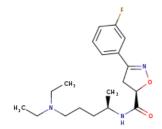
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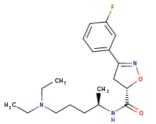
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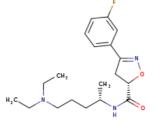
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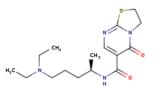
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ZINC000042537100 Score: 0.312









⊕ ∂ ○ Σ ♣ ⊚

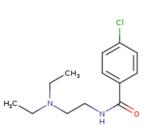
⊕ ⊘ ○ ∑ **↓ ○**

⊕ ∂ ○ Σ ♣ ⊚

⊕ 6 0 Σ **↓ 0** ZINC000019633255

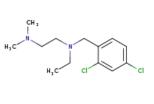
ZINC000001760515 Score: 0.311

ZINC000005453448 Score: 0.311



Score: 0.311

ZINC000001406292



 $\oplus \bullet \bullet \bigcirc \Sigma \bullet \odot$

⊕ 6 0 Σ **↓ 0**

⊕ ⊘ ○ ∑ **↓ ⊙**

 $\bullet \bullet \bullet \bigcirc \Sigma \bullet \odot$

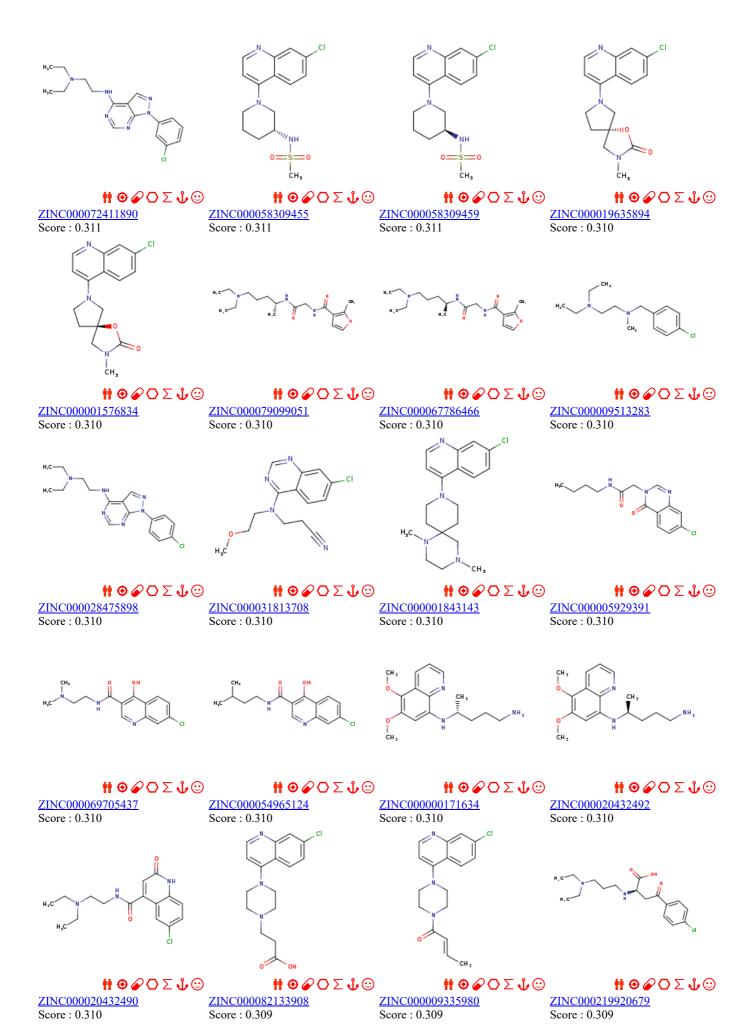
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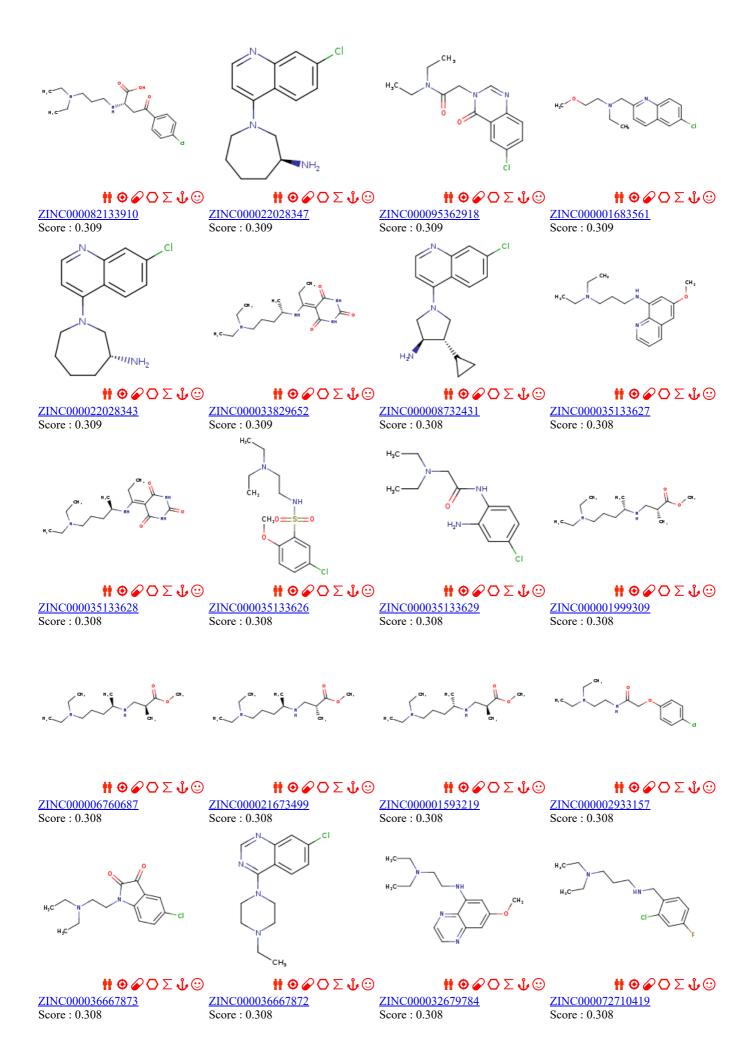
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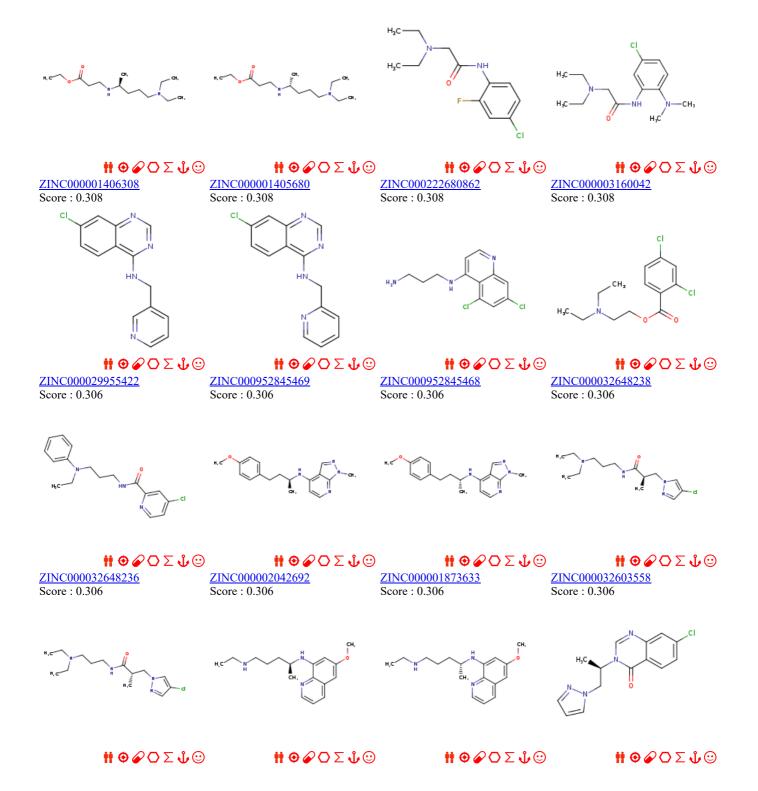
ZINC000131350722 Score: 0.311

ZINC000072411891 Score: 0.311

Score: 0.311









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