| | | | |
|---|---|---|---|
| CODE | 3K5C (PDB) | Resolution | 2.1 |
| Name | | Ring size | 16 |
| Formula | C35H45N3O4 | # Ligand atoms | 42 |
| Type | Macrocycle | Scorpion Score | 12.5 |

| | | | |
|---|---|---|---|
| Mol. Weight (Da) | 571,34 | Saturated/ Unsaturated | U |
| cLogP | 5.8919 | | |
| tPSA | 91.85 | Chiral centres.ring | 1 |
| #HBD's | 3 | Chiral centres.sub | 1 |
| #HBA's | 3 | | |
| $N_{RB\ (RING)}$ | 11 | $N_{RB\ (SUBSTITUENT)}$ | 8 |

| | | | |
|---|---|---|---|
| Number of substituents | 3 | P/NP balance, substituents | 3/22 |
| *Large (≥5HA)* | 2 | P/NP balance, peripheral groups | 1/0 |
| *Small (2-4HA)* | 1 | | |
| Proportion HA in substituents | 60% | Degrees of unsaturation ring | 15 |
| Number of peripheral groups | 1 | N:O ratio | 3:3 |
| | | Chiral centres | 2 |

Polarity distribution ligand atoms

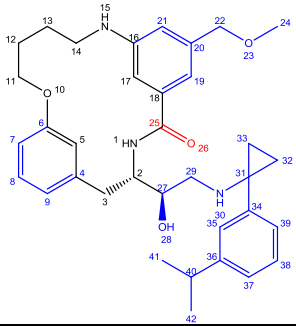
| | All | | Contact | |
|---|---|---|---|---|
| | *Polar* | *Nonpolar* | *Polar* | *Nonpolar* |
| Ring | 3 | 13 | 1 | 5 |
| Substituent | 3 | 22 | 2 | 10 |
| Peripheral groups | 1 | - | 1 | - |
| Total | 7 | 35 | 4 | 15 |

| | |
|---|---|
| Protein name | BACE-1 |
| Organism | Homo sapien |
| Classification | Hydrolase/ Hydrolase inhibitor |
| Binding mode | Face on |
| Receptor secondary structure topology | |
| Number of residue 'hotspots' | 21 |

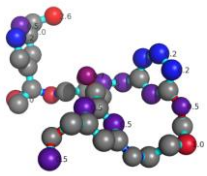
Number of protein-ligand interactions* ('Database link')

| | | | |
|---|---|---|---|
| Hydrogen bond | 3 | Hydrogen donor-π | 1 |
| Ionic interaction | 1 | π-π | 5 |
| Cation-dipole | - | VdW interaction | 17 |
| Cation-π | - | Unfavourable | 6 |
| Dipolar interaction | 1 | Poor-angle | 2 |
| Halogen bond | | Unclassified | 2 |
| Water-mediated interaction | | | |

2D-STRUCTURE LIGAND



3D-STRUCTURE LIGAND +SCORPIONSCORE ('Scorpion link')

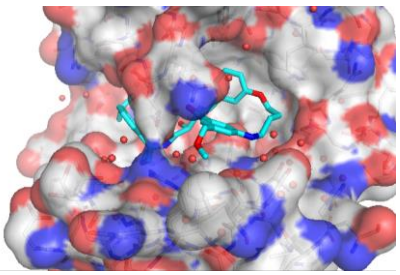


Physicochemical properties

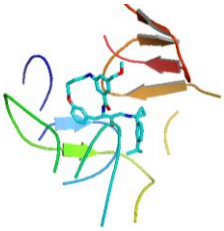
'click for publication'

| IC50 (nM): | |
|---|---|
| BACE-1 | 17 |
| CHO | 20 |
| CathD | 1 |
| CathE | 0.4 |

LIGAND-PROTEIN COMPLEX (I) ('Pymol link')



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis