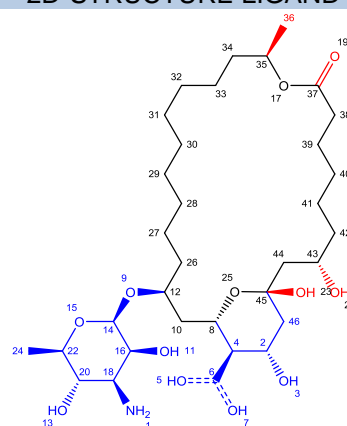
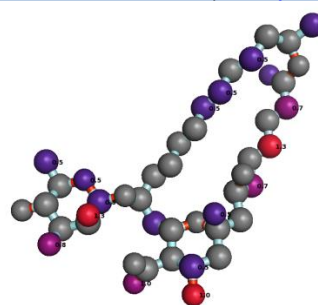


| | | | | |
|--|--|---------------------------------|---------|----------|
| CODE | 2XBK(PDB) | Resolution | 1.95 | |
| Name | | Ring size | 24 | |
| Formula | C ₃₃ H ₆₀ NO ₁₂ | # Ligand atoms | 46 | |
| Type | Macrocycle | Scorpion Score | 12.2 | |
| Mol. Weight (Da) | 663 | Saturated/ Unsaturated | S | |
| cLogP | 1.07 | Chiral centres.ring | 5 | |
| tPSA | 224 | Chiral centres.sub | 7 | |
| #HBD's | 9 | | | |
| #HBA's | 13 | | | |
| NRB (RING) | 22 | NRB (SUBSTITUENT) | 3 | |
| Number of substituents | 2 | P/NP balance, substituents | 2/5 | |
| Large (≥5HA) | 2 | P/NP balance, peripheral groups | 3/1 | |
| Small (2-4HA) | - | Degrees of unsaturation ring | 4.5 | |
| Proportion HA in substituents | 39% | N:O ratio | 1:12 | |
| Number of peripheral groups | 4 | Chiral centres | 12 | |
| Polarity distribution ligand atoms | | | | |
| | All | | Contact | |
| | Polar | Nonpolar | Polar | Nonpolar |
| Ring | 2 | 22 | - | 7 |
| Substituent | 8 | 10 | 5 | 3 |
| Peripheral groups | 3 | 1 | 2 | 1 |
| Total | 13 | 33 | 7 | 11 |
| | | | | |
| | | | | |
| | | | | |
| Protein name | Cytochrome P450 | | | |
| Organism | Streptomyces natalensis | | | |
| Classification | Oxidoreductase | | | |
| Binding mode | Compact | | | |
| Receptor secondary structure topology | | | | |
| Number of residue 'hotspots' | 13 | | | |
| Number of protein-ligand interactions* ('Database link') | | | | |
| Hydrogen bond | 7 | Hydrogen donor-π | - | |
| Ionic interaction | - | π-π | - | |
| Cation-dipole | 1 | VdW interaction | 12 | |
| Cation-π | - | Unfavourable | 1 | |
| Dipolar interaction | - | Poor-angle | - | |
| Halogen bond | - | Unclassified | 1 | |
| Water-mediated interaction | 10 | | | |
| | | | | |
| | | | | |
| | | | | |

2D-STRUCTURE LIGAND

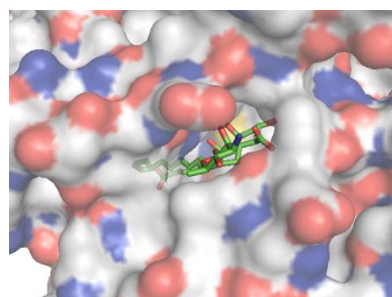


3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')

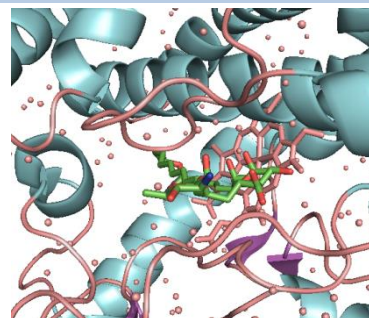


Physicochemical properties 'click for publication'

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



LIGAND-PROTEIN COMPLEX (II)



*Based on Scorpion® analysis