

|         |            |                |      |
|---------|------------|----------------|------|
| CODE    | 2FKE(PDB)  | Resolution     | 1.7  |
| Name    |            | Ring size      | 21   |
| Formula | C44H75NO12 | # Ligand atoms | 57   |
| Type    | Macrocycle | Scorpion Score | 13.4 |

|                        |     |                               |    |
|------------------------|-----|-------------------------------|----|
| Mol. Weight (Da)       | 810 | Saturated/Unsaturated         | S  |
| cLogP                  | 6.8 | Chiral centres.ring           | 10 |
| tPSA                   | 178 | Chiral centres.sub            | 6  |
| #HBD's                 | 3   |                               |    |
| #HBA's                 | 13  |                               |    |
| N <sub>RB</sub> (RING) | 17  | N <sub>RB</sub> (SUBSTITUENT) | 8  |

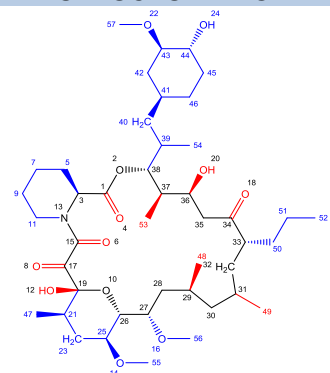
|                               |       |                                 |      |
|-------------------------------|-------|---------------------------------|------|
| Number of substituents        | 5     | P/NP balance, substituents      | 4/23 |
| Large (≥5HA)                  | 2     | P/NP balance, peripheral groups | 6/3  |
| Small (2-4HA)                 | 3     | Degrees of unsaturation ring    | 8    |
| Proportion HA in substituents | 47.4% | N:O ratio                       | 1:12 |
| Number of peripheral groups   | 9     | Chiral centres                  | 16   |

| Polarity distribution ligand atoms |       |          |         |          |
|------------------------------------|-------|----------|---------|----------|
|                                    | All   |          | Contact |          |
|                                    | Polar | Nonpolar | Polar   | Nonpolar |
| Ring                               | 3     | 18       | -       | -        |
| Substituent                        | 4     | 23       | -       | 6        |
| Peripheral groups                  | 6     | 3        | 4       | 2        |
| Total                              | 13    | 44       | 4       | 8        |
|                                    |       |          |         |          |
|                                    |       |          |         |          |

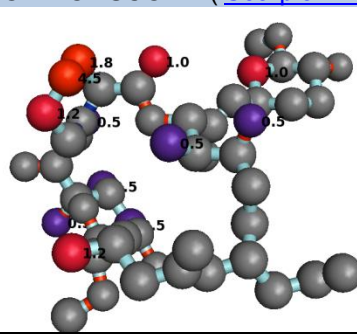
|                                       |                        |  |  |
|---------------------------------------|------------------------|--|--|
| Protein name                          | FK-506-BINDING PROTEIN |  |  |
| Organism                              | Homo sapiens           |  |  |
| Classification                        | CIS-TRANS ISOMERASE    |  |  |
| Binding mode                          | Compact                |  |  |
| Receptor secondary structure topology |                        |  |  |
| Number of residue 'hotspots'          | 14                     |  |  |

| Number of protein-ligand interactions* ('Database link') |   |                  |    |
|--|---|------------------|----|
| Hydrogen bond  | 5 | Hydrogen donor-π | -  |
| Ionic interaction  | - | π-π              | -  |
| Cation-dipole  | - | VdW interaction  | 15 |
| Cation-π   | - | Unfavourable     | 4  |
| Dipolar interaction                                      | - | Poor-angle       | 1  |
| Halogen bond   | - | Unclassified     | -  |
| Water-mediated interaction                               | - |                  |    |
|  |   |                  |    |
|  |   |                  |    |

## 2D-STRUCTURE LIGAND



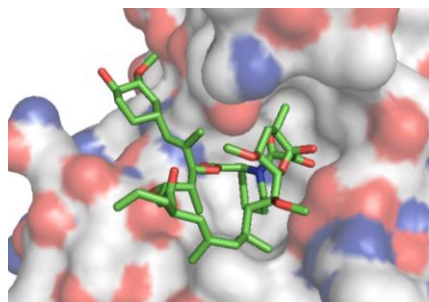
## 3D-STRUCTURE LIGAND +SCORPIONSORE ('Scorpion link')



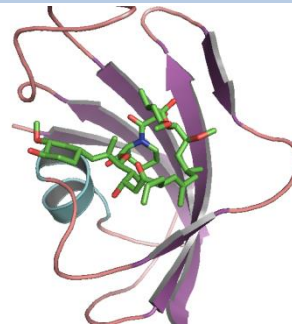
## Physicochemical properties

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



## LIGAND-PROTEIN COMPLEX (II)



\*Based on Scorpion® analysis