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## Supplementary material:

MolDock scoring function, $E_{score}$is:
$E_{score} = E_{inter} + E_{intra}$
$E_{inter}$is defined as ligand-protein interaction energy:

$$E_{inter} = \sum_{i \in ligand} \sum_{j \in protein} \left[ E_{PLP}(r_{ij}) + 332.0 \frac{q_i q_j}{4r_{ij}^2} \right]$$

$E_{PLP}$term: a piecewise linear potential
The second term describes the electrostatic interactions between charged atoms
$E_{intra}$is the internal energy of the ligand:

$$E_{intra} = \sum_{i \in ligand} \sum_{j \in ligand} E_{PLP}(r_{ij}) + \sum_{flexible\ bonds} A[1 - \cos(m \cdot \theta - \theta_0)] + E_{clash}$$

**Table 1:** binding energy level of top five poses of Hexadecanal to CCRL1

| Ligand name | MolDock Score | Rerank Score | HBond |
|---|---|---|---|
| Hexadecanal | -142.991 | -70.069 | 8.45892 |
| Hexadecanal | -129.6428 | -7.03469 | -2.5 |
| Hexadecanal | -128.2786 | -71.6903 | 0 |
| Hexadecanal | -127.4818 | -73.7083 | 0 |
| Hexadecanal | -127.3446 | -70.2874 | 0 |

For more information see supplementary data