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N-[[2-(4-Phenyl-piperazin-1-yl)-ethyl]-phenyl]-arylamides with dopamine D₂ and 5-hydroxytryptamine 5HT_{1A} activity: Synthesis, testing and molecular modeling

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Table 2: List of amino acids considered to be part of the arylpiperazine binding site in the D₂ DAR and 5HT_{1A} receptor.

| D ₂ Receptor | 5HT _{1A} receptor | Ballesteros-Weinstein amino acids numbering |
|-------------------------|----------------------------|---|
| ASP 114 | ASP 116 | 3.32 |
| SER 167 | | 4.57 |
| ILE 166 | | 4.58 |
| LEU 170 | | 4.61 |
| LEU 171 | | 4.62 |
| ASN 175 | | 4.66 |
| PHE 189 | | 5.38 |
| VAL 190 | | 5.39 |
| | SER 199 | 5.42 |
| SER 194 | THR 200 | 5.43 |
| SER 197 | | 5.46 |
| | PHE 204 | 5.47 |
| TRP 386 | TRP 358 | 6.48 |
| | PHE 361 | 6.51 |
| PHE 390 | PHE 362 | 6.52 |
| ILE 397 | | 6.59 |
| HIS 398 | | 6.60 |
| TYR 420 | TYR 390 | 7.43 |

Conformational energy diagram for compounds **4a**, **6a** and **7a**

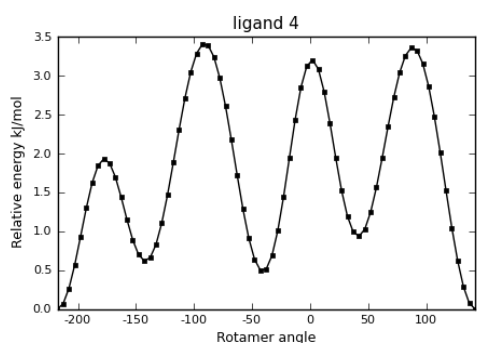


Figure 1: Conformational energy diagram for compound **4a**

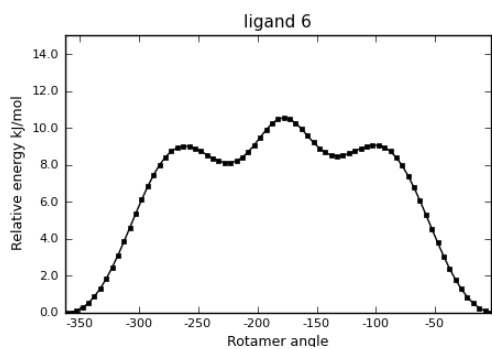


Figure 2: Conformational energy diagram for compound **6a**

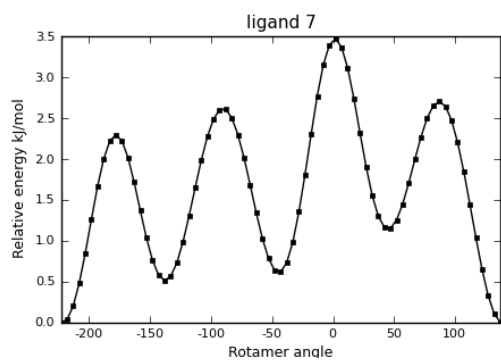


Figure 3: Conformational energy diagram for compound **7a**