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N-{[2-(4-Phenyl-piperazin-1-yl)-ethyl]-phenyl}-arylamides with dopamine D_2 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 D_2 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**

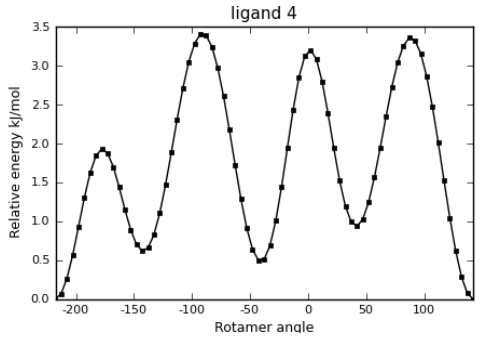

Figure 1: Conformational energy diagram for compound **4a**

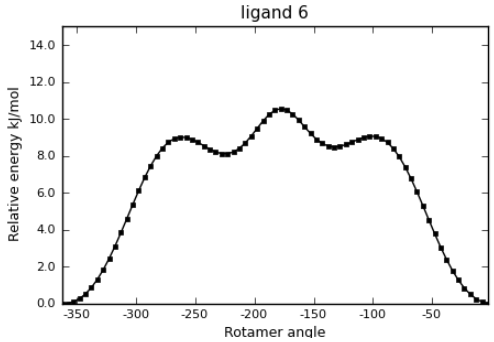

Figure 2: Conformational energy diagram for compound **6a**

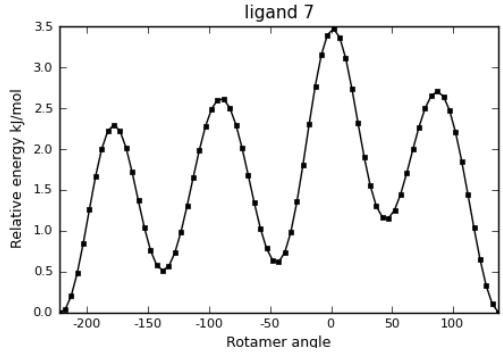

Figure 3: Conformational energy diagram for compound **7a**