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Supporting Information_1

Sequential ligand- and structure-based virtual screening approach for the identification of potential G protein-coupled estrogen receptor-1 (GPER-1) modulators

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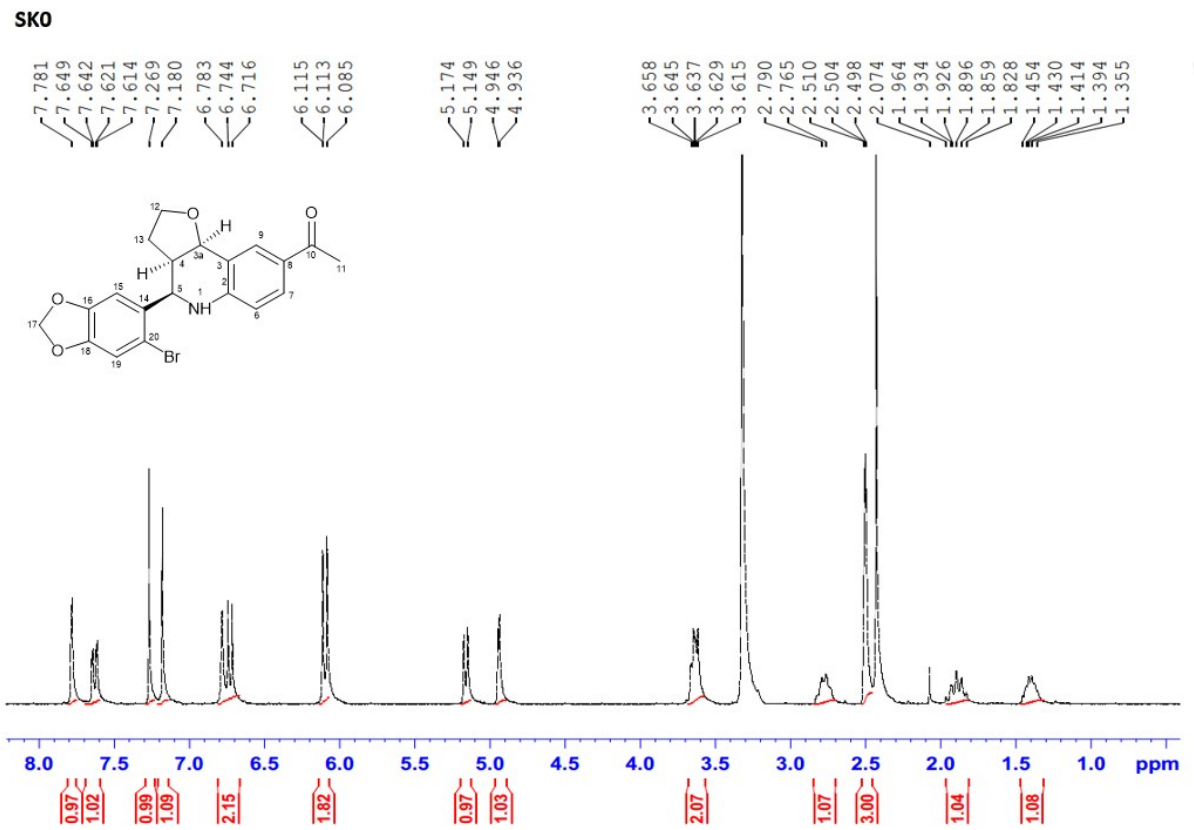
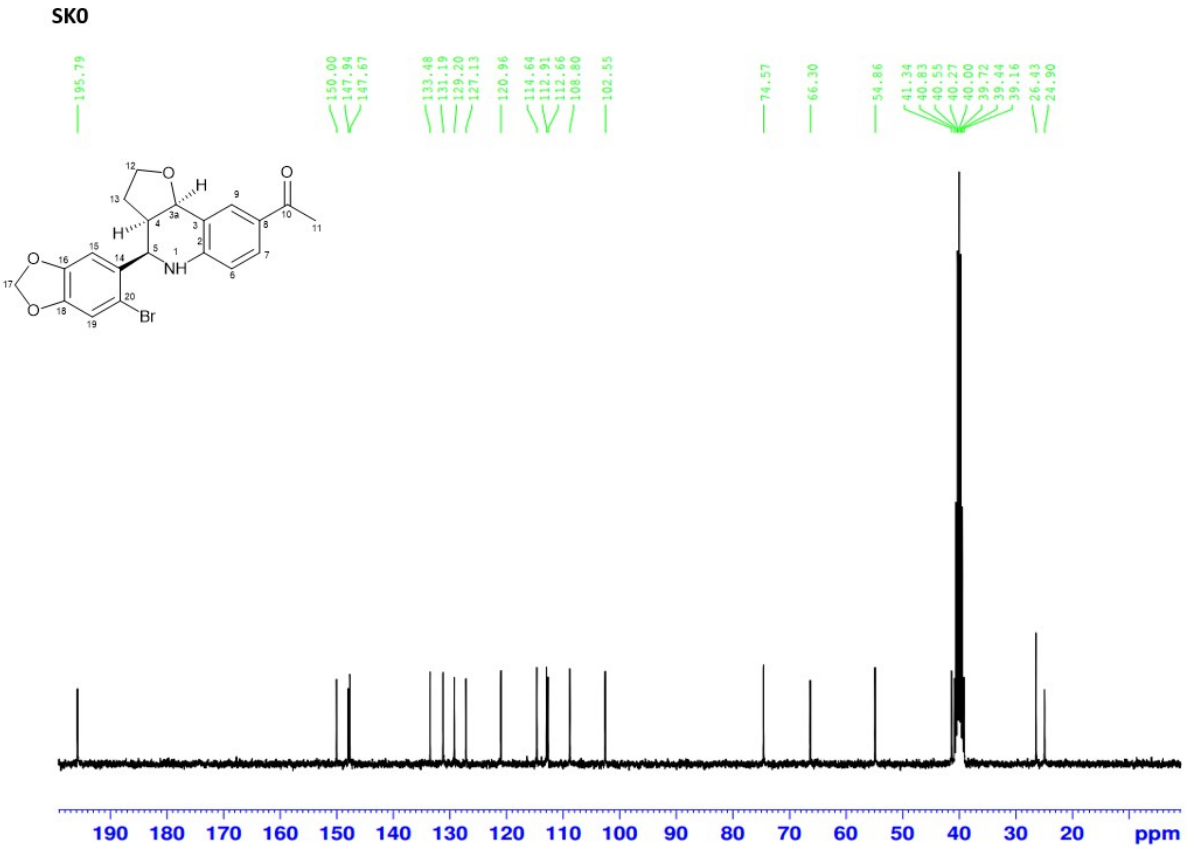
S1: Table 1. The enrichment factor (EF) 0.5%, 1% and 2% and the area under ROC curves (AUC) of the 3D virtual screening protocols for the selection of query model

Statistical Matrices	G1_conformer#1	G1_conformer#2	G1_conformer#3	G1_conformer#4
ROCS_TanimotoColour				
AUC	0.754	0.749	0.746	0.732
0.5% Enrichment	42.6	43.1	43.6	43.6
1.0% Enrichment	21.3	21.6	21.9	21.8
2.0% Enrichment	10.7	10.8	12.3	11.3
ROCS_ShapeTanimoto				
AUC	0.767	0.7311	0.731	0.757
0.5% Enrichment	52.2	52.7	42.6	44.4
1.0% Enrichment	28.4	28.0	22.5	25.3
2.0% Enrichment	16.3	14.1	14.4	18.1
ROC_TanimotoCombo				
AUC	0.797	0.766	0.777	0.798
0.5% Enrichment	56.1	58.9	48.5	49.9
1.0% Enrichment	28.2	29.6	28.3	29.9
2.0% Enrichment	15.6	16.5	17.0	17.3
Electrostatics Potential Similarity Virtual Screening				
AUC	0.649			
0.5% Enrichment	35.7			
1.0% Enrichment	21.4			
2.0% Enrichment	10.7			
Structure Based Virtual Screening Using Homology Model of GPER-1and Diverse Dataset of Active and Decoy GPER-1				
AUC	0.546			
0.5% Enrichment	10.0			
1.0% Enrichment	6.7			
2.0% Enrichment	3.3			
Structure Based Virtual Screening Using Homology Model of GPER-1 and selective Dataset of Active and Decoy GPER-1				
AUC	0.660			
0.5% Enrichment	14.0			
1.0% Enrichment	7.6			
2.0% Enrichment	5.6			

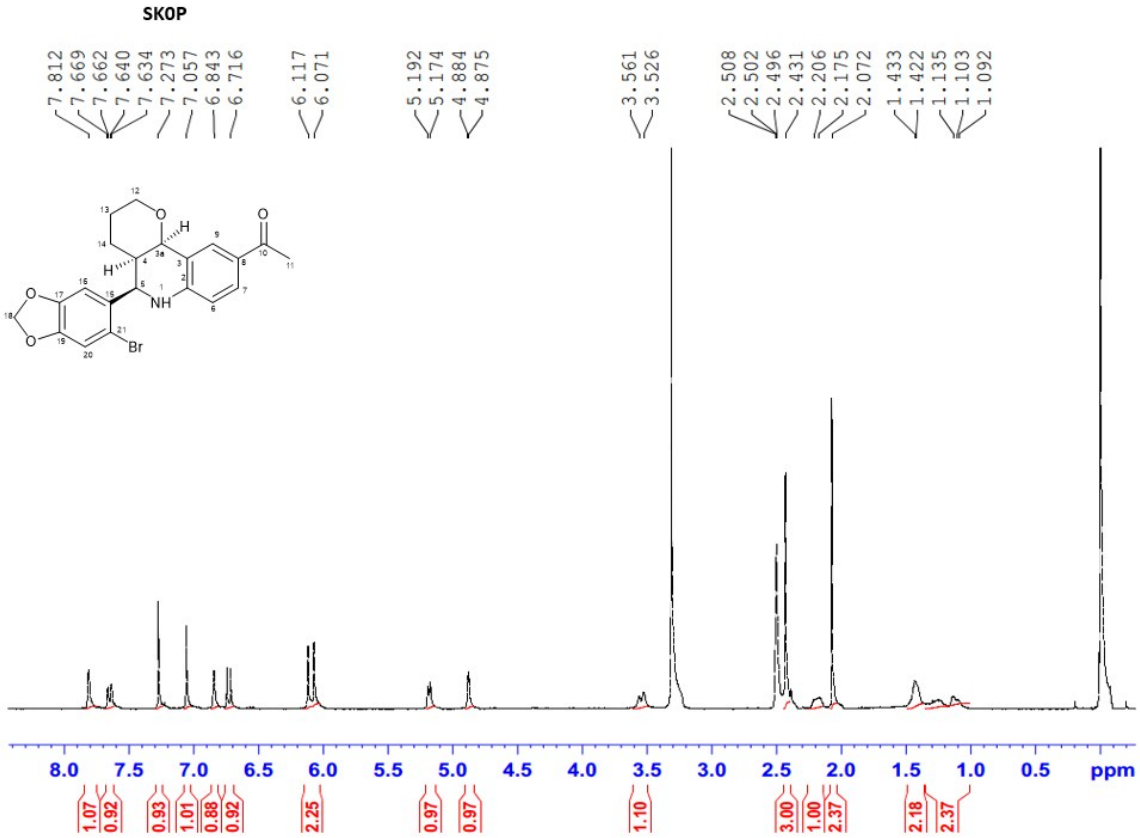
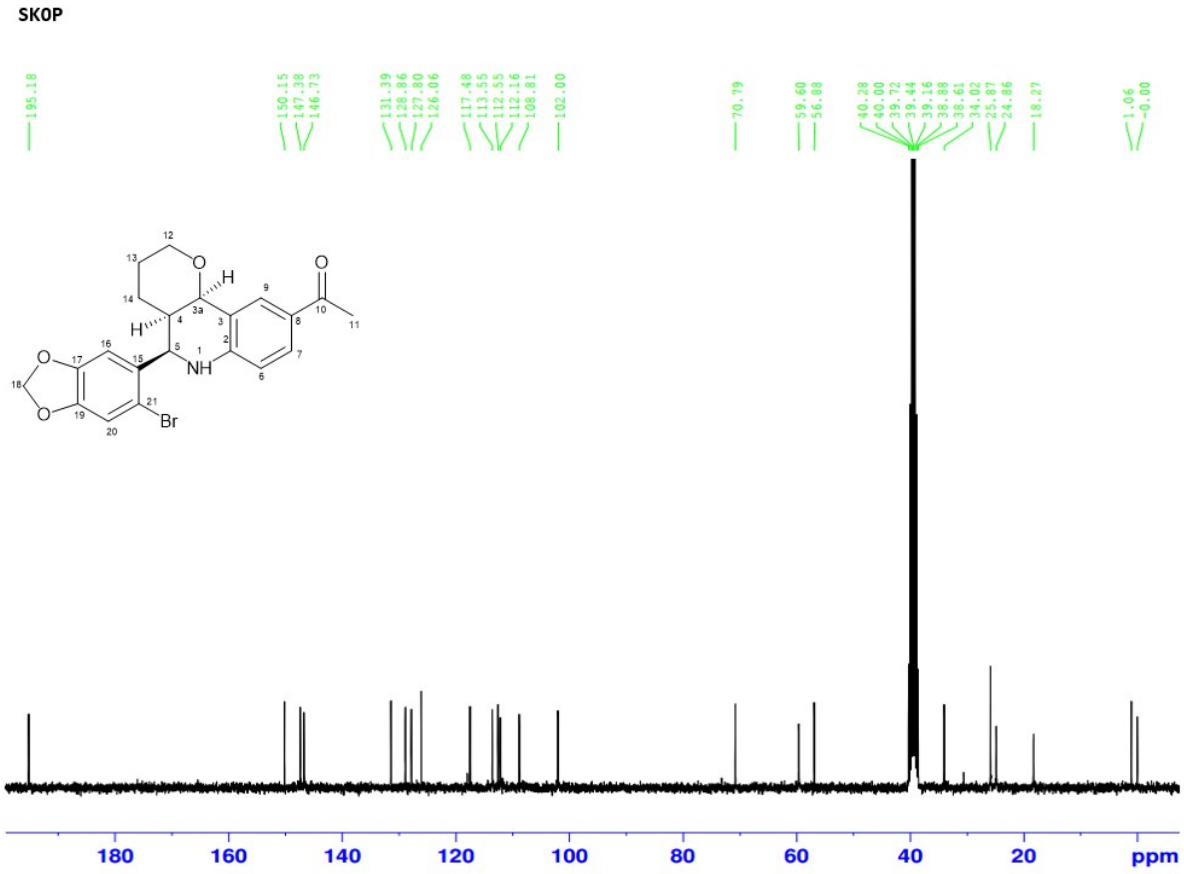
S2: ^{1}H NMR Spectra of Compound SK0



S3: ^{13}C NMR Spectra of Compound SK0



S4: ^{1}H NMR Spectra of Compound SK0P



S5: ^{13}C NMR Spectra of Compound SK0P