

Supplementary Information

Synthesis, Experimental and Computational Evaluation of SERAAK1 as a 5-HT_{2A} Receptor Ligand

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Supplementary Figures

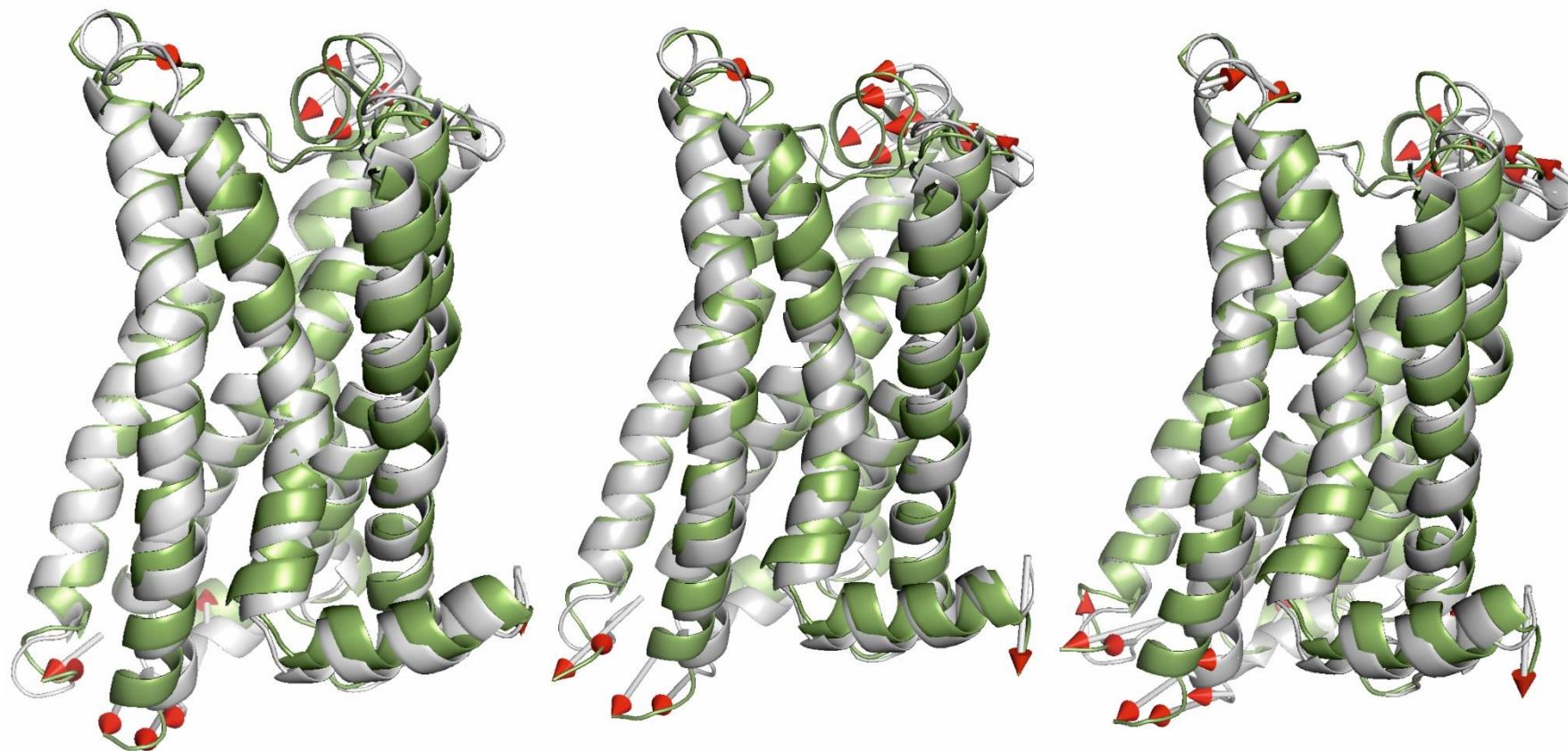
Figure S1. Porcupine plots obtained for protein – ligand complexes after molecular dynamics simulations.

Figure S2. High- Resolution Mass Spectrometry (HRMS) Analysis of SERAAK1.

Figure S3. ^1H NMR Spectrum of SERAAK1 (600 MHz, MeOD).

Figure S4. ^{13}C NMR Spectrum of SERAAK1 (151 MHz, CDCl_3).

Figure S5. Chromatogram of SERAAK1.



PCA 1

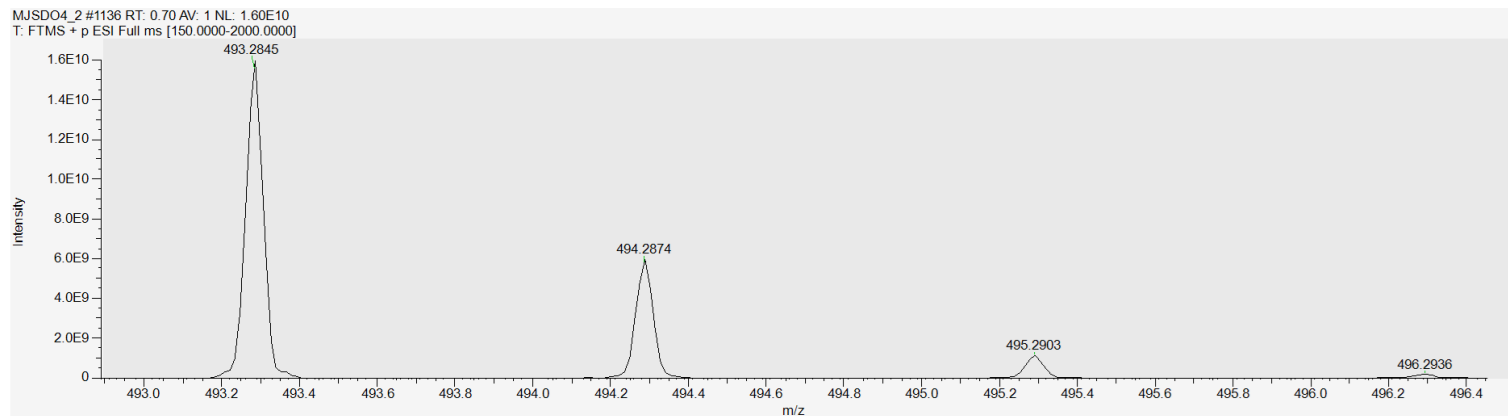
PCA 2

PCA 3

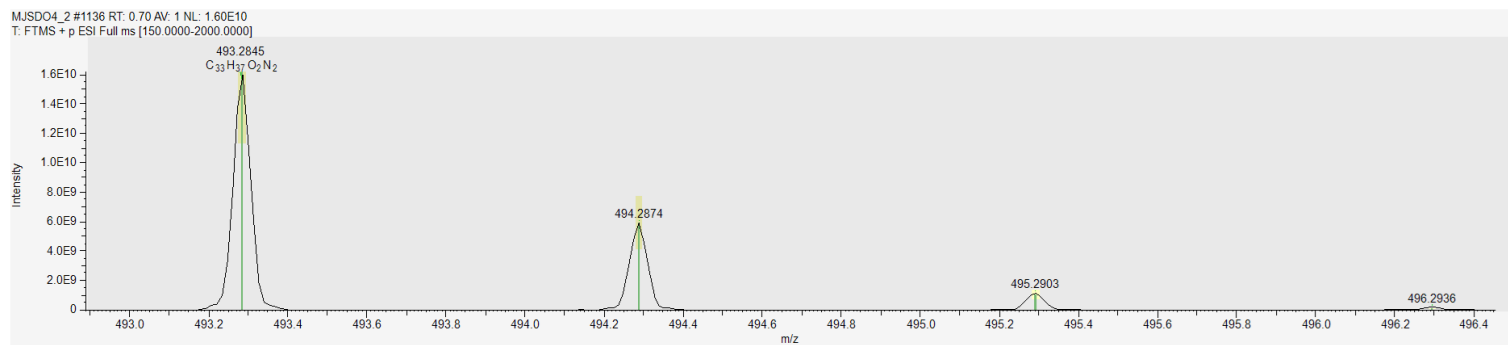
Figure S1. Porcupine plots obtained for protein – ligand complexes after molecular dynamics simulations.

IUPAC NAME	1-(benzhydryloxy)-3-(4-benzhydrylpiperazin-1-yl)propan-2-ol
Chemical Formula	C ₃₃ H ₃₆ N ₂ O ₂
Monoisotopic Mass:	492.2777 Da
[M+H]⁺	493.2855 Da

Measured HRMS spectrum



Measured Mass (Da): 493.2845



Isotopic pattern match score: 98.77%

Figure S2. High- Resolution Mass Spectrometry (HRMS) Analysis of SERAAK1.

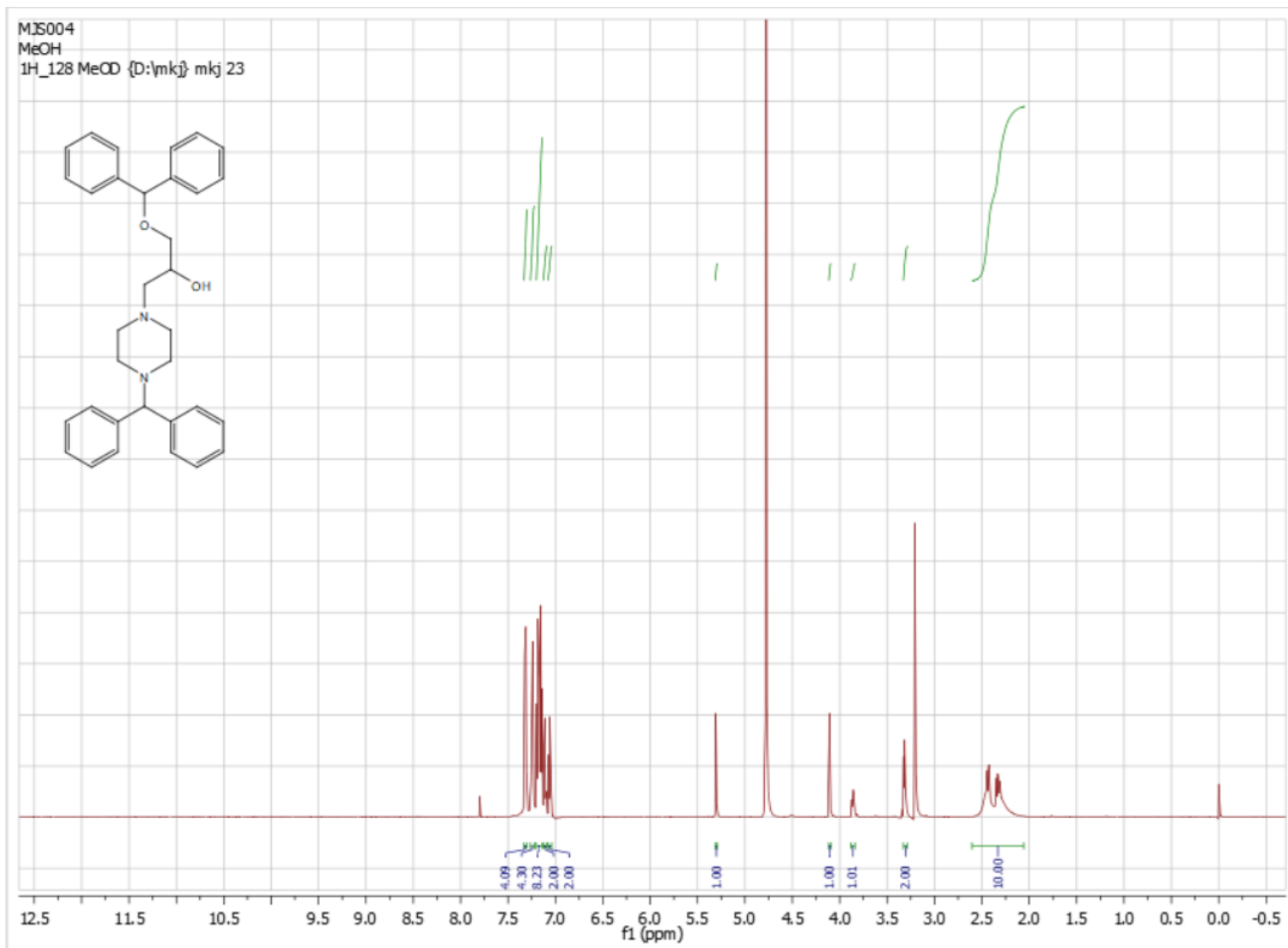


Figure S3. ¹H NMR Spectrum of SERAAK1 (600 MHz, MeOD).

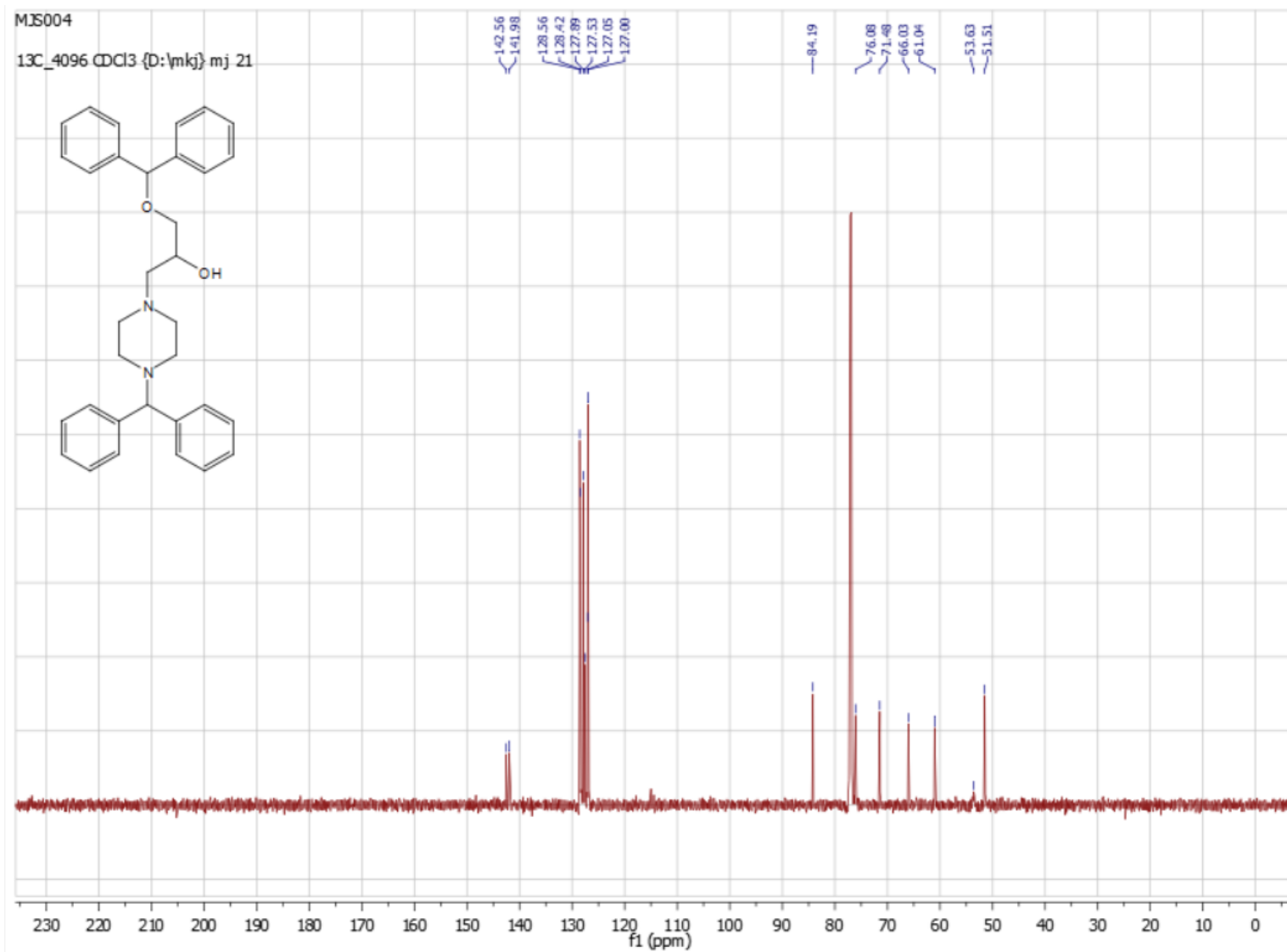


Figure S4. ^{13}C NMR Spectrum of SERAAK1 (151 MHz, CDCl_3).

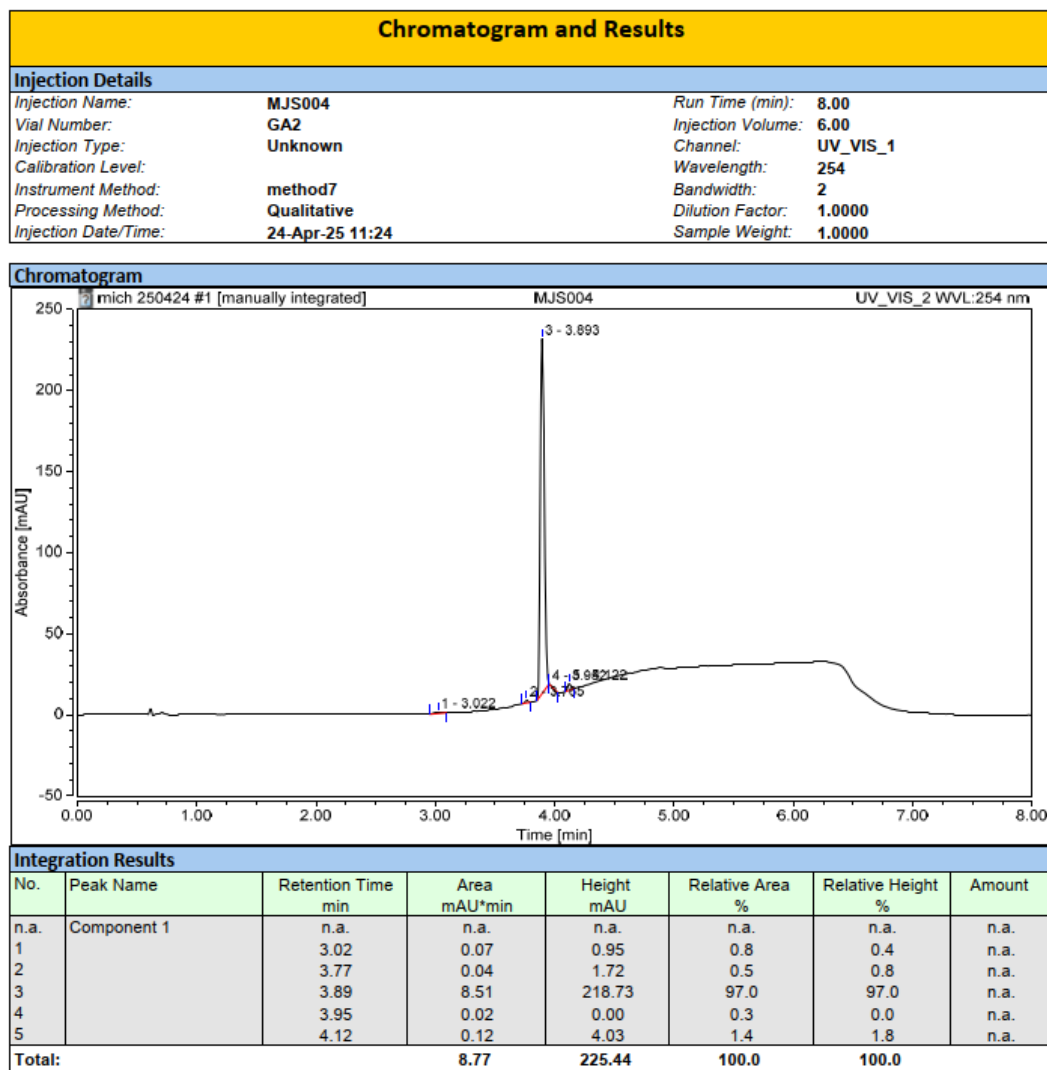


Figure S5. Chromatogram of SERAAK1.