

Supplementary Materials

Figure S1. ^1H -NMR spectrum of compound **3**.

Figure S2. ^{13}C -NMR spectrum of compound **3**.

Figure S3. Mass spectrum of compound **3**.

Figure S4. All possible intermolecular interactions and their contribution to the overall molecular packing interactions.

Figure S5. Hirshfeld surfaces mapped with d_{norm} , shape index and curvedness (A). Hirshfeld surface mapped over d_{norm} highlighting the area of intermolecular $\text{C-H}\cdots\text{O}$ contacts, where two molecules formed inversion dimer linkage through dark red spots on the d_{norm} Hirshfeld surface (B).

Figure S6. 3D image obtained from nine iterated docking results between compound **3** and glutathione S-transferase containing glutathione (red color) generated by PyMol.

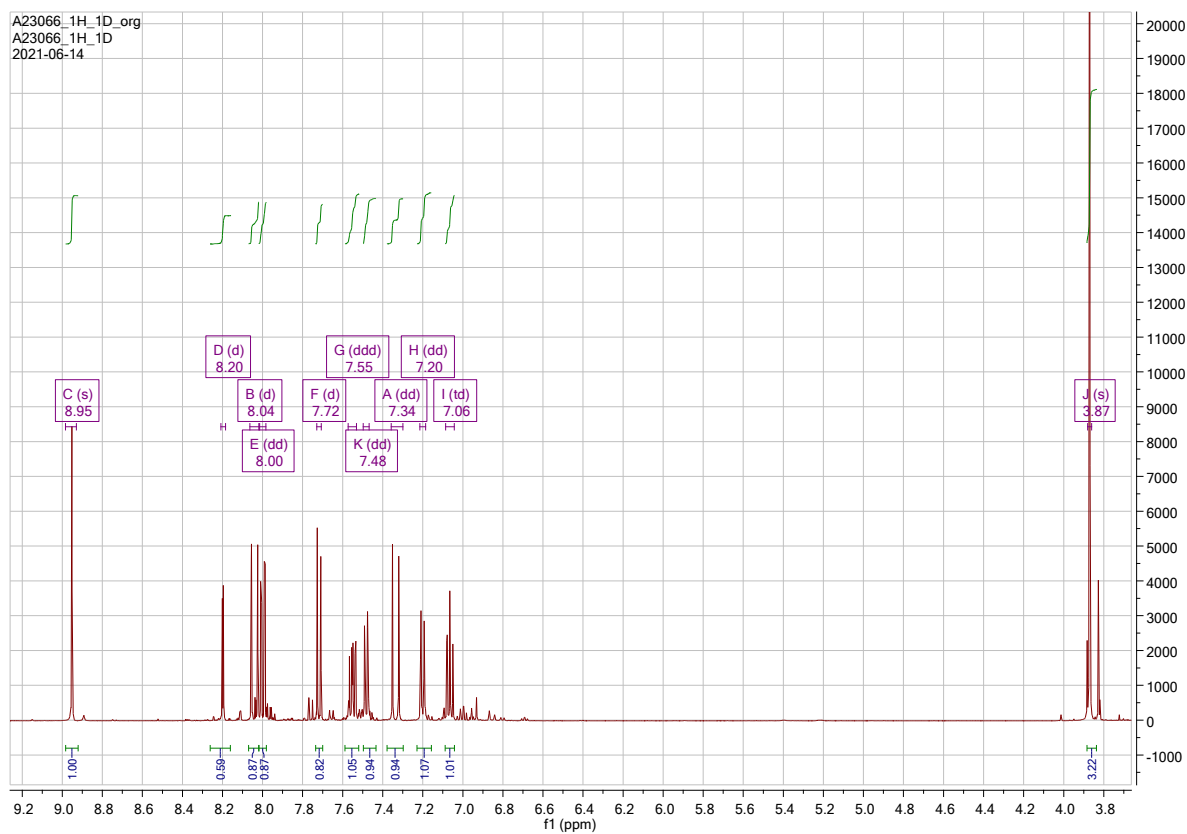


Figure S1. ^1H -NMR spectrum of compound **3**.

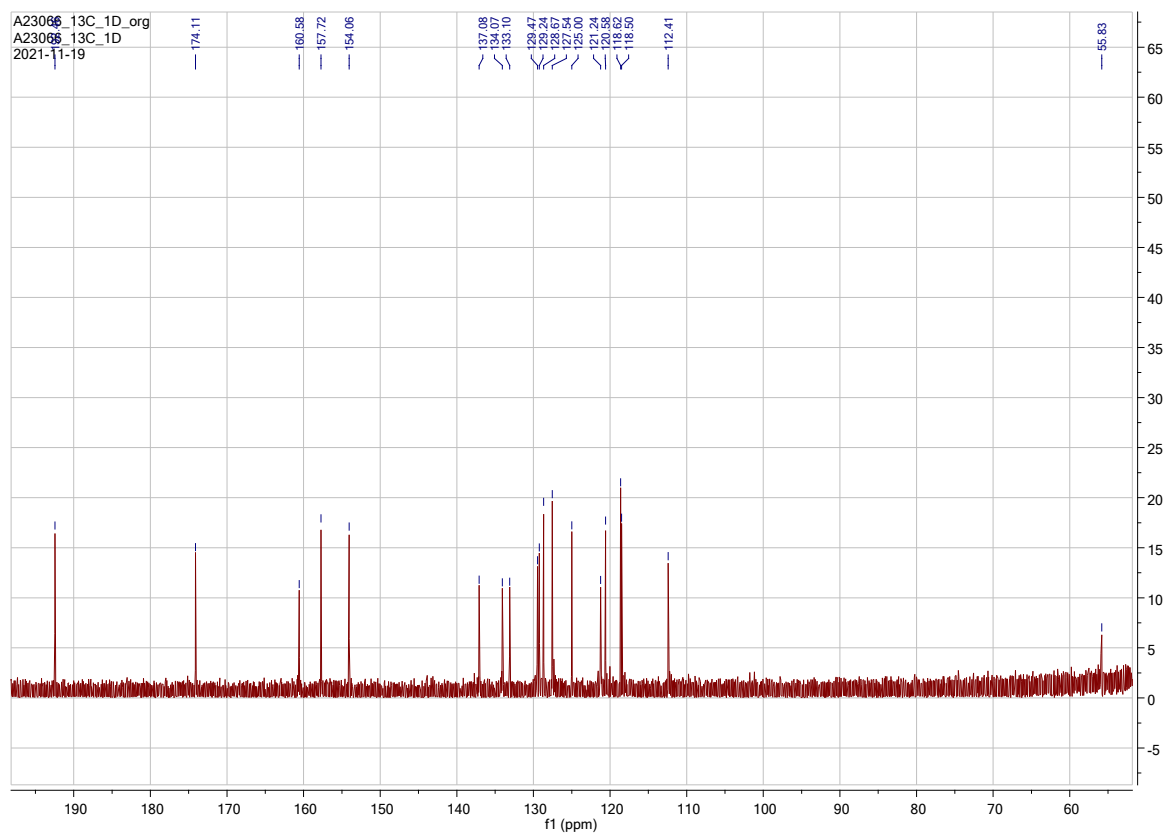


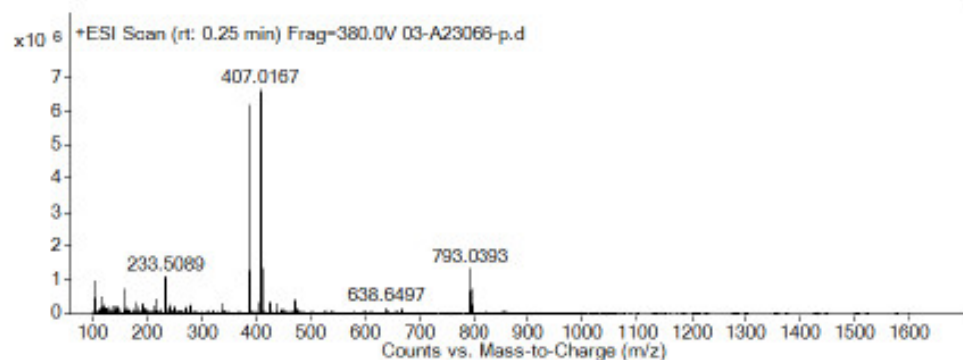
Figure S2. ^{13}C -NMR spectrum of compound **3**.

Data Filename	03-A23066-p.d	Sample Name	03-A23066-p
Sample Type	Sample	Position	P1-D1
Instrument Name	Instrument 1	User Name	
Acq Method	DirectMS-2min-p.m	Acquired Time	11/23/2021 11:02:24 AM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500
		Version	series Q-TOF B.06.01 (B6172 SP1)

Data Filename	13-A23066-n.d	Sample Name	13-A23066-n
Sample Type	Sample	Position	P1-D1
Instrument Name	Instrument 1	User Name	
Acq Method	DirectMS-2min-n.m	Acquired Time	11/23/2021 11:32:19 AM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500
		Version	series Q-TOF B.06.01 (B6172 SP1)



m/z	z	Abund
233.5089	2	1076724.25
385.0332	1	6192467
386.0358	1	1191099.25
387.0315	1	6104703.5
388.0341	1	1240823.63
407.0167	1	6650736
408.0191	1	1358013.13
409.015	1	6568515.5
410.0175	1	1316316.88
793.0393	1	1318459.63

Figure S3. Mass spectrum of compound 3.

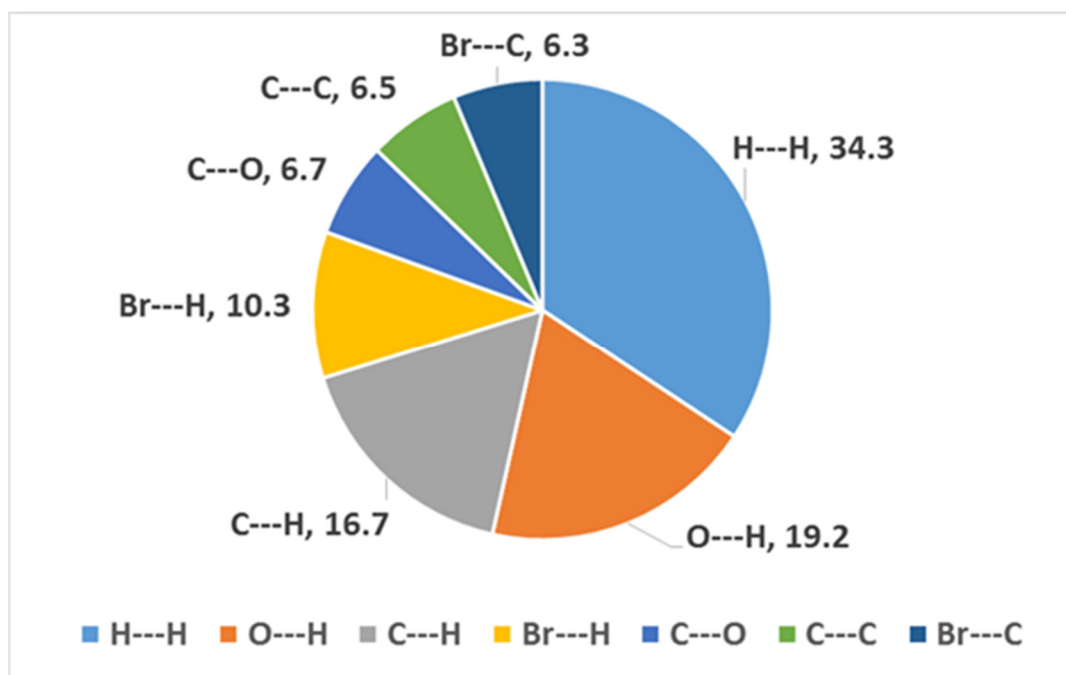


Figure S4. All possible intermolecular interactions and their contribution to the overall molecular packing interactions.

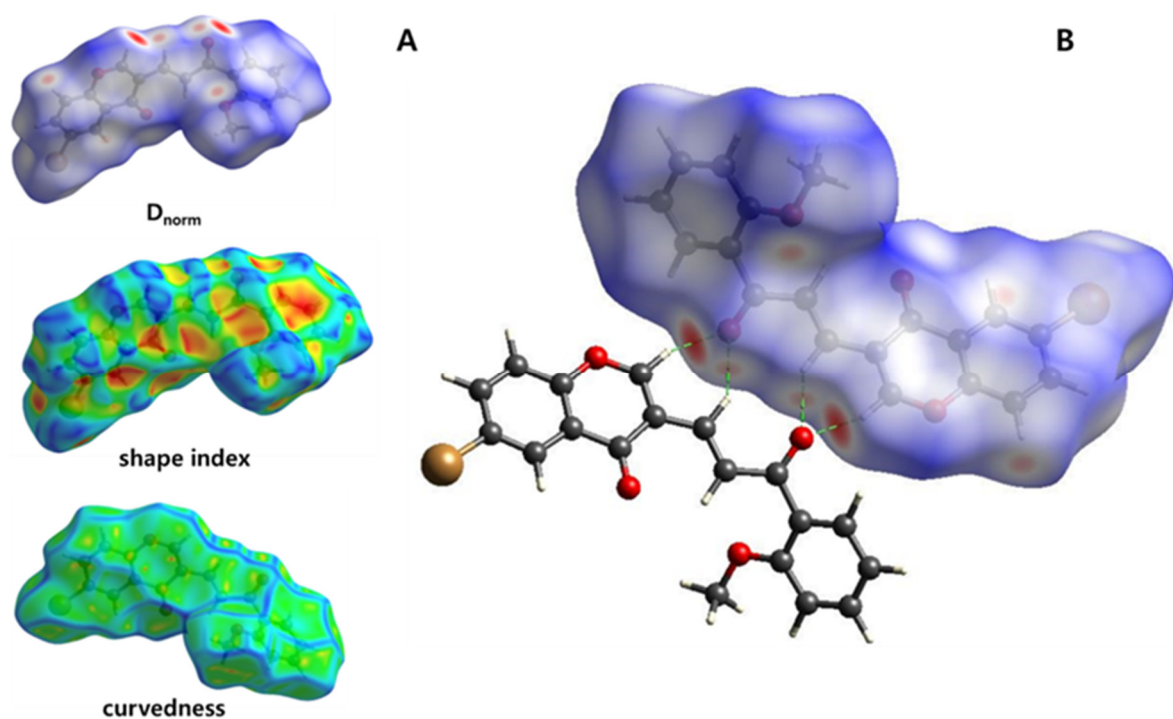


Figure S5. Hirshfeld surfaces mapped with d_{norm} , shape index and curvedness (A). Hirshfeld surface mapped over d_{norm} highlighting the area of intermolecular $\text{C-H}\cdots\text{O}$ contacts, where two molecules formed inversion dimer linkage through dark red spots on the d_{norm} Hirshfeld surface (B).



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