

Supporting Information

Synthesis, Characterization, and Crystal Structure of *N*-(3-nitrophenyl)cinnamamide

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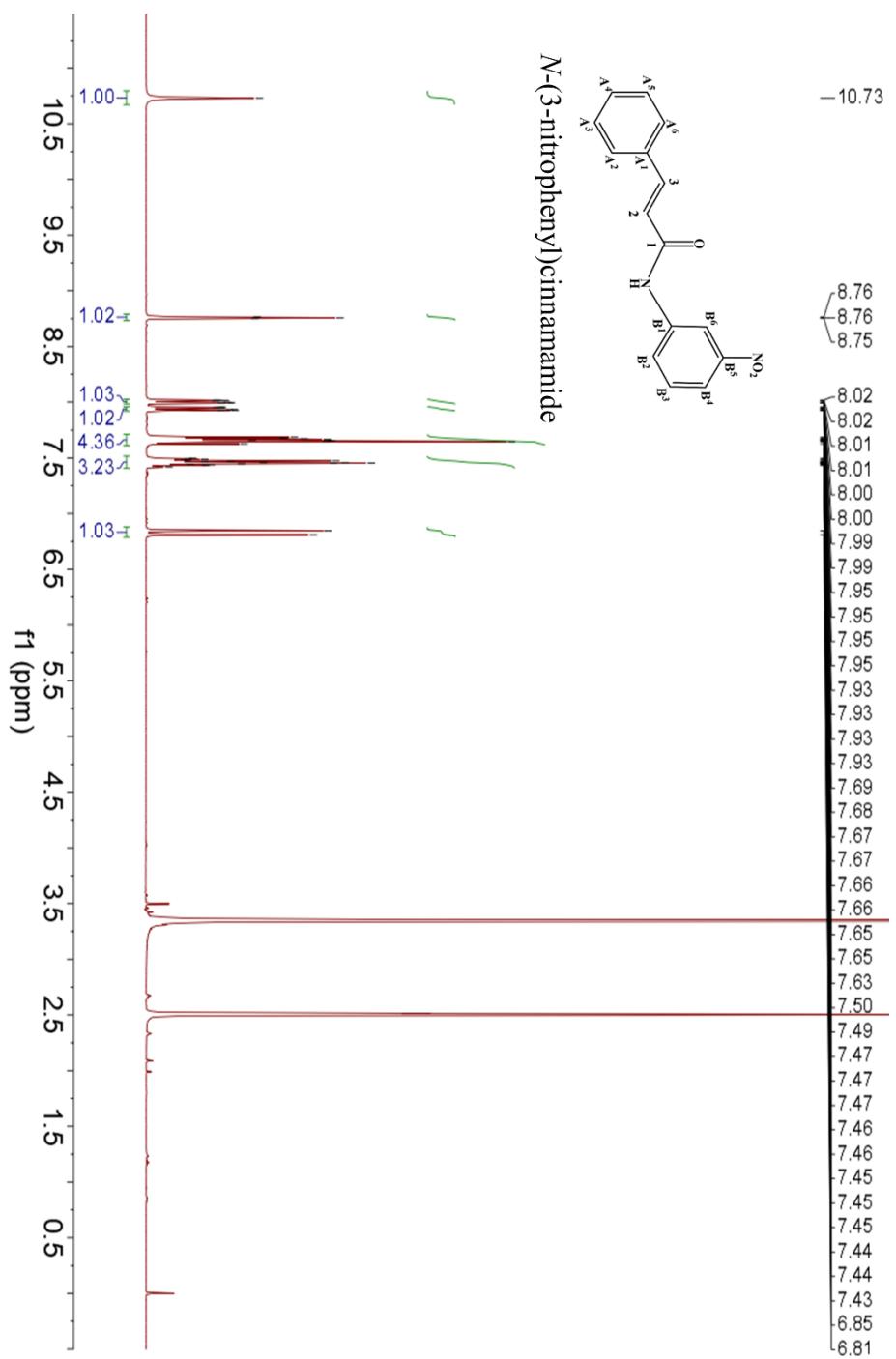


Figure S1: ^1H NMR spectra of compound 1

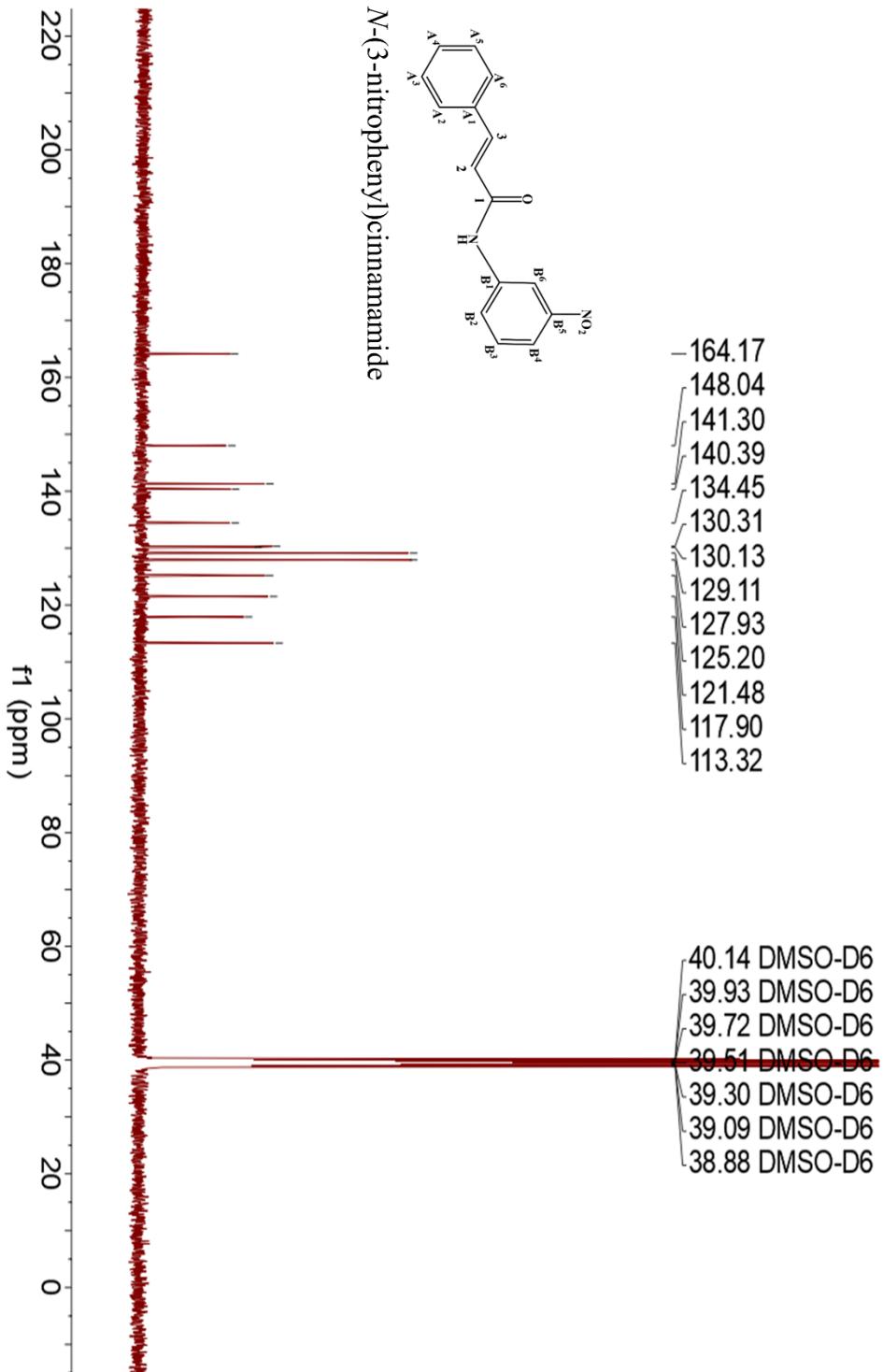
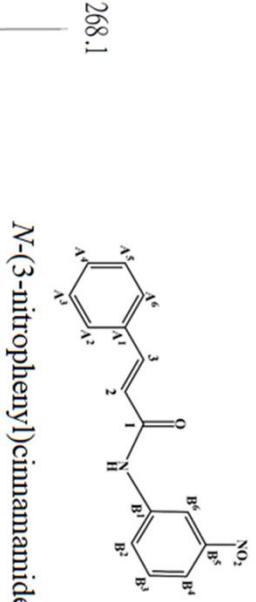


Figure S2: ^{13}C NMR spectra of compound 1

[Mass Spectrum] Scan#: 37
 RT : 1.38 min
 Elements : C 15/0, H 31/0, N 2/0, O 3/0
 Mass Tolerance : 1000ppm, 5mmu if $m/z < 5$, 50mmu if $m/z > 50$
 Unsaturation (U.S.) : -0.5 - 20.0



Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
1 268.0847	100.00	-0.3 / -0.1	11.0	C15 H12 N2 O3

Figure S3: Mass spectra of compound 1

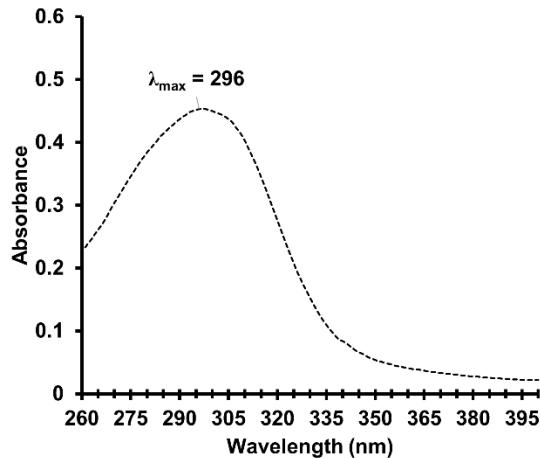


Figure S4: UV absorbance spectra of compound 1

Table S1. Calculated inter-molecular potentials energies obtained by UNI forcefield calculations

mol1	mol2	Distance	Energy (kJ/mol)
0	1	4.02201	-58.5595
0	2	9.00783	-49.8388
0	3	7.71775	-39.0104
0	4	5.55739	-36.3843
0	5	8.2079	-24.0213
0	6	8.2079	-24.0213
0	7	10.1371	-13.122