The Influence of Intermolecular Interactions and Molecular Packings on Mechanochromism and Mechanoluminescence — A Tetraphenylethylene Derivatives Case

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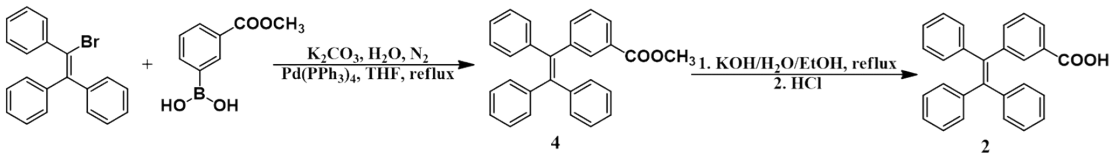
Scheme 1. The synthetic route of compound **4** and **2**.


Br
COOCH3
HO
B
OH
K2CO3, H2O, N2
Pd(PPh3)4, THF, reflux
COOCH3
1. KOH/H2O/EtOH, reflux
2. HCl
COOH

4

2

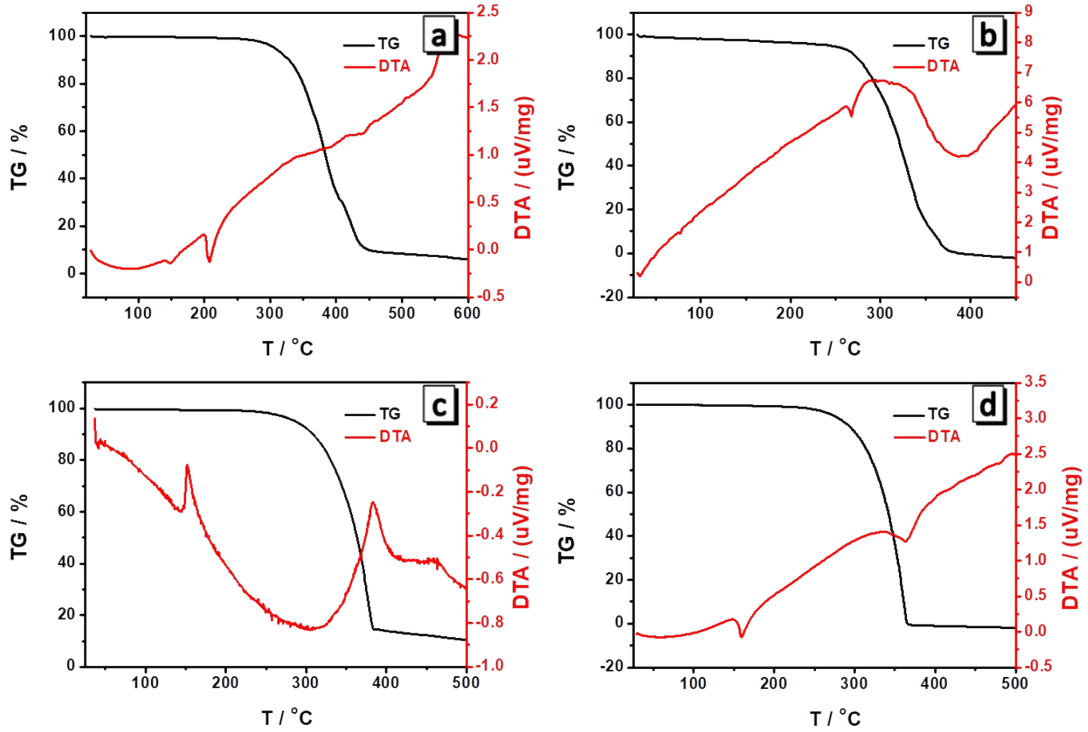


Figure S1. TG and DTA curves of **1**-**4**.

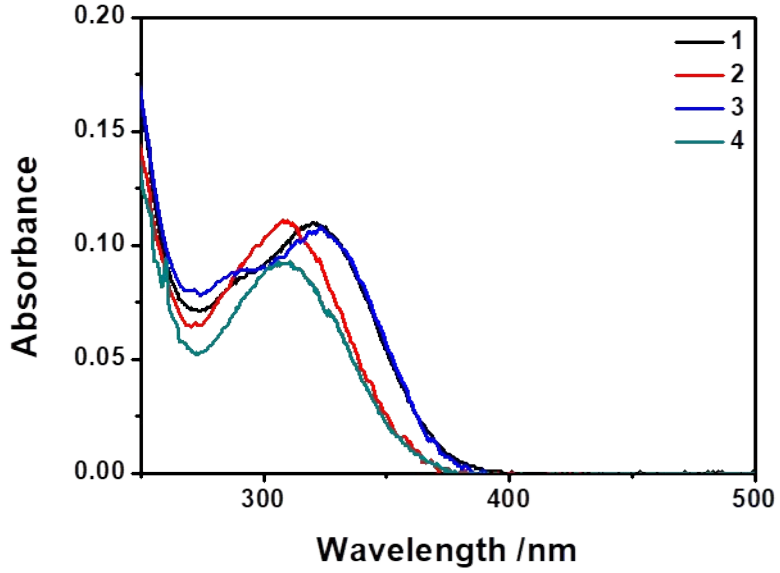


Figure S2. The absorption spectra of **1**-**4** in THF solution, concentration: 10 μM.

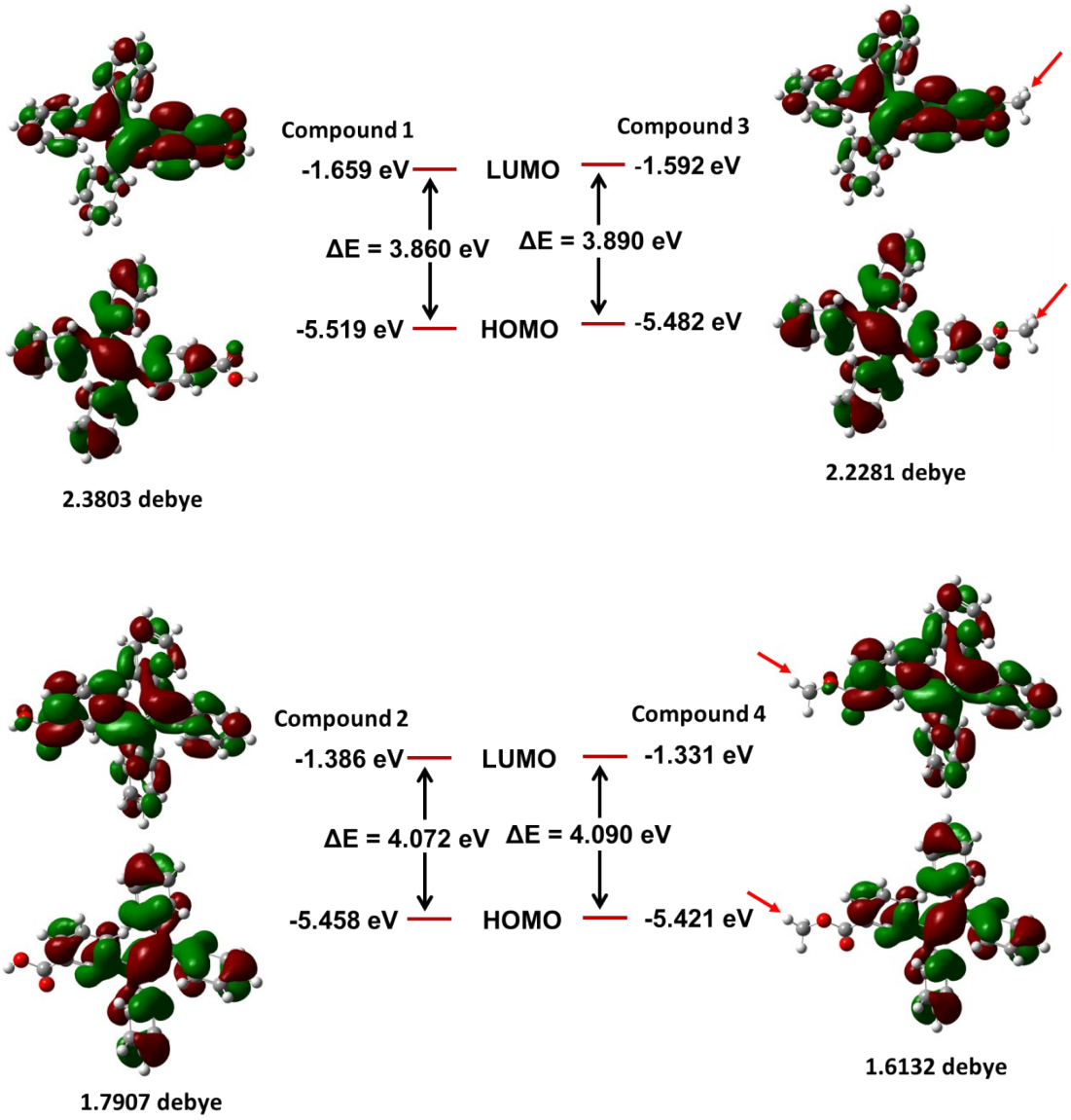


Figure S3. The HOMO and LUMO orbital distribution and dipole moment of **1**-**4** calculated by B3LYP/6-31+G(d). The red arrows indicated the methyl group.

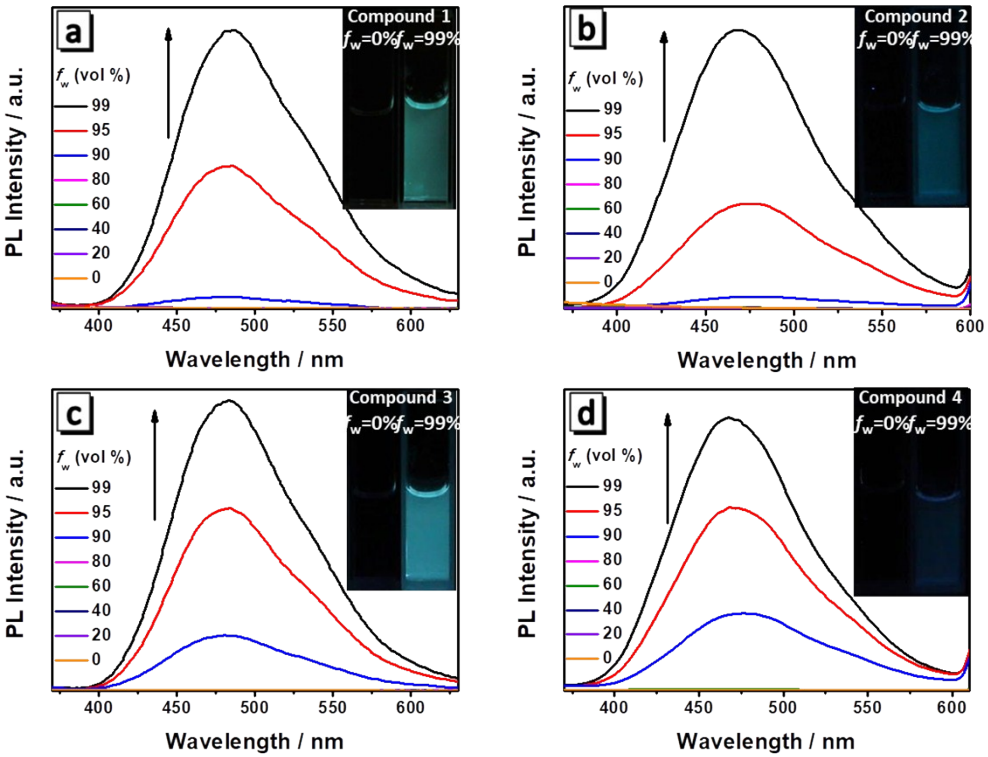


Figure S4. The fluorescence spectra of (a) **1**, (b) **2**, (c) **3** and (d) **4** in THF/water mixtures with different water fractions (f_w), concentration: 10 μM.

Table S1. Single crystal data of **1-3**

	1	**2**	**3**
CCDC Number	1904515	1904516	1904514
Formula	C27H20O2	C27H20O2	C28H22O2
Formula Weight /g•mol^{-1}	376.43	376.43	390.46
Crystal system	monoclinic	monoclinic	monoclinic
Space group	P21/c	P21/c	P21
T/K	150	169.99	293.15
Z	8	4	4
a/Å	9.68410(10)	19.8069(10)	9.7794(2)
b/Å	9.40430(10)	5.4313(3)	9.5115(2)
c/Å	51.7692(6)	19.6647(9)	23.9482(5)
α/°	90	90	90
β/°	90.9180(10)	102.555(4)	101.228(2)
γ/°	90	90	90
V/Å^3	4714.13(9)	2064.89(18)	2184.95(8)
ρ_c/g•cm^{-3}	1.061	1.208	1.187
μ/mm^{-1}	0.517	0.590	0.575
F(000)	1584	788	824
Reflections collected	28098	14694	13022
Independent reflections	9296	3496	6238
R_{int}	0.0272	0.0528	0.0312
$R_1(I > 2\sigma(I))$	0.0424	0.0727	0.0479
wR_2	0.1105	0.2303	0.1390
GOOF	1.041	1.051	1.046

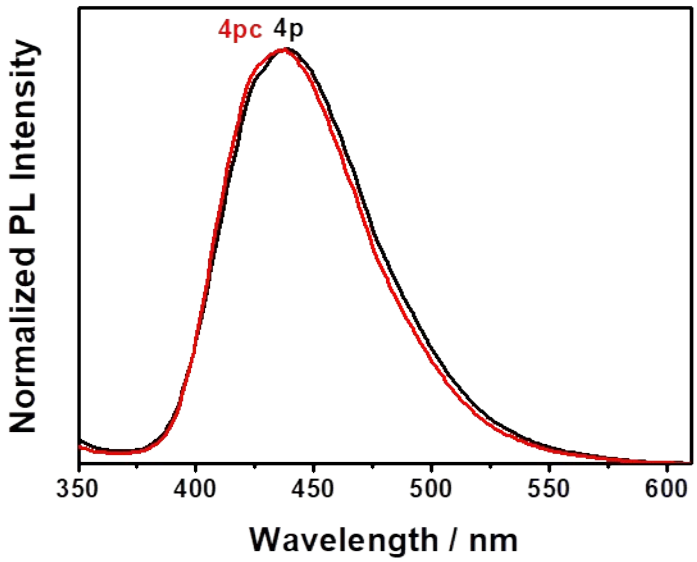


Figure S5. Normalized PL intensity of as-prepared powder (**4p**) and polycrystal (**4pc**) of **4**.

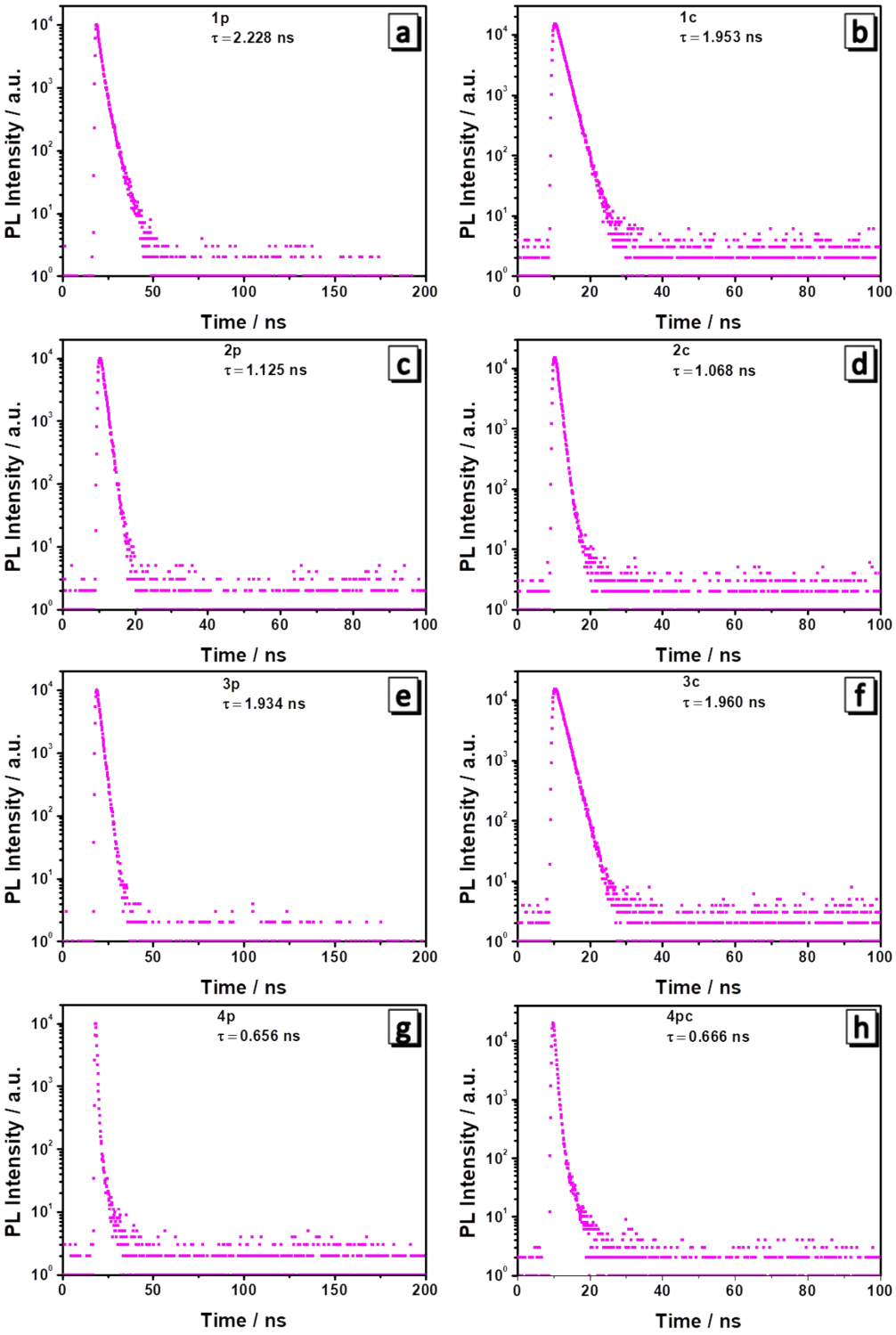


Figure S6. Fluorescence decay curves of (a) **1p**, (b) **1c**, (c) **2p**, (d) **2c**, (e) **3p**, (f) **3c**, (g) **4p** and (h) **4pc**.

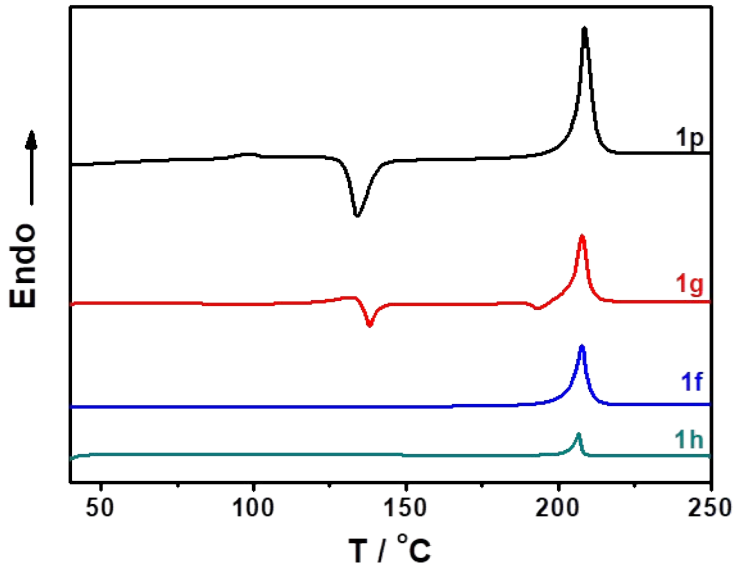


Figure S7. DSC curves of the as-prepared powder (**1p**), ground powder (**1g**), fumed powder (**1f**) and heated powder (**1h**) of **1**.

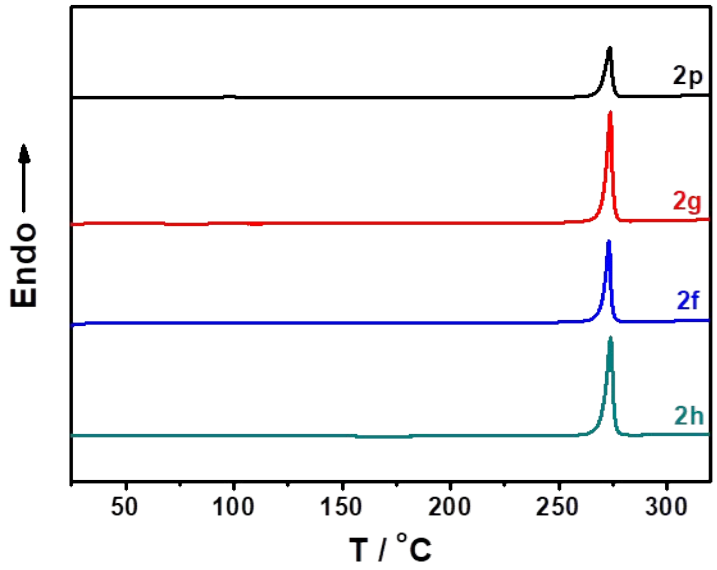


Figure S8. DSC curves of the as-prepared powder (**2p**), ground powder (**2g**), fumed powder (**2f**) and heated powder (**2h**) of **2**.

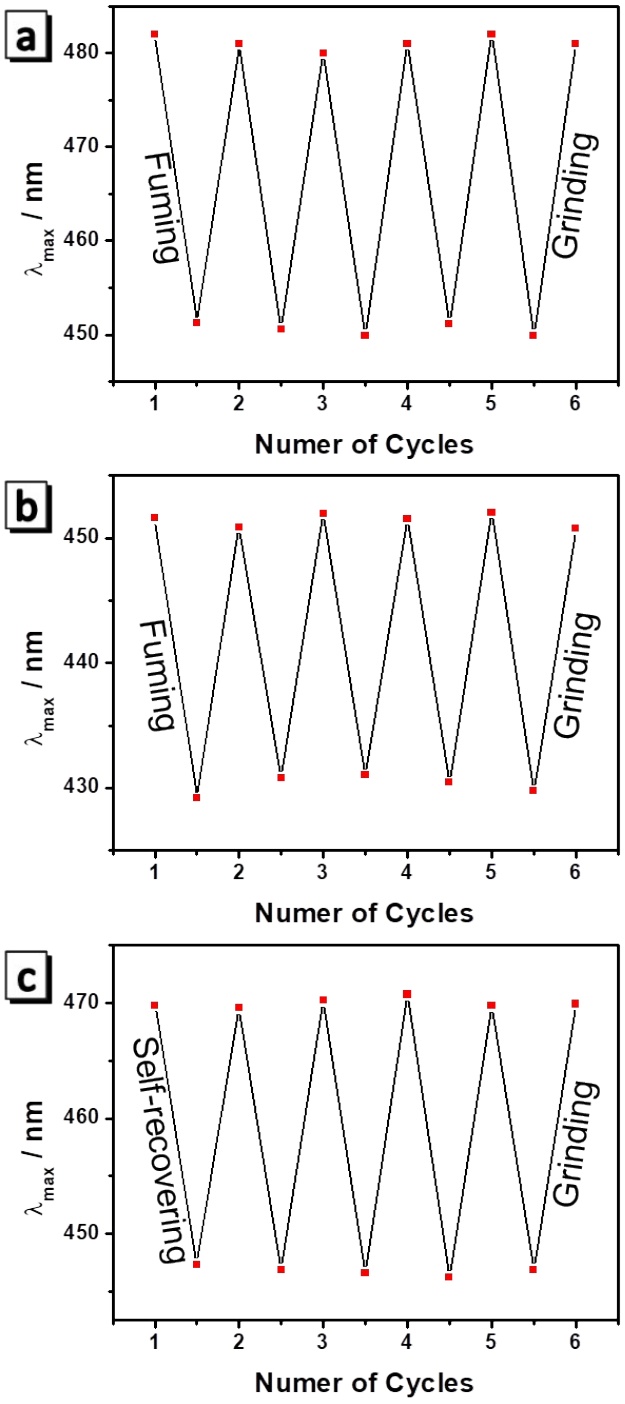


Figure S9. Maximum emission wavelength changes of (a) **1** and (b) **2** cast weighing paper versus dichloromethane fuming/grinding cycles. Maximum emission wavelength changes of (c) **3** cast weighing paper versus self-recovering/grinding cycles.

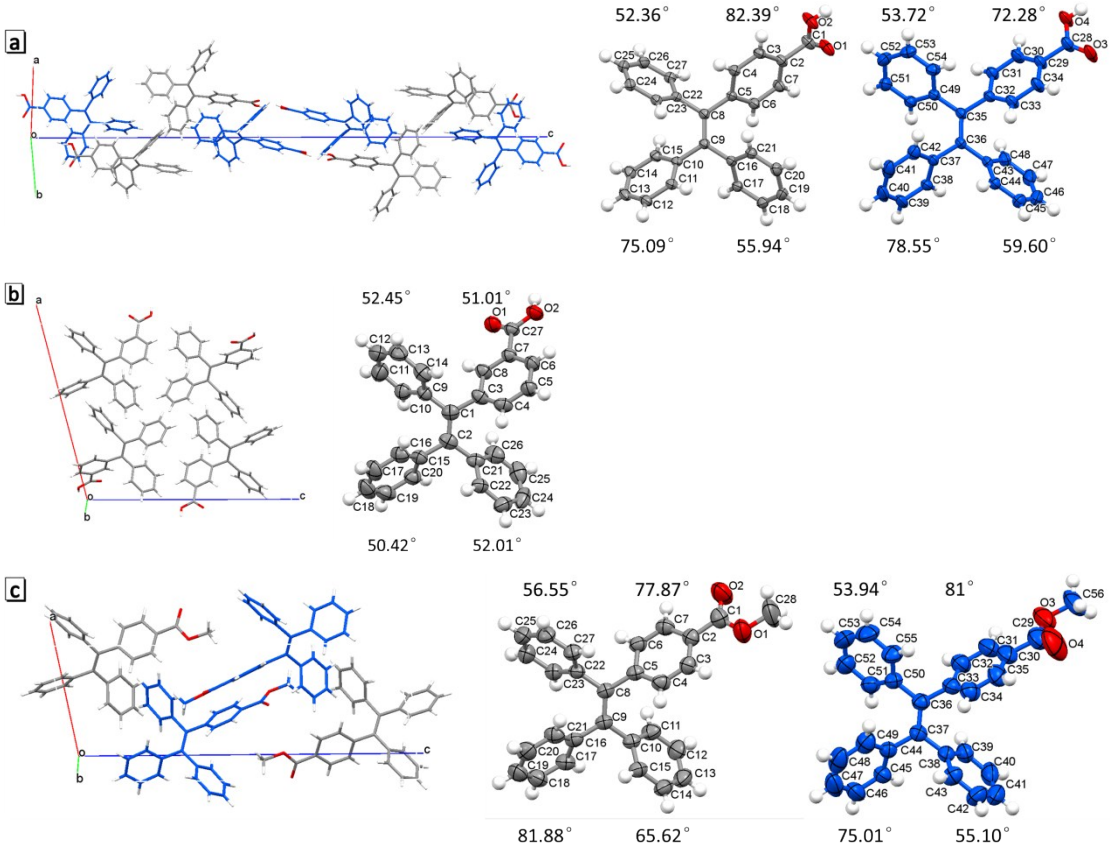


Figure S10. The unit cell and molecular conformations with labels of carbon/oxygen atoms and dihedral angles (between the phenyl ring and central ethene group) of single cyrstals (a) **1**, (b) **2** and (c) **3**. Ellipsoids represent the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radii.

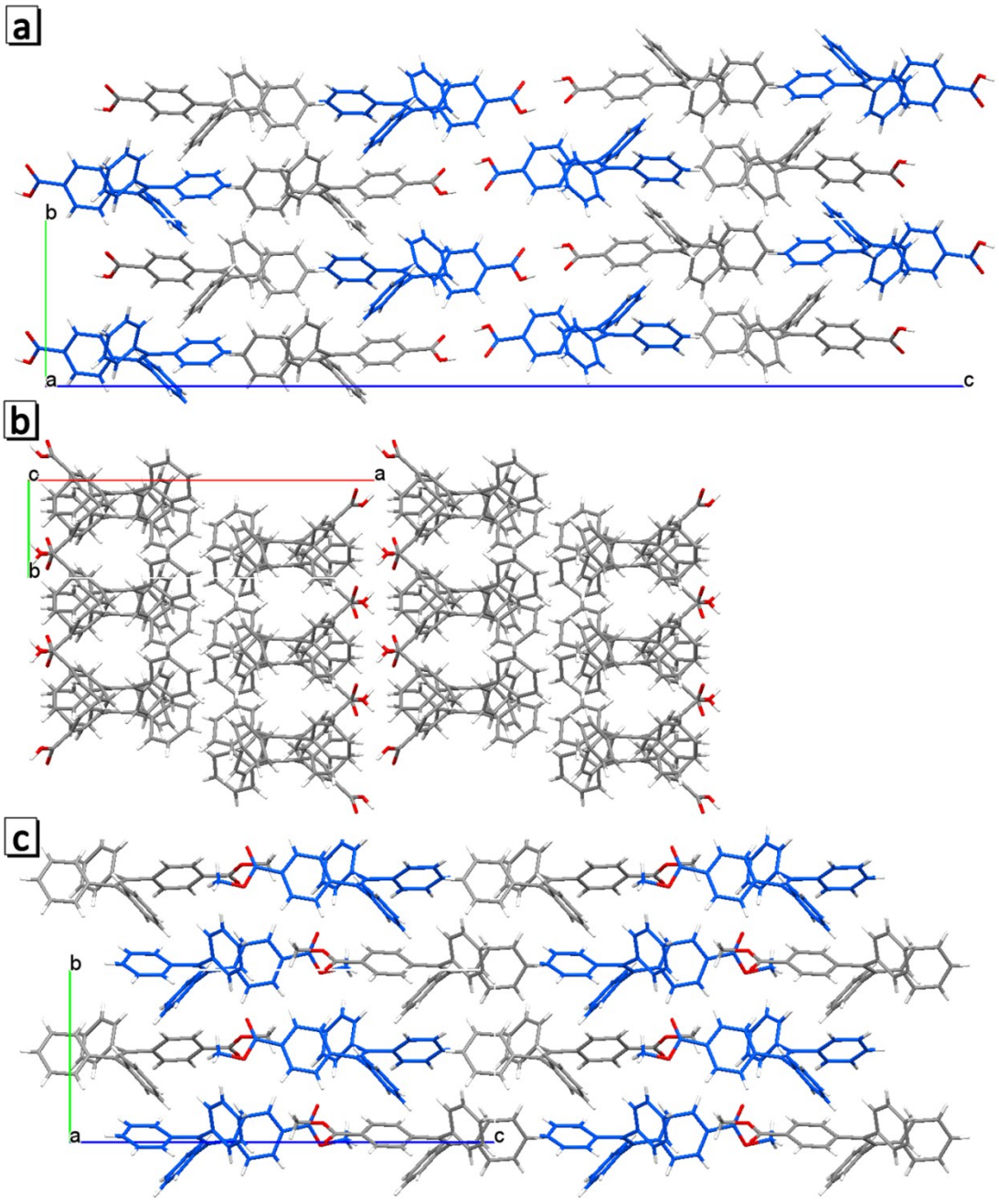


Figure S11. The lamellar stacking in single crystals (a) **1**, (b) **2** and (c) **3**.

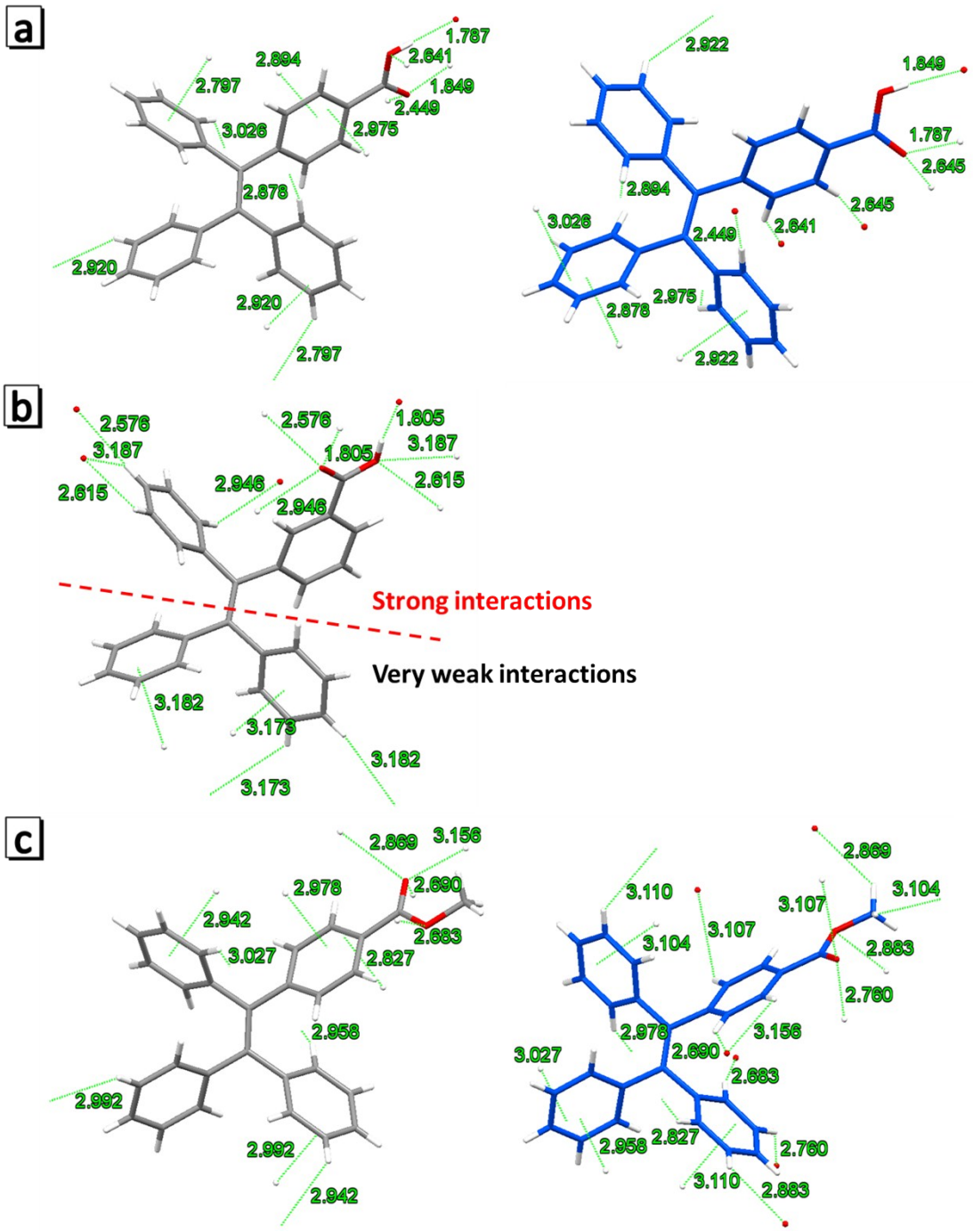


Figure S12. The detailed intermolecular interactions of every conformation in single crystals (a) **1**, (b) **2** and (c) **3**. Bond length of C-H···π interaction is the distance between hydrogen atom and the plane of benzene ring.

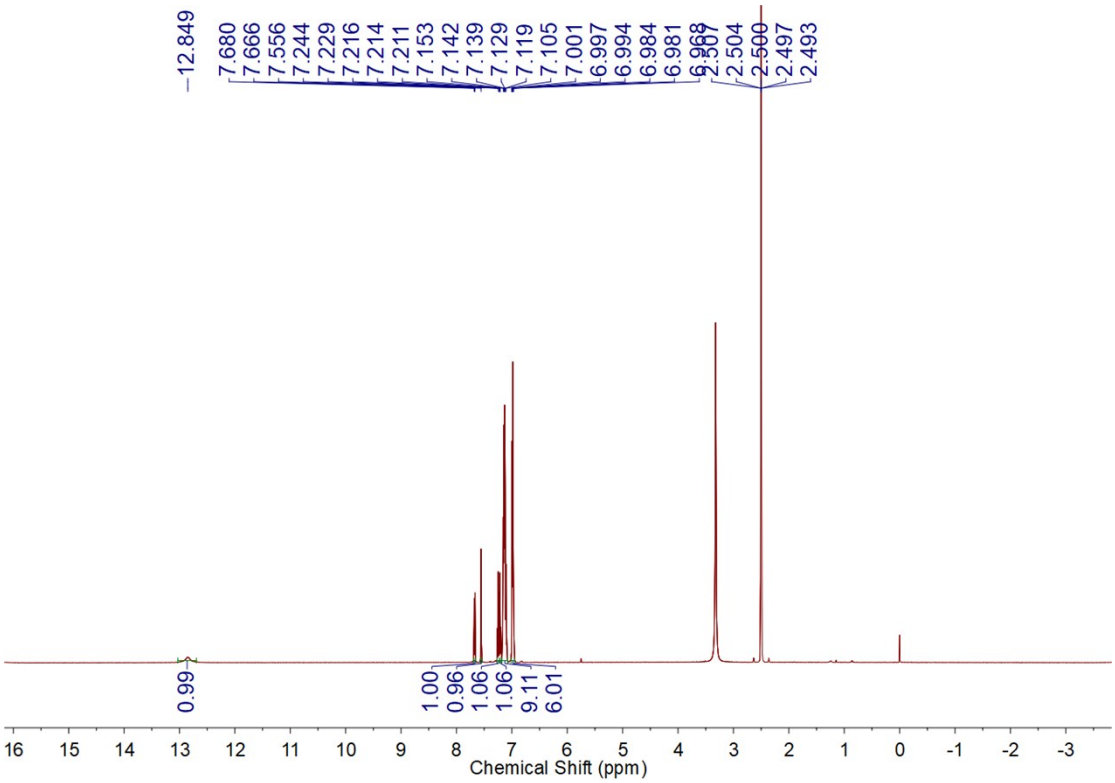


Figure S13. 1H NMR of compound **2**.

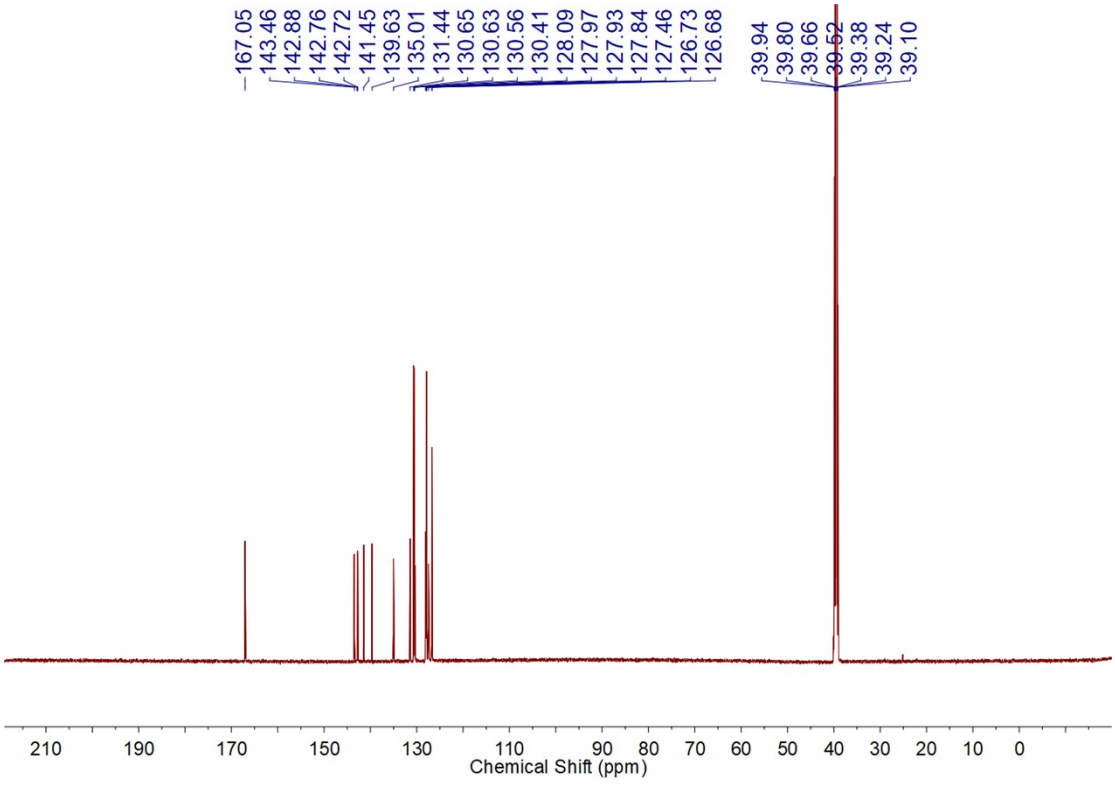


Figure S14. ^{13}C NMR of compound **2**.

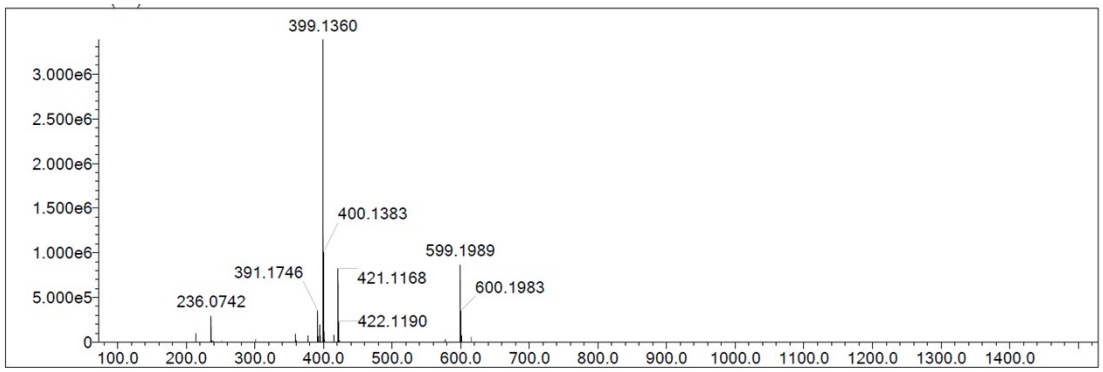


Figure S15. HRMS of compound **2**.

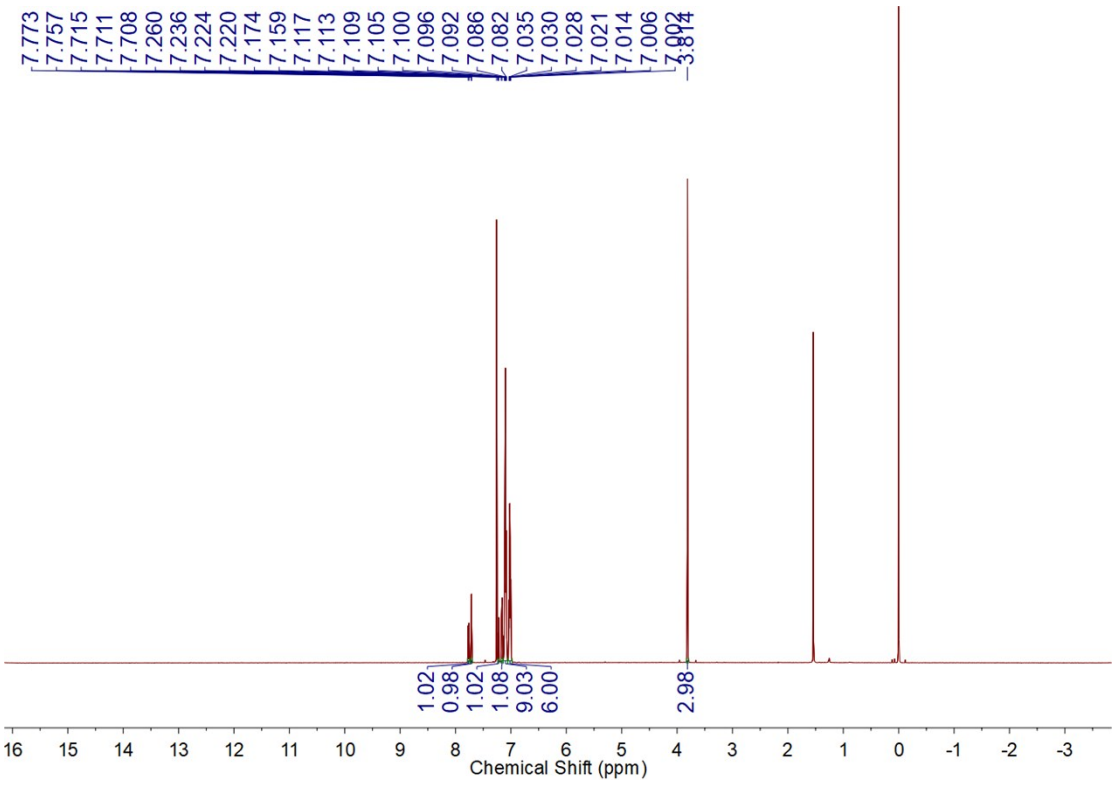


Figure S16. 1H NMR of compound **4**.

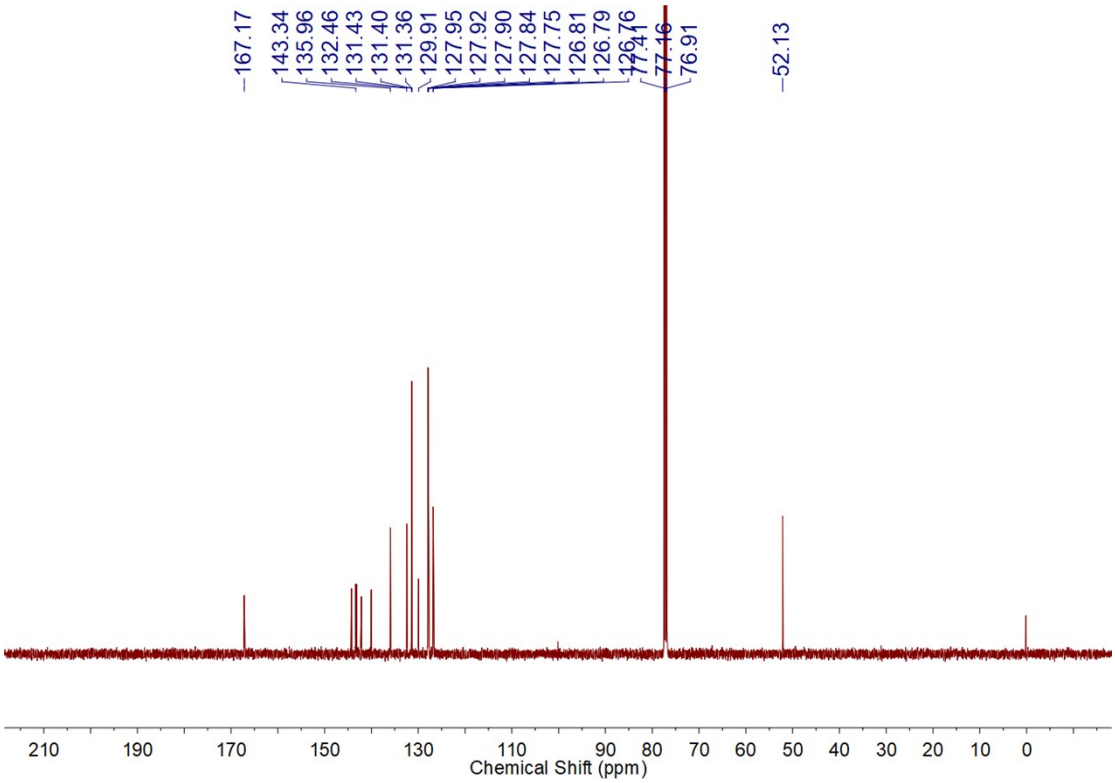


Figure S17. ^{13}C NMR of compound **4**.

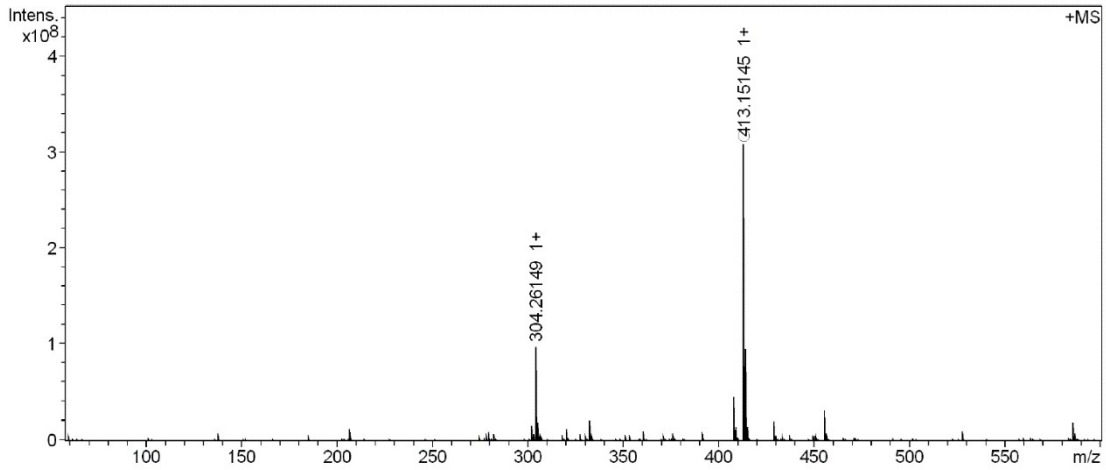


Figure S18. HRMS of compound **4**.