

Hydrogen-bond-driven supramolecular self-assembly of diacetylene derivatives for topochemical polymerization in solution

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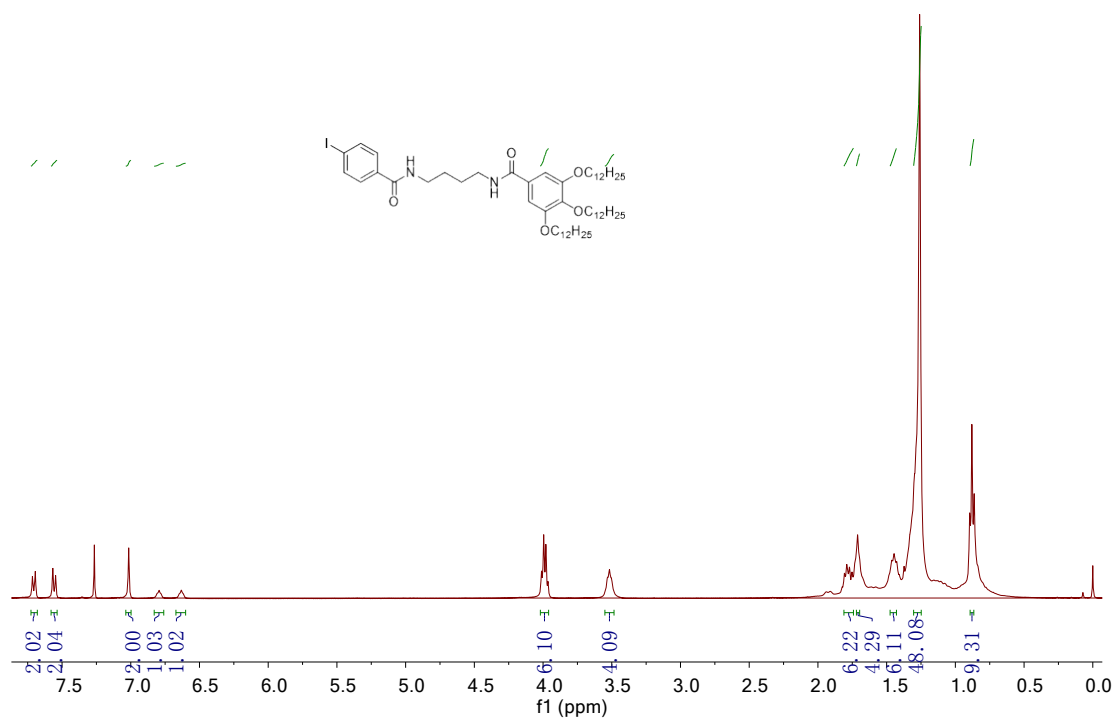


Fig. S1. ¹H NMR spectrum of **4** at 25 °C in CDCl₃.

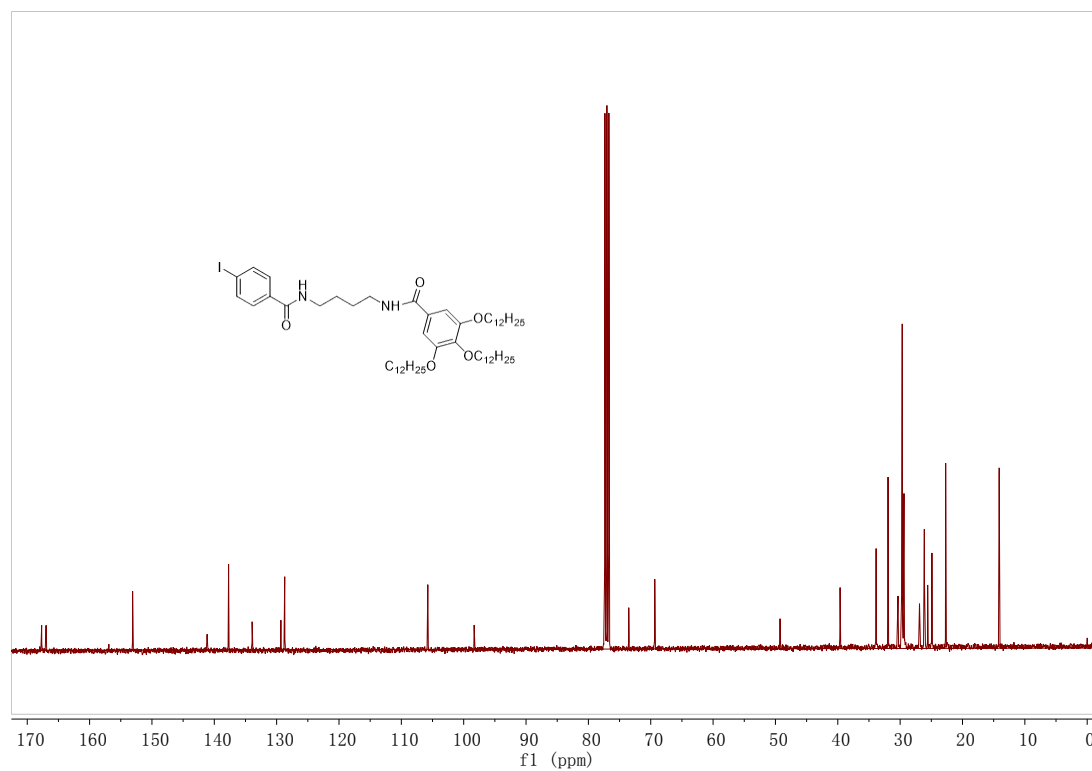


Fig. S2. ¹³C NMR spectrum of 4 at 25 °C in CDCl₃.

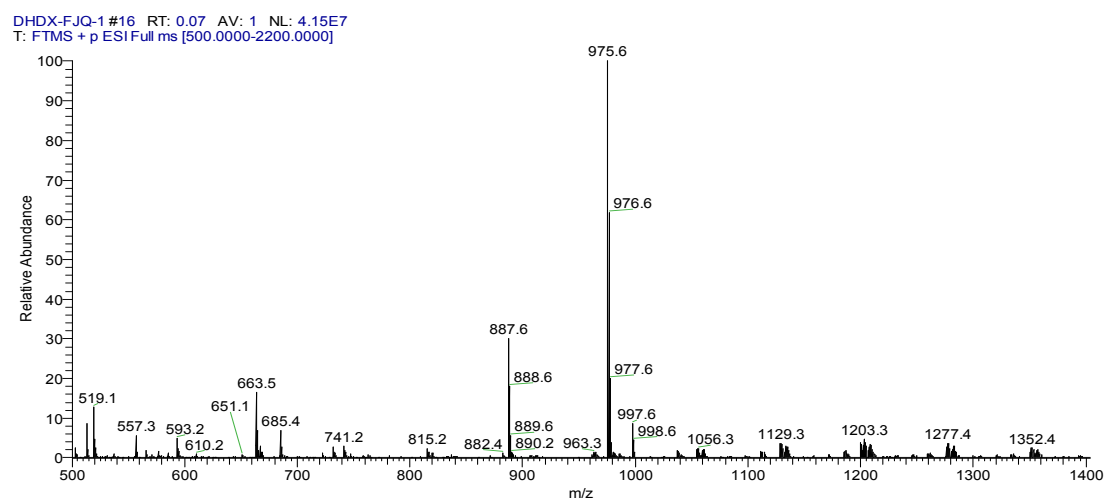


Fig. S3. ESI mass spectrum of 4.

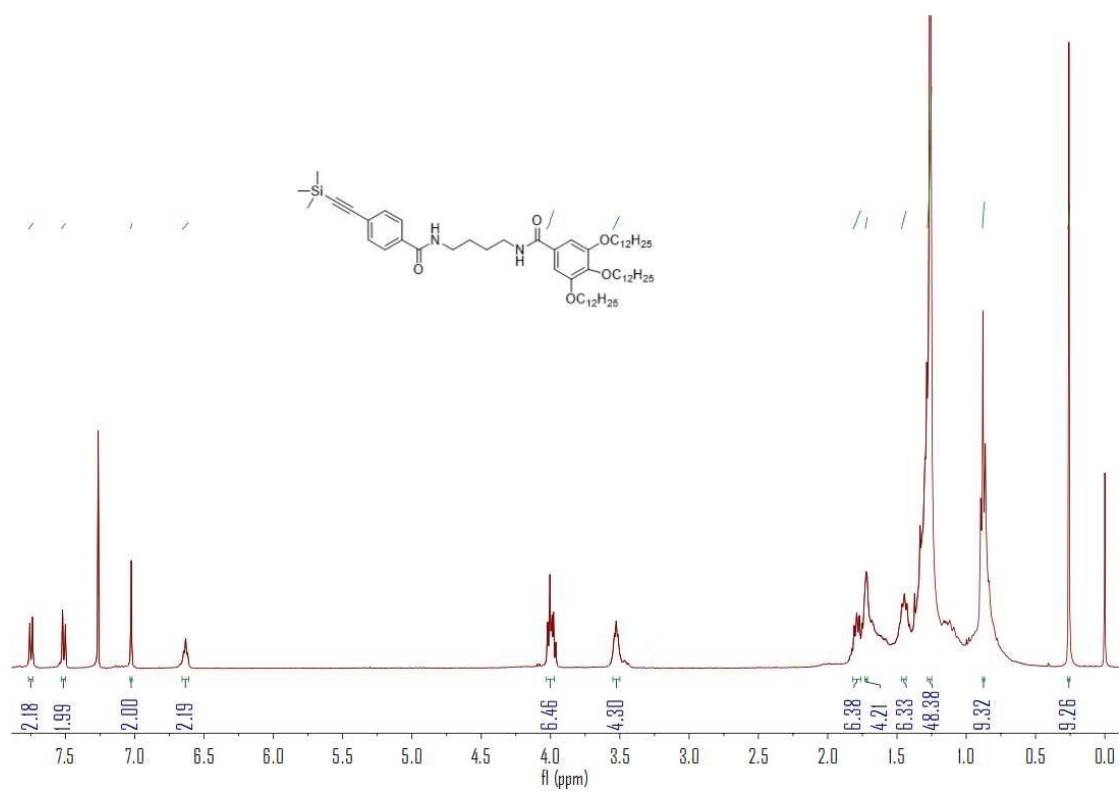


Fig. S4. ¹H NMR spectrum of **5** at 25 °C in CDCl₃.

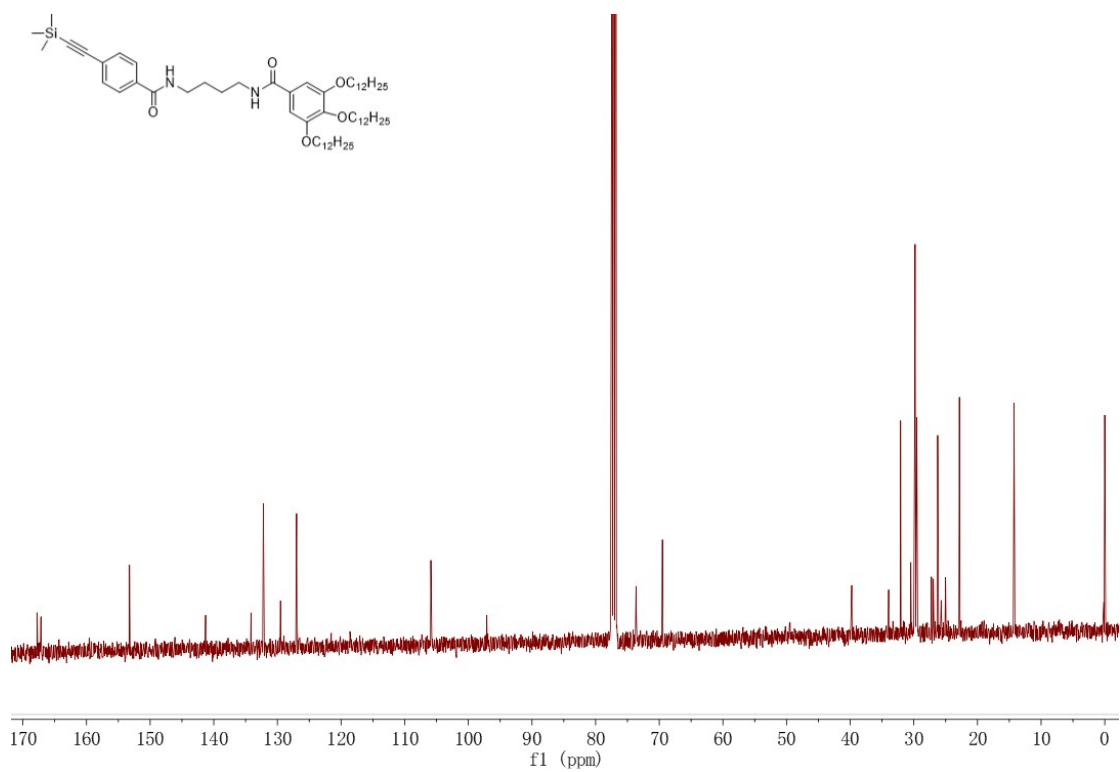


Fig. S5. ¹³C NMR spectrum of **5** at 25 °C in CDCl₃.

DHDX-FJQ-2 #16 RT: 0.07 AV: 1 NL: 1.18E8
T: FTMS + p ESI Full ms [500.0000-2200.0000]

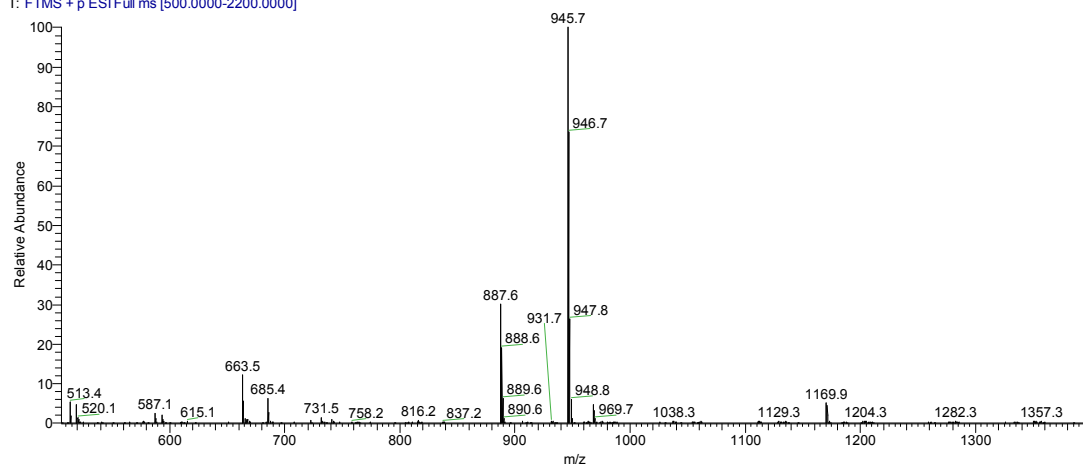


Fig. S6. ESI mass spectrum of **5**.

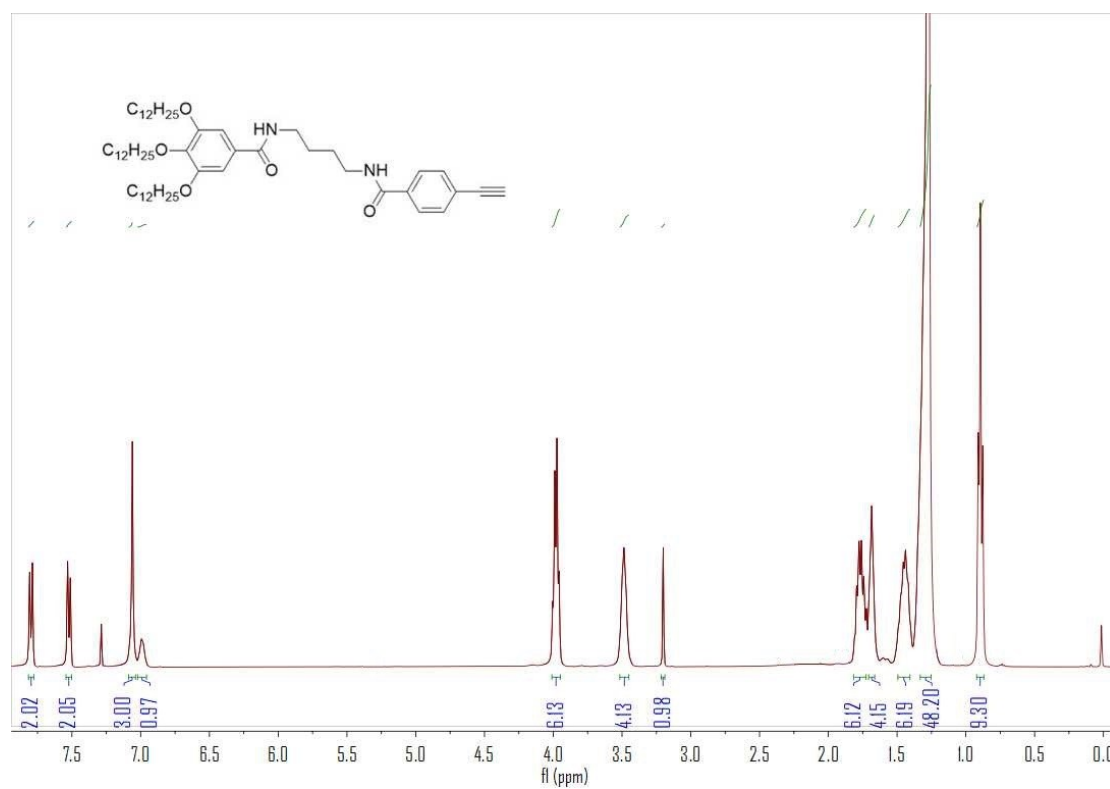


Fig. S7. ¹H NMR spectrum of **6** at 25 °C in CDCl₃.

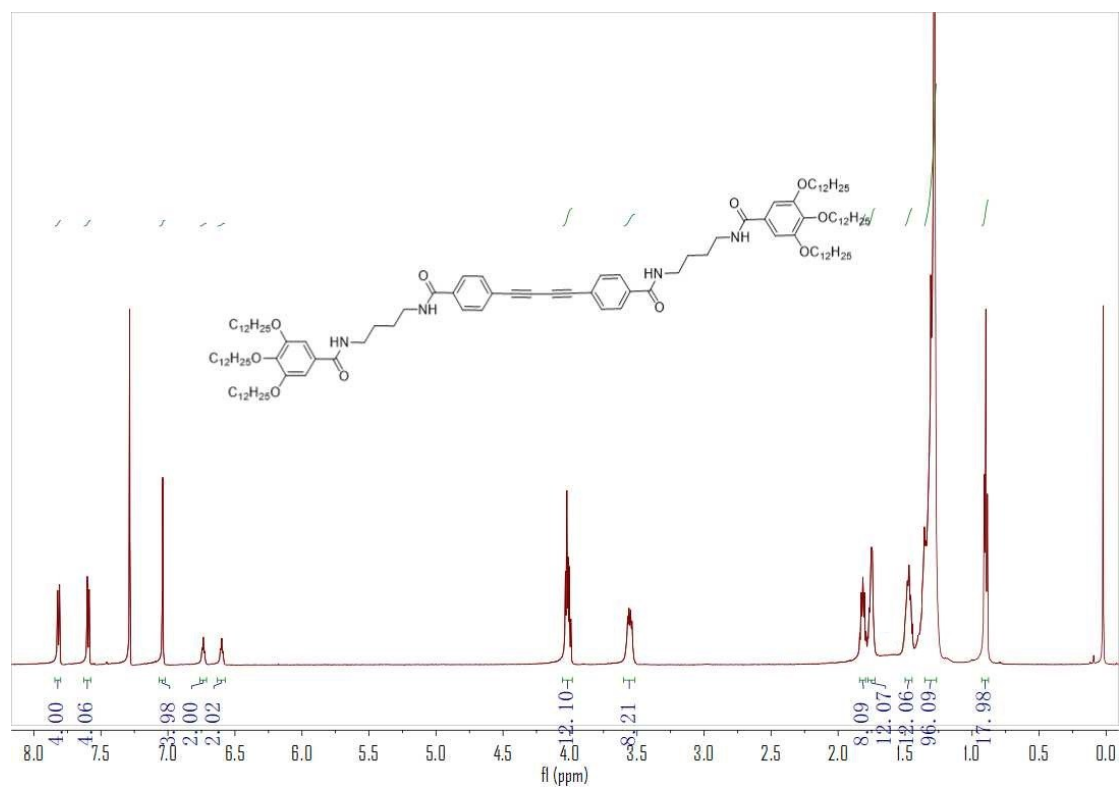


Fig. S8. ¹H NMR spectrum of **1** at 25 °C in CDCl₃.

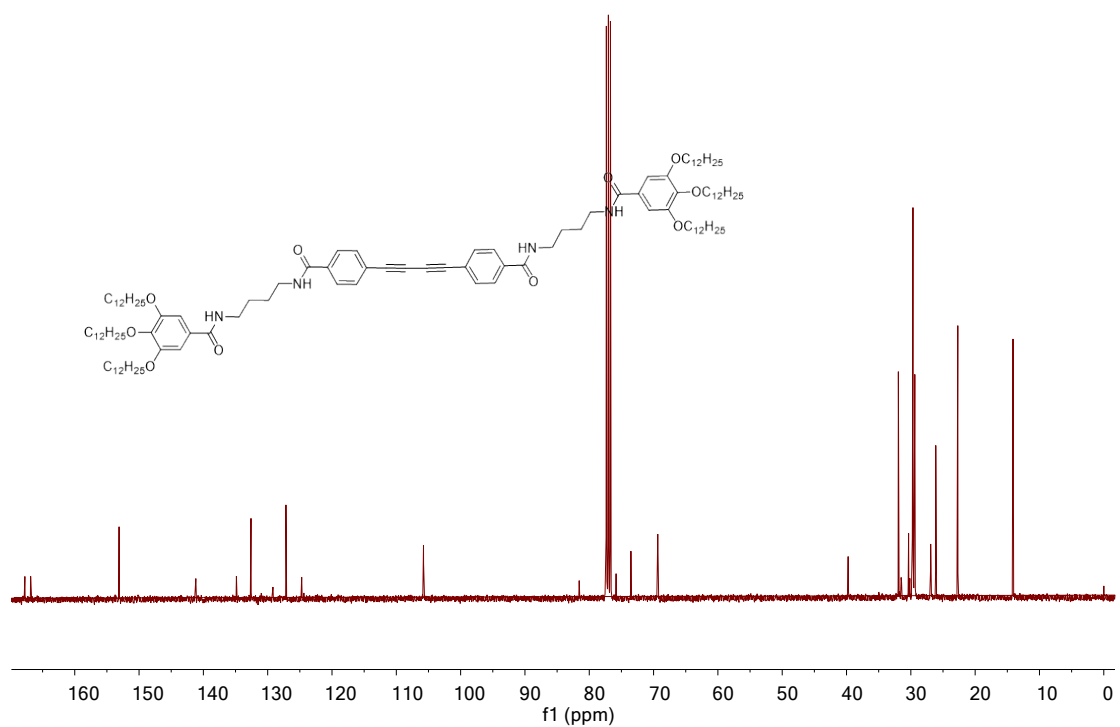


Fig. S9. ¹³C NMR spectrum of **1** at 25 °C in CDCl₃.

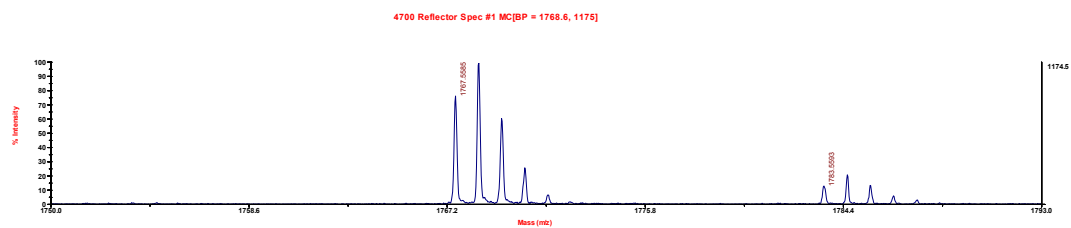


Fig. S10. MALDI-TOF mass spectrum of **1**.

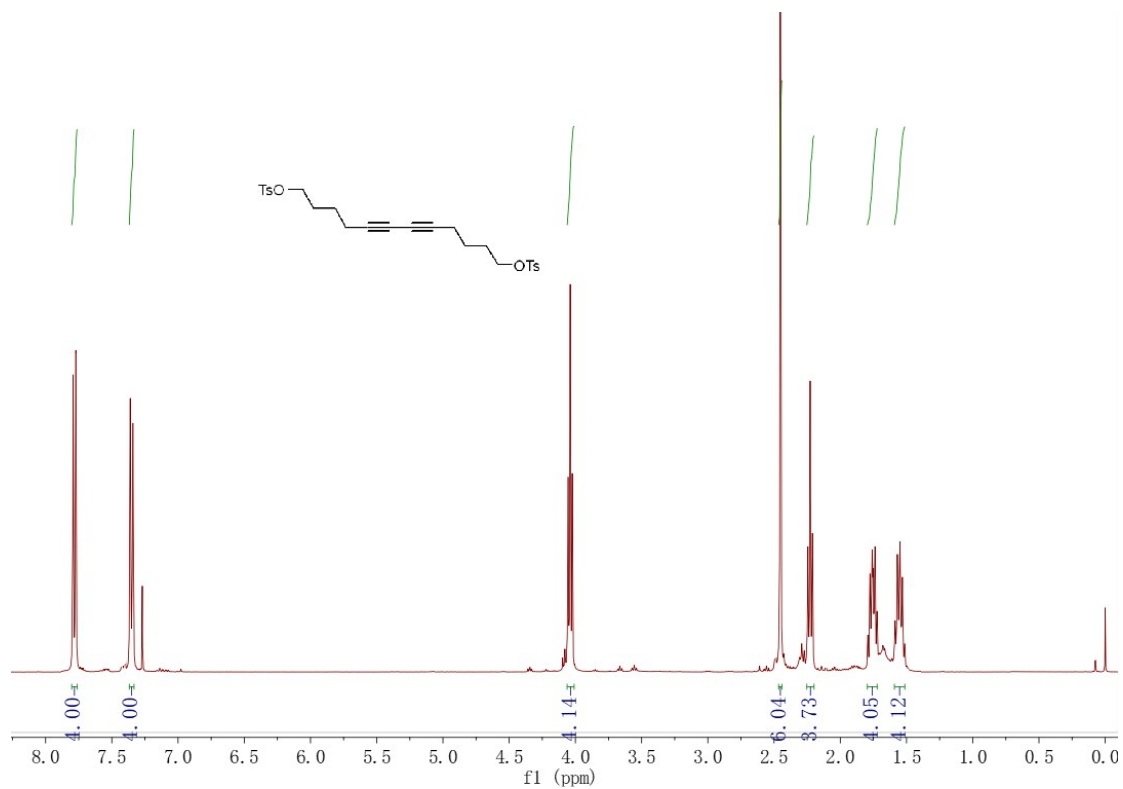


Fig. S11. ^1H NMR spectrum of **8** at 25 °C in CDCl_3 .

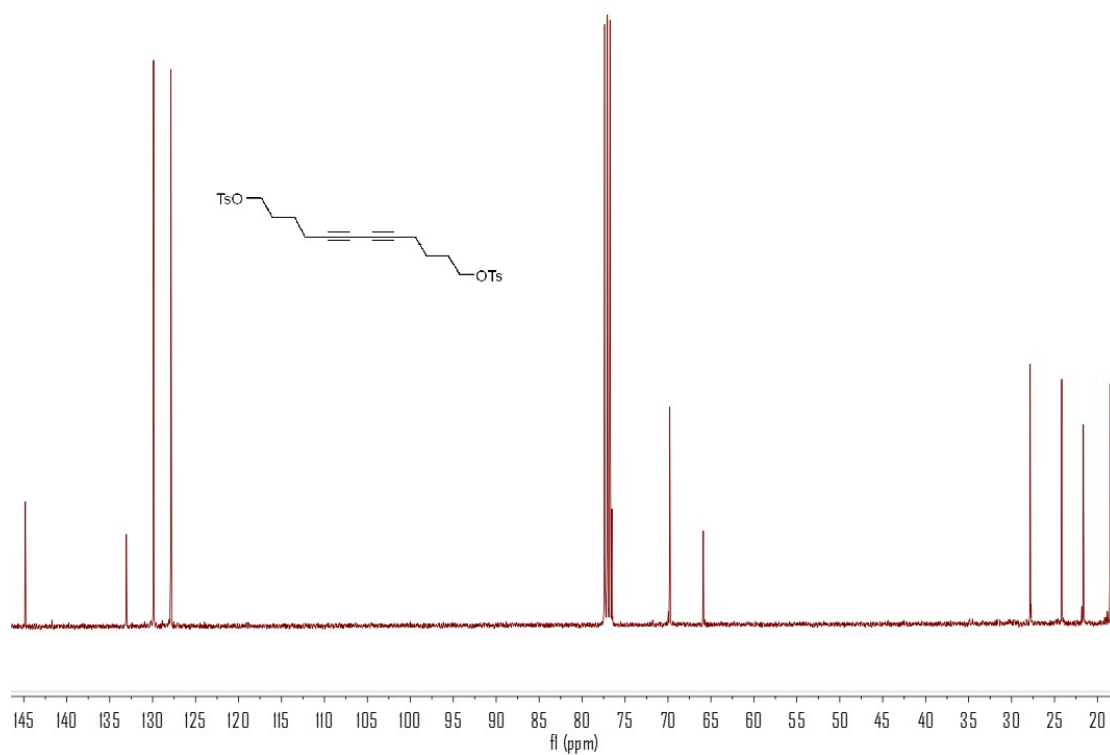


Fig. S12. ¹³C NMR spectrum of **8** at 25 °C in CDCl₃.

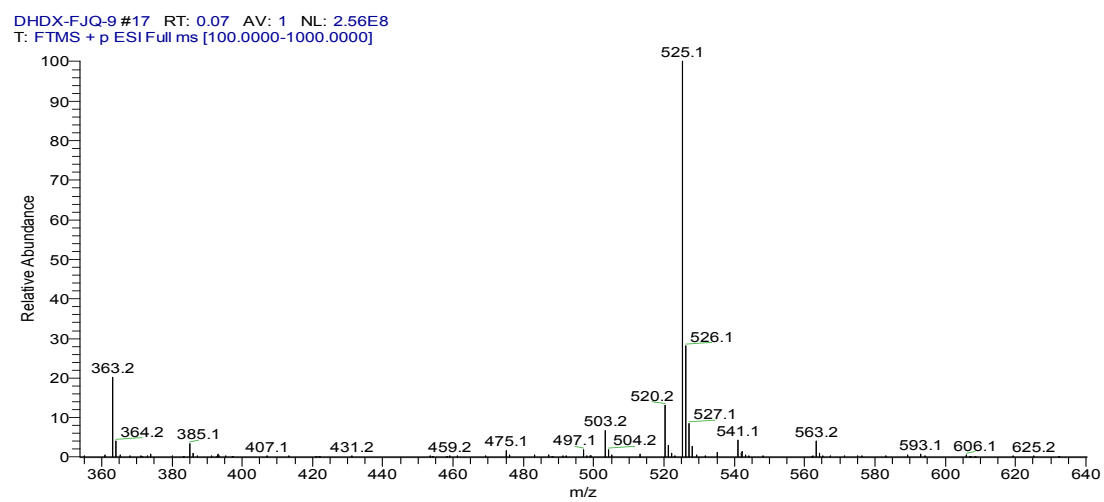


Fig. S13. ESI mass spectrum of **8**.

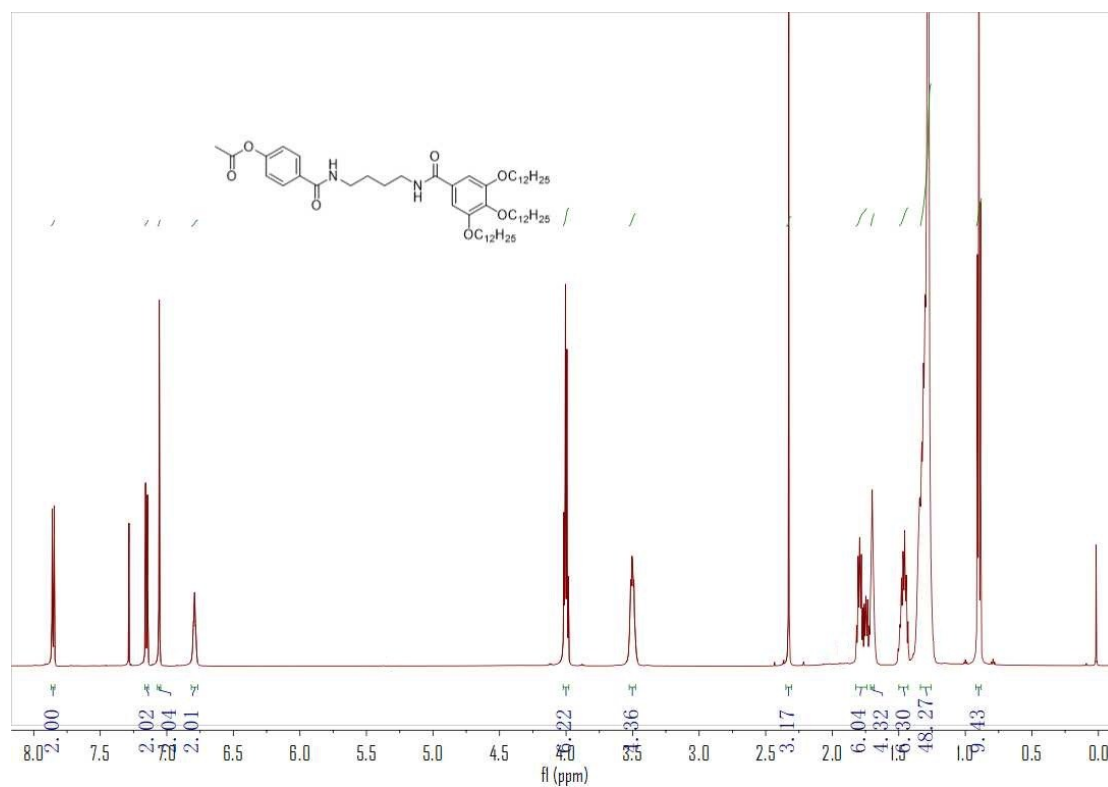


Fig. S14. ¹H NMR spectrum of **9** at 25 °C in CDCl₃.

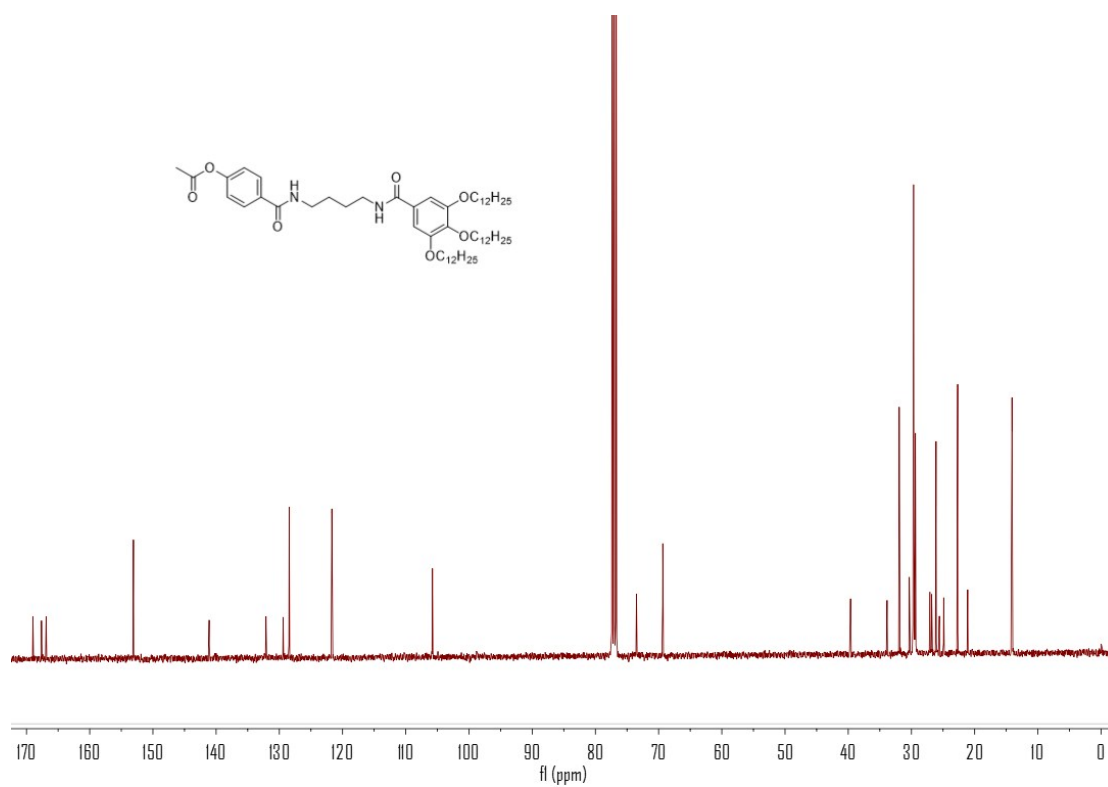


Fig. S15. ¹³C NMR spectrum of **9** at 25 °C in CDCl₃.

DHDX-FJQ-6 #17 RT: 0.07 AV: 1 NL: 4.22E7
T: FTMS + p ESI Full ms [500.0000-2200.0000]

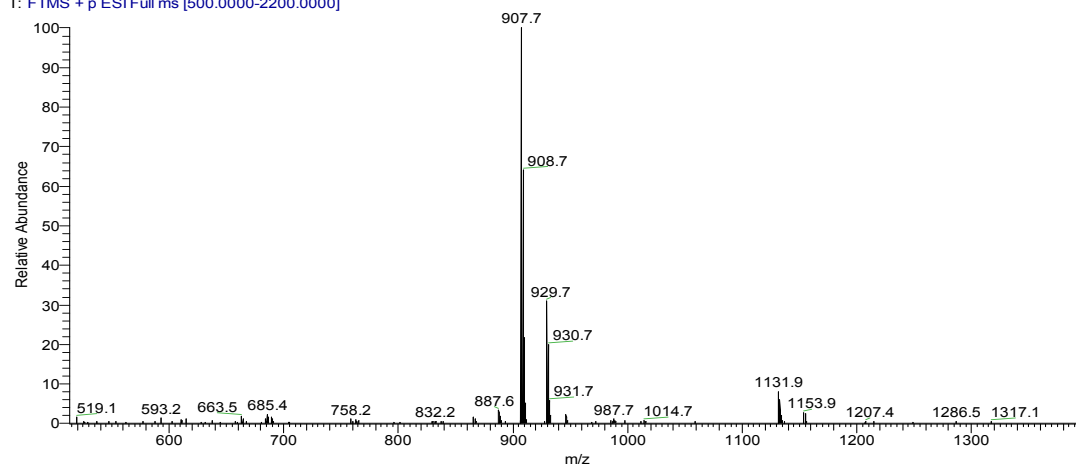


Fig. S16. ESI mass spectrum of **9**.

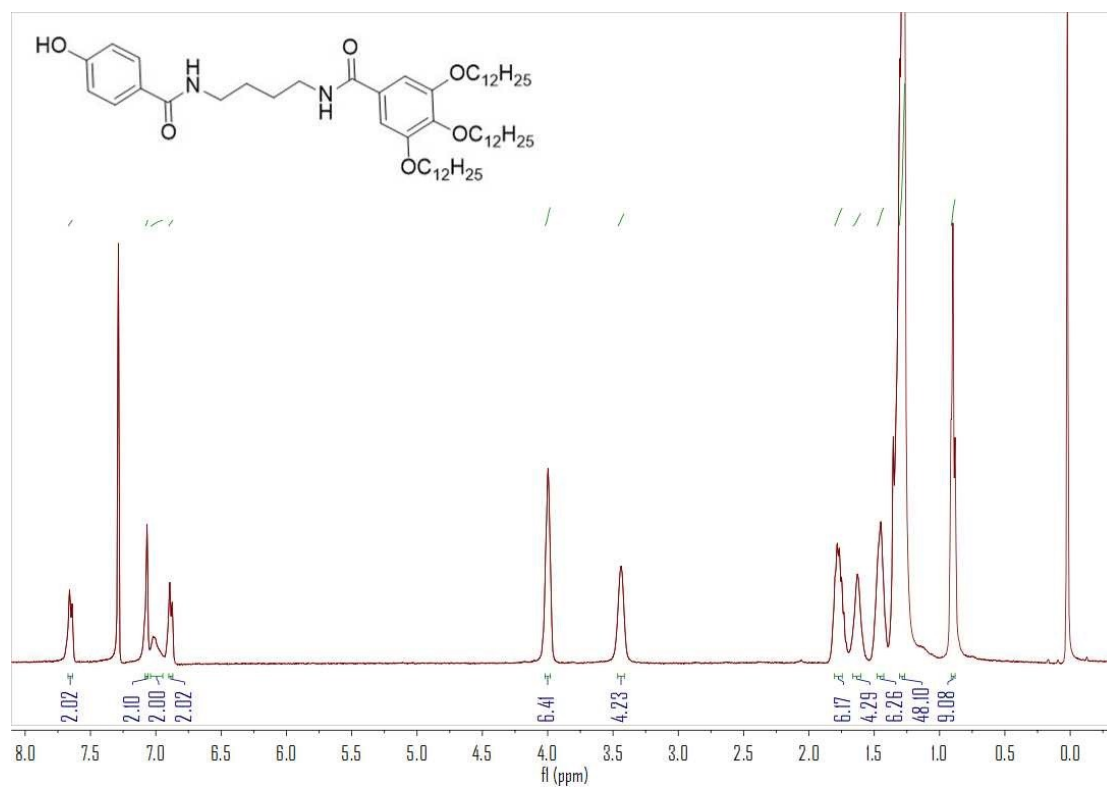


Fig. S17. ¹H NMR spectrum of **10** at 25 °C in CDCl₃.

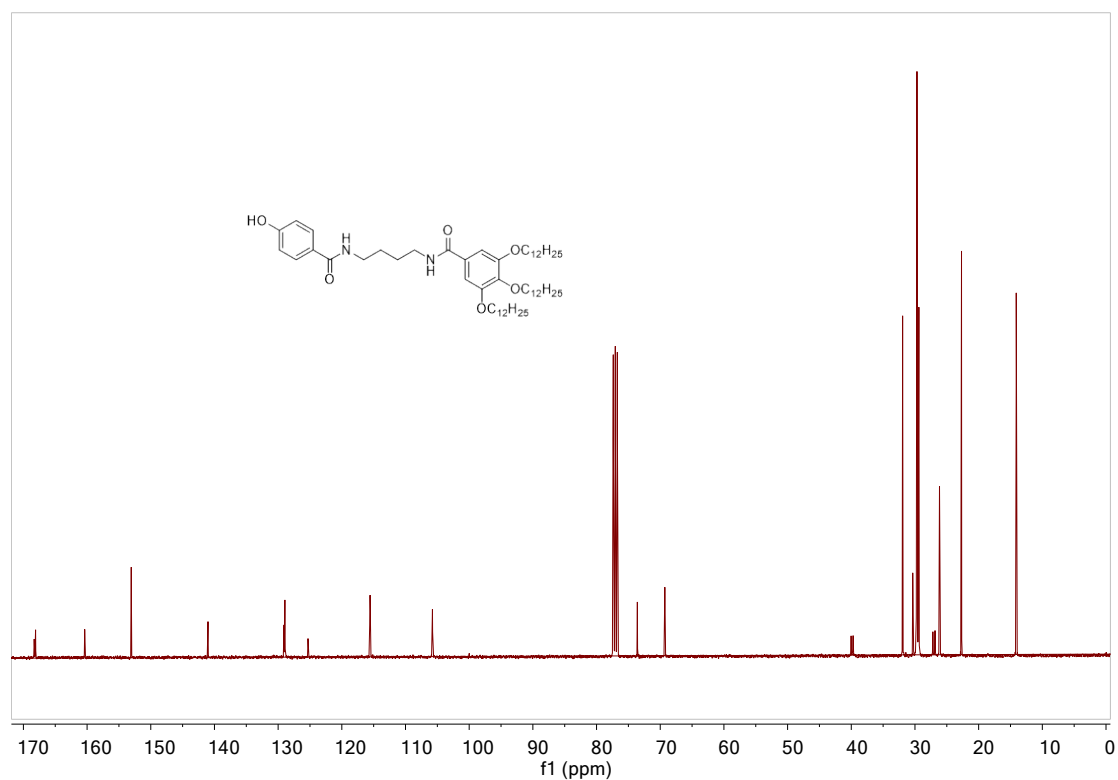


Fig. S18. ¹³C NMR spectrum of **10** at 25 °C in CDCl₃.

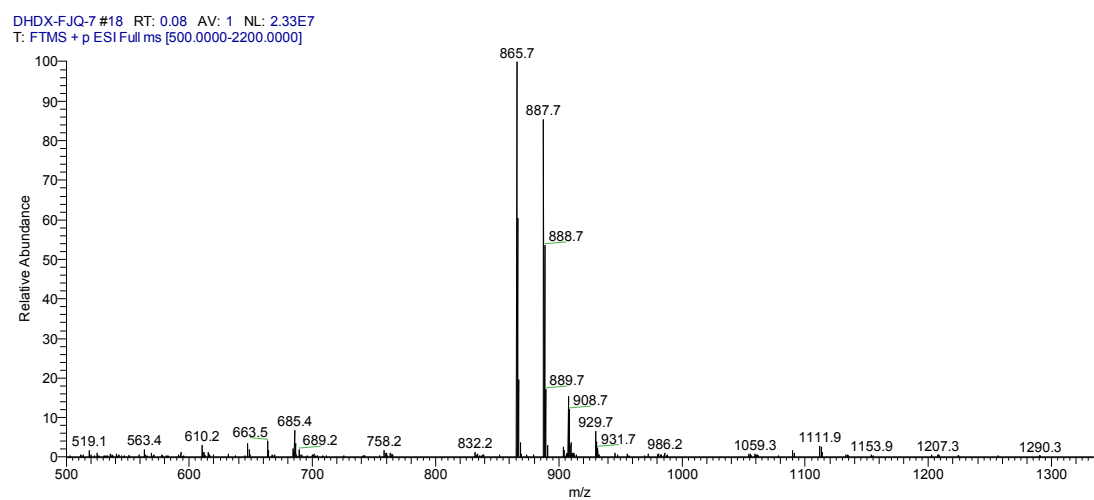


Fig. S19. ESI mass spectrum of **10**.

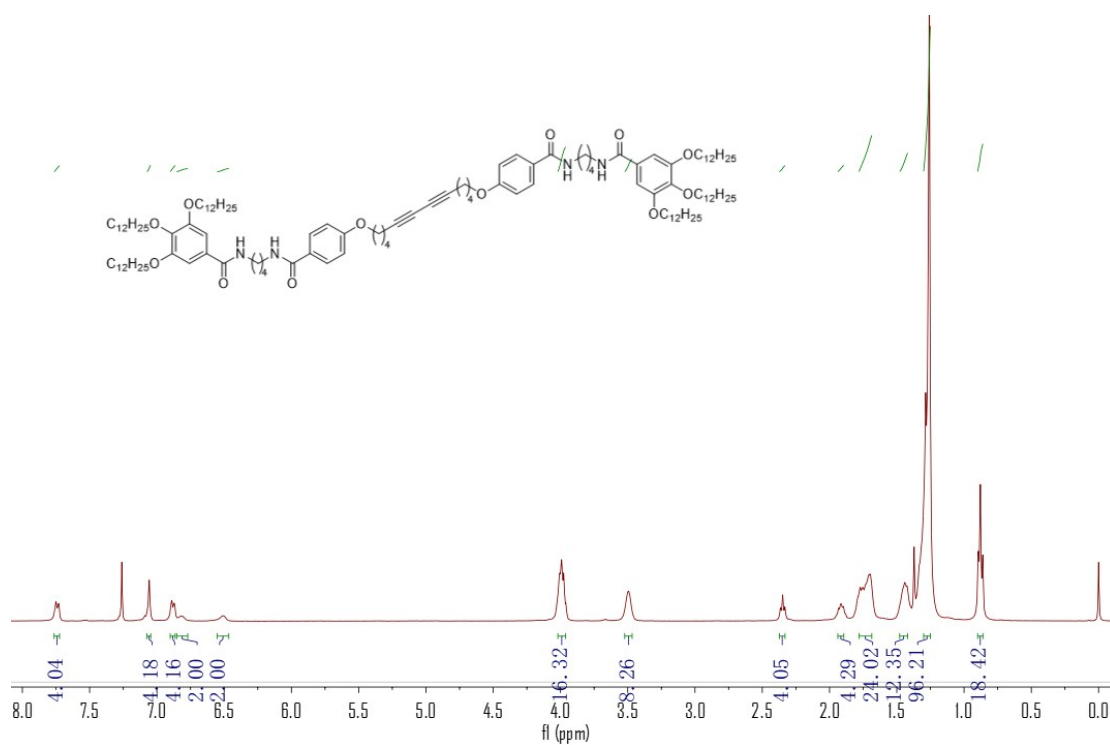


Fig. S20. ^1H NMR spectrum of **2** at 25 °C in CDCl_3 .

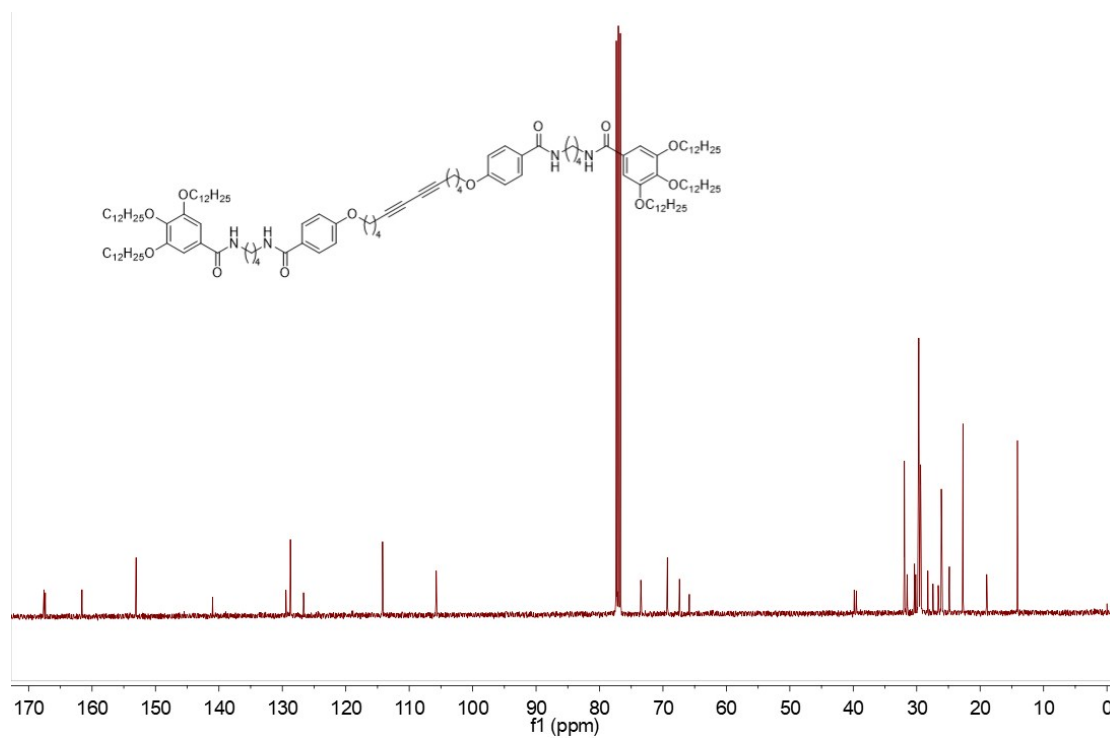


Fig. S21. ^{13}C NMR spectrum of **2** at 25 °C in CDCl_3 .

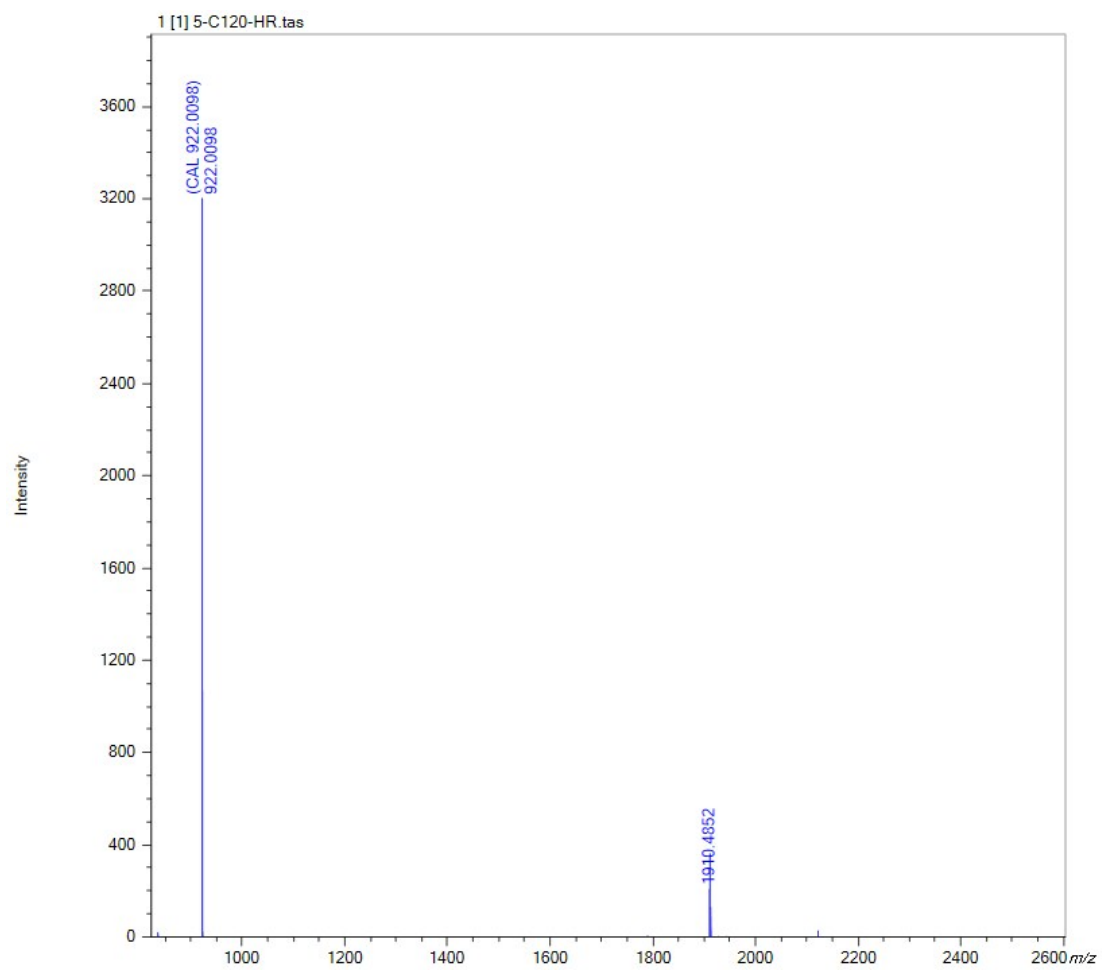


Fig. S22. MALDI-TOF mass spectrum of **2**.

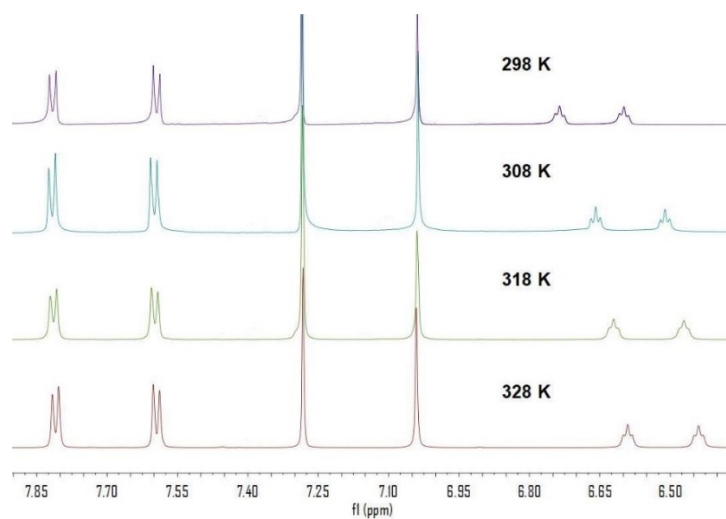


Fig. S23. The variable-temperature ^1H NMR spectra of **1** in CDCl_3 from 298 to 328 K.

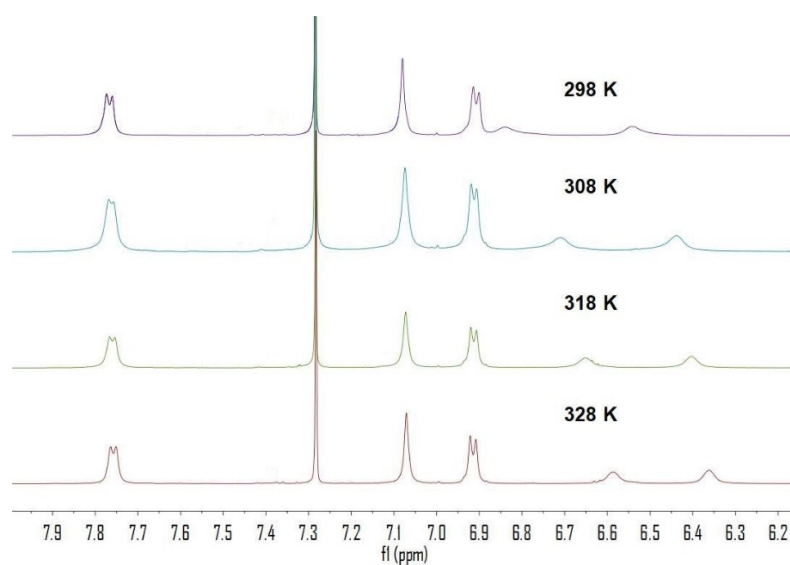


Fig. S24. The variable-temperature ^1H NMR spectra of **2** in CDCl_3 from 298 to 328 K.

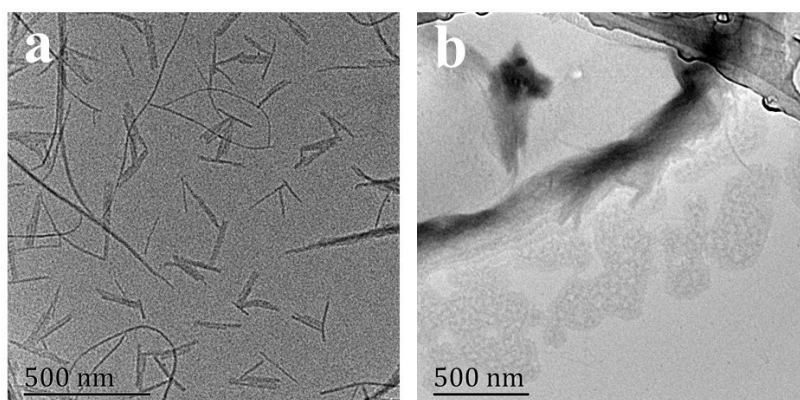


Fig. S25. TEM images of **1** (a) and **2** (b) in CHCl_3 .

Table S1. Hansen solubility parameters of the solvents¹

Solvent	MCH	toluene	CHCl_3	CH_2Cl_2	dioxane	THF
δ_{H}	1.0	2.0	5.7	6.1	7.4	8.0

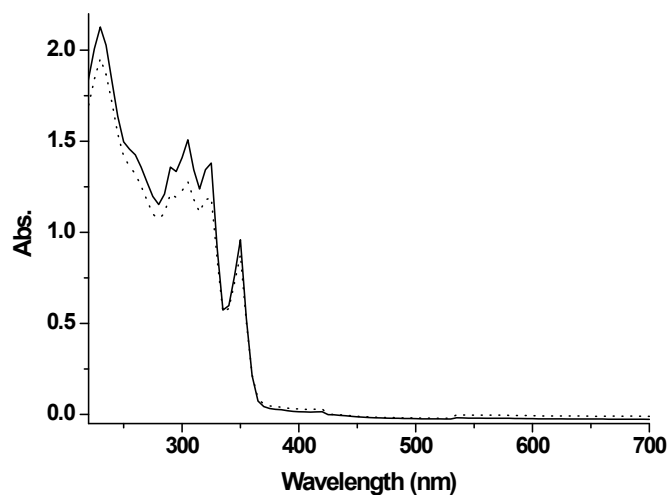


Fig. S26. UV/Vis absorption spectra of **1** (2 mg/mL) in MCH before (dotted line) and after 5 min of irradiation at 254 nm (full line).

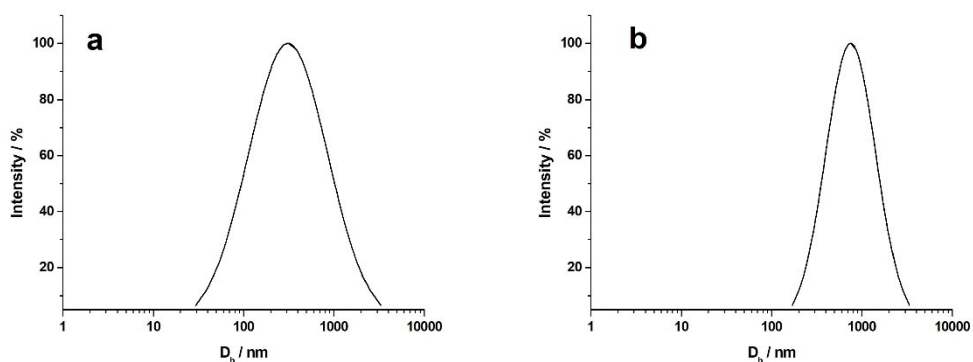


Fig. S27. Size distributions of **2** before (a) and after (b) irradiation at 254 nm ($c = 0.23$ mg/L) in methylcyclohexane.

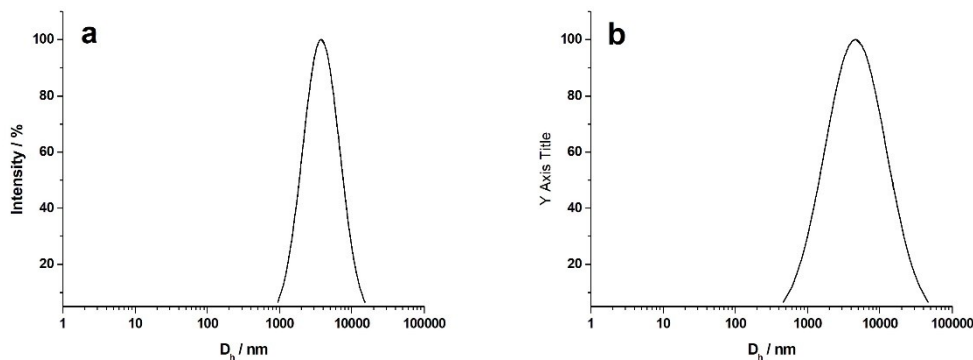


Fig. S28. Size distributions of **1** before (a) and after (b) irradiation at 254 nm ($c = 0.23$ mg/L) in methylcyclohexane.

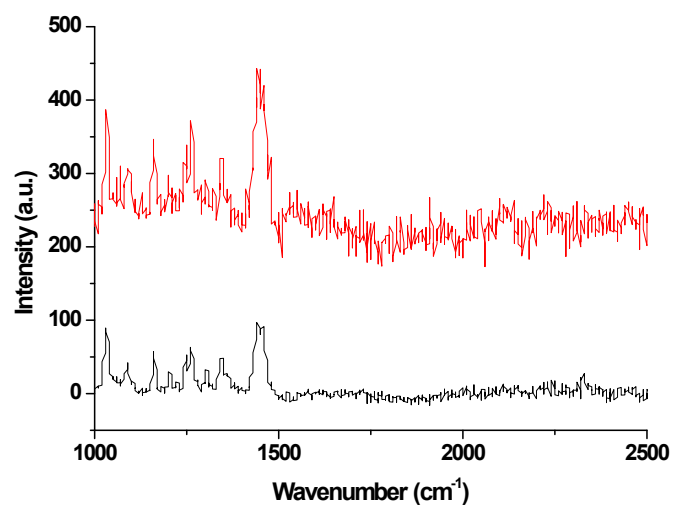


Fig. S29. Raman spectra of **1** before (black) and after irradiation for 2 min (red) at 254 nm.

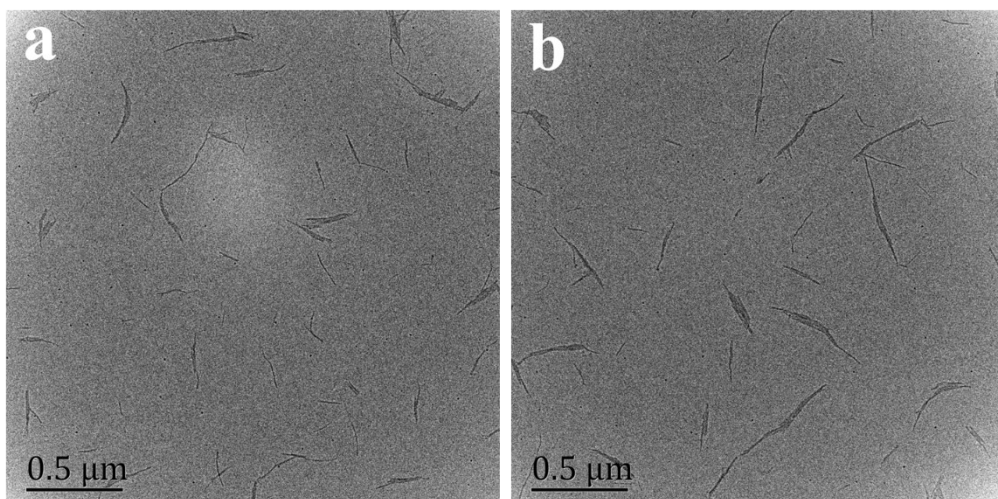


Fig. S30 TEM images of **1**: nonirradiated (a) and irradiated (b). Irradiated samples were exposed (254 nm) for 2 min.

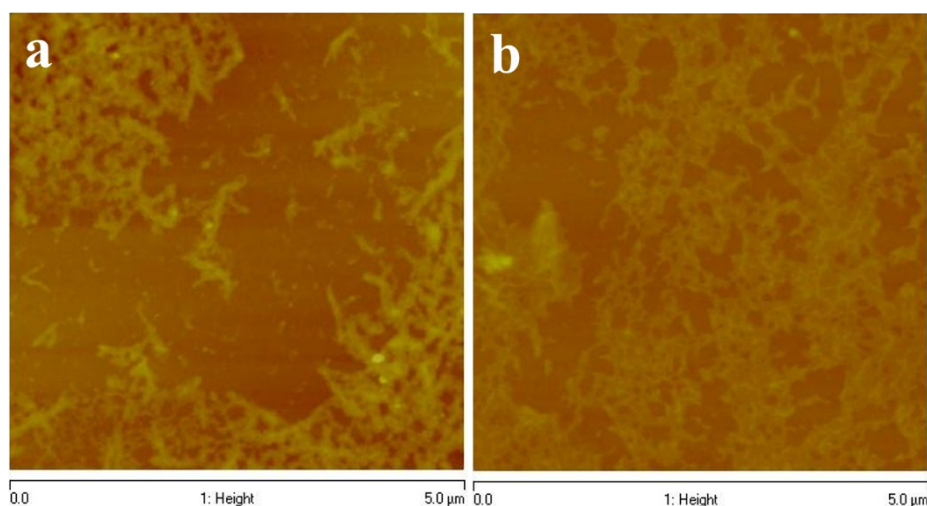


Fig. S31 AFM height profiles of **1** nonirradiated (a) and irradiated (b). Samples were drop-casted and imaged on silicon substrates after 2 min of irradiation.

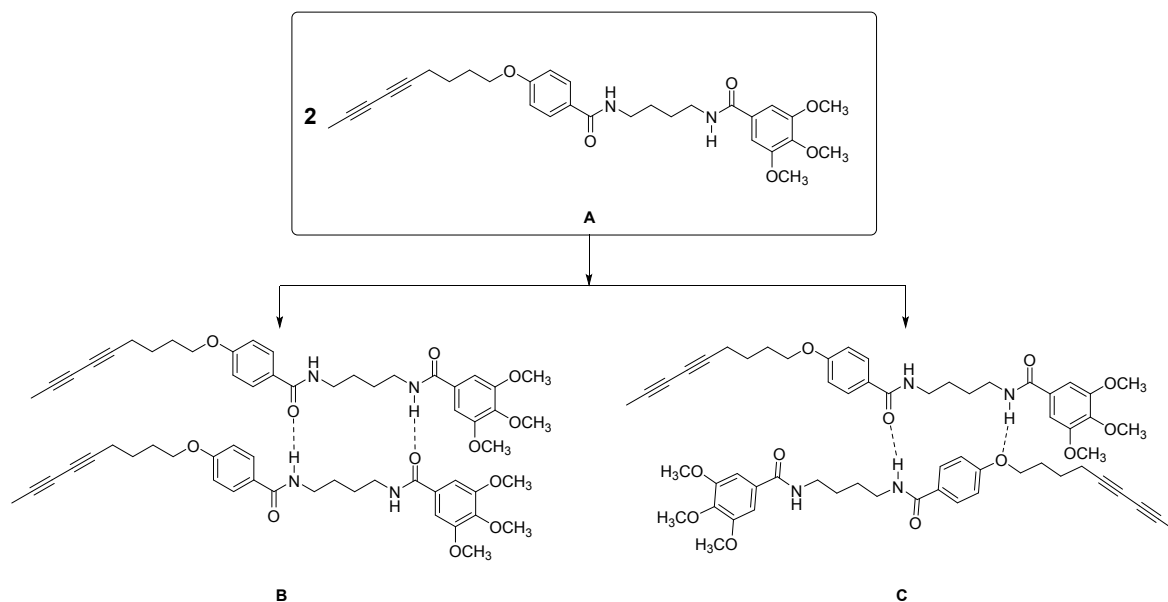


Fig. S32. Possible molecular packing modes.

In order to understand the interaction between diacetylenes, density functional theory (DFT) computations were carried out. All calculations were carried out by using the Gaussian 09 program.² Geometry optimizations were carried out in gas phase at the M06-2X³ level with 6-31G(d,p)⁴ basis set. All optimized structures were characterized as energy minimums without imaginary frequencies by frequency calculations. Zero-point vibrational energies and thermodynamic corrections were

calculated at the level of geometry optimization at 298.15 K under 1 atm. With M06-2X/6-31G(d,p) geometries, the energies were further refined by single-point calculations at the M06-2X/Def2-TZVP⁵ level. For simplicity, one-half of each structure is shown and the dodecyl groups are replaced by -OCH₃ (Fig. S32, **A**). The optimized structures were displayed by the CYLview visualization program.⁶

As shown in Fig. S32, two interaction modes were considered for evaluating the hydrogen bonding interaction between diacetylenes. For the mode **B**, two H-bonds were formed between amide groups. For the mode **C**, one H-bond was formed between amide groups and one H-bond was formed between hydrogen of amide group and oxygen of phenoxyl group.

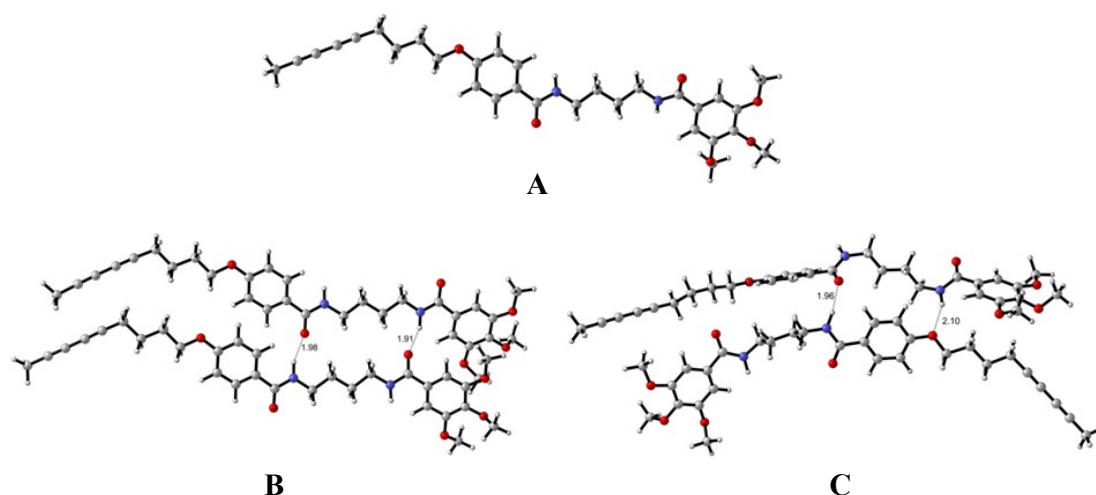


Fig. S33. Optimized structures of **A**, **B** and **C**

The optimized structures of **A**, **B** and **C** were shown in Fig. S33. It was found that the formation Gibbs free energy ΔG of **B** and **C** from two molecular of **A** is -20.9 kJ/mol and -14.1 kJ/mol, respectively. Therefore, the formation of **B** was more favorable than **C** by 6.8 kJ/mol. This was in good agreement with our previous assumption.

Table S2. Cartesian coordinates for all optimized structures and the energetic data

A E = -1724.909632 ZPE = 0.622166
--

Nimag = 0			
Htot = -1724.245856			
Gtot = -1724.371015			
SP(M06-2X/Def2-TZVP) = -1725.544008			
C	-13.17363300	-0.66922200	0.38720600
C	-14.18294700	-0.00139100	0.34832400
C	-15.33661700	0.75360200	0.30582200
C	-16.34841800	1.41670300	0.26932300
C	-17.56788400	2.21628000	0.22590300
C	-11.92865100	-1.43430800	0.42580900
C	-10.69906600	-0.56339100	0.12987400
C	-9.40582300	-1.37140100	0.18670400
C	-8.19194500	-0.50625900	-0.09116000
O	-7.04415900	-1.33141100	0.00679500
C	-5.82890100	-0.75876300	-0.17480700
C	-5.62908800	0.59363200	-0.46484100
C	-4.33269300	1.07173800	-0.62400800
C	-3.23203600	0.23065300	-0.48890400
C	-3.44627800	-1.12625100	-0.21821000
C	-4.72993700	-1.61880200	-0.06158100
C	-1.87366800	0.83642300	-0.66295800
N	-0.82867500	0.12458200	-0.14039200
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C	7.93593100	0.88588300	-0.00397600
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C	10.16308200	-0.79772400	0.20620400
C	8.88713400	-1.34087500	0.09332000
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H	3.07957600	0.90061200	0.77837400
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H	9.00767200	3.23223200	2.02153500
H	10.73049600	2.99437400	1.59554700
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H	12.41561300	0.22598500	-1.30417900
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E = -3449.876847			
ZPE = 1.247932			
Nimag = 0			
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Gtot = -3448.761465			
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C	16.91169600	3.33620800	-1.17834600
C	18.10745700	4.10704500	-1.50266300
C	12.58626200	0.57245700	-0.01293500
C	11.35282700	1.48642700	-0.00652600
C	10.06652600	0.73538700	0.32926200
C	8.87416800	1.67178100	0.29548600
O	7.71235700	0.94212800	0.64923200
C	6.52378200	1.60862600	0.61964100
C	6.38224600	2.94865700	0.24898600
C	5.11194600	3.51414900	0.21594300
C	3.97921400	2.76742200	0.52737100
C	4.13520700	1.43547000	0.92616400
C	5.39726200	0.86470300	0.98324000
C	2.65129000	3.45862500	0.42673600
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O	2.56782200	4.68068800	0.41596200
C	0.24916300	3.26188100	0.20184500

C	-0.83973900	2.21452800	0.38593100
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N	-4.64424900	2.26970000	0.39017200
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C	-8.63915400	3.78737300	-0.13286000
C	-9.67329600	3.00797800	0.38951100
C	-9.39496200	1.73273100	0.92010700
C	-8.09278500	1.25219000	0.93437400
H	1.65087700	1.66905200	0.13998800
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C	-9.96235500	5.32157300	-1.41688100
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O	-10.96536800	3.46029100	0.37494400
C	-11.38793700	3.97975600	1.63171200
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H	12.70714600	0.08754200	0.96356200
H	12.45409300	-0.24124400	-0.73705000
H	11.26110100	1.96321900	-0.98928600
H	11.51310300	2.29262100	0.71830800
H	10.13812600	0.28035600	1.32437400
H	9.90206400	-0.07746300	-0.38862300
H	8.75792100	2.09858400	-0.71103000
H	9.02011000	2.50515600	0.99805400
H	7.24076800	3.55329600	-0.01528100
H	4.97363000	4.55423500	-0.06069900
H	3.27038200	0.83358900	1.19512900
H	5.53455800	-0.16433500	1.29710600
H	0.15691300	4.05950900	0.94660700
H	0.15195200	3.74460100	-0.78147300
H	-0.71092500	1.42266400	-0.36164100
H	-0.70805900	1.73503900	1.36446700
H	-2.37405900	3.57871800	1.05358000
H	-2.37453900	3.29810800	-0.68921800
H	-3.20188200	0.96973800	-0.33655300
H	-3.15260500	1.19995900	1.40665000
H	-4.79050800	3.24594800	0.60068800
H	-6.56146200	3.90130000	-0.59652900

H	-7.84903400	0.27016800	1.31964800
H	-9.67863800	6.15185100	-2.06560300
H	-10.23635400	4.45609800	-2.02680700
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H	-11.20062100	-0.50440500	2.42481600
H	-9.71186500	-0.88208900	1.52654400
H	-9.62269500	0.09721300	3.02354800
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H	-10.77991400	4.84792600	1.91210400
H	-11.32052400	3.21177600	2.40788800
C	12.48550800	-3.41006000	0.29217500
C	13.51266000	-2.76907500	0.25661200
C	14.66939000	-2.01959700	0.21607100
C	15.66806600	-1.33565800	0.17845800
C	16.85821800	-0.49521600	0.13005800
C	11.21554300	-4.13150200	0.33115600
C	10.02602400	-3.22855000	-0.02666000
C	8.70096800	-3.97348700	0.09181200
C	7.51761200	-3.10936800	-0.30048500
O	6.34799300	-3.87503300	-0.04759700
C	5.14545700	-3.26433600	-0.14938800
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C	2.79046900	-3.41860100	0.34497500
C	4.05399200	-3.97975100	0.36161600
C	1.26348100	-1.45321500	-0.17075100
N	0.16704500	-2.24829700	-0.15753600
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C	-4.72337700	-3.19174700	0.21733800
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C	-7.13124200	-3.38071800	0.00176600
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C	-10.95643900	-1.60824000	-0.83862600
C	-10.84112800	-2.85525000	-0.18586400
C	-9.59738600	-3.40226600	0.09104700
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C	-12.83407400	-1.74236700	-2.21603900
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H	10.16366300	-2.84573400	-1.04526400
H	10.02834900	-2.35864700	0.64022600
H	8.55204400	-4.31030800	1.12405300
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H	7.57005100	-2.83487700	-1.36370700
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H	3.51845400	-0.44610700	-1.10636000
H	1.96497300	-3.96067200	0.79791600
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H	-1.22794500	-0.91007700	0.59255600
H	-1.34396400	-1.17051600	-1.14491400
H	-2.11631700	-3.54257800	-0.71586700
H	-2.06582300	-3.22061100	1.01881900
H	-3.73275300	-1.34142100	0.68003700
H	-3.79032900	-1.71656800	-1.02982400
H	-4.62690500	-4.04540000	-0.46328800
H	-4.63729600	-3.59737000	1.23531800
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H	-11.63427400	0.73694600	-2.63545700
H	-11.38083300	1.24597300	-0.94088000
H	-13.00335100	-5.01486600	0.90542000
H	-11.46353500	-5.44730200	0.10931100
H	-11.45011900	-4.65188800	1.70666300
H	-13.81643200	-1.27921600	-2.32029900
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H	-12.25004600	-1.57221400	-3.12954700
C			
E = -3449.878715			
ZP E= 1.248778			
Nimag = 0			

Htot = -3448.548316

Gtot = -3448.760535

SP(M06-2X/Def2-TZVP) = -3451.134355

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C	-14.39015200	7.72451600	-0.18039000
C	-10.24648800	2.45442700	0.29513000
C	-8.77559300	2.89218900	0.19644700
C	-7.85015300	1.69520400	0.38624300
C	-6.38001500	2.04501300	0.28059300
O	-5.64414300	0.85834900	0.57038300
C	-4.28132500	0.93682300	0.61160400
C	-3.61602500	-0.20812700	1.06281000
C	-2.22959600	-0.23970700	1.11557600
C	-1.48609700	0.88259600	0.72812400
C	-2.16268000	2.02134900	0.29664900
C	-3.55134500	2.06202700	0.22852400
C	0.01321600	0.98288600	0.79593200
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C	2.90762700	0.02227700	-0.09451100
C	4.37117100	0.39759900	0.12423100
C	5.17761400	0.41832700	-1.17883000
N	6.32956300	1.30475700	-1.12294500
C	7.57386500	0.89755500	-0.77387600
O	7.83992900	-0.27249600	-0.51128000
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C	8.47244200	3.19155800	-1.38045300
C	9.47635100	4.15327200	-1.28633300
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C	10.78446600	2.66030400	0.10446700
C	9.78489700	1.69433000	0.00329200
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O	9.35067200	5.32166100	-1.98513700
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O	11.94770000	2.51262700	0.77760300
C	12.23395500	1.22656200	1.29843300
O	11.58476800	4.86645800	-0.42401500
C	12.68064000	4.65905900	-1.30959800
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C	13.26004200	-1.89092300	2.06849300
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C	7.94823600	-3.14992500	-1.05409500
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H	-13.71503900	-1.47288200	0.30661500

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