Supporting Information

Trace mild acid-catalysed *Z* →*E* isomerization of norbornene-fused stilbene derivatives: intelligent chiral molecular photoswitches with controllable self-recovery

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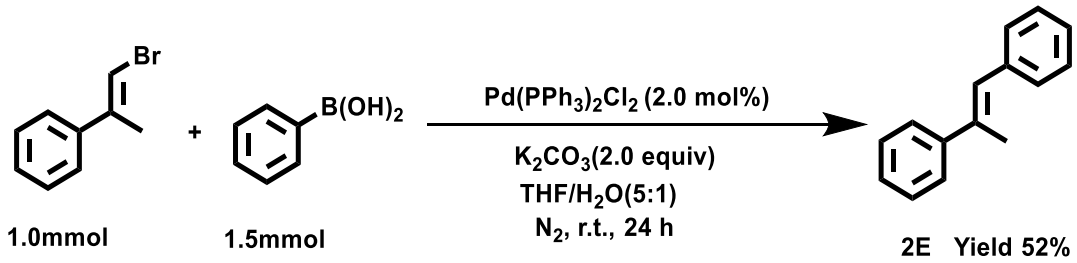
1. General Methods

All solvents, reagents, and deuterated solvents were purchased from Aldrich, Adamas, or TCI. Column chromatography was performed with silica gel (Merck, 300−400 mesh). ^{1}HNMR spectra were recorded on Bruker Avance 400 or 600 MHz spectrometers. Chemical shifts were reported in ppm with 7.26 ppm of $CDCl_3$ (2.50 ppm of DMSO-d6) as reference. The following abbreviations are used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet. Coupling constants, *J*, are reported in hertz unit (Hz). ^{13}C NMR spectra were recorded on Bruker Avance 100 or 150 MHz spectrometers and were fully decoupled by broad band proton decoupling. Chemical shifts are reported in ppm with the signal of $CDCl_3$ at 77.16 ppm (or of DMSO-d_6 at 39.52 ppm) as the reference. HRMS was recorded on a in a Waters–Q–TOF Premiers apparatus (ESI Source). Melting points were obtained on a XT4A micro melting point measurement instrument. UV-vis. spectra were recorded in a JASCO V650 spectrometer. Circular dichroism spectra were measured on a JASCO J-1500 spectrometer. Fluorescence spectra were taken on a Fluoromax-4 spectrofluorometer or a JASCO FP-8500 spectrofluorometer.

2. Synthesis and Characterization

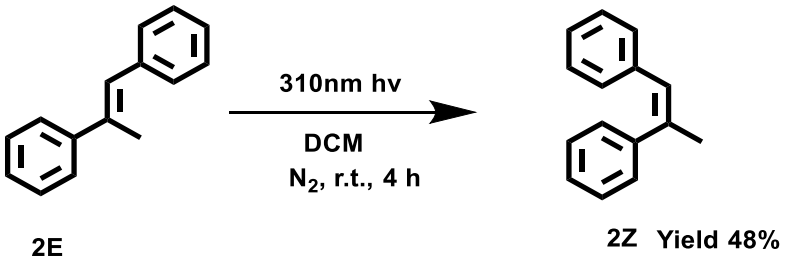
Scheme S1. Synthesis of **2E**



Adapted from a previously reported procedure[1] with some modification: styryl bromide (1.0 mmol), phenylboronic acid (1.5 mmol), $Pd(PPh_3)_2Cl_2$ (2.0 mol%, 14.0 mg), K_2CO_3(2.0 mmol, 276 mg) was added in a dried 25 mL Schlenk tube equipped with a magnetic stirring bar under N_2 atmosphere, H_2O (0.4 mL) and distilled THF (2.0 mL) were then added by syringe. The resulting solution was stirred at r.t. for 24 h. The mixture was then diluted by 10 mL DCM and was filtered through silica gel. The solvent was removed in vacuo to afford the crude product. The crude product was finally purified by chromatography using petroleum ether/DCM (10:1) as the eluent to afford the desired product **2E** in 52% yield.

(*E*)-prop-1-ene-1,2-diyldibenzene (2E).[2] White solid (yield: 100.5 mg, 52%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.2 Hz, 2H), 7.42 – 7.37 (m, 6H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.28 – 7.23 (m, 1H), 6.86 (d, *J* = 1.1 Hz, 1H), 2.30 (d, *J* = 1.3 Hz, 3H).

Scheme S2. Synthesis of **2Z**

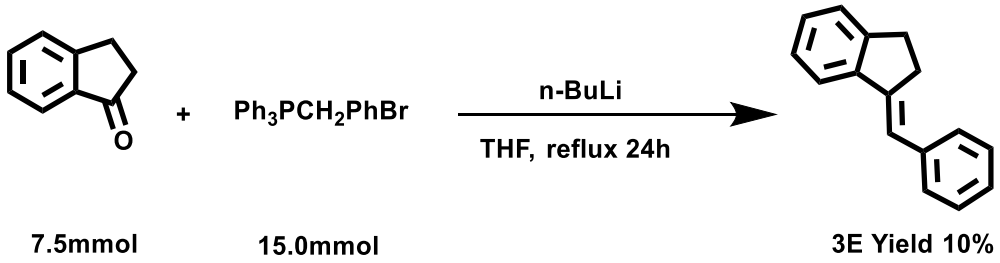


20 mg **2E** in 10 ml DCM was irradiated with 310 nm UV light for 4 h, then the solvent was removed in vacuo to afford the mixture of **2E**/**2Z**, then **2E** and **2Z** was isolated by HPLC with n-hexane as the eluent, to afford the desired product **2Z** in 48% yield.

(*Z*)-prop-1-ene-1,2-diyldibenzene (2Z).[2] Colorless oil (yield: 9.5 mg, 48%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.17 (m, 2H),

7.13 – 7.04 (m, 3H), 6.94 (d, *J* = 7.3 Hz, 2H), 6.48 (s, 1H), 2.21 (d, *J* = 1.5 Hz, 3H).

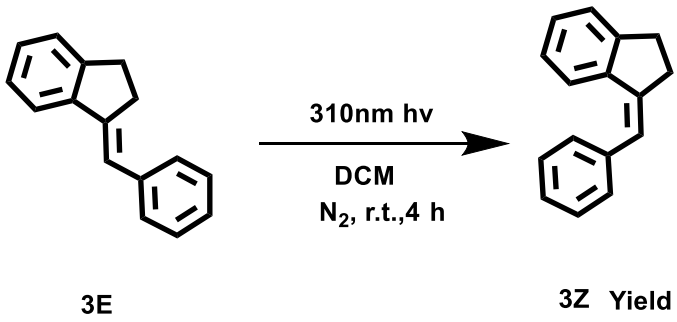
Scheme S3. Synthesis of **3E**



Adapted from a previously reported procedure[3] with some modification: To a suspension of benzyltriphenylphosphonium bromide (15.0 mmol) in THF (40 mL) was dropwise added n-BuLi (6.1 mL, 2.5 M in n-hexanes). After the system was stirred at room temperature for 2 h, indanone (7.5 mmol) in THF (10 mL) was added. The reaction mixture was stirred to reflux for 24 h. Then, the mixture was cooled to room temperature and quenched with water (20 mL). n-Hexane (4 × 30 mL) was added to extract the product. The organic layers were combined, washed with water, dried with Na_2SO_4 and filtered, the filtrate was concentrated under reduced pressure. The residue was purified with silica gel column chromatography (n-hexane) to give the corresponding products.

(*E*)-1-benzylidene-2,3-dihydro-1H-indene (3E).[3] White solid (yield: 154.5 mg, 10%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (m, 1H), 7.50 (d, *J* = 7.5 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.33 – 7.28 (m, 1H), 7.25 – 7.20 (m, 3H), 6.98 (s, 1H), 3.12 (s, 4H).

Scheme S4. Synthesis of **3Z**

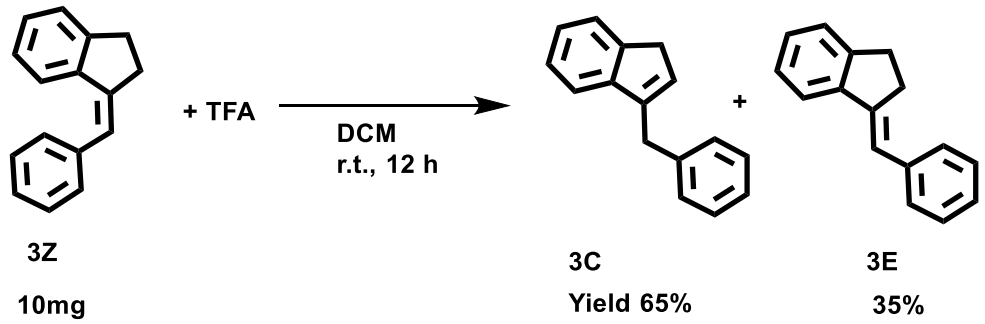


30 mg **3E** in 15 ml DCM was irradiated with 310 nm UV light for 4 h, and the solvent were removed in vacuo, then the mixture of **3E/3Z** was isolated by HPLC with a mixture solvent of n-hexane: DCM (95:5) as the eluent, to afford desired product **3Z** in 52% yield.

(*Z*)-1-benzylidene-2,3-dihydro-1H-indene (3Z).[4] Colorless oil (yield: 15.6 mg, 52%)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.31(m, 4H), 7.30 – 7.27 (m, 1H), 7.25 – 7.23 (m, 1H)7.22 – 7.17 (m,1H), 7.13 (t, *J* = 7.4 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.61 (s, 1H), 3.02 – 2.96 (m, 2H), 2.93 – 2.87 (m, 2H).

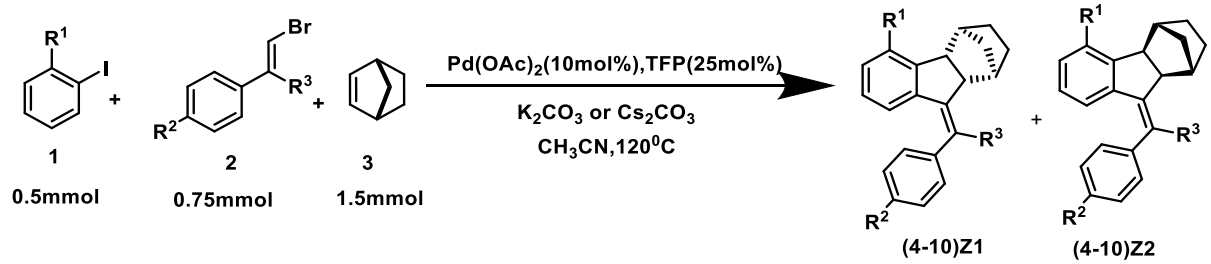
Scheme S5. Synthesis of **3C**



10 mg **3Z** in 2.0 mL DCM was added 5.0 ul TFA (1.5 equiv.), the mixture was stirred for 12 h. Then the solvent was removed in vacuo, and the mixture of **3C**/**3E** was then isolated by HPLC with n-hexane as the eluent, to afford desired product **3C** in 65% yield.

3-benzyl-1H-indene (3C).[5] Colorless oil (yield: 6.5 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.2 Hz, 1H), 7.35 – 7.28 (m, 5H), 7.25 – 7.17 (m, 3H), 6.14 (s, 1H), 3.92 (s, 2H), 3.36 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 144.7, 143.6, 139.5, 130.2, 129.1, 128.5, 126.3, 126.2, 124.7, 123.9, 119.5, 37.9, 34.6.

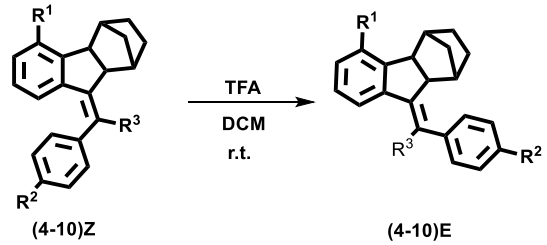
Scheme S6. General Procedure for the Synthesis of **4Z** – **10Z**



A dried 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with **1** (0.5 mmol), **2** (0.75 mmol), **3** (1.5 mmol), $Pd(OAc)_2$ (11.2 mg, 0.05 mmol), TFP (29.5 mg, 0.125 mmol), K_2CO_3 (332.5 mg, 2.5 mmol) or Cs_2CO_3(326 mg 1.0 mmol) , and CH_3CN (3.0 mL). The tube was sealed well, then the solution was stirred at 120 °C for 12 h. The reaction mixture was cooled down to room temperature, washed with DCM,

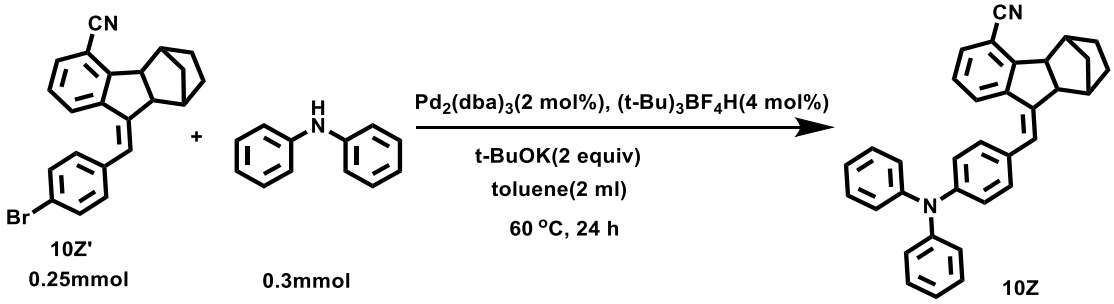
filtered, and then the solvent was evaporated in vacuum. The crude product was finally purified by chromatography using petroleum ether/ethyl acetate (50:1) as the eluent to afford the desired products.

Scheme S7. General Procedure for the Synthesis of **4E – 10E**



0.2 mmol **(4-10) Z** in 1.0 ml DCM was added 0.5 equiv TFA, the solution was stirred at room temperature until the isomerization reaction was finished which was monitored by TLC (silica gel, PE:DCM = 5:1). Then the solvent was evaporated in vacuum to afford the desired *E* isomer without further purified process.

Scheme S8. Synthesis of **10Z**



A dried 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with **10Z'** (0.25 mmol), diphenylamine (0.3 mmol), $Pd_2(dba)_3$ (5.2 mg, 0.005 mmol), (t-Bu)$_3BF_4H$(3.0 mg, 0.01 mmol), t-BuOK (56.5 mg, 0.5 mmol) and toluene (2.0 mL) under N_2 , then the solution was stirred at 60 °C for 24 h. The reaction mixture was cooled down to room temperature, washed with DCM (10 mL), filtered, and then the solvent was evaporated in vacuum. The crude product was finally purified by chromatography using petroleum ether/ethyl acetate (20:1) as the eluent to afford the desired products.

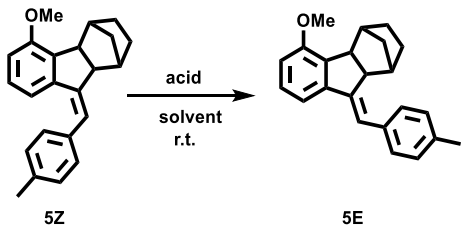
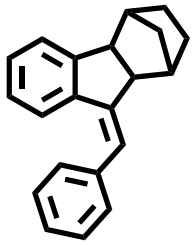


Table S1. Optimization of the acid-catalyzed isomerization of **5Z** [a]

Entry	acids	solvents	time	the ratio of *E*:*Z* [b]
1	TFA	DCM	2h	>99%
2	HCl(aq)	DCM	3.5h	>99%
3	HBr(aq)	DCM	3.5h	>99%
4	H_2SO_4(98%aq)	DCM	3.5h	>99%
5	H_3PO_4	DCM	24h	NR[c]
6	HCOOH	DCM	24h	NR
7	CH_3COOH	DCM	24h	NR
8	$H_2C_2O_4$	DCM	24h	NR
9	Ph-COOH	DCM	24h	NR
10	$F_2CHCOOH$	DCM	80h	>99%
11	$Cl_2CHCOOH$	DCM	126h	>99%
10	TFA	CCl_4	6h	>99%
11	TFA	$CHCl_3$	2h	>99%
12	TFA	n-hexane	8h	>99%
13	TFA	toluene	8h	>99%
14	TFA	Et_2O	72h	NR
15	TFA	THF	72h	NR
16	TFA	dioxane	72h	NR
17	TFA	EA	72h	NR
18	TFA	CH_3CN	56h	>99%
19	TFA	MeOH	72h	NR
20	TFA	EtOH	72h	NR
21	TFA	DMSO	72h	NR
22	TFA	DMF	72h	NR
23	TFA	DMA	72h	NR
24[d]	TFA	DCM	32h	>99%

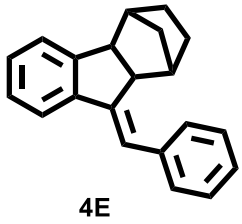
[a] Rection conditions: 0.2 mmol **5Z** in 1.0 mL different solvent, with 0.5 equiv different kinds of acid; [b] the ratio of *E*:*Z* was determined by HPLC using a mixed solvent system of n-hexane and DCM ($V_{n\text{-hexane}}$: V_{DCM} = 80:20); [c] no isomerization reaction occurred. [d] 5 mmol **5Z** with 0.01 equiv TFA.

(*Z*)-9-benzylidene-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene(4Z).[6] Yellow



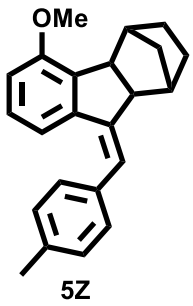
oil (yield: 85.5 mg, 62%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.14 (m, 5H), 7.11 (d, *J* = 7.5 Hz, 1H), 7.07 – 7.00 (m, 2H), 6.77 (t, *J* = 7.5 Hz, 1H), 6.50 (d, *J* = 1.8 Hz, 1H), 2.95 (d, *J* = 7.1 Hz, 1H), 2.81 (d, *J* = 7.1 Hz, 1H), 2.20 (dd, *J* = 15.2, 3.2 Hz, 2H), 1.61 – 1.49 (m, 2H), 1.40 – 1.27 (m, 2H), 1.06 (d, *J* = 10.0 Hz, 1H), 0.90 (d, *J* = 10.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9, 147.6, 141.5, 138.9, 128.8, 128.6, 126.9, 126.2, 125.4, 123.8, 123.1, 53.7, 51.9, 45.7, 42.9, 32.5, 29.7, 28.8.

(*E*)-9-benzylidene-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene (4E).



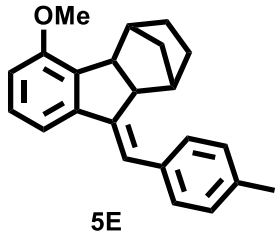
White solid (yield: 54.4 mg, >99%). m.p. 78.9 – 79.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.53 (m, 3H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.32 – 7.27 (m, 1H), 7.24 – 7.19 (m, 3H), 6.92 (d, *J* = 2.1 Hz, 1H), 3.35 (d, *J* = 6.8 Hz, 1H), 3.23 (d, *J* = 6.8 Hz, 1H), 2.44 (d, *J* = 3.7 Hz, 1H), 2.36 (d, *J* = 3.9 Hz, 1H), 1.71 – 1.58 (m, 2H), 1.52 – 1.45 (m, 2H), 1.03 (d, *J* = 10.2 Hz, 1H), 0.92 (d, *J* = 10.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 147.2, 144.4, 137.7, 128.9, 128.6, 128.5, 126.9, 126.4, 125.1, 119.6, 119.4, 53.5, 50.9, 43.1, 40.5, 32.8, 29.1, 28.9. HRMS (ESI) m/z: calcd for $C_{21}H_{20}$ [M + H]+:273.1638; found:273.1635.

(*Z*)-5-methoxy-9-(4-methylbenzylidene)-2,3,4,4a,9,9a-hexahydro-1H-1,4-



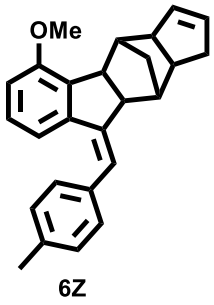
methanofluorene (5Z).[6] White solid (yield: 146.9 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 7.9 Hz, 2H), 7.17 (d, *J* = 7.9 Hz, 2H), 6.90 (t, *J* = 7.9 Hz, 1H), 6.81 (d, *J* = 7.8 Hz, 1H), 6.65 (d, *J* = 7.9 Hz, 1H), 6.58 (s, 1H), 3.83 (s, 3H), 3.09 (d, *J* = 7.1 Hz, 1H), 2.90 (d, *J* = 7.1 Hz, 1H), 2.52 (d, *J* = 2.5 Hz, 1H), 2.39 (s, 3H), 2.31 (d, *J* = 2.7 Hz, 1H), 1.71 – 1.56 (m, 2H), 1.52 – 1.42 (m, 1H), 1.40 – 1.33 (m, 1H), 1.19 (d, *J* = 10.0 Hz, 1H), 1.00 (d, *J* = 10.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 147.6, 143.3, 138.3, 136.3, 135.8, 129.2, 128.7, 127.5, 123.2, 116.3, 109.5, 55.2, 53.7, 49.4, 45.6, 40.0, 32.6, 29.8, 28.6, 21.5.

(*E*)-5-methoxy-9-(4-methylbenzylidene)-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene (5E). White solid (yield: 63.2 mg, >99%). m.p. 153.2 – 155.6 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 6.8 Hz, 2H), 7.24 – 7.14 (m, 4H), 6.87 (s, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 3.87 (s, 3H), 3.33 (d, *J* = 6.5 Hz, 1H), 3.26 (d, *J* = 6.6 Hz, 1H), 2.59 (s, 1H), 2.44 (s, 1H), 2.38 (s, 3H), 1.72 – 1.54 (m, 2H), 1.56 – 1.40 (m, 2H), 1.04 (d, *J* = 10.1 Hz, 1H), 0.91 (d, *J* = 10.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 146.6, 146.4, 136.2, 135.6, 134.8, 129.3, 128.8, 128.4, 119.5, 111.9, 109.3, 55.3, 51.4, 51.0, 40.4, 40.3, 33.0, 29.0, 28.9, 21.4. HRMS (ESI) m/z: calcd for $C_{23}H_{24}O$ $[M+H]^+$:317.1900; found: 317.1905



5E

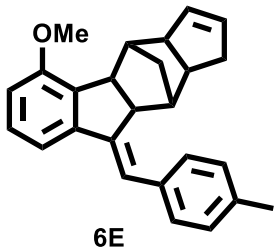
(*Z*)-5-methoxy-9-(4-methylbenzylidene)-1,3a,4,4a,9,9a,10,10a-octahydro-4,10-methanocyclopenta[b]fluorene (6Z).[6]



6Z

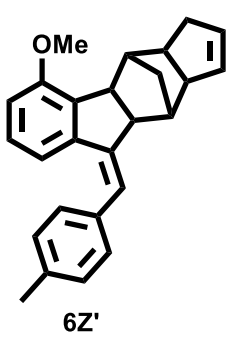
White solid (yield: 109.6 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.9 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 6.93 (t, *J* = 7.8 Hz, 1H), 6.87 (d, *J* = 7.7 Hz, 1H), 6.67 (d, *J* = 7.7 Hz, 1H), 6.54 (s, 1H), 5.85 – 5.79 (m, 2H), 3.85 (s, 3H), 3.32 – 3.26 (m, 1H), 3.22 (d, *J* = 7.1 Hz, 1H), 2.97 (d, *J* = 7.1 Hz, 1H), 2.73 – 2.64 (m, 2H), 2.56 – 2.45 (m, 2H), 2.43 (s, 3H), 2.27 (d, *J* = 4.1 Hz, 1H), 1.35 (d, *J* = 9.9 Hz, 1H), 1.28 (d, *J* = 10.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 148.2, 143.5, 138.8, 136.3, 135.8, 132.8, 131.1, 129.2, 128.7, 127.2, 122.8, 116.4, 109.5, 55.2, 53.9, 50.7, 46.0, 44.9, 42.6, 42.1, 35.7, 32.4, 21.4.

(*E*)-5-methoxy-9-(4-methylbenzylidene)-1,3a,4,4a,9,9a,10,10a-octahydro-4,10-methanocyclopenta[b]fluorene (6E). White solid (yield: 70.7 mg, >99%). m.p. 163.1 –164.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.1 Hz, 2H), 7.18 – 7.08 (m, 4H), 6.80 (d, *J* = 2.3 Hz, 1H), 6.65 (d, *J* = 8.6 Hz, 1H), 5.87 – 5.70 (m, 2H), 3.80 (s, 3H), 3.39 (d, *J* = 6.8 Hz, 1H), 3.29 (d, *J* = 6.8 Hz, 1H), 3.12 – 3.10 (m, 1H), 2.68 – 2.60 (m, 1H), 2.54 – 2.44 (m, 4H), 2.33 (s, 3H), 1.13 (d, *J* = 10.1 Hz, 1H), 1.08 (d, *J* = 10.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 147.5, 146.6, 136.0, 135.8, 134.7, 132.0, 131.6, 129.1, 128.5, 127.9, 118.7, 111.8, 109.1, 55.1, 53.1, 46.2, 44.9, 43.6, 42.7, 42.1, 35.9, 32.2, 21.2. HRMS (ESI) m/z: calcd for $C_{26}H_{26}O$ [M + H]+:355.2056; found: 355.2051.



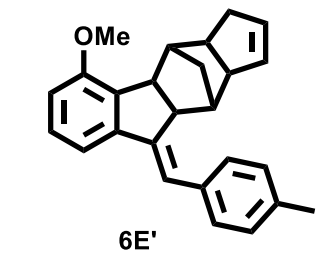
6E

(*Z*)-5-methoxy-9-(4-methylbenzylidene)-3,3a,4,4a,9,9a,10,10a-octahydro-4,10-methanocyclopenta[b]fluorene (6Z'). [6] White solid (yield: 53.2 mg, 30%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 6.88 (t, *J* = 7.9 Hz, 1H), 6.80 (d, *J* = 7.8 Hz, 1H), 6.63 (d, *J* = 7.8 Hz, 1H), 6.49 (s, 1H), 5.78 – 5.69 (m, 1H), 3.81 (s, 1H), 3.22 – 3.12 (m, 1H), 2.91 (d, *J* = 7.1 Hz, 1H), 2.73 – 2.64 (m, 1H), 2.52 (d, *J* = 17.4 Hz, 1H), 2.44 (d, *J* = 5.0 Hz, 1H), 2.41 (d, *J* = 2.5 Hz, 1H), 2.38 (s, 1H), 2.34 – 2.22 (m, 1H), 1.36 (d, *J* = 10.0 Hz, 1H), 1.23 (d, *J* = 10.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 148.2, 143.7, 138.7, 136.3, 135.8, 132.4, 131.2, 129.1, 128.7, 127.3, 122.4, 116.4, 109.5, 55.3, 52.9, 49.1, 48.4, 44.8, 43.0, 41.7, 35.5, 32.6, 21.4.



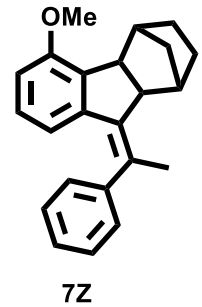
6Z'

(*E*)-5-methoxy-9-(4-methylbenzylidene)-3,3a,4,4a,9,9a,10,10a-octahydro-4,10-methanocyclopenta[b]fluorene (6E'). white solid (yield: 70.7mg, >99%). m.p. 163.5-164.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.09 (m, 4H), 6.83 (s, 1H), 6.65 (d, *J* = 8.2 Hz, 1H), 5.82 – 5.74 (m, 2H), 3.81 (s, 3H), 3.33 (d, *J* = 6.2 Hz, 1H), 3.27 (d, *J* = 6.4 Hz, 1H), 3.20 – 3.13 (m, 1H), 2.67 (d, *J* = 4.5 Hz, 1H), 2.58 – 2.49 (m, 2H), 2.43 – 2.37 (m, 1H), 2.34 (s, 3H), 2.24 (d, *J* = 3.6 Hz, 1H), 1.15 – 1.06 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 147.7, 146.8, 136.3, 136.2, 134.9, 132.9, 131.1, 129.3, 128.8, 128.2, 119.2, 112.1, 109.4, 55.4, 53.6, 46.7, 44.9, 43.4, 42.4, 36.2, 32.4, 21.5. HRMS (ESI) m/z: calcd for $C_{26}H_{26}O$ [M + H]+:355.2056; found: 355.2053.



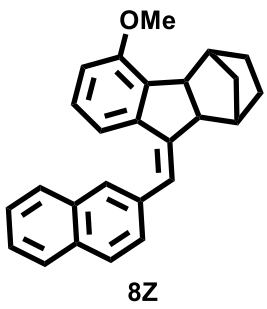
6E'

(*Z*)-5-methoxy-9-(1-phenylethylidene)-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene（7Z）.[6] White solid (yield: 99.5 mg, 63%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (t, *J* = 7.6 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.23 – 7.08 (m, 1H), 6.72 (t, *J* = 8.0 Hz, 1H), 6.53 (d, *J* = 8.0 Hz, 1H), 5.75 (d, *J* = 7.9 Hz, 1H), 3.79 (s, 2H), 3.15 (d, *J* = 7.2 Hz, 1H), 2. 95 (d, *J* = 7.2 Hz, 1H), 2.54 (d, *J* = 3.5 Hz, 1H), 2.44 (d, *J* = 3.2 Hz, 1H), 2.17 (s, 2H), 1.67 – 1.54 (m, 1H), 1.50 – 1.38 (m, 1H), 1.12 (d, *J* = 10.0 Hz, 1H), 0.97 (d, *J* = 10.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 145.0, 144.3, 141.6, 137.0, 131.5, 129.0, 127.3, 126.8, 116.2, 108.3, 55.2, 51.6, 49.5, 42.3, 40.1, 32.7, 29.1, 29.0, 24.7.



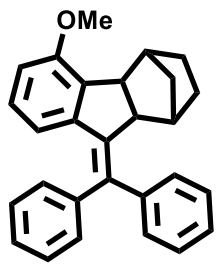
7Z

(*Z*)-5-methoxy-9-(naphthalen-2-ylmethylene)-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene（8Z）.[6] White solid (yield:114.5 mg, 65%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.8 Hz, 2H), 7.80 – 7.62 (m, 2H), 7.50 – 7.43 (m, 2H), 7.40 – 7.26 (m, 1H), 6.60 (t, *J* = 8.0 Hz, 1H), 6.49 (d, *J* = 8.0 Hz, 1H), 5.78 (d, *J* = 7.8 Hz, 1H), 3.77 (s, 3H), 3.16 (d, *J* = 7.2 Hz, 1H), 3.00 (s, 1H), 2.55 (s, 1H), 2.48 (s, 1H), 2.22 (s, 3H), 1.69 – 1.56 (m, 2H), 1.51 – 1.39 (m, 2H), 1.16 (d, *J* = 9.7 Hz, 1H), 0.99 (d, *J* = 10.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 144.2, 142.5, 142.0, 137.1, 134.1, 132.5, 131.2, 128.7, 128.2, 127.9, 127.4, 127.0, 126.0, 125.6, 116.3, 108.4, 55.2, 51.7, 49.5, 42.3, 40.1, 32.8, 29.1, 29.0.



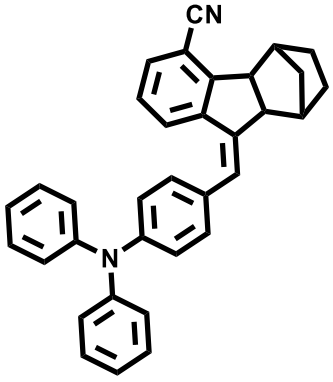
8Z

9-(diphenylmethylene)-5-methoxy-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene (9).[6] White solid (yield:132.5 mg, 70%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.27 (m, 8H), 7.21 – 7.16 (m, 1H), 7.12 – 6.96 (m, 1H), 6.77 (t, *J* = 8.0 Hz, 1H), 6.58 (d, *J* = 8.0 Hz, 1H), 5.94 (d, *J* = 7.9 Hz, 1H), 3.80 (s, 3H), 3.28 (d, *J* = 7.3 Hz, 1H), 3.05 (d, *J* = 7.2 Hz, 1H), 2.48 (s, 1H), 1.95 (s, 1H), 1.55 – 1.47 (m, 1H), 1.36 – 1.25 (m, 2H), 1.20 (d, *J* = 10.0 Hz, 1H), 0.97 – 0.90 (m, 1H), 0.87 (d, J = 11.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 144.9, 144.7, 144.4, 143.8, 138.1, 136.9, 129.3, 128.4, 127.5, 127.2, 126.7, 117.1, 109.2, 55.4, 51.9, 49.7, 41.9, 40.7, 32.7, 29.5, 28.7.



9

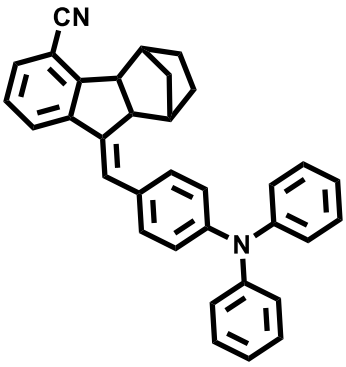
(*Z*)-9-(4-(diphenylamino)benzylidene)-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene-5-carbonitrile (10Z). Yellow solid (yield:92.8 mg, 80%); m.p. 112.3 – 113.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.9 Hz, 1H), 7.42 (d, *J* = 7.4 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 4H), 7.21 (d, *J* = 8.3 Hz, 2H), 7.14 (d, *J* = 7.6 Hz, 4H), 7.09 – 7.02 (m, 5H), 6.65 (s, 1H), 3.25 (d, *J* = 7.3 Hz, 1H), 3.00 (d, *J* = 7.2 Hz, 1H), 2.66 (d, *J* = 3.5 Hz, 1H), 2.35 (d, *J* = 3.5 Hz, 1H), 1.75 – 1.53 (m, 3H), 1.47 – 1.35 (m, 1H), 1.18 – 1.03 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.9, 147.7, 147.1, 145.1, 143.1, 131.9, 131.6, 129.5, 129.4, 127.5, 126.9, 125.5, 124.6, 123.5, 123.2, 117.9, 109.6, 53.5,



10Z

51.4, 45.8, 41.5, 32.6, 29.7, 28.4. HRMS (ESI) m/z: calcd for $C_{34}H_{28}N_2$ [M + H]+:465.2325; found: 465.2340.

(*E*)-9-(4-(diphenylamino)benzylidene)-2,3,4,4a,9,9a-hexahydro-1H-1,4-methanofluorene-5-carbonitrile (10E). Yellow solid (yield:46.5 mg, 99%); m.p. 169.5-171.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.9 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 8.7 Hz, 2H), 7.33 – 7.28 (m, 5H), 7.14 (d, *J* = 7.6 Hz, 4H), 7.10 – 7.03 (m, 4H), 6.88 (d, *J* = 1.9 Hz, 1H), 3.41 (d, *J* = 7.0 Hz, 1H), 3.33 (d, *J* = 6.8 Hz, 1H), 2.73 (d, *J* = 4.0 Hz, 1H), 2.54 (d, *J* = 2.9 Hz, 1H), 1.82 – 1.70 (m, 1H), 1.65 – 1.52 (m, 2H), 1.50 – 1.42 (m, 1H), 1.10 – 0.93 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0, 147.5, 146.9, 146.4, 142.8, 131.5, 130.6, 130.1, 129.5, 127.6, 124.9, 123.4, 123.4, 123.0, 121.3, 117.9, 109.4, 53.2, 50.9, 41.7, 40.5, 33.1, 28.9, 28.8. HRMS (ESI) m/z:calcd for $C_{34}H_{28}N_2$ [M + H]+:465.2325; found: 465.2342.



10E

3. ^{1}H NMR and ^{13}C NMR Spectra

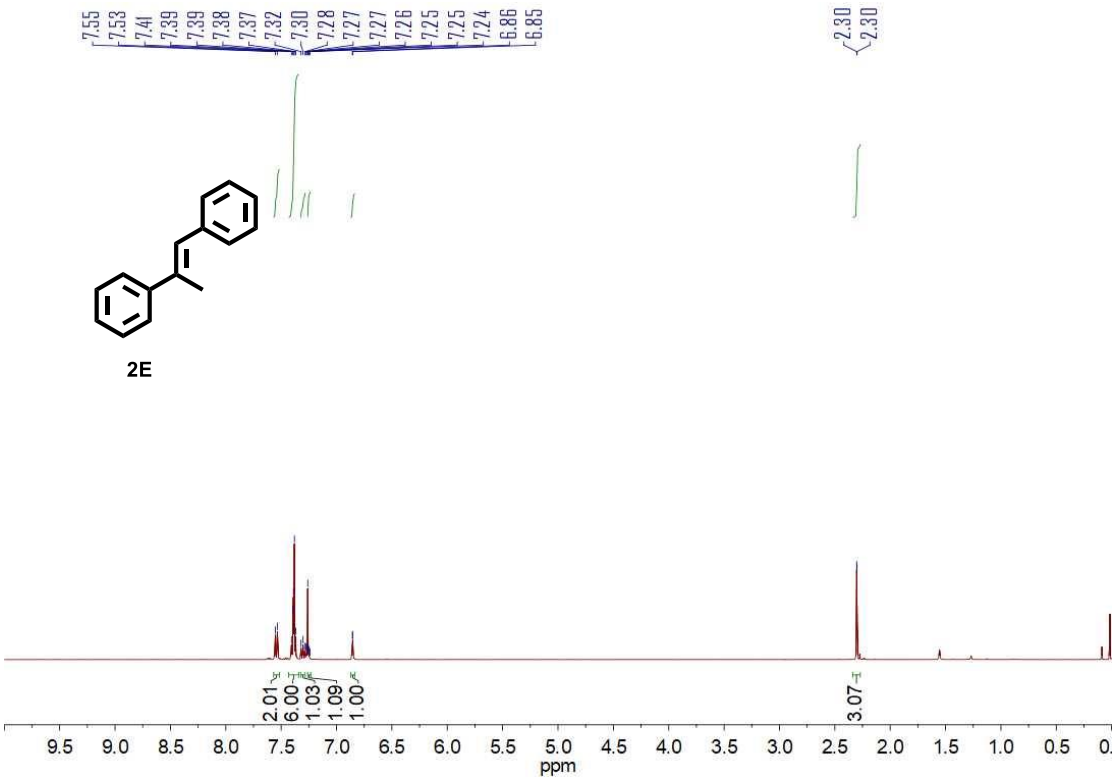


Figure S1. ^{1}H NMR spectrum of **2E** in $CDCl_3$

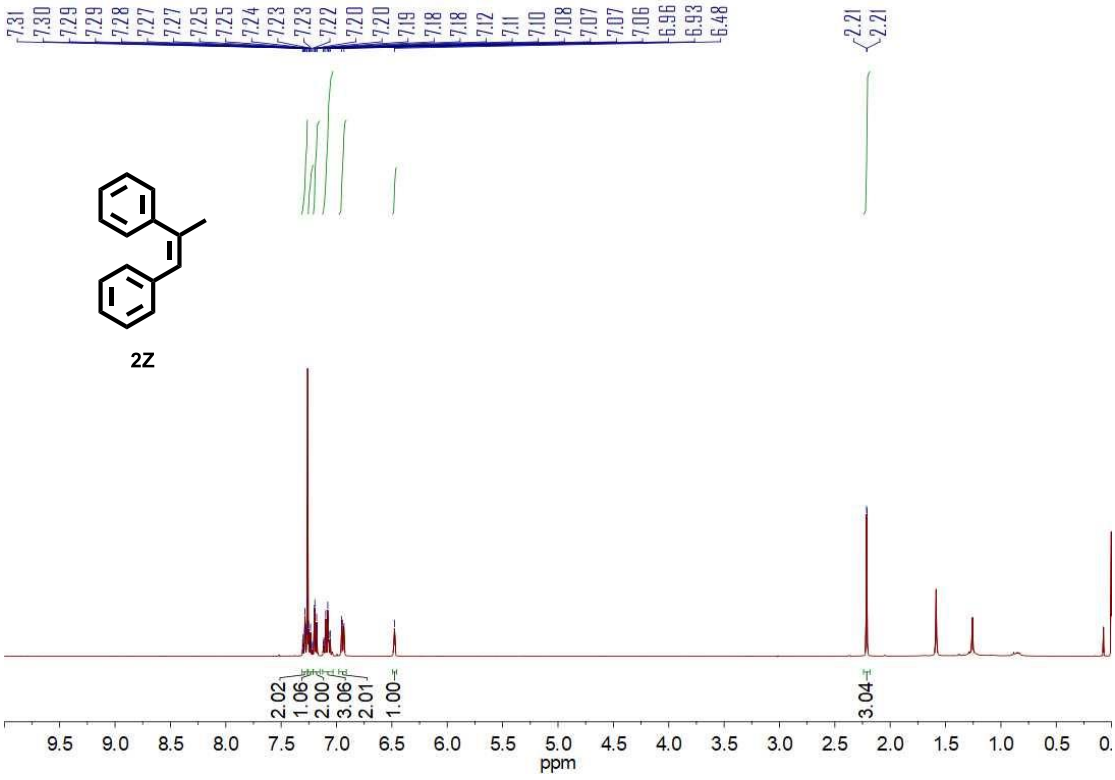


Figure S2. ^{1}H NMR spectrum of **2Z** in $CDCl_3$

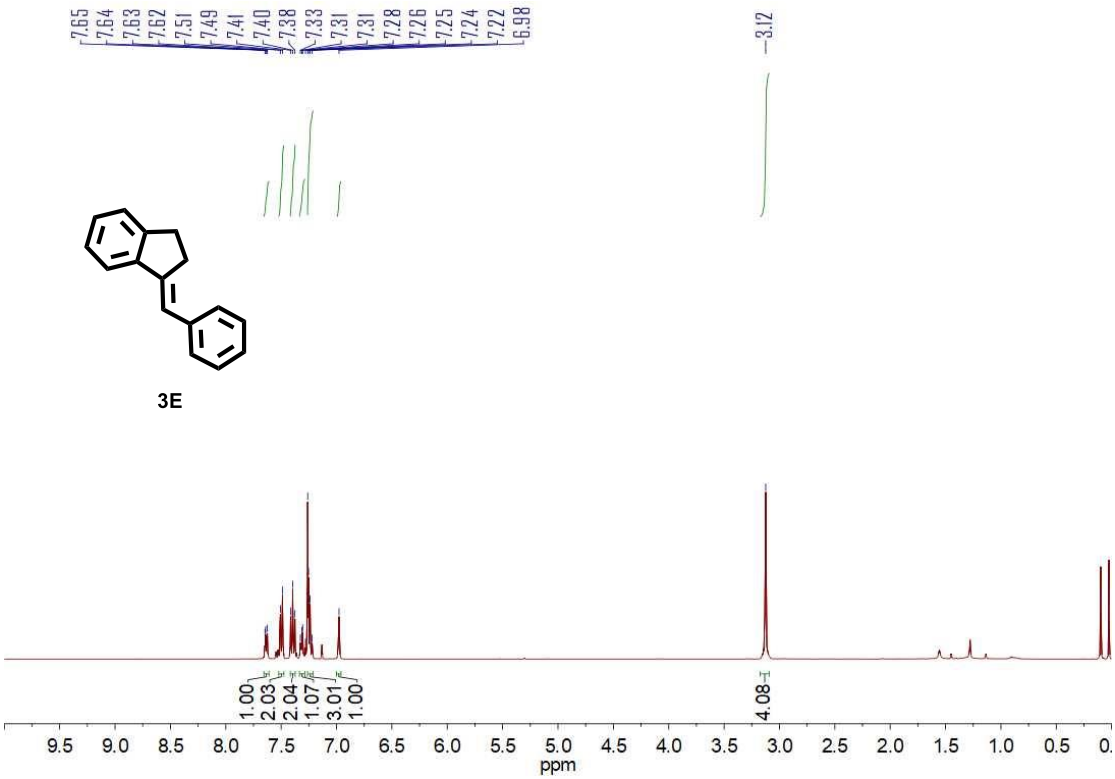


Figure S3. ^{1}H NMR spectrum of **3E** in $CDCl_3$

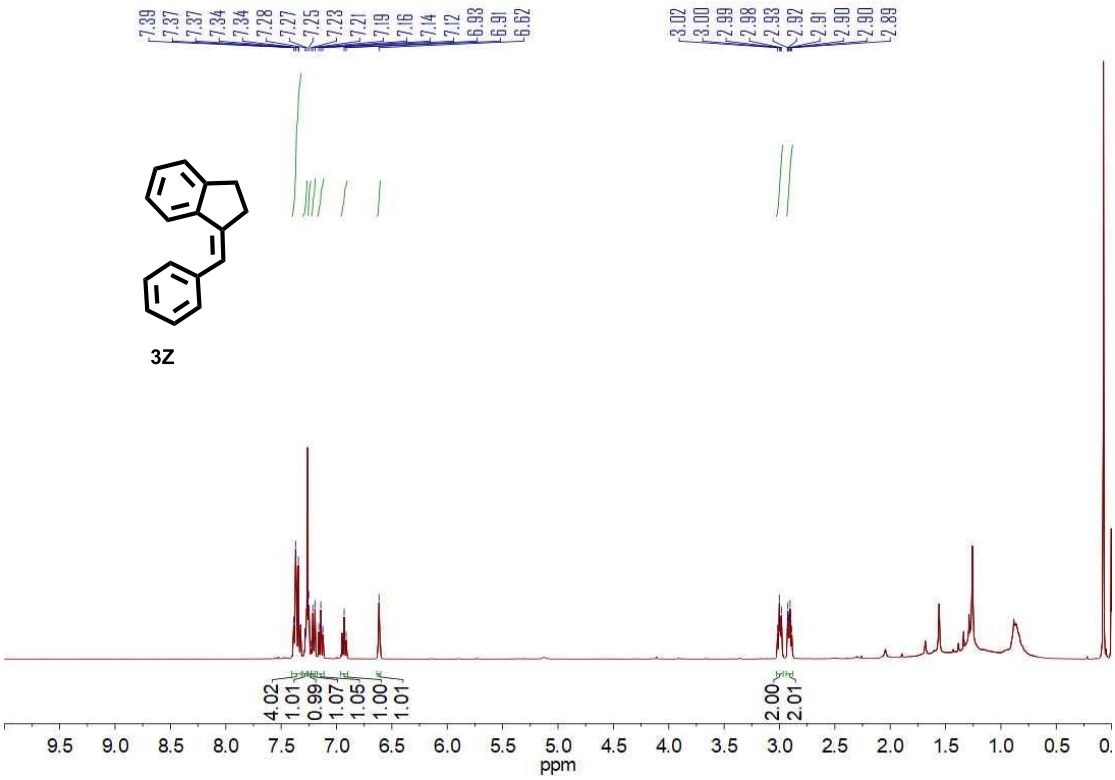


Figure S4. ^{1}H NMR spectrum of **3Z** in $CDCl_3$

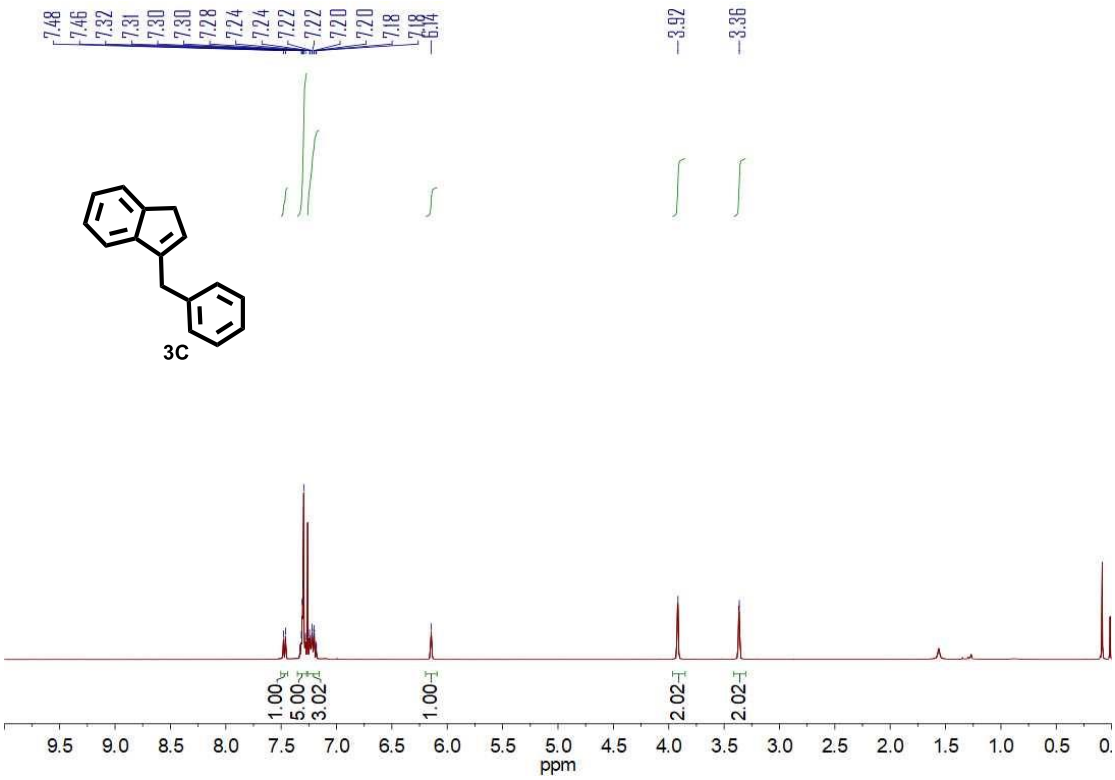


Figure S5. ^{1}H NMR spectrum of **3C** in $CDCl_3$

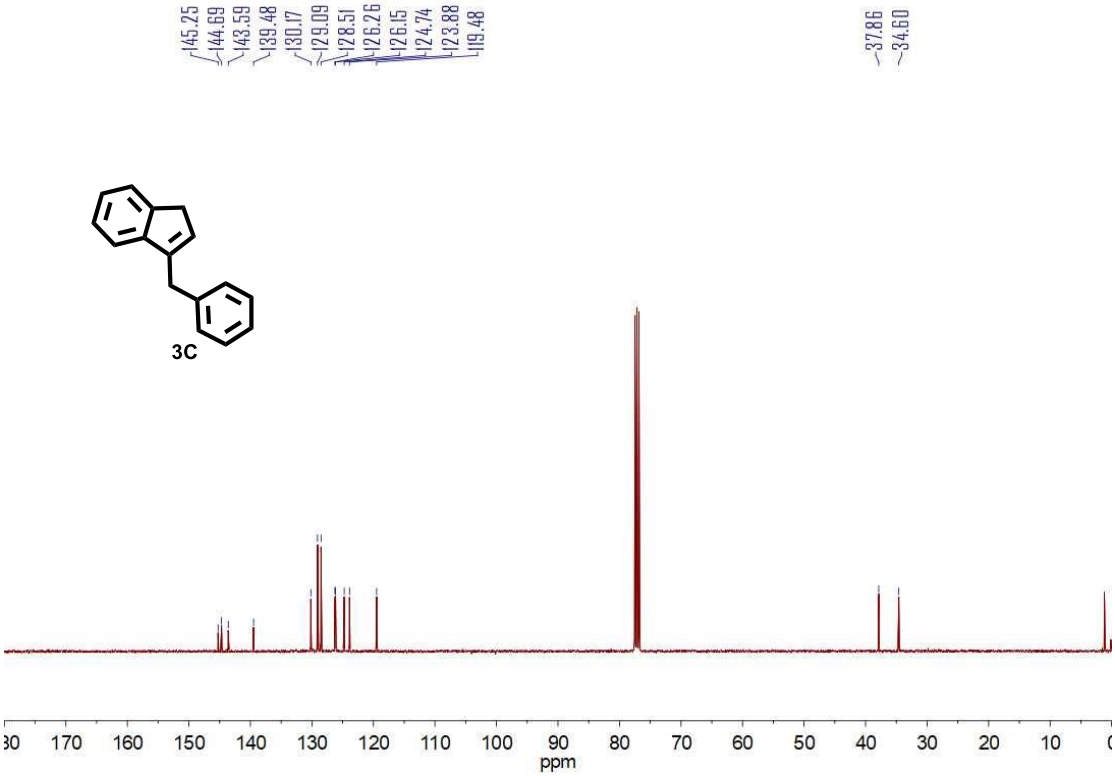


Figure S6. ^{13}C NMR spectrum of **3C** in $CDCl_3$

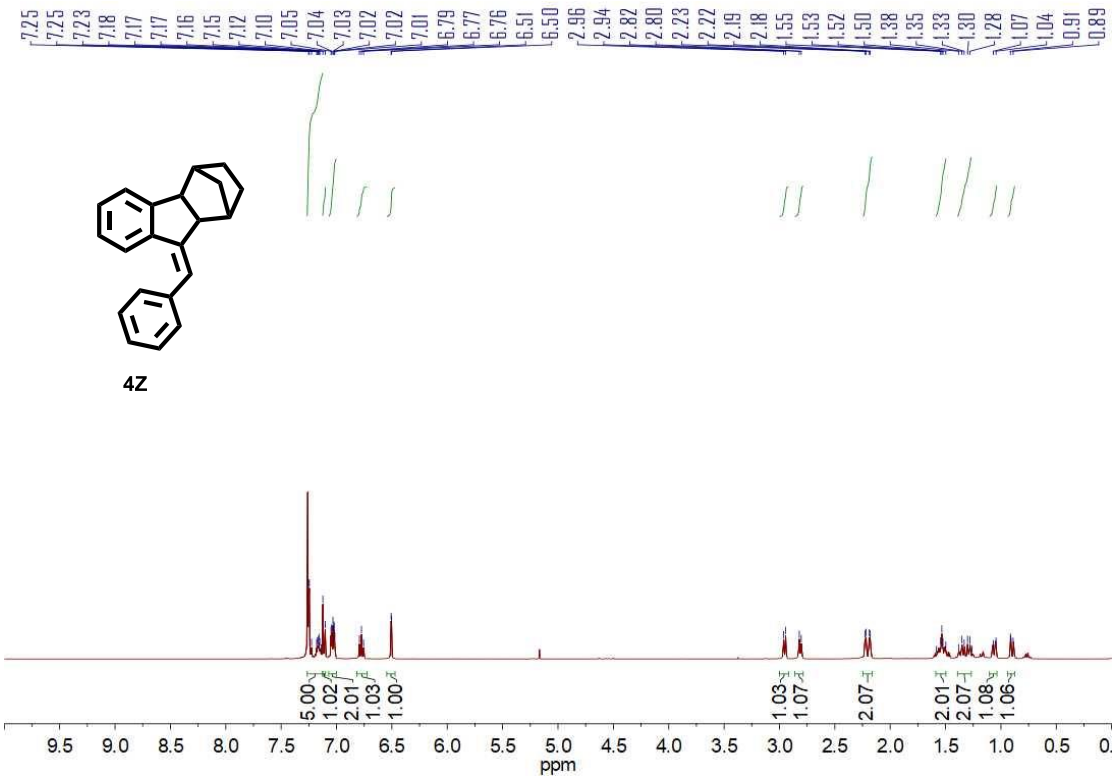


Figure S7. ^{1}H NMR spectrum of **4Z** in $CDCl_3$

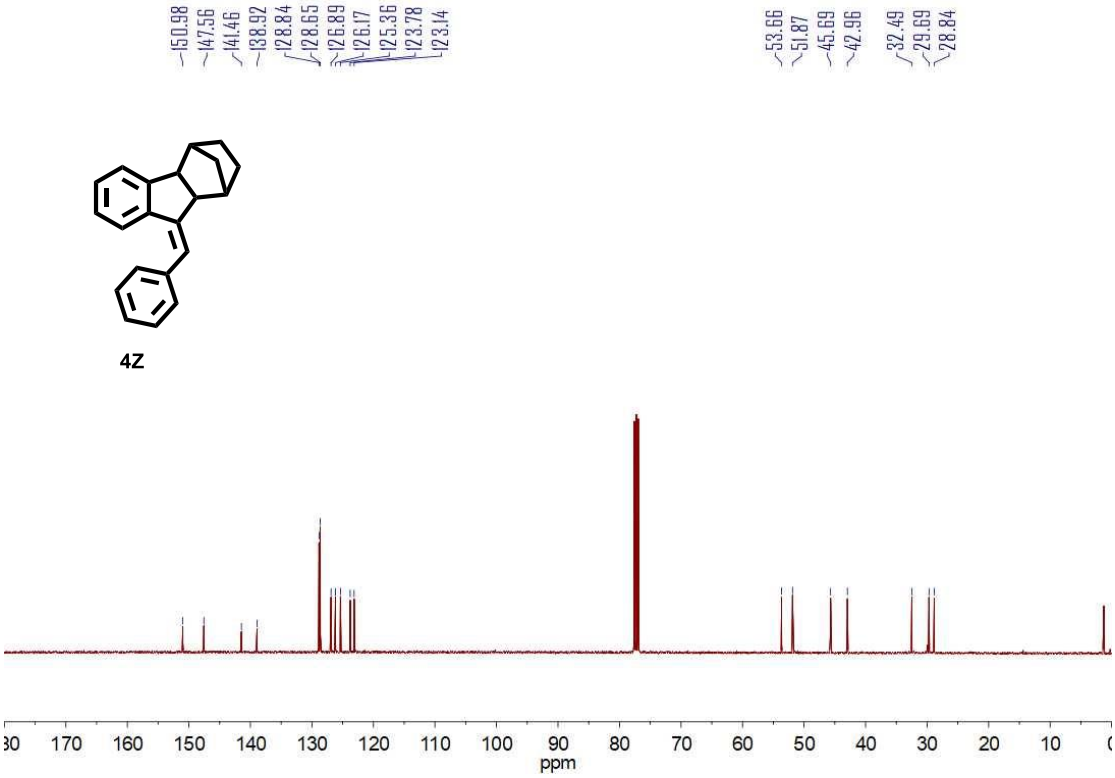


Figure S8. ^{13}C NMR spectrum of **4Z** in $CDCl_3$

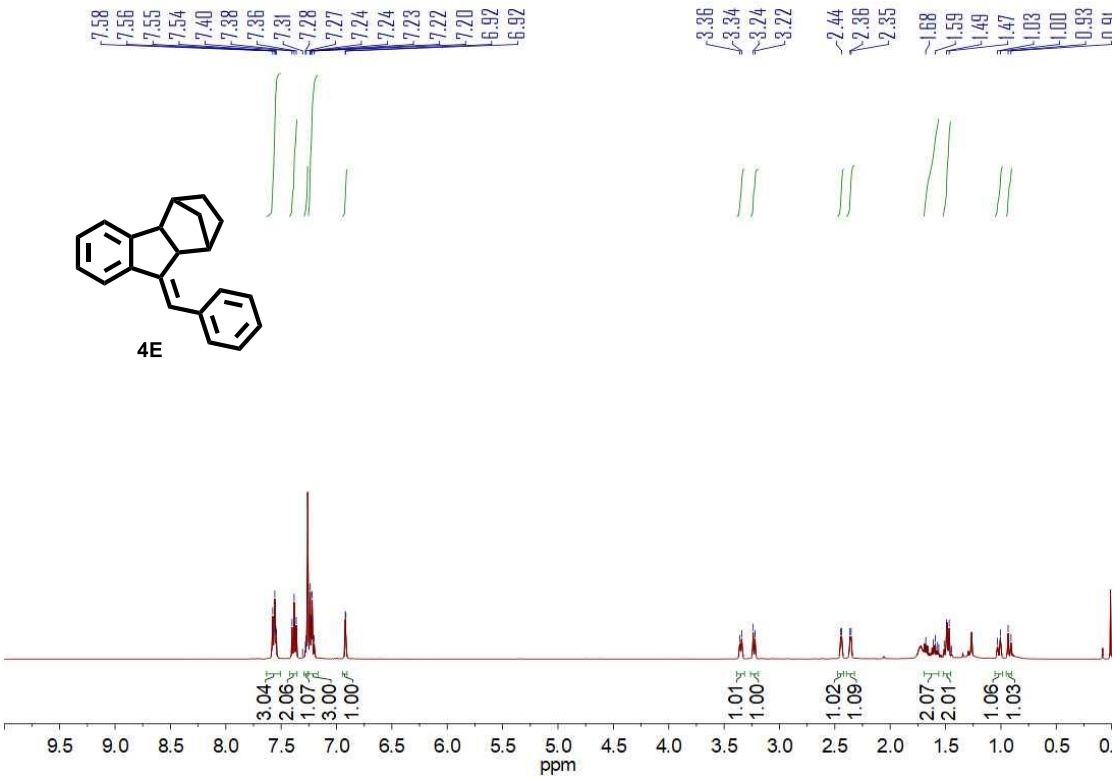


Figure S9. ^{1}H NMR spectrum of **4E** in $CDCl_3$

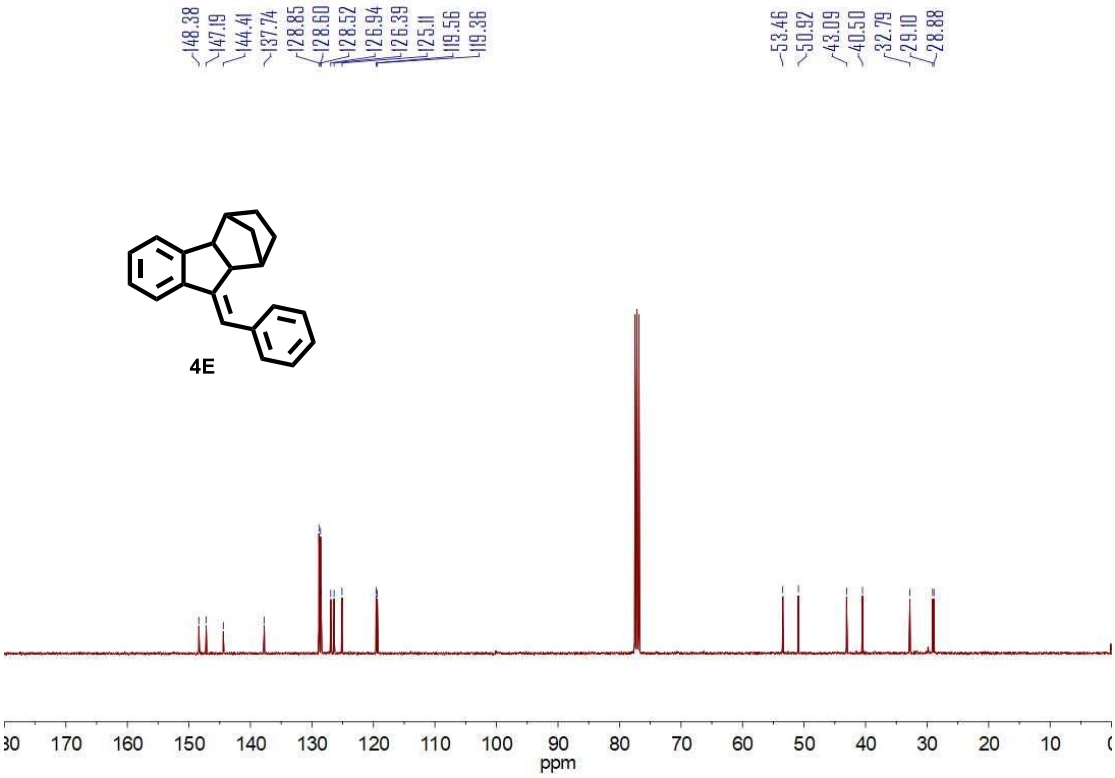


Figure S10. ^{13}C NMR spectrum of **4E** in $CDCl_3$

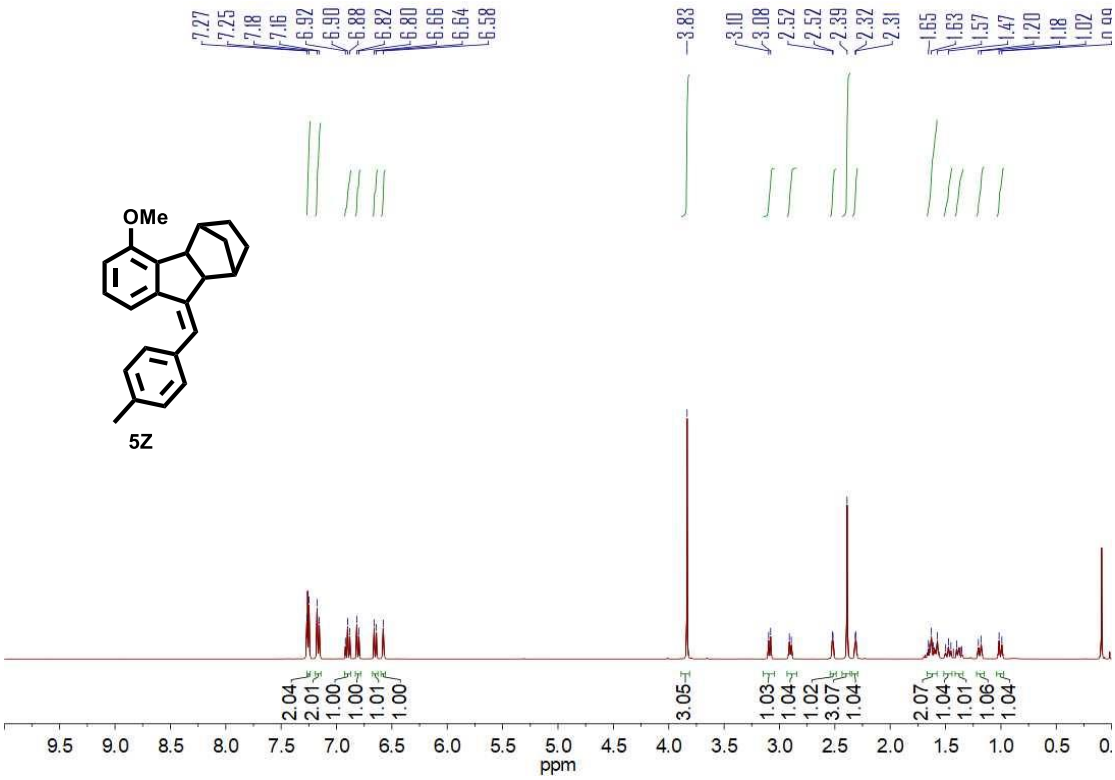


Figure S11. ^{1}H NMR spectrum of **5Z** in $CDCl_3$

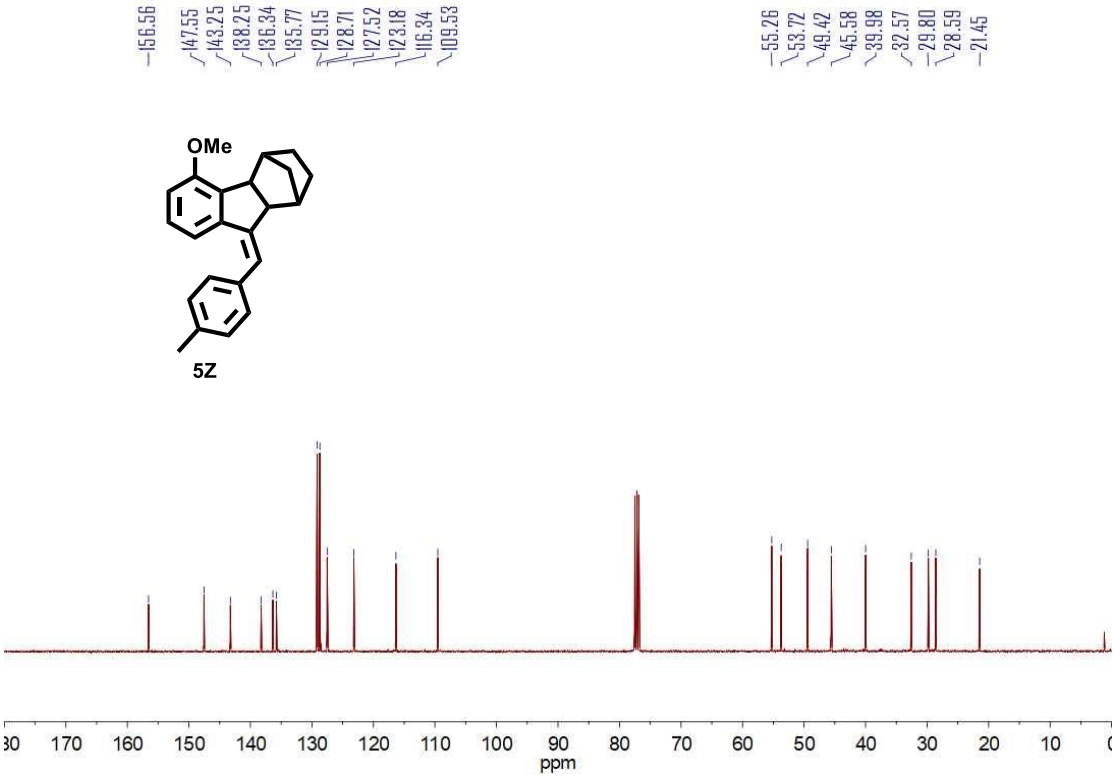


Figure S12. ^{13}C NMR spectrum of **5Z** in $CDCl_3$

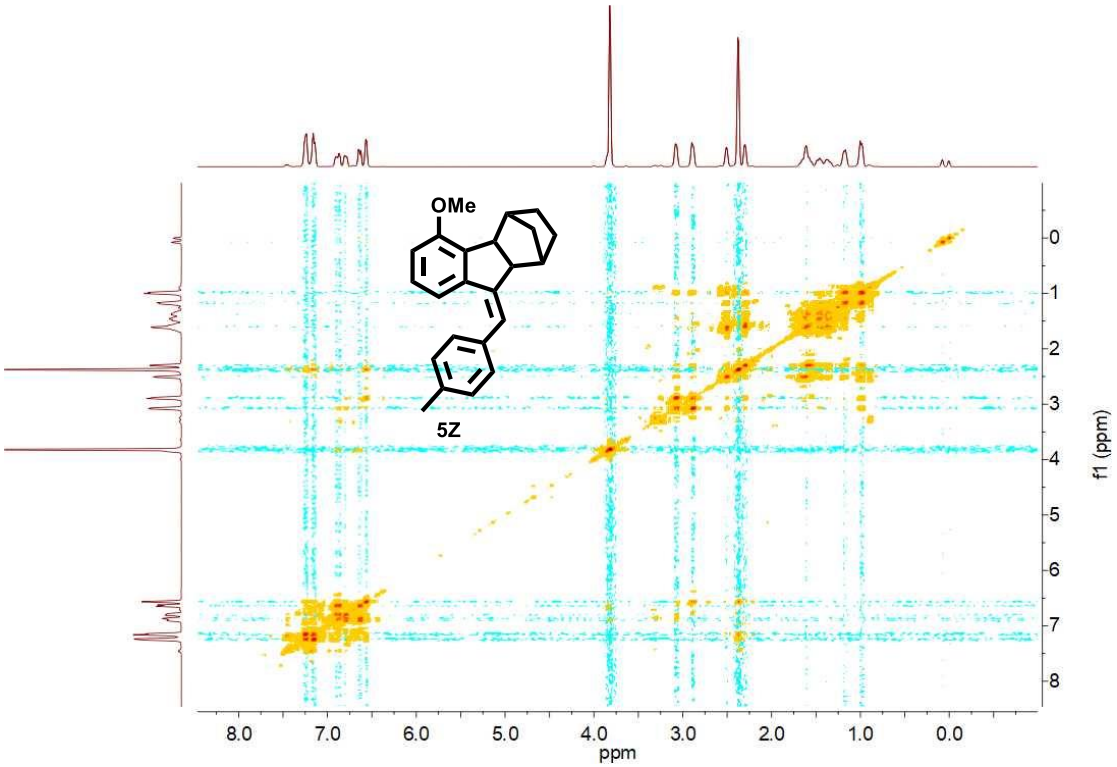


Figure S13. $^{1}H,^{1}H$-COSY NMR spectrum of **5Z** in $CDCl_3$

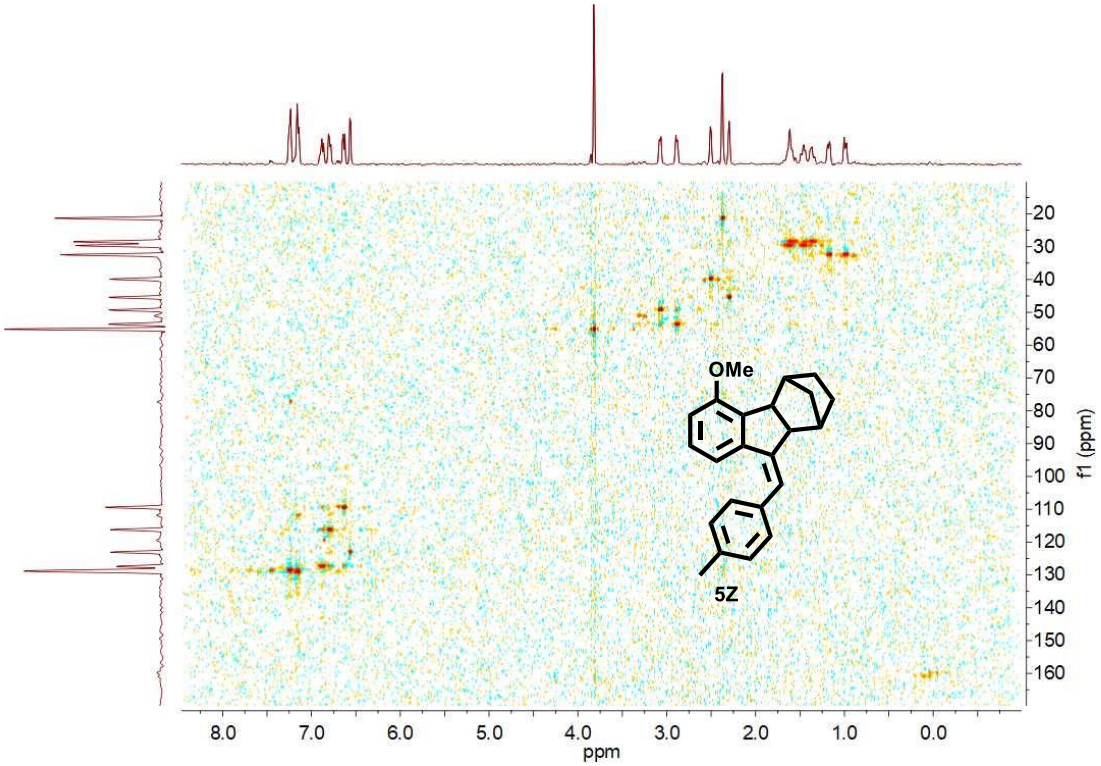


Figure S14. $^{1}H,^{13}C$-COSY NMR spectrum of **5Z** in $CDCl_3$

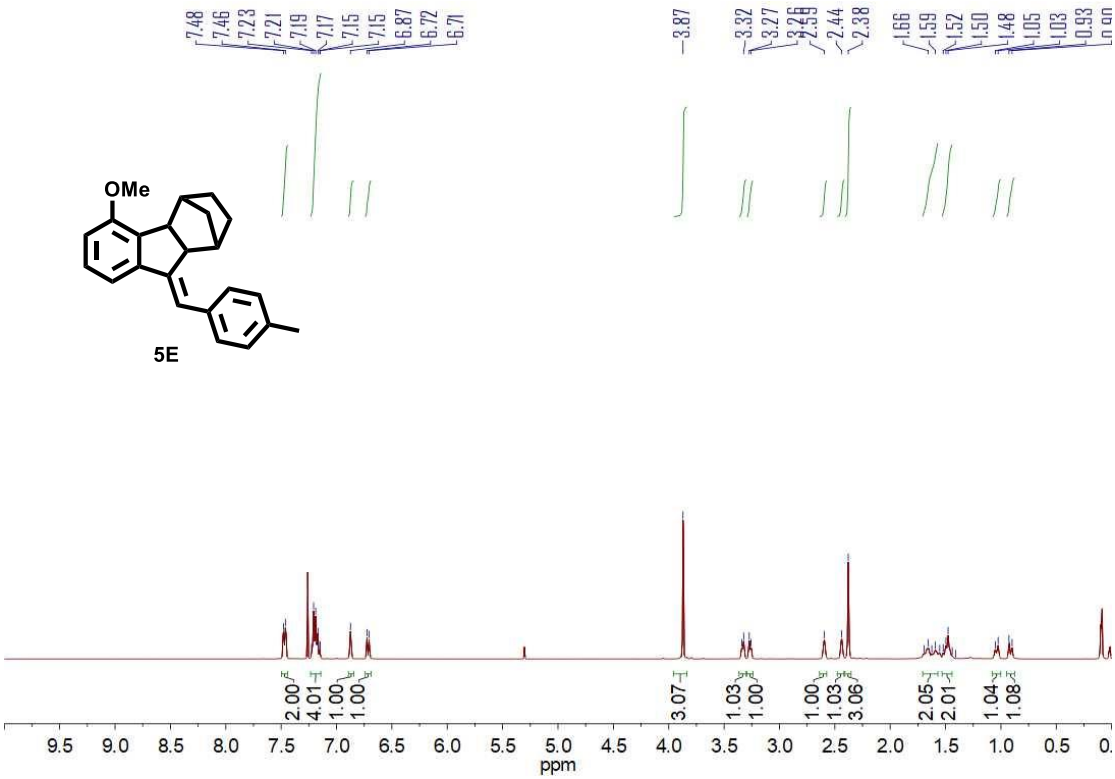


Figure S15. ^{1}H NMR spectrum of **5E** in $CDCl_3$

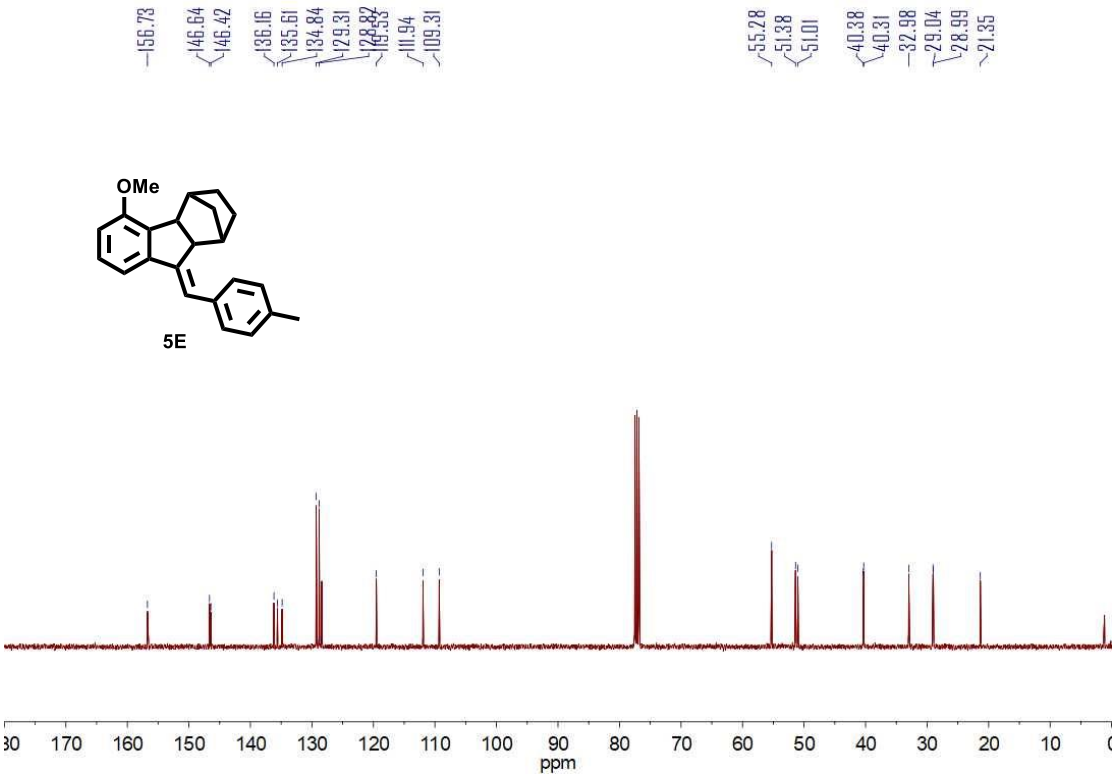


Figure S16. ^{13}C NMR spectrum of **5E** in $CDCl_3$

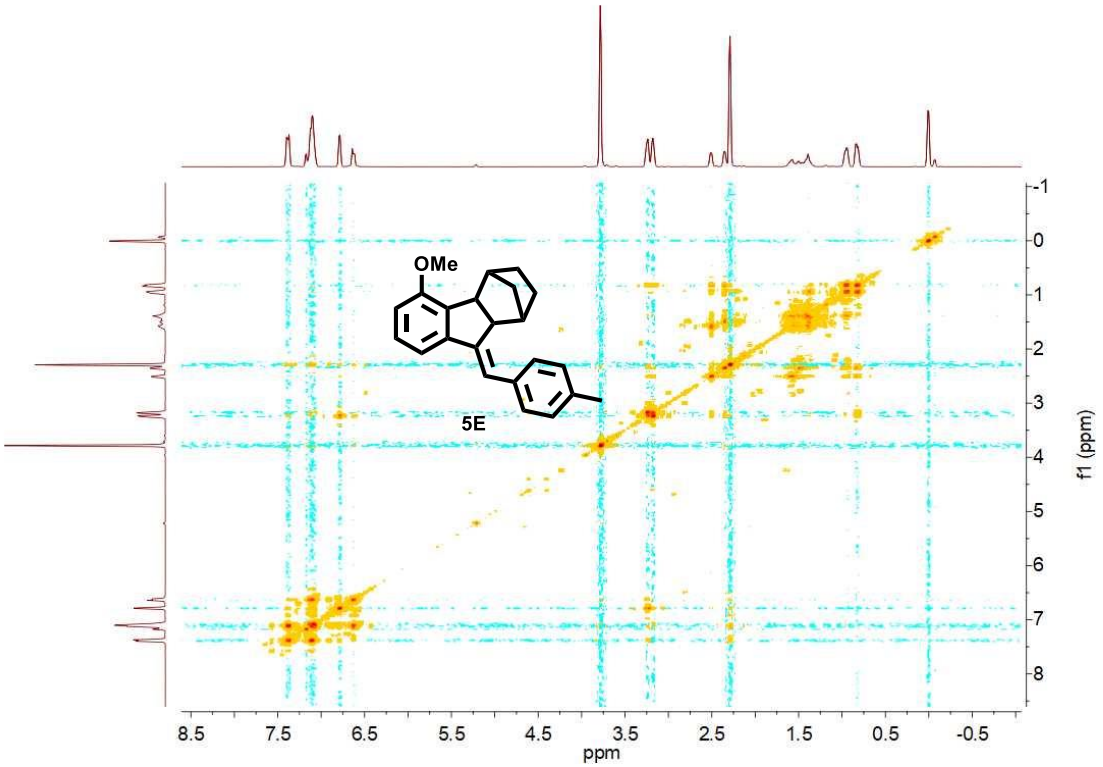


Figure S17. $^{1}H,^{1}H$-COSY NMR spectrum of **5E** in $CDCl_3$

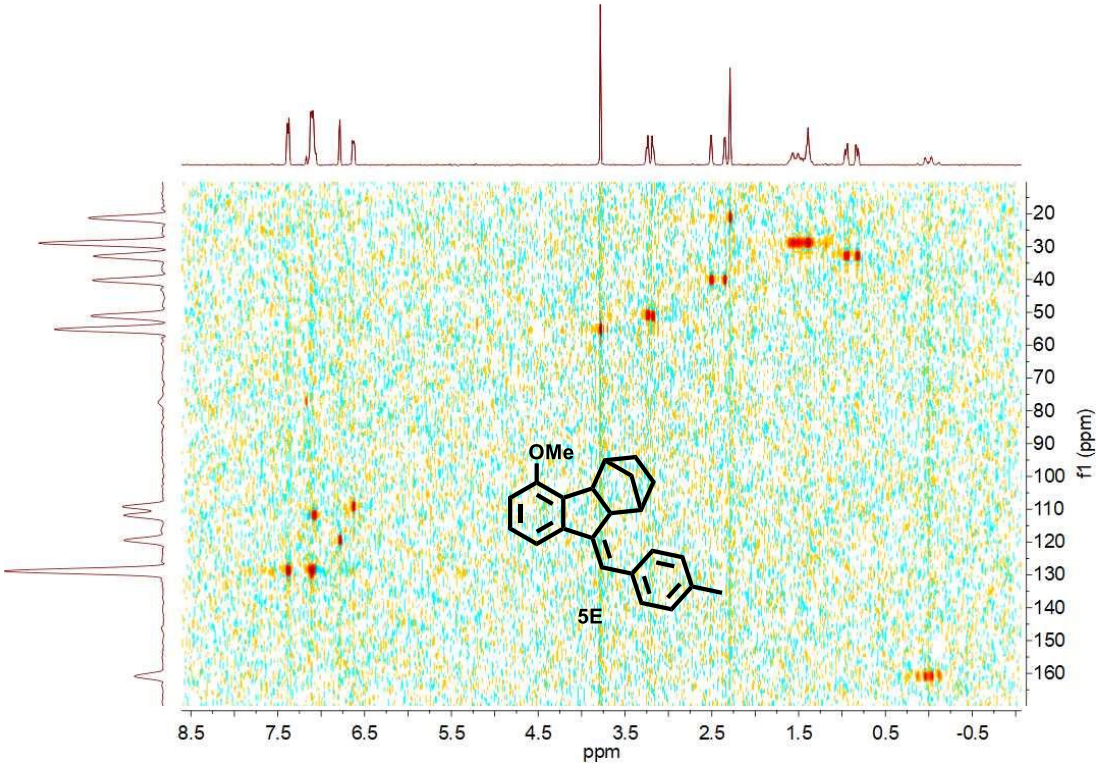


Figure S18. $^{1}H,^{13}C$-COSY NMR spectrum of **5E** in $CDCl_3$

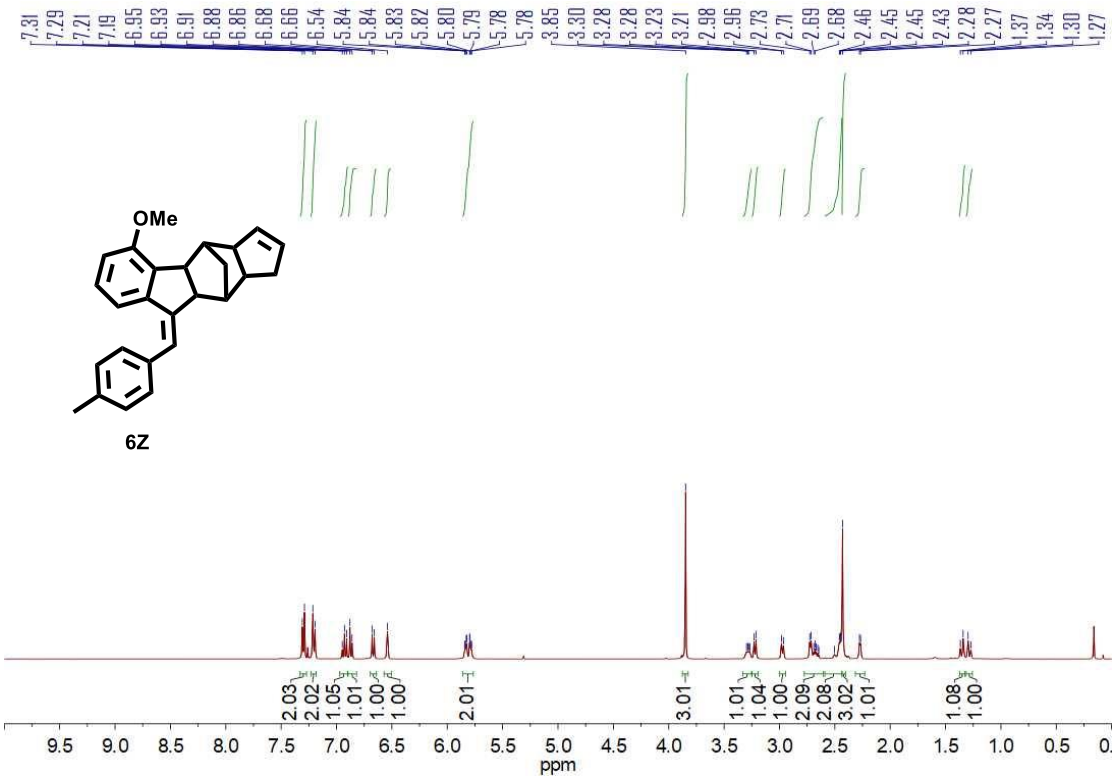


Figure S19. ^{1}H NMR spectrum of **6Z** in $CDCl_3$

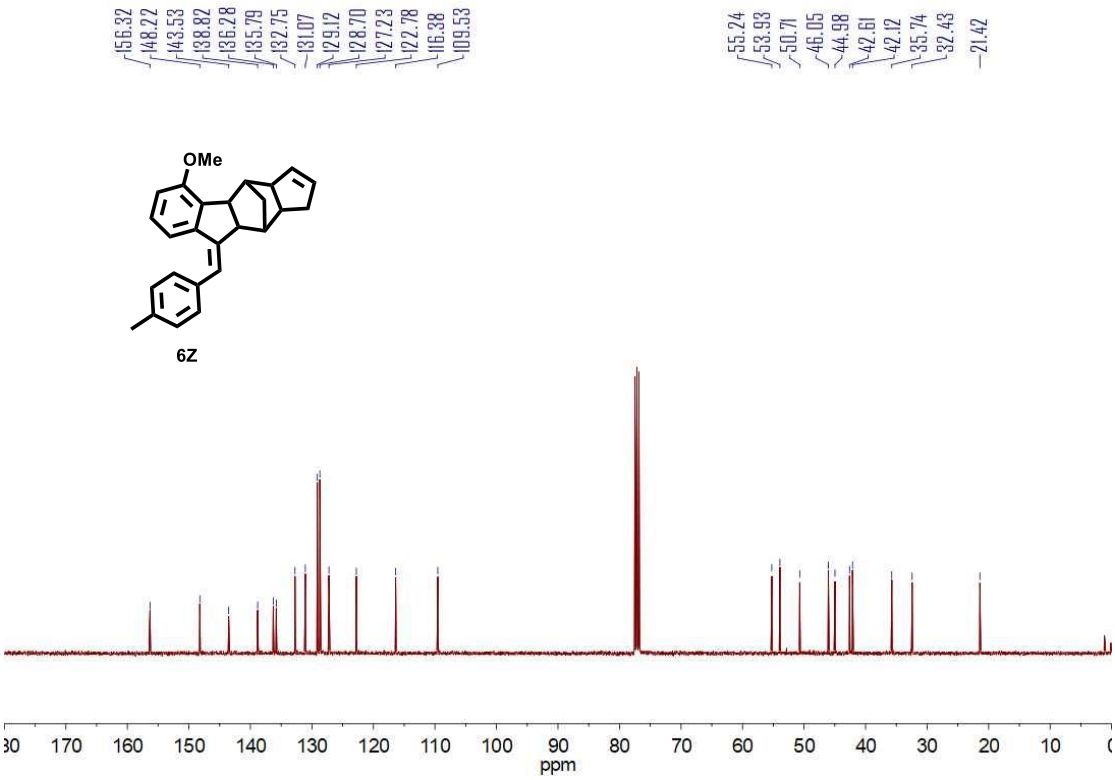


Figure S20. ^{13}C NMR spectrum of **6Z** in $CDCl_3$

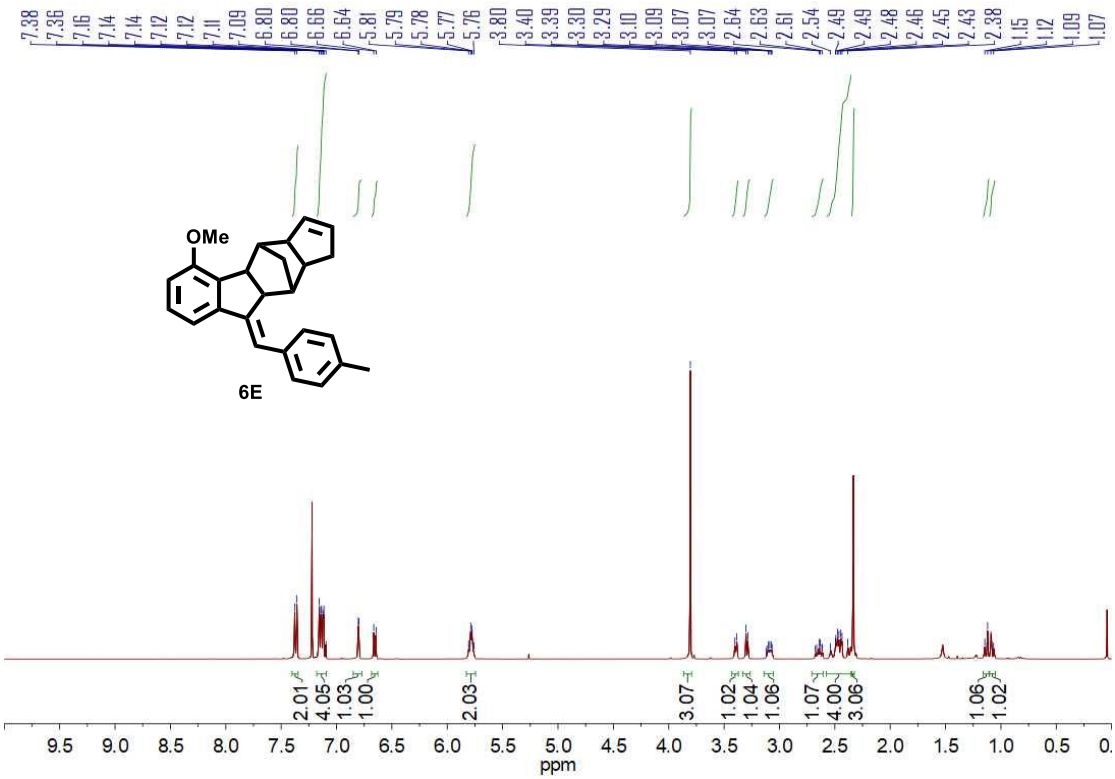


Figure S21. ^{1}H NMR spectrum of **6E** in $CDCl_3$

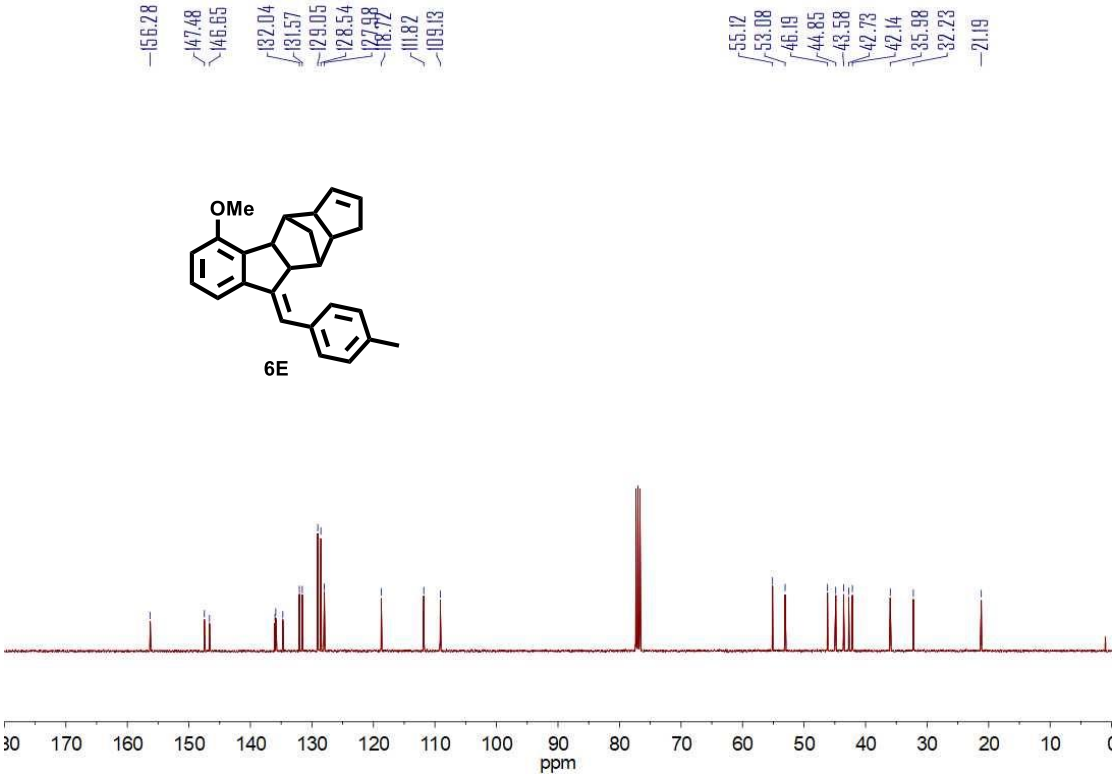


Figure S22. ^{13}C NMR spectrum of **6E** in $CDCl_3$

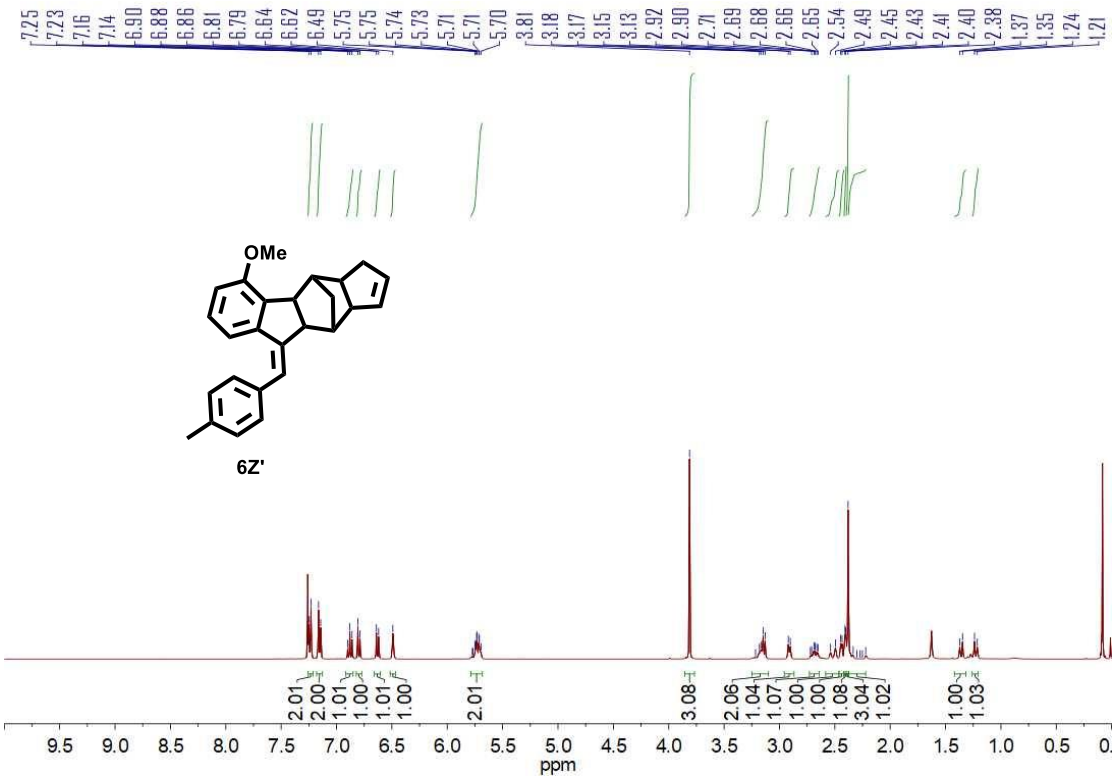


Figure S23. ^{1}H NMR spectrum of **6Z'** in $CDCl_3$

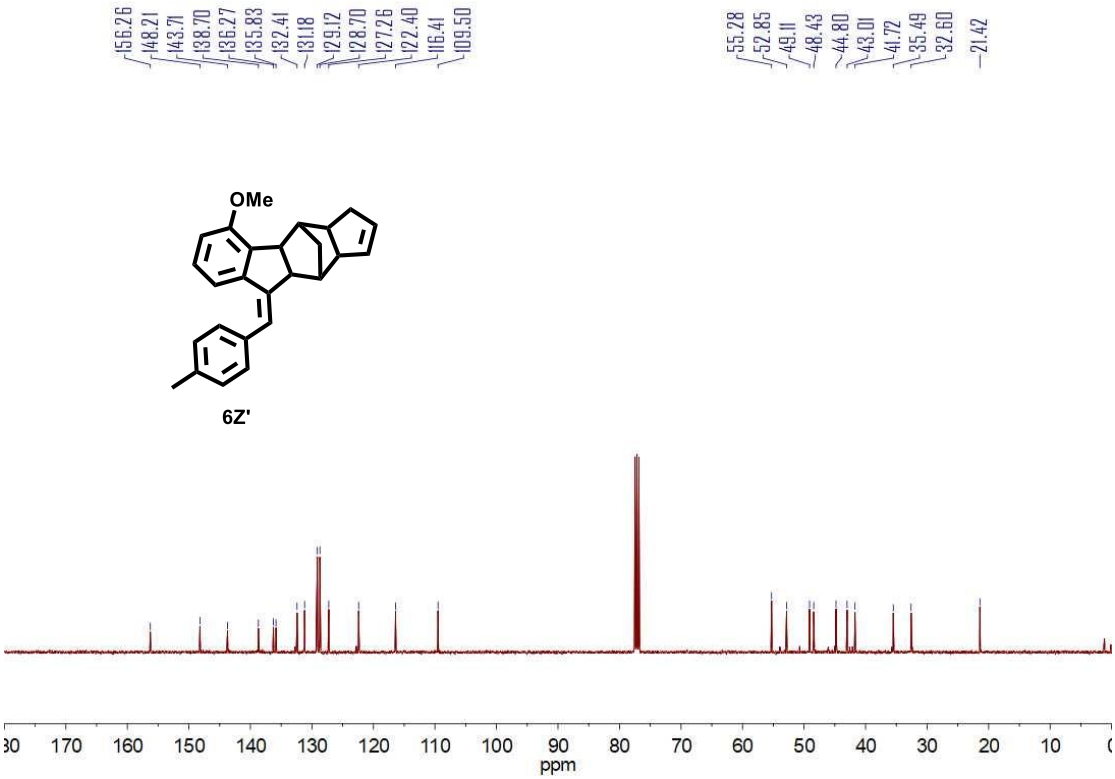


Figure S24. ^{13}C NMR spectrum of **6Z'** in $CDCl_3$

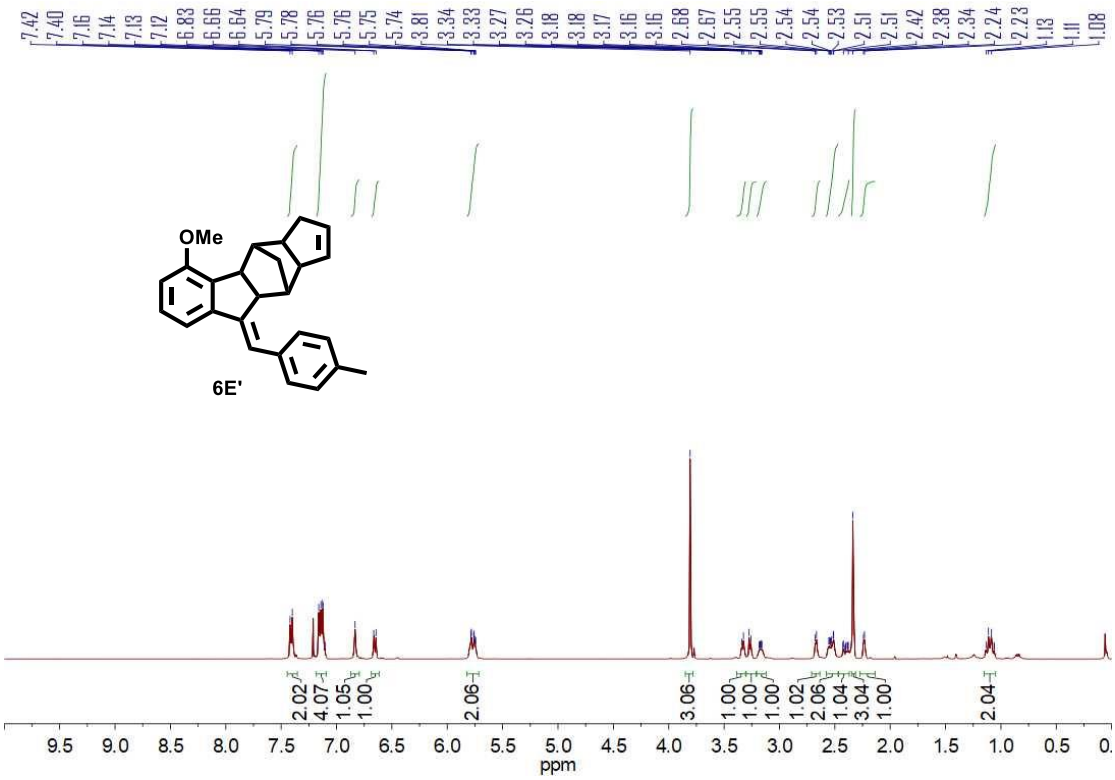


Figure S25. ^{1}H NMR spectrum of **6E'** in $CDCl_3$

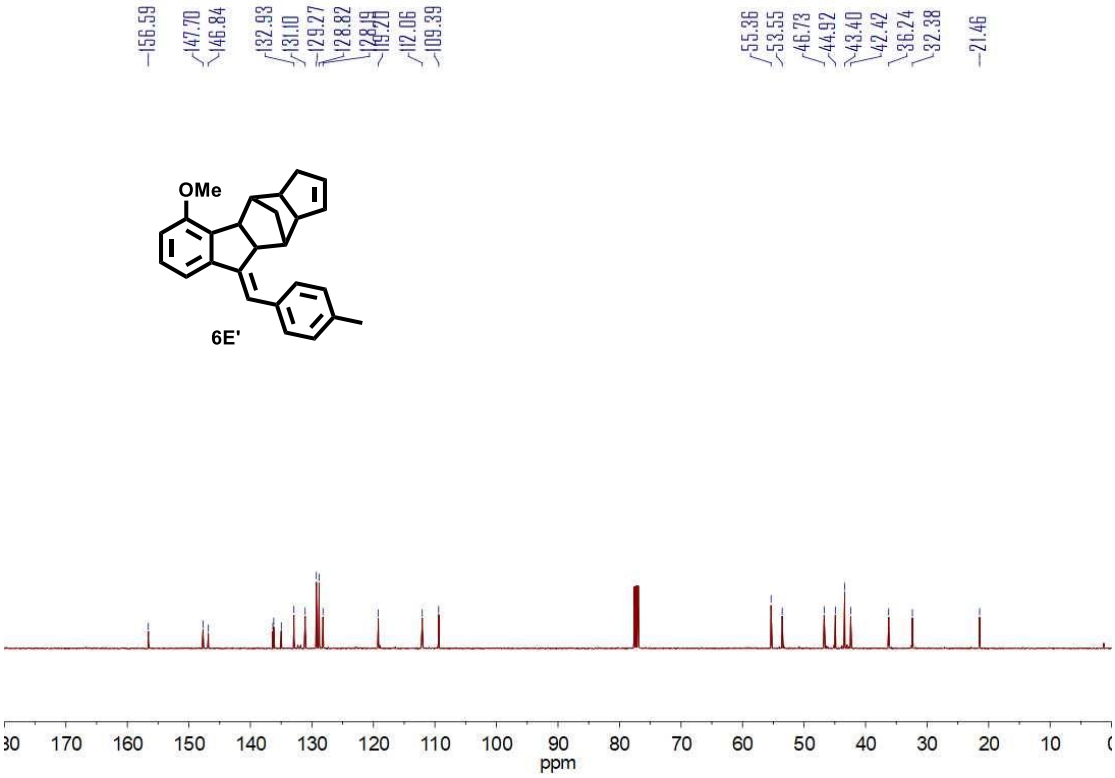


Figure S26. ^{13}C NMR spectrum of **6E'** in $CDCl_3$

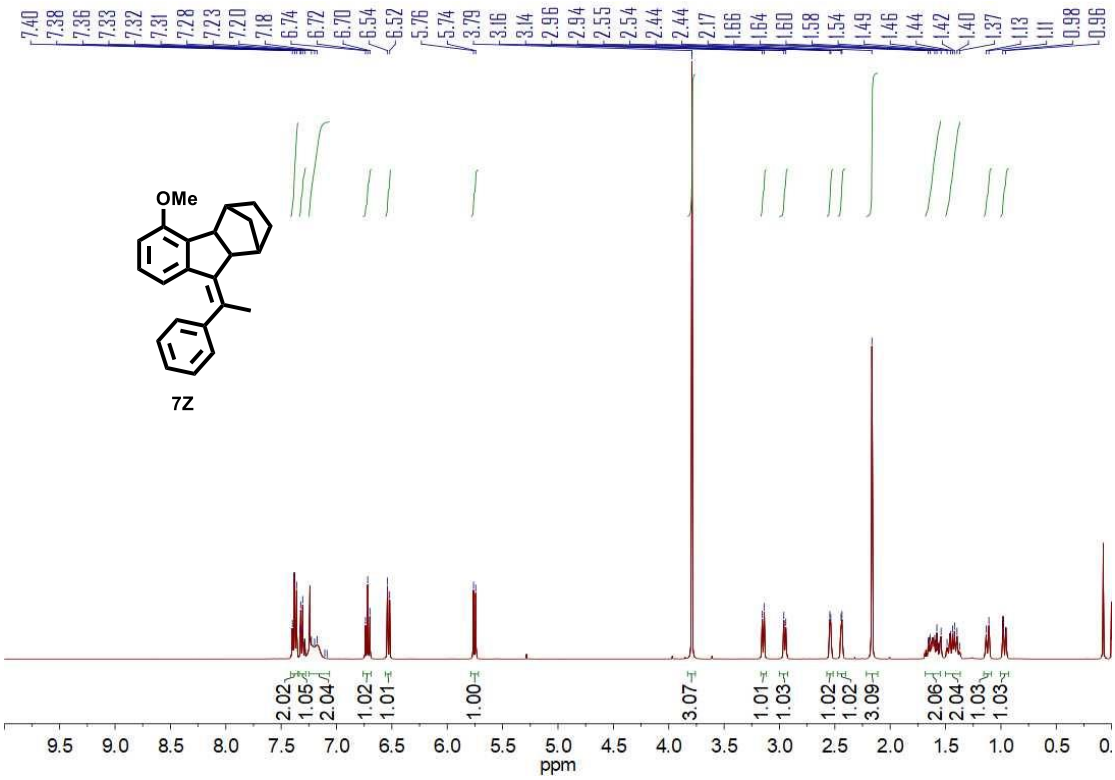


Figure S27. ^{1}H NMR spectrum of **7Z** in $CDCl_3$

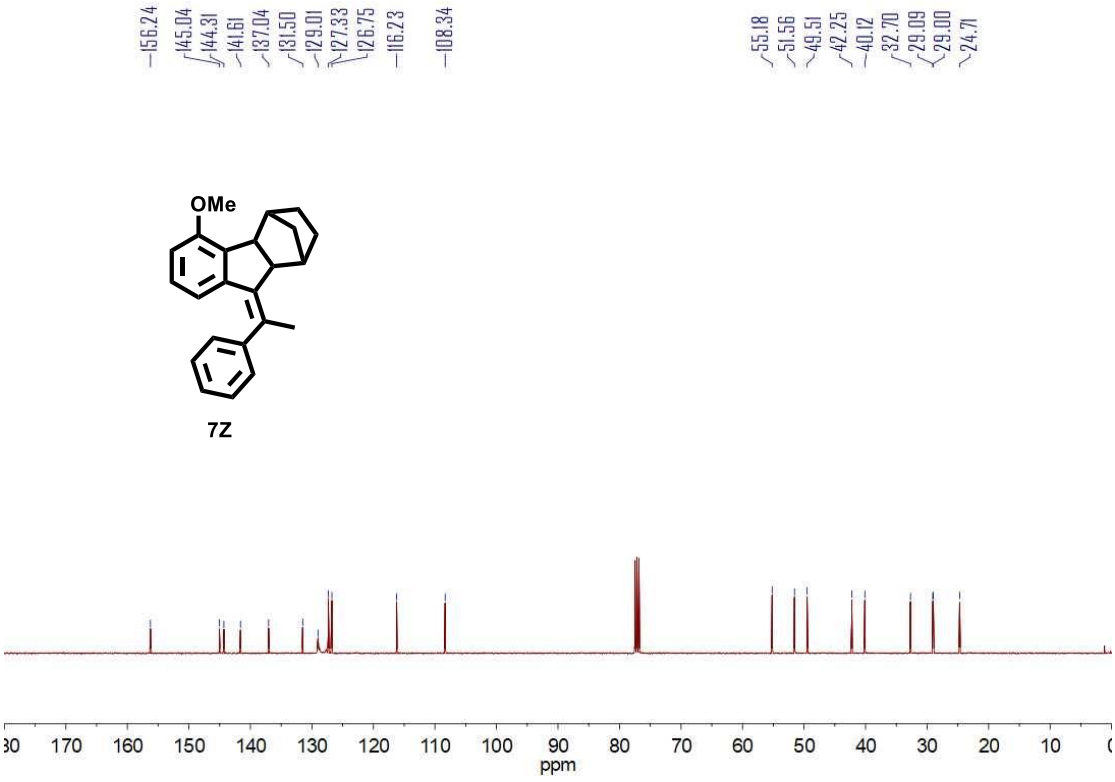


Figure S28. ^{13}C NMR spectrum of **7Z** in $CDCl_3$

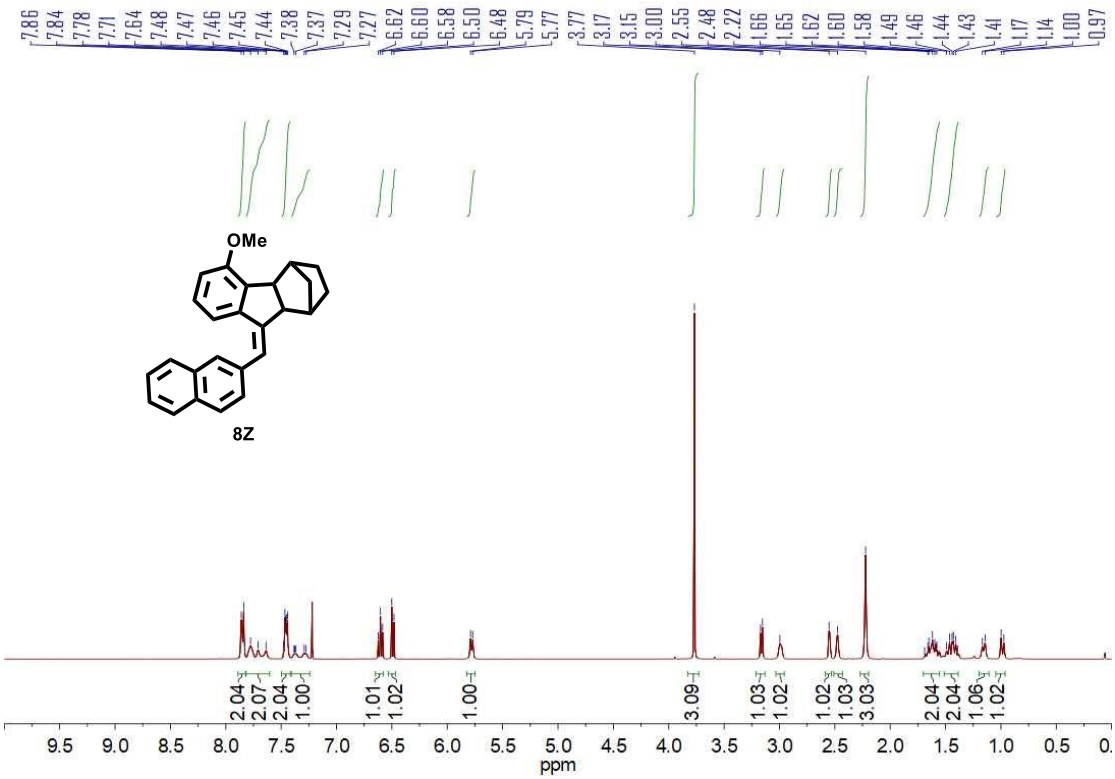


Figure S29. ^{1}H NMR spectrum of **8Z** in $CDCl_3$

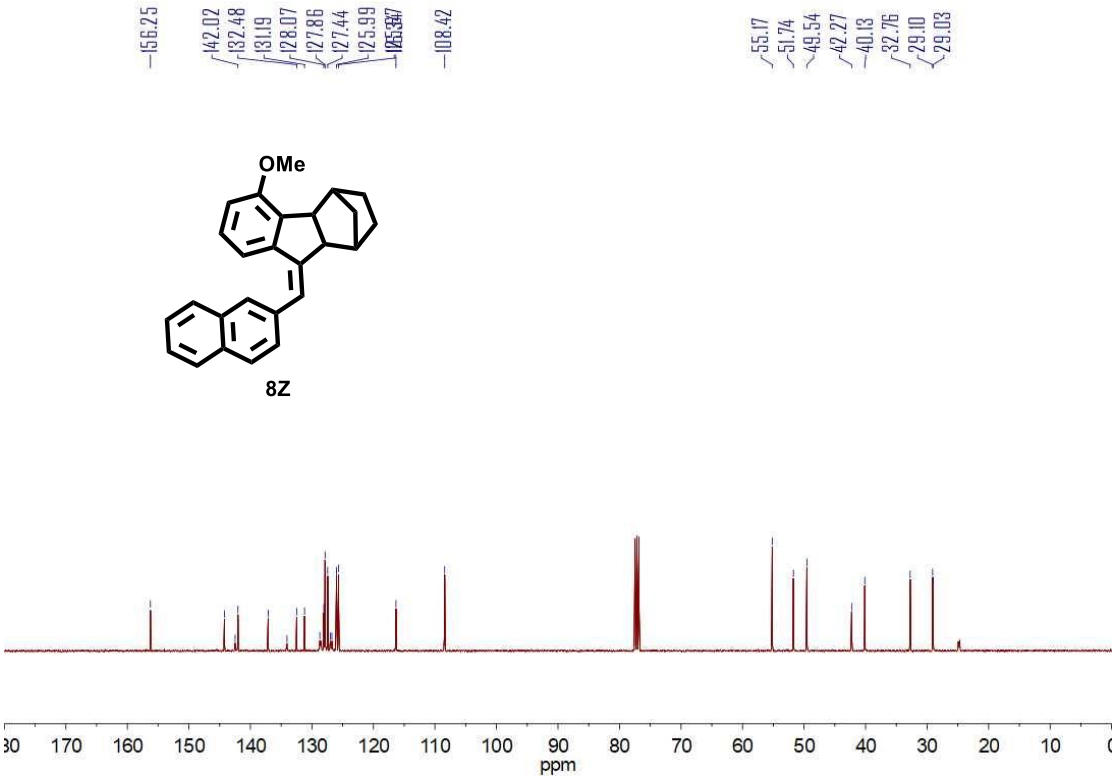


Figure S30. ^{13}C NMR spectrum of **8Z** in $CDCl_3$

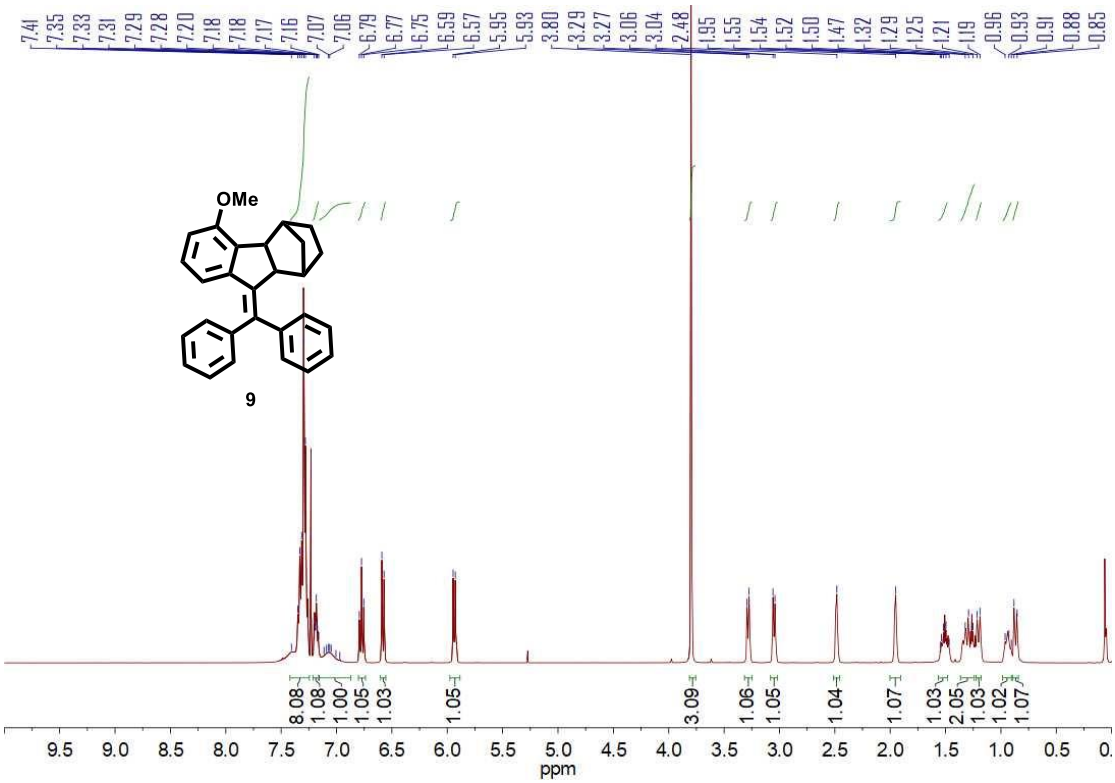


Figure S31. ^{1}H NMR spectrum of **9** in $CDCl_3$

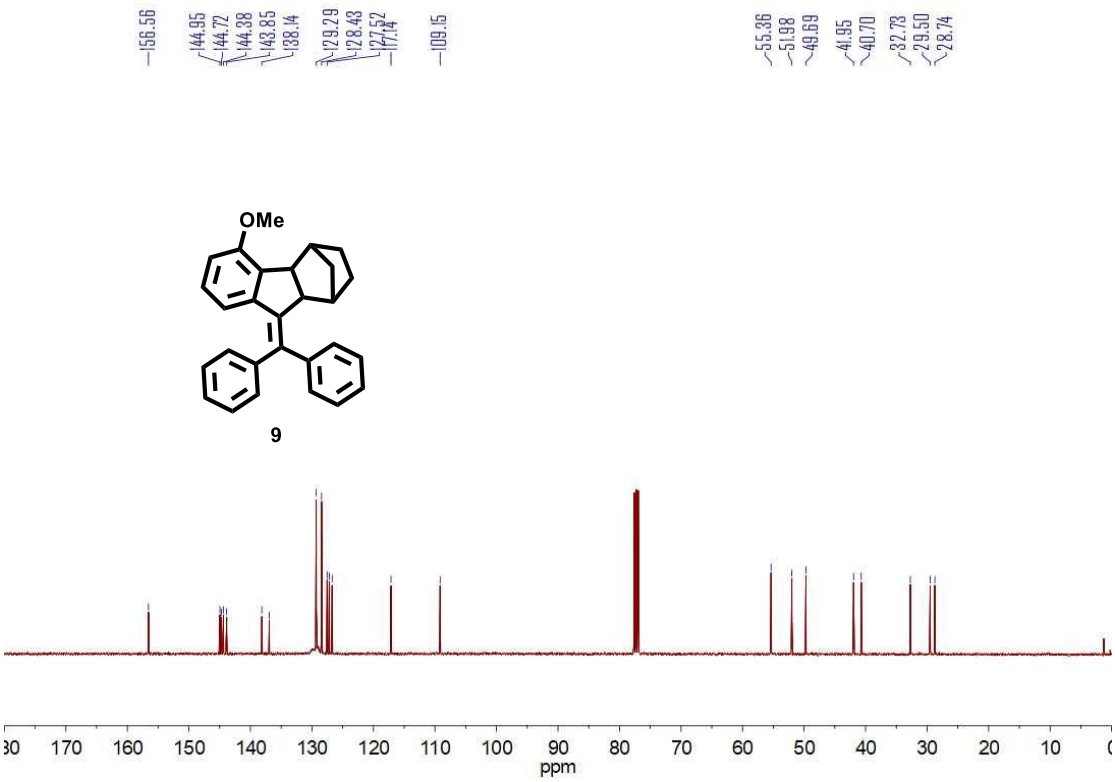


Figure S32. ^{13}C NMR spectrum of **9** in $CDCl_3$

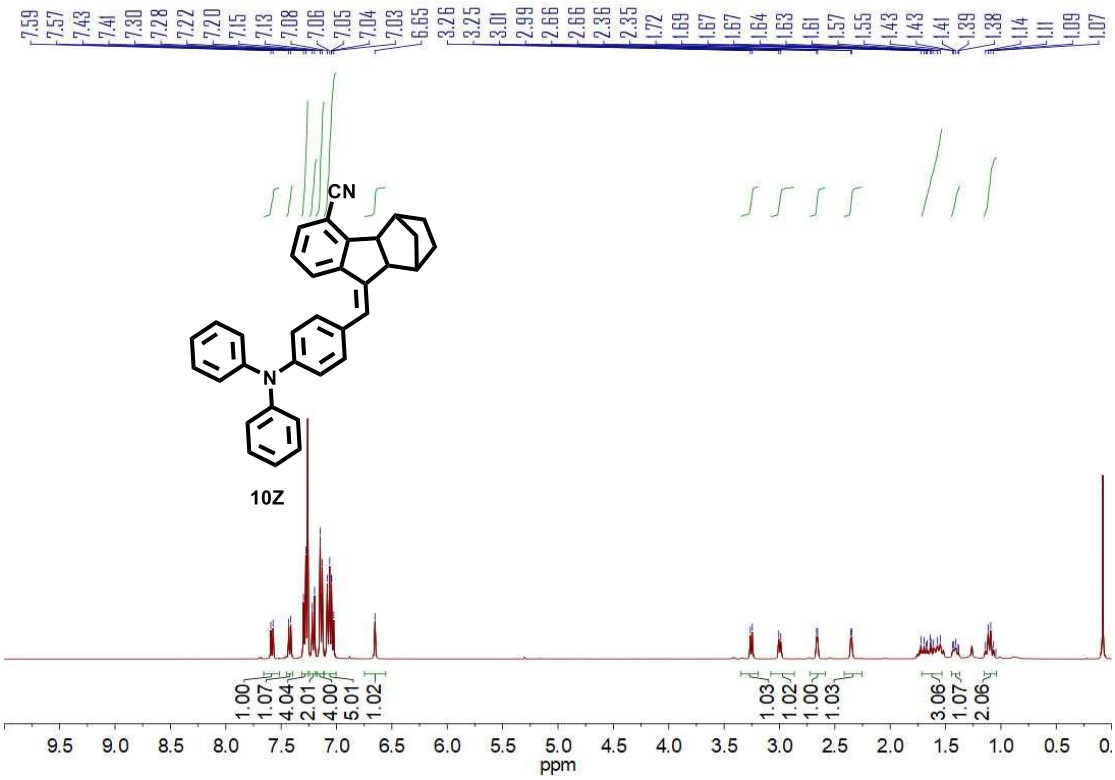


Figure S33. ^{1}H NMR spectrum of **10Z** in $CDCl_3$

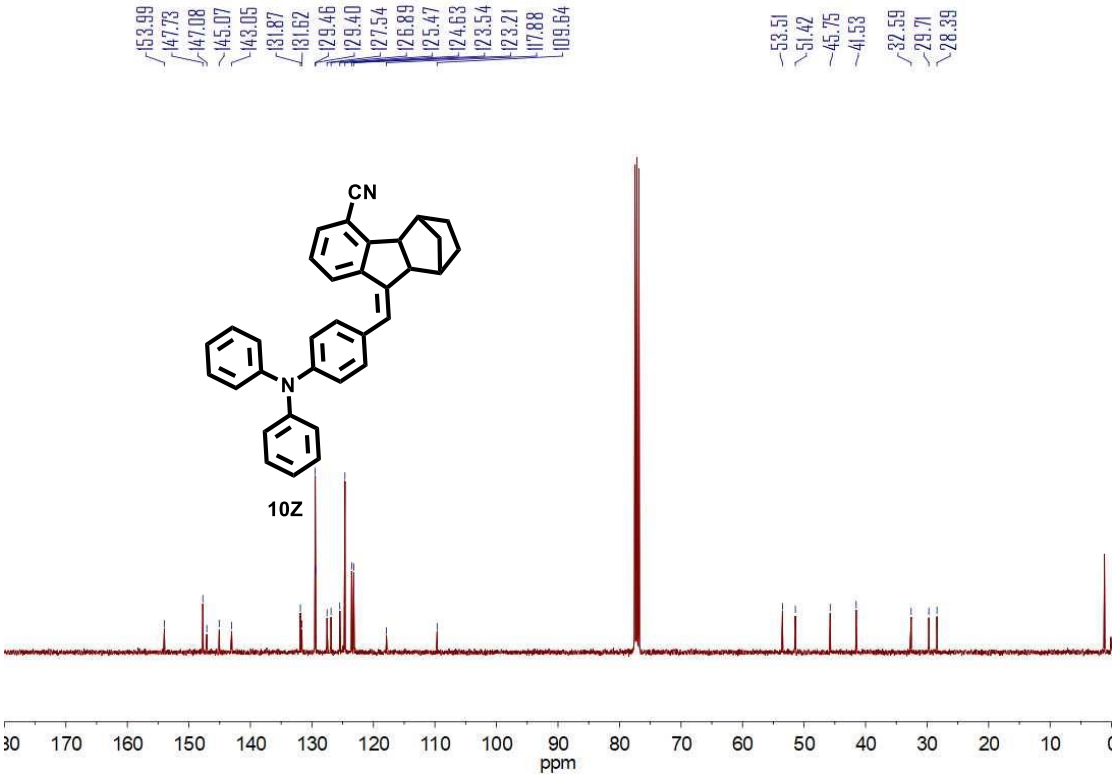


Figure S34. ^{13}C NMR spectrum of **10Z** in $CDCl_3$

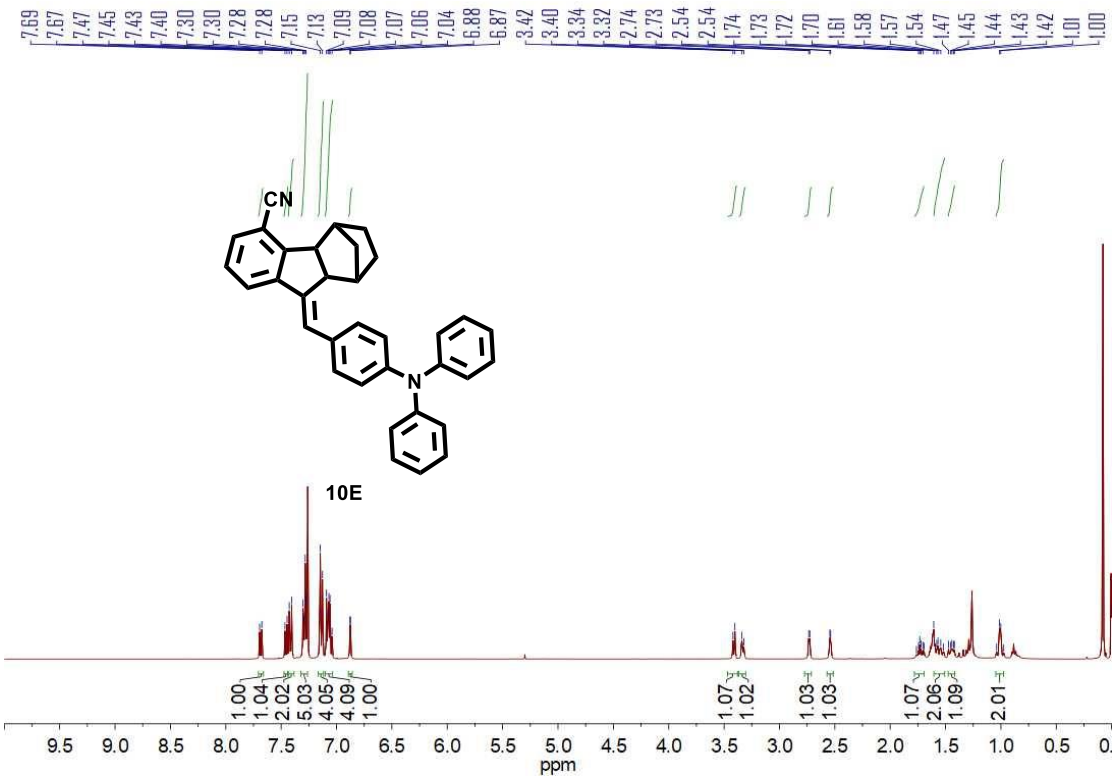


Figure S35. ^{1}H NMR spectrum of **10E** in $CDCl_3$

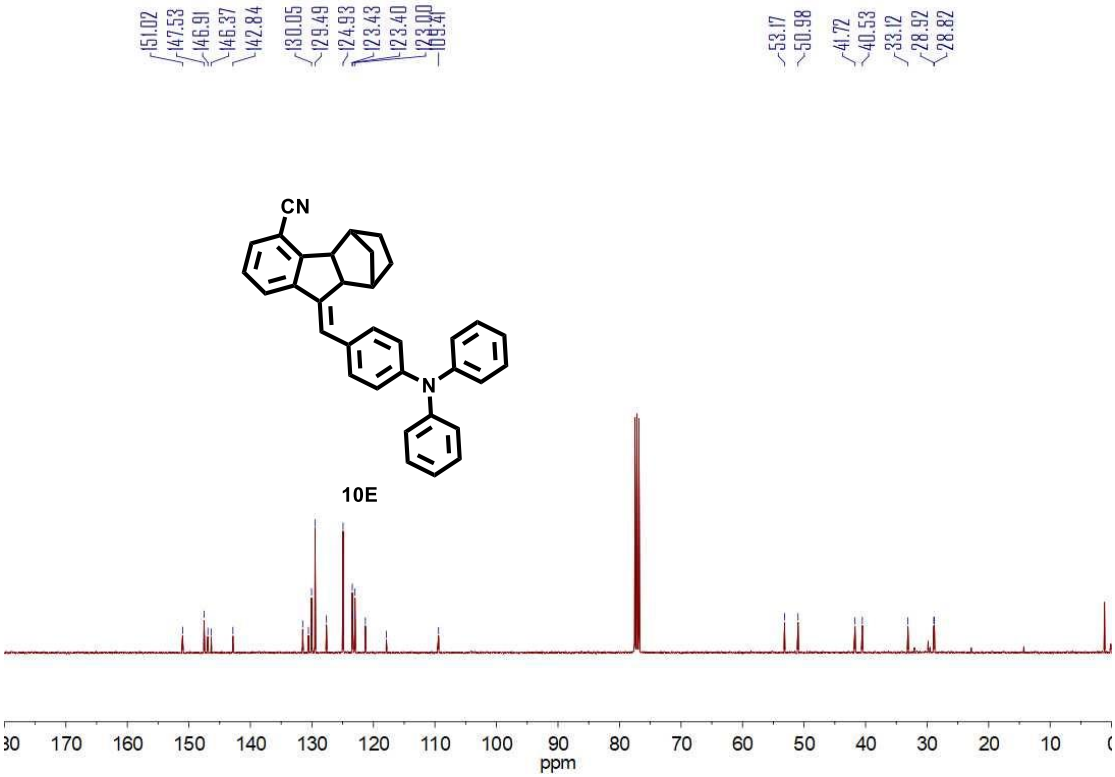


Figure S36. ^{13}C NMR spectrum of **10E** in $CDCl_3$

4. Dynamic Changes of ^{1}H NMR Spectra

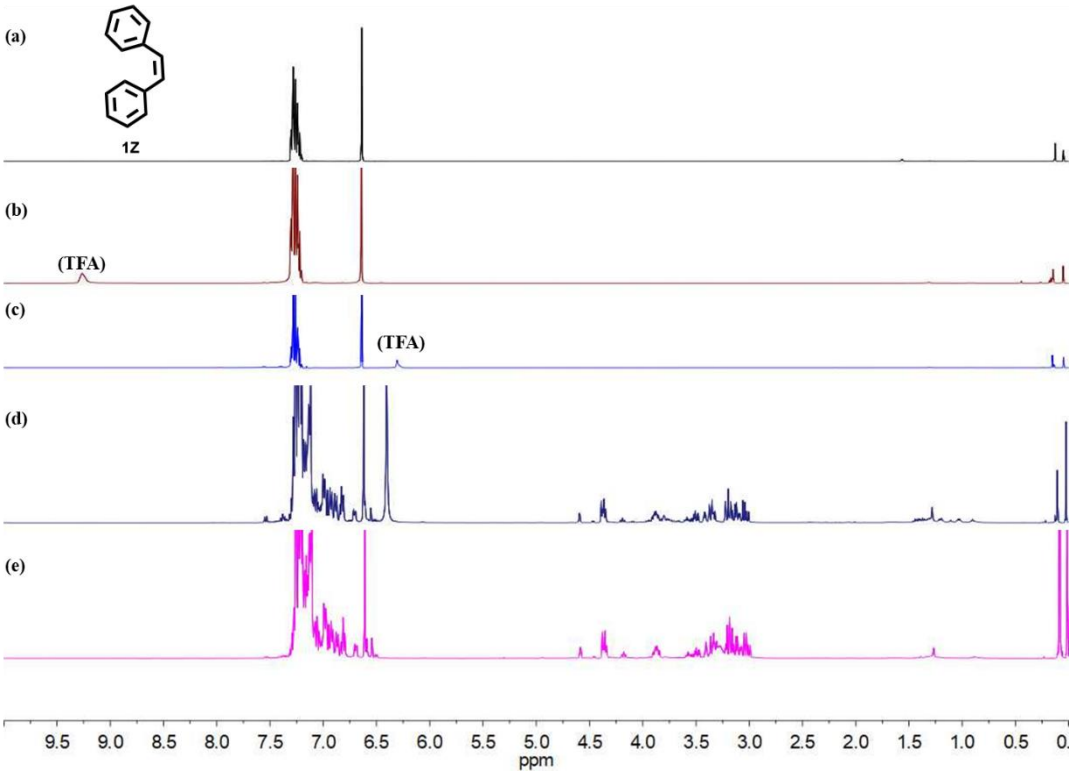


Figure S37. Comparison of the ^{1}H NMR spectra in $CDCl_3$. a) **1Z**; b) upon addition of 0.5 equiv TFA to **1Z** after 24 h; c) upon addition of 0.5 equiv TFA to **1Z** after 1 week; (d) ^{1}HNMR of the product prepared by the following steps: 20 mg **1Z** was dissolved in 1.0 ml TFA and was stirred for 12h at r.t., TFA was evaporated in vacuum to offer the product without further purification; (e) ^{1}HNMR of the product prepared with similar steps with (d) except for the long reaction time of 48 h.

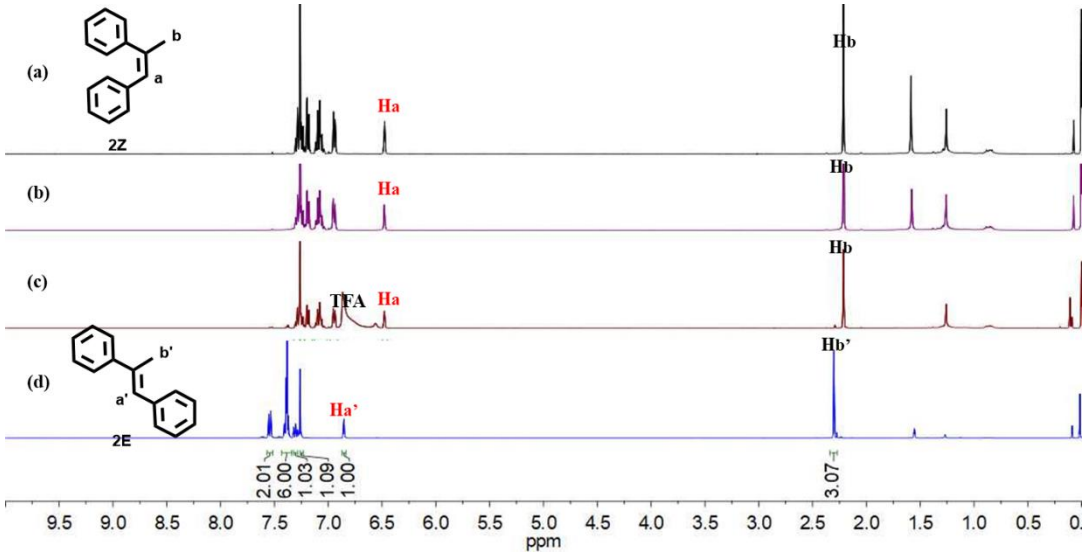


Figure S38. Comparison of the ^{1}H NMR spectra in $CDCl_3$. a) **2Z**; b) after 48h; c) 1 week later after addition of 0.5 equiv TFA to **2Z**; d) **2E**.

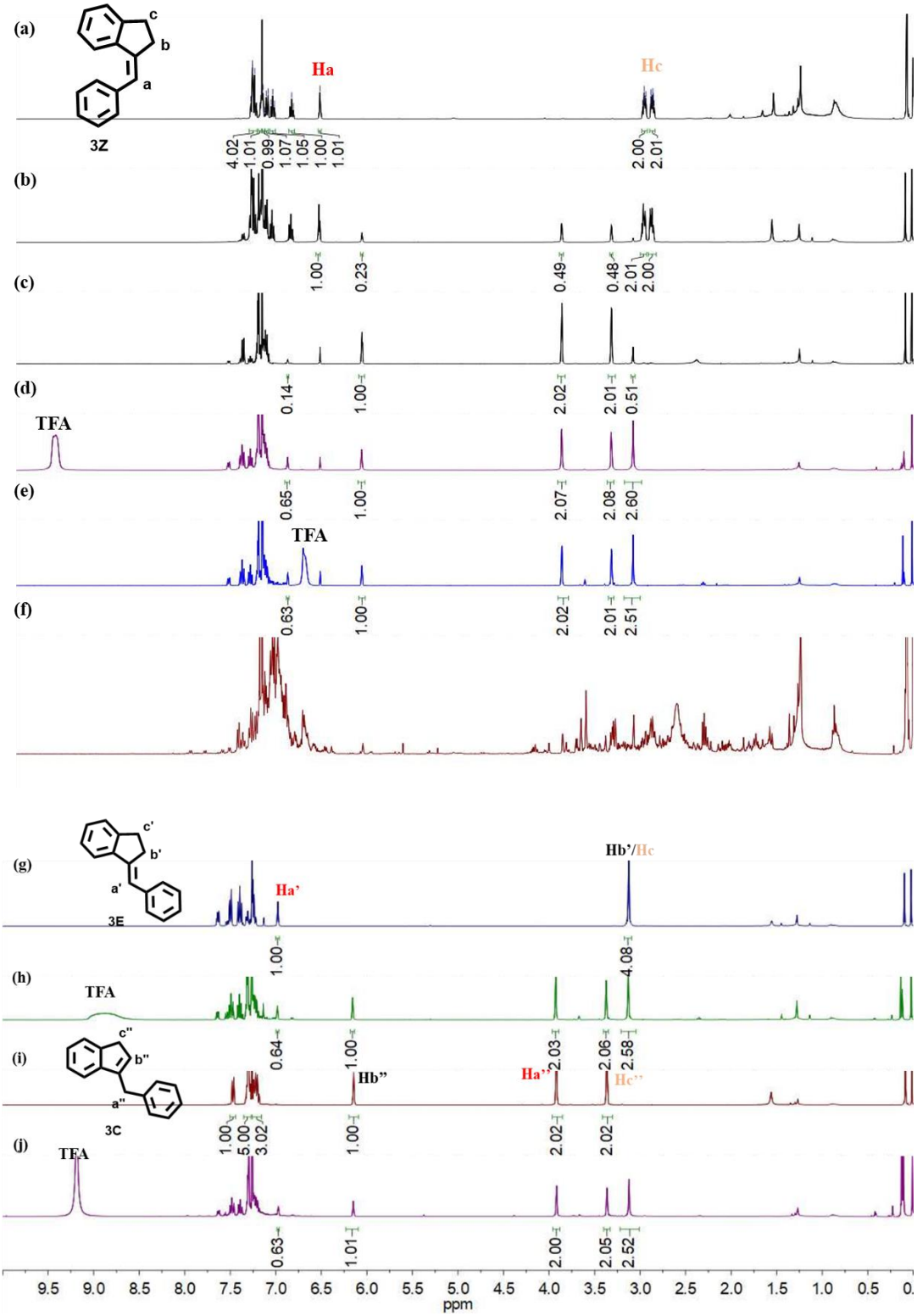
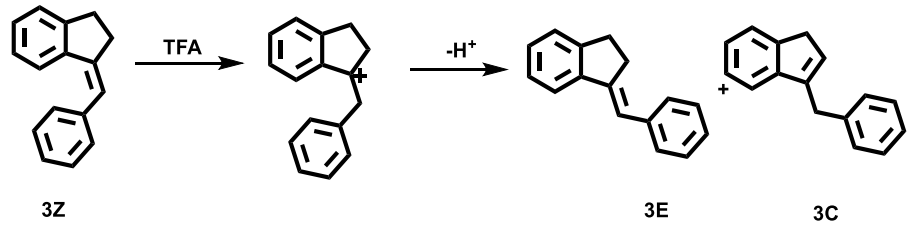


Figure S39. Comparison of the ^{1}H NMR spectra in $CDCl_3$. a) **3Z** in $CDCl_3$ with K_2CO_3 added to remove the tiny acid in the solvent; b) solution of **a** after 24 h; c) solution of **a** after 144 h; d) 24 h after addition of 0.5 equiv TFA to **3Z**; e) 96 h after addition of 0.5 equiv TFA to **3Z**; f) ^{1}HNMR of

the product prepared by the following steps:10 mg **3Z** dissolved in 1.0 ml TFA and was stirred for 12 h at r.t., TFA was evaporated in vacuum to offer the products without further purification; g) **3E** in $CDCl_3$ with K_2CO_3 added to remove the tiny acid in the solvent; h) 24 h after addition of 0.5 equiv TFA to **3E**; i) **3C** in $CDCl_3$ with K_2CO_3 added to remove tiny acid in solvent; j) 24 h after addition of 0.5 equiv TFA to **3C**.

Scheme S9. Possible mechanism of **3Z** transform to **3E** and **3C**



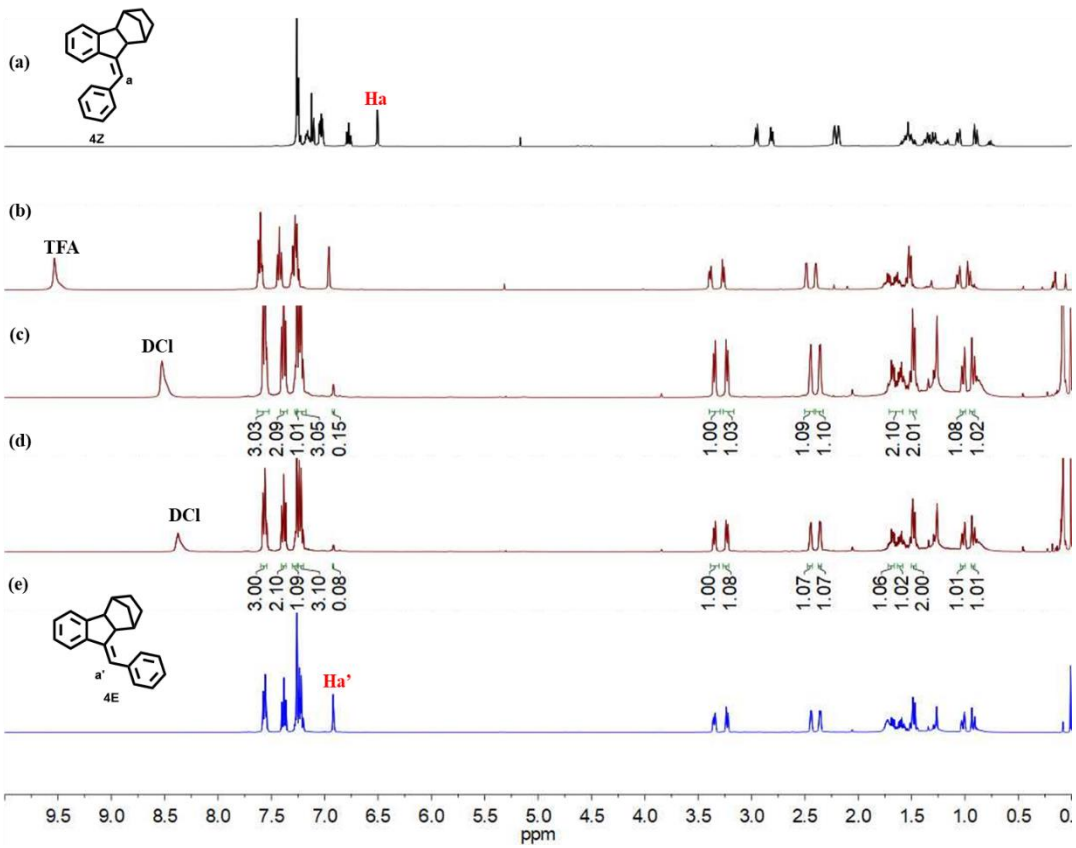


Figure S40. Comparison of the ^{1}H NMR spectra in $CDCl_3$. a) **4Z** in $CDCl_3$ with K_2CO_3 added to remove tiny acid in the solvent; b) upon addition of 0.5 equiv TFA to **4Z**; (c) 8 h later upon addition of 2.0 equiv DCl to **4Z**; d) 48h later .e) **4E** in $CDCl_3$.

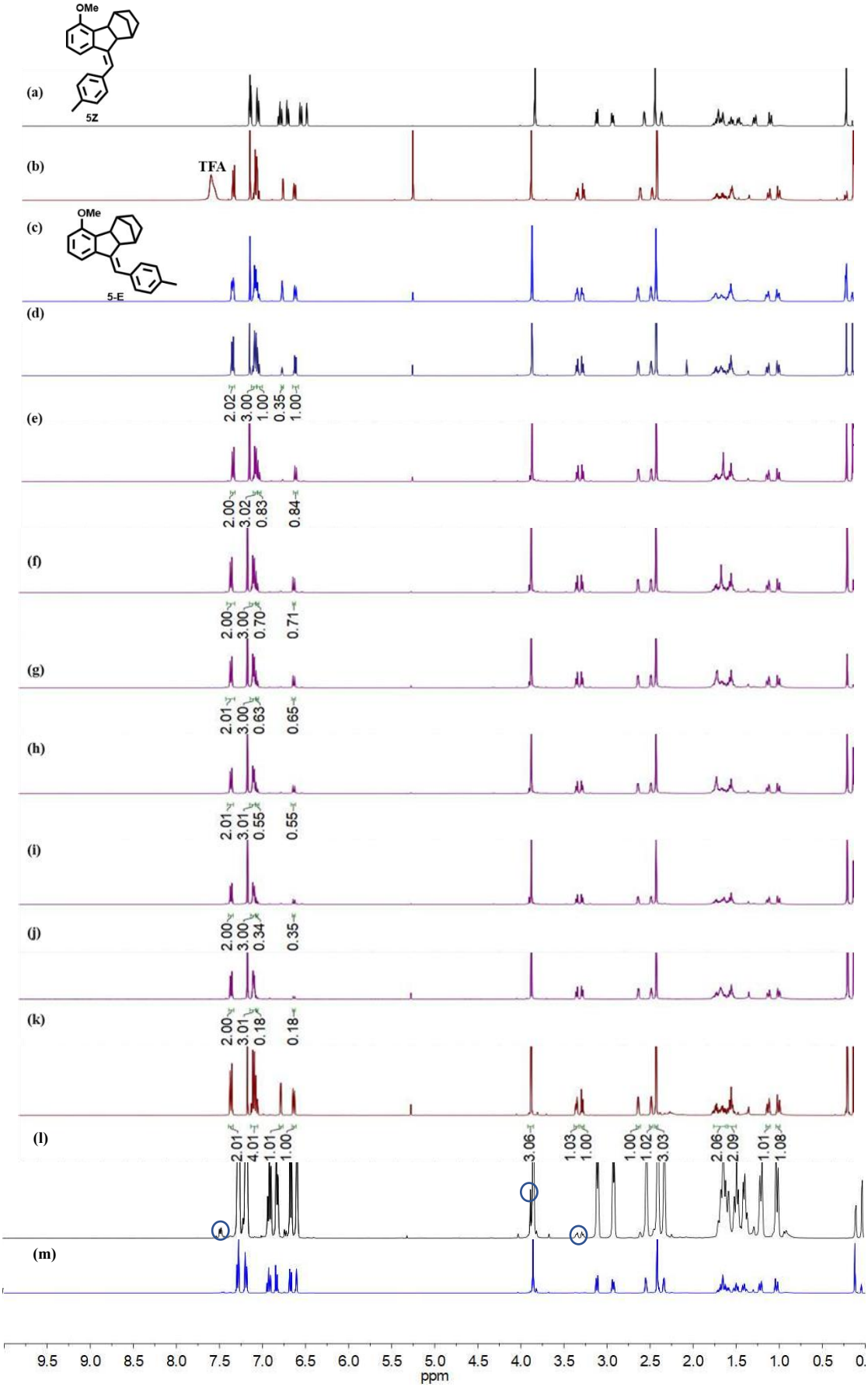
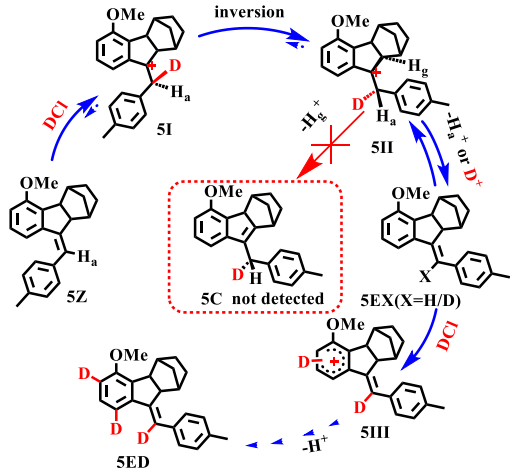

OMe
5Z
(a)
(b)
TFA
OMe
5-E
(c)
(d)
(e)
2.02
3.00
1.00
0.35
1.00
(f)
2.00
3.02
0.83
0.84
(g)
2.00
3.00
0.70
0.71
(h)
2.01
3.00
0.63
0.65
(i)
2.01
3.01
0.55
0.55
(j)
2.00
3.00
0.34
0.35
(k)
2.00
3.01
0.18
0.18
(l)
2.01
4.01
1.01
1.00
3.06
1.03
1.00
1.00
1.02
3.03
2.06
2.09
1.01
1.08
(m)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
ppm

Figure S41. Comparison of the ^{1}H NMR spectra in $CDCl_3$. a) **5Z** in $CDCl_3$ with K_2CO_3 added to remove tiny acid in the solvent); b) upon addition of 0.5 equiv TFA to **5Z**; c) **5E**; d) 2 h later upon addition of 2.0 equiv **DCl** to **5E**; e) 2 h later upon addition of 20.0 equiv **DCl** to **5Z**; f) 4 h later; g) 8 h later; h) 16 h later; i) 24 h later; j) 48 h later; (k) ^{1}HNMR of the product prepared by the following steps: 20 mg **5Z** dissolved in 1.0 ml TFA and was stirred for 12 h at r.t., TFA was evaporated in vacuum to offer the products without further purification; (l) **5Z** in new opened $CDCl_3$; (m) bubbling oxygen to the solution of **5Z** in $CDCl_3$.

Scheme S10. Proposed mechanism for the *Z*→*E* isomerization of **5Z**.



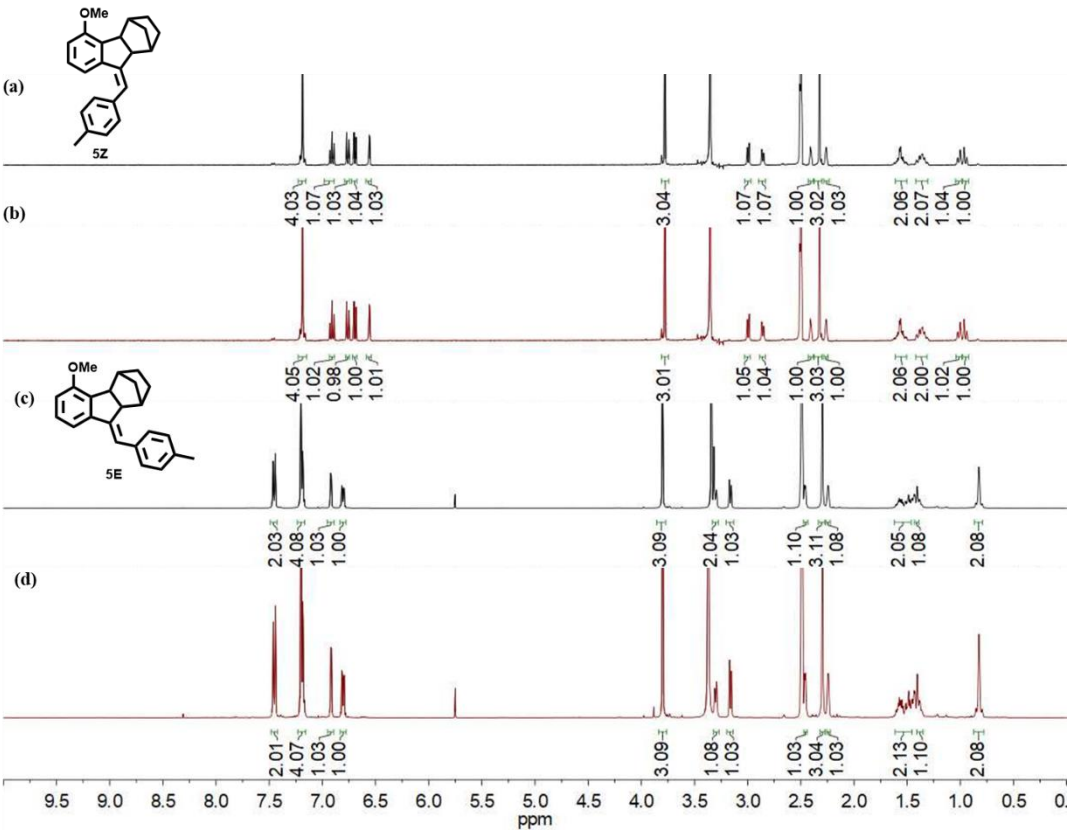


Figure S42. Comparison of the ^{1}H NMR spectra. a) **5Z** in DMSO; b) **5Z** in DMSO after heating at 130°C for 24 h; c) **5E** in DMSO; d) **5E** in DMSO after heating at 130°C for 24 h.

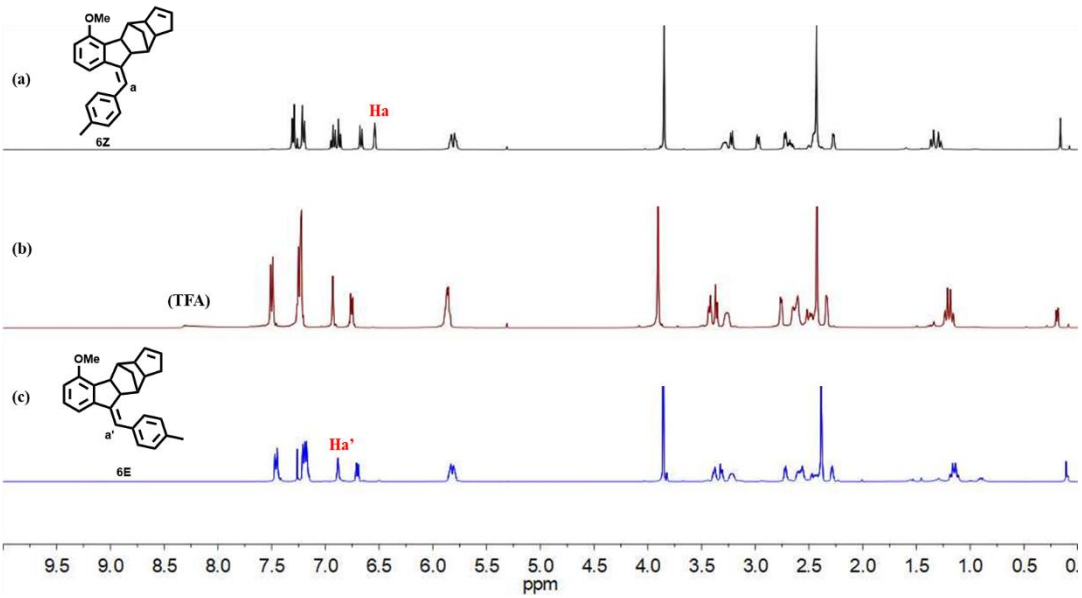


Figure S43. Comparison of the ^{1}H NMR spectra in $CDCl_3$: a) **6Z** in $CDCl_3$ with K_2CO_3 added to remove tiny acid in the solvent; b) upon addition of 0.5 equiv TFA to **6Z**; c) **6E**.

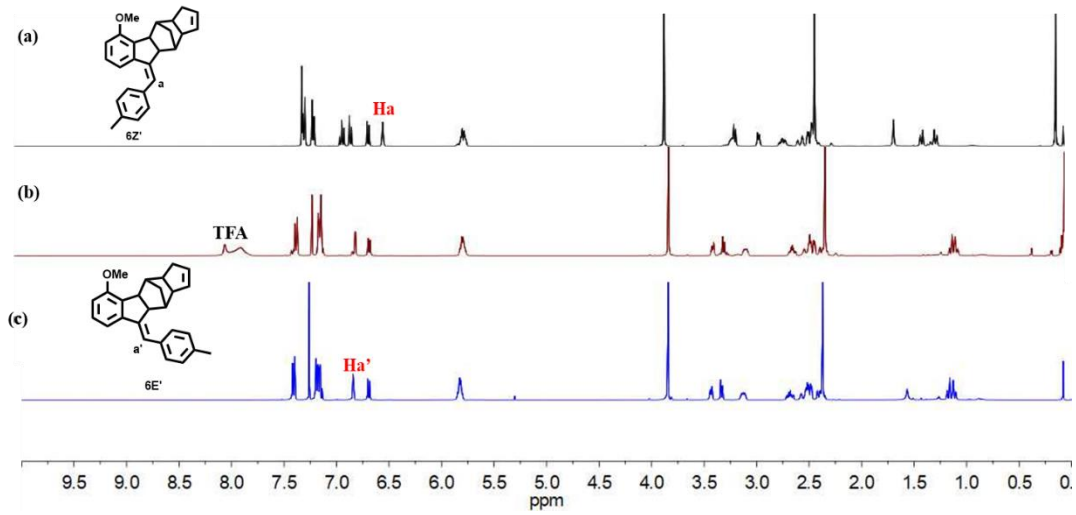


Figure S44. Comparison of the ^{1}H NMR spectra in $CDCl_3$. a) **6Z'** in $CDCl_3$ with K_2CO_3 added to remove tiny acid in the solvent); b) upon addition of 0.5 equiv TFA to **6Z'**; c) **6E'**.

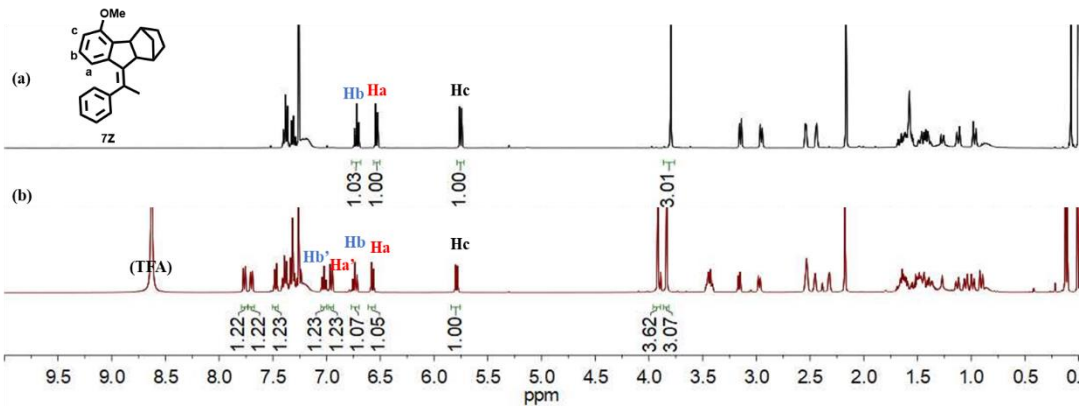


Figure S45. Comparison of ^{1}H NMR spectra in $CDCl_3$. a) **7Z**; b) upon addition of 0.5 equiv TFA to **7Z**.

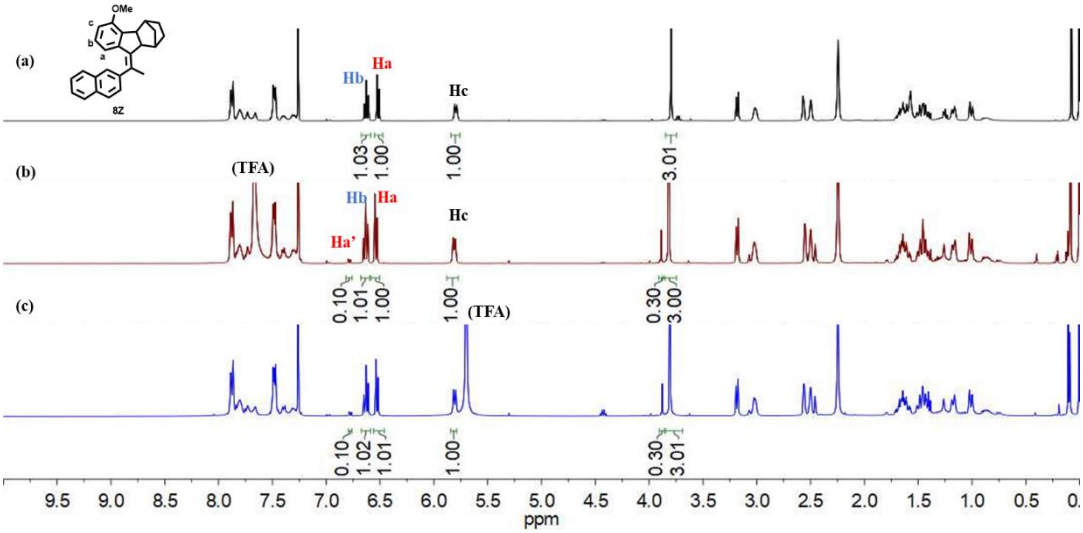


Figure S46. Comparison of ^{1}H NMR spectra in $CDCl_3$. a) **8Z**; b) 24 h later upon addition of 0.5 equiv TFA to **8Z**; c) 96 h later.

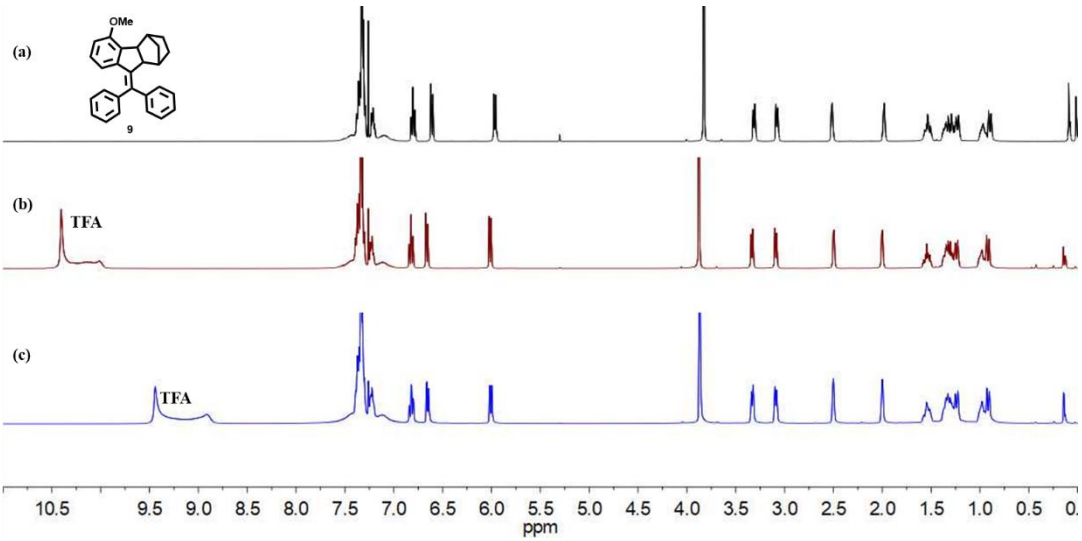


Figure S47. Comparison of ^{1}H NMR spectra in $CDCl_3$. a) **9**; b) 24 h later upon addition of 2.0 equiv TFA to **9**; c) 96 h later.

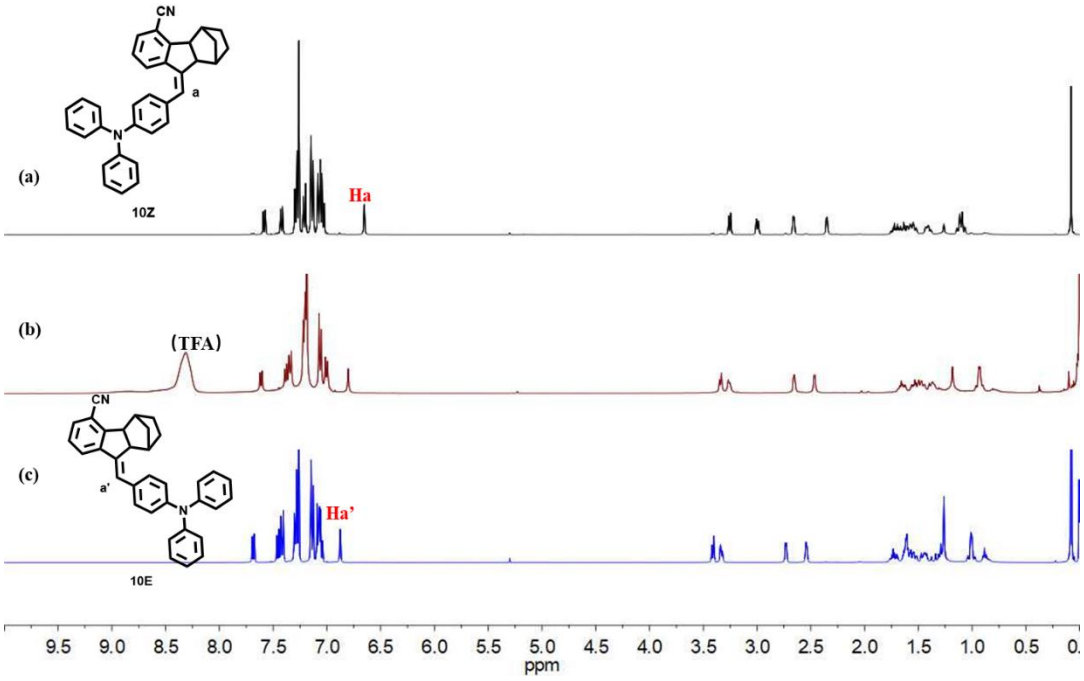


Figure S48. Comparison of ^{1}H NMR spectra in $CDCl_3$. a) **10Z**; b) upon addition of 0.5 equiv. TFA to **10Z**; c) **10E**.

5 . X-ray Data of Compounds 5Z, 5E1, 5E2 6Z, 6E, 7Z and 9 .

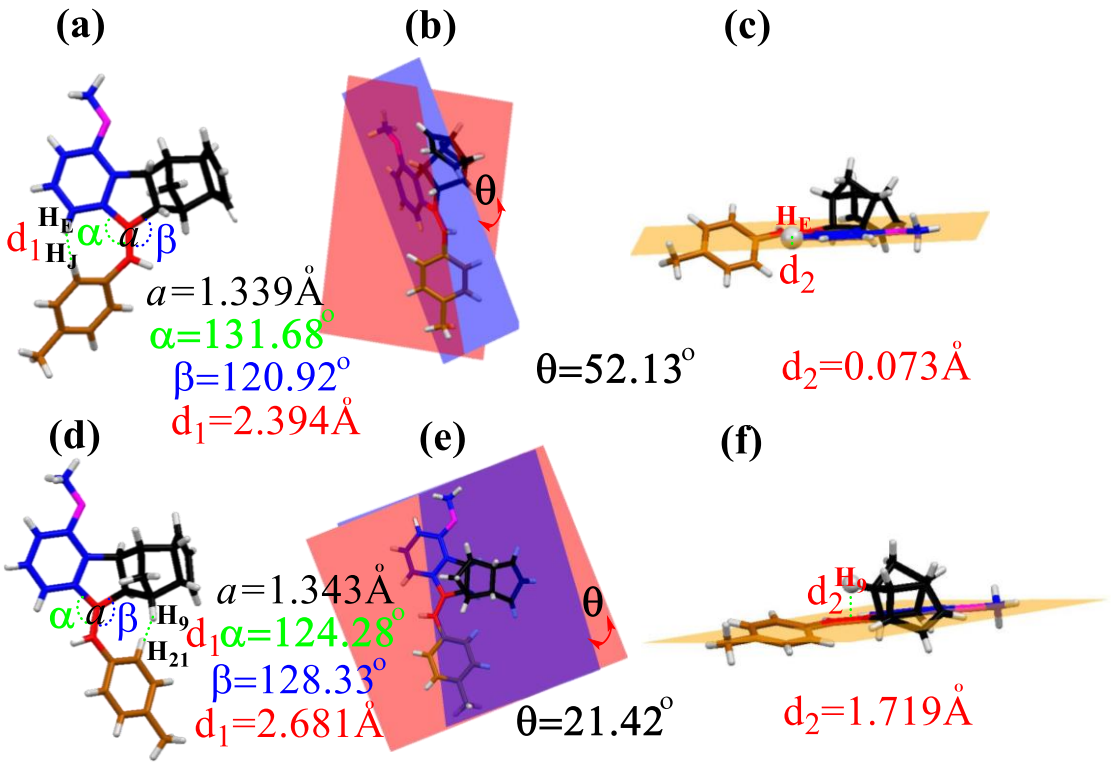


Figure S49. Single crystal structures of **6Z**, **6E** (thermal ellipsoid plots at the 50% probability level). (a)The studied parameter for **6Z**:the length of C=C(*a*); bond angle(α,β); the distance between H_E-H_J(d_1) ; (b) dihedral angle(θ) of two benzene ring planes in **6Z**; (c) the distance H_E to C=C plane(d_2); (d) ,(e), (f) The studied parameter for **6E**.

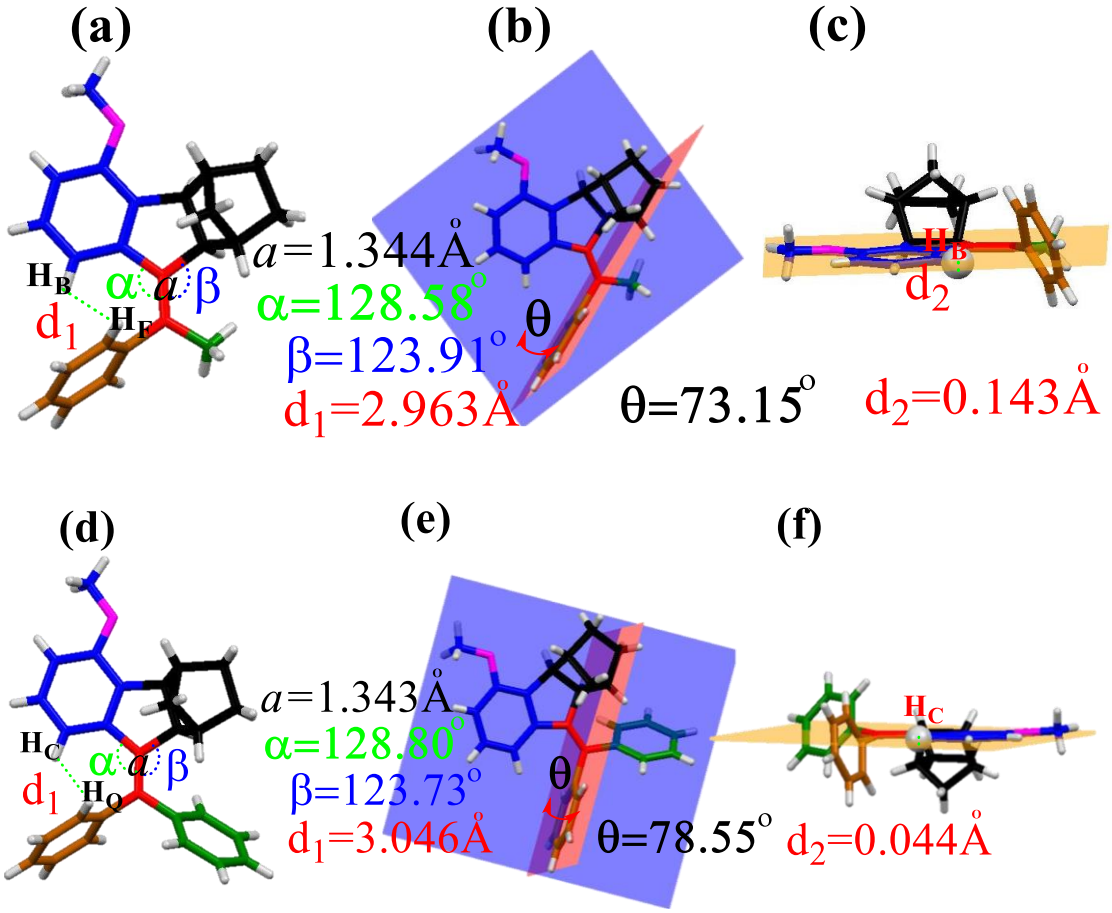


Figure S50. Single crystal structures of **7Z**, **9** (thermal ellipsoid plots at the 50% probability level). (a)The studied parameter for **7Z**: the length of C=C(*a*); bond angle(α,β); the distance between H_B-H_F(d_1) ; (b) dihedral angle(θ) of two benzene ring planes in **7Z**; (c) the distance H_B to C=C plane(d_2); (d) ,(e), (f) The studied parameter for **9**.

Table S2 : The studied parameter for **5Z**, **5E**, **6Z**, **6E**, **7Z** and **9**.

Parameter / Molecular	Bond lengths	Bond angles		Dihedral angles	Distance	
	a (Å)	α (°)	β (°)	θ (°)	d1 (Å)	d2 (Å)
5Z	1.336	130.53	121.65	56.15	2.533	0.162
5E	1.344	124.00	128.12	36.48	2.718	1.613
6Z	1.339	131.68	120.92	52.13	2.394	0.073
6E	1.343	124.28	128.33	21.42	2.681	1.719
7Z	1.344	128.58	123.91	73.55	2.963	0.143
9	1.343	128.80	123.73	78.55	3.046	0.044

5.1. X-ray Data of Compounds 5Z. Ellipsoids drawn at the 50% probability level.

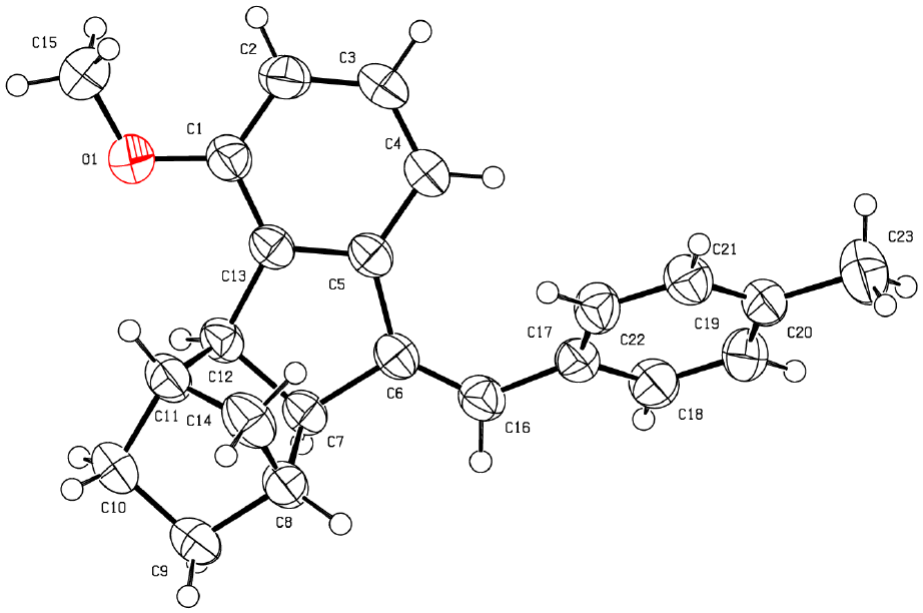


Table S3. Crystal data and structure refinement for **5Z**.

Identification code	1949916
Empirical formula	$C_{23}H_{24}O$
Formula weight	316.42
Temperature/K	293.15
Crystal system	triclinic
Space group	P-1
a/Å	9.4684(6)
b/Å	10.1128(6)
c/Å	11.1589(9)
α/°	111.746(7)
β/°	114.773(7)
γ/°	91.316(5)
Volume/Å^3	880.77(12)
Z	2
ρcalcg/cm^3	1.193
μ/mm^{-1}	0.071
F(000)	340.0
Crystal size/mm^3	0.35 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.972 to 52.742
Index ranges	-11 ⩽ h ⩽ 11, -12 ⩽ k ⩽ 12, -13 ⩽ l ⩽ 13
Reflections collected	6849

Independent reflections	3587 [R_{int} = 0.0144, R_{sigma} = 0.0301]
Data/restraints/parameters	3587/0/219
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0473, wR_2 = 0.1125
Final R indexes [all data]	R_1 = 0.0685, wR_2 = 0.1276
Largest diff. peak/hole / e $Å^{-3}$	0.20/-0.17

5.2. X-ray Data of Compounds 5E1. Ellipsoids drawn at the 50% probability level.

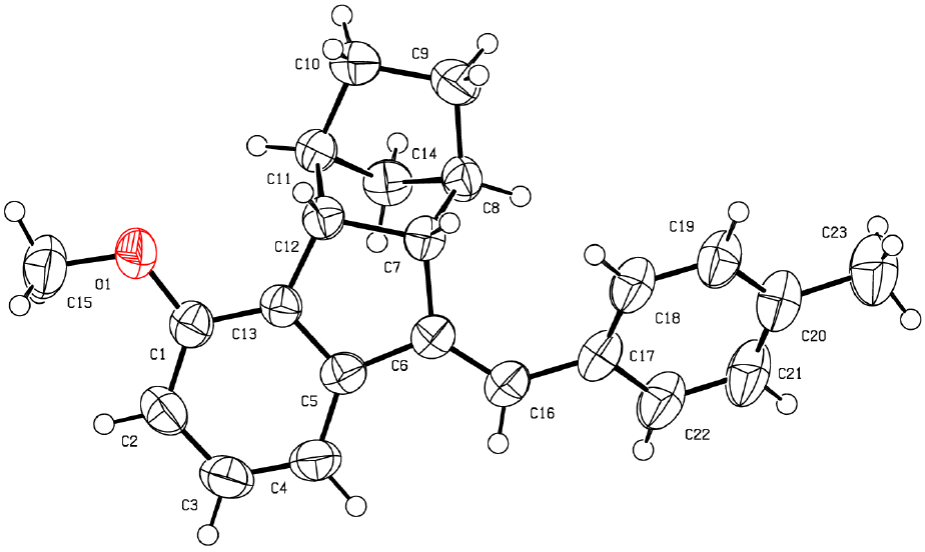


Table S4. Crystal data and structure refinement for **5E1.**

Identification code	1949886
Empirical formula	$C_{23}H_{24}O$
Formula weight	316.42
Temperature/K	293.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.0878(5)
b/Å	7.9427(6)
c/Å	36.134(3)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	1747.2(3)
Z	4
ρcalcg/cm^3	1.203
μ/mm^{-1}	0.071
F(000)	680.0
Crystal size/mm^3	0.4 × 0.15 × 0.05

Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.144 to 52.728
Index ranges	-7 ⩽ h ⩽ 6, -9 ⩽ k ⩽ 9, -41 ⩽ l ⩽ 44
Reflections collected	7936
Independent reflections	3276 [R_{int} = 0.0325, R_{sigma} = 0.0508]
Data/restraints/parameters	3276/0/219
Goodness-of-fit on F^2	1.012
Final R indexes [I>=2σ (I)]	R_1 = 0.0495, wR_2 = 0.0975
Final R indexes [all data]	R_1 = 0.0754, wR_2 = 0.1095
Largest diff. peak/hole / e $Å^{-3}$	0.12/-0.15

5.3. X-ray Data of Compounds 5E2. Ellipsoids drawn at the 50% probability level.

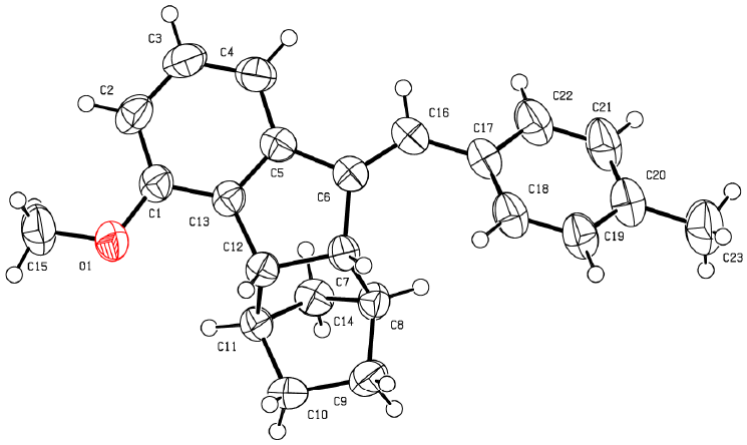


Table S5. Crystal data and structure refinement for **5E2.**

Identification code	1949886
Empirical formula	$C_{23}H_{24}O$
Formula weight	316.42
Temperature/K	293.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.0783(3)
b/Å	7.9438(4)
c/Å	36.1259(16)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	1744.33(13)
Z	4
ρcalcg/cm^3	1.205
μ/mm^{-1}	0.072
F(000)	680.0

Crystal size/mm^3	0.35 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.144 to 52.744
Index ranges	-7 ≤ h ≤ 6, -9 ≤ k ≤ 9, -45 ≤ l ≤ 41
Reflections collected	9136
Independent reflections	3468 [R_{int} = 0.0278, R_{sigma} = 0.0429]
Data/restraints/parameters	3468/0/219
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0498, wR_2 = 0.1034
Final R indexes [all data]	R_1 = 0.0697, wR_2 = 0.1167
Largest diff. peak/hole / e Å^{-3}	0.14/-0.19

5.4. X-ray Data of Compounds 6E. Ellipsoids drawn at the 50% probability level.

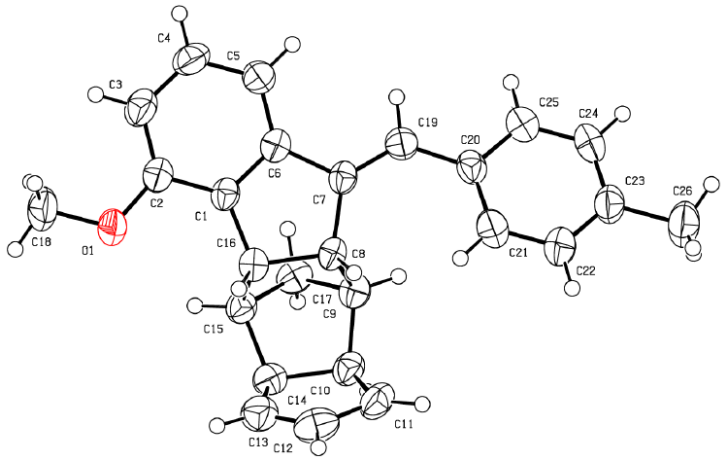


Table S6. Crystal data and structure refinement for **6E.**

Identification code	1949917
Empirical formula	$C_{26}H_{25}O$
Formula weight	353.46
Temperature/K	293.15
Crystal system	monoclinic
Space group	I2
a/Å	11.9345(13)
b/Å	7.2394(8)
c/Å	22.679(2)
α/°	90
β/°	99.029(11)
γ/°	90
Volume/Å^3	1935.2(4)
Z	4
ρcalcg/cm^3	1.213

μ/mm^{-1}	0.072
F(000)	756.0
Crystal size/mm^3	0.35 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.914 to 52.734
Index ranges	-14 ≤ h ≤ 14, -7 ≤ k ≤ 9, -28 ≤ l ≤ 28
Reflections collected	4757
Independent reflections	3120 [R_{int} = 0.0273, R_{sigma} = 0.0523]
Data/restraints/parameters	3120/1/246
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0530, wR_2 = 0.1194
Final R indexes [all data]	R_1 = 0.0749, wR_2 = 0.1344
Largest diff. peak/hole / e $Å^{-3}$	0.27/-0.16

6. Photophysical and Chiral Optical Properties

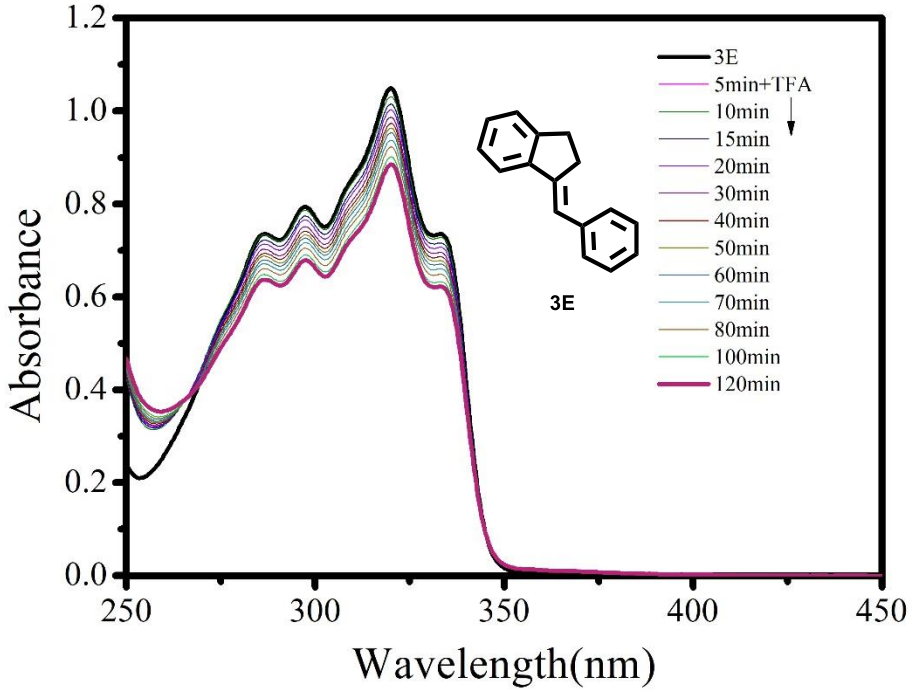


Figure S51. Changes of UV−vis spectra of **3E** (5×10^{-5} M in DCM) after addition of TFA (V_{TFA} : V_{DCM} = 0.0033) for different time periods.

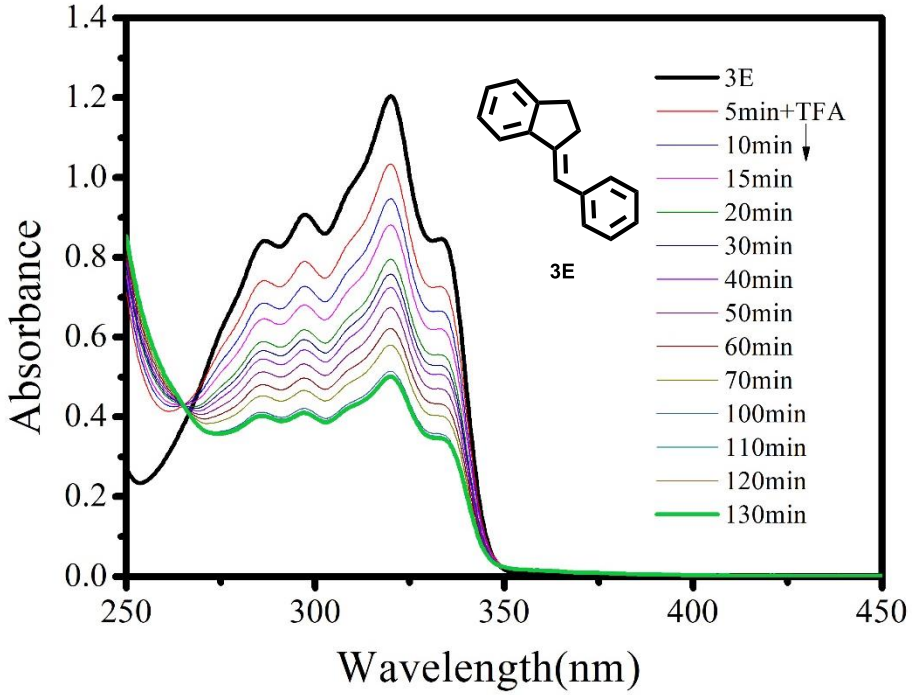


Figure S52. Changes of UV−vis spectra of **3E** (5×10^{-5} M in DCM) after addition of TFA (V_{TFA} : V_{DCM} = 0.033) for different time periods.

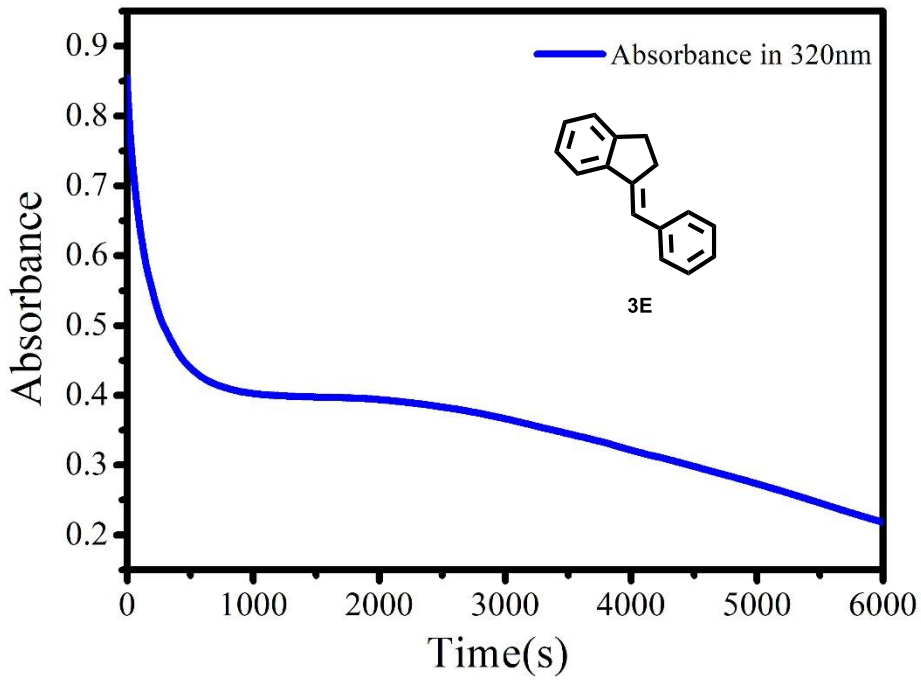


Figure S53. Changes in time for **3E** (5×10^{-5} M in DCM) absorbance in 320 nm after addition of TFA (V_{TFA} : V_{DCM} = 0.033).

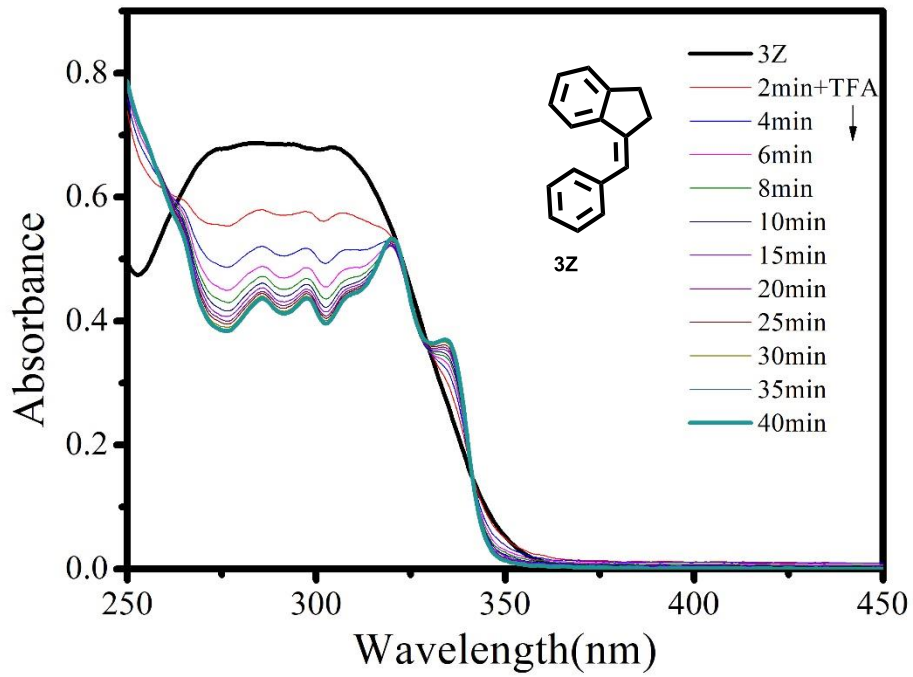


Figure S54. Changes of UV−vis spectra of **3Z** (5×10^{-5} M in DCM) after addition of TFA (V_{TFA} : V_{DCM} = 0.0033) for different time periods.

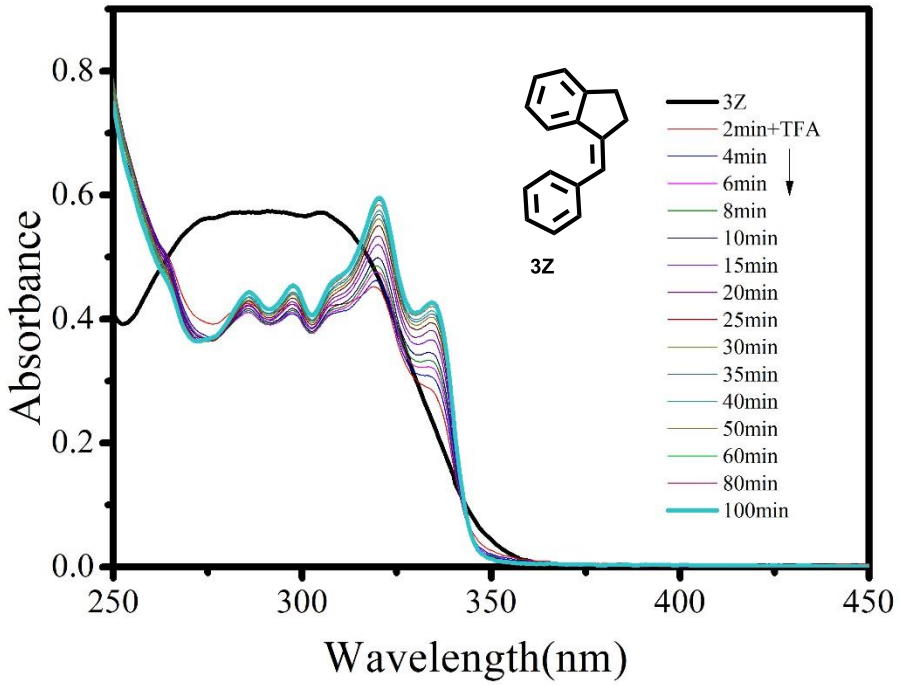


Figure S55. Changes of UV−vis spectra of **3Z** (5×10^{-5} M in DCM) after addition of TFA (V_{TFA} : V_{DCM} = 0.0066) for different time periods.

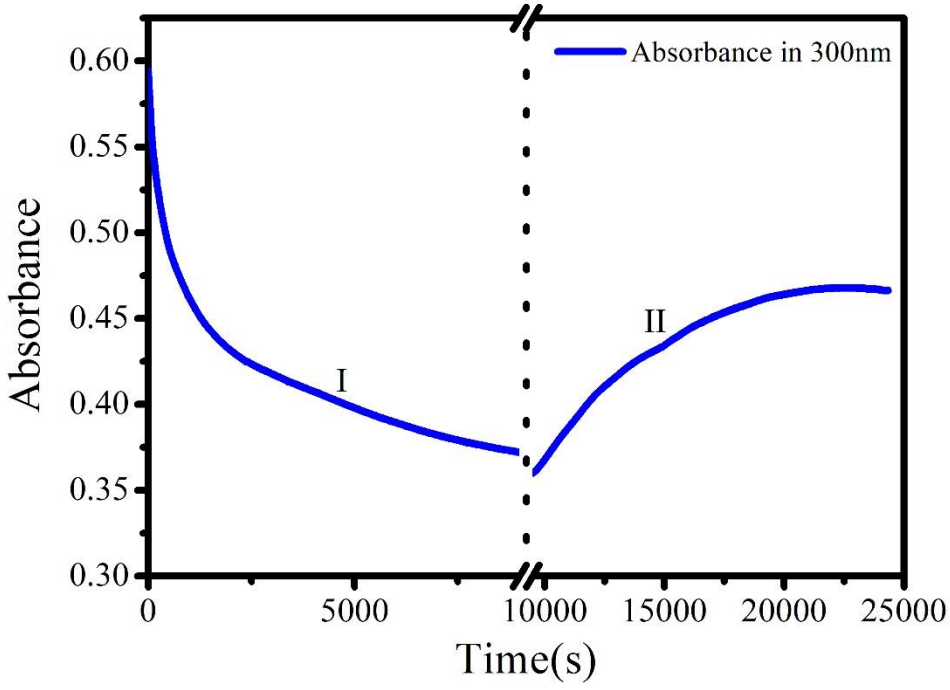


Figure S56. Changes in time for **3Z** (5×10^{-5} M in DCM) absorbance in 320nm after addition of TFA. I (V_{TFA} : V_{DCM} = 0.0033); II. addition TFA again.

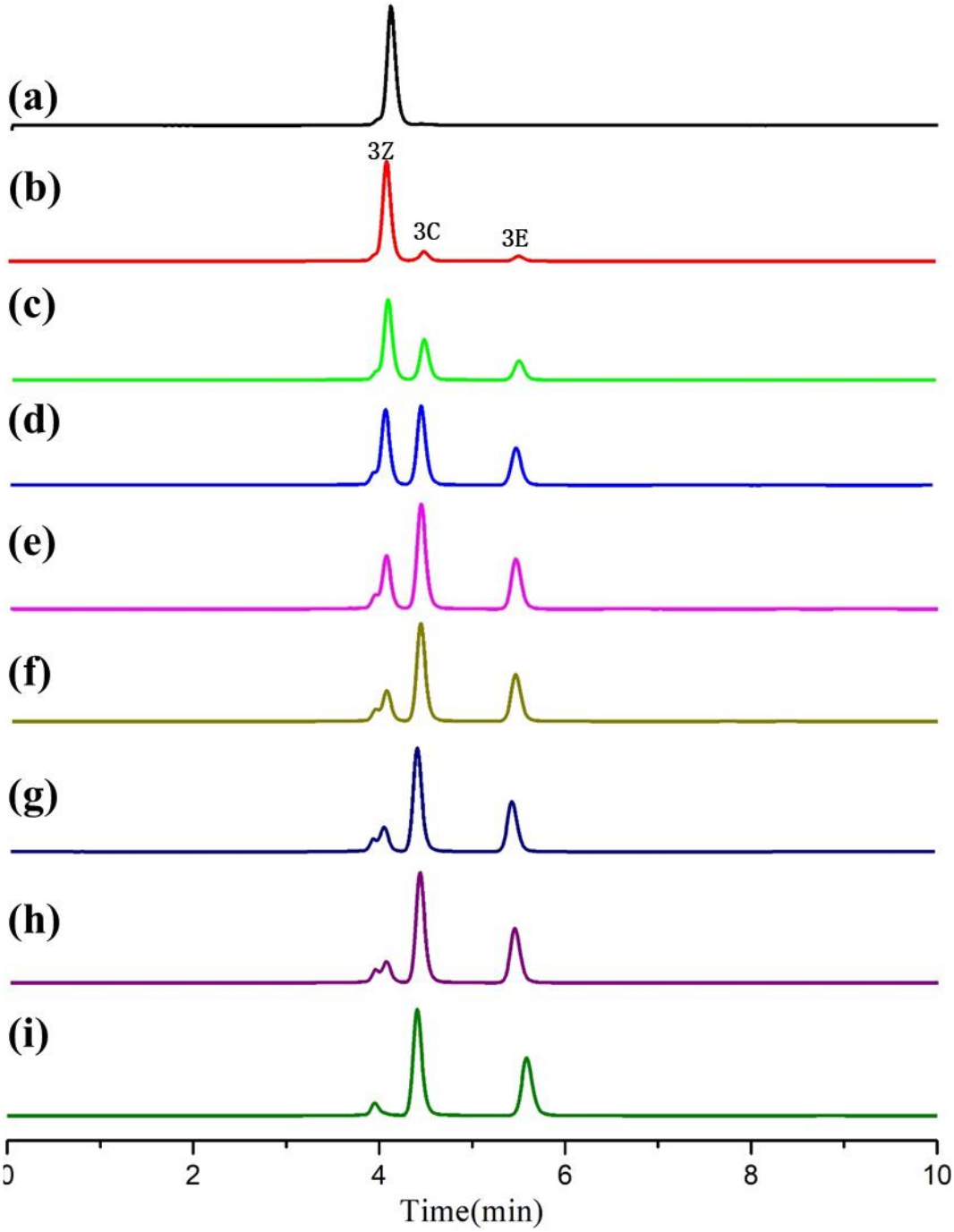


Figure S57. HPLC traces with the absorbance at 265nm. (a) **3Z**; addition of 2 equiv TFA after (b) 2 min ; (c)15 min ; (d) 25 min; (e) 40 min; (f) 55 min; (g) 70 min; (h) 85 min; (i) 22h;

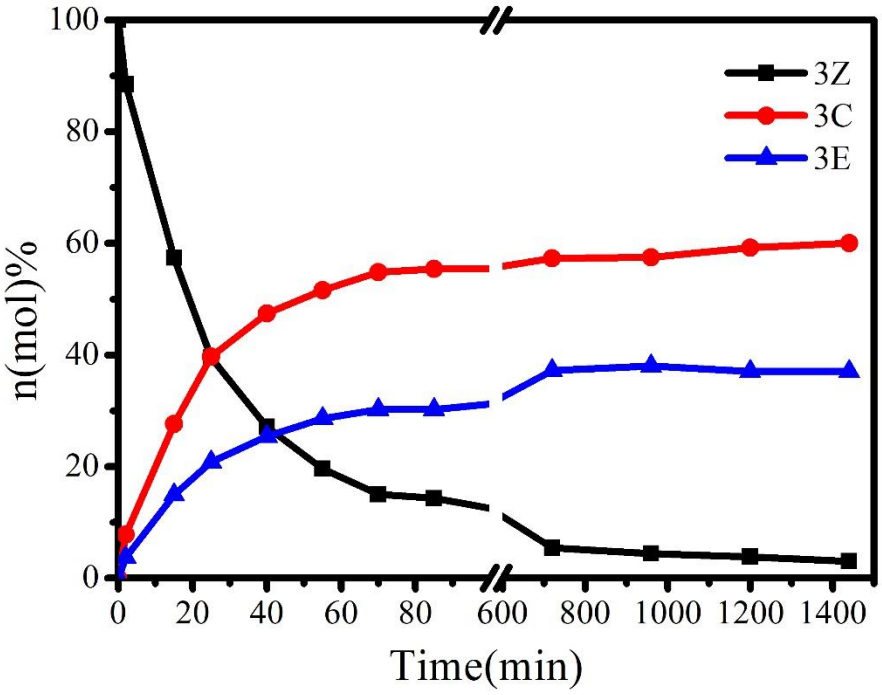


Figure S58. Change of the ratio of **3Z**, **3E**, **3C** over time after addition of 2.0 equiv TFA to **3Z** (1 × 10^{-1} M in DCM), the ratio was detected by HPLC.

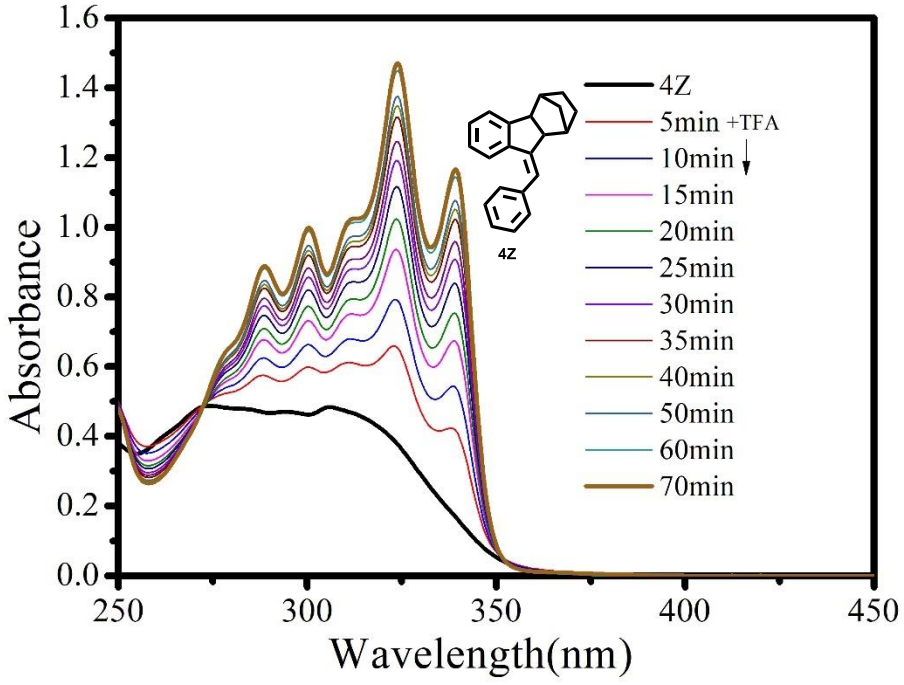


Figure S59. Changes of UV−vis spectra of **4Z** (5 × 10^{-5} M in DCM) after addition of TFA (V_{TFA} : V_{DCM} = 0.0033) for different time periods.

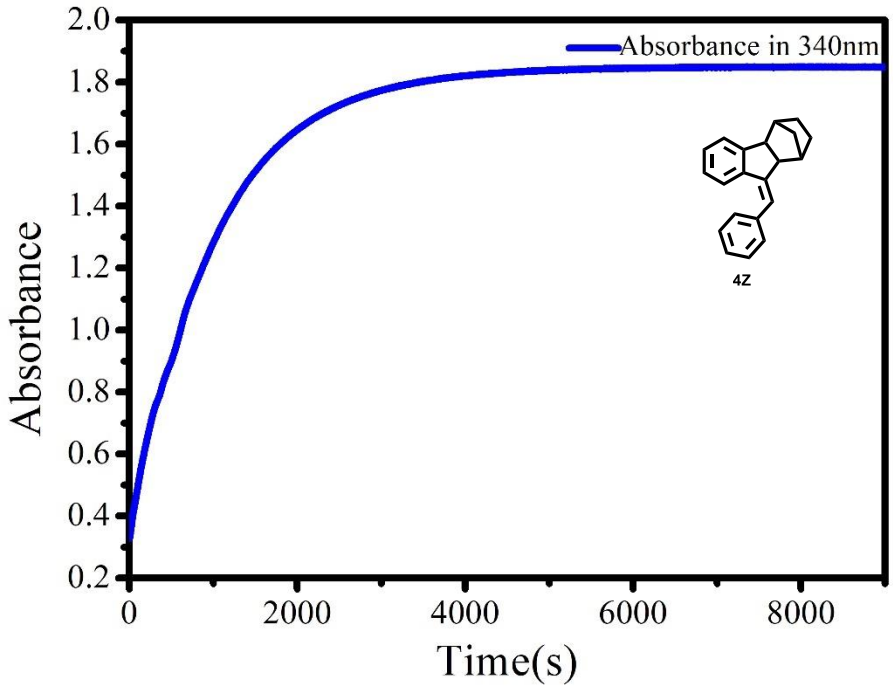


Figure S60. Changes in time for **4Z** (1x10^{-4} M in DCM) absorbance in 340 nm after addition of TFA (V_{TFA} : V_{DCM} = 0.0033).

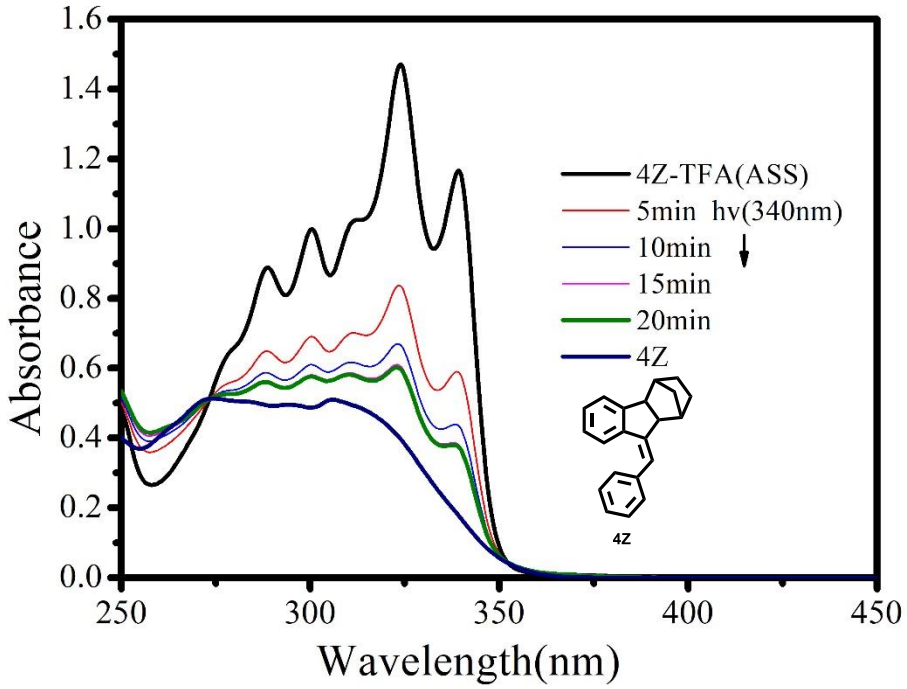


Figure S61. Changes of UV−vis spectra of **4Z** (5 × 10^{-5} M in DCM) after addition of TFA (V_{TFA} : V_{DCM} = 0.0033) to stable state (ASS) then the solution was irradiated with 340 nm UV light for different time periods.

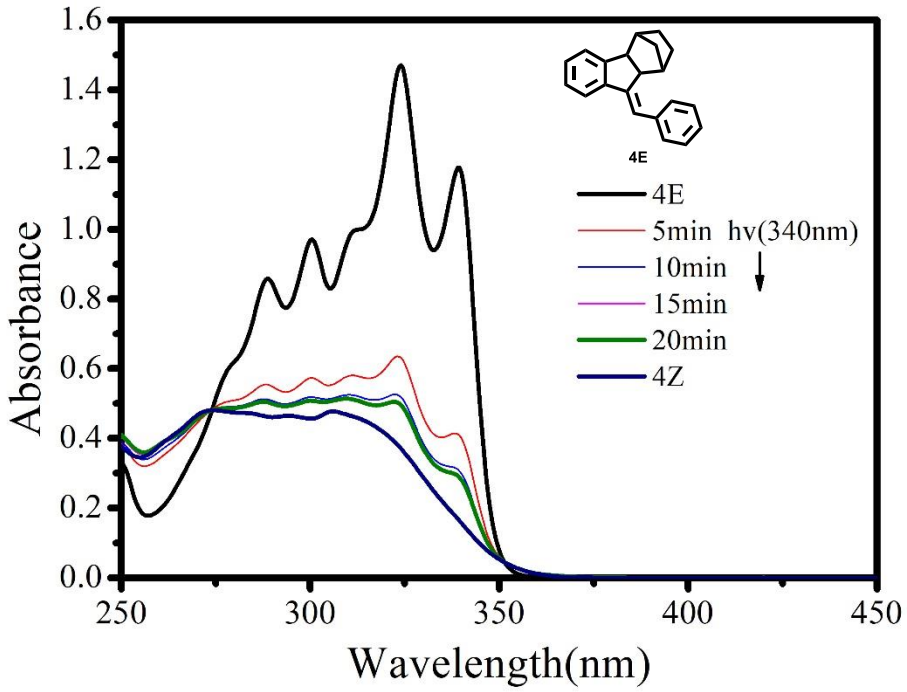


Figure S62. Changes of UV−vis spectra of **4E** (5×10^{-5} M in DCM) upon irradiation with 340 nm UV light for different time periods. PSS(**4Z:4E** = 88:12).

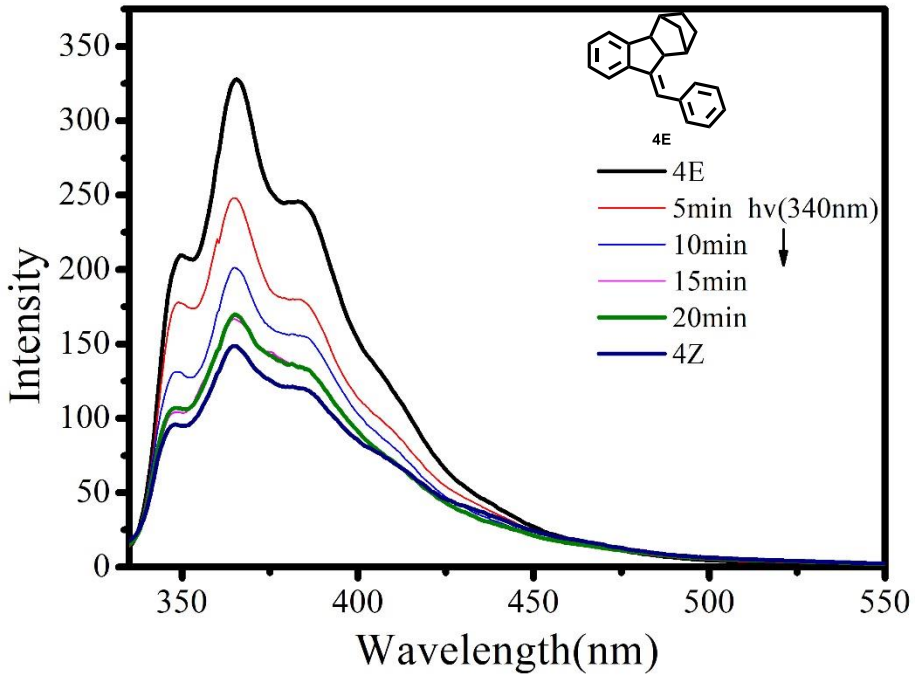


Figure S63. Changes of the photoluminescence intensity of **4E** (5×10^{-5} M in DCM) upon 340nm UV light irradiation for different time periods, λ_{ex} = 310 nm.

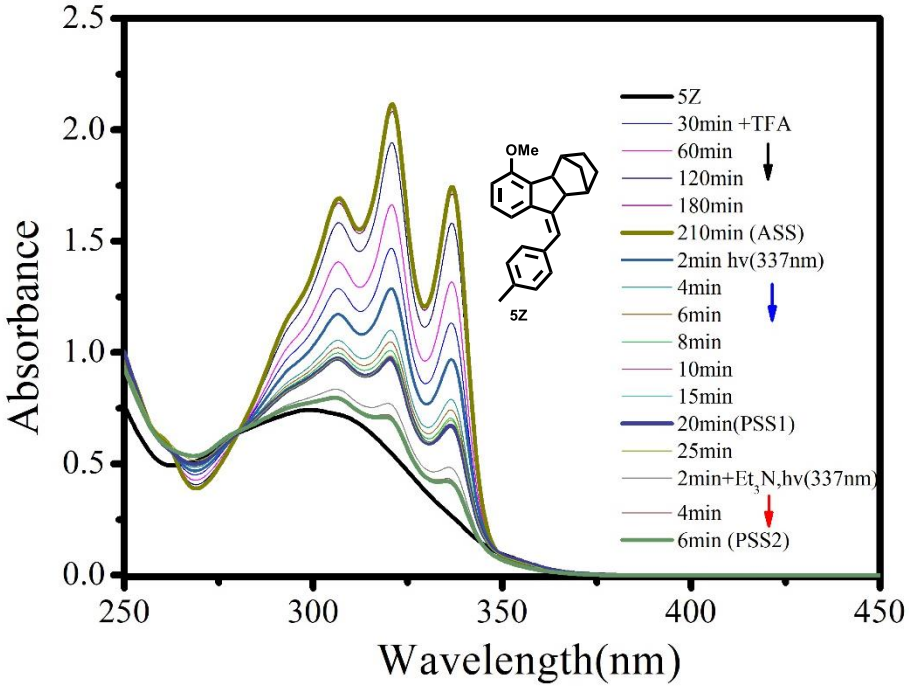


Figure S64. Changes of UV−vis spectra of **5Z** (5×10^{-5} M in DCM) after addition of TFA (V_{TFA} : V_{DCM} = 0.0016) to stable state (ASS) then irradiation of the solution with 337 nm UV light. about 20 min the system reached at PSS1, then Et_3N was added, continuous irradiation with 337 nm UV light to reach another photo stable state PSS2.

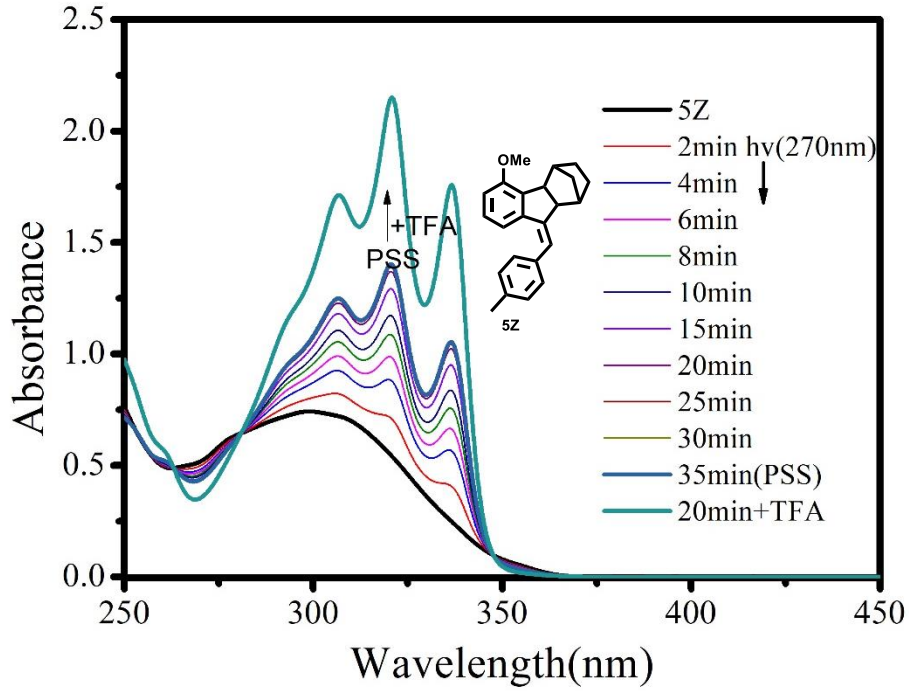


Figure S65. Changes of UV−vis spectra of **5Z** (5×10^{-5} M in DCM) upon irradiation with 270 nm UV light. After 35 min the solution reach to PSS (**5E:5Z** = 53:47), then addition of TFA (V_{TFA}:V_{DCM} = 0.0033) to reach a stable state.

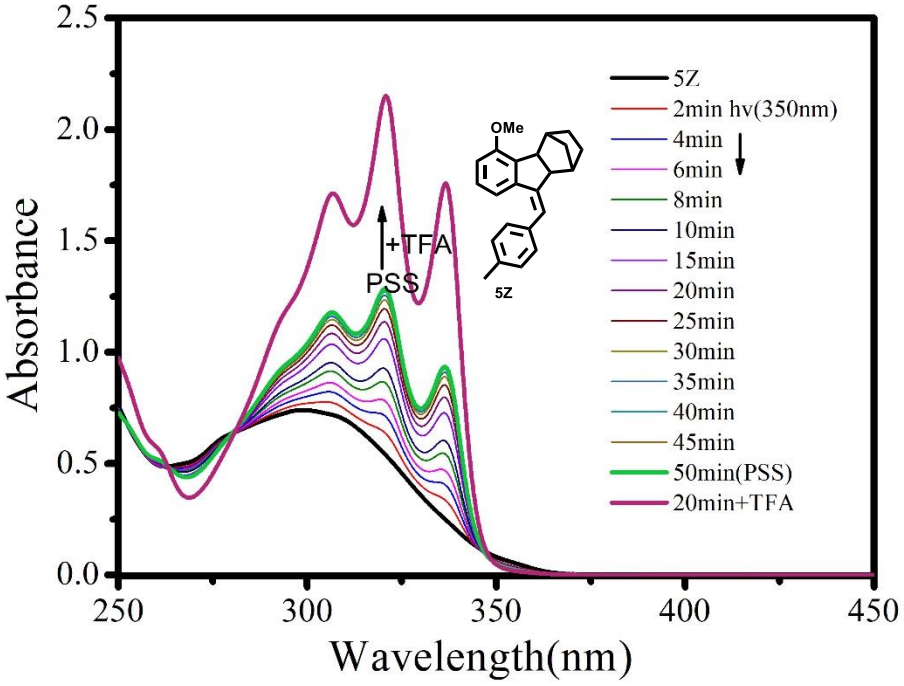


Figure S66. Changes of UV−vis spectra of **5Z** (5×10^{-5} M in DCM) upon irradiation with350 nm UV light. After 50 min the solution reach to PSS (**5E:5Z** = 53:47), then addition of TFA (V_{TFA}:V_{DCM} = 0.0033) to reach a stable state.

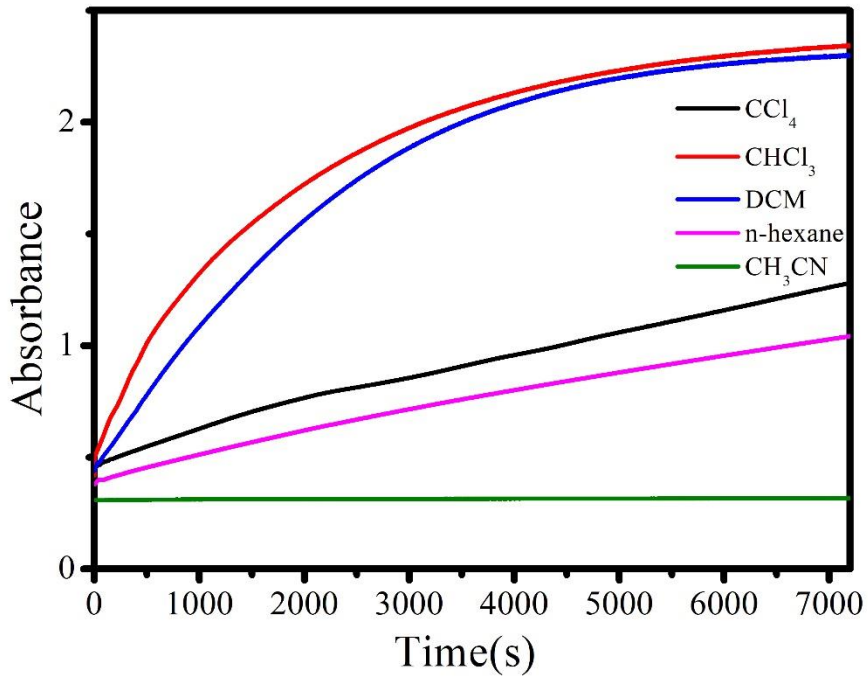


Figure S67. Changes in time for **5Z** (1×10^{-4} M in different solvents) absorbance in 337 nm after addition TFA.

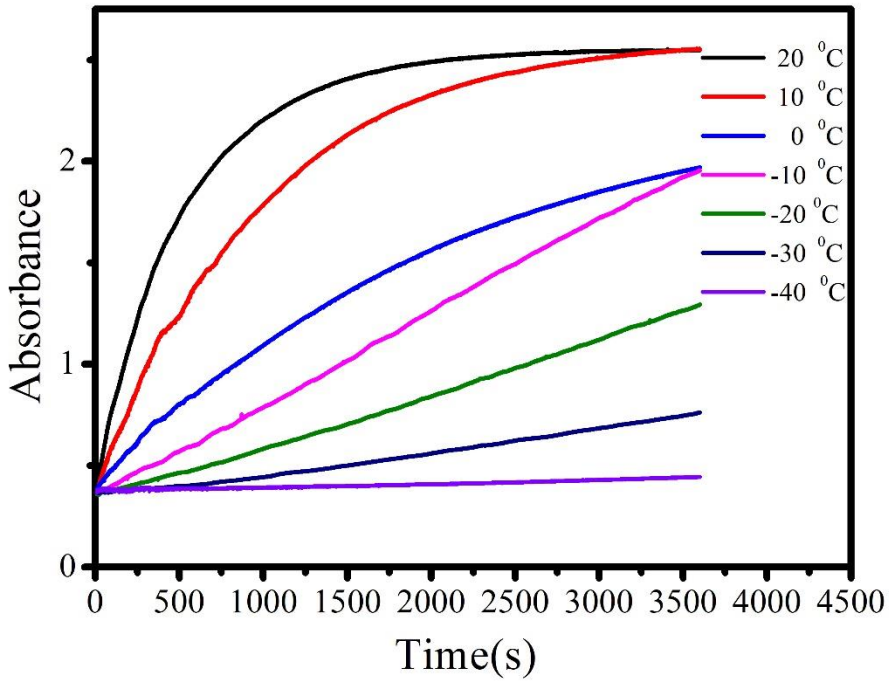


Figure S68. Changes in time for **5Z** absorbance in 337 nm after addition of TFA (V_{TFA} : V_{DCM} = 0.0066) under different temperature.

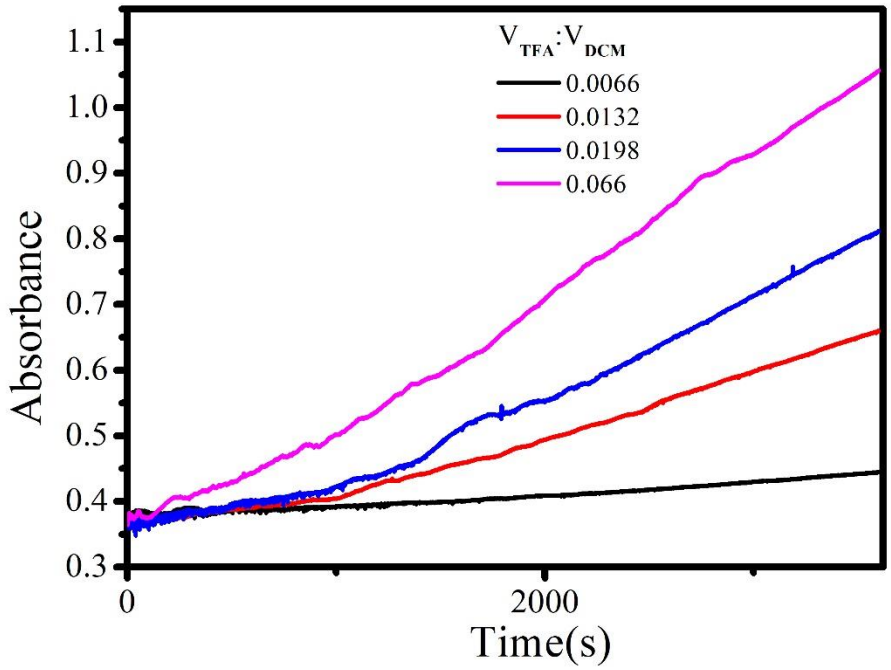


Figure S69. Changes in time for **5Z (** $1x10^{-4}$ M in DCM) absorbance in 337 nm after addition of different amounts of TFA under -40 ^{0}C.

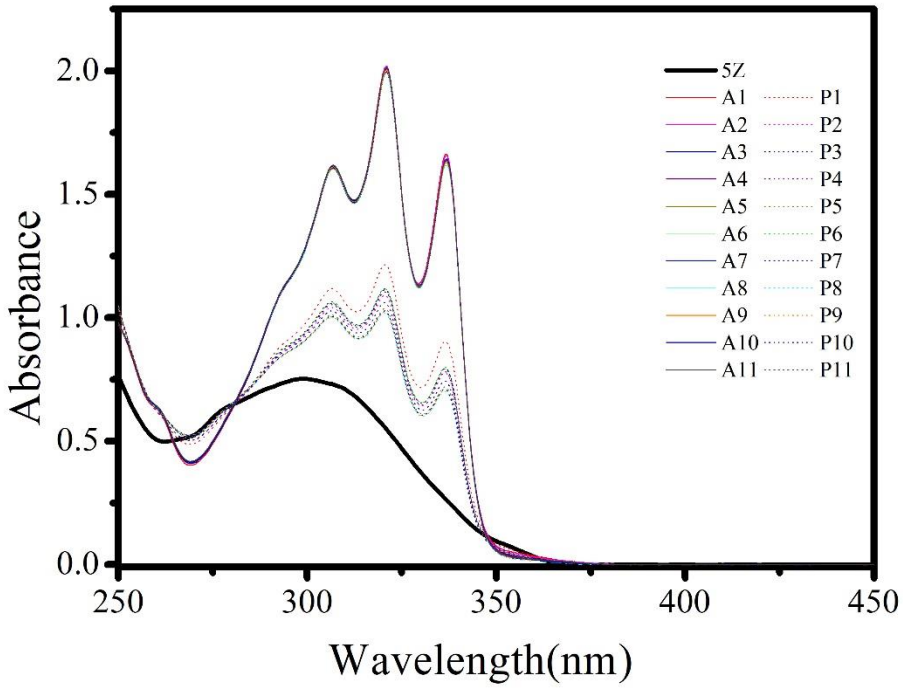


Figure S70. Changes of UV−vis spectra of **5Z** (5×10^{-5} M in DCM) after addition TFA (V_{TFA}:V_{DCM} = 0.0033) to stable state(ASS) about 80 min, then irradiation with 337 nm UV light, about 10 min the system at PSS. A1-A11 means the acid -catalyzed process and P1-P11measns photo irradiation with 337 nm UV light.

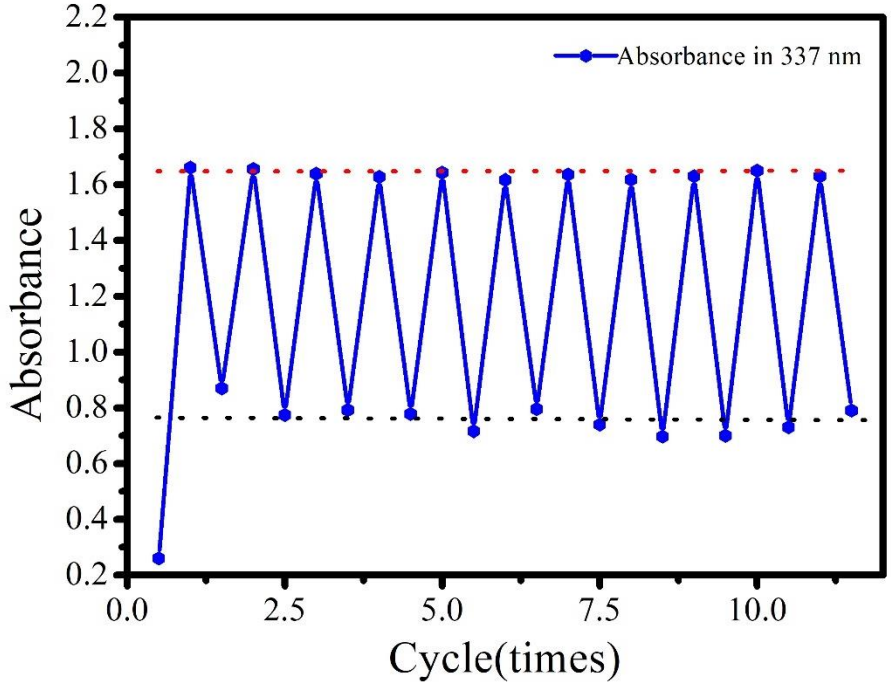


Figure S71. Changes of absorbance of **5Z** (5×10^{-5} M in DCM) in 337 nm after addition TFA (V_{TFA}:V_{DCM} = 0.0033) to stable state (ASS) about 80 min , then irradiation with 337 nm UV light , about 10 min the system at PSS, over 11 cycles.

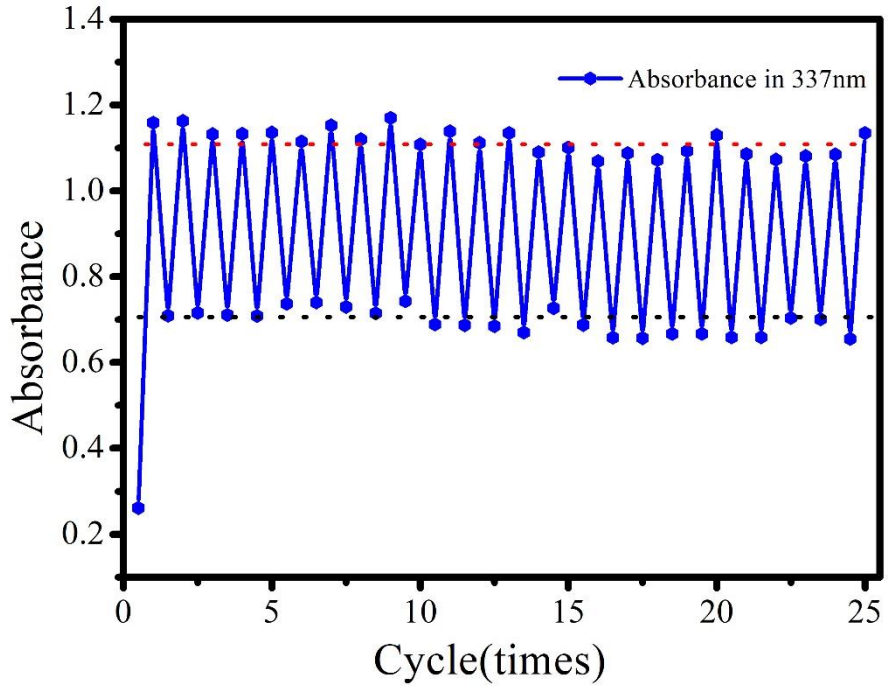


Figure S72. Changes of absorbance of **5Z** (5×10^{-5} M in DCM) in 337 nm after addition of TFA (V_{TFA}:V_{DCM} = 0.0066) for 10 min, and then irradiation with 337 nm UV light for 5 min over 25 cycles.

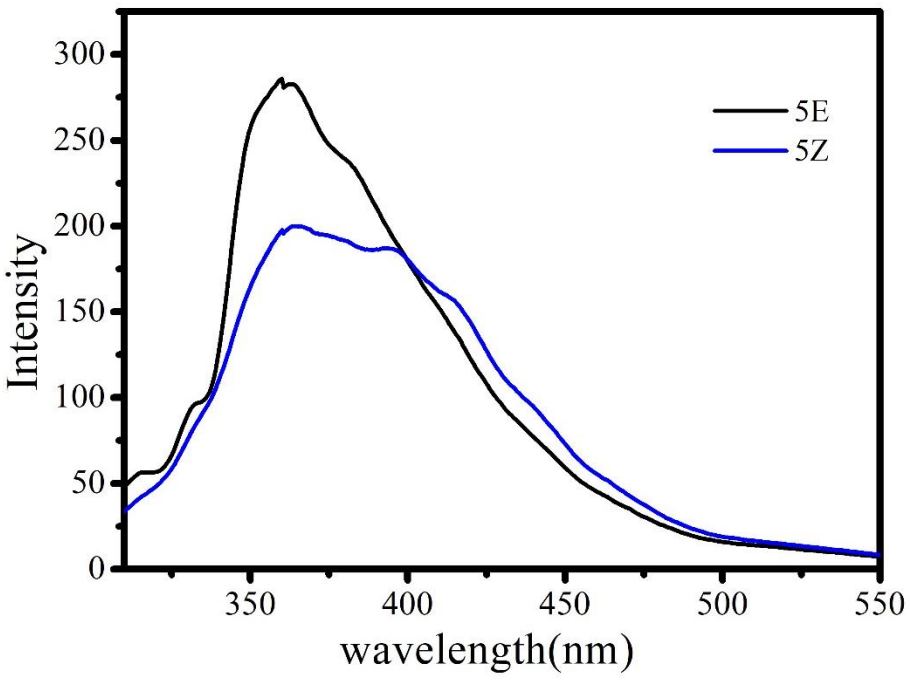


Figure S73. Photoluminescence spectra of **5Z** and **5E** (5×10^{-5} M in DCM), λ_{ex} = 310 nm.

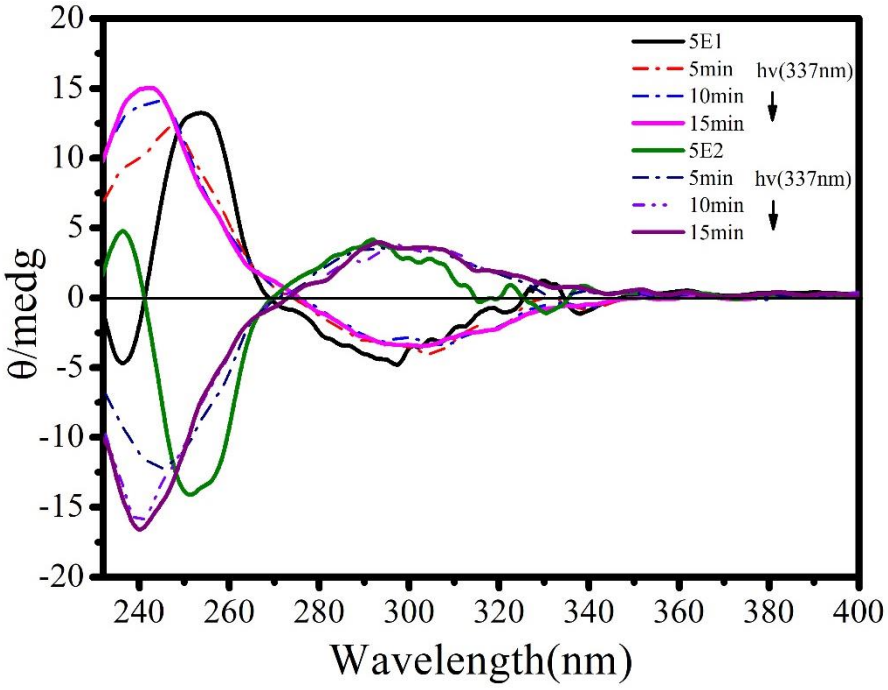


Figure S74. Changes of circular dichroism (CD) spectra of **5E1** and **5E2** (5×10^{-5} M in n-hexane) upon 337 nm UV light irradiation for different time periods.

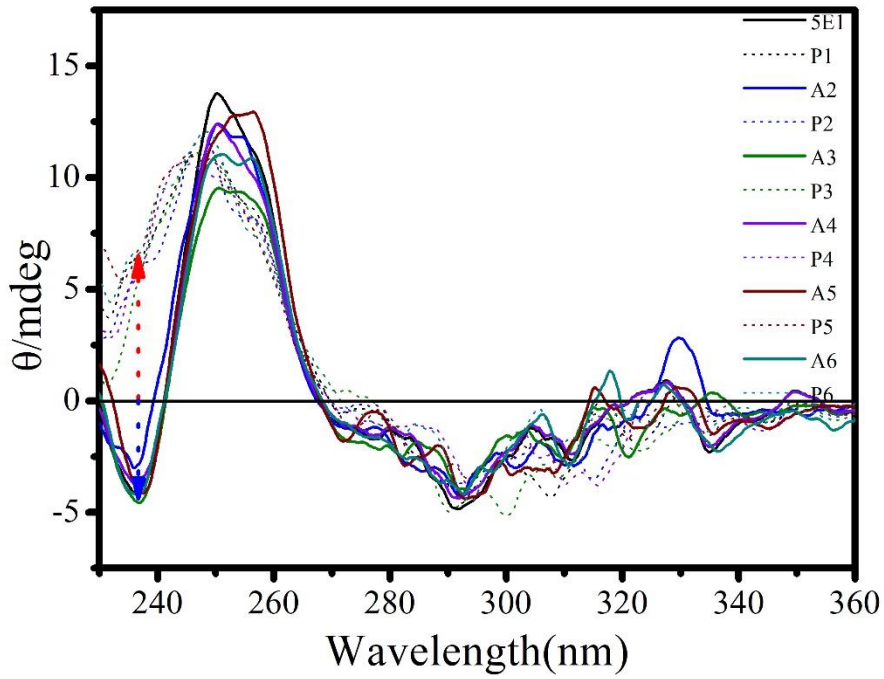


Figure S75. Changes of circular dichroism (CD) spectra of **5E1** (5×10^{-5} M in n-hexane) after irradiation with 337 nm 10 min then addition of TFA (V_{TFA}:$V_{n\text{-}hexane}$ = 0.0066) about 80 min to stable state, and irradiation with 337 nm 10 min again then await 80 min to stable state, the process cycled a few times.

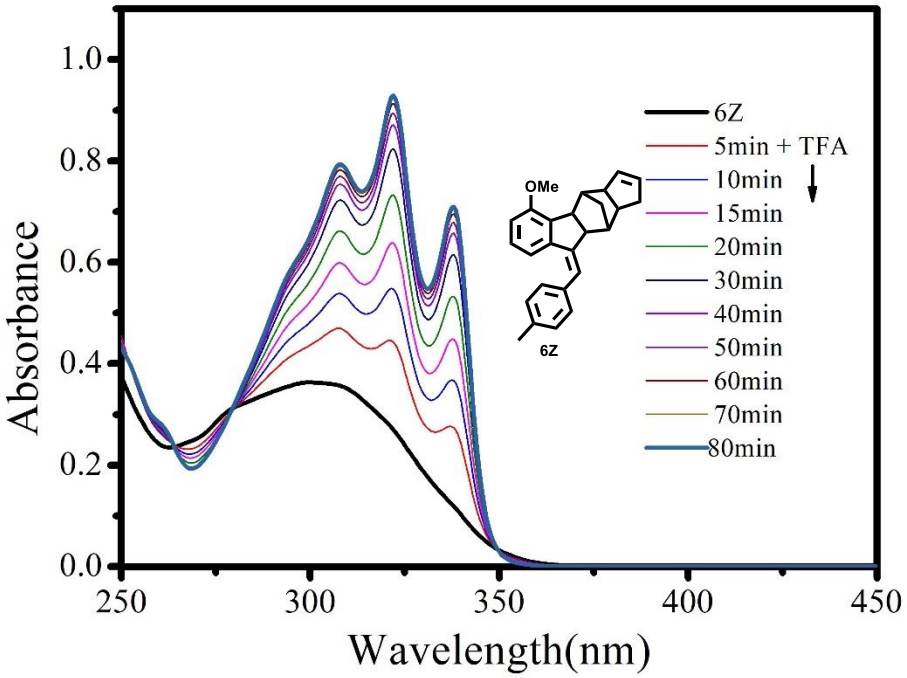


Figure S76. Change of UV−vis spectra of **6Z** (2.5×10^{-5} M in DCM) after addition of TFA (V_{TFA}:V_{DCM} = 0.0016) for different time periods.

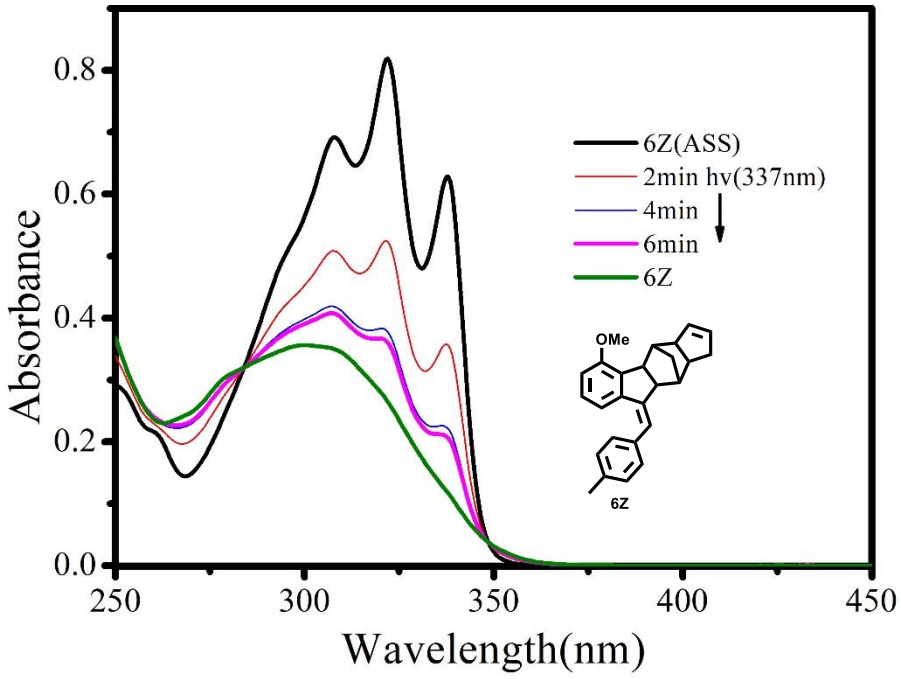


Figure S77. Change of UV−vis spectra of **6Z** (2.5×10^{-5} M in DCM) after addition of TFA (V_{TFA}:V_{DCM} = 0.0016) to stable state (ASS) then irradiation with 337 nm UV light for different time periods.

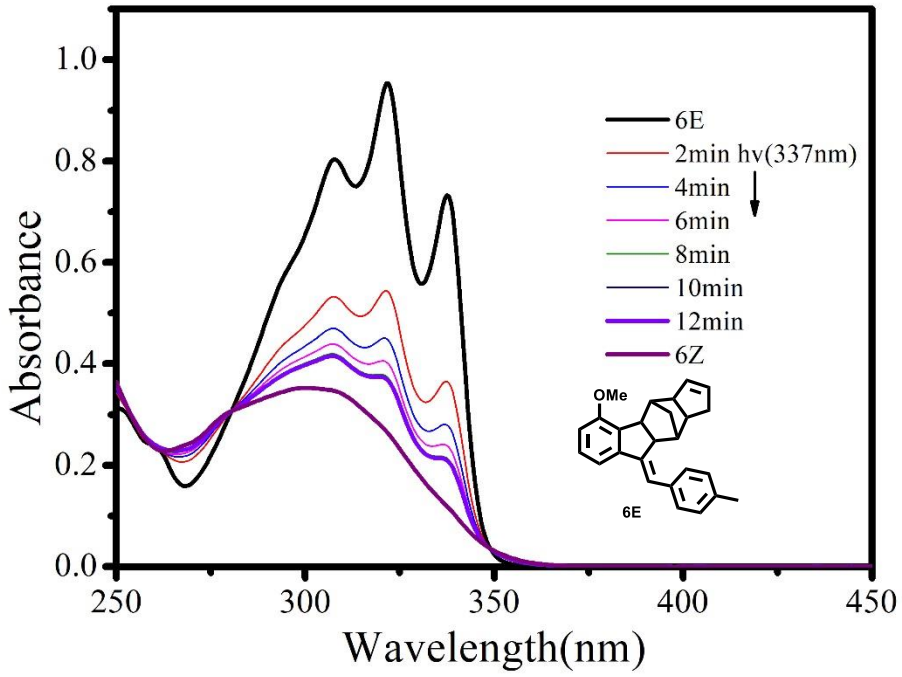


Figure S78. Changes of UV−vis spectra of **6E** (2.5×10^{-5} M in DCM) upon 337 nm UV light irradiation for different time periods. PSS (**6Z:6E** = 86:14).

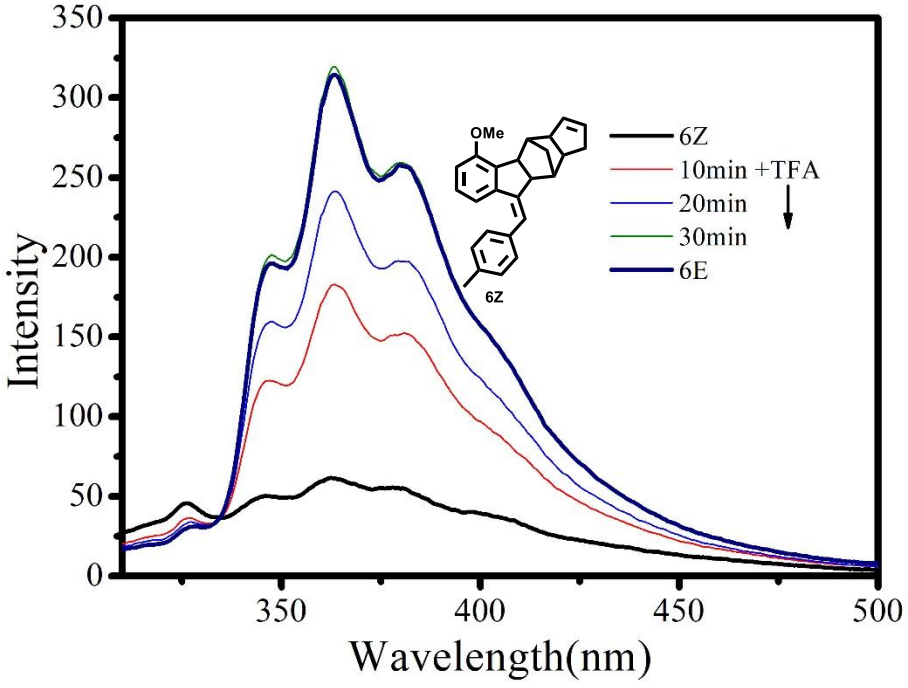


Figure S79. Changes of photoluminescence intensity of **6Z** (2.5×10^{-5} M in DCM) after addition of TFA (V_{TFA}:V_{DCM} = 0.0016) for different time periods, λ_{ex} = 295 nm.

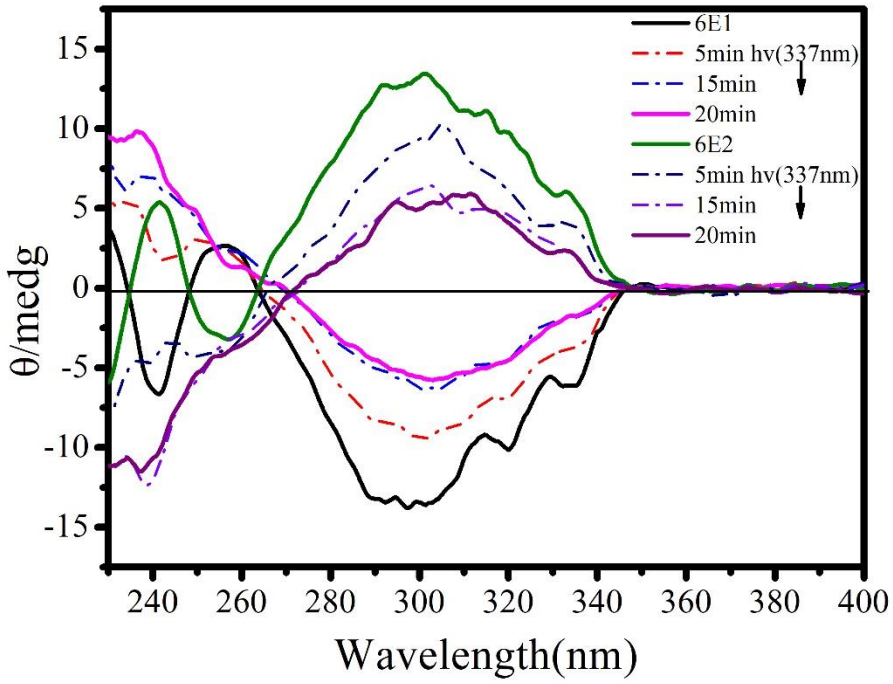


Figure S80. Changes of circular dichroism (CD) spectra of **6E1** and **6E2** (5×10^{-5} M in n-hexane) upon 337 nm UV light irradiation for different time periods.

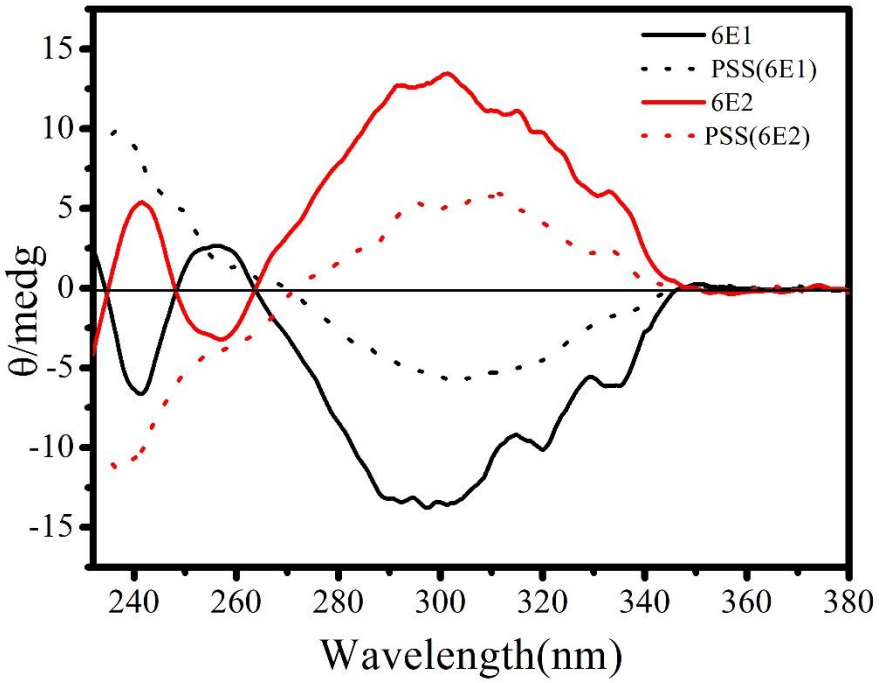


Figure S81. Circular dichroism (CD) spectra of **6E1** and **6E2** (5×10^{-5} M in n-hexane) (solid) and at PSS (dot).

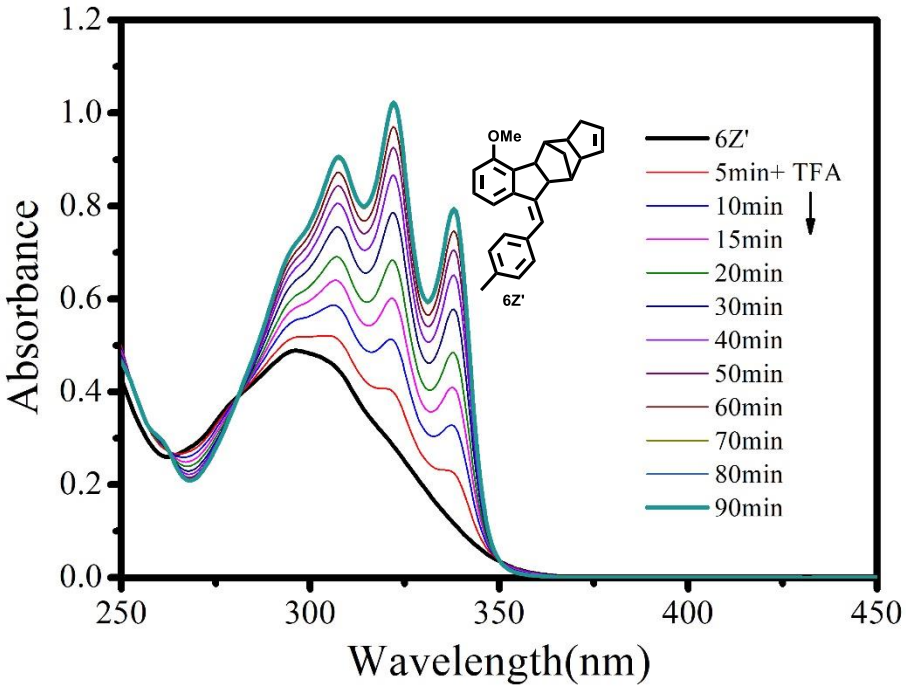


Figure S82. Changes of UV−vis spectra of **6Z'** (2.5×10^{-5} M in DCM) after addition of TFA (V_{TFA}:V_{DCM} = 0.0016) for different time periods.

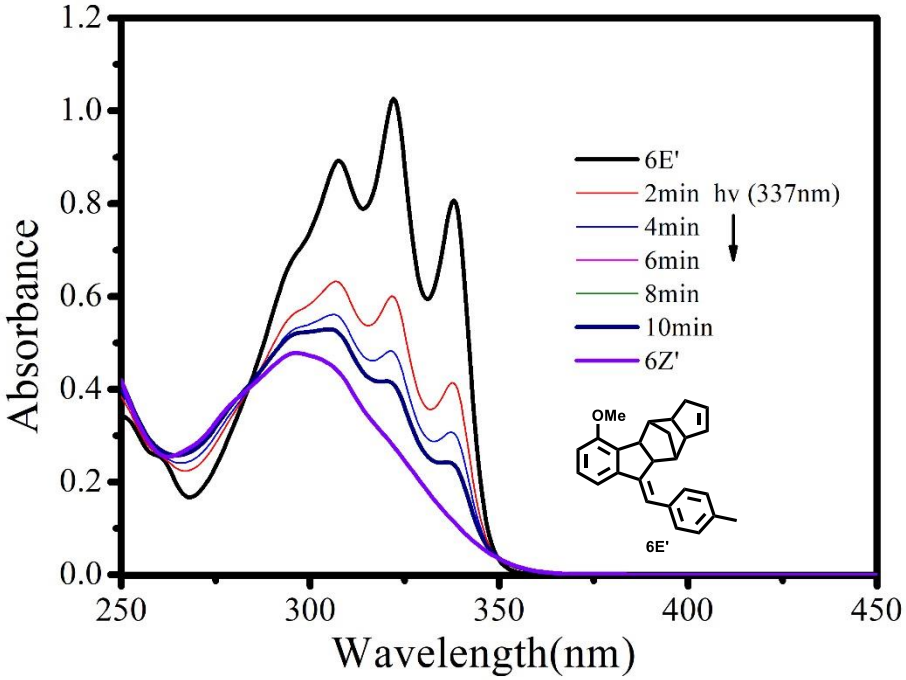


Figure S83. Changes of UV−vis spectra of **6E'** (2.5×10^{-5} M in DCM) upon 337nm UV light irradiation for different time periods. PSS(**6Z': 6E'** = 85:15).

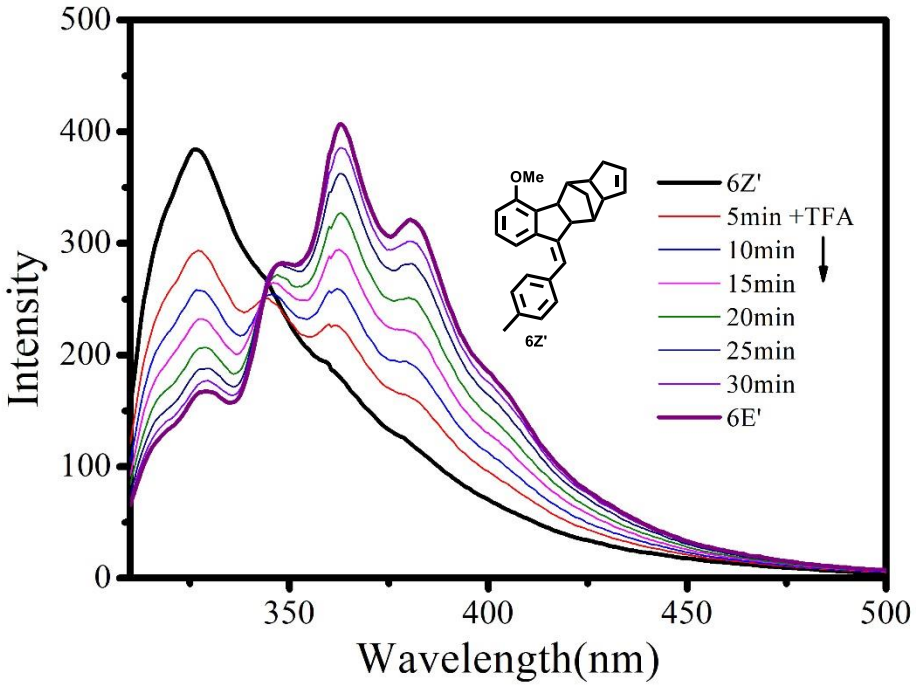


Figure S84. Changes of the photoluminescence intensity of **6Z'** (2.5×10^{-5} M in DCM) after addition of TFA (V_{TFA}: V_{DCM} = 0.0033) for different time periods, λ_{ex} = 295 nm.

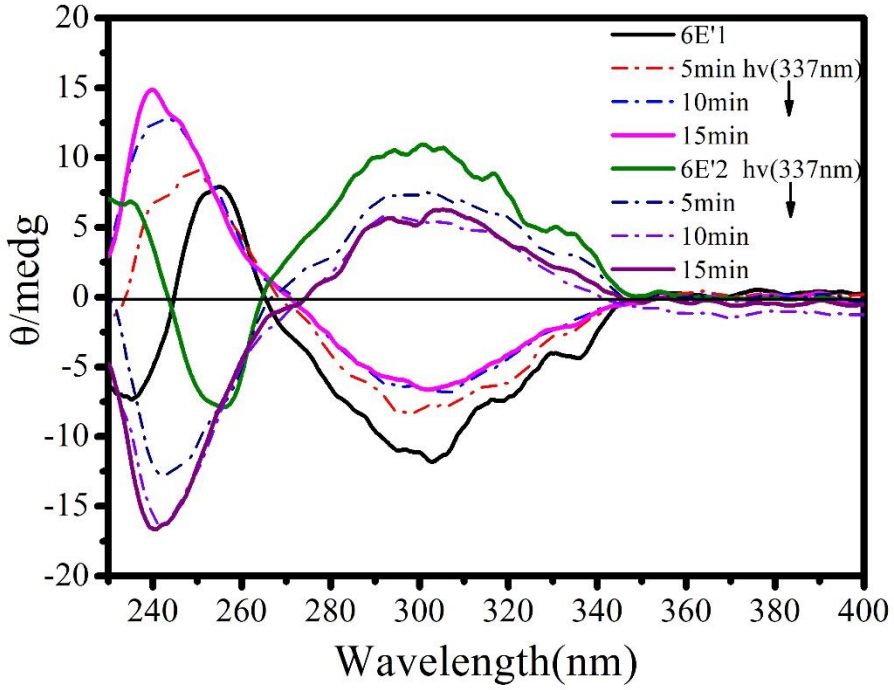


Figure S85. Changes of circular dichroism (CD) spectra of **6E'1** and **6E'2** (5×10^{-5} M in n-hexane) upon 337 nm UV light irradiation for different time periods.

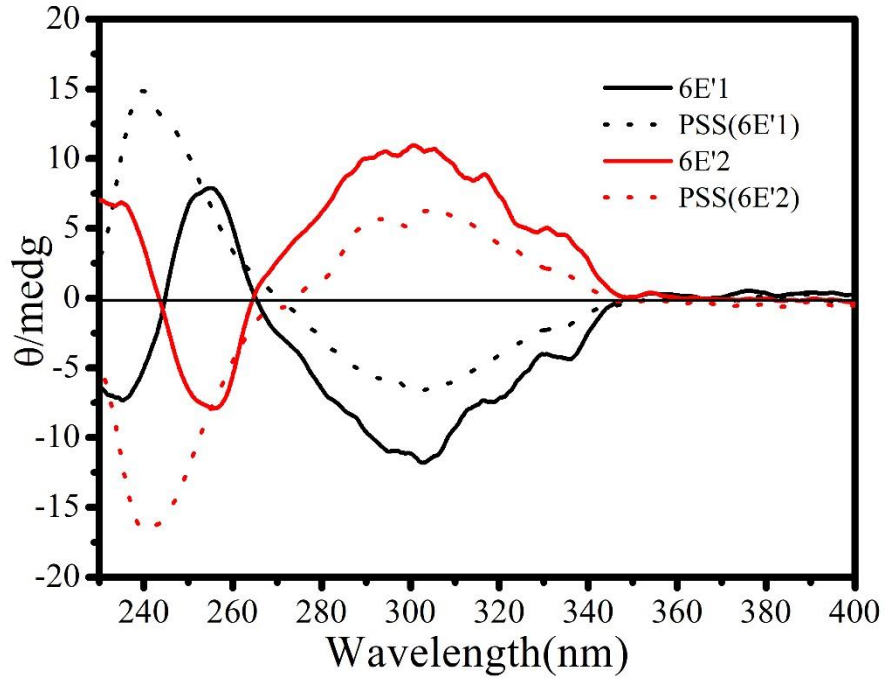


Figure S86. Circular dichroism (CD) spectra of **6E'1** and **6E'2** (5×10^{-5} M in n-hexane) (solid) and at PSS (dot).

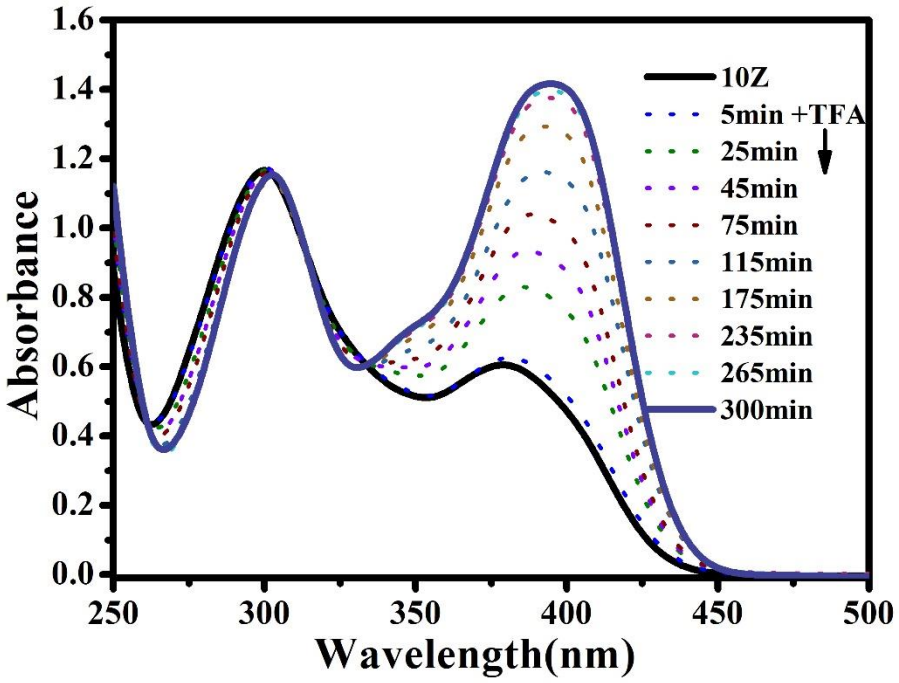


Figure 87. Changes of UV−vis spectra of **10Z** (5×10^{-5} M in DCM) after addition of TFA. (V_{TFA}:V_{DCM} = 0.0016) for different time periods.

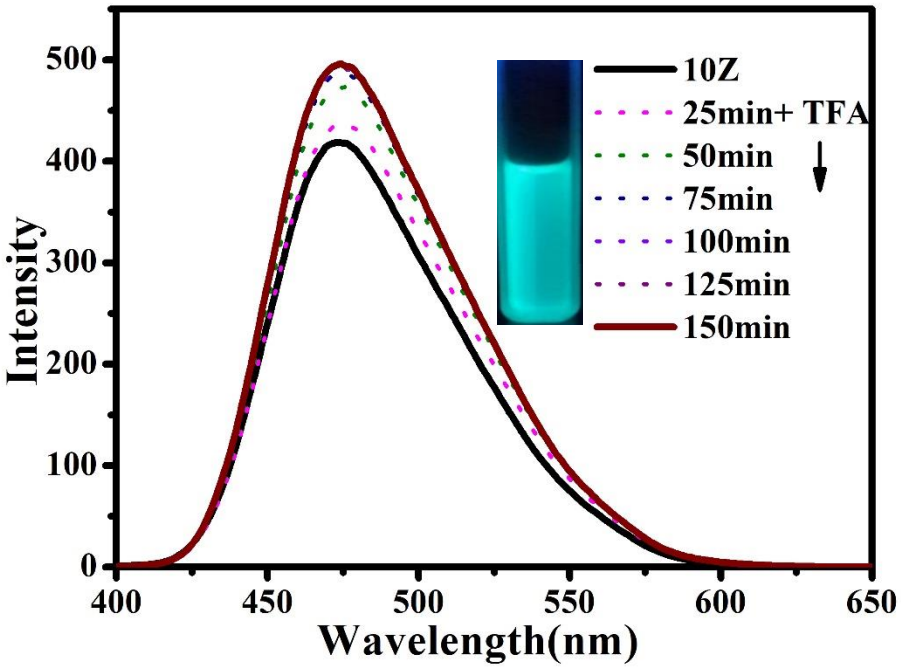


Figure S88. Changes of the photoluminescence intensity of **10Z** (5×10^{-5} M in DCM) after addition of TFA (V_{TFA}:V_{DCM} = 0.0016) for different time periods, λ_{ex} = 380 nm. insert: the fluorescence image of **10Z** (5×10^{-5} M in DCM).

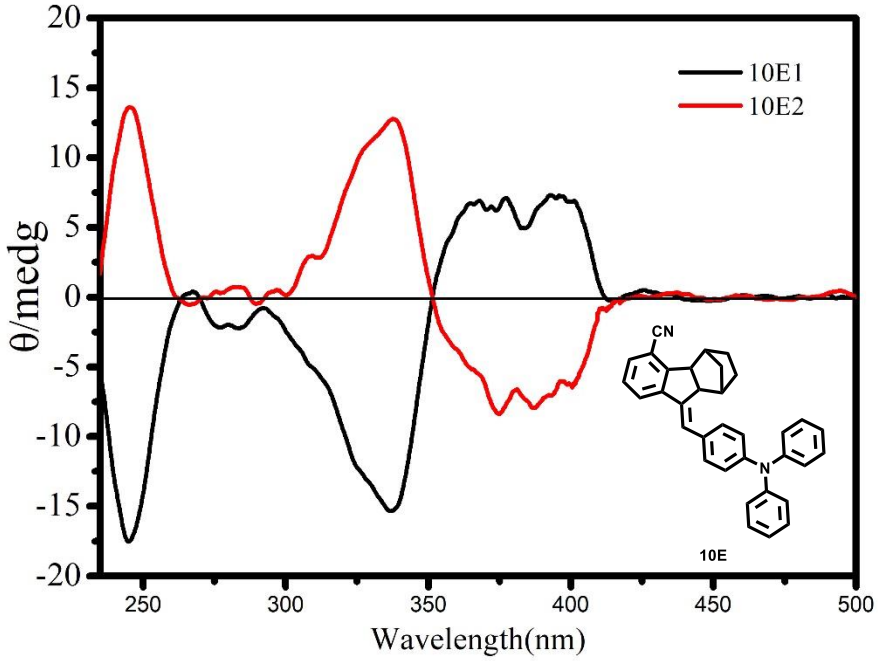


Figure S89. Circular dichroism (CD) spectra of **10E1** and **10E2** (5×10^{-5} M in n-hexane).

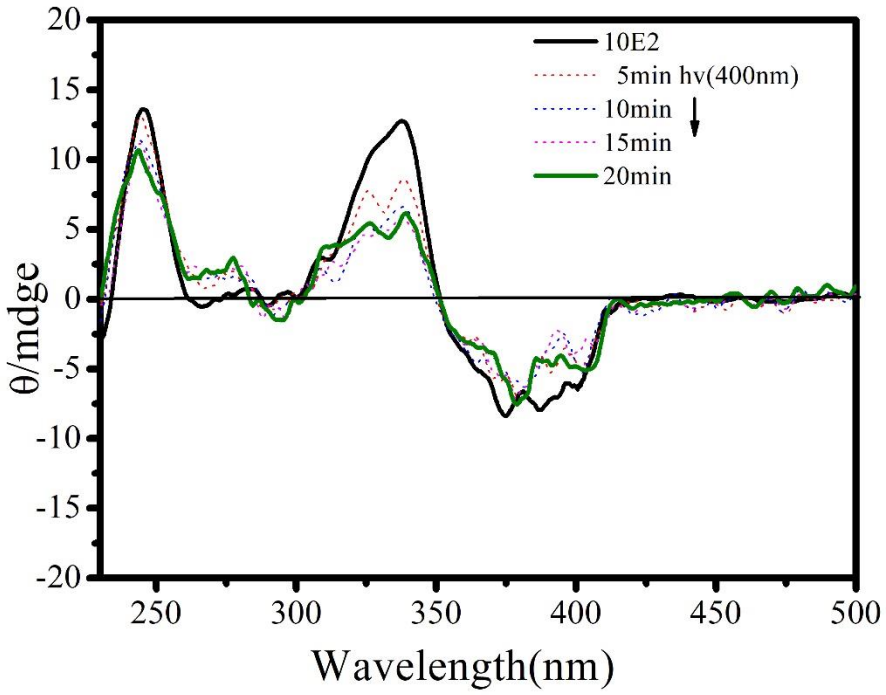
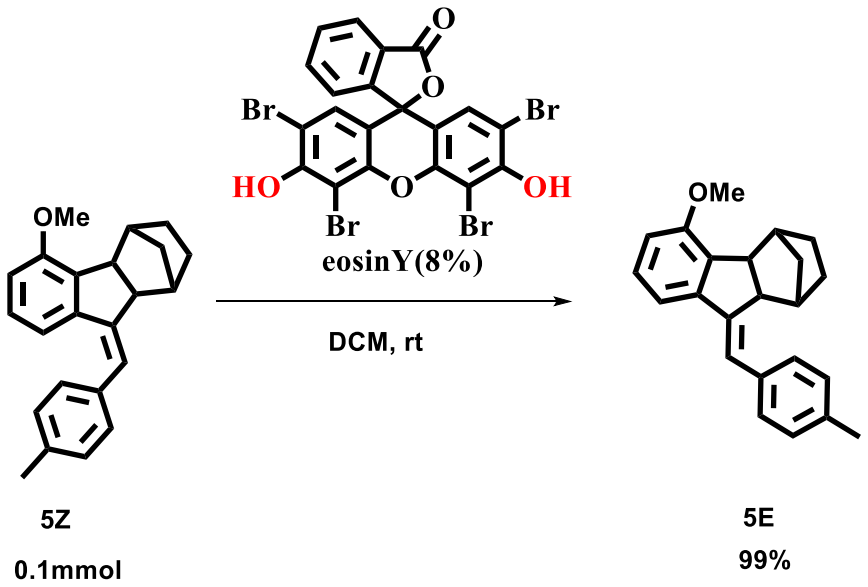
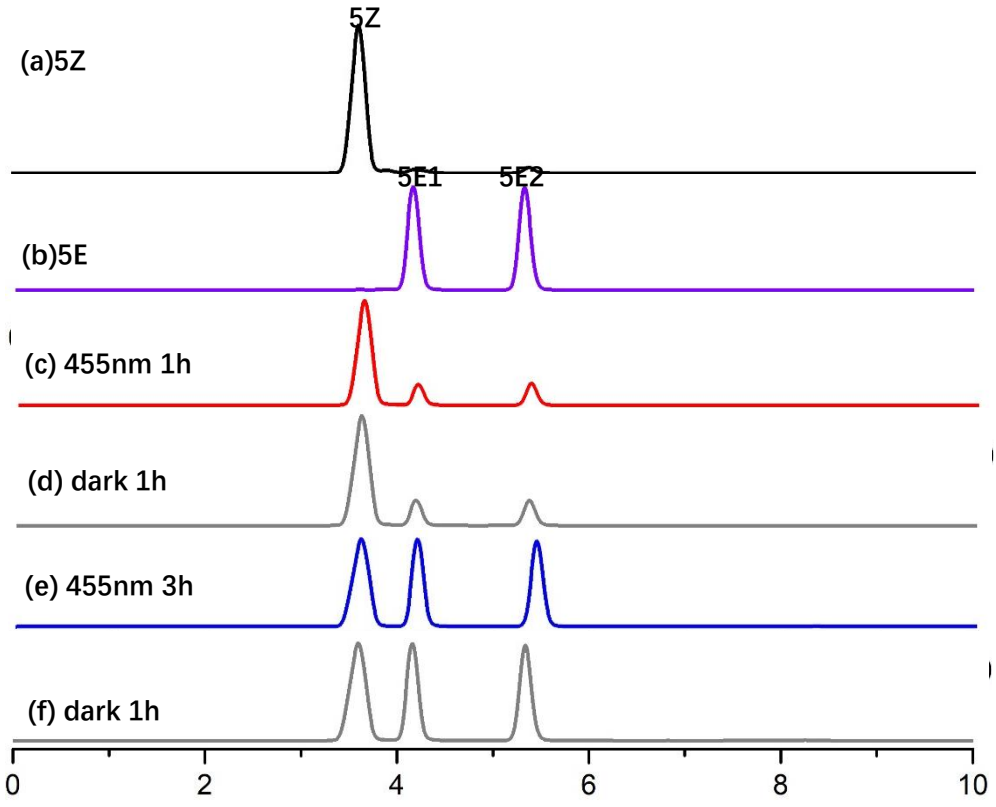


Figure 90. Changes of circular dichroism (CD) spectra of **10E2** (5×10^{-5} M in n-hexane) upon 400 nm light irradiated for different time periods.

7. Eosin Y catalyzed isomerization of 5Z



Procedure A: In a dried 10 mL glass bottle equipped with a magnetic stirring bar, was added 0.1 mmol **5Z**, 8 mmol% of eosin Y and 3.0 ml degassed DCM, then the solution was irradiated with 455 nm OLED for different time, the sample was then taken out by micro-syringe and analyzed with HPLC using a mixed solvent system of n-hexane and DCM ($V_{n\text{-}hexane}$: V_{DCM} = 80:20) as the eluent.



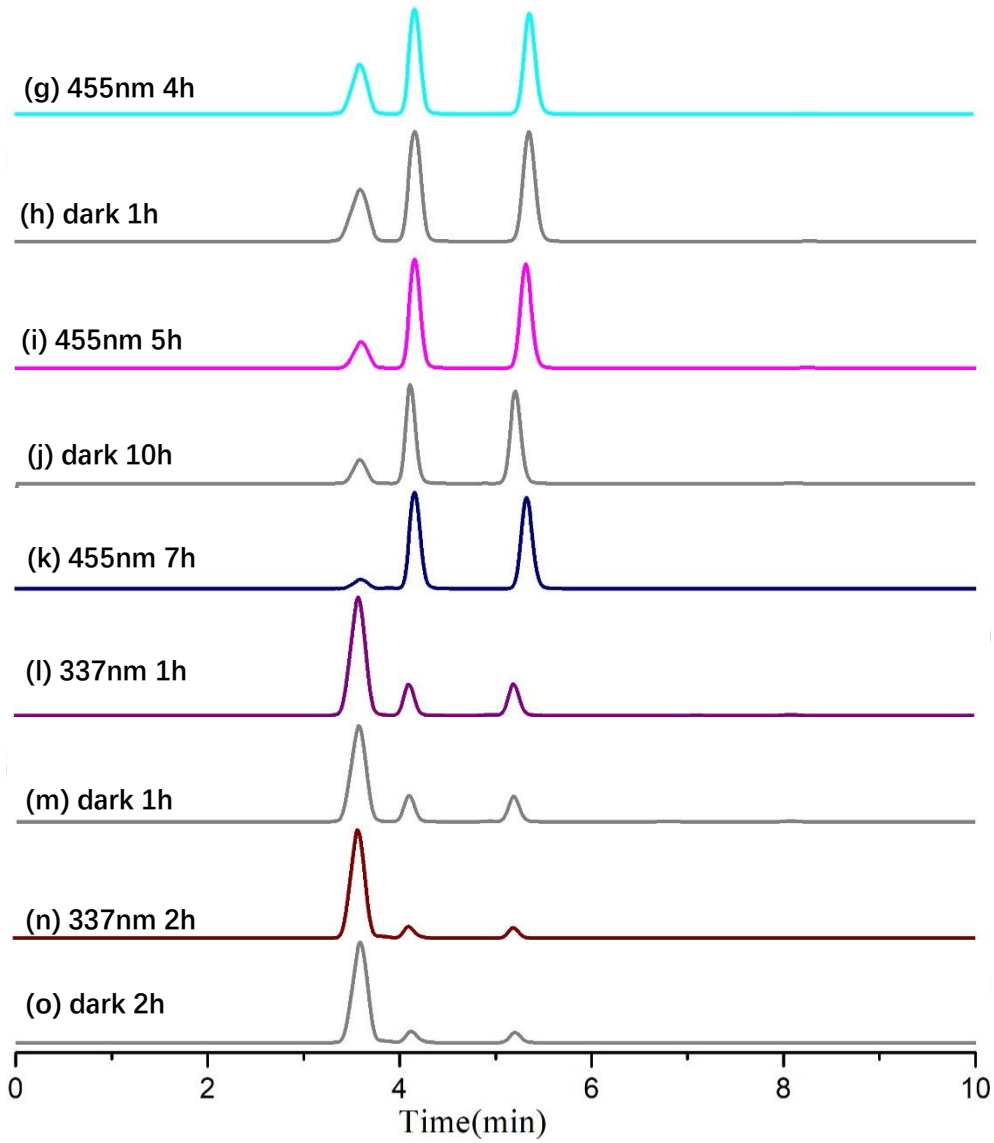


Figure S91. HPLC traces at the absorbance at 300 nm : (a) **5Z**; (b) **5E** (the chiral column was used hence **5E** exist two peaks) ; (c) irradiation with 455 nm OLED for 1 h; (d) under dark for 1 h;(e) irradiation with 455 nm OLED for 3 h; (f) under dark for 1 h; (g) irradiation with 455 nm OLED for 4 h; (h) under dark for 1 h; (i) irradiation with 455 nm OLED for 5 h; (j) under dark for 10 h; (k) irradiation with 455 nm OLED for 7 h; (l) after the sample was irradiation with 455 nm OLED for 9 h, then the solution was diluted 30 times and then was irradiated with 337 nm UV light for 1 h; (m) under dark for 1 h; (n) the sample l was continuously irradiated with 337 nm UV light for 1 h; (o) under dark for 2 h.

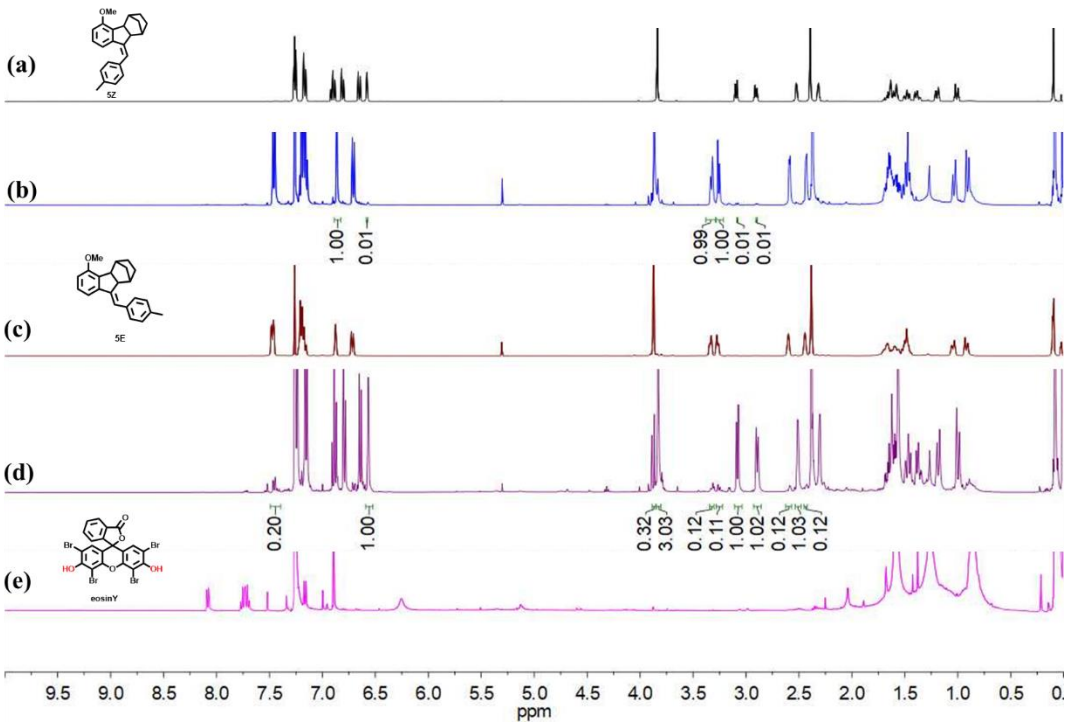


Figure S92. Comparison of the ^{1}HNMR spectrum in $CDCl_3$: (a) **5Z**; (b) the sample of Procedure A after 9 h irradiation with 455 nm OLED light and then the solvent was evaporated in vacuum to offer desired product without further purification; (c) **5E**; (d) the sample of (b) diluted 30 times irradiation with 337 nm UV light 2 h then the solvent was evaporated in vacuum to offer desired product without further purification; (e) eosin Y.

Using the absorbance in 300nm to calculate the *E*/*Z* ratio

ξ_{5E}（300 nm）/ξ_{5Z}（300 nm）= 1.41

$A_{5E}=\xi_{5E}$（300 nm）b c_{5E} ; $A_{5Z}=\xi_{5Z}$（300 nm）b c_{5Z}

$A_{5E}/A_{5Z}=(\xi_{5E}$（300 nm）$c_{5E})/(\xi_{5Z}$（300 nm）$c_{5Z})$

$c_{5E}/c_{5Z}=(A_{5E}/A_{5Z})$* 0.709

5E% =（$c_{5E}/c_{5Z}+c_{5E}$）= $0.709A_{5E}/(0.709A_{5E}+A_{5Z})$

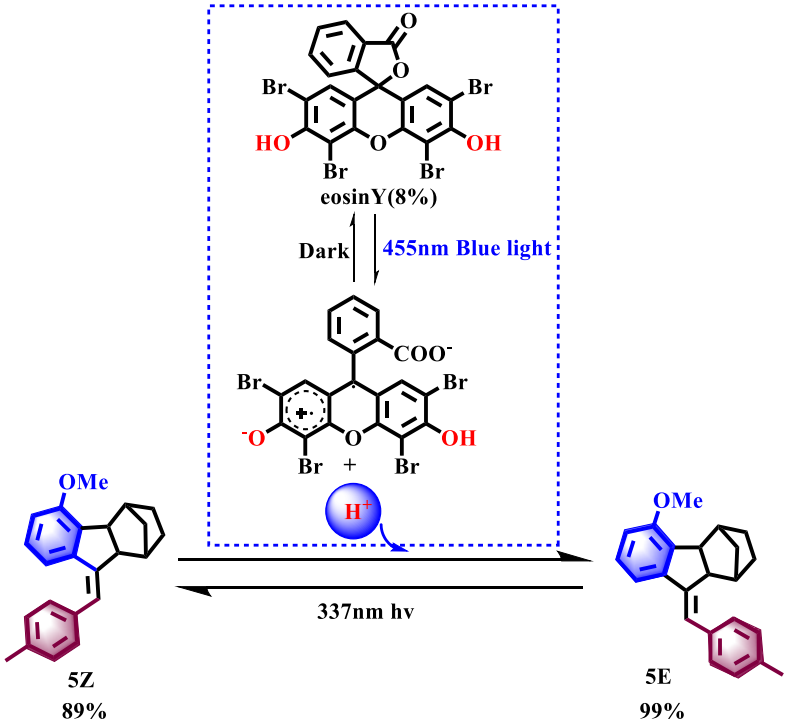


Figure S93. Possible mechanism of *Z*→*E* isomerization of **5Z** catalyzed by eosin Y.

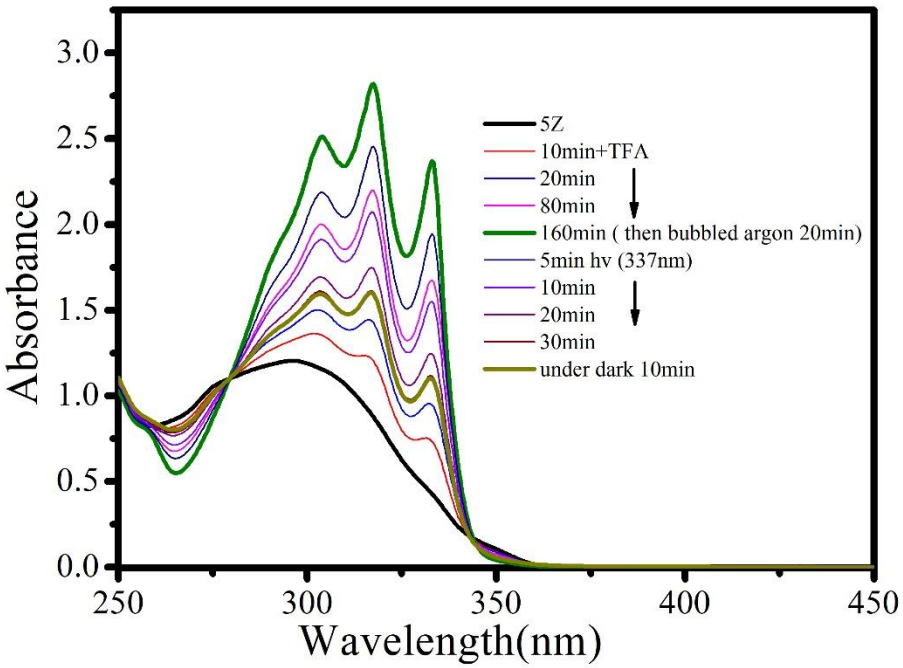


Figure S94. Change of UV−vis spectra of **5Z** (5×10^{-5} M in n-hexane) after addition of TFA (V_{TFA}:V_{DCM} = 0.0033) to stable state, then irradiation with 337 nm UV light after bubbling with nitrogen 20 min under 0 ^{0}C.

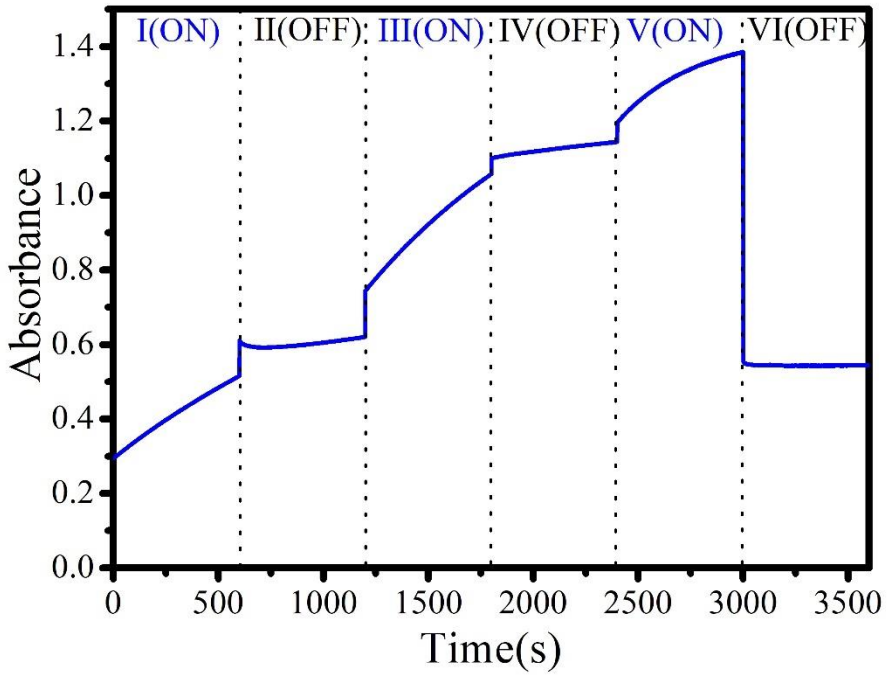


Figure S95. Control of the isomerization rate of **5Z** (5×10^{-5} M in n-hexane) by the addition of TFA or bubbling with nitrogen. Conditions: stage I: addition of TFA (V_{TFA}:V_{DCM} = 0.0033); stage II: bubbling with nitrogen for 5 min under 0 ^{0}C; stage III: addition of TFA (V_{TFA}:V_{DCM} = 0.0033); stage IV: bubbling with nitrogen 5 min under 0 ^{0}C; stage V: addition of TFA (V_{TFA}:V_{DCM} = 0.0066); Stage VI: irradiation with 337 nm UV light after bubbling with nitrogen 20 min under 0 ^{0}C .

8 DFT studies

1. Computational Methods

All of the DFT calculations were carried out with the Gaussian 09.[7] The geometries of intermediates and transition states were optimized using the M06-2X[8] with 6-31G(d, p) basis set. Vibrational frequency calculations were performed to confirm that the optimized structures were either a local minimum or a transition state. The solvation single-point energy calculations were calculated at the level of M06-2X/6-311+G(d, p)/SMD[9] in the dichloromethane solvent based on the gas-phase optimized geometries. Intrinsic reaction coordinate (IRC) calculations were calculated to obtain stable intermediates or complexes connected by corresponding transition states.

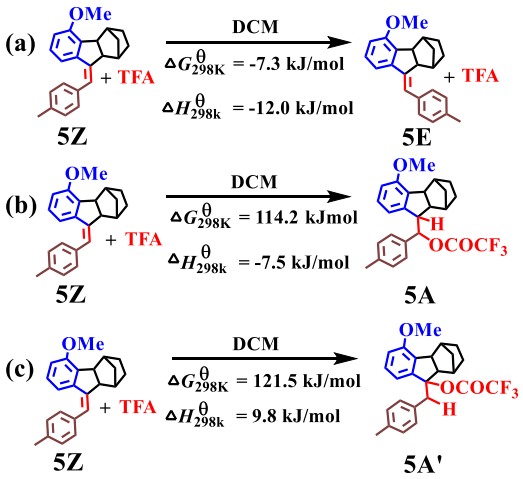


Figure S96. Three possible reactions of **5Z** catalyzed by acid. The enthalpy changes and the changes in Gibbs free energy were calculated at 298K and 1 atmosphere of pressure for the three reactions.

To estimate the bulk solvent effects on the reaction, all the structures were optimized in dichloromethane (DCM) with the polarized continuum model using the integral equation formalism variant (IEFPCM). The temperature-dependent enthalpy corrections and the entropy effects were calculated at 298 K and 1 atmosphere of pressure.

As depicted in **Figure S96**, the reactions **a** and **b** are exothermic reactions on the basis of the calculated enthalpy changes, and the absolute enthalpy change of the reaction is 4.5 kJ/mol which is larger than that of the reaction **b**, while the reaction **c** is an endothermic reaction and has the change in enthalpy of 9.8 kJ/mol. At 298 K and 1 atm, the computed change in the Gibbs free energy for reaction **a** is –7.3 kJ/mol, with a negative $\Delta G^{\theta}_{298\mathrm{K}}$ value, suggesting that reaction is spontaneous. For reactions **b** and **c**, $\Delta G^{\theta}_{298\mathrm{K}}$ were calculated to be 114.2 kJ/mol and 121.5 kJ/mol, respectively, suggesting that reactions **b** and **c** are not thermodynamically viable. The present theoretical calculations provide a rational explanation as to why only the isomerized

product could be observed for **5Z** under acidic conditions.

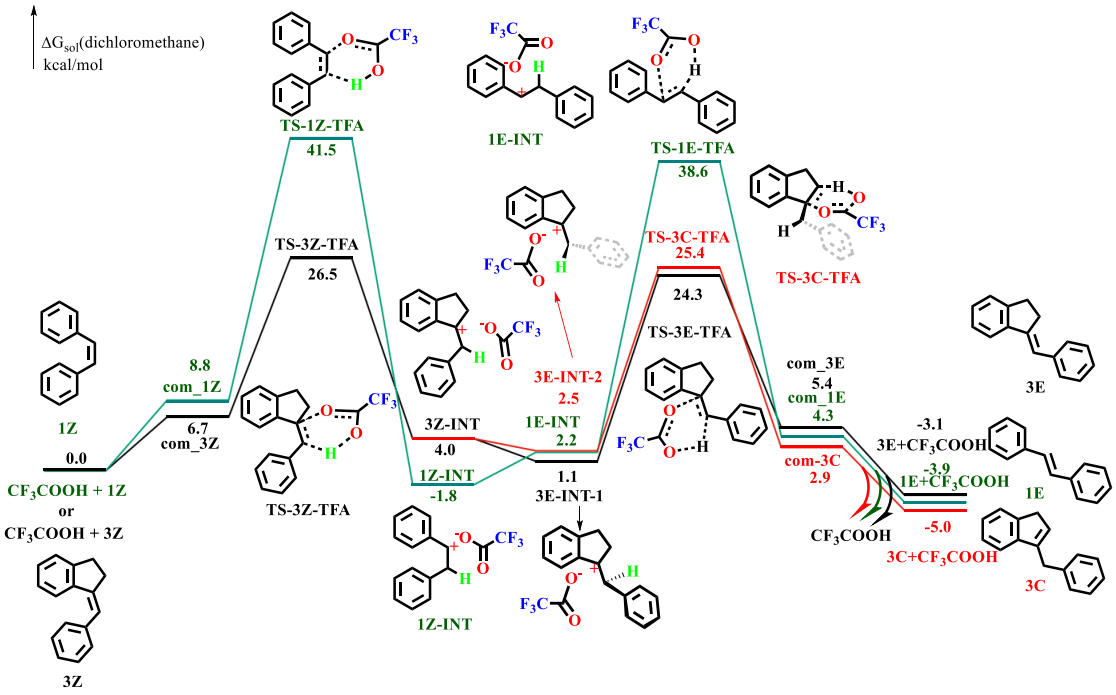


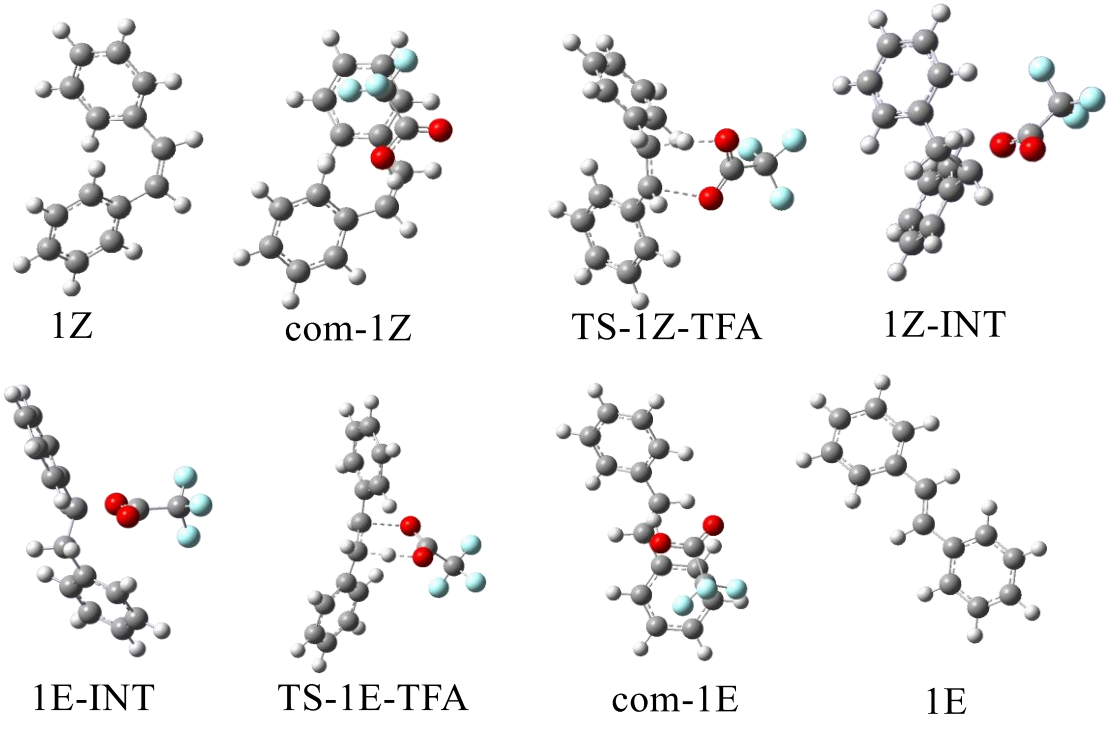
Figure S97. Calculated energy profiles of **1Z** to **1E** and **3Z** to **3E/ 3C**

2. Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	*E*(elec-M06-2X)[1]	*G*(corr-M06-2X)[2]	*H*(corr-M06-2X)[3]	*E*(solv,M06-2X)[4]	IF[5]
1Z	-540.474118	0.178702	0.229126	-540.6173175	—
com-1Z	-1067.099922	0.20886	0.278858	-1067.420611	—
TS-1Z-TFA	-1067.039861	0.205102	0.272833	-1067.364775	-1079.76
1Z-INT	-1067.120443	0.210328	0.280034	-1067.438876	—
1E-INT	-1067.116364	0.212613	0.280306	-1067.434805	—
TS-1E-TFA	-1067.045097	0.205552	0.272827	-1067.369821	-1259.91
com-1E	-1067.105719	0.208909	0.278677	-1067.427776	—
1E	-540.478827	0.178033	0.229114	-540.6228809	—
3Z	-617.873408	0.213425	0.26623	-618.0329792	—
com-3Z	-1144.499379	0.240573	0.315742	-1144.836675	—
TS-3Z-TFA	-1144.455258	0.241435	0.311467	-1144.805946	-233.44
3Z-INT	-1144.514657	0.247972	0.316902	-1144.84835	—
3E-INT-1	-1144.519319	0.248345	0.316845	-1144.853264	—
3E-INT-2	-1144.514521	0.246973	0.316753	-1144.84967	—
TS-3E-TFA	-1144.45905	0.240736	0.310426	-1144.808653	-279.60
TS-3C-TFA	-1144.452997	0.239772	0.310982	-1144.806068	-228.44
com-3E	-1144.505251	0.243879	0.315574	-1144.842044	—
com-3C	-1144.504294	0.241175	0.315152	-1144.843295	—

3E	-617.877497	0.21364	0.266349	-618.0380497	—
3C	-617.876442	0.211003	0.265593	-618.0384872	—
4Z	-811.950743	0.310599	0.37087	-812.1539596	—
com-4Z	-1338.578051	0.338711	0.420342	-1338.959473	—
TS-4Z-TFA	-1338.533017	0.339943	0.415945	-1338.926959	-206.79
4Z-INT	-1338.582599	0.346	0.421656	-1338.960416	—
4E-INT-1	-1338.590248	0.347546	0.420693	-1338.966456	—
4E-INT-2	-1338.584198	0.345934	0.421349	-1338.963024	—
TS-4E-TFA	-1338.196109	0.340051	0.415768	-1338.929311	-245.36
TS-4C-TFA	-1338.526159	0.337177	0.414739	-1338.918672	-256.57
com-4E	-1338.682463	0.340515	0.420391	-1338.963535	—
com-4C	-1338.586139	0.336929	0.420052	-1338.944631	—
4E	-811.955099	0.311415	0.371255	-812.1587678	—
4C	-811.99399	0.309491	0.370545	-812.1380778	—

[1]The electronic energy calculated by M06-2X in gas phase. [2]The thermal correction to Gibbs free energy calculated by M06-2X in gas phase. [3]The thermal correction to enthalpy calculated by M06-2X in gas phase. [4]The electronic energy calculated by M06-2X in solvent. [5]The M06-2X calculated imaginary frequencies for the transition states.



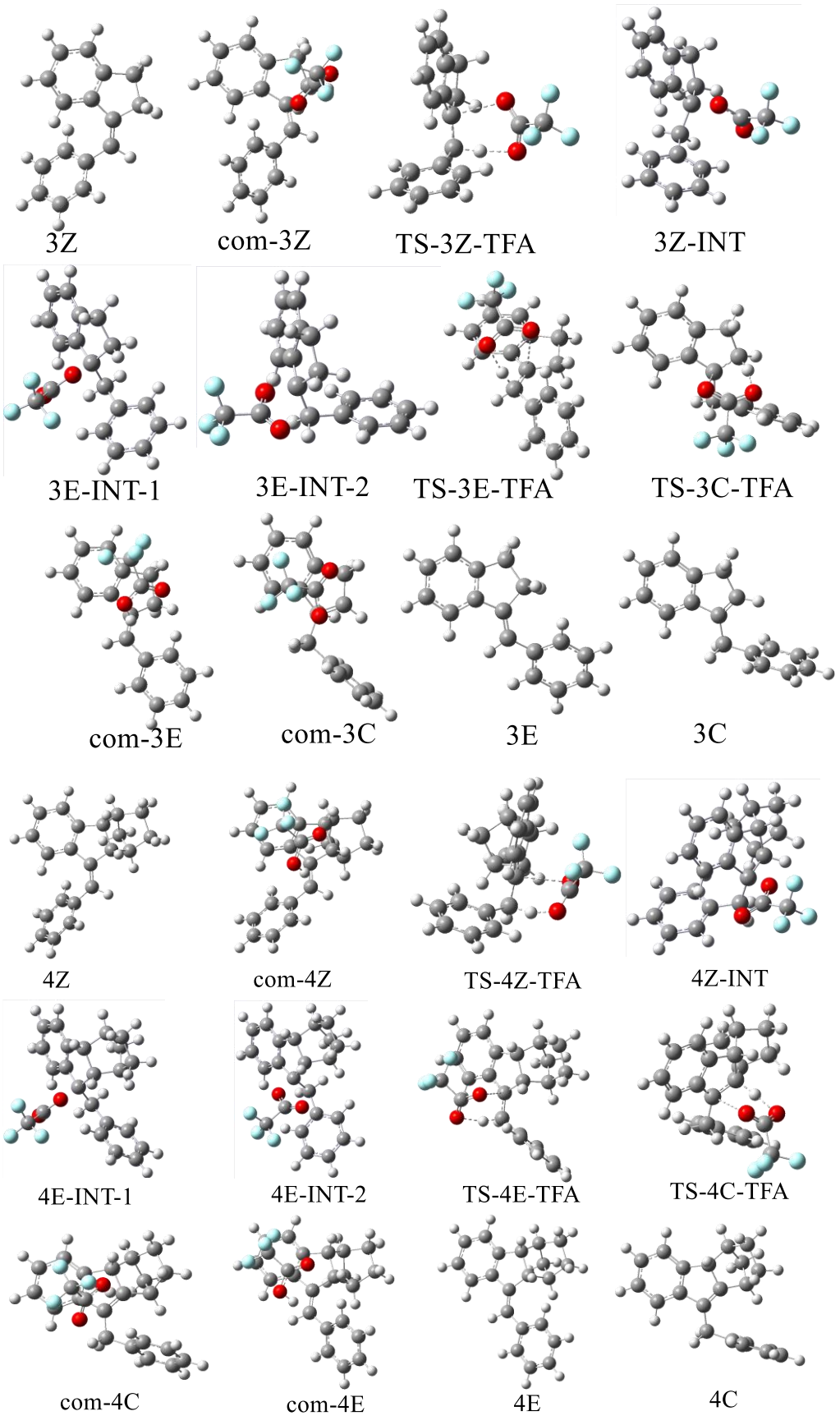


Figure S98. Optimized geometric structures of the compounds at ground state and some important

transition state. The dark grey atoms represent carbon, red atoms represent oxygen and blue atoms represent fluorine.

3.M06-2X Geometries for All the Optimized Compounds and Transition State

1Z

C	1.59149800	0.75838300	0.08899800
C	2.80690800	0.80505300	-0.60334700
C	3.70985300	-0.25112500	-0.53381000
C	3.41830800	-1.36582600	0.24693700
C	2.22182400	-1.41360500	0.96072000
C	1.31752200	-0.36144000	0.88579200
C	0.67027100	1.91116600	0.01104700
H	4.64351500	-0.20038400	-1.08487600
H	4.12309900	-2.18872400	0.30816200
H	1.99591600	-2.27210000	1.58520900
H	0.39134100	-0.39657900	1.45056800
C	-0.67032400	1.91122100	-0.01108700
H	-1.16154900	2.88268600	0.01631500
C	-1.59151000	0.75846400	-0.08909800
C	-2.80678400	0.80501400	0.60350100
C	-1.31768900	-0.36123600	-0.88613200
C	-3.70965800	-0.25123700	0.53412900
H	-3.03866500	1.67817100	1.20755700
C	-2.22195100	-1.41344000	-0.96093700
H	-0.39170500	-0.39622300	-1.45123700
C	-3.41823800	-1.36582900	-0.24681200
H	-4.64318400	-0.20061500	1.08543600
H	-1.99617500	-2.27182700	-1.58562300
H	-4.12299600	-2.18876100	-0.30795500
H	1.16136000	2.88273200	-0.01565600
H	3.03886000	1.67825700	-1.20730800

Com-1Z

C	1.33159300	1.56443200	0.68093300
C	0.83145700	2.85998200	0.48805900
C	1.49015700	3.75222100	-0.35149900
C	2.65903100	3.36775400	-1.00488300
C	3.15329800	2.07823800	-0.83181000
C	2.49432100	1.18484000	0.00101900
C	0.78669000	0.68115700	1.73291700
H	1.09869900	4.75569200	-0.48433400
H	3.18440400	4.07181200	-1.64216500
H	4.06743200	1.77194600	-1.32996400

H	2.91257700	0.19833100	0.16597100
C	0.83103000	-0.65872200	1.79687300
H	0.58195800	-1.12276100	2.75569200
C	1.25459400	-1.59094900	0.72960400
C	2.20619100	-2.56562000	1.04108300
C	0.76964700	-1.51005200	-0.58195700
C	2.71136800	-3.40613800	0.05669000
H	2.57621400	-2.63527300	2.06039600
C	1.26372700	-2.36329900	-1.56390600
H	0.03131200	-0.75556000	-0.83857200
C	2.24472000	-3.30269800	-1.25093800
H	3.47012900	-4.13969400	0.30954600
H	0.88715000	-2.28887200	-2.57893200
H	2.63838800	-3.95624000	-2.02251800
H	-1.23182900	-0.83197300	1.98056000
C	-2.10755900	0.12595100	0.65492000
C	-3.06835900	-0.04653800	-0.51367600
F	-4.03844100	-0.91408100	-0.24832400
F	-2.38401500	-0.47459800	-1.58127000
F	-3.59910800	1.13693000	-0.79467300
O	-2.00313600	-0.96242000	1.39942200
O	-1.53018900	1.16883200	0.78074500
H	0.37716700	1.20781700	2.59297800
H	-0.07056700	3.16386600	1.00882600

TS-1Z-TFA

C	1.17444300	1.57957500	0.63797600
C	0.71283800	2.89406500	0.46029500
C	1.39745400	3.77174600	-0.36491500
C	2.56680800	3.35624300	-1.00303500
C	3.04628200	2.06326500	-0.81363400
C	2.35208200	1.17061000	-0.00452800
C	0.48977500	0.71854900	1.60332800
H	1.02548400	4.78006100	-0.51061500
H	3.10694600	4.04504100	-1.64477700
H	3.96248300	1.74517800	-1.29916100
H	2.73516600	0.16831400	0.14524700
C	0.54592800	-0.69392900	1.74818100
H	0.71694900	-0.99428900	2.78623200
C	1.12361400	-1.59262500	0.70487400
C	2.09843300	-2.53797100	1.02736100
C	0.65328000	-1.52229300	-0.61181700
C	2.61269900	-3.38561900	0.04882300
H	2.45925100	-2.60690200	2.05019900
C	1.16949100	-2.36574500	-1.58780700

H	-0.10899200	-0.79319900	-0.87442200
C	2.15223300	-3.29916100	-1.26136400
H	3.37247200	-4.11429600	0.31277600
H	0.79733500	-2.29945900	-2.60492100
H	2.55098100	-3.95999100	-2.02396500
H	-0.68693500	-0.88874700	1.73510500
C	-2.15489100	0.06025700	0.69066200
C	-3.13638100	-0.03538600	-0.49642400
F	-4.12171500	-0.89571200	-0.25597900
F	-2.47058100	-0.45953300	-1.58540600
F	-3.66937100	1.15225700	-0.78272000
O	-2.06332200	-0.95041000	1.42893600
O	-1.47073000	1.10235800	0.75423800
H	0.07790000	1.24428700	2.46072900
H	-0.20616200	3.19583700	0.95128100

1Z-INT

C	1.48020600	1.30528100	0.23569900
C	1.67294600	0.82912100	-1.06152200
C	2.87311300	1.07641100	-1.72150700
C	3.88915800	1.78907800	-1.09026100
C	3.70105600	2.26165800	0.20612800
C	2.49851700	2.02276500	0.86384400
C	0.23033300	0.98879700	1.01480800
H	3.01586800	0.70573400	-2.73130800
H	4.82396100	1.97862500	-1.60767500
H	4.48598200	2.82326100	0.70206400
H	2.34783900	2.39827700	1.87340300
C	0.35652200	-0.29761600	1.85503500
H	1.19133900	-0.14544900	2.54690800
C	0.58075200	-1.52524300	1.01021800
C	1.87170800	-1.93559900	0.66822200
C	-0.50830500	-2.24127200	0.50855100
C	2.06980300	-3.03922300	-0.15572600
H	2.72525300	-1.37591800	1.04306500
C	-0.31417600	-3.34303800	-0.31922500
H	-1.51795900	-1.93652000	0.77179200
C	0.97664200	-3.74452700	-0.65270800
H	3.07861100	-3.34748800	-0.41091700
H	-1.17119700	-3.88862600	-0.70074200
H	1.13027400	-4.60565200	-1.29501800
H	-0.55339200	-0.40029300	2.45394100
C	-2.07923300	0.94187000	0.54504000
C	-3.09274200	0.65471800	-0.57674800
F	-4.32200600	0.93182300	-0.16696900

F	-3.03341400	-0.63936900	-0.91080100
F	-2.82362800	1.37866600	-1.66210100
O	-2.40526500	1.19142000	1.67208400
O	-0.84967900	0.83515100	0.06537900
H	-0.02726300	1.81899300	1.68022100
H	0.88386700	0.26333500	-1.54567800

1E-INT

C	-2.15688800	-0.81552500	-0.16669300
C	-2.99054100	-0.97270500	-1.27614100
C	-4.37375100	-0.91038900	-1.14224700
C	-4.93813200	-0.69263000	0.11125600
C	-4.11469100	-0.53490500	1.22301900
C	-2.73099700	-0.59416800	1.08780500
C	-0.65993000	-0.89576400	-0.37815900
H	-5.00816700	-1.03530800	-2.01356400
H	-6.01665700	-0.64565900	0.22203900
H	-4.55046900	-0.36112900	2.20142900
H	-2.09853800	-0.44635500	1.95550200
C	0.13375300	-1.60372700	0.72624200
H	-0.05905900	-1.13817100	1.69355400
C	0.00557000	1.32153100	0.26385100
C	0.74468300	2.55447300	-0.28966300
F	2.03731100	2.25943900	-0.45397000
F	0.64565800	3.56781700	0.56123500
F	0.24650300	2.93087700	-1.46684500
O	-0.34624000	1.24926600	1.41044200
O	-0.10221100	0.41549700	-0.68934500
C	1.61468900	-1.60521200	0.43281200
C	2.16167900	-2.53394600	-0.45565000
C	2.45256000	-0.64519300	1.00337400
C	3.51663500	-2.50461000	-0.76890600
H	1.51909800	-3.29076900	-0.90016400
C	3.80833900	-0.61012500	0.68865300
H	2.03752100	0.07761000	1.70150800
C	4.34335900	-1.53964200	-0.19804500
H	3.92846500	-3.23633300	-1.45661400
H	4.44595200	0.14436200	1.13798500
H	5.40033500	-1.51476600	-0.44217600
H	-0.25176800	-2.62816300	0.76929900
H	-0.47381100	-1.42609600	-1.31632200
H	-2.54856400	-1.14530300	-2.25408300

TS-1E-TFA

C	2.30052900	0.78971600	-0.26432500
C	3.14871600	0.95982400	-1.36316400

C	4.52804700	0.91452000	-1.19581400
C	5.06419300	0.66929500	0.06535400
C	4.22271000	0.46611600	1.16026100
C	2.84637200	0.52800000	1.00030900
C	0.85763100	0.89239000	-0.45923100
H	5.18251400	1.05959300	-2.04843800
H	6.14049700	0.62257700	0.19564700
H	4.64401500	0.25072600	2.13627800
H	2.18698400	0.33181100	1.84069200
C	-0.02300500	1.32301600	0.56426200
H	-0.08218300	0.20698200	1.17530500
C	-0.17080900	-1.59906900	0.31897000
C	-1.12868900	-2.77049200	0.01793000
F	-2.20671300	-2.30987700	-0.63637100
F	-1.54200500	-3.36880300	1.13038000
F	-0.53703300	-3.67797500	-0.75967100
O	-0.19471700	-1.11887400	1.48283500
O	0.49146700	-1.16912900	-0.64722400
C	-1.42538300	1.68664000	0.21496200
C	-2.06365100	2.74755600	0.86281700
C	-2.13919000	0.94618300	-0.73420400
C	-3.38027700	3.07458400	0.55789200
H	-1.52002600	3.32216000	1.60800100
C	-3.45624900	1.27575100	-1.03883700
H	-1.67142800	0.09706000	-1.22527200
C	-4.08087200	2.34110400	-0.39665400
H	-3.85976800	3.90493800	1.06636900
H	-3.99776800	0.68859100	-1.77348300
H	-5.10923000	2.59397000	-0.63251100
H	0.45163400	1.93072900	1.33610200
H	0.51066200	0.89724300	-1.48993300
H	2.72142000	1.13671600	-2.34584500

Com-1E

C	-2.83240400	-0.44913800	-0.35798900
C	-3.38700300	0.74045600	-0.85116400
C	-4.69138800	1.10291400	-0.53140500
C	-5.46597600	0.27718100	0.27888400
C	-4.92915100	-0.91461300	0.76428100
C	-3.62569400	-1.27690700	0.44860100
C	-1.43038800	-0.75782600	-0.68013900
H	-5.10345500	2.02988500	-0.91698100
H	-6.48564800	0.55478200	0.52473000
H	-5.53432400	-1.56933500	1.38320900
H	-3.22316000	-2.22015100	0.80569600

C	-0.59741200	-1.45219000	0.10993500
H	-0.84697300	1.20807000	0.94277600
C	0.74313900	1.61652100	0.05266100
C	2.25248900	1.71900300	0.33000000
F	2.67596100	0.70004300	1.07235500
F	2.50394800	2.85386000	0.99196100
F	2.92681700	1.73691100	-0.81207400
O	0.08596800	1.36021300	1.17527100
O	0.26327800	1.78653200	-1.03423900
C	0.84076500	-1.65709900	-0.11081100
C	1.58410000	-2.31674400	0.87686600
C	1.51679700	-1.18148200	-1.24556700
C	2.95526500	-2.49803600	0.74205100
H	1.07408900	-2.68505500	1.76294100
C	2.88828500	-1.35942300	-1.37779200
H	0.97349500	-0.65896500	-2.02621500
C	3.61337200	-2.01735900	-0.38621900
H	3.51102800	-3.00982400	1.52103600
H	3.39441100	-0.97439300	-2.25699700
H	4.68486300	-2.15102200	-0.49232200
H	-0.98087400	-1.85605000	1.04691400
H	-1.05142400	-0.29558500	-1.58847100
H	-2.77529700	1.38481500	-1.47791600

1E

C	-1.92832100	0.20644300	0.01830700
C	-2.80498100	1.23351700	-0.35387500
C	-4.17979300	1.02800500	-0.38359400
C	-4.70673900	-0.21135700	-0.03244700
C	-3.84754500	-1.23856600	0.35526600
C	-2.47480400	-1.03157500	0.38597400
C	-0.48207100	0.46558500	0.01421400
H	-4.83990400	1.83681600	-0.68014200
H	-5.77926700	-0.37467300	-0.05098500
H	-4.25172300	-2.20298500	0.64615000
H	-1.82031200	-1.83092500	0.71918900
C	0.48211900	-0.46579700	0.01430300
C	1.92835100	-0.20657100	0.01834700
C	2.80510500	-1.23354800	-0.35385900
C	2.47468900	1.03149800	0.38605100
C	4.17989000	-1.02786700	-0.38362200
H	2.39629200	-2.20158100	-0.63100400
C	3.84740400	1.23865600	0.35530300
H	1.82007200	1.83072600	0.71932900
C	4.70669900	0.21155100	-0.03246900

H	4.84009400	-1.83658800	-0.68021100
H	4.25148600	2.20310700	0.64620900
H	5.77920800	0.37499100	-0.05104100
H	0.20110900	-1.51716400	-0.02678500
H	-0.20100500	1.51693400	-0.02707700
H	-2.39606800	2.20150800	-0.63102100

3Z

C	-1.29348200	-0.01457300	-0.15636000
C	-2.64694200	-0.20035200	0.16282100
C	-3.53662900	0.86633500	0.13918300
C	-3.07085000	2.12751400	-0.22601500
C	-1.73028200	2.31240700	-0.56959500
C	-0.83425000	1.24838900	-0.53869600
C	-0.59566200	-1.31864800	-0.08931800
C	-1.69102500	-2.37506500	-0.06996300
C	-2.92450600	-1.64620700	0.50263300
H	-4.58303400	0.71636800	0.38956200
H	-3.75592700	2.96888700	-0.25668400
H	-1.38396300	3.29522500	-0.87283600
H	0.20191100	1.39830500	-0.82092900
H	-1.40488400	-3.26288900	0.49779800
H	-3.86823900	-2.00501900	0.08386500
C	0.71149500	-1.61540400	-0.04650100
H	0.97500400	-2.67304600	-0.06670700
C	1.85895800	-0.68933100	0.03907600
C	1.86634500	0.39452700	0.92666900
C	3.00445400	-0.92882800	-0.72934500
C	2.97182400	1.23299600	1.01462300
H	0.99468800	0.57103000	1.54997200
C	4.11085100	-0.09020200	-0.64315500
H	3.01866400	-1.77899200	-1.40595800
C	4.09684200	0.99679100	0.22686800
H	2.95956500	2.06762900	1.70857200
H	4.98618700	-0.28737200	-1.25396600
H	4.96038100	1.65005900	0.29856700
H	-1.90444800	-2.68820400	-1.09914900
H	-2.97874800	-1.77407500	1.59035000

com-3Z

C	1.02263000	1.78632100	0.16354600
C	0.07686600	2.81856900	0.25933100
C	0.05107600	3.84472000	-0.67766200
C	0.99196600	3.84806000	-1.70393000
C	1.95514400	2.83973000	-1.78470500
C	1.97917600	1.80490000	-0.85628900

C	0.84316200	0.86087800	1.30475000
C	-0.06306700	1.57802900	2.29732100
C	-0.81445500	2.63391600	1.46322800
H	-0.68497700	4.63973400	-0.60159100
H	0.98727200	4.64713200	-2.43849000
H	2.69761000	2.86713900	-2.57549300
H	2.74108300	1.03619800	-0.91709700
H	0.56780000	2.07591300	3.04317300
H	-1.79572600	2.25057900	1.16382000
C	1.33760700	-0.37265700	1.53751100
H	1.10712900	-0.80362600	2.51287700
C	2.18283400	-1.22547700	0.67353500
C	3.21520800	-1.96932100	1.25866000
C	1.94461700	-1.37943400	-0.69880100
C	4.01288200	-2.81077800	0.49144100
H	3.39391800	-1.87620100	2.32636700
C	2.73868600	-2.22537600	-1.46538100
H	1.12652800	-0.83901600	-1.16700300
C	3.77907700	-2.93912400	-0.87525400
H	4.81429300	-3.37097300	0.96226200
H	2.53589300	-2.33503300	-2.52579800
H	4.39601700	-3.60015400	-1.47501000
H	-0.73455100	0.89156400	2.81565100
H	-0.97703600	3.56867100	2.00589200
H	-0.53249200	-0.81881400	0.51029600
C	-2.41335200	-0.77449000	0.37800700
C	-3.53883600	-1.31990800	-0.51782200
F	-4.71432500	-0.85860400	-0.11442900
F	-3.55809300	-2.65331800	-0.46670600
F	-3.34264000	-0.95144700	-1.78486800
O	-1.23936700	-1.18291000	-0.06830500
O	-2.62495500	-0.08635800	1.33946200

TS-3Z-TFA

C	0.68270700	1.59826400	0.06685000
C	0.05100200	2.85998300	0.11945600
C	0.13714700	3.73174300	-0.95740800
C	0.84678100	3.32739100	-2.08383800
C	1.46401100	2.06990100	-2.14813900
C	1.38808200	1.19029300	-1.08264400
C	0.45985900	0.92697000	1.31790900
C	-0.17527000	1.88414100	2.27623700
C	-0.69215500	3.04088100	1.41069900
H	-0.34526000	4.70315300	-0.92551900
H	0.92274200	3.99747800	-2.93480400

H	2.00476400	1.78475600	-3.04354100
H	1.86323900	0.21902200	-1.13754200
H	0.61790200	2.22297900	2.95829600
H	-1.75980600	2.89570100	1.22108300
C	0.83110500	-0.40067000	1.74898900
H	1.11464500	-0.37961000	2.80839500
C	1.76290400	-1.20860400	0.88680200
C	3.14365900	-1.00544300	0.95091700
C	1.24650400	-2.13744000	-0.01994600
C	3.99949000	-1.70326700	0.10459100
H	3.54696700	-0.28640800	1.65986700
C	2.10455100	-2.83148500	-0.87023800
H	0.17360400	-2.30375800	-0.06013100
C	3.47893700	-2.61312000	-0.81392200
H	5.07049900	-1.53628700	0.15950000
H	1.69546400	-3.54592500	-1.57718400
H	4.14439800	-3.15543500	-1.47786300
H	-0.94195600	1.38010600	2.86676900
H	-0.53973700	4.02747600	1.85467700
H	-0.20953000	-0.91790200	1.77522700
C	-2.07674100	-0.72451400	0.60903600
C	-2.87563900	-1.30669300	-0.57925900
F	-3.49704300	-0.36783100	-1.29485800
F	-3.79085800	-2.19296800	-0.17657600
F	-2.02849500	-1.95233300	-1.40752600
O	-1.65563800	-1.58636600	1.41589100
O	-1.86585900	0.50171900	0.60246600

3Z-INT

C	1.89518600	-0.04879100	0.03549500
C	2.94358200	0.86280300	0.17024800
C	4.12074000	0.69556000	-0.55108600
C	4.22960400	-0.38478900	-1.42302700
C	3.16467700	-1.27063600	-1.58930400
C	1.98378800	-1.10412700	-0.86881500
C	0.72237200	0.35864000	0.90968000
C	1.33810500	1.43248700	1.83592500
C	2.56772500	1.98852300	1.10086000
H	4.93923800	1.40102300	-0.44157300
H	5.14424300	-0.53089900	-1.98901000
H	3.25332900	-2.09347500	-2.29108100
H	1.14916600	-1.77779500	-1.02314700
H	1.66117400	0.92086900	2.74804600
H	2.31276400	2.88072500	0.51747700
C	0.03885600	-0.75657800	1.72557000

H	0.83994700	-1.23609900	2.29728100
C	-0.72305200	-1.80591100	0.95147700
C	-0.15931500	-3.06198700	0.70906600
C	-2.01592000	-1.55571100	0.48378000
C	-0.85181200	-4.03007100	-0.01217400
H	0.83877000	-3.27631400	1.08338300
C	-2.70962900	-2.51803300	-0.24372600
H	-2.50020900	-0.61212600	0.71522000
C	-2.12734200	-3.75632800	-0.49921300
H	-0.39642900	-4.99909500	-0.19010400
H	-3.71006100	-2.30049200	-0.60363600
H	-2.66917500	-4.50841500	-1.06335000
H	0.60592500	2.18475500	2.12843900
H	3.37282200	2.26770200	1.78569000
H	-0.62808600	-0.27147800	2.44469200
C	-1.30886500	1.57274200	0.39400800
C	-2.14390700	2.03485300	-0.81678300
F	-1.38830400	2.66747500	-1.71310400
F	-3.11253000	2.85071200	-0.42130000
F	-2.69749400	0.97074700	-1.40784600
O	-1.68071200	1.74023400	1.52493800
O	-0.22144000	0.96412100	-0.03868300

3E-INT-1

C	2.01555300	-0.66971100	-0.28981300
C	2.77974900	-0.95528400	0.84467000
C	4.16652100	-0.88948300	0.78833000
C	4.77558200	-0.54327400	-0.41724800
C	4.00927800	-0.26101600	-1.54808900
C	2.61755000	-0.31726500	-1.49235500
C	0.54015300	-0.80914000	0.03903500
C	0.56168500	-1.66486200	1.31511100
C	1.88813900	-1.31106500	2.01121900
H	4.76735600	-1.11354100	1.66485000
H	5.85834400	-0.49666600	-0.47816700
H	4.50008700	0.00637500	-2.47800500
H	2.01772800	-0.07723900	-2.36365600
H	0.57951800	-2.71712200	1.01331300
H	1.76155000	-0.44439600	2.66980800
C	-0.34698400	-1.36152000	-1.08370900
H	-0.32979600	-1.49431300	1.92136000
H	2.28123600	-2.13223500	2.61574800
H	-0.21634100	-0.74857500	-1.97845300
C	-0.06413900	1.50417100	-0.31814300
C	-0.71567600	2.69538800	0.41003300

F	-2.01118500	2.43555800	0.61503200
F	-0.61570300	3.79473400	-0.32541000
F	-0.14015200	2.91471800	1.59224100
O	0.24383600	1.55712000	-1.47833500
O	0.02093100	0.48353100	0.51263500
C	-1.80705200	-1.42210700	-0.70324200
C	-2.34065700	-2.54641300	-0.06838700
C	-2.64439000	-0.33072000	-0.94750800
C	-3.67541000	-2.57560700	0.32482500
H	-1.70503600	-3.40984800	0.11231100
C	-3.97805100	-0.35390400	-0.55161400
H	-2.24951000	0.53996700	-1.46488700
C	-4.49665400	-1.47638300	0.08804900
H	-4.07517400	-3.45878500	0.81289500
H	-4.61215700	0.50501500	-0.74643100
H	-5.53733600	-1.49749600	0.39459900
H	0.03356900	-2.36228200	-1.31341600

3E-INT2

C	-0.38597500	-1.36063500	-0.11497600
C	-0.44533600	-2.07073200	1.08286100
C	-0.81150600	-3.41247500	1.08185000
C	-1.10614300	-4.03024100	-0.13186600
C	-1.01970500	-3.32279500	-1.33205400
C	-0.64960700	-1.97981500	-1.33109200
C	0.07293300	0.06185100	0.13543600
C	-0.14220800	0.22380800	1.65201600
C	-0.02959500	-1.19508500	2.23969900
H	-0.86700500	-3.97133700	2.01137100
H	-1.40046800	-5.07486300	-0.14613800
H	-1.24008800	-3.82252200	-2.26952400
H	-0.56847500	-1.43277800	-2.26660600
H	-1.16278800	0.58888900	1.79466200
H	1.00326300	-1.42567200	2.52621100
C	-0.56351100	1.13203700	-0.76702900
H	0.53861900	0.95204700	2.09227100
H	-0.65346100	-1.33046200	3.12683200
H	-0.02486300	2.06949100	-0.61200000
C	2.29645400	1.03837900	0.09893900
C	3.73947000	0.68674100	-0.31336300
F	4.16405700	-0.38546600	0.35912200
F	4.55250700	1.70178000	-0.05480500
F	3.79626100	0.41232000	-1.61836500
O	2.00965200	2.09576000	0.59147600
O	1.51330100	0.01015200	-0.17839500

C	-2.03488800	1.36130100	-0.51086500
C	-3.01543500	0.53990100	-1.07223100
C	-2.43837400	2.41623300	0.31318500
C	-4.36436700	0.76409500	-0.81172800
H	-2.72152800	-0.28203700	-1.71794100
C	-3.78583400	2.64231900	0.57724300
H	-1.68282300	3.06532400	0.74945500
C	-4.75359400	1.81439900	0.01483700
H	-5.11277100	0.11739100	-1.25845200
H	-4.07923200	3.46800500	1.21757400
H	-5.80548100	1.98961200	0.21583000
H	-0.39862000	0.82820500	-1.80694700

TS-3E-TFA

C	0.84898100	-1.33498800	-0.33196200
C	1.46650200	-1.80359600	0.84281700
C	2.79194100	-2.21728500	0.80560700
C	3.48581000	-2.10001200	-0.39492300
C	2.88797500	-1.57137400	-1.55082400
C	1.56099300	-1.18431100	-1.53405200
C	-0.50448500	-0.96924100	-0.04158500
C	-0.81778200	-1.33272800	1.36962700
C	0.54063100	-1.65063500	2.01441300
H	3.28805300	-2.58637600	1.69703400
H	4.52807000	-2.40129400	-0.43581400
H	3.47672300	-1.45842400	-2.45385300
H	1.09069500	-0.74534600	-2.40803300
H	-1.47161400	-2.21722400	1.32203100
H	0.87341600	-0.77185000	2.57925700
C	-1.39709600	-0.36175200	-0.98847400
H	-1.38024300	-0.54119100	1.86470400
H	0.52659200	-2.51593200	2.68079500
H	-0.83133800	0.66520100	-1.14023300
C	0.77193600	1.62211800	-0.03457000
C	2.30602500	1.80009800	0.08182100
F	2.61462400	2.98904200	0.61551800
F	2.92035700	1.71038900	-1.10189400
F	2.83518900	0.85406500	0.87876200
O	0.28669300	1.80276500	-1.17597300
O	0.19195300	1.26125600	1.00550600
C	-2.81560900	-0.11988900	-0.56051600
C	-3.86505700	-0.89136700	-1.06011200
C	-3.08769400	0.90394700	0.35282400
C	-5.17337100	-0.65124200	-0.64753400
H	-3.65759800	-1.68034500	-1.77859400

C	-4.39493700	1.13896200	0.76652100
H	-2.25890600	1.50324400	0.72461900
C	-5.43966000	0.36271600	0.26808900
H	-5.98387300	-1.25486800	-1.04339100
H	-4.60015600	1.93658300	1.47331900
H	-6.45919700	0.55153400	0.58836900
H	-1.29193200	-0.81385500	-1.98095000

TS-3C-TFA

C	2.07717500	-0.89285600	-0.29050500
C	2.77493400	-0.92317700	0.93156700
C	4.16522200	-0.88474000	0.93215700
C	4.82488800	-0.82808700	-0.29053500
C	4.12675400	-0.79439800	-1.51093200
C	2.74609500	-0.82046000	-1.52334100
C	0.67712000	-0.90413500	-0.01629100
C	0.43830300	-0.93797200	1.41157500
C	1.81393400	-0.96050400	2.08283900
H	4.72445900	-0.89774300	1.86181600
H	5.91022700	-0.80466800	-0.30717000
H	4.68066900	-0.73740600	-2.44112900
H	2.19385800	-0.77260300	-2.45626300
H	-0.29111900	-1.69759300	1.70916600
H	1.95179300	-0.07690300	2.71618200
C	-0.39201900	-0.89074500	-1.05162400
H	-0.09391400	0.06216800	1.63590000
H	1.96345300	-1.84528300	2.70941800
H	-0.50149800	0.17221900	-1.31707300
C	-0.11829800	2.02476200	0.58756500
C	-0.95807000	2.99398100	-0.27707200
F	-0.20857400	3.80831500	-1.02065000
F	-1.80491500	3.73899500	0.43254700
F	-1.70491500	2.24762100	-1.13375700
O	-0.68316100	1.62529800	1.63458400
O	0.95478200	1.65109000	0.08694300
C	-1.71739000	-1.46497500	-0.60452600
C	-2.06514800	-2.77064500	-0.95235700
C	-2.59060600	-0.70549600	0.17866700
C	-3.27271700	-3.31682700	-0.52601800
H	-1.38926900	-3.36193800	-1.56528400
C	-3.79477500	-1.25585300	0.60789500
H	-2.32113900	0.30893100	0.46125600
C	-4.13930300	-2.55897600	0.25630900
H	-3.53576700	-4.33163000	-0.80659100
H	-4.46716100	-0.65962400	1.21586300

H	-5.08182100	-2.98165500	0.58889700
H	-0.02670700	-1.39513600	-1.95270600

com-3E

C	0.76118600	-1.48251300	-0.05564800
C	1.58069700	-1.36289600	1.07262300
C	2.93002100	-1.69819500	1.00007700
C	3.44773800	-2.16300200	-0.20483700
C	2.62981900	-2.28014000	-1.33333500
C	1.28681200	-1.93348300	-1.26916800
C	-0.61007000	-1.04590300	0.26997100
C	-0.66270200	-0.83957900	1.77757700
C	0.80852200	-0.82517300	2.25210400
H	3.56901300	-1.59746700	1.87254000
H	4.49696600	-2.43207200	-0.27318700
H	3.05035300	-2.63942400	-2.26683700
H	0.65724400	-2.02096200	-2.14993700
H	-1.19831300	-1.69177500	2.21204900
H	1.13471400	0.19612900	2.47484200
C	-1.60111900	-0.89718800	-0.62634700
H	-1.19642100	0.06225800	2.07071100
H	0.96392300	-1.42602400	3.15248200
H	-0.51197700	1.17713900	-1.36806400
C	0.90951700	1.62996600	-0.25359200
C	2.44388700	1.72899600	-0.26185700
F	2.80714700	2.94544800	-0.68185900
F	2.98807300	0.82590200	-1.06893700
F	2.91190300	1.55116000	0.96939200
O	0.44062800	1.36235300	-1.46209200
O	0.26193800	1.81727200	0.74107400
C	-2.96178000	-0.38633400	-0.35750600
C	-4.07477200	-1.04290800	-0.89752200
C	-3.16915200	0.78473000	0.38390900
C	-5.36114700	-0.56650100	-0.67141500
H	-3.92339800	-1.94108200	-1.48998100
C	-4.45672800	1.26269000	0.60670200
H	-2.30955600	1.33482900	0.75808800
C	-5.55686500	0.58588000	0.08661000
H	-6.21275700	-1.09383100	-1.08945600
H	-4.59949400	2.17337200	1.17976800
H	-6.56038400	0.96010700	0.26091300
H	-1.40774700	-1.21147600	-1.65321500

com-3C

C	0.67153100	-1.48033900	-0.53170700
C	1.18371700	-2.16114500	0.58350000

C	2.53019100	-2.48010400	0.65508500
C	3.36613800	-2.09935000	-0.39644600
C	2.86007200	-1.40789200	-1.49767100
C	1.50327200	-1.09371100	-1.57870300
C	-0.75652700	-1.20172200	-0.29555600
C	-1.09149700	-1.66110500	0.92709900
C	0.08384700	-2.32692900	1.59936200
H	2.93633600	-2.99113300	1.52290700
H	4.42578400	-2.32839800	-0.34995000
H	3.53051000	-1.10461000	-2.29528000
H	1.11482100	-0.54349300	-2.43086500
H	-2.07702000	-1.58953300	1.37356200
H	0.34919700	-1.83025800	2.54071300
C	-1.61083800	-0.47547200	-1.30060000
H	-0.45117700	0.90160400	0.90781300
H	-0.12254200	-3.37841000	1.83382200
H	-1.04191200	0.38365400	-1.67708900
C	1.39980000	1.20578400	0.86726900
C	2.44693800	1.95239500	0.02437600
F	3.64514400	1.41510800	0.19863800
F	2.49040900	3.23346200	0.40713200
F	2.14077500	1.91983800	-1.27315400
O	0.17298800	1.48276900	0.43227900
O	1.68747800	0.51776100	1.80383400
C	-2.92755500	-0.00619800	-0.73347400
C	-3.99348600	-0.89688100	-0.58112400
C	-3.08664600	1.31323100	-0.30461700
C	-5.19162000	-0.47886800	-0.01071200
H	-3.87685900	-1.92560700	-0.91316000
C	-4.28543700	1.73474800	0.26651000
H	-2.26737400	2.01738900	-0.43150200
C	-5.34007200	0.83931000	0.41604300
H	-6.01204900	-1.18114000	0.09802200
H	-4.39585500	2.76501300	0.58959700
H	-6.27525100	1.16676400	0.85831500
H	-1.77826900	-1.13626000	-2.16116100

3E

C	-1.80004900	-0.27955200	0.10274900
C	-2.61173800	0.81840000	-0.20511800
C	-3.99263300	0.67909000	-0.27035200
C	-4.55934100	-0.56930500	-0.01957000
C	-3.75085900	-1.66543200	0.29061500
C	-2.36822000	-1.52852100	0.35488100
C	-0.38284300	0.12637200	0.10535800

C	-0.36405400	1.64438300	0.03603600
C	-1.77100700	2.04563500	-0.46637300
H	-4.62292400	1.53075000	-0.51037600
H	-5.63711800	-0.69077500	-0.05955600
H	-4.20691100	-2.62936400	0.49221100
H	-1.74465500	-2.37903700	0.61462800
H	0.44275600	2.01732800	-0.60025300
H	-2.15861000	2.93600200	0.03596200
C	0.65389000	-0.72753500	0.09540200
H	-0.20422400	2.05680300	1.03972500
H	-1.75181300	2.26389400	-1.54028100
C	2.08779600	-0.41469300	0.06457200
C	2.97015800	-1.36345000	-0.47499500
C	2.63078000	0.77745700	0.56681800
C	4.33556700	-1.11996200	-0.54403700
H	2.56769800	-2.29977300	-0.85223200
C	3.99872500	1.02024800	0.50106300
H	1.98382200	1.50594900	1.04144500
C	4.85653900	0.07818100	-0.05996900
H	4.99563700	-1.86688900	-0.97357000
H	4.39753000	1.94743700	0.90055300
H	5.92323000	0.27072400	-0.10965900
H	0.41931700	-1.79094200	0.05893100

3C

C	1.81648600	-0.28342200	-0.00007800
C	2.47977800	0.95437700	0.00024800
C	3.86430000	1.01080700	0.00030200
C	4.58582800	-0.18575400	0.00002600
C	3.92658500	-1.41496700	-0.00029800
C	2.53317200	-1.47594400	-0.00035300
C	0.36397500	-0.03615800	-0.00005200
C	0.14817000	1.29060400	0.00027500
C	1.44813300	2.05474200	0.00049500
H	4.38338600	1.96520000	0.00055600
H	5.67079300	-0.15927300	0.00006600
H	4.50559400	-2.33303300	-0.00050800
H	2.02269400	-2.43513900	-0.00060600
H	-0.82636600	1.76487900	0.00037300
H	1.54125500	2.70402400	-0.87907600
C	-0.64717100	-1.14933700	-0.00035000
H	1.54121200	2.70358900	0.88039200
H	-0.46886600	-1.78573100	-0.87711400
C	-2.07283300	-0.65717700	-0.00019900
C	-2.73495900	-0.39798300	1.20118000

C	-2.73471300	-0.39659300	-1.20141900
C	-4.03435400	0.10113300	1.20385200
H	-2.22356800	-0.58973600	2.14103200
C	-4.03410300	0.10252900	-1.20378000
H	-2.22312000	-0.58724900	-2.14138500
C	-4.68796300	0.35181800	0.00011400
H	-4.53731600	0.29286600	2.14642100
H	-4.53687000	0.29536000	-2.14623000
H	-5.70196400	0.73840800	0.00023300
H	-0.46885100	-1.78621800	0.87605700

4Z

C	-1.85660900	2.74462100	-0.20994900
C	-0.86377000	3.70542400	-0.04274100
H	-1.13347800	4.74961100	0.08017500
C	0.48170000	3.33129900	-0.05146700
H	1.25092900	4.08921100	0.05746400
C	0.85105700	1.99924300	-0.20327800
H	1.90003600	1.72874300	-0.21948600
C	-0.14420200	1.02505900	-0.34483700
C	-0.04403400	-0.43592300	-0.55246900
C	-1.45375600	-0.97372100	-0.78807600
H	-1.52651800	-1.44051200	-1.77621200
C	-1.93389500	-1.93827900	0.31915700
H	-1.20010400	-2.70881600	0.56656800
C	-3.31813100	-2.48192500	-0.08430300
H	-3.60917100	-3.31182700	0.56584000
H	-3.32653800	-2.85257500	-1.11359300
C	-4.25803100	-1.25589200	0.12081100
H	-4.79001000	-0.97265100	-0.79211500
H	-5.00898200	-1.46190200	0.88890300
C	-3.29142400	-0.15333500	0.59069800
H	-3.77632500	0.69713300	1.07656400
C	-2.41558600	0.24849200	-0.62016300
H	-3.03915600	0.43277000	-1.50220900
C	-1.49189200	1.41243600	-0.37289000
C	-2.29963700	-0.95792400	1.44745400
H	-2.77716800	-1.44832100	2.30139200
H	-1.44876000	-0.36736000	1.80021400
C	1.02309400	-1.25035900	-0.55485200
H	0.84216900	-2.28934400	-0.83456000
C	2.42247900	-0.93668800	-0.19810400
C	3.47157700	-1.34436300	-1.03004100
H	3.24057100	-1.85680900	-1.95981800
C	4.79506400	-1.09058700	-0.68458100

H	5.59527100	-1.40530500	-1.34699800
C	5.09305400	-0.43751200	0.50868100
C	4.05896000	-0.04622100	1.35659800
H	4.28357800	0.44894600	2.29609700
C	2.73656600	-0.29953600	1.00896300
H	1.92785700	-0.00494200	1.67221400
H	-2.90496900	3.03058700	-0.22903900
H	6.12526300	-0.24251000	0.78094700

com-4Z

C	0.28271300	0.07479600	0.79495200
C	1.52517700	-0.55319400	0.97094700
C	1.69202800	-1.54858500	1.92739000
C	0.59932100	-1.94671500	2.69142000
C	-0.65117000	-1.35872600	2.48945300
C	-0.82036000	-0.35041400	1.54642300
C	0.37589600	1.04085500	-0.32310200
C	1.79021200	0.97124400	-0.88906300
C	2.55719300	-0.06704300	-0.01011100
H	2.65838600	-2.02917500	2.05207500
H	0.71159800	-2.73435700	3.42963500
H	-1.50616600	-1.70013200	3.06357200
H	-1.80392200	0.07384600	1.38343400
H	2.94852000	-0.90892900	-0.59071900
C	-0.54976000	1.86027100	-0.86104800
H	-1.33616900	-0.23062000	-1.65946000
C	-0.63175500	-1.92791800	-1.32107600
C	-1.00562900	-3.25995800	-0.64742700
F	-2.01434400	-3.12312500	0.20869000
F	0.04797700	-3.74296600	0.00082400
F	-1.36812900	-4.14287900	-1.58483900
O	-1.66671900	-1.10259500	-1.36892500
O	0.46866600	-1.72821600	-1.75698000
C	2.60385600	2.26784000	-0.67687600
H	2.05539100	3.17287900	-0.94913700
C	3.95525800	2.10099200	-1.39824400
H	4.48736500	3.05560600	-1.43987500
H	3.82812700	1.74950700	-2.42619000
C	4.71477900	1.07689200	-0.50238700
H	5.00759300	0.17469700	-1.04682300
H	5.62328800	1.51976600	-0.08443500
C	3.69847800	0.77071500	0.61330900
H	4.13240700	0.31763000	1.50821800
C	3.02147100	2.13969800	0.79880100
H	3.72061600	2.92060100	1.11352800

H	2.17348700	2.11637400	1.49015600
H	1.75703500	0.68339800	-1.94406900
C	-1.90975600	2.16809300	-0.36725400
C	-2.13614600	2.51607800	0.97040600
C	-2.99256800	2.18697700	-1.25460100
C	-3.41406800	2.83669300	1.41385100
H	-1.29514100	2.53286900	1.65796600
C	-4.27271000	2.50417100	-0.81180800
H	-2.82715100	1.94879700	-2.30291300
C	-4.48768700	2.82649400	0.52527700
H	-3.57157000	3.10398400	2.45390600
H	-5.10172000	2.50259700	-1.51207300
H	-5.48462800	3.07791700	0.87193300
H	-0.25109500	2.40442200	-1.75895800

TS-4Z-TFA

C	0.18699400	-0.08644300	0.69790600
C	1.37068400	-0.73831400	1.10530000
C	1.38215900	-1.48739800	2.27349600
C	0.19546200	-1.61282800	2.99071700
C	-0.99481400	-1.00487500	2.56296900
C	-1.01558000	-0.23055300	1.41773000
C	0.42792800	0.57897100	-0.54464500
C	1.85195700	0.40729300	-0.95022400
C	2.48867300	-0.51443900	0.12821000
H	2.28461800	-1.99244600	2.60285200
H	0.18275000	-2.21362600	3.89509100
H	-1.90592800	-1.15370700	3.13098800
H	-1.93095200	0.23326600	1.06898800
H	2.82958500	-1.47008000	-0.28159700
C	-0.53783700	1.28208700	-1.34619500
H	-1.11226800	0.35973700	-1.78244300
C	-1.03596300	-1.79241200	-1.46599900
C	-1.39441200	-2.97336200	-0.52873000
F	-2.49161600	-2.73088200	0.19999600
F	-0.39311000	-3.21937200	0.33332700
F	-1.60898900	-4.09881500	-1.22379500
O	-1.98519200	-1.01780400	-1.74514300
O	0.15707600	-1.70604800	-1.79114600
C	2.68468600	1.71720600	-0.83345100
H	2.18477300	2.59606600	-1.24817100
C	4.06119400	1.41539400	-1.45789200
H	4.63739700	2.33943300	-1.55626700
H	3.97152200	0.97180000	-2.45246600
C	4.71741400	0.45541000	-0.42141200

H	4.96209700	-0.52089900	-0.84816500
H	5.64050300	0.88228400	-0.02072700
C	3.64916600	0.34534800	0.68434200
H	4.02897000	-0.00449800	1.64694300
C	3.03334400	1.75603900	0.66511400
H	3.75905700	2.53845400	0.90495600
H	2.16509700	1.86311800	1.32252300
H	1.86848200	-0.00162800	-1.96444500
C	-1.56927900	2.12450300	-0.63018600
C	-1.16213600	3.17098000	0.20180400
C	-2.93259600	1.87288100	-0.79830800
C	-2.10293900	3.95794400	0.85803200
H	-0.09967700	3.36646300	0.33389600
C	-3.87317600	2.66232500	-0.14053600
H	-3.24175200	1.03791300	-1.42024600
C	-3.46195500	3.70415800	0.68685800
H	-1.77615300	4.76752400	1.50281100
H	-4.93088700	2.45821400	-0.27212600
H	-4.19754500	4.31593300	1.19898600
H	-0.06518300	1.79963300	-2.18623500

4Z-INT

C	0.18141100	-0.01781800	0.95125600
C	0.51486100	-1.24787200	1.52260700
C	0.77159700	-1.34976000	2.88660700
C	0.69617900	-0.20615300	3.67589400
C	0.36949700	1.02421200	3.10476100
C	0.10332600	1.12884900	1.74227900
C	-0.14921200	-0.21144700	-0.52130800
C	0.44830700	-1.60275500	-0.86146700
C	0.62083200	-2.35095100	0.50082800
H	1.03291400	-2.30836000	3.32631800
H	0.89695500	-0.26994700	4.74078900
H	0.31716800	1.91080900	3.72794600
H	-0.16413100	2.08360600	1.30867600
H	-0.13009900	-3.13137400	0.66501300
C	0.15133900	0.90015700	-1.56237700
H	-0.79599300	1.33266700	-1.88424000
C	-2.47271400	0.42989000	-0.26691100
C	-3.89460600	-0.16030900	-0.32423500
F	-4.79044400	0.76086600	0.00297400
F	-4.00789100	-1.18911300	0.51760600
F	-4.16167200	-0.59900300	-1.55784600
O	-2.26407900	1.57867100	0.01662600
O	-1.60350000	-0.50878800	-0.59041000

C	1.87145200	-1.69419000	-1.46686600
H	2.10681100	-0.93584900	-2.21633500
C	2.01240900	-3.13373100	-2.00574700
H	2.94134100	-3.23039400	-2.57481700
H	1.18790000	-3.41023900	-2.66834300
C	2.06497600	-3.99324700	-0.70774000
H	1.21806600	-4.68093600	-0.62513000
H	2.97906400	-4.59138600	-0.66619600
C	2.04788900	-2.93317200	0.41042900
H	2.43443300	-3.28183500	1.37111800
C	2.80201700	-1.76270900	-0.24080100
H	3.83007500	-2.01773900	-0.51665400
H	2.80684100	-0.86044900	0.37579400
H	-0.26244800	-2.09425300	-1.53198000
C	1.04827200	2.03062700	-1.11351100
C	2.41822000	1.84561100	-0.91491300
C	0.50425400	3.29815000	-0.89124400
C	3.22301200	2.89769300	-0.48753500
H	2.86195200	0.87102400	-1.09685900
C	1.30679200	4.35314600	-0.46628800
H	-0.56342000	3.44560600	-1.03085500
C	2.66911300	4.15455200	-0.25941300
H	4.28536200	2.73546800	-0.33526100
H	0.86635300	5.33034700	-0.29539600
H	3.29639900	4.97487700	0.07401500
H	0.57980500	0.42190100	-2.44777700

4E-INT-1

C	1.59017100	-0.62667100	0.80285500
C	2.61755400	-0.26683500	-0.06826800
C	3.91505600	-0.71920800	0.15442800
C	4.17038800	-1.52314400	1.26241900
C	3.14339200	-1.86334600	2.14430500
C	1.84252400	-1.41952000	1.92045700
C	0.26691000	-0.05872300	0.32578700
C	0.65863200	0.98414500	-0.75237200
C	2.15073300	0.68879800	-1.13596400
H	4.71901200	-0.44007800	-0.52101400
H	5.17803800	-1.88179800	1.44756900
H	3.35847800	-2.48318300	3.00844100
H	1.04029700	-1.70078500	2.59333800
H	2.26712800	0.26711400	-2.14021900
C	-0.64626100	0.44578700	1.44241400
H	-0.88213700	-0.39423600	2.10332800
C	-0.86046100	-2.21541800	0.07821200

C	-1.51447300	-3.07464200	-1.02168500
F	-2.01697200	-4.18638200	-0.50532800
F	-0.62080500	-3.39874500	-1.95740100
F	-2.50326700	-2.39095300	-1.61081500
O	-0.82239100	-2.56407000	1.22593400
O	-0.40850500	-1.10522600	-0.47533100
C	-1.92829200	1.15402900	1.04467600
C	-2.39678400	2.17780900	1.87654000
C	-2.68277300	0.82565700	-0.08611500
C	-3.57832000	2.85423400	1.59561600
H	-1.81993700	2.44809400	2.75787100
C	-3.86505400	1.50692800	-0.37126200
H	-2.36050400	0.03496700	-0.75295600
C	-4.31896800	2.52091900	0.46457200
H	-3.91720500	3.64476700	2.25768900
H	-4.43379200	1.23624400	-1.25527700
H	-5.24019800	3.04748500	0.23787700
H	-0.03620200	1.13678800	2.03562700
C	0.71086700	2.47337100	-0.33184800
H	-0.11315100	2.79275700	0.30687000
C	0.81901500	3.28857400	-1.63622100
H	0.70406100	4.35470200	-1.42168200
H	0.04606000	3.01267800	-2.35855900
C	2.26109600	2.97481400	-2.13434000
H	2.27155700	2.47040600	-3.10514800
H	2.85315500	3.88866800	-2.23320200
C	2.82490100	2.07431900	-1.01869400
H	3.91603400	2.02131000	-0.98782700
C	2.13318800	2.64263200	0.23173200
H	2.38485200	3.69134800	0.41684100
H	2.33077400	2.06239200	1.13762600
H	-0.02801700	0.86238500	-1.59358100

4E-INT-2

C	1.57305900	1.22057600	-0.64363500
C	2.77099200	0.94835200	0.00506000
C	3.87777400	1.77267100	-0.19221500
C	3.75818100	2.87748900	-1.02877200
C	2.54376700	3.16315400	-1.65878200
C	1.44338300	2.33399300	-1.47048200
C	0.49524500	0.20425800	-0.31340700
C	1.20819000	-0.79231000	0.66260200
C	2.66787200	-0.26158900	0.88908200
H	4.81767400	1.55962600	0.30946500
H	4.61146400	3.52905800	-1.18826800

H	2.45979100	4.03703600	-2.29633000
H	0.49514600	2.56181300	-1.95004500
H	2.85696800	0.01294700	1.93325900
C	-0.13099000	-0.35696900	-1.62805200
H	0.64848600	-0.83466100	1.59394600
H	-0.06877900	0.44696900	-2.36715900
C	-1.49011000	0.39348600	1.08546200
C	-2.49311800	1.46601200	1.55591700
F	-1.95385400	2.18221700	2.54809800
F	-3.60129600	0.89009800	2.00143500
F	-2.81791000	2.30755000	0.57070600
O	-1.60140600	-0.75711400	1.40181800
O	-0.53563600	0.98468100	0.37488700
C	-1.56918300	-0.81177000	-1.56522500
C	-1.92599000	-2.15662300	-1.47099500
C	-2.58553600	0.14940800	-1.58004000
C	-3.26076100	-2.53060900	-1.34446100
H	-1.15609200	-2.92219300	-1.49494400
C	-3.91950800	-0.21806500	-1.43598500
H	-2.32177100	1.19948000	-1.67341100
C	-4.25997400	-1.56253400	-1.31101900
H	-3.51953600	-3.58151400	-1.26442600
H	-4.69041400	0.54594900	-1.42412600
H	-5.29868300	-1.85436600	-1.19641100
H	0.51332900	-1.15918900	-1.99486100
C	1.45864000	-2.22060800	0.14086100
H	0.59672000	-2.66359800	-0.35747500
C	1.96625900	-3.06584100	1.32699600
H	1.97243700	-4.12600400	1.05898700
H	1.32701400	-2.95296100	2.20660800
C	3.41485300	-2.54116400	1.55380100
H	3.56754000	-2.13908100	2.55948300
H	4.14995900	-3.33645300	1.40215400
C	3.55729600	-1.45492300	0.47289500
H	4.58809800	-1.16983800	0.24773300
C	2.74882200	-2.05749100	-0.68709400
H	3.15289200	-3.01199800	-1.03812100
H	2.65667100	-1.37376600	-1.53692500

TS-4E-TFA

C	0.98923600	0.56329600	0.98481200
C	1.31917700	1.69119600	0.20970000
C	2.54393200	2.31942300	0.39636300
C	3.43512600	1.77091400	1.31434400
C	3.12687700	0.61390500	2.04814900

C	1.89771500	-0.00096800	1.89769400
C	-0.30376800	0.08366300	0.60276100
C	-0.87551500	0.96311100	-0.45683300
C	0.22738000	2.01763000	-0.76865500
H	2.81738500	3.19369900	-0.18570500
H	4.40711100	2.23479300	1.45188000
H	3.86484100	0.19580300	2.72305800
H	1.65723300	-0.91764500	2.42640900
H	0.60654100	1.94029100	-1.79272200
C	-0.93064000	-1.07428700	1.18964000
H	-0.16544100	-1.90169700	0.85537300
C	1.44380800	-1.90309200	-0.61881300
C	2.95358500	-1.65059000	-0.85674800
F	3.70612100	-2.02416800	0.18347600
F	3.18585100	-0.34169400	-1.06507900
F	3.39130900	-2.30984500	-1.93731200
O	1.15994300	-2.66367900	0.33635300
O	0.67516600	-1.26788400	-1.36188200
C	-2.31472500	-1.43619000	0.73440000
C	-3.41164600	-1.32716100	1.59019400
C	-2.50519100	-1.89863900	-0.57172500
C	-4.68947700	-1.65437000	1.14327300
H	-3.26403900	-0.98208600	2.61069800
C	-3.78342000	-2.22140400	-1.01674000
H	-1.63554700	-2.00633100	-1.21709500
C	-4.87779200	-2.09733100	-0.16301800
H	-5.53627500	-1.56541900	1.81633800
H	-3.92429600	-2.58162000	-2.03086200
H	-5.87297800	-2.35341900	-0.51188000
H	-0.79891900	-1.08059100	2.27784600
C	-2.06772900	1.83526400	0.04562300
H	-2.79616200	1.28181700	0.64029800
C	-2.65477900	2.51510200	-1.20580800
H	-3.59092800	3.01880000	-0.94997700
H	-2.87188300	1.79399900	-1.99762100
C	-1.55564600	3.54674100	-1.59861300
H	-1.14612900	3.36783900	-2.59657100
H	-1.94959100	4.56629600	-1.58151500
C	-0.48813500	3.36252200	-0.50108800
H	0.19687500	4.20636600	-0.39039600
C	-1.35317000	3.01699400	0.72378400
H	-2.04407000	3.82051800	0.99487500
H	-0.76962700	2.73952700	1.60663400
H	-1.16571900	0.34855300	-1.31077400

TS-4C-TFA

C	1.90070600	0.37795800	-1.11152900
C	2.74739600	0.22460000	0.00435900
C	4.07130100	0.64342600	-0.06913300
C	4.52615200	1.19657500	-1.26173100
C	3.67905600	1.35850400	-2.37124600
C	2.35717600	0.95862000	-2.30554600
C	0.61111500	-0.15881500	-0.78577600
C	0.58444400	-0.62791500	0.56633300
C	1.98070100	-0.34221100	1.15903600
H	4.73546000	0.54234200	0.78332600
H	5.56043300	1.51738700	-1.33998300
H	4.06873300	1.80490700	-3.27931600
H	1.69412700	1.09209100	-3.15431300
H	1.92256900	0.42366200	1.94390800
C	-0.55998000	-0.10036500	-1.70704300
H	-0.25459800	0.06916700	1.07635100
H	-0.98041200	0.90482200	-1.53643400
C	-0.84605900	2.08836200	0.91544800
C	-2.01625500	3.01910000	0.52504400
F	-1.60854700	4.22952500	0.14976400
F	-2.91755000	3.16358700	1.49735700
F	-2.65757100	2.46312500	-0.53453900
O	-1.20280800	1.09013800	1.61243200
O	0.25426500	2.33074000	0.41927600
C	-1.61036600	-1.15829000	-1.46897100
C	-1.54817600	-2.36581700	-2.16563400
C	-2.60234000	-0.96790300	-0.50521600
C	-2.45732500	-3.38397900	-1.89298200
H	-0.77700900	-2.51313000	-2.91796100
C	-3.50849900	-1.98884300	-0.23157100
H	-2.64403400	-0.03330800	0.04666000
C	-3.43642000	-3.19785500	-0.91988300
H	-2.40051400	-4.32072800	-2.43804800
H	-4.27261000	-1.83716100	0.52373100
H	-4.14455800	-3.99104900	-0.70299100
H	-0.21315400	-0.11351800	-2.74552000
C	0.31345000	-2.11407700	0.93919900
H	-0.49093300	-2.58306400	0.37538100
C	0.13786800	-2.16703900	2.46921100
H	-0.24573900	-3.14585600	2.76911900
H	-0.56680100	-1.40750900	2.81640400
C	1.58313900	-1.94338600	3.00809700
H	1.65055500	-1.09557400	3.69469800

H	1.94564600	-2.82947900	3.53685900
C	2.40823100	-1.71591800	1.72628200
H	3.48735300	-1.82725000	1.85646500
C	1.72901900	-2.69727400	0.75319700
H	1.80628400	-3.73882200	1.08109900
H	2.09456500	-2.61584000	-0.27601400

com-4E

C	0.90778600	0.44995800	1.05623300
C	1.37177900	1.58890000	0.38722100
C	2.62901000	2.10927800	0.67234300
C	3.43294700	1.46392100	1.60910400
C	2.98575800	0.30655300	2.25109900
C	1.72223500	-0.20859300	1.98059900
C	-0.44928300	0.10694700	0.59293900
C	-0.83223600	1.08976000	-0.50584700
C	0.36925000	2.08988300	-0.61831000
H	2.98703900	2.99556100	0.15578500
H	4.42243300	1.85120800	1.83017000
H	3.63310200	-0.20080000	2.95881000
H	1.38821200	-1.11989600	2.46837700
H	0.81220900	2.10364300	-1.62025400
C	-1.20995200	-0.86626700	1.12869600
H	0.02980800	-2.52629400	-0.15325800
C	1.52265000	-1.76414700	-0.96667500
C	3.05661200	-1.71087400	-0.85891900
F	3.50083900	-2.20614000	0.29227600
F	3.46742500	-0.45369600	-0.97776300
F	3.58787600	-2.42592800	-1.85628600
O	0.99816400	-2.62788500	-0.10919300
O	0.92550600	-1.10499000	-1.77316700
C	-2.54307100	-1.30275700	0.67191400
C	-3.51643200	-1.66369700	1.61361400
C	-2.85866900	-1.41583000	-0.68966800
C	-4.77787700	-2.08504600	1.20998600
H	-3.27703000	-1.59875800	2.67151300
C	-4.11987000	-1.84185300	-1.09318800
H	-2.09751900	-1.19592300	-1.43248900
C	-5.08642200	-2.17033700	-0.14608400
H	-5.52158700	-2.35026000	1.95468200
H	-4.34447000	-1.92674200	-2.15166100
H	-6.07009900	-2.50161000	-0.46220300
H	-0.82679900	-1.37962600	2.01142200
C	-2.01335400	2.01005100	-0.11872100
H	-2.85769700	1.47131400	0.31649400

C	-2.36857400	2.86070500	-1.35260200
H	-3.30982400	3.39379000	-1.19145300
H	-2.48812200	2.24641100	-2.24983200
C	-1.17424000	3.85672900	-1.45707800
H	-0.64613300	3.78562800	-2.41233300
H	-1.51474900	4.89007200	-1.34521300
C	-0.27642600	3.45168900	-0.27243600
H	0.44817800	4.21356000	0.02637400
C	-1.31999600	3.04764600	0.78282400
H	-1.98020200	3.87378400	1.06475600
H	-0.88074900	2.61438100	1.68639400
H	-1.01036700	0.57972900	-1.45352000

com-4C

C	-0.66369600	1.30269300	-1.27682800
C	-0.84047900	2.30233500	-0.30012600
C	-1.86348600	3.22873400	-0.41997000
C	-2.68893900	3.17552200	-1.54668700
C	-2.51777800	2.18136100	-2.50955300
C	-1.50812100	1.22672600	-2.37935900
C	0.52183700	0.48562800	-0.93032000
C	0.97971000	0.90359800	0.27346300
C	0.10480900	2.01532000	0.83859400
H	-2.01627700	3.98991300	0.33984400
H	-3.47695800	3.91131200	-1.67079700
H	-3.18048700	2.14812600	-3.36828800
H	-1.38661200	0.44323600	-3.12163600
H	-0.52234500	1.64149600	1.66438900
C	1.09862500	-0.51362800	-1.89640700
H	-0.53653500	-0.55994700	0.76499000
H	0.28905000	-1.19311200	-2.19121400
C	-2.03455000	-1.57937900	0.25403400
C	-3.39972000	-2.02175800	0.80749100
F	-4.05564500	-2.73600200	-0.09600500
F	-4.13503800	-0.95829500	1.13471000
F	-3.22870100	-2.76587000	1.90314600
O	-1.37728600	-0.88263600	1.16479900
O	-1.65977700	-1.86431600	-0.85094500
C	2.24916300	-1.30314600	-1.32574200
C	3.56340000	-1.06822500	-1.72712400
C	2.00747700	-2.25218400	-0.32823900
C	4.62143600	-1.75259400	-1.13121000
H	3.76030800	-0.33340200	-2.50348300
C	3.05996800	-2.93398500	0.27185800
H	0.98088000	-2.45354800	-0.02922300

C	4.37246800	-2.68115400	-0.12517700
H	5.63985700	-1.55743200	-1.45199200
H	2.85816900	-3.66613100	1.04731200
H	5.19508900	-3.21184000	0.34298200
H	1.41086700	0.01813500	-2.80436200
C	2.33498300	1.05510800	0.91346000
H	3.12482900	0.42612100	0.50616400
C	2.19765200	1.01313500	2.45498400
H	3.18104300	0.91982100	2.92204000
H	1.60015000	0.15555800	2.77752800
C	1.52835900	2.37662900	2.81343800
H	0.64838800	2.26142800	3.45188000
H	2.23476700	3.02915000	3.33474500
C	1.18081200	2.96556400	1.43196600
H	0.90913600	4.02273200	1.44115000
C	2.45930400	2.58577200	0.65115800
H	3.36231300	3.02180200	1.09155600
H	2.41591900	2.83128700	-0.41327900

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C	1.42823400	-1.32237800	-0.14966900
C	2.43308500	-0.38481300	-0.41414200
C	3.77359600	-0.75338500	-0.37877900
C	4.10735700	-2.07242500	-0.08179500
C	3.10592600	-3.01164500	0.17866200
C	1.76541900	-2.64512700	0.14669600
C	0.09887700	-0.68809900	-0.23812500
C	0.30904500	0.77977700	-0.57387800
C	1.85986700	0.97847100	-0.70261000
H	4.55009100	-0.02123600	-0.58399100
H	5.14933200	-2.37470500	-0.05391100
H	3.37766900	-4.03723500	0.40715000
H	0.99611600	-3.38412200	0.35013400
H	2.16390200	1.32887000	-1.69551100
C	-1.05497600	-1.34189300	-0.01074800
C	-2.44841600	-0.88163400	-0.05967000
C	-3.43318900	-1.75591500	0.42986900
C	-2.87659500	0.35317300	-0.57594700
C	-4.77912800	-1.41467900	0.42343400
H	-3.12586500	-2.72080900	0.82426300
C	-4.22451900	0.69341000	-0.58694600
H	-2.15954600	1.05538500	-0.98121300
C	-5.18303500	-0.18314700	-0.08522700
H	-5.51367800	-2.11194800	0.81365200
H	-4.52756500	1.65292300	-0.99414300

H	-6.23323100	0.08938800	-0.09438200
H	-0.96354900	-2.39186000	0.26568500
C	-0.06385300	1.74658600	0.57876300
H	-1.01934600	1.51333200	1.05229800
C	0.05033400	3.18419600	0.03864700
H	-0.37037800	3.89685200	0.75359700
H	-0.48645000	3.31208100	-0.90678400
C	1.58916800	3.38592000	-0.11106300
H	1.88787700	3.61132600	-1.13908900
H	1.93955600	4.20727000	0.52032000
C	2.16860200	2.04303600	0.37435000
H	3.22402300	2.08234500	0.65581800
C	1.17722100	1.65811800	1.48362000
H	1.15259900	2.38280500	2.30337600
H	1.34675000	0.65791500	1.89224700
H	-0.20643800	1.04613800	-1.50217600

4C

C	1.81261400	-1.11586300	-0.16593800
C	2.51123600	0.10853300	-0.14105200
C	3.89194600	0.13055100	-0.05097100
C	4.58061200	-1.08281100	0.05867200
C	3.89130200	-2.29298800	0.03690700
C	2.49975600	-2.32176100	-0.08374300
C	0.35802600	-0.84735800	-0.20119200
C	0.18098200	0.48639900	-0.27633500
C	1.51258100	1.21330300	-0.37815700
H	4.43342800	1.07262100	-0.04861100
H	5.66105200	-1.08150400	0.16117100
H	4.44245000	-3.22486600	0.11577100
H	1.96936100	-3.26998500	-0.10344900
H	1.68077200	1.56201900	-1.40915200
C	-0.64804500	-1.95390400	-0.03198200
H	-0.49693100	-2.68264200	-0.84108400
C	-2.07777000	-1.47512900	-0.03625900
C	-2.83312400	-1.45137000	1.13518000
C	-2.64621500	-0.98114500	-1.21402400
C	-4.12693800	-0.93263500	1.13783000
H	-2.39867900	-1.83009100	2.05662400
C	-3.93534900	-0.46093800	-1.21589400
H	-2.05840300	-0.98816700	-2.12843900
C	-4.67916200	-0.43156800	-0.03677900
H	-4.70090600	-0.91773100	2.05900200
H	-4.36161200	-0.07564200	-2.13683500
H	-5.68476200	-0.02360900	-0.03651400

H	-0.43325200	-2.49364100	0.89954200
C	-0.80607300	1.48023100	0.27939900
H	-1.77731800	1.07925500	0.56533100
C	-0.86355200	2.73595000	-0.62451100
H	-1.70757500	3.36976400	-0.34069200
H	-0.99611500	2.46361200	-1.67490300
C	0.49588700	3.45570500	-0.35931700
H	1.03661500	3.69191400	-1.27996300
H	0.33843700	4.39269800	0.18314400
C	1.25570200	2.44823800	0.52640900
H	2.13987700	2.85386300	1.02220600
C	0.10392000	1.97711700	1.44209800
H	-0.34161200	2.80062300	2.01100300
H	0.38514100	1.17017700	2.12381600

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