Electronic Supplementary Information

Multiple Photoluminescence of Spiro[acridine-fluorene]-based *o*-Carboranyl Compounds and Potential as a Visual Sensory Material

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General synthetic method for 10-phenyl-10H-spiro[acridine-9,9'-fluorene] (SA) and bromo-10-phenyl-10H-spiro[acridine-9,9'-fluorene] precursors (*p*-BrSA and *o*-BrSA)

n-BuLi (1.6 M in *n*-hexane) was added dropwise to a THF solution (100 mL) of 2-bromo-N,N-diphenylaniline at −78 °C. The reaction mixture was stirred for 1 h. The THF solutions (10 mL) of either 9H-fluoren-9-one (for **SA**) or bromo-9H-fluoren-9-one (for *p*-**BrSA** and *o*-**BrSA**) were added dropwise to the reaction mixture. The solution was stirred for 1 h at −78 °C, after which the mixture was slowly heated to 25 °C and stirred for 20 h. The mixture was quenched using a saturated aqueous NaCl solution (100 mL) and extracted with diethyl ether (50 mL × 3). The organic layer was dried over $MgSO_4$. The volatiles were removed via rotary evaporation to produce a pale gray residue. The crude product was used *in situ* without any purification, where it was dissolved in an acidic mixture solvent of acetic acid and saturated aqueous hydrochloric acid solution (v/v = 10/1, 77 mL). The acid solution was stirred and refluxed for 2 h at 100 °C and cooled to ambient temperature. Saturated aqueous $NaHCO_3$ solution (100 mL) was slowly added and the reaction mixture was extracted with saturated aqueous $NaHCO_3$ solution (50 mL × 3) and $CHCl_3$ (50 mL × 3). The organic layer was dried over $MgSO_4$. The volatiles were removed via rotary evaporation to produce an ivory residue. The remaining solid was purified via column chromatography on silica (DCM/*n*-hexane = 1/4, v/v) to produce solid bromo-precursors.

Data for 10-phenyl-10H-spiro[acridine-9,9'-fluorene], SA

n-BuLi (1.9 mL, 3.0 mmol), 2-bromo-*N,N*-diphenylaniline (0.74 g, 2.3 mmol) and 9H-fluoren-9-one (0.50 g, 2.8 mmol) afforded **SA** as a white solid. Yield = 59 % (0.55 g). ^{1}H NMR (CD_2Cl_2): δ 7.90 (d, *J* = 7.5 Hz, 2H), 7.79 (t, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 8.1 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.46 (t, *J* = 8.2 Hz, 2H), 7.34 (td, *J* = 7.5, 1.1 Hz, 2H), 6.97 (td, *J* = 8.6, 1.6 Hz, 2H), 6.61 (td, *J* = 7.9, 1.2 Hz, 2H), 6.43 (d, *J* = 8.0 Hz 4H). ^{13}C NMR (CD_2Cl_2): δ 156.62, 141.44, 141.03, 139.27, 131.17, 131.16, 128.57, 128.41, 127.75, 127.48, 127.29, 125.58, 124.78, 120.45, 120.10, 114.81, 56.86 (spiro-*C*). Anal. Calcd for $C_{31}H_{21}N$: C, 91.37; H, 5.19; N, 3.44. Found: C, 91.02; H, 5.05; N, 3.20.

Data for 2'-bromo10-phenyl-10H-spiro[acridine-9,9'-fluorene], *p*-BrSA

n-BuLi (8.1 mL, 13.0 mmol), 2-bromo-*N,N*-diphenylaniline (3.2 g, 10.0 mmol) and 2-bromo-9*H*-fluoren-9-one (2.2 g, 12.0 mmol) afforded *p*-**BrSA** as a white solid. Yield = 52 % (2.5 g). ^{1}H NMR ($CDCl_3$): δ 7.79 (d, *J* = 8.2 Hz, 1H), 7.73 (t, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.59 (m, 2H), 7.51 (m, 3H), 7.41 (m, 2H), 7.31 (td, *J* = 8.0, 2.4 Hz, 1H), 6.95 (t, *J* = 8.1 Hz, 2H), 6.60 (t, 7.4 Hz, 2H), 6.40 (dd, *J* = 12.5, 8.1 Hz, 4H). ^{13}C NMR ($CDCl_3$): δ 158.55, 156.29, 141.31, 140.96, 138.40, 138.15, 131.23, 130.94, 129.13, 128.92, 128.65, 127.90, 127.82, 127.57, 126.07, 123.99, 121.94, 121.41, 120.73, 120.05, 114.92, 57.01 (spiro-*C*). Anal. Calcd for $C_{31}H_{20}BrN$: C, 76.55; H, 4.14; N, 2.88. Found: C, 76.34; H, 4.01; N, 2.78.

Data for 4'-bromo10-phenyl-10H-spiro[acridine-9,9'-fluorene], *o*-BrSA

n-BuLi (5.2 mL, 8.3 mmol), 2-bromo-*N,N*-diphenylaniline (2.2 g, 6.4 mmol) and 4-bromo-9*H*-fluoren-9-one (2.0 g, 7.7 mmol) afforded *o*-BrSA as a white solid. Yield = 73 % (2.3 g). ^{1}H NMR ($CDCl_3$): δ 8.65 (m, *J* = 8.4 Hz, 1H), 7.71 (t, *J* = 8.2 Hz, 2H), 7.58 (t, *J* = 7.0 Hz, 1H), 7.50 (t, *J* = 8.2 Hz, 3H), 7.45 (d, *J* = 4.1 Hz, 1H), 7.43 (t, *J* = 2.3 Hz, 1H), 7.38 (d, *J* = 8.2 Hz, 1H), 7.34 (t, *J* = 8.6 Hz, 1H), 7.09 (t, *J* = 7.7 Hz, 1H), 6.93 (td, *J* = 8.5, 1.6 Hz, 2H), 6.57 (td, *J* = 7.6, 1.2 Hz, 2H), 6.39 (dd, *J* = 12.0, 4.2 Hz, 2H) 6.35 (dd, *J* = 12.6, 8.1, 4H). ^{13}C NMR ($CDCl_3$): δ 159.68, 156.98, 141.22, 141.01, 138.73, 137.32, 132.43, 131.23, 131.20, 129.33, 129.14, 128.62, 127.95, 127.49, 127.45, 125.96, 124.90, 124.33, 123.48, 120.67, 116.73, 114.84, 56.88 (spiro-*C*). Anal. Calcd for $C_{31}H_{20}BrN$: C, 76.55; H, 4.14; N, 2.88. Found: C, 76.40; H, 4.12; N, 2.82.

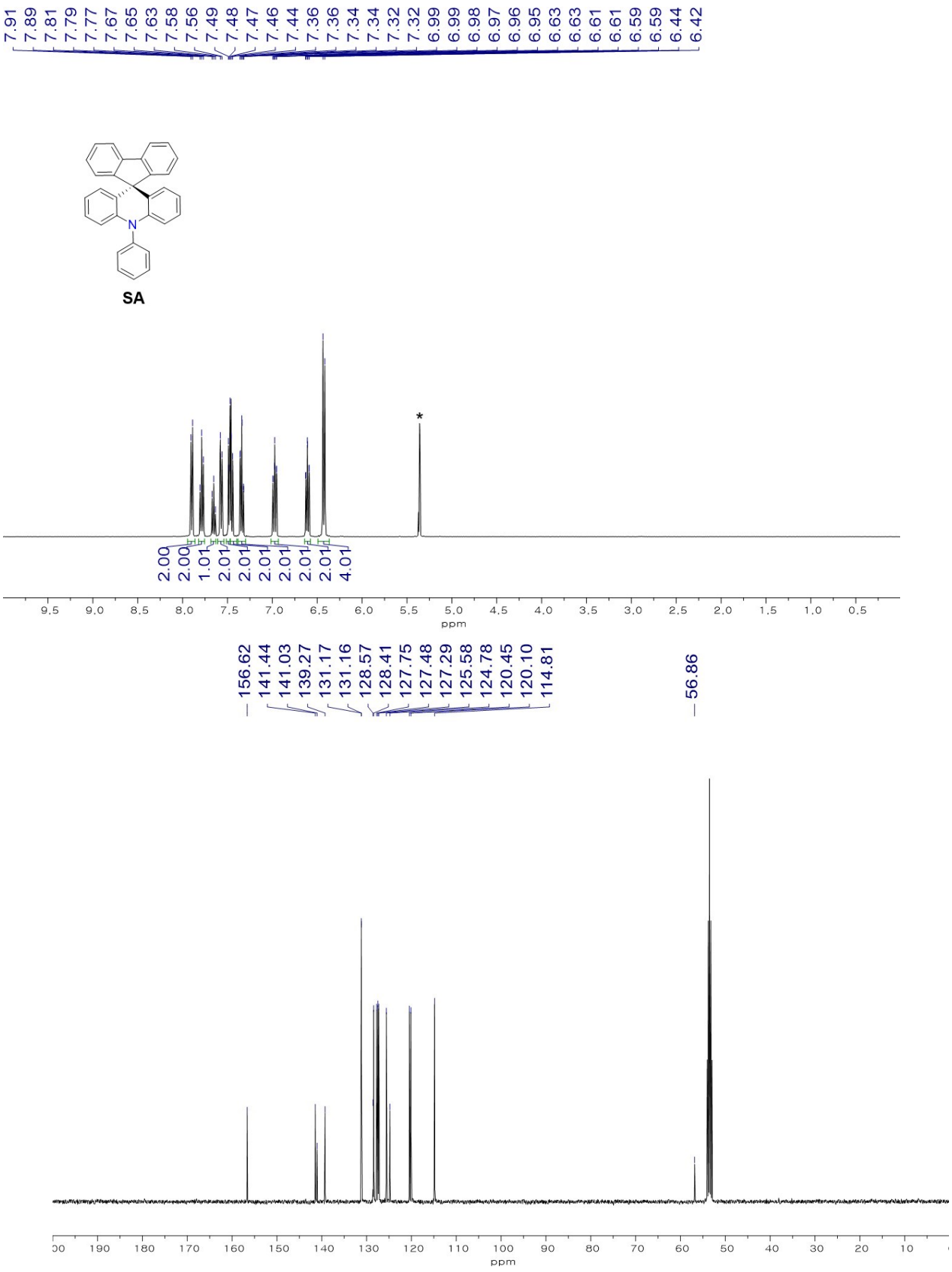
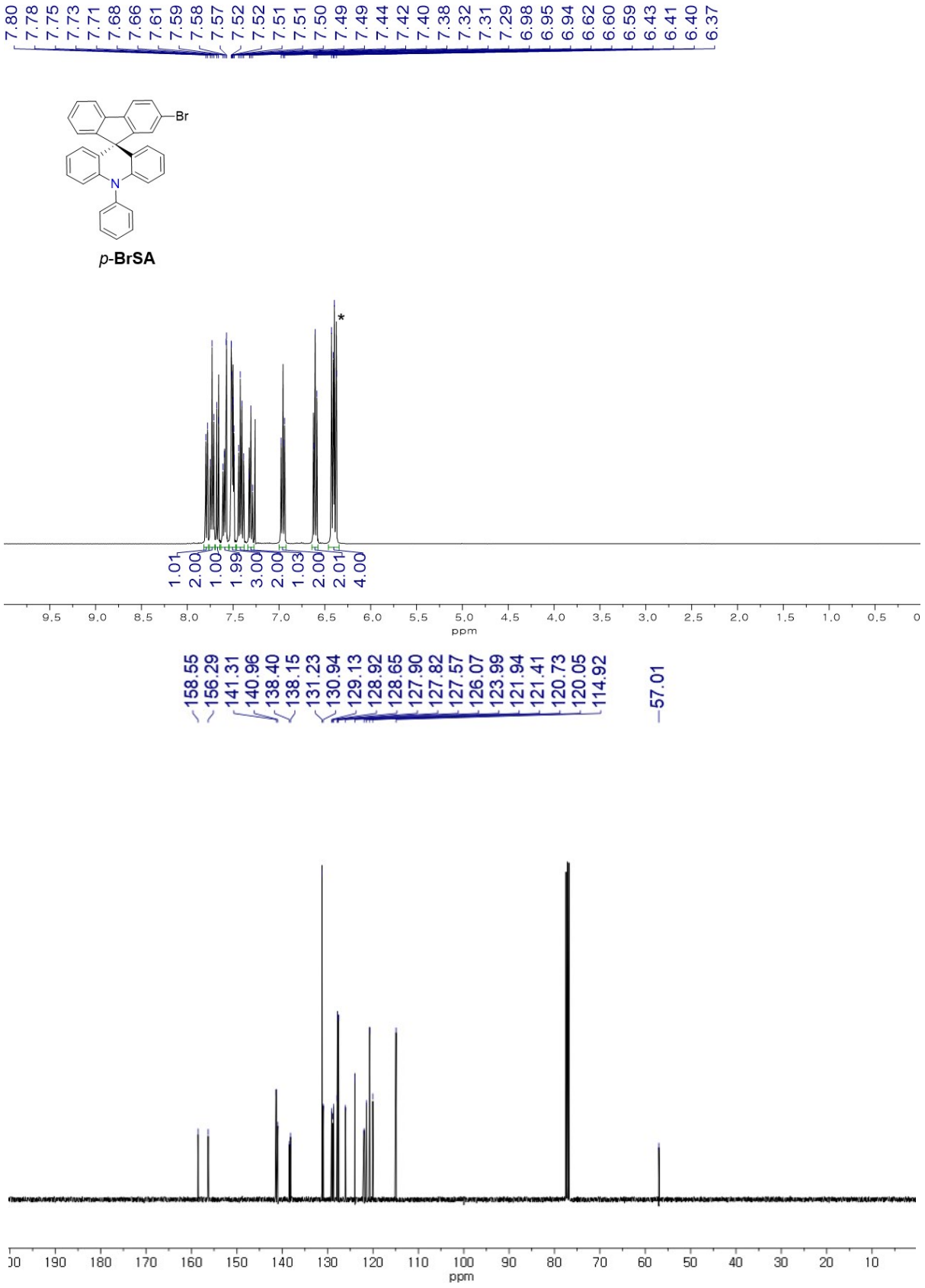


Fig. S1 ^{1}H (top) and ^{13}C (bottom) NMR spectra of **SA** (∗ from residual CH_2Cl_2 in CD_2Cl_2).



p-**BrSA**

Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectra of *p*-**BrSA** (∗ from residual $CHCl_3$ in $CDCl_3$).

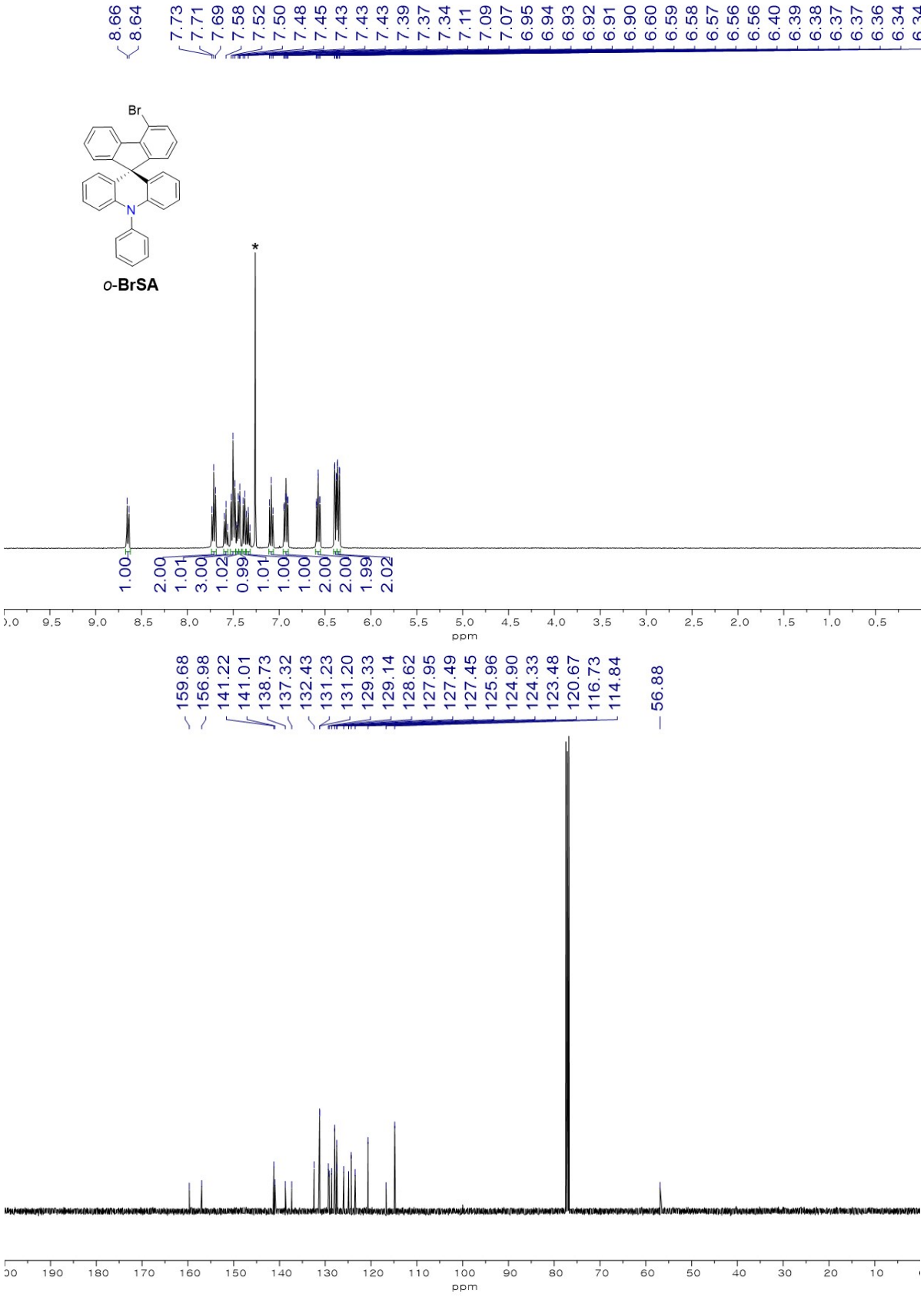


Fig. S3 ^{1}H (top) and ^{13}C (bottom) NMR spectra of *o*-**BrSA** (∗ from residual $CHCl_3$ in $CDCl_3$).

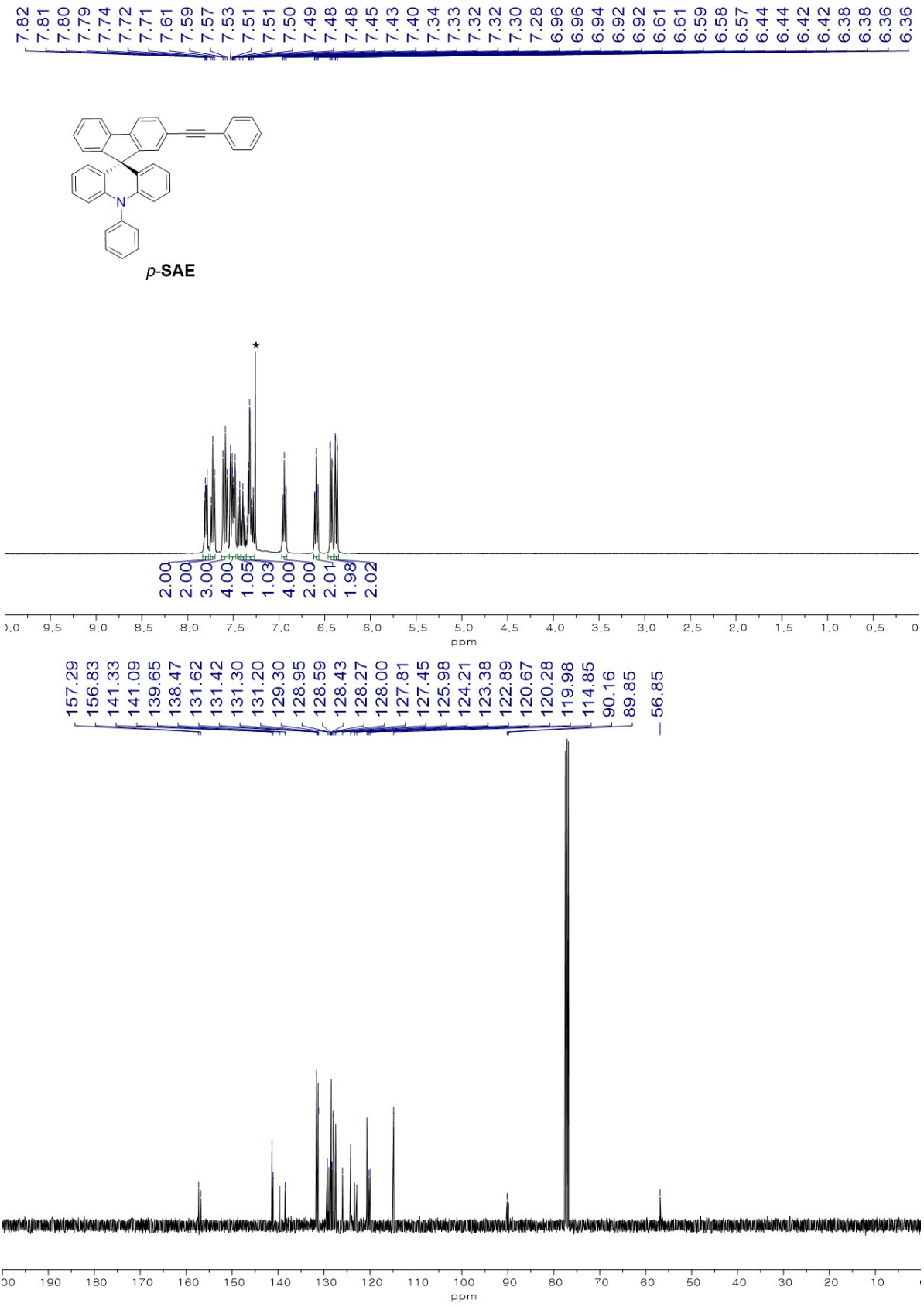


Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectra of *p*-**SAE** (∗ from residual $CHCl_3$ in $CDCl_3$).

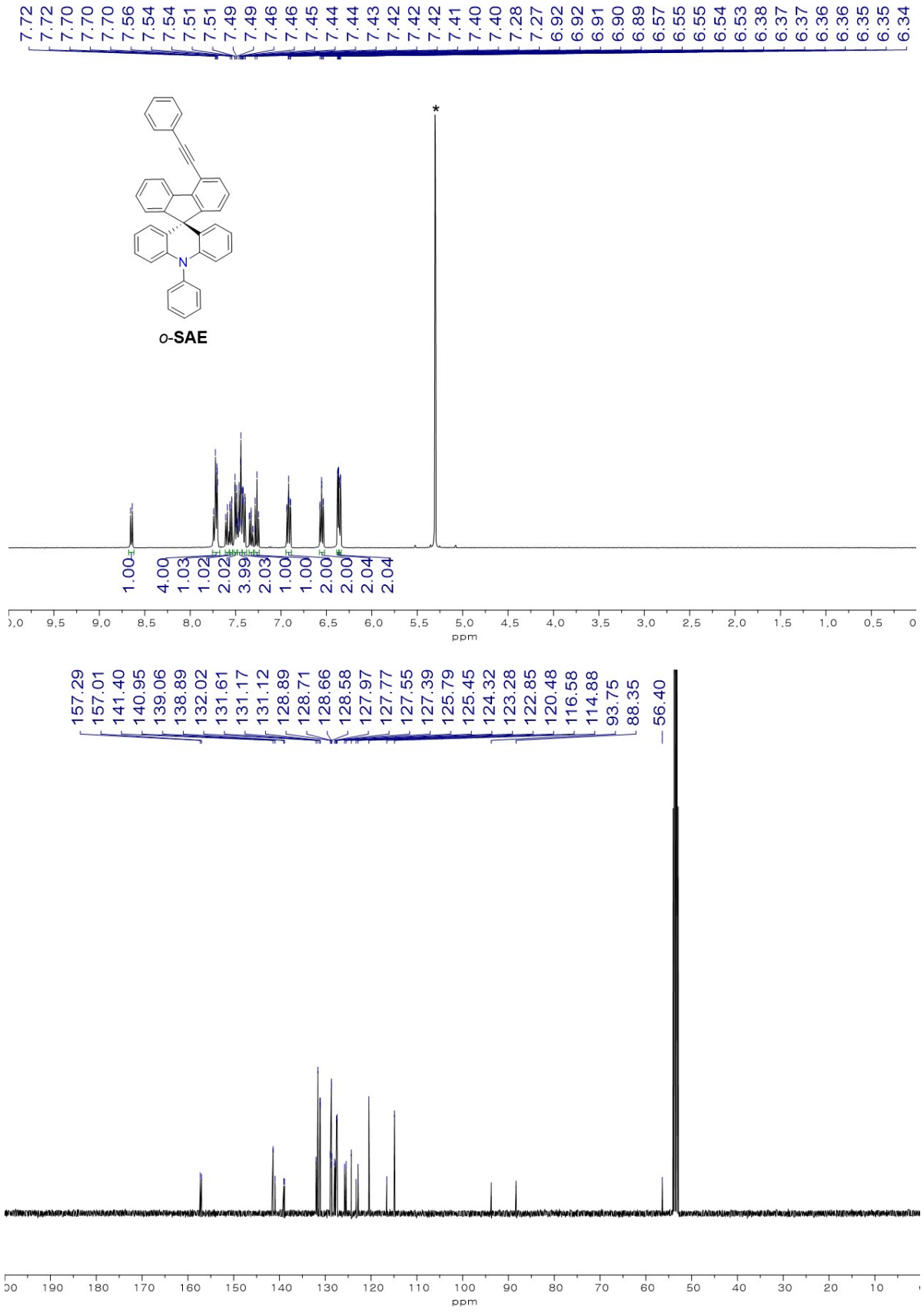


Fig. S5 ^{1}H (top) and ^{13}C (bottom) NMR spectra of *o*-**SAE** (∗ from residual CH_2Cl_2 in CD_2Cl_2).

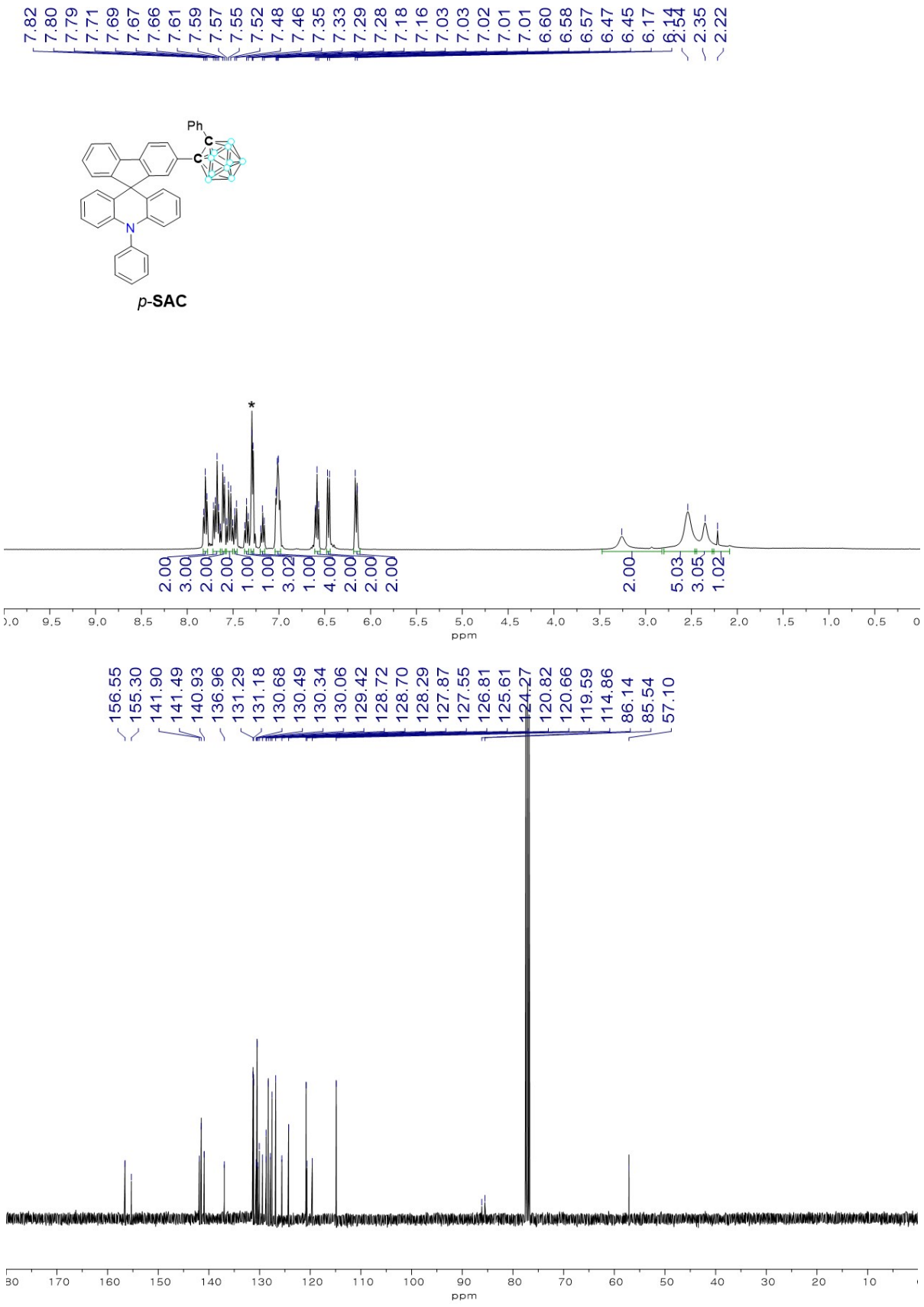


Fig. S6 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of *p*-**SAC** (∗ from residual $CHCl_3$ in $CDCl_3$).

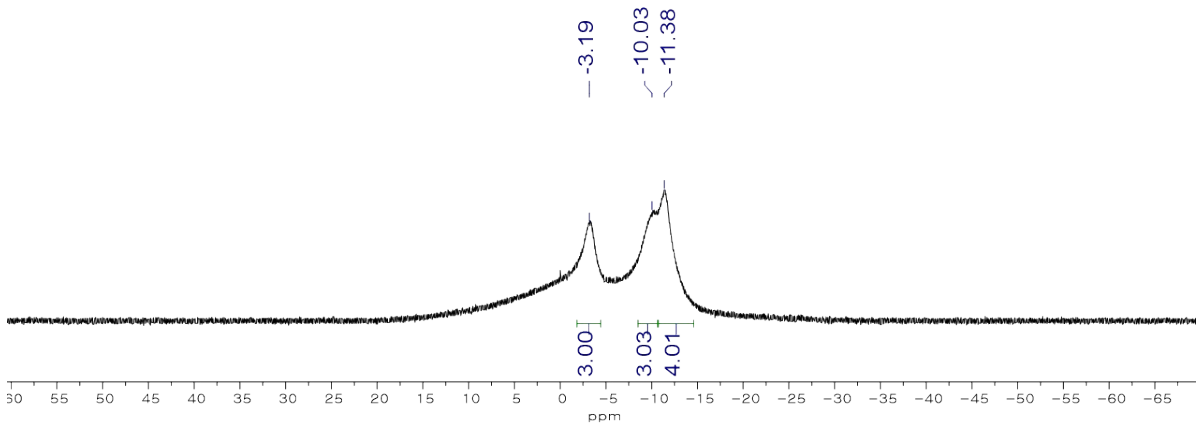


Fig. S7 $^{11}B\{^{1}H\}$ NMR spectra of *p*-**SAC**.

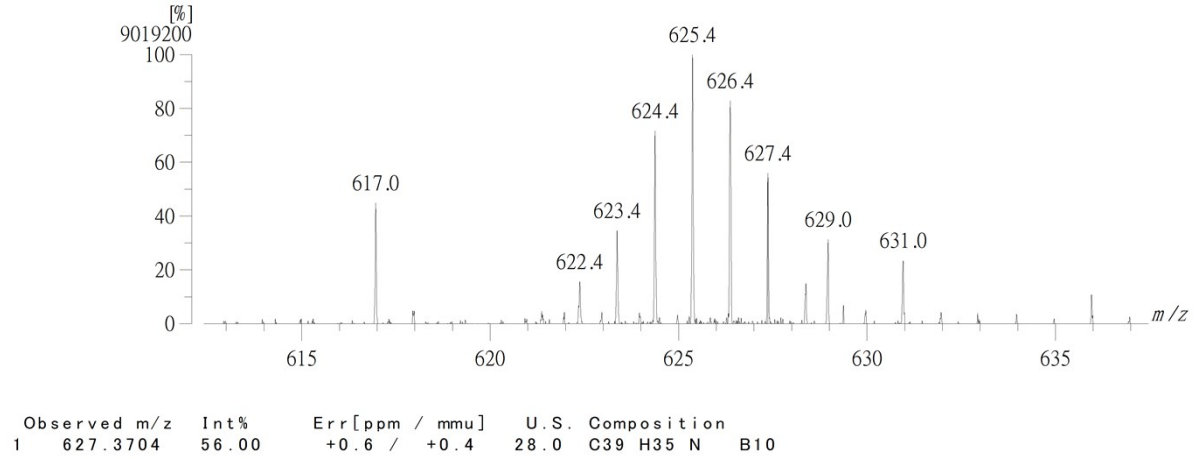


Fig. S8 HR-mass spectrum for *p*-**SAC** (Calcd. for $C_{39}H_{35}B_{10}N$: 627.3700. Found: 627.3704).

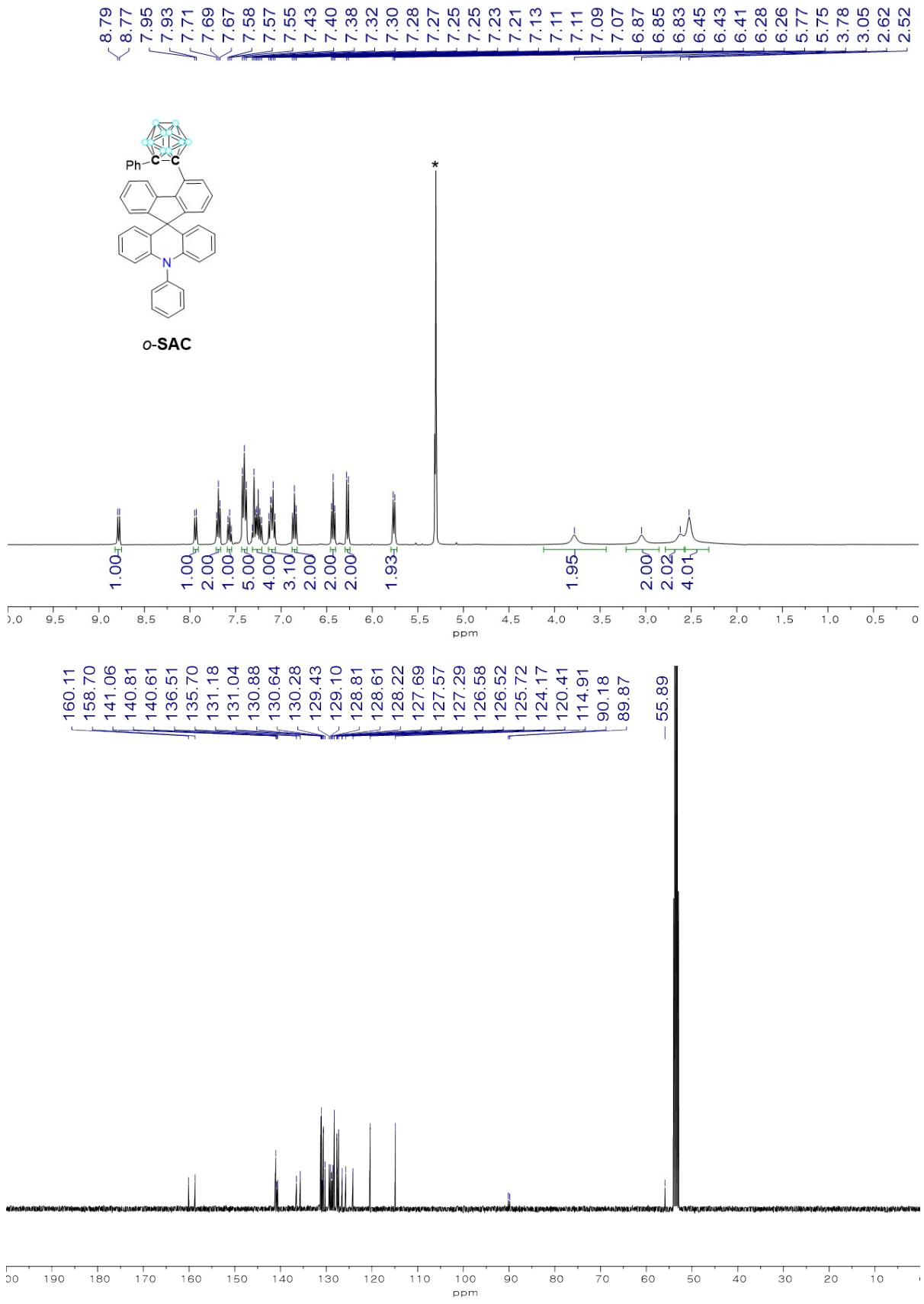


Fig. S9 $^{1}H\{^{11}B\}$ (top) and ^{13}C (bottom) NMR spectra of *o*-**SAC** (∗ from residual CH_2Cl_2 in CD_2Cl_2).

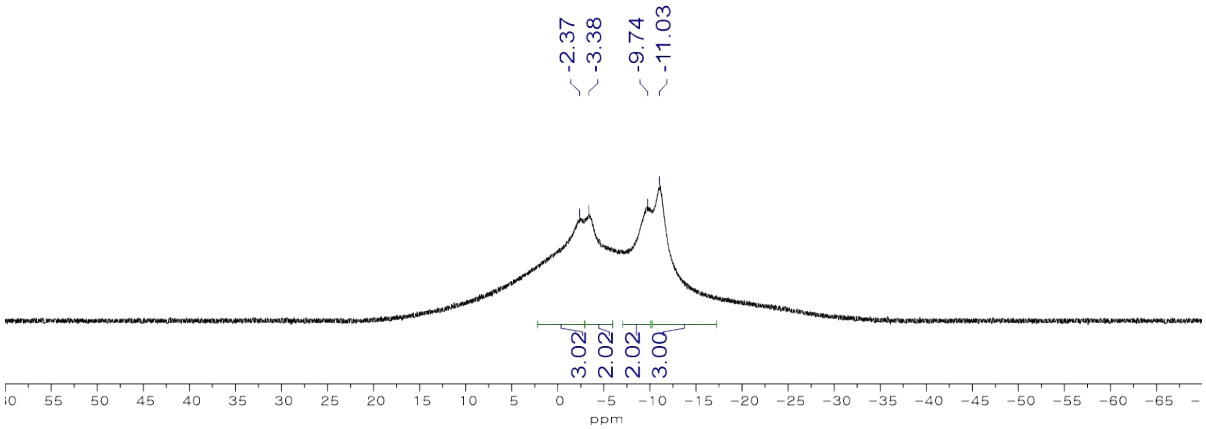
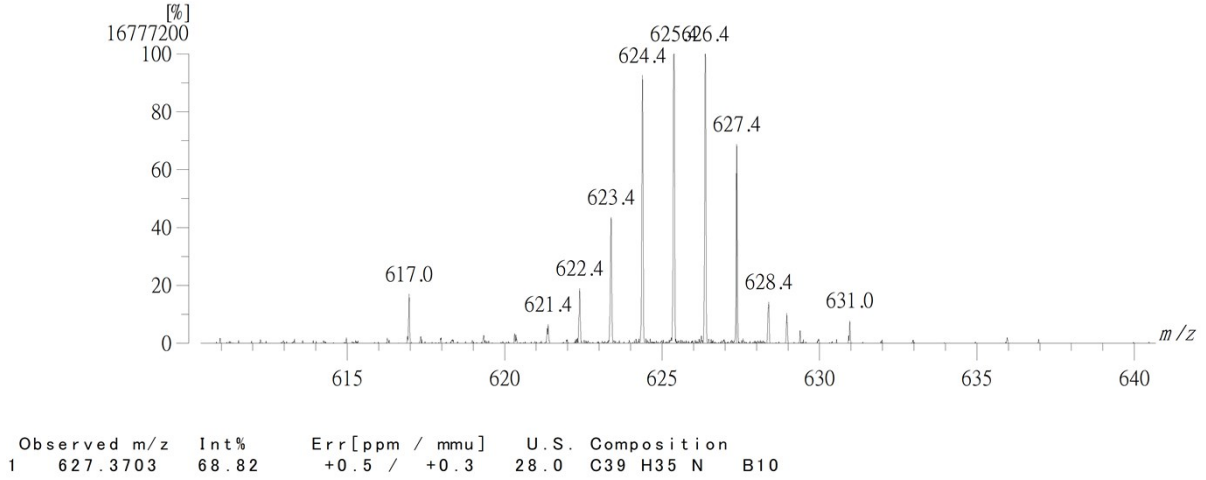


Fig. S10 $^{11}B\{^{1}H\}$ NMR spectra of ***o*-SAC**.



Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1 627.3703	68.82	+0.5 / +0.3	28.0	C39 H35 N B10

Fig. S11 HR-mass spectrum for ***o*-SAC** (Calcd. for $C_{39}H_{35}B_{10}N$: 627.3700. Found: 627.3703).

Table S1 Crystallographic data and parameters for *o*-**SAC**.

Compound	2(*o*-**SAC**·CH_2Cl_2)
Formula	2($C_{39}H_{35}B_{10}$·CH_2Cl_2)
Formula weight	1421.41
Crystal system	Triclinic
Space group	P_{-1}
a (Å)	13.970(3)
b (Å)	15.150(3)
c (Å)	19.772(4)
α (°)	101.81(3)
β (°)	108.00(3)
γ (°)	100.13(3)
V (Å^3)	3764.9(15)
Z	2
ρ_{calc}(g cm^{-3})	1.254
μ (mm^{-1})	0.204
F(000)	1472
T (K)	153(2)
Scan mode	*multi-scan*
hkl range	−17 < h < 18, −19 < k < 19, −25 < l < 25
Measd reflns	38062
Unique reflns [R_{int}]	17206 [0.1496]
Reflns used for refinement	17206
Refined parameters	955
R_1[a] (I > 2σ(I))	0.0868
wR_2[b] all data	0.1837
GOF on F^2	1.005
ρ_{fin} (max/min) (e Å^{-3})	0.357, −0.502

[a]$R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b]$wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

Table S2 Selected bond lengths (Å) and angles (°) for *o*-**SAC**

bond lengths (Å)	
C1–C2	1.754(11)
C1–C3	1.506(10)
C2–C34	1.507(10)
angles (°)	
C2–C1–C3	119.1(6)
C1–C2–C34	117.3(7)
C7–C15–C14	100.8(6)
C7–C15–C16	110.3(6)
C7–C15–C22	108.6(7)
C14–C15–C16	110.4(7)
C14–C15–C22	113.0(6)
C16–C15–C22	113.1(7)
C17–N–C27	120.8(7)
C17–N–C28	120.0(7)
C27–N–C28	119.1(7)

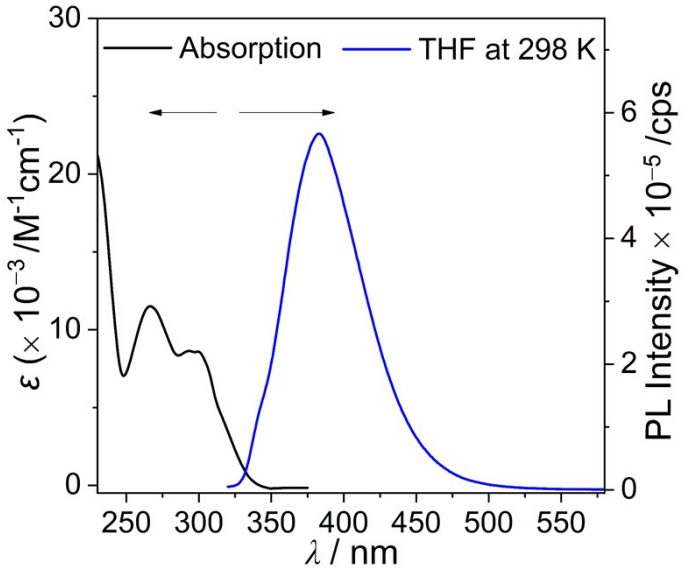


Fig. S12 UV-vis absorption and PL spectra (λ_{ex} = 310 nm) for **SA** in THF (5.0×10^{-5} M). λ_{abs} = 268 nm (ε = 11,500 M^{-1} cm^{-1}), 297 nm (8,600 M^{-1} cm^{-1}). λ_{em} = 387 nm.

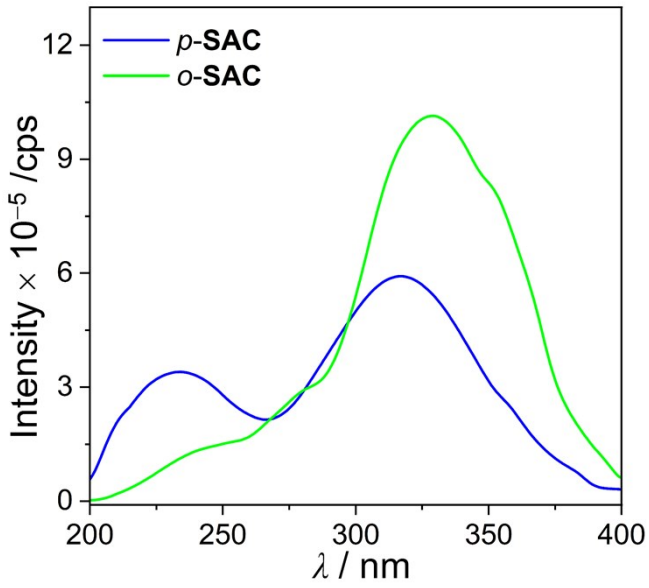


Fig. S13 Excitation graphs in THF (5.0×10^{-5} M) of *p*-**SAC** and *o*-**SAC**.

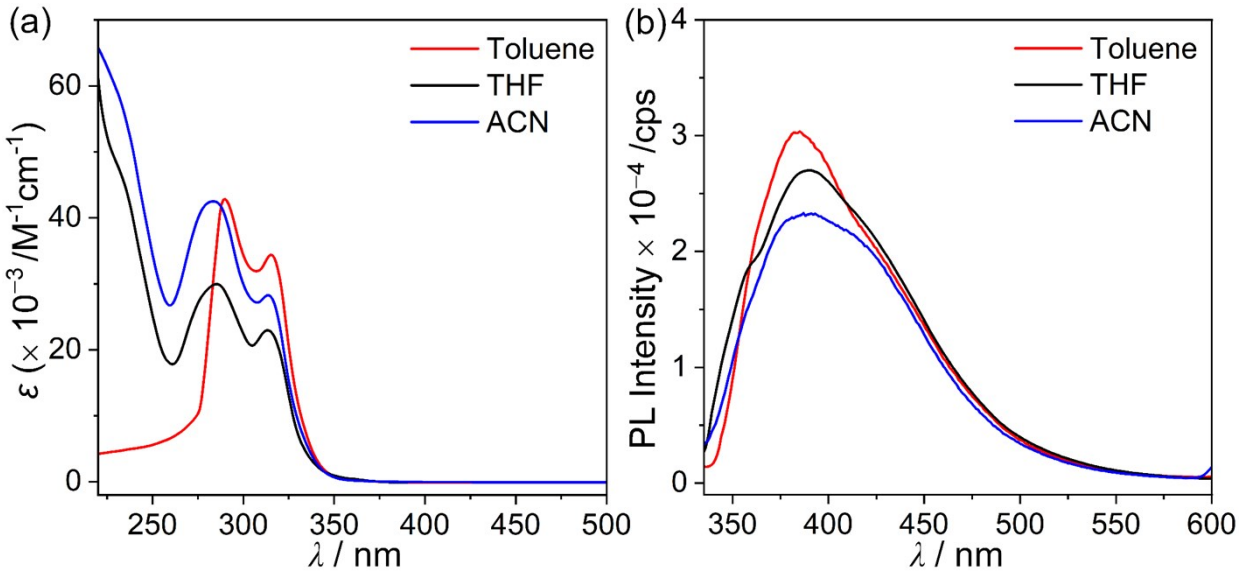


Fig. S14 (a) UV−vis absorption and (b) PL spectra of *p*-**SAC** (5.0×10^{-5} M, λ_{ex} = 313 nm) in various organic solvents.

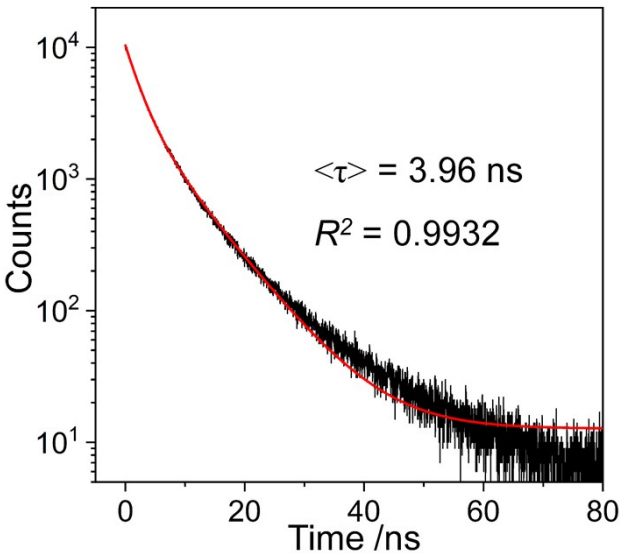


Fig. S15 Emission decay curve for *p*-**SAC** in the film state (5 wt% doped in PMMA) detected at 428 nm at 298 K. The red-line is its single exponential fitting curve.

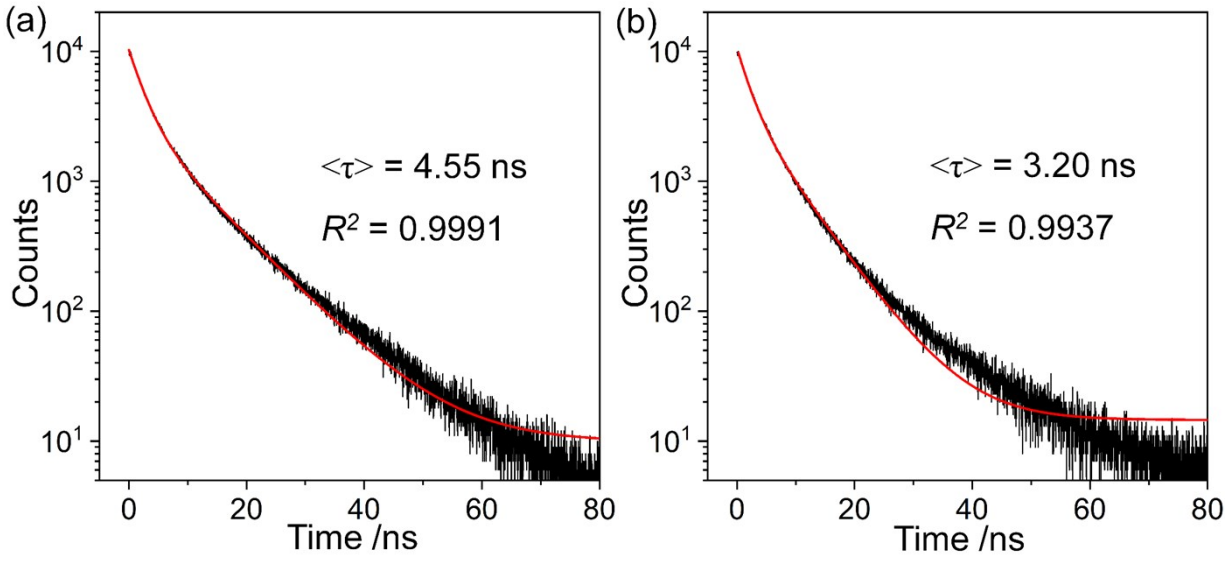


Fig. S16 Emission decay curves for *o*-**SAC** in (a) THF (5.0×10^{-5} M) detected at 461nm and (b) the film state (5 wt% doped in PMMA) detected at 440 nm at 298 K. Each red-line is its single exponential fitting curve.

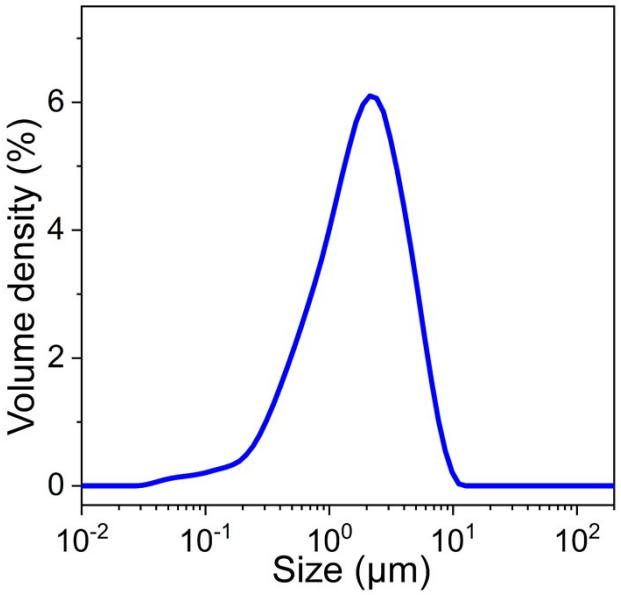


Fig. S17 Dynamic light scattering (DLS) data for *o*-**SAC** in acetonitrile (7.0×10^{-4} M) at 20 °C.

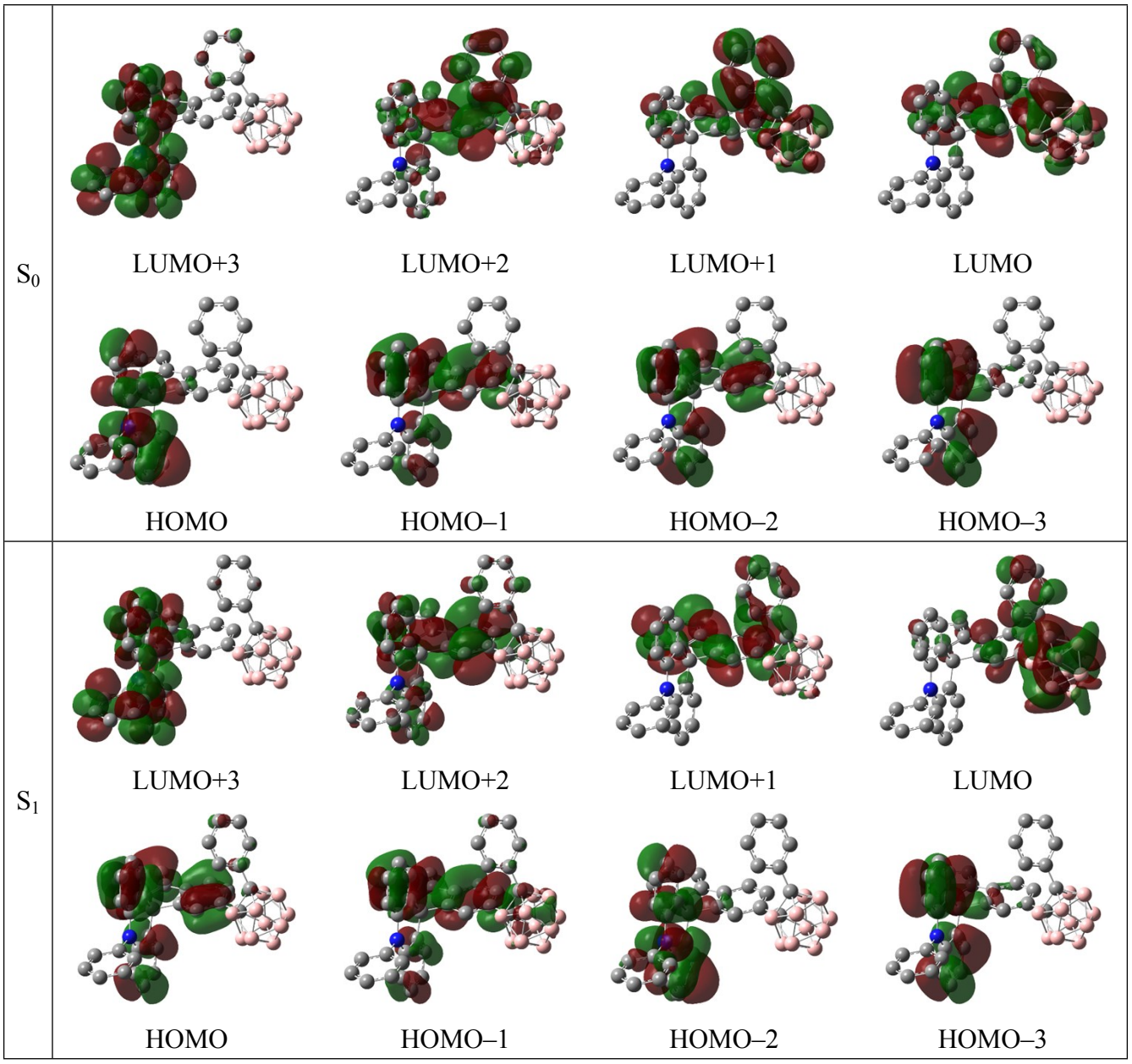


Fig. S18 The selected frontier orbitals of *p*-**SAC** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

Table S3 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for *p*-**SAC** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF

state	λ_{calc} (/nm)	f_{calc}	Major contribution
			S_0
1	336.44	0.0639	HOMO → LUMO (98.6%)
2	326.58	0.0079	HOMO → LUMO+1 (93.8%)
			HOMO → LUMO+2 (4.9%)
3	316.03	0.0001	HOMO → LUMO+1 (4.8%)
			HOMO → LUMO+2 (90.8%)
4	305.21	0.3799	HOMO−1 → LUMO (94.9%)
5	302.42	0.0236	HOMO → LUMO+3 (91.9%)
			S_1
1	475.68	0.3534	HOMO → LUMO (99.9%)
2	453.45	0.0827	HOMO−1 → LUMO (99.0%)
3	443.48	0.0031	HOMO−3 → LUMO (4.5%)
			HOMO−2 → LUMO (93.6%)
4	400.05	0.0010	HOMO−3 → LUMO (97.3%)
5	392.94	0.2903	HOMO−1 → LUMO+1 (99.3%)

Table S4 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of *p*-**SAC** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF

	E (eV)	Carborane	Car-phenyl	Car-fluorene	tripheylamine
			S_0		
LUMO+3	−0.54	0.2	2.7	16.6	80.5
LUMO+2	−0.79	8.5	19.0	62.2	10.3
LUMO+1	−1.04	20.9	51.8	26.8	0.5
LUMO	−1.60	27.4	8.7	63.3	0.6
HOMO	−5.08	0.0	0.1	3.5	96.4
HOMO−1	−5.55	2.7	0.1	78.2	19.0
HOMO−2	−6.60	1.3	0.3	57.8	40.5
HOMO−3	−6.65	0.1	0.2	7.5	92.2
			S_1		
LUMO+3	−0.54	0.3	1.2	27.3	71.2
LUMO+2	−0.76	4.5	3.4	68.0	24.1
LUMO+1	−1.19	6.2	8.1	84.7	1.0
LUMO	−3.45	72.8	11.8	15.3	0.1
HOMO	−6.07	2.5	2.3	62.7	32.5
HOMO−1	−6.30	5.7	1.9	74.0	18.4
HOMO−2	−6.63	0.0	0.0	3.7	96.3
HOMO−3	−6.69	0.1	0.0	6.6	93.3

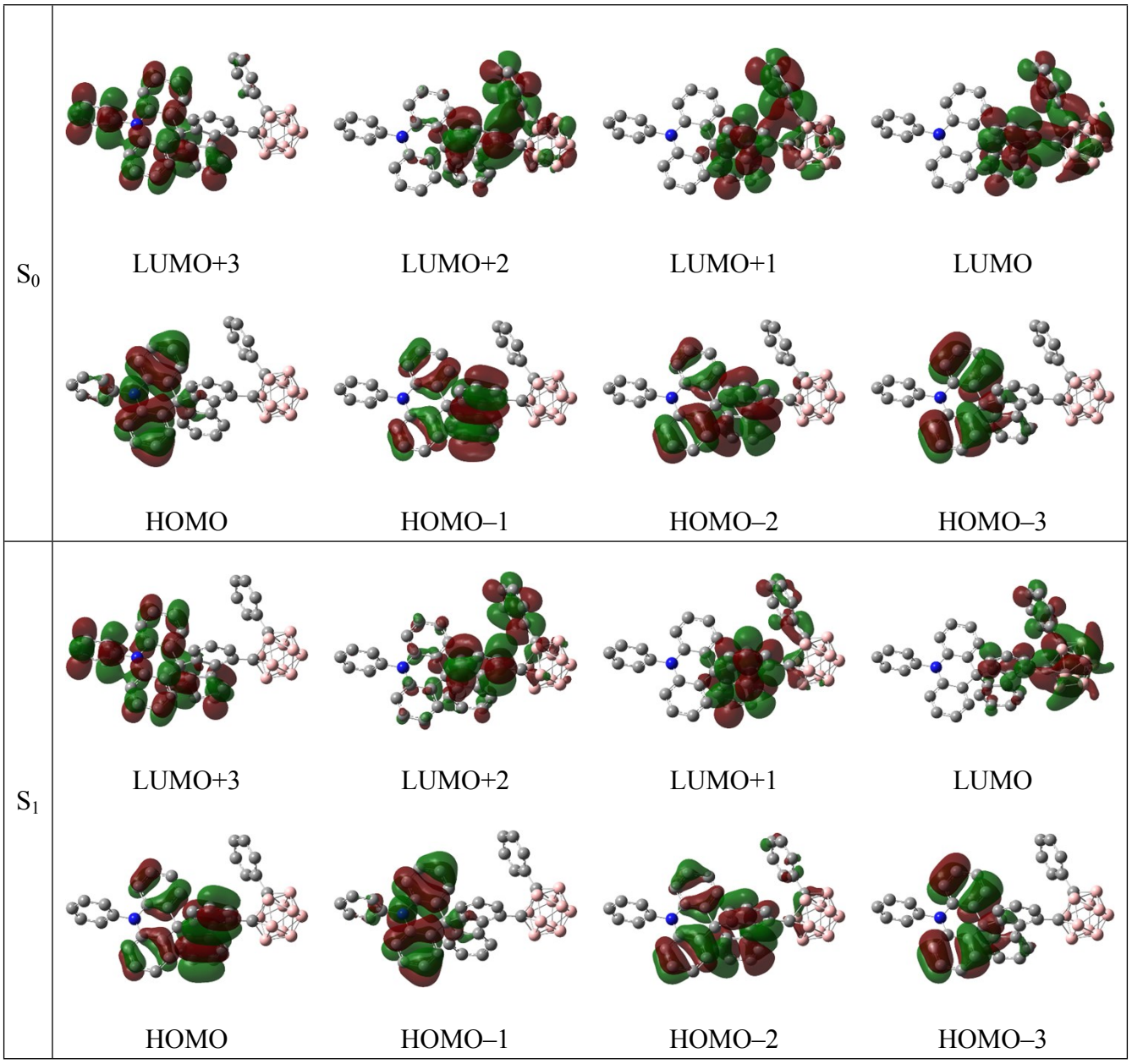


Fig. S19 The selected frontier orbitals of *o*-**SAC** from B3LYP calculations (Isovalue = 0.04 a.u.) at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF.

Table S5 Computed absorption wavelengths (λ_{calc} in nm) and oscillator strengths ($f_{calc.}$) for *o*-**SAC** from TD-B3LYP calculations using the B3LYP geometries at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF

state	λ_{calc} (/nm)	f_{calc}	Major contribution
			S_0
1	338.66	0.1227	HOMO → LUMO (98.3%)
2	305.83	0.0065	HOMO → LUMO+1 (91.6%)
			HOMO → LUMO+2 (5.7%)
3	298.70	0.0895	HOMO−1 → LUMO (97.1%)
4	284.54	0.0756	HOMO → LUMO+1 (6.0%)
			HOMO → LUMO+2 (91.0%)
5	279.99	0.0149	HOMO → LUMO+3 (92.6%)
			HOMO → LUMO+5 (4.8%)
			S_1
1	482.81	0.1605	HOMO → LUMO (99.9%)
2	465.10	0.0746	HOMO−1 → LUMO (99.3%)
3	421.88	0.0017	HOMO−2 → LUMO (95.7%)
4	407.80	0.0291	HOMO−3 → LUMO (97.1%)
5	394.27	0.2143	HOMO → LUMO+1 (94.6%)

Table S6 Molecular orbital energies (in eV) and molecular orbital distributions (in %) of *o*-**SAC** at the ground state (S_0) and first singlet excited state (S_1) optimized geometries in THF

	E (eV)	Carborane	Car-phenyl	Car-fluorene	tripheylamine
			S_0		
LUMO+3	−0.56	0.9	1.6	21.1	76.4
LUMO+2	−0.82	10.9	26.1	56.0	7.0
LUMO+1	−1.16	16.3	32.2	50.1	1.4
LUMO	−1.83	29.3	7.7	63.6	0.5
HOMO	−5.18	0.0	0.0	3.4	96.5
HOMO−1	−5.68	0.5	0.1	77.4	22.0
HOMO−2	−6.57	2.1	0.2	65.3	32.4
HOMO−3	−6.66	0.1	0.1	7.7	92.2
			S_1		
LUMO+3	−0.58	0.4	0.7	22.5	76.4
LUMO+2	−0.73	6.3	18.5	63.5	11.7
LUMO+1	−1.24	5.7	5.7	87.2	1.3
LUMO	−3.55	73.4	11.1	15.4	0.1
HOMO	−5.98	0.9	0.3	77.2	21.7
HOMO−1	−6.29	0.0	0.0	3.8	96.2
HOMO−2	−6.60	3.8	2.8	61.6	31.7
HOMO−3	−6.70	0.1	0.0	8.0	91.9

Table S7 Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of *p*-**SAC** from B3LYP calculations (in Å)

Atom	X	Y	Z
C	4.061657	-1.023781	0.224913
C	3.173202	-0.405422	-1.174200
B	5.616568	-1.515836	-0.274505
B	4.329956	-2.697912	0.025894
B	5.704389	-1.214361	-2.021439
B	5.368277	-2.858708	-1.409291
B	4.475435	-2.239339	-2.813455
B	3.610199	-3.137719	-1.536580
B	4.167937	-0.507201	-2.557468
B	2.879106	-1.689201	-2.257199
B	2.807198	-1.953255	-0.501500
B	4.853894	-0.071931	-0.977072
H	6.501696	-1.365676	0.494866
H	4.318174	-3.359773	1.006085
H	6.161120	-3.738952	-1.483292
H	6.728708	-0.904708	-2.533772
H	5.188909	1.019706	-0.695002
H	1.793098	-2.107667	0.071716
H	3.125772	-4.207936	-1.702314
H	4.615497	-2.670389	-3.910489
H	4.042173	0.344176	-3.368649
H	1.862445	-1.655632	-2.860248
C	3.834794	-0.393364	1.574840
C	4.765907	0.526870	2.083139
C	2.726702	-0.733753	2.365071
C	4.587631	1.096114	3.342552
H	5.638460	0.795689	1.500225
C	2.547262	-0.157151	3.621967
H	2.000101	-1.451743	2.007881
C	3.474983	0.760374	4.115227
H	5.321082	1.803130	3.717247
H	1.676507	-0.427444	4.210524
H	3.334610	1.207403	5.094531
C	2.184281	0.714145	-0.988016
C	0.832416	0.433065	-0.717155
C	2.586896	2.053933	-1.136348
C	-0.069878	1.475472	-0.577594
H	0.490819	-0.590797	-0.625121
C	1.678716	3.102272	-1.000262
H	3.618692	2.284201	-1.369625
C	-1.577666	1.388578	-0.272866
C	0.343662	2.812770	-0.712926
H	2.017335	4.126615	-1.121094
C	-1.944677	2.883343	-0.256677
C	-2.319386	0.646546	-1.390377
C	-1.820648	0.741715	1.095704
C	-0.818478	3.687877	-0.514114
C	-3.188084	3.462135	-0.029763
C	-2.245600	1.143784	-2.698625
C	-2.578077	-0.437126	1.248641
C	-1.256076	1.332584	2.234004
C	-0.930255	5.080703	-0.546523
C	-3.300281	4.856311	-0.061887
H	-4.059365	2.844661	0.168884
C	-3.700459	-1.163588	-2.238415
C	-2.876621	0.516700	-3.766865
H	-1.673394	2.049749	-2.875068
C	-2.739120	-0.982472	2.540863
C	-1.417318	0.795094	3.506354
H	-0.674154	2.240880	2.109362
C	-2.180731	5.658055	-0.318126
H	-0.064195	5.705388	-0.745014
H	-4.265511	5.321973	0.113357
C	-3.608254	-0.648166	-3.524583
H	-4.272211	-2.066218	-2.066277
H	-2.798297	0.927667	-4.768130
C	-2.167071	-0.374730	3.650839
H	-3.319031	-1.887205	2.669020
H	-0.969313	1.280467	4.367347
H	-2.286726	6.738479	-0.339403
H	-4.112119	-1.161331	-4.338366
H	-2.312016	-0.818675	4.631383
N	-3.168977	-1.067434	0.140961
C	-3.928322	-2.273906	0.339326
C	-3.294532	-3.517411	0.256264
C	-5.297617	-2.201258	0.614114
C	-4.031543	-4.687309	0.448268
H	-2.231326	-3.559347	0.041716
C	-6.031023	-3.373374	0.805508
H	-5.777136	-1.229384	0.675622
C	-5.399249	-4.616525	0.722820
H	-3.537405	-5.651782	0.382962
H	-7.093984	-3.314822	1.018521
H	-5.971192	-5.527291	0.871692
C	-3.060438	-0.528114	-1.152547

Table S8 Cartesian coordinates of the first excited state (S_1) fully optimized geometry in THF of ***p*-SAC** from B3LYP calculations (in Å)

Atom	X	Y	Z
C	4.371215	-0.795613	0.023861
C	2.845087	0.206576	-1.525066
B	5.702124	-0.929548	-0.914246
B	4.548065	-2.275893	-0.645280
B	5.415506	-0.294894	-2.535577
B	5.323854	-2.063860	-2.229490
B	4.201589	-1.328216	-3.366440
B	3.570765	-2.442863	-2.104786
B	3.794396	0.322568	-2.849357
B	2.638460	-1.024010	-2.579606
B	2.943834	-1.347841	-0.773950
B	4.508623	0.476250	-1.139389
H	6.757058	-0.805656	-0.379713
H	4.711683	-3.190691	0.096847
H	6.144427	-2.843314	-2.604431
H	6.330263	0.200313	-3.117336
H	4.813482	1.554461	-0.745709
H	2.030321	-1.689982	-0.095356
H	3.134136	-3.519793	-2.371188
H	4.246383	-1.599285	-4.526704
H	3.613530	1.255444	-3.564701
H	1.567098	-1.127418	-3.086583
C	4.390703	-0.522708	1.475761
C	5.174276	0.518497	2.011860
C	3.635991	-1.303235	2.373923
C	5.201374	0.766625	3.382679
H	5.768721	1.132643	1.344101
C	3.664712	-1.053906	3.744583
H	3.028047	-2.114985	1.989157
C	4.445665	-0.016045	4.259564
H	5.817450	1.574549	3.767681
H	3.075773	-1.675246	4.413748
H	4.467362	0.178227	5.327741
C	1.797378	1.175318	-1.156047
C	0.507110	0.734240	-0.790866
C	2.047593	2.565815	-1.162602
C	-0.463693	1.660603	-0.452484
H	0.291152	-0.328451	-0.781080
C	1.066629	3.493567	-0.821542
H	3.033527	2.918031	-1.444447
C	-1.927086	1.386295	-0.026120
C	-0.205947	3.042301	-0.459553
H	1.295553	4.555183	-0.840646
C	-2.440093	2.821869	0.201391
C	-2.674954	0.697393	-1.156335
C	-1.946640	0.573858	1.258844
C	-1.420969	3.759356	-0.057317
C	-3.706279	3.227287	0.602486
C	-2.856753	1.355042	-2.372167
C	-2.454619	-0.749974	1.302207
C	-1.409902	1.109537	2.428377
C	-1.677505	5.125160	0.089590
C	-3.958669	4.597155	0.748784
H	-4.489742	2.501425	0.800838
C	-3.801390	-1.258768	-2.134039
C	-3.491107	0.737562	-3.447262
H	-2.488872	2.369051	-2.477599
C	-2.401489	-1.496812	2.507651
C	-1.363416	0.376423	3.611846
H	-1.016369	2.119141	2.408076
C	-2.951393	5.533772	0.493746
H	-0.901983	5.859536	-0.106299
H	-4.942316	4.932648	1.062246
C	-3.963388	-0.577560	-3.323574
H	-4.165934	-2.271274	-2.036644
H	-3.615263	1.276152	-4.380068
C	-1.861736	-0.934610	3.646647
H	-2.787284	-2.505814	2.532838
H	-0.937883	0.822011	4.503984
H	-3.161493	6.592645	0.611265
H	-4.455600	-1.064088	-4.157795
H	-1.825796	-1.510542	4.564207
N	-3.013722	-1.324059	0.163360
C	-3.481379	-2.700127	0.233804
C	-2.597656	-3.730493	-0.086497
C	-4.798004	-2.954467	0.618532
C	-3.049678	-5.048986	-0.018038
H	-1.579408	-3.502288	-0.382528
C	-5.235981	-4.277797	0.682620
H	-5.462224	-2.131977	0.861745
C	-4.364491	-5.322048	0.365226
H	-2.371839	-5.859084	-0.264877
H	-6.257560	-4.488879	0.980475
H	-4.710390	-6.349236	0.416545
C	-3.159519	-0.630019	-1.036258

Table S9 Cartesian coordinates of the ground state (S_0) fully optimized geometry in THF of *o*-**SAC** from B3LYP calculations (in Å)

Atom	X	Y	Z
C	4.567789	-0.709686	-0.084242
C	3.714577	0.822252	-0.632257
B	5.708975	-0.292547	1.102749
B	6.201432	-0.648925	-0.559395
B	5.628598	1.469609	1.295584
B	6.914763	0.735976	0.298683
B	6.107327	2.208922	-0.261561
B	6.422356	0.886396	-1.412541
B	4.398103	2.124247	0.201065
B	4.872033	1.755334	-1.463622
B	4.917156	-0.015189	-1.608042
B	4.141729	0.542870	1.005108
H	5.872290	-1.063993	1.983932
H	6.700633	-1.678840	-0.858006
H	8.051523	0.710577	0.639086
H	5.830394	1.974313	2.350172
H	3.291783	0.319160	1.779414
H	4.602041	-0.583447	-2.585136
H	7.188235	0.974693	-2.314326
H	6.652564	3.261182	-0.326865
H	3.689921	3.038809	0.435531
H	4.481441	2.395173	-2.378327
C	3.799784	-2.000990	-0.015247
C	3.252294	-2.434135	1.203837
C	3.671535	-2.829661	-1.141079
C	2.587251	-3.656216	1.289834
H	3.355722	-1.825348	2.093475
C	3.002616	-4.049561	-1.052741
H	4.101915	-2.531871	-2.088625
C	2.455586	-4.466802	0.160907
H	2.178430	-3.975024	2.243490
H	2.914694	-4.674559	-1.935736
H	1.938299	-5.418777	0.228800
C	-0.279972	0.150143	-2.214558
C	2.092531	0.406702	-2.449827
C	-0.147184	0.526134	-0.887502
H	-1.257115	-0.101536	-2.615095
C	2.271653	0.725408	-1.087259
H	2.958937	0.360761	-3.092548
C	-1.318008	0.611370	0.093062
C	1.091264	0.885401	-0.294129
C	-0.613896	1.191998	1.313738
C	-2.402526	1.570573	-0.410913
C	-1.886973	-0.784873	0.380267
C	0.764268	1.392220	1.078819
C	-1.222401	1.559911	2.507880
C	-2.032844	2.866021	-0.797905
C	-3.264553	-1.068969	0.288526
C	-1.012830	-1.807682	0.771938
C	1.499122	2.070842	2.064480
C	-0.462577	2.184302	3.497056
H	-2.283441	1.380612	2.655250
C	-4.703506	2.156465	-0.926412
C	-2.960993	3.800624	-1.241993
H	-0.983673	3.141203	-0.742616
C	-3.715901	-2.370107	0.598781
C	-1.459385	-3.088989	1.074410
H	0.048087	-1.586778	0.839157
C	0.886980	2.454168	3.258860
H	2.533238	2.332447	1.919366
H	-0.922871	2.481407	4.434469
C	-4.307476	3.433274	-1.301971
H	-5.750054	1.886018	-0.980397
H	-2.641064	4.795739	-1.533488
C	-2.825882	-3.363273	0.985832
H	-4.771826	-2.597908	0.532192
H	-0.753198	-3.857327	1.371496
H	1.475460	2.975896	4.007503
H	-5.056751	4.141336	-1.643663
H	-3.205459	-4.354400	1.216441
N	-4.184462	-0.081962	-0.104871
C	-5.585043	-0.407647	-0.163598
C	-6.135529	-0.924457	-1.340791
C	-6.393581	-0.206096	0.959084
C	-7.494489	-1.238990	-1.392794
H	-5.496700	-1.076019	-2.205200
C	-7.752189	-0.521903	0.903115
H	-5.953139	0.195707	1.866171
C	-8.303507	-1.038268	-0.271798
H	-7.919785	-1.640052	-2.307657
H	-8.378062	-0.364574	1.776160
H	-9.360343	-1.283445	-0.313812
C	-3.761694	1.205517	-0.476806
C	0.853848	0.137061	-3.018616
H	0.787800	-0.103338	-4.074582

Table S10 Cartesian coordinates of the first excited state (S_1) fully optimized geometry in THF of *o*-**SAC** from B3LYP calculations (in Å)

Atom	X	Y	Z
C	4.801428	-0.789855	-0.052148
C	3.520124	1.172492	-0.671893
B	5.811616	-0.138095	1.051507
B	6.280266	-0.431906	-0.653013
B	5.525380	1.593959	1.242960
B	6.867930	1.011047	0.200056
B	5.953529	2.428109	-0.291984
B	6.248155	1.121363	-1.484181
B	4.265270	2.305106	0.231160
B	4.701014	1.975326	-1.473701
B	4.718326	0.127848	-1.486484
B	4.091606	0.522047	0.813007
H	6.115654	-0.814457	1.980962
H	6.942780	-1.337452	-1.046676
H	8.019763	1.105091	0.492659
H	5.727324	2.081539	2.311815
H	3.293527	0.234957	1.637157
H	4.362005	-0.430834	-2.469709
H	6.962957	1.280629	-2.424413
H	6.472905	3.500095	-0.342741
H	3.623298	3.231966	0.603933
H	4.369327	2.633530	-2.406753
C	4.231925	-2.153399	0.031621
C	3.663613	-2.633981	1.227943
C	4.247232	-3.019253	-1.079497
C	3.132611	-3.920630	1.307531
H	3.646455	-1.992748	2.102430
C	3.716656	-4.305231	-0.998567
H	4.684090	-2.677917	-2.011711
C	3.152471	-4.765044	0.194301
H	2.707789	-4.266491	2.245982
H	3.746000	-4.951685	-1.871326
H	2.740957	-5.768062	0.257088
C	-0.452931	0.530257	-2.293859
C	1.917251	0.894707	-2.521944
C	-0.302090	0.773680	-0.937914
H	-1.421997	0.282892	-2.715930
C	2.113948	1.093264	-1.132868
H	2.786566	0.927066	-3.165810
C	-1.439966	0.695296	0.090290
C	0.931548	1.111529	-0.330889
C	-0.725027	1.189732	1.354064
C	-2.589521	1.617666	-0.272972
C	-1.887769	-0.749062	0.269901
C	0.639069	1.438592	1.094262
C	-1.303915	1.412553	2.596238
C	-2.339341	2.967043	-0.521568
C	-3.251063	-1.131515	0.173353
C	-0.946816	-1.738755	0.551314
C	1.407952	1.986181	2.130417
C	-0.513119	1.929801	3.625517
H	-2.357323	1.205038	2.762618
C	-4.974202	2.063549	-0.672139
C	-3.366540	3.852226	-0.837259
H	-1.318216	3.326564	-0.464672
C	-3.628735	-2.486788	0.366674
C	-1.319197	-3.067798	0.735008
H	0.098924	-1.463977	0.623294
C	0.829426	2.223375	3.380010
H	2.442999	2.243876	1.977638
H	-0.945718	2.116805	4.603421
C	-4.690501	3.393266	-0.911104
H	-5.993414	1.709209	-0.730580
H	-3.139615	4.895792	-1.024773
C	-2.670028	-3.439371	0.643212
H	-4.668703	-2.770979	0.293281
H	-0.559238	-3.811761	0.946066
H	1.441460	2.647695	4.170315
H	-5.494718	4.077605	-1.156065
H	-2.965256	-4.472503	0.786293
N	-4.226240	-0.182306	-0.117619
C	-5.615762	-0.608041	-0.185003
C	-6.138770	-1.035134	-1.405567
C	-6.390439	-0.577240	0.974574
C	-7.472662	-1.441313	-1.460734
H	-5.512217	-1.048162	-2.290964
C	-7.722759	-0.986245	0.904686
H	-5.956567	-0.239792	1.909812
C	-8.262467	-1.417092	-0.309174
H	-7.890860	-1.775824	-2.404145
H	-8.335442	-0.966986	1.799698
H	-9.299035	-1.734127	-0.357754
C	-3.928295	1.160093	-0.352008
C	0.681886	0.633592	-3.099037
H	0.610413	0.486629	-4.172391