Electronic Supporting Information

Solid-state white-light emission from a pyrylium dye obtained in one synthetic step

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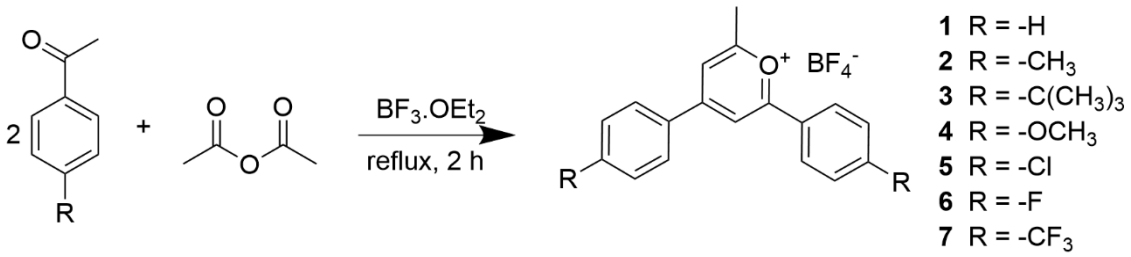
Experimental Section

All commercially available reagents and solvents were used as received. ^{1}H and ^{13}C NMR spectra were recorded with a Bruker Advance III HD spectrometer (400 MHz for ^{1}H and 101 MHz for ^{13}C). High resolution mass spectra were obtained with a Waters Q-Tof Premier mass spectrometer with an electrospray source. UV-vis spectra were obtained with a Jasco V-630 UV-vis spectrophotometer. Steady-state emission (solution) was recorded with an Agilent Cary-Eclipse spectrofluorometer. Time resolved fluorescence experiments (solution) were performed with an IBH5000U apparatus by using 372 nm (fwhm 1.3 ns) and 464 nm (fwhm 1.4 ns) nanoLEDs as excitation sources. Solid-state measurements where recorded in a C13534-01 apparatus from Hamamatsu Photonics K.K. TGA/DSC measurements were performed on a Mettler Toledo TGA/SDTA851e/LF/1600 instrument at a heating rate of 10ºC/min under N_2 atmosphere.

<u>Synthetic procedures and chemical characterization</u>



Scheme S1. Synthetic process for compounds **1**-**7**.

General procedure for the synthesis of compounds 1-7.[1] To a solution of the correspondent *para*-substituted acetophenone (10 mmol) in acetic anhydride (20 mmol, 1.89 mL), BF_3 diethyl etherate (7 mmol, 0.88 mL) was added dropwise under continuous stirring at room temperature. Then, the solution was heated to reflux in a silicone oil bath for 2 hours. After cooling to room temperature, the reaction mixture was poured into 200 ml of diethyl ether, and the formed precipitate was recovered by filtration and washed

with diethyl ether. For compounds **3**, **4**, **5** and **7**, further purification by recrystallization in acetic acid was needed. All the obtained solids were dried under vacuum before use.

Compound 1 (Yellow solid, yield 32%): ^{1}H NMR (400 MHz, CD_3CN) δ 8.67 (d, *J* = 1.7 Hz, 1H), 8.36 – 8.32 (m, 2H), 8.23 – 8.17 (m, 3H), 7.86 – 7.81 (m, 2H), 7.77 – 7.71 (m, 4H), 3.00 (s, 3H). ^{13}C NMR (101 MHz, CD_3CN) δ 178.78, 173.27, 167.67, 136.58, 133.68, 131.39, 131.20, 130.74, 130.08, 129.73, 120.11, 116.51, 22.12. HRMS (ESI-TOF)$^{+}$ calculated for $C_{18}H_{15}O^{+}$ (M^{+}) (m/z): 247.1120; experimental (M^{+}) (m/z): 247.1123.

Compound 2 (Yellow solid, yield 20%): ^{1}H NMR (400 MHz, CD_3CN) δ 8.56 (d, *J* = 1.8 Hz, 1H), 8.25 – 8.17 (m, 2H), 8.14 – 8.06 (m, 3H), 7.55 (dd, *J* = 8.0, 0.6 Hz, 4H), 2.94 (s, 3H), 2.51 (s, 6H). ^{13}C NMR (101 MHz, CD_3CN) δ 177.28, 172.89, 166.62, 148.62, 148.35, 131.91, 131.68, 130.55, 129.45, 127.20, 118.59, 115.03, 22.01, 21.96, 21.71. HRMS (ESI-TOF)$^{+}$ calculated for $C_{20}H_{19}O^{+}$ (M^{+}) (m/z): 275.1436; experimental (M^{+}) (m/z): 247.1438.

Compound 3 (Light orange solid, yield 24%): ^{1}H NMR (400 MHz, CD_3CN) δ 8.61 (d, *J* = 1.7 Hz, 1H), 8.31 – 8.22 (m, 2H), 8.20 – 8.11 (m, 3H), 7.86 – 7.71 (m, 4H), 2.95 (s, 3H), 1.40 (s, 18H). ^{13}C NMR (101 MHz, CD_3CN) δ 177.38, 177.38, 172.78, 166.47, 161.15, 160.90, 130.59, 130.50, 129.41, 128.34, 128.11, 127.24, 118.75, 115.31, 36.30, 36.28, 31.12, 31.11, 21.73. HRMS (ESI-TOF)$^{+}$ calculated for $C_{26}H_{31}O^{+}$ (M^{+}) (m/z): 359.2375; experimental (M^{+}) (m/z): 359.2383.

Compound 4 (Red solid, yield 35%): ^{1}H NMR (400 MHz, CD_3CN) δ 8.38 (d, *J* = 1.8 Hz, 1H), 8.29 – 8.24 (m, 2H), 8.22 – 8.17 (m, 2H), 7.93 (d, *J* = 1.8 Hz, 1H), 7.25 – 7.17 (m, 4H), 3.95 (s, 3H), 3.95 (s, 3H), 2.86 (s, 3H). ^{13}C NMR (101 MHz, CD_3CN) δ 175.30, 171.90, 167.20, 166.64, 164.66, 133.03, 131.73, 125.26, 122.20, 116.80, 116.54, 116.48,

113.02, 57.01, 56.94, 21.42. HRMS (ESI-TOF)$^+$ calculated for $C_{20}H_{19}O_3^+$ (M^+) (m/z): 307.1334; experimental (M^+) (m/z): 307.1332.

Compound 5 (Yellow solid, yield 30%): ^{1}H NMR (400 MHz, CD_3CN) δ 8.63 (d, *J* = 1.7 Hz, 1H), 8.33 – 8.28 (m, 2H), 8.20 (d, *J* = 1.4 Hz, 1H), 8.19 – 8.14 (m, 2H), 7.78 – 7.73 (m, 4H), 2.99 (s, 3H). ^{13}C NMR (101 MHz, CD3CN) δ 178.92, 171.91, 166.08, 142.55, 142.42, 132.26, 132.07, 131.94, 131.31, 131.27, 131.18, 130.98, 128.42, 119.91, 116.94, 116.32, 21.92. HRMS (ESI-TOF)$^+$ calculated for $C_{18}H_{13}Cl_2O^+$ (M^+) (m/z): 315.0343; experimental (M^+) (m/z): 315.0347.

Compound 6 (Yellow solid, yield 27%): ^{1}H NMR (400 MHz, CD_3CN) δ 8.59 (d, *J* = 1.3 Hz, 1H), 8.49 – 8.33 (m, 2H), 8.33 – 8.21 (m, 2H), 8.16 (s, 1H), 7.48 (t, *J* = 8.6 Hz, 4H), 2.98 (s, 3H). ^{13}C NMR (101 MHz, CD_3CN) δ 178.19, 171.77, 169.25, 169.03, 166.69, 166.47, 165.85, 133.47, 133.37, 132.42, 132.32, 129.65, 126.22, 119.26, 118.39, 118.28, 115.73, 21.69. HRMS (ESI-TOF)$^+$ calculated for $C_{18}H_{13}F_2O^+$ (M^+) (m/z): 283.0934; experimental (M^+) (m/z): 283.0934.

Compound 7 (Yellow solid, yield 28%): ^{1}H NMR (400 MHz, CD_3CN) δ 8.81 (d, *J* = 1.7 Hz, 1H), 8.51 (dd, *J* = 8.9, 0.7 Hz, 2H), 8.36 (d, *J* = 1.5 Hz, 1H), 8.34 (dd, *J* = 8.9, 0.7 Hz, 2H), 8.09 – 8.03 (m, 4H), 3.08 (s, 3H). ^{13}C NMR (101 MHz, CD_3CN) δ 180.92, 171.82, 166.78, 137.11, 136.41, 136.25, 136.09, 135.92, 133.17, 131.33, 130.35, 127.96-127.86 (m), 122.05, 22.36. (ESI-TOF)$^+$ calculated for $C_{20}H_{13}F_6O^+$ (M^+) (m/z): 383.0871; experimental (M^+) (m/z): 383.0866.

Absorption and Fluorometric studies in solution

1mM stock solutions of compounds **1**-**7** were prepared in acetonitrile. For the measurements of the absorption spectra, the correspondent stock solution for each compound was diluted to reach a final concentration of 10 μM, both in dichloromethane

and acetonitrile. For emission spectra, concentration was adjusted to reach a value of 0.1 in absorbance, in order to minimize the primary inner filter effect. λ_{exc} was set at 340 nm for all compounds, except for compound **4** (360 nm).

Fluorescence Quantum Yield Measurements (ϕ_F). The fluorescence quantum yields of all compounds were determined in dichloromethane and acetonitrile, under a N_2 atmosphere. Quinine sulfate (ϕ_F = 0.55 in 0.5 M H_2SO_4)[2] was used as a reference for compounds **1**-**3**, **5**-**7** and Acridine Orange (ϕ_F = 0.2 in ethanol; 0.01 M KOH)[3] was used as a reference for compound **4**.

The concentration of the reference and the studied compounds were adjusted to obtain the same absorption at the excitation wavelength. Fluorescence quantum yields were calculated by using [**Equation (1)**]:

$$\phi_F = \phi_R \cdot (A_R \cdot F_S / A_S \cdot F_R) \cdot (n_S^2 / n_R^2) \qquad (1)$$

where ϕ_F is the fluorescence quantum yield, F is the integral of the emission spectrum, A is the absorption intensity, and n is the refractive index. The subindex R refers to the reference compound and S to the studied pyrylium salt.

Fluorescence Lifetime Measurements (τ_F). The fluorescence lifetimes of all compounds were determined in dichloromethane and acetonitrile, under a N_2 atmosphere. For this purpose, solutions were prepared similarly to those used to obtain the emission spectra. Fluorescence lifetimes were determined by using the technique of time-correlated single-photon counting (TCSPC). Data obtained from the experiments were adjusted to a single exponential model by using the software IBH DAS6.

Fluorometric studies in the solid state

The fluorescence quantum yields and fluorescence spectra in the solid state were obtained with an absolute PL quantum yield measurement system (C13534-01) from Hamamatsu Photonics K.K. The 1931 x,y chromaticity diagram was obtained from the Konica-Minolta website.

Thermogravimetric analysis (TGA) and Differential Scanning Calorimetry (DSC)

Table S1. Melting temperatures (T_m from DSC) and thermal decomposition temperatures (T_{ds} from TGA) of **1**–**7**.

Comp.	**1**	**2**	**3**	**4**	**5**	**6**	**7**
T_m (ºC)	246	258	240	249	267	251	243
T_{ds} (ºC)[a]	245	253	240	261	241	247	234

(a) 5% weight loss

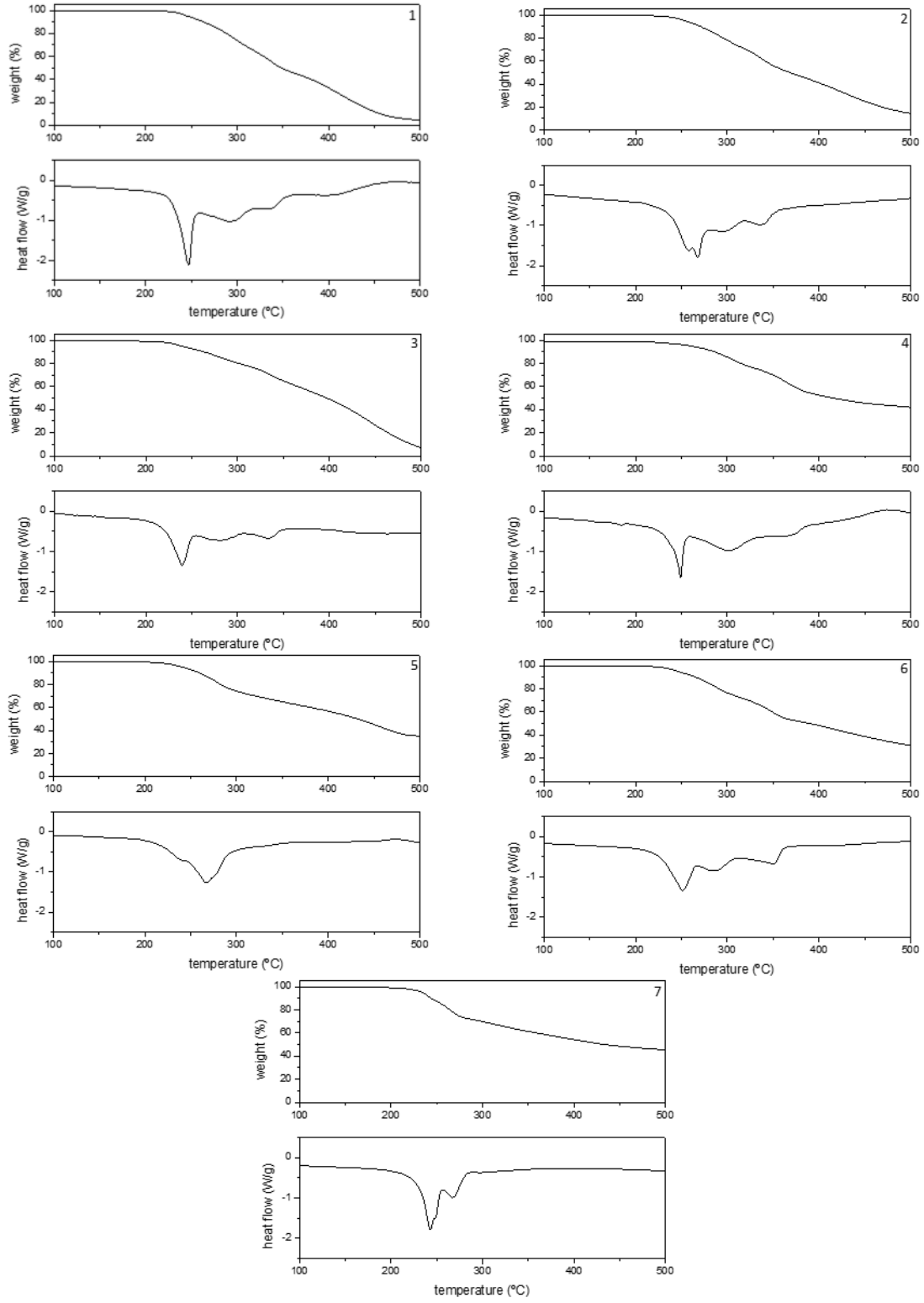


Figure S1. TGA plots (up) and DSC thermograms (down) for compounds **1**-**7** obtained at a heating rate of 10ºC/min under N_2 atmosphere. For DSC: exothermic up.

Spectroscopic data of compounds 1-7

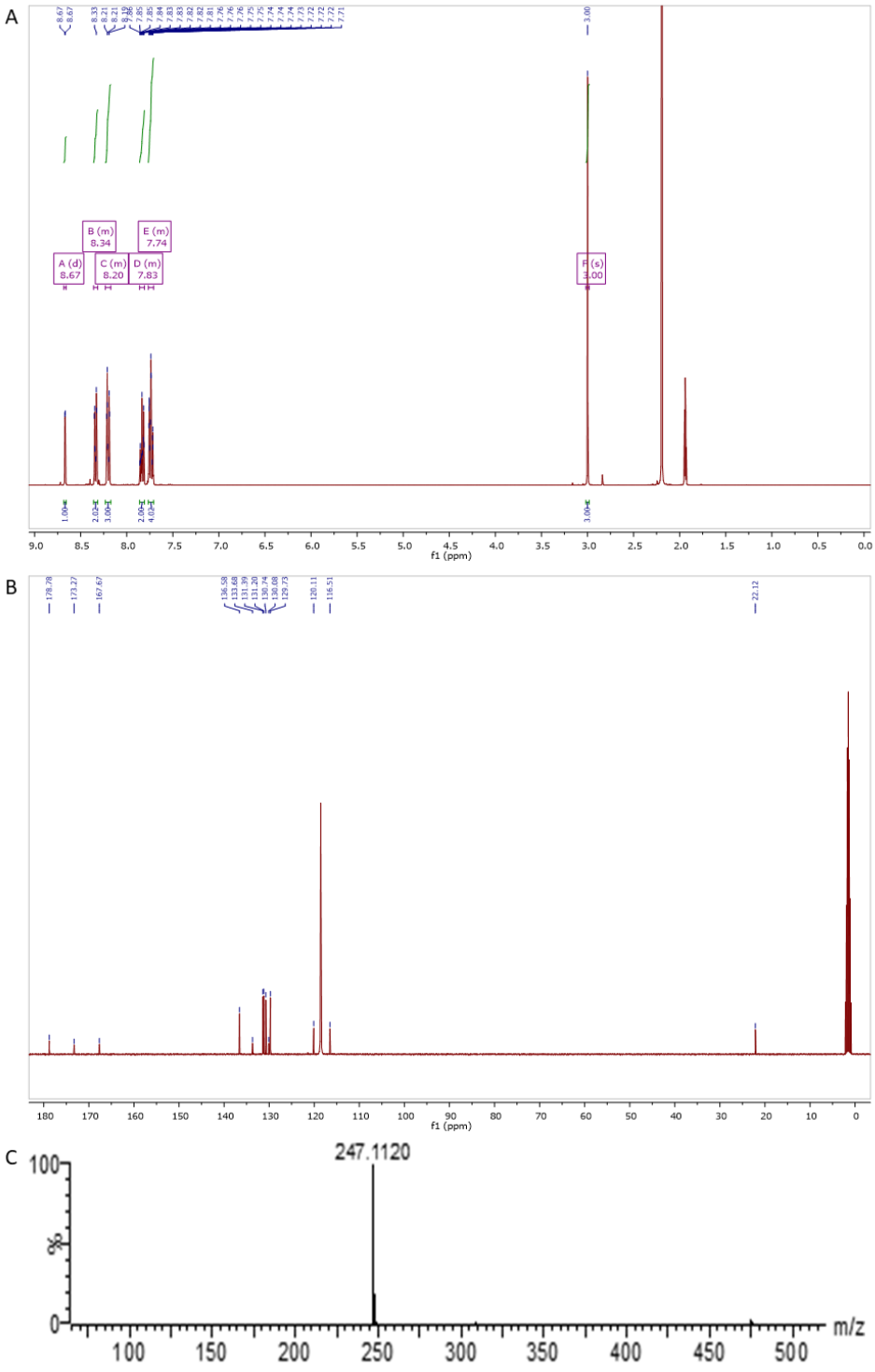


Figure S2. A) ^{1}H NMR (CD_3CN) spectrum of compound **1** B) ^{13}C NMR (CD_3CN) spectrum of compound **1** C) HRMS spectrum of compound **1**.

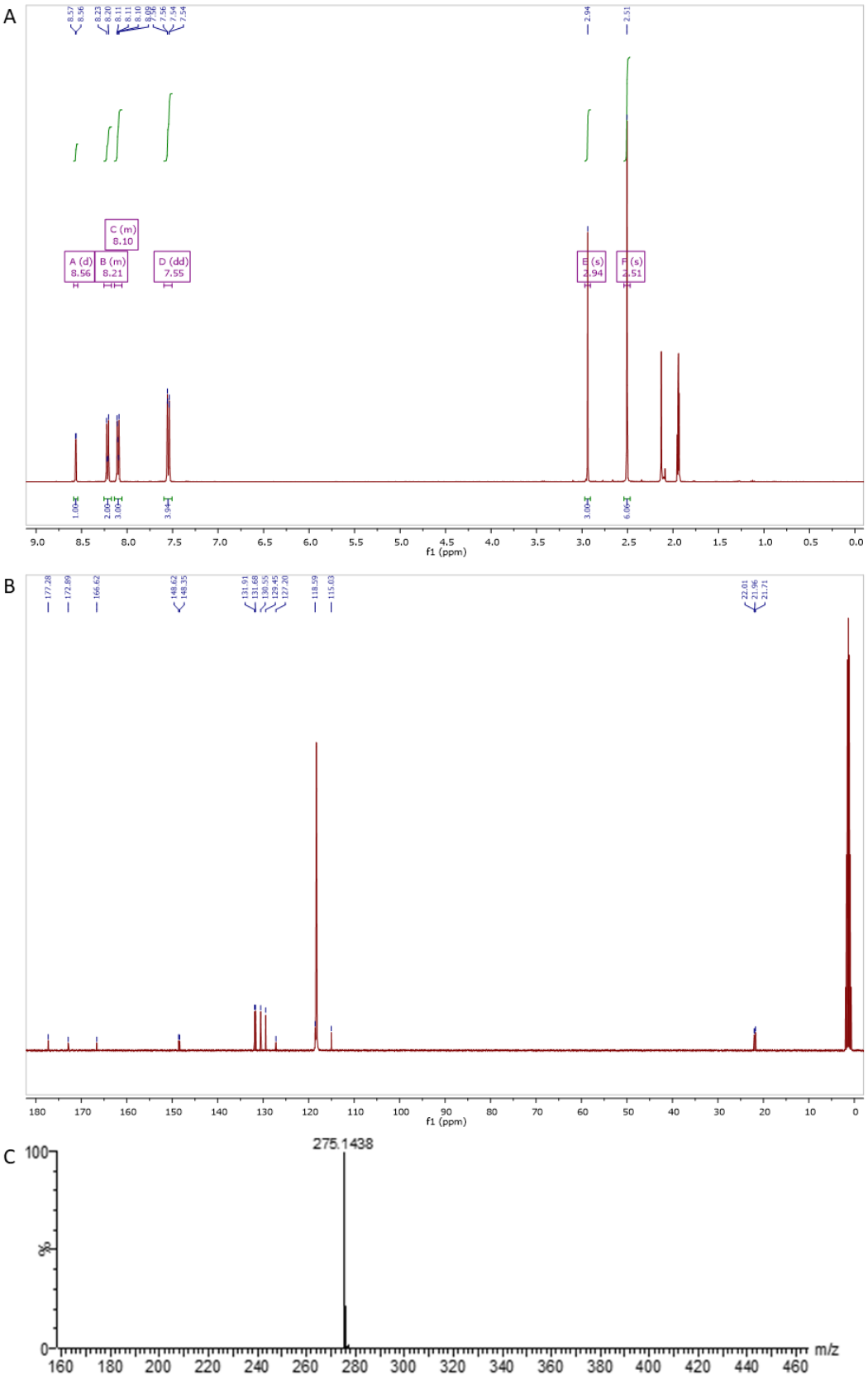


Figure S3. A) ^{1}H NMR (CD_3CN) spectrum of compound **2** B) ^{13}C NMR (CD_3CN) spectrum of compound **2** C) HRMS spectrum of compound **2**.

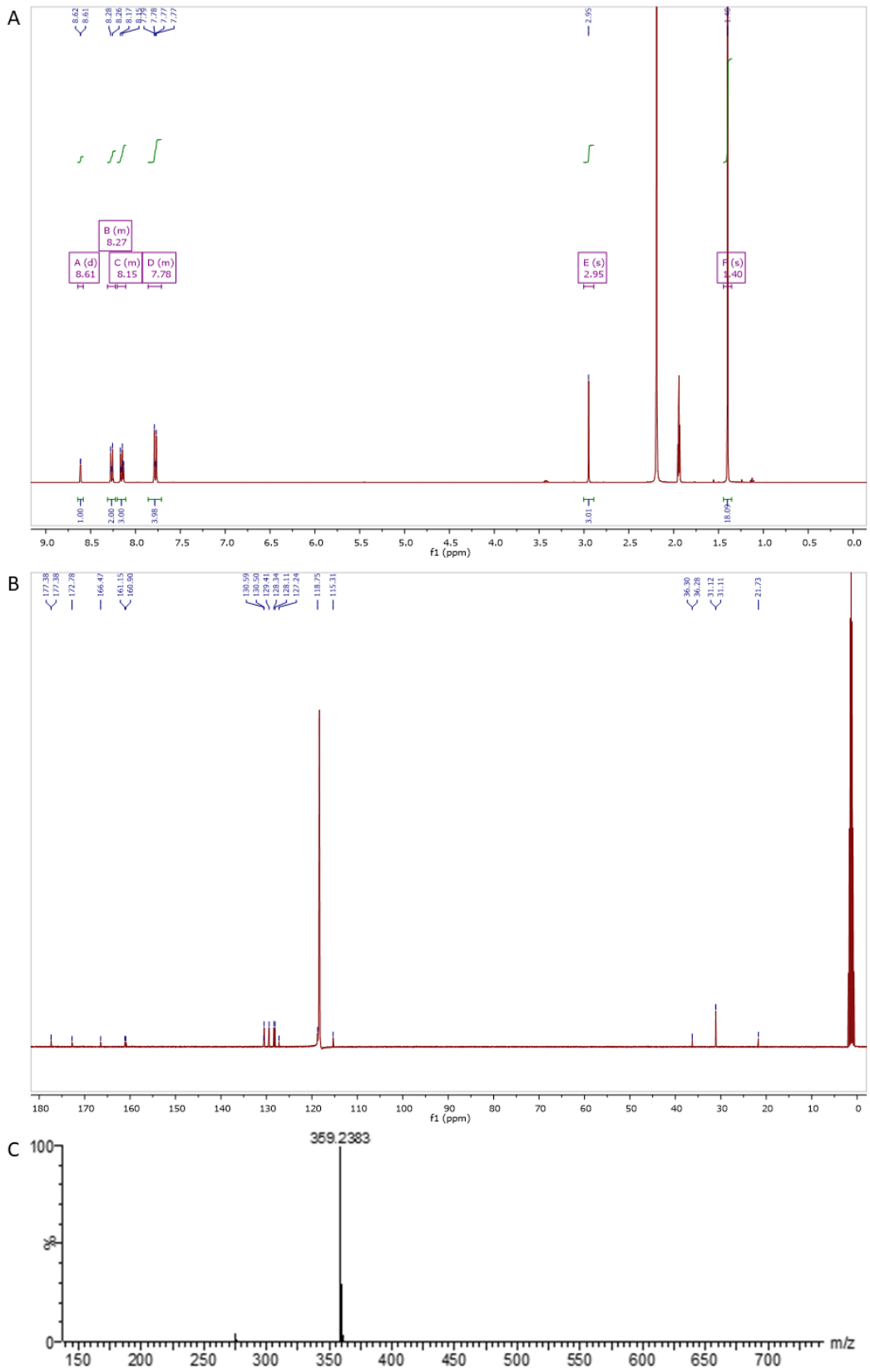


Figure S4. A) ^{1}H NMR (CD_3CN) spectrum of compound **3** B) ^{13}C NMR (CD_3CN) spectrum of compound **3** C) HRMS spectrum of compound **3**.

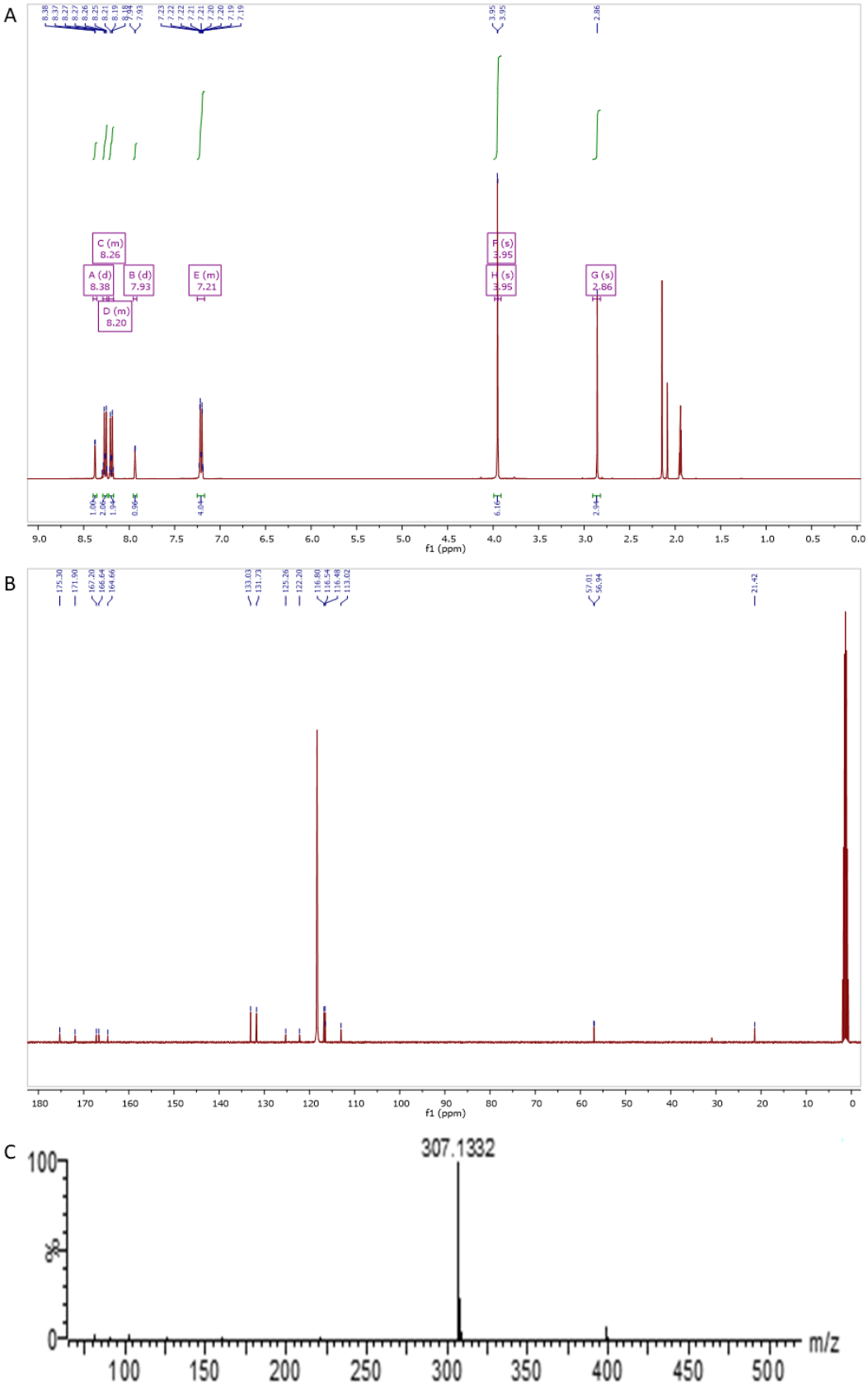


Figure S5. A) ^{1}H NMR (CD_3CN) spectrum of compound **4** B) ^{13}C NMR (CD_3CN) spectrum of compound **4** C) HRMS spectrum of compound **4**.

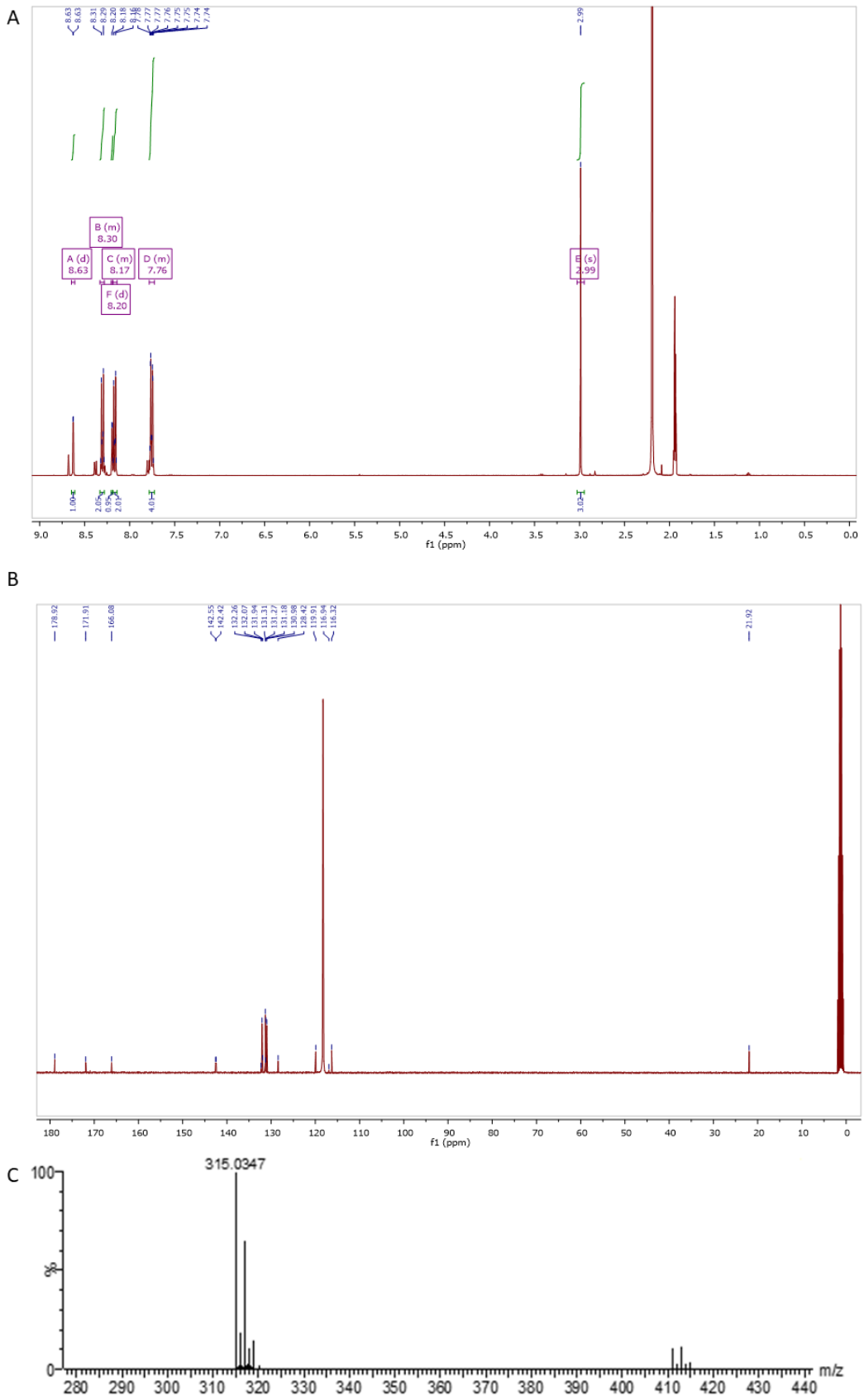


Figure S6. A) ^{1}H NMR (CD_3CN) spectrum of compound **5** B) ^{13}C NMR (CD_3CN) spectrum of compound **5** C) HRMS spectrum of compound **5**.

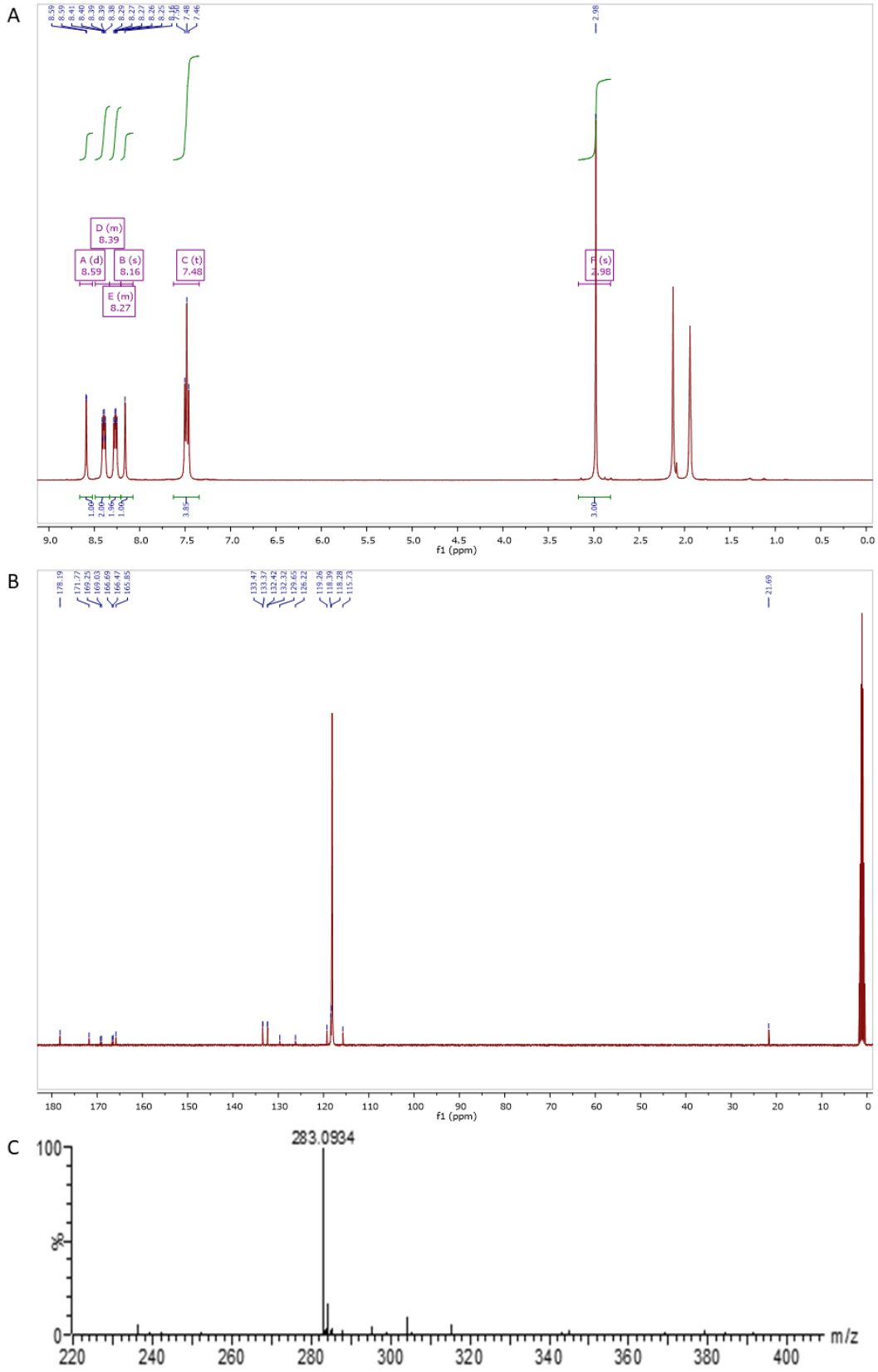


Figure S7. A) ^{1}H NMR (CD_3CN) spectrum of compound **6** B) ^{13}C NMR (CD_3CN) spectrum of compound **6** C) HRMS spectrum of compound **6**.

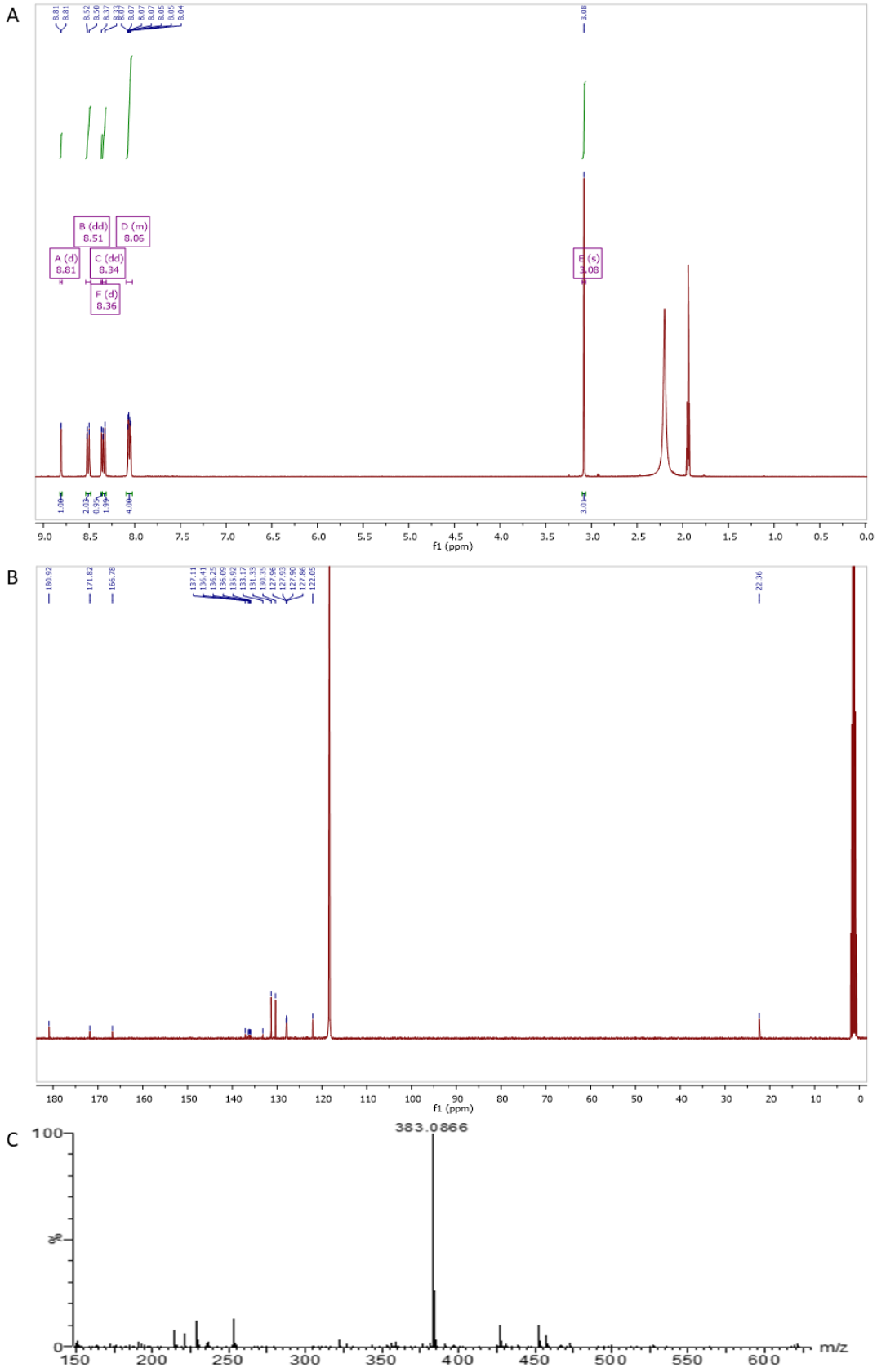


Figure S8. A) ^{1}H NMR (CD_3CN) spectrum of compound **7** B) ^{13}C NMR (CD_3CN) spectrum of compound **7** C) HRMS spectrum of compound **7**.

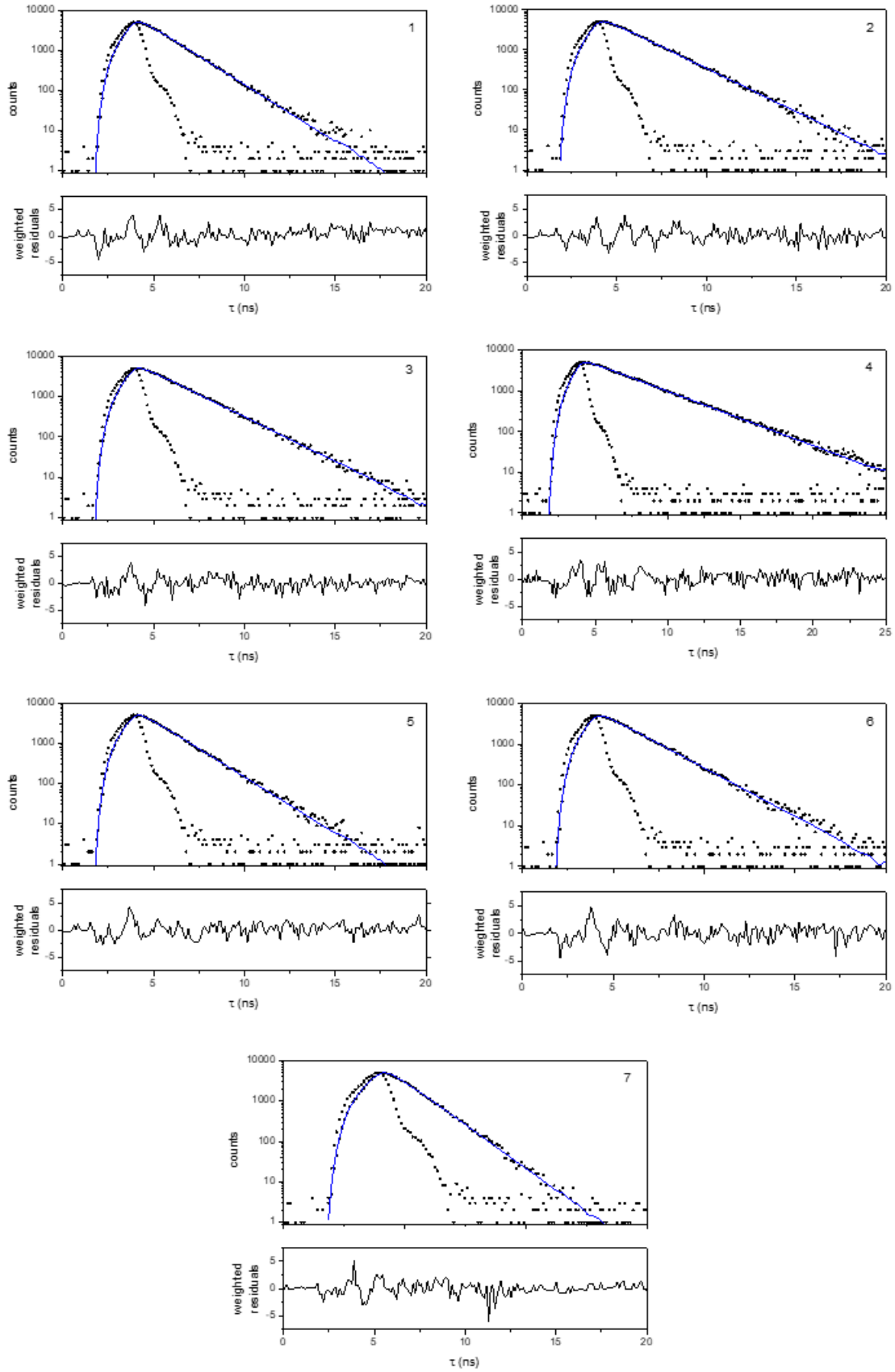


Figure S9. Fluorescence decay curves for compounds **1**-**7** in dichloromethane at 295 K. λ_{exc} was set at 372 nm (464 nm for compound **4**). λ_{em} was set at the emission maximum for each compound. The incident light pulse and the residuals are also shown.

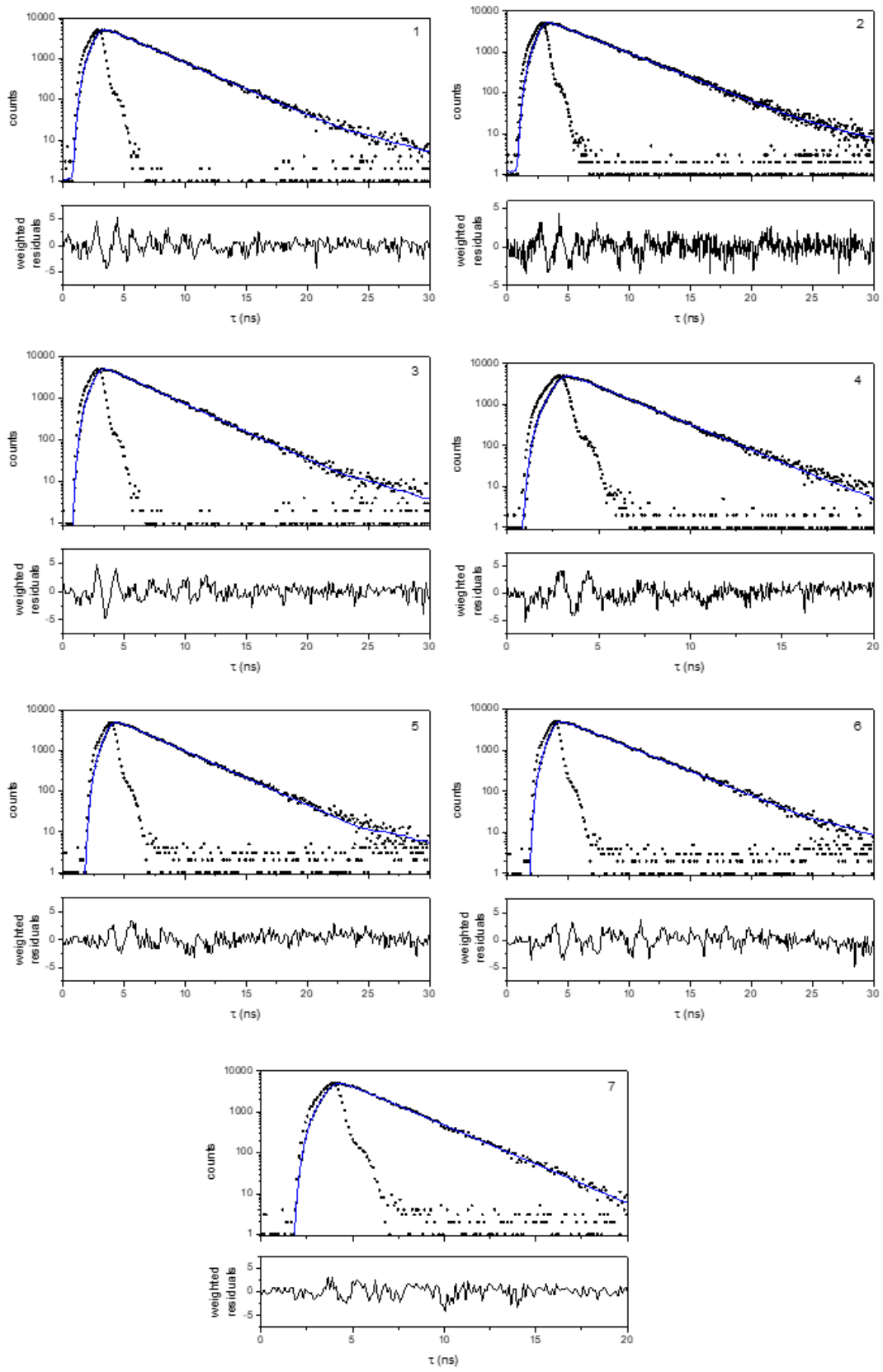


Figure S10. Fluorescence decay curves for compounds **1**-**7** in acetonitrile at 295 K. λ_{exc} was set at 372 nm (464 nm for compound **4**). λ_{em} was set at the emission maximum for each compound. The incident light pulse and the residuals are also shown.

DFT calculations

Results of DFT and TD-DFT calculations (atom coordinates and sum of electronic and zero-point energies)

The calculation was carried out at the DFT level, using the Gaussian 09 software package. The geometries of the studied compounds **1-7** ignored with the counter anion, BF_4^- were fully optimized by using the 6-31+G(d) base set at the B3LYP, CAM-B3LYP and PBE0 methods on the CPCM model considering dielectric constants of DCM and ACN.[4] The results are summarized in **Tables S2-4**. Atom coordinates for the optimized geometries of the compounds are listed in **Tables S5-46**. The calculated molecular orbital diagrams of the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) in DCM and ACN are shown in **Figures S11-16**, respectively.

Table S2. Calculation results for compounds **1-7** in DCM based on B3LYP method.[a]

Compound	HOMO / eV	LUMO / eV	λ_{tr} [b]/ nm	f [c]	Coefficient[d]
1	-7.60 (-7.35)	-3.86 (-3.59)	383 (379)	0.7036 (0.6800)	0.70369 (0.70526)
2	-7.29 (-7.05)	-3.75 (-3.49)	405 (400)	0.8509 (0.8253)	0.70191 (0.70518)
3	-7.28 (-7.06)	-3.75 (-3.50)	408 (403)	0.9282 (0.9050)	0.70514 (0.70507)
4	-6.82 (-6.60)	-3.60 (-3.35)	442 (436)	0.9712 (0.9437)	0.70518 (0.70507)
5	-7.50 (-7.26)	-3.98 (-3.64)	406 (400)	0.8691 (0.8408)	0.70539 (0.70518)
6	-7.57 (-7.32)	-3.90 (-3.62)	389 (384)	0.7352 (0.7101)	0.70520 (0.70498)
7	-8.05 (-7.77)	-4.18 (-3.88)	368 (365)	0.7256 (0.7052)	0.69963 (0.69854)

[a] In parentheses, data in ACN.
[b] Wavelength estimated from the HOMO-LUMO energy gap.
[c] Oscillator strength for the $S_0 \rightarrow S_1$ transition.
[d] For the HOMO-LUMO transition.

Table S3. Calculation results for compounds **1-7** in DCM based on CAM-B3LYP method.[a]

Compound	HOMO / eV	LUMO / eV	λ_{tr} [b]/ nm	f [c]	Coefficient[d]
1	-8.90 (-8.65)	-2.83 (-2.56)	347 (345)	0.8279 (0.8020)	0.68788 (0.68808)
2	-8.57 (-8.33)	-2.74 (-2.48)	364 (361)	1.0105 (0.9843)	0.68685 (0.68695)
3	-8.55 (-8.35)	-2.75 (-2.47)	367 (357)	1.1061 (1.0533)	0.68607 (0.68550)
4	-8.12 (-7.88)	-2.55 (-2.35)	397 (382)	1.1460 (1.1379)	0.68431 (0.68489)
5	-8.63 (-7.88)	-3.08 (-2.35)	403 (358)	1.1940 (1.0074)	0.68488 (0.68068)
6	-8.85 (-8.59)	-2.87 (-2.59)	353 (349)	0.8672 (0.8393)	0.68725 (0.68742)
7	-9.39 (-9.06)	-3.11 (-2.84)	332 (336)	0.7952 (0.7971)	0.68673 (0.69854)

[a] In parentheses, data in ACN.
[b] Wavelength estimated from the HOMO-LUMO energy gap.
[c] Oscillator strength for the $S_0 \rightarrow S_1$ transition.
[d] For the HOMO-LUMO transition.

Table S4. Calculation results for compounds **1-7** in DCM based on PBE0 method.[a]

Compound	HOMO / eV	LUMO / eV	λ_{tr} [b]/ nm	f [c]	Coefficient[d]
1	-6.94 (-6.69)	-4.42 (-4.15)	432 (428)	0.0477 (0.0422)	0.28077 (0.27092)
2	-6.63 (-6.40)	-4.28 (-4.04)	456 (452)	0.7043 (0.6830)	0.69809 (0.69723)
3	-6.62 (-6.41)	-4.29 (-4.03)	463 (403)	0.7653 (0.6940)	0.69521 (0.69272)
4	-6.12 (-5.89)	-4.11 (-3.83)	456 (507)	0.7574 (0.7239)	0.69589 (0.69421)
5	-6.77 (-6.53)	-4.50 (-4.23)	476 (469)	0.7252 (0.7022)	0.69852 (0.69730)
6	-6.28 (-6.57)	-4.42 (-4.14)	444 (439)	0.6154 (0.5960)	0.69726 (0.69624)
7	-7.36 (-7.04)	-4.71 (-4.42)	424 (422)	0.0029 (0.0043)	0.11236 (0.12859)

[a] In parentheses, data in ACN.
[b] Wavelength estimated from the HOMO-LUMO energy gap.
[c] Oscillator strength for the $S_0 \rightarrow S_1$ transition.
[d] For the HOMO-LUMO transition.

Table S5. Atom coordinates for the optimized geometry of compound **1** in DCM based on B3LYP method.

Atom	X	Y	Z
C	-0.118041	2.397679	-0.196117
C	1.125362	1.823614	-0.152059
C	1.258245	0.416891	-0.047185
C	0.073812	-0.340189	0.012433
C	-1.162776	0.276775	-0.038352
H	1.991924	2.467706	-0.228243
H	0.115926	-1.411781	0.148229
C	-2.472457	-0.368053	0.028690
C	-3.632690	0.397543	0.266933
C	-2.591264	-1.762521	-0.144139
C	-4.877594	-0.222408	0.339462
H	-3.556195	1.470170	0.405576
C	-3.840470	-2.373472	-0.073868
H	-1.718776	-2.372125	-0.353056
C	-4.985835	-1.607311	0.170253
H	-5.763963	0.375017	0.530867
H	-3.920736	-3.447097	-0.214918
H	-5.958603	-2.087410	0.226343
C	2.579636	-0.224229	0.007946
C	2.762493	-1.535600	-0.478438
C	3.688035	0.461555	0.546893
C	4.017897	-2.137671	-0.432876
H	1.933330	-2.073664	-0.927132
C	4.937779	-0.151408	0.606192
H	3.569120	1.460779	0.953775
C	5.107396	-1.449913	0.113243
H	4.147352	-3.141316	-0.827025
H	5.778276	0.382485	1.039648
H	6.084193	-1.923528	0.153606
O	-1.219386	1.621270	-0.141877
C	-0.432980	3.846527	-0.317331
H	-1.021968	4.179118	0.545336

H	0.485419	4.433573	-0.369924
H	-1.029489	4.031045	-1.218134

Sum of electronic and zero-point energies = -770.032536037 Hartree

Table S6. Atom coordinates for the optimized geometry of compound **1** in ACN based on B3LYP method.

Atom	X	Y	Z
C	-0.118041	2.397679	-0.196117
C	1.125362	1.823614	-0.152059
C	1.258245	0.416891	-0.047185
C	0.073812	-0.340189	0.012433
C	-1.162776	0.276775	-0.038352
H	1.991924	2.467706	-0.228243
H	0.115926	-1.411781	0.148229
C	-2.472457	-0.368053	0.028690
C	-3.632690	0.397543	0.266933
C	-2.591264	-1.762521	-0.144139
C	-4.877594	-0.222408	0.339462
H	-3.556195	1.470170	0.405576
C	-3.840470	-2.373472	-0.073868
H	-1.718776	-2.372125	-0.353056
C	-4.985835	-1.607311	0.170253
H	-5.763963	0.375017	0.530867
H	-3.920736	-3.447097	-0.214918
H	-5.958603	-2.087410	0.226343
C	2.579636	-0.224229	0.007946
C	2.762493	-1.535600	-0.478438
C	3.688035	0.461555	0.546893
C	4.017897	-2.137671	-0.432876
H	1.933330	-2.073664	-0.927132
C	4.937779	-0.151408	0.606192
H	3.569120	1.460779	0.953775

C	5.107396	-1.449913	0.113243
H	4.147352	-3.141316	-0.827025
H	5.778276	0.382485	1.039648
H	6.084193	-1.923528	0.153606
O	-1.219386	1.621270	-0.141877
C	-0.432980	3.846527	-0.317331
H	-1.021968	4.179118	0.545336
H	0.485419	4.433573	-0.369924
H	-1.029489	4.031045	-1.218134

Sum of electronic and zero-point energies = -770.038032849Hartree

Table S7. Atom coordinates for the optimized geometry of compound **2** in DCM based on B3LYP method.

Atom	X	Y	Z
C	0.113383	2.652752	0.158875
C	-1.126121	2.073935	0.127576
O	-1.255916	0.662382	0.052746
C	-0.066802	-0.088669	0.009803
C	1.168690	0.533148	0.047248
C	-1.993888	2.717546	0.190380
C	-0.103474	-1.163217	-0.100206
C	2.478050	-0.106223	-0.002628
C	3.644387	0.659188	-0.208284
C	2.606585	-1.502662	0.150716
C	4.889684	0.042691	-0.265587
C	3.573424	1.733626	-0.336105
C	3.857668	-2.104992	0.094921
C	1.735882	-2.124672	0.328664
C	5.024034	-1.347716	-0.113493
C	5.774316	0.650733	-0.435676
C	3.932543	-3.182256	0.218316

C	-2.571910	0.017188	0.012329
C	-2.747896	-1.304521	0.475954
C	-3.699913	0.700810	-0.486916
C	-3.999813	-1.907718	0.445462
H	-1.912522	-1.852556	0.900533
H	-4.945617	0.082211	-0.529018
H	-3.603507	1.709016	-0.877300
H	-5.122694	-1.231186	-0.063507
H	-4.111600	-2.918804	0.828803
H	-5.795315	0.627192	-0.931924
H	1.220435	1.881320	0.121373
H	0.422348	4.105673	0.249014
H	1.010875	4.422515	-0.619857
H	-0.498609	4.689925	0.287767
H	1.016711	4.312666	1.146385
H	-6.469326	-1.905852	-0.125048
H	-6.527905	-2.569557	-0.998241
H	-6.646576	-2.523083	0.762253
H	-7.280160	-1.175937	-0.209543
H	6.378836	-2.007258	-0.146045
H	6.764334	-2.142842	0.873598
H	6.329796	-2.998624	-0.608584
H	7.106254	-1.401308	-0.694944

Sum of electronic and zero-point energies = -848.673120662 Hartree

Table S8. Atom coordinates for the optimized geometry of compound **2** in ACN based on B3LYP method.

Atom	X	Y	Z
C	0.113779	2.652457	0.160769
C	-1.126119	2.073699	0.128907
O	-1.255559	0.662823	0.052939
C	-0.066865	-0.088895	0.009518

C	1.168100	0.533176	0.047845
C	-1.993688	2.717510	0.191682
C	-0.103547	-1.163337	-0.101281
C	2.477962	-0.106335	-0.002381
C	3.643238	0.658582	-0.214384
C	2.607045	-1.501858	0.156955
C	4.888804	0.042130	-0.272128
C	3.571327	1.732391	-0.346973
C	3.858372	-2.104134	0.100623
C	1.736832	-2.122982	0.340132
C	5.023892	-1.347463	-0.114146
C	5.772737	0.649809	-0.447266
C	3.933738	-3.180838	0.228747
C	-2.571966	0.017291	0.011801
C	-2.747974	-1.303855	0.476442
C	-3.699378	0.700538	-0.488808
C	-4.000064	-1.907226	0.445657
H	-1.912619	-1.851629	0.901305
H	-4.945265	0.081849	-0.530933
H	-3.602640	1.708554	-0.879500
H	-5.122554	-1.231113	-0.064426
H	-4.111805	-2.918138	0.829532
H	-5.794731	0.626733	-0.934547
H	1.220191	1.880797	0.122997
H	0.422800	4.105088	0.251927
H	1.012118	4.421841	-0.616383
H	-0.498207	4.689162	0.290278
H	1.016513	4.311022	1.149933
H	-6.469382	-1.905835	-0.126313
H	-6.529030	-2.567437	-1.001040

H	-6.645685	-2.525165	0.759736
H	-7.280179	-1.175502	-0.208291
H	6.378938	-2.006978	-0.147384
H	6.765105	-2.142992	0.871939
H	6.329521	-2.998269	-0.610171
H	7.105895	-1.400765	-0.696675

Sum of electronic and zero-point energies = -848.678306249 Hartree

Table S9. Atom coordinates for the optimized geometry of compound **3** in DCM based on B3LYP method.

Atom	X	Y	Z
C	-0.061905	0.463951	-0.034785
C	1.178078	1.083339	-0.060915
O	1.228220	2.437171	-0.104524
C	0.115802	3.207269	-0.123287
C	-1.120514	2.628206	-0.100076
C	-1.254514	1.210187	-0.055865
C	-2.567179	0.569027	-0.025875
C	2.482524	0.443748	-0.029654
C	2.611702	-0.952402	-0.170889
C	3.862996	-1.557972	-0.140537
C	5.042449	-0.810987	0.033701
C	4.900074	0.585819	0.173547
C	3.660004	1.204930	0.140732
C	-3.699623	1.246883	0.468887
C	-4.946313	0.630092	0.508023
C	-5.135875	-0.682147	0.038968
C	-3.999742	-1.351178	-0.464397
C	-2.749144	-0.752996	-0.490480
C	0.424590	4.663654	-0.186054
C	-6.500006	-1.385427	0.054150
C	-6.892909	-1.757892	-1.398464
C	-7.612083	-0.498518	0.646524
C	-6.397227	-2.675327	0.907283
C	6.436794	-1.450193	0.073844

C	6.388960	-2.980096	-0.105618
C	7.096491	-1.138283	1.441605
C	7.302075	-0.851511	-1.064401
H	-0.096695	-0.613039	0.051349
H	-1.989803	3.271471	-0.149652
H	1.739050	-1.579518	-0.323499
H	3.913256	-2.633723	-0.259791
H	5.779551	1.206018	0.313441
H	3.599134	2.281504	0.255625
H	-3.606992	2.251951	0.869593
H	-5.780635	1.187398	0.917323
H	-4.095752	-2.360456	-0.851805
H	-1.916386	-1.304034	-0.917498
H	1.018431	4.967333	0.684321
H	-0.495709	5.250934	-0.207001
H	1.012267	4.892886	-1.082863
H	-7.867859	-2.258515	-1.401606
H	-6.170384	-2.439043	-1.860651
H	-6.969608	-0.865347	-2.030147
H	-8.559200	-1.048029	0.635363
H	-7.761599	0.419155	0.065492
H	-7.408602	-0.222129	1.687883
H	-7.366817	-3.185793	0.924045
H	-6.118473	-2.445038	1.942066
H	-5.660493	-3.379432	0.506228
H	7.406929	-3.381946	-0.069560
H	5.959928	-3.268987	-1.072454
H	5.817111	-3.471880	0.690213
H	8.094624	-1.588831	1.481797
H	6.506527	-1.548613	2.269287
H	7.212567	-0.062216	1.609032
H	8.300450	-1.303161	-1.046582
H	7.428037	0.231647	-0.962884
H	6.858363	-1.050990	-2.046670

Sum of electronic and zero-point energies = -1084.55255836 Hartree

Table S10. Atom coordinates for the optimized geometry of compound **3** in ACN based on B3LYP method.

Atom	X	Y	Z
C	0.110892	3.229345	0.138035
C	-1.125878	2.643313	0.109884
O	-1.247756	1.230827	0.057866
C	-0.054651	0.485003	0.034670
C	1.176357	1.114552	0.068845
C	-1.997123	3.283565	0.155943
C	-0.083450	-0.591511	-0.056644
C	2.488753	0.479503	0.036452
C	3.650851	1.236613	-0.200328
C	2.627147	-0.908998	0.241514
C	4.901109	0.623542	-0.240542
C	3.578627	2.306051	-0.365504
C	3.880419	-1.504870	0.203342
C	1.761896	-1.529116	0.450735
C	5.052295	-0.759705	-0.041884
C	5.766380	1.246502	-0.434733
C	3.942298	-2.575112	0.373712
C	-2.560219	0.577383	0.021288
C	-2.732255	-0.740917	0.494643
C	-3.691651	1.243685	-0.486074
C	-3.980078	-1.349717	0.466329
C	-1.895966	-1.284715	0.922795
C	-4.935754	0.617120	-0.524971
C	-3.604168	2.247558	-0.889692
C	-5.117069	-0.691706	-0.046005
C	-4.066283	-2.358344	0.858281
C	-5.770469	1.168727	-0.941443
H	1.221659	2.463397	0.120003

H	0.411133	4.685058	0.205730
H	1.009576	4.988928	-0.660878
H	-0.513351	5.264624	0.222112
H	0.992505	4.910768	1.107126
H	-6.478186	-1.404838	-0.059078
H	6.416699	-1.464817	-0.082535
H	6.401955	-2.538032	-1.199861
H	7.371662	-3.048848	-1.237519
H	5.631204	-3.297544	-1.030477
H	6.219624	-2.081969	-2.180172
H	6.678627	-2.148652	1.282897
H	7.648967	-2.659214	1.262949
H	6.698785	-1.411149	2.094020
H	5.913525	-2.894954	1.521584
H	7.575320	-0.488960	-0.365384
H	7.465029	0.007886	-1.336423
H	7.661643	0.282062	0.409299
H	8.519904	-1.044018	-0.384499
H	-6.368435	-2.702678	-0.897874
H	-5.626203	-3.395567	-0.487628
H	-7.335677	-3.219244	-0.911206
H	-6.088265	-2.478324	-1.933915
H	-6.876492	-1.766125	1.394170
H	-6.962358	-0.865620	2.013832
H	-7.847764	-2.275455	1.398246
H	-6.147461	-2.434086	1.865266
H	-7.594169	-0.531126	-0.663854
H	-7.747586	0.392062	-0.092784
H	-7.384837	-0.261837	-1.705822
H	-8.537729	-1.088082	-0.650222

Sum of electronic and zero-point energies = -1084.55765955 Hartree

Table S11. Atom coordinates for the optimized geometry of compound **4** in DCM based on B3LYP method.

Atom	X	Y	Z
C	-0.031120	2.870830	-0.130319
C	1.176586	2.233815	-0.123517
O	1.242089	0.812334	-0.075202
C	0.016391	0.122542	-0.030859
C	-1.189838	0.802922	-0.043956
C	2.071963	2.838177	-0.185832
C	-0.000825	-0.954087	0.059142
C	-2.523876	0.229210	0.005949
C	-3.661154	1.054546	0.179778
C	-2.723395	-1.160449	-0.120625
C	-4.930971	0.510290	0.232121
C	-3.541403	2.127153	0.281496
C	-3.996081	-1.716492	-0.071374
C	-1.883532	-1.828986	-0.275561
C	-5.113891	-0.881862	0.108503
C	-5.802262	1.142378	0.371693
C	-4.108979	-2.788387	-0.178745
C	2.521465	0.107166	-0.065303
C	2.621813	-1.241194	-0.488736
O	3.702594	0.745108	0.367930
C	3.833567	-1.906792	-0.482909
O	1.748664	-1.765396	-0.863106
C	4.925004	0.082834	0.394279
H	3.672486	1.768083	0.728289
H	5.000196	-1.253328	-0.036837
H	3.907235	-2.933519	-0.827398
H	5.803087	0.605745	0.753694

H	-1.178181	2.155463	-0.093596
H	-0.270254	4.338992	-0.191909
H	-0.842336	4.667671	0.683504
H	0.677730	4.879134	-0.220826
H	-0.853932	4.592373	-1.084493
H	6.132680	-1.987322	-0.062261
H	-6.389789	-1.316681	0.172737
H	7.367031	-1.391122	0.364182
H	7.309441	-1.088602	1.415078
H	8.120314	-2.169501	0.245029
H	7.619655	-0.530638	-0.264211
H	-6.660534	-2.722117	0.061715
H	-7.742923	-2.815475	0.146353
H	-6.330048	-3.105535	-0.909320
H	-6.175760	-3.275659	0.872689

Sum of electronic and zero-point energies = -999.097283675 Hartree

Table S12. Atom coordinates for the optimized geometry of compound **4** in ACN based on B3LYP method.

Atom	X	Y	Z
C	-0.031223	2.870419	-0.132851
C	1.176776	2.233178	-0.125855
O	1.241599	0.812434	-0.076070
C	0.016246	0.122088	-0.030660
C	-1.189285	0.802980	-0.044461
C	2.072189	2.837393	-0.188435
C	-0.000993	-0.954438	0.060425
C	-2.524014	0.229358	0.006180
C	-3.660132	1.054434	0.186211
C	-2.724011	-1.159441	-0.125867
C	-4.930298	0.510164	0.239368
C	-3.539538	2.126529	0.292356

C	-3.997054	-1.715338	-0.075900
C	-1.884706	-1.827381	-0.285933
C	-5.113771	-0.881172	0.110302
C	-5.800678	1.142482	0.383923
C	-4.110273	-2.786714	-0.187746
C	2.521415	0.106733	-0.065514
C	2.621790	-1.240799	-0.490562
O	3.701721	0.744252	0.369763
C	3.833961	-1.906419	-0.484359
O	1.748861	-1.764628	-0.865854
C	4.924365	0.081866	0.396308
H	3.671220	1.766878	0.730930
H	4.999816	-1.253442	-0.036480
H	3.907224	-2.932859	-0.829948
H	5.801947	0.604661	0.757047
H	-1.177701	2.154932	-0.095411
H	-0.270161	4.338371	-0.195048
H	-0.839225	4.667507	0.682139
H	0.677949	4.877953	-0.227568
H	-0.856891	4.590606	-1.085884
H	6.133650	-1.987552	-0.061676
H	-6.390590	-1.316705	0.175916
H	7.366516	-1.389713	0.367052
H	7.307114	-1.088125	1.418079
H	8.121469	-2.166583	0.248174
H	7.618541	-0.528021	-0.259862
H	-6.659668	-2.722164	0.059701
H	-7.741742	-2.817652	0.146553
H	-6.330849	-3.101246	-0.913553
H	-6.172012	-3.278498	0.866972

Sum of electronic and zero-point energies = -999.102591885 Hartree

Table S13. Atom coordinates for the optimized geometry of compound **5** in DCM based on B3LYP method.

Atom	X	Y	Z
C	0.113252	2.854160	0.162413
C	-1.126942	2.271680	0.132275
O	-1.251041	0.862288	0.063940
C	-0.062719	0.109742	0.026945
C	1.169533	0.735851	0.063221
C	-1.996853	2.913061	0.191023
C	-0.098735	-0.965310	-0.080114
C	2.482782	0.098777	0.017356
C	3.641586	0.867067	-0.215519
C	2.612872	-1.291812	0.206577
C	4.893545	0.263970	-0.268029
C	3.565413	1.937699	-0.366843
C	3.861802	-1.900995	0.159012
C	1.746622	-1.910986	0.411274
C	4.994255	-1.117430	-0.080677
C	5.780868	0.858799	-0.455104
C	3.955521	-2.970491	0.311995
C	-2.567993	0.212860	0.022719
C	-2.746532	-1.089088	0.533442
Cl	-3.681875	0.878755	-0.528000
Cl	-3.993535	-1.705043	0.504195
H	-1.918665	-1.618986	0.993157
H	-4.929794	0.265591	-0.578229
H	-3.575514	1.870061	-0.956159
H	-5.076367	-1.022538	-0.056770
H	-4.124575	-2.699838	0.916001
H	-5.776654	0.779284	-1.020195

H	1.218777	2.082558	0.129993
H	0.419457	4.307137	0.245883
H	1.010429	4.619596	-0.622893
H	-0.502408	4.890053	0.278933
H	1.011071	4.518755	1.144001
H	6.567520	-1.880248	-0.144302
H	-6.646369	-1.795517	-0.105670

Sum of electronic and zero-point energies = -1689.22105919 Hartree

Table S14. Atom coordinates for the optimized geometry of compound **5** in ACN based on B3LYP method.

Atom	X	Y	Z
C	0.113740	2.853584	0.164476
C	-1.126983	2.271163	0.133952
O	-1.250527	0.862627	0.064410
C	-0.062797	0.109211	0.026805
C	1.168801	0.735678	0.063754
C	-1.996746	2.912668	0.192780
C	-0.098961	-0.965763	-0.080732
C	2.482747	0.098518	0.017603
C	3.640327	0.866505	-0.220580
C	2.613226	-1.291015	0.211748
C	4.892689	0.263626	-0.273549
C	3.563217	1.936503	-0.375784
C	3.862486	-1.900205	0.163797
C	1.747472	-1.909361	0.420692
C	4.993397	-1.116747	-0.081255
C	5.779180	0.858361	-0.464753
C	3.956409	-2.969108	0.320653
C	-2.568087	0.212867	0.022556
C	-2.747213	-1.087365	0.536582
Cl	-3.680387	0.877616	-0.531930

Cl	-3.994509	-1.703428	0.506943
H	-1.919929	-1.616263	0.998349
H	-4.928697	0.264621	-0.582354
H	-3.572912	1.867898	-0.962034
H	-5.075544	-1.021725	-0.057515
H	-4.125863	-2.697242	0.920976
H	-5.774558	0.777738	-1.026867
H	1.218380	2.081711	0.131553
H	0.420051	4.306241	0.248655
H	1.010676	4.618554	-0.620351
H	-0.501851	4.888911	0.282487
H	1.012220	4.516698	1.146625
H	6.568638	-1.880175	-0.145534
H	-6.647562	-1.795349	-0.106763

Sum of electronic and zero-point energies = -1689.22719988 Hartree

Table S15. Atom coordinates for the optimized geometry of compound **6** in DCM based on B3LYP method.

Atom	X	Y	Z
C	0.113239	2.854085	0.162284
C	-1.126948	2.271604	0.132137
O	-1.251050	0.862207	0.063833
C	-0.062720	0.109670	0.026839
C	1.169540	0.735785	0.063035
C	-1.996862	2.912984	0.190861
C	-0.098750	-0.965389	-0.080133
C	2.482806	0.098731	0.017251
C	3.641686	0.867162	-0.214802
C	2.612859	-1.291967	0.205700
C	4.893677	0.264121	-0.267212
C	3.565561	1.937880	-0.365521
C	3.861816	-1.901099	0.158252

C	1.746564	-1.911295	0.409727
C	4.994335	-1.117382	-0.080617
C	5.781057	0.859074	-0.453608
C	3.955500	-2.970680	0.310653
C	-2.568010	0.212806	0.022680
C	-2.746576	-1.089144	0.533406
F	-3.681908	0.878757	-0.527939
F	-3.993606	-1.705054	0.504222
H	-1.918714	-1.619078	0.993084
H	-4.929850	0.265642	-0.578107
H	-3.575536	1.870072	-0.956082
H	-5.076442	-1.022491	-0.056663
H	-4.124664	-2.699845	0.916029
H	-5.776720	0.779376	-1.020004
H	1.218768	2.082489	0.129834
H	0.419439	4.307065	0.245693
H	1.010333	4.619520	-0.623139
H	-0.502430	4.889973	0.278804
H	1.011126	4.518713	1.143756
H	6.567642	-1.880147	-0.144121
H	-6.646485	-1.795395	-0.105470

Sum of electronic and zero-point energies = -1689.22105920 Hartree

Table S16. Atom coordinates for the optimized geometry of compound **6** in ACN based on B3LYP method.

Atom	X	Y	Z
C	0.114942	2.628401	0.179585
C	-1.126452	2.049399	0.143108
O	-1.253849	0.641212	0.057411
C	-0.067366	-0.113449	0.009373
C	1.166158	0.509474	0.052875

C	-1.994496	2.692301	0.210822
C	-0.105541	-1.186789	-0.112391
C	2.478090	-0.129712	-0.002339
C	3.636514	0.640025	-0.238764
C	2.604440	-1.522366	0.181586
C	4.888059	0.036513	-0.300128
C	3.558186	1.711000	-0.385473
C	3.851469	-2.135177	0.124930
C	1.736502	-2.137961	0.388890
C	4.967615	-1.340387	-0.117130
C	5.785876	0.615272	-0.488659
C	3.962451	-3.204118	0.271406
C	-2.572260	-0.004800	0.009702
C	-2.750601	-1.313614	0.505720
F	-3.685071	0.672458	-0.532028
F	-3.998323	-1.928365	0.470788
H	-1.921454	-1.848404	0.956839
H	-4.935167	0.063845	-0.588456
H	-3.574535	1.668725	-0.946766
H	-5.064087	-1.224857	-0.080980
H	-4.148647	-2.927305	0.866059
H	-5.792391	0.570121	-1.019220
H	1.218768	1.854798	0.137075
H	0.424865	4.079440	0.280802
H	1.014748	4.401055	-0.585327
H	-0.495637	4.663840	0.323092
H	1.018830	4.277981	1.180284
H	-6.281136	-1.820691	-0.124925
H	6.184702	-1.932904	-0.174241

Sum of electronic and zero-point energies = -968.521466297 Hartree

Table S17. Atom coordinates for the optimized geometry of compound **7** in DCM based on B3LYP method.

Atom	X	Y	Z
C	0.118658	3.193569	0.166044
C	-1.124908	2.610631	0.143812
O	-1.246862	1.204588	0.087114
C	-0.061592	0.446697	0.053592
C	1.169083	1.073524	0.079922
C	-1.995859	3.251397	0.197805
C	-0.101162	-0.629536	-0.042457
C	2.485855	0.433812	0.032033
C	3.635055	1.194298	-0.256186
C	2.615519	-0.947628	0.270958
C	4.884146	0.584002	-0.313852
C	3.553196	2.257755	-0.44812
C	3.865095	-1.555622	0.215809
C	1.752394	-1.555229	0.518054
C	4.998752	-0.790499	-0.080503
C	5.761393	1.177544	-0.546857
C	3.95255	-2.620229	0.404074
C	-2.568012	0.552895	0.051873
C	-2.75599	-0.716955	0.632309
F	-3.661562	1.190568	-0.562213
C	-4.00489	-1.327951	0.604492
F	-1.938149	-1.217395	1.140184
F	-4.908933	0.572401	-0.606938
F	-3.538827	2.157497	-1.038741
C	-5.08054	-0.684202	-0.019417
F	-4.140341	-2.297614	1.072365
F	-5.738771	1.069419	-1.096758
H	1.21913	2.418678	0.135474

H	0.426101	4.64602	0.236582
H	1.015904	4.949775	-0.636066
H	-0.495047	5.229961	0.26683
H	1.020246	4.863633	1.131631
H	-6.41514	-1.383738	-0.080559
H	6.35679	-1.446973	-0.098543
H	6.299427	-2.731518	-0.526486
H	7.23312	-0.797313	-0.900777
H	6.914462	-1.476344	1.143486
H	-6.413739	-2.384073	-1.004378
H	-6.741215	-1.95928	1.104759
H	-7.427645	-0.549587	-0.41035

Sum of electronic and zero-point energies = -1444.14561897 Hartree

Table S18. Atom coordinates for the optimized geometry of compound **7** in ACN based on B3LYP method.

Atom	X	Y	Z
C	0.119138	3.192843	0.167083
C	-1.124905	2.609990	0.144585
O	-1.246384	1.204691	0.087205
C	-0.061675	0.445986	0.053466
C	1.168374	1.073176	0.080242
C	-1.995630	3.250988	0.198369
C	-0.101356	-0.630207	-0.042356
C	2.485749	0.433386	0.032337
C	3.634116	1.193881	-0.258185
C	2.615849	-0.947339	0.273611
C	4.883518	0.584032	-0.315988
C	3.551451	2.256950	-0.451771
C	3.865621	-1.555160	0.218260
C	1.753042	-1.554564	0.522408
C	4.998741	-0.790126	-0.080556

C	5.759982	1.178059	-0.550622
C	3.952909	-2.619424	0.408483
C	-2.568057	0.552790	0.051568
C	-2.756584	-0.715742	0.634159
F	-3.660497	1.189596	-0.564880
C	-4.005616	-1.326704	0.606195
F	-1.939096	-1.215667	1.142952
F	-4.908156	0.571828	-0.609514
F	-3.536917	2.155831	-1.042427
C	-5.080592	-0.683688	-0.019732
F	-4.140919	-2.295715	1.075446
F	-5.737019	1.068780	-1.101005
H	1.218830	2.417709	0.136249
H	0.426794	4.644987	0.237970
H	1.016803	4.948155	-0.634667
H	-0.494342	5.228799	0.268250
H	1.020948	4.861657	1.133181
H	-6.414515	-1.382486	-0.080700
H	6.356052	-1.445907	-0.099016
H	6.300663	-2.731432	-0.526557
H	7.233758	-0.797223	-0.901724
H	6.916948	-1.476214	1.142583
H	-6.415269	-2.385714	-1.002760
H	-6.743666	-1.957028	1.105155
H	-7.428249	-0.549669	-0.412797

Sum of electronic and zero-point energies = -1444.15263283 Hartree

Table S19. Atom coordinates for the optimized geometry of compound **1** in DCM based on CAM-B3LYP method.

Atom	X	Y	Z
C	-0.119246	2.383562	-0.210701
C	1.120929	.815230	-0.164894

C	1.250496	.416540	-0.050305
C	0.074269	0.341440	0.015721
C	-1.154112	0.275353	-0.039639
H	1.987574	.457753	-0.244726
H	0.117435	1.411480	0.159065
C	-2.464395	0.368622	0.030298
C	-3.610514	0.392318	0.300909
C	-2.584841	1.750531	-0.172190
C	-4.851817	0.223820	0.376732
H	-3.527573	1.460852	0.462081
C	-3.829923	2.358740	-0.098697
H	-1.715838	2.354521	-0.407505
C	-4.964447	1.598376	0.177977
H	-5.733435	0.370189	0.593852
H	-3.915249	3.427712	-0.263285
H	-5.936830	2.077092	0.236417
C	2.571832	0.223058	0.009296
C	2.758097	1.518109	-0.495427
C	3.664074	0.453476	0.571064
C	4.009338	2.117667	-0.445190
H	1.933682	2.048618	-0.960189
C	4.909881	0.156258	0.634709
H	3.537110	1.445897	0.990469
C	5.086031	1.440359	0.123513
H	4.144902	3.113822	-0.853559
H	5.743928	0.370891	1.086268
H	6.062227	1.912932	0.167678
O	-1.210422	1.608339	-0.150857
C	-0.437696	3.826726	-0.338205
H	-1.023598	4.158974	0.524481
H	0.477586	4.415754	-0.396659
H	-1.036282	4.001794	-1.237357

Sum of electronic and zero-point energies = -769.593134008 Hartree

Table S20. Atom coordinates for the optimized geometry of compound **1** in ACN based on CAM-B3LYP method.

Atom	X	Y	Z
C	-0.119740	2.383153	-0.211944
C	1.120895	1.814950	-0.165688
C	1.250163	0.416979	-0.050395
C	0.074367	-0.341735	0.015985
C	-1.153483	0.275211	-0.039932
H	1.987237	2.457835	-0.245339
H	0.117621	-1.411753	0.159327
C	-2.464306	-0.368807	0.030282
C	-3.609573	0.391996	0.304116
C	-2.585336	-1.750049	-0.175073
C	-4.851168	-0.223896	0.380239
H	-3.525703	1.460126	0.467534
C	-3.830706	-2.358063	-0.101175
H	-1.716651	-2.353530	-0.412710
C	-4.964698	-1.598017	0.178645
H	-5.732181	0.370152	0.599857
H	-3.916358	-3.426699	-0.267946
H	-5.937209	-2.076525	0.237350
C	2.571959	-0.222889	0.009625
C	2.758427	-1.517410	-0.495978
C	3.663651	0.453276	0.572539
C	4.009810	-2.117061	-0.445427
H	1.934033	-2.047749	-0.960880
C	4.909667	-0.156405	0.636202
H	3.536251	1.445569	0.992003
C	5.086312	-1.440169	0.124207
H	4.145298	-3.113086	-0.854220
H	5.743395	0.370800	1.088365

H	6.062559	-1.912725	0.168515
O	-1.210223	1.607736	-0.151923
C	-0.438293	3.826041	-0.339867
H	-1.024060	4.157940	0.522992
H	0.477018	4.414868	-0.398691
H	-1.037153	4.000241	-1.238948

Sum of electronic and zero-point energies = -769.598724972 Hartree

Table S21. Atom coordinates for the optimized geometry of compound **2** in DCM based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.114378	2.638258	0.172160
C	-1.121958	2.065063	0.139905
O	-1.248004	0.661251	0.057750
C	-0.067425	-0.091119	0.010155
C	1.159995	0.530815	0.051064
C	-1.990132	2.706829	0.205584
C	-0.105559	-1.164349	-0.106561
C	2.469996	-0.107884	-0.001437
C	3.623117	0.653392	-0.236608
C	2.598794	-1.493080	0.178533
C	4.865150	0.040139	-0.297616
C	3.546791	1.724407	-0.384408
C	3.845626	-2.092626	0.119003
C	1.730880	-2.110282	0.381598
C	5.001398	-1.339845	-0.119716
C	5.746317	0.644639	-0.490951
C	3.925792	-3.166032	0.263839
C	-2.564029	0.017290	0.013423
C	-2.744049	-1.285325	0.503763
C	-3.674394	0.688870	-0.517078

C	-3.992027	-1.886078	0.468561
H	-1.914280	-1.822650	0.950959
H	-4.916338	0.072818	-0.563516
H	-3.568498	1.687704	-0.927075
H	-5.099704	-1.222608	-0.071386
H	-4.112025	-2.887288	0.872454
H	-5.759212	0.607789	-0.991138
H	1.210973	1.867331	0.130665
H	0.427205	4.085651	0.266392
H	1.011292	4.400900	-0.603854
H	-0.490510	4.672160	0.311665
H	1.025183	4.284129	1.161095
H	-6.442561	-1.896116	-0.136541
H	-6.485375	-2.585038	-0.988252
H	-6.636275	-2.482808	0.766039
H	-7.249110	-1.168607	-0.257382
H	6.352064	-1.998856	-0.158713
H	6.719546	-2.179397	0.858271
H	6.306779	-2.967514	-0.664676
H	7.087201	-1.373307	-0.671110

Sum of electronic and zero-point energies = -848.183055662 Hartree

Table S22. Atom coordinates for the optimized geometry of compound **2** in ACN based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.114472	2.665427	0.161471
C	-1.131270	2.080333	0.130083
O	-1.262900	0.663983	0.054588
C	-0.067552	0.088116	0.010792
C	1.174952	0.535682	0.048660
C	-2.005512	2.730151	0.195449
C	-0.102658	1.171586	-0.104944

C	2.484590	0.104523	-0.002827
C	3.656201	0.661472	0.224575
C	2.613245	-1.506078	0.166601
C	4.905185	0.040455	-0.282525
C	3.583304	1.742887	-0.366997
C	3.868791	-2.112109	0.110148
C	1.735705	-2.129084	0.360847
C	5.040747	-1.355270	-0.114648
C	5.796771	0.649524	-0.467173
C	3.945089	-3.196259	0.247255
C	-2.579019	0.017786	0.012780
C	-2.753042	-1.314656	0.467635
C	-3.714962	0.708340	-0.478945
C	-4.009534	-1.920895	0.435824
H	-1.909041	-1.867734	0.891394
H	-4.964810	0.086255	-0.522833
H	-3.618077	1.727012	-0.866671
H	-5.140666	-1.238101	-0.066158
H	-4.121467	-2.942699	0.814996
H	-5.823577	0.636776	-0.922215
H	1.233628	1.894721	0.124062
H	0.420648	4.118469	0.252703
H	1.015821	4.441731	-0.619468
H	-0.507851	4.705485	0.289580
H	1.017646	4.330987	1.156878
H	-6.486096	-1.913087	-0.129572
H	-6.544605	-2.577121	-1.012676
H	-6.663013	-2.543428	0.758327
H	-7.305082	-1.180287	-0.211591
H	6.394313	-2.015546	-0.147315

H	6.791616	-2.131609	0.878942
H	6.342000	-3.024553	-0.589418
H	7.124146	-1.416894	-0.716329

Sum of electronic and zero-point energies = -847.583469052 Hartree

Table S23. Atom coordinates for the optimized geometry of compound **3** in DCM based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.112593	3.203850	0.107223
C	-1.121831	2.626467	0.084954
O	-1.242185	1.220535	0.041727
C	-0.059379	0.471081	0.020868
C	1.166694	1.097159	0.042499
C	-1.992514	3.266511	0.130738
C	-0.096762	0.606065	-0.045562
C	2.480392	0.463908	0.013685
C	3.644605	1.239365	-0.021224
C	2.609476	-0.933233	0.022229
C	4.894732	0.636008	-0.047243
C	3.578353	2.320983	-0.030314
C	3.861295	-1.520670	-0.003351
C	1.736574	-1.575076	0.052418
C	5.037155	-0.754927	-0.038548
C	5.768274	1.275129	-0.075214
C	3.919384	-2.603731	0.005840
C	-2.556207	0.571101	0.017381
C	-2.735215	-0.718932	0.540086
C	-3.669345	1.219641	-0.528792
C	-3.980811	-1.321645	0.520333
C	-1.905413	-1.246165	0.999125
C	-4.911604	0.598647	-0.559084
C	-3.570166	2.206420	-0.968902
C	-5.101378	-0.682519	-0.032069
C	-4.078636	-2.312563	0.950860
C	-5.739198	1.134340	-1.007286

H	1.211288	2.435547	0.085817
H	0.420871	4.654014	0.167268
H	1.017479	4.947631	-0.701916
H	-0.498791	5.238976	0.183384
H	1.004511	4.877838	1.065567
H	-6.459038	-1.389493	-0.035079
H	6.399809	-1.450727	-0.064249
H	6.487413	-2.347465	-1.314044
H	7.458703	-2.852783	-1.341411
H	5.710643	-3.117712	-1.320837
H	6.386632	-1.755547	-2.229988
H	6.548683	-2.318677	1.200052
H	7.521460	-2.821840	1.192656
H	6.490082	-1.706425	2.106255
H	5.775056	-3.089718	1.261213
H	7.563942	-0.452936	-0.103722
H	7.533580	0.177487	-0.998620
H	7.576562	0.197310	0.777331
H	8.510154	-1.002700	-0.120464
H	-6.342084	-2.712453	-0.815797
H	-5.608630	-3.389445	-0.368040
H	-7.309053	-3.226704	-0.822653
H	-6.046618	-2.530778	-1.854628
H	-6.876181	-1.688840	1.417700
H	-6.966445	-0.765054	1.999029
H	-7.848158	-2.193681	1.429281
H	-6.157246	-2.339300	1.924570
H	-7.557383	-0.540632	-0.686876
H	-7.715651	0.403524	-0.155230
H	-7.332648	-0.313966	-1.734406
H	-8.501932	-1.093042	-0.664893

Sum of electronic and zero-point energies = -1083.91577040 Hartree

Table S24. Atom coordinates for the optimized geometry of compound **3** in ACN based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.110867	3.229405	0.138236
C	-1.125881	2.643355	0.110052
O	-1.247743	1.230854	0.057926
C	-0.054618	0.485071	0.034672
C	1.176380	1.114633	0.068919
C	-1.997153	3.283565	0.156167
C	-0.083360	0.591437	-0.056787
C	2.488745	0.479589	0.036479
C	3.650764	1.236527	-0.201257
C	2.627194	-0.908777	0.242451
C	4.900995	0.623415	-0.241519
C	3.578469	2.305848	-0.367174
C	3.880444	-1.504684	0.204240
C	1.761988	-1.528691	0.452483
C	5.052237	-0.759699	-0.041947
C	5.766207	1.246216	-0.436477
C	3.942419	-2.574801	0.375364
C	-2.560179	0.577399	0.021299
C	-2.732205	-0.740917	0.494628
C	-3.691615	1.243690	-0.486085
C	-3.980014	-1.349732	0.466284
C	-1.895901	-1.284690	0.922783
C	-4.935701	0.617108	-0.525020
C	-3.604119	2.247566	-0.889693
C	-5.117007	-0.691727	-0.046060
C	-4.066232	-2.358370	0.858210
C	-5.770426	1.168686	-0.941511
H	1.221667	2.463494	0.120183

H	0.411060	4.685122	0.206015
H	1.009381	4.989092	-0.660644
H	-0.513443	5.264657	0.222554
H	0.992536	4.910790	1.107354
H	-6.478101	-1.404892	-0.059180
H	6.416604	-1.464874	-0.082601
H	6.401333	-2.539030	-1.199005
H	7.370991	-3.049945	-1.236624
H	5.630594	-3.298344	-1.028666
H	6.218638	-2.083779	-2.179626
H	6.679092	-2.147558	1.283297
H	7.649429	-2.658128	1.263392
H	6.699565	-1.409377	2.093795
H	5.914094	-2.893669	1.522923
H	7.575137	-0.489291	-0.366774
H	7.464551	0.006608	-1.338264
H	7.661726	0.282484	0.407130
H	8.519718	-1.044369	-0.385657
H	-6.368306	-2.702638	-0.898110
H	-5.626045	-3.395543	-0.487940
H	-7.335527	-3.219244	-0.911493
H	-6.088148	-2.478166	-1.934128
H	-6.876356	-1.766356	1.394036
H	-6.962248	-0.865923	2.013800
H	-7.847606	-2.275731	1.398079
H	-6.147290	-2.434340	1.865047
H	-7.594132	-0.531157	-0.663835
H	-7.747657	0.391910	-0.092597
H	-7.384792	-0.261655	-1.705747
H	-8.537651	-1.088190	-0.650348

Sum of electronic and zero-point energies = -1084.55765958 Hartree

Table S25. Atom coordinates for the optimized geometry of compound **4** in DCM based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.001402	0.027048	0.000810
C	0.003048	0.021065	1.361118
O	1.228234	0.002808	2.070721
C	2.405908	-0.009984	1.312731
C	2.357459	0.002989	0.064475
C	-0.947259	0.058567	1.875839
C	3.368481	-0.076936	1.797668
C	3.484181	-0.017305	-0.982211
C	3.282697	-0.228802	-2.359765
C	4.792801	0.174612	-0.520853
C	4.349515	-0.254864	-3.231014
C	2.280975	-0.381342	-2.743748
C	5.872477	0.152768	-1.389517
C	4.988675	0.361045	0.528860
C	5.655640	-0.065671	-2.754636
C	4.199985	-0.423952	-4.291853
C	6.869159	0.311248	-0.998547
C	1.260187	-0.010762	3.531014
C	2.376107	0.477151	4.239230
O	0.181818	-0.513245	4.272038
C	2.404882	0.466692	5.616868
O	3.219818	0.903728	3.707824
C	0.204004	-0.545008	5.658362
H	-0.686201	-0.923670	3.767846
H	1.319597	-0.049130	6.340898
H	3.256838	0.859886	6.160964
H	-0.641807	-0.958719	6.192353

H	1.162819	0.020741	-0.674274
H	-1.183630	0.055480	-0.892571
H	-1.183730	-0.823070	-1.545229
H	-2.102915	0.064492	-0.306689
H	-1.154919	0.945478	-1.528705
H	1.440865	-0.024337	7.680989
H	6.631245	-0.108378	-3.679434
H	0.372310	-0.522482	8.483269
H	0.197417	-1.583844	8.282905
H	0.694578	-0.392661	9.515095
H	-0.544064	0.049237	8.308614
H	7.985507	0.069828	-3.269021
H	8.580239	-0.009147	-4.177497
H	8.128810	1.056998	-2.819603
H	8.283832	-0.711837	-2.564038

Sum of electronic and zero-point energies = -998.566799668 Hartree

Table S26. Atom coordinates for the optimized geometry of compound **4** in ACN based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.013755	0.026765	0.007308
C	0.010056	0.028891	1.368043
O	1.232070	0.017311	2.081641
C	2.413196	0.002739	1.329019
C	2.369430	0.007708	-0.047983
C	-0.942361	0.066822	1.878763
C	3.374018	0.058889	1.818114
C	3.500199	0.015441	-0.961830
C	3.304696	0.241402	-2.337592
C	4.805682	0.187926	-0.497375
C	4.375251	-0.270344	-3.204765
C	2.305144	-0.403087	-2.723522

C	5.888924	0.163292	-1.362000
C	4.996387	0.385691	0.551171
C	5.678252	-0.069633	-2.725356
C	4.229884	-0.450745	-4.264374
C	6.883123	0.330925	-0.968578
C	1.258514	0.011955	3.542845
C	2.369028	0.509506	4.252179
O	0.179826	-0.491793	4.282061
C	2.392128	0.507180	5.630363
O	3.213015	0.936455	3.721569
C	0.196479	-0.515137	5.668907
H	-0.684145	-0.909178	3.776718
H	1.306576	-0.009590	6.352712
H	3.240467	0.907649	6.174910
H	-0.649682	-0.929805	6.201575
H	1.177691	0.019188	-0.662506
H	-1.167699	0.046913	-0.890661
H	-1.162652	-0.835662	-1.537781
H	-2.089064	0.057229	-0.308197
H	-1.138178	0.933177	-1.531883
H	1.421803	0.023628	7.694413
H	6.658769	-0.116263	-3.646554
H	0.350994	-0.475376	8.493353
H	0.182120	-1.538560	8.297735
H	0.666480	-0.338464	9.526407
H	-0.567203	0.090666	8.310235
H	8.009993	0.072714	-3.230475
H	8.610310	-0.011857	-4.134816
H	8.145944	1.064667	-2.789494
H	8.308361	-0.700472	-2.516289

Sum of electronic and zero-point energies = -998.572275442 Hartree

Table S27. Atom coordinates for the optimized geometry of compound **5** in DCM based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.015395	0.070712	0.003869
C	0.010867	0.056813	1.369324
O	1.228590	0.012664	2.075872
C	2.414105	-0.016676	1.329898
C	2.368305	0.004761	-0.044482
C	-0.939687	0.107054	1.883394
C	3.371702	-0.105415	1.822412
C	3.504637	-0.033679	-0.962185
C	3.306934	-0.322001	-2.319302
C	4.802237	0.217394	-0.497212
C	4.382526	-0.369017	-3.192157
C	2.310726	-0.521045	-2.695967
C	5.881626	0.175779	-1.365299
C	4.984389	0.466993	0.541544
C	5.662492	-0.120053	-2.707112
C	4.229198	-0.599501	-4.240040
C	6.883619	0.376918	-1.004560
C	1.254661	-0.012960	3.544293
C	2.326321	0.552184	4.248982
Cl	0.207380	-0.603059	4.264819
Cl	2.351190	0.537223	5.635270
H	3.137189	1.041016	3.720015
H	0.230797	-0.638242	5.650848
H	-0.622576	-1.071270	3.747085
H	1.302852	-0.062930	6.325010
H	3.174494	0.990443	6.175324
H	-0.573978	-1.110435	6.202476

H	1.179753	0.047290	-0.658023
H	-1.163675	0.125079	-0.893874
H	-1.178910	-0.753732	-1.546034
H	-2.085021	0.154769	-0.312315
H	-1.110643	1.013861	-1.530092
H	7.015245	-0.176323	-3.800012
H	1.332653	-0.093554	8.065628

Sum of electronic and zero-point energies = -1688.78752667 Hartree

Table S28. Atom coordinates for the optimized geometry of compound **5** in ACN based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.016107	0.073329	0.003722
C	0.011315	0.058757	1.369654
O	1.228471	0.013005	2.075356
C	2.414545	-0.017106	1.330225
C	2.368164	0.005225	-0.043654
C	-0.939327	0.109153	1.883468
C	3.372021	-0.106467	1.822824
C	3.504798	-0.033829	-0.962047
C	3.306721	-0.326648	-2.317881
C	4.801688	0.221054	-0.498087
C	4.382157	-0.374385	-3.191292
C	2.310619	-0.528663	-2.693224
C	5.881108	0.178699	-1.366549
C	4.983364	0.474040	0.539882
C	5.661311	-0.121598	-2.706920
C	4.228421	-0.608365	-4.238333
C	6.882698	0.382738	-1.006349
C	1.254605	-0.013474	3.544476
C	2.324850	0.553796	4.249082
Cl	0.208651	-0.606381	4.264109

Cl	2.349710	0.538228	5.635637
H	3.134953	1.043915	3.720251
H	0.231702	-0.641959	5.650376
H	-0.620255	-1.075597	3.745721
H	1.302442	-0.064458	6.324156
H	3.172330	0.992799	6.175577
H	-0.572477	-1.115980	6.201291
H	1.180270	0.049246	-0.657321
H	-1.162659	0.128983	-0.893939
H	-1.178022	-0.749766	-1.546095
H	-2.083797	0.159353	-0.312223
H	-1.108196	1.017912	-1.529751
H	7.015150	-0.178849	-3.801366
H	1.331957	-0.095643	8.066624

Sum of electronic and zero-point energies = -1688.79382443 Hartree

Table S29. Atom coordinates for the optimized geometry of compound **6** in DCM based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.014255	0.054701	0.003614
C	0.009407	0.043777	1.368211
O	1.227721	0.009434	2.076613
C	2.412860	-0.014599	1.330056
C	2.367967	0.003788	-0.044825
C	-0.941867	0.089617	1.881246
C	3.370986	-0.098032	1.822348
C	3.504221	-0.029853	-0.961236
C	3.307620	-0.327163	-2.318159
C	4.800127	0.235480	-0.495044
C	4.382208	-0.369212	-3.192165
C	2.312288	-0.536406	-2.691342
C	5.881469	0.198957	-1.360626

C	4.976811	0.491898	0.542902
C	5.646888	-0.105183	-2.691933
C	4.250331	-0.604172	-4.242097
C	6.888501	0.408040	-1.018612
C	1.253363	-0.012065	3.544011
C	2.327506	0.554980	4.246508
F	0.203458	-0.599614	4.265825
F	2.354769	0.544616	5.632618
H	3.137449	1.041047	3.713883
H	0.224876	-0.631783	5.651795
H	-0.626082	-1.067589	3.747534
H	1.301483	-0.053990	6.304228
H	3.170108	0.993846	6.188050
H	-0.571453	-1.097088	6.221394
H	1.179156	0.037834	-0.659072
H	-1.164872	0.099378	-0.894985
H	-1.174574	-0.781274	-1.544775
H	-2.086694	0.124850	-0.313917
H	-1.117409	0.986729	-1.533608
H	1.324866	-0.074127	7.652032
H	6.694856	-0.142880	-3.537599

Sum of electronic and zero-point energies = -968.042071581 Hartree

Table S30. Atom coordinates for the optimized geometry of compound **6** in ACN based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.014790	0.057230	0.003398
C	0.009666	0.045629	1.368427
O	1.227456	0.009832	2.076062
C	2.413122	0.014866	1.330322
C	2.367698	0.004416	-0.044089

C	-0.941713	0.091534	1.881187
C	3.371149	0.098854	1.822674
C	3.504284	0.029832	-0.961082
C	3.307527	0.331749	-2.316689
C	4.799421	0.239358	-0.495886
C	4.382118	-0.374583	-3.191085
C	2.312377	-0.544019	-2.688641
C	5.880829	0.202033	-1.361830
C	4.975549	0.499265	0.541240
C	5.646014	-0.106688	-2.691706
C	4.249818	-0.613143	-4.240157
C	6.887366	0.414058	-1.020164
C	1.253229	-0.012521	3.544124
C	2.326221	0.556202	4.246487
F	0.204541	-0.602497	4.265202
F	2.353546	0.545131	5.632878
H	3.135528	1.043313	3.713955
H	0.225862	-0.635135	5.651431
H	-0.624212	-1.071185	3.746411
H	1.301340	-0.055642	6.303601
H	3.168522	0.995411	6.188003
H	-0.570054	-1.102064	6.220292
H	1.179523	0.039856	-0.658491
H	-1.164044	0.103036	-0.895166
H	-1.173814	-0.777620	-1.544870
H	-2.085681	0.129172	-0.313962
H	-1.115232	0.990480	-1.533476
H	1.324720	-0.076397	7.653166
H	6.695133	-0.145219	-3.538689

Sum of electronic and zero-point energies = -968.048355968 Hartree

Table S31. Atom coordinates for the optimized geometry of compound **7** in DCM based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.119773	3.173837	0.176813
C	-1.120569	2.596459	0.153147
O	-1.239414	1.198100	0.089142
C	-0.061886	0.439148	0.050721
C	1.160387	1.065671	0.080641
C	-1.991390	3.236200	0.209211
C	-0.102465	-0.636096	-0.050050
C	2.478311	0.426973	0.031397
C	3.613050	1.182473	-0.286300
C	2.609410	-0.940998	0.298416
C	4.859025	0.576245	-0.344927
C	3.523733	2.240713	-0.499952
C	3.855502	-1.545332	0.242485
C	1.749308	-1.542252	0.568244
C	4.976743	-0.785566	-0.081887
C	5.732841	1.163978	-0.601599
C	3.950381	-2.604697	0.452297
C	-2.560589	0.547703	0.051562
C	-2.750667	-0.705395	0.648644
F	-3.639145	1.176023	-0.580315
C	-3.995718	-1.313442	0.619295
F	-1.936242	-1.197744	1.168593
F	-4.882898	0.561062	-0.625839
F	-3.509114	2.135946	-1.067630
C	-5.058129	-0.679770	-0.022195
F	-4.138674	-2.275040	1.100046
F	-5.709093	1.049972	-1.128577
H	1.210302	2.400316	0.142199

H	0.430516	4.621125	0.252077
H	1.016194	4.923894	-0.621520
H	-0.487575	5.207224	0.288557
H	1.027647	4.830257	1.144996
H	-6.389189	-1.375060	-0.084103
H	6.331455	-1.437390	-0.100280
H	6.271935	-2.720607	-0.506701
H	7.194136	-0.800806	-0.914516
H	6.894730	-1.447551	1.129735
H	-6.389241	-2.369081	-1.001841
H	-6.714823	-1.945180	1.094448
H	-7.392709	-0.541896	-0.413477

Sum of electronic and zero-point energies = -1443.55949260 Hartree

Table S32. Atom coordinates for the optimized geometry of compound **7** in ACN based on CAM-B3LYP method.

Atom	X	Y	Z
C	0.022048	0.054442	0.004982
C	0.015819	0.043512	1.373719
O	1.230685	0.010856	2.076843
C	2.420232	0.010367	1.336091
C	2.373346	0.005699	-0.036363
C	-0.935178	0.084564	1.888048
C	3.377397	0.086212	1.832014
C	3.513768	0.028975	-0.956686
C	3.319999	0.364774	-2.301527
C	4.801098	0.270085	-0.495684
C	4.400071	-0.409618	-3.170417
C	2.329105	-0.603134	-2.668622
C	5.879676	0.227761	-1.365314
C	4.972764	0.553971	0.535765
C	5.676602	-0.114846	-2.699888

C	4.245192	-0.680222	-4.208512
C	6.873654	0.462450	-1.001746
C	1.256764	-0.012140	3.550070
C	2.295706	0.614943	4.249893
F	0.242972	-0.659868	4.263850
C	2.315764	0.599357	5.635637
F	3.076887	1.146416	3.717744
F	0.269760	-0.691229	5.651525
F	-0.559055	-1.169501	3.741647
C	1.303909	-0.057833	6.332903
F	3.114386	1.102842	6.169428
F	-0.513798	-1.206194	6.194838
H	1.186800	0.037406	-0.650909
H	-1.155806	0.097202	-0.893339
H	-1.160770	-0.782202	-1.544751
H	-2.077694	0.118914	-0.312639
H	-1.108818	0.986164	-1.529777
H	1.366662	-0.103655	7.833047
H	6.842629	-0.118637	-3.647693
H	7.988672	-0.492407	-3.044508
H	6.653506	-0.949673	-4.690631
H	7.066279	1.110340	-4.169508
H	2.287051	-0.995928	8.268286
H	1.716103	1.088355	8.361213
H	0.193480	-0.455134	8.390926

Sum of electronic and zero-point energies = -1443.56658858 Hartree

Table S33. Atom coordinates for the optimized geometry of compound **1** in DCM based on BPE0 method.

Atom	X	Y	Z
C	-0.119067	2.409397	-0.198299
C	1.130633	1.829197	-0.153764

C	1.265188	0.417554	-0.049229
C	0.074780	0.340921	0.009890
C	-1.168905	0.278100	-0.040745
H	2.003841	2.479302	-0.231735
H	0.115852	1.421434	0.150271
C	-2.478824	-0.367442	0.028231
C	-3.644552	0.399189	0.277365
C	-2.597148	-1.767690	-0.154401
C	-4.893252	-0.225624	0.351236
H	-3.566627	1.479381	0.425548
C	-3.850881	-2.382423	-0.082710
H	-1.717619	-2.378637	-0.375493
C	-5.001205	-1.615835	0.172568
H	-5.786225	0.373985	0.552637
H	-3.931285	-3.463314	-0.232630
H	-5.980650	-2.101184	0.230286
C	2.586623	-0.224453	0.007564
C	2.768258	-1.545353	-0.473594
C	3.701743	0.467218	0.543256
C	4.028496	-2.150296	-0.425867
H	1.931213	-2.087205	-0.924629
C	4.955825	-0.149485	0.605100
H	3.581067	1.475648	0.950544
C	5.124171	-1.457035	0.117409
H	4.158113	-3.163601	-0.818421
H	5.803713	0.389618	1.038780
H	6.108078	-1.935063	0.159783
O	-1.232262	1.633167	-0.144971
C	-0.431477	3.858200	-0.319711
H	-1.026724	4.196641	0.546669
H	0.494281	4.448310	-0.370753
H	-1.031373	4.048427	-1.226890

Sum of electronic and zero-point energies = -769.055809833 Hartree

Table S34. Atom coordinates for the optimized geometry of compound **1** in ACN based on BPE0 method.

Atom	X	Y	Z
C	-0.119498	2.409079	-0.199370
C	1.130596	1.829022	-0.154450
C	1.264828	0.417964	-0.049251
C	0.074908	-0.341211	0.010210
C	-1.168319	0.278047	-0.040947
H	2.003529	2.479434	-0.232234
H	0.116084	-1.421678	0.150591
C	-2.478670	-0.367588	0.028229
C	-3.643747	0.398990	0.279790
C	-2.597341	-1.767341	-0.156551
C	-4.892700	-0.225668	0.353892
H	-3.565137	1.478907	0.429656
C	-3.851326	-2.381945	-0.084510
H	-1.718042	-2.377926	-0.379337
C	-5.001308	-1.615595	0.173115
H	-5.785221	0.374039	0.557171
H	-3.931867	-3.462629	-0.236034
H	-5.980851	-2.100805	0.231052
C	2.586662	-0.224286	0.007876
C	2.768425	-1.544633	-0.474302
C	3.701236	0.467011	0.544768
C	4.028825	-2.149659	-0.426363
H	1.931378	-2.086331	-0.925414
C	4.955528	-0.149668	0.606512
H	3.580209	1.475302	0.952169
C	5.124325	-1.456845	0.117874
H	4.158328	-3.162821	-0.819405
H	5.803128	0.389463	1.040799

H	6.108283	-1.934860	0.160308
O	-1.232026	1.632545	-0.145859
C	-0.432061	3.857578	-0.321077
H	-1.027250	4.195552	0.545470
H	0.493715	4.447503	-0.372410
H	-1.032256	4.046993	-1.228171

Sum of electronic and zero-point energies = -769.061246810 Hartree

Table S35. Atom coordinates for the optimized geometry of compound **2** in DCM based on BPE0 method.

Atom	X	Y	Z
C	0.114472	2.665427	0.161471
C	-1.131270	2.080333	0.130083
O	-1.262900	0.663983	0.054588
C	-0.067552	-0.088116	0.010792
C	1.174952	0.535682	0.048660
C	-2.005512	2.730151	0.195449
C	-0.102658	-1.171586	-0.104944
C	2.484590	0.104523	0.002827
C	3.656201	0.661472	0.224575
C	2.613245	-1.506078	0.166601
C	4.905185	0.040455	-0.282525
C	3.583304	1.742887	-0.366997
C	3.868791	-2.112109	0.110148
C	1.735705	-2.129084	0.360847
C	5.040747	-1.355270	-0.114648
C	5.796771	0.649524	-0.467173
C	3.945089	-3.196259	0.247255
C	-2.579019	0.017786	0.012780
C	-2.753042	-1.314656	0.467635
C	-3.714962	0.708340	-0.478945

C	-4.009534	-1.920895	0.435824
H	-1.909041	-1.867734	0.891394
H	-4.964810	0.086255	-0.522833
H	-3.618077	1.727012	-0.866671
H	-5.140666	-1.238101	-0.066158
H	-4.121467	-2.942699	0.814996
H	-5.823577	0.636776	-0.922215
H	1.233628	1.894721	0.124062
H	0.420648	4.118469	0.252703
H	1.015821	4.441731	-0.619468
H	-0.507851	4.705485	0.289580
H	1.017646	4.330987	1.156878
H	-6.486096	-1.913087	-0.129572
H	-6.544605	-2.577121	-1.012676
H	-6.663013	-2.543428	0.758327
H	-7.305082	-1.180287	-0.211591
H	6.394313	-2.015546	-0.147315
H	6.791616	-2.131609	0.878942
H	6.342000	-3.024553	-0.589418
H	7.124146	-1.416894	-0.716329

Sum of electronic and zero-point energies = -847.583469052 Hartree

Table S36. Atom coordinates for the optimized geometry of compound **2** in ACN based on BPE0 method.

Atom	X	Y	Z
C	0.114884	2.665143	0.162695
C	-1.131226	2.080158	0.130895
O	-1.262562	0.664386	0.054550
C	-0.067674	0.088405	0.010353
C	1.174381	0.535633	0.048860
C	-2.005212	2.730254	0.196117
C	-0.102887	1.171801	-0.105668

C	2.484465	0.104693	-0.002826
C	3.655322	0.661116	-0.228116
C	2.613450	-1.505640	0.169921
C	4.904589	0.040184	-0.286191
C	3.581714	1.742133	-0.373246
C	3.869268	-2.111570	0.113271
C	1.736200	-2.128132	0.366882
C	5.040653	-1.355009	-0.114950
C	5.795713	0.649126	-0.473637
C	3.945819	-3.195393	0.252992
C	-2.579077	0.017923	0.012332
C	-2.753023	-1.314156	0.467823
C	-3.714607	0.708286	-0.480164
C	-4.009695	-1.920516	0.435896
H	-1.908946	-1.867209	0.891363
H	-4.964667	0.086139	-0.523873
H	-3.617579	1.726912	-0.867864
H	-5.140606	-1.237928	-0.066597
H	-4.121474	-2.942289	0.815259
H	-5.823313	0.636727	-0.923505
H	1.233400	1.894096	0.125071
H	0.421233	4.117871	0.254485
H	1.016792	4.440761	-0.617503
H	-0.507273	4.704753	0.291281
H	1.018091	4.329476	1.158919
H	-6.486267	-1.912998	-0.130010
H	-6.544772	-2.577673	-1.012617
H	-6.663349	-2.542668	0.758367
H	-7.304992	-1.179910	-0.212697
H	6.394522	-2.015211	-0.147755

H	6.791420	-2.132902	0.878455
H	6.342254	-3.023618	-0.591344
H	7.124413	-1.415582	-0.715726

Sum of electronic and zero-point energies = -847.588582090 Hartree

Table S37. Atom coordinates for the optimized geometry of compound **3** in DCM based on BPE0 method.

Atom	X	Y	Z
C	0.111476	3.244825	0.137005
C	-1.131028	2.652431	0.109420
O	-1.254962	1.234290	0.060292
C	-0.055239	0.488130	0.038479
C	1.183405	1.119428	0.071528
C	-2.009138	3.298643	0.156313
C	-0.082585	-0.597643	-0.055794
C	2.495572	0.483775	0.038110
C	3.664645	1.242904	-0.203247
C	2.632921	-0.911500	0.247565
C	4.918233	0.625224	-0.244254
C	3.591577	2.320475	-0.373400
C	3.890508	-1.511197	0.208375
C	1.759910	-1.533827	0.464037
C	5.068239	-0.764626	-0.041979
C	5.793061	1.249135	-0.443576
C	3.953520	-2.589753	0.383420
C	-2.567037	0.580064	0.023556
C	-2.737482	-0.748046	0.491501
C	-3.706303	1.252210	-0.479598
C	-3.989749	-1.360033	0.461889
C	-1.892958	-1.295391	0.921711
C	-4.954078	0.621866	-0.520545
C	-3.617505	2.265272	-0.883994
C	-5.133526	-0.696638	-0.046884
C	-4.077090	-2.378753	0.852482
C	-5.798805	1.176426	-0.936693

H	1.235072	2.479846	0.121119
H	0.408964	4.701004	0.203201
H	1.016343	5.009762	-0.665709
H	-0.522938	5.283654	0.213935
H	0.990404	4.934851	1.112331
H	-6.493749	-1.410035	-0.061304
H	6.431241	-1.470917	-0.084074
H	6.408597	-2.549575	-1.198187
H	7.383962	-3.066800	-1.234933
H	5.630431	-3.311926	-1.022345
H	6.224681	-2.093664	-2.187005
H	6.692539	-2.151425	1.285038
H	7.667661	-2.669879	1.262708
H	6.718540	-1.405824	2.099179
H	5.919327	-2.899435	1.529714
H	7.591356	-0.497496	-0.373702
H	7.479150	-0.000841	-1.353822
H	7.683356	0.281242	0.404213
H	8.541375	-1.058989	-0.393801
H	-6.380284	-2.707542	-0.903071
H	-5.630354	-3.404562	-0.492057
H	-7.353647	-3.229551	-0.914062
H	-6.101434	-2.479211	-1.946854
H	-6.886988	-1.775573	1.394110
H	-6.974850	-0.870303	2.020381
H	-7.863957	-2.291178	1.397641
H	-6.150003	-2.448210	1.865215
H	-7.611731	-0.535589	-0.663271
H	-7.768813	0.391868	-0.084484
H	-7.402168	-0.261364	-1.712500
H	-8.560873	-1.098756	-0.650912

Sum of electronic and zero-point energies = -1083.12227283 Hartree

Table S38. Atom coordinates for the optimized geometry of compound **3** in ACN based on BPE0 method.

Atom	X	Y	Z
C	0.111917	3.244237	0.138613
C	-1.130995	2.651934	0.110273
O	-1.254581	1.234431	0.059635
C	-0.055316	0.487535	0.037104
C	1.182815	1.119101	0.071280
C	-2.008867	3.298376	0.157281
C	-0.082743	0.598140	-0.057890
C	2.495537	0.483408	0.037772
C	3.663829	1.242371	0.206772
C	2.633208	-0.911127	0.250465
C	4.917754	0.624879	-0.247667
C	3.590066	2.319483	-0.379544
C	3.891122	-1.510696	0.211276
C	1.760469	-1.532904	0.469374
C	5.068210	-0.764362	-0.042168
C	5.791965	1.248878	-0.449500
C	3.954240	-2.588853	0.388899
C	-2.567100	0.579911	0.022347
C	-2.737461	-0.747750	0.491046
C	-3.705894	1.251860	-0.481630
C	-3.989977	-1.359772	0.461620
C	-1.892863	-1.295130	0.920946
C	-4.953964	0.621587	-0.522116
C	-3.616936	2.264790	-0.886195
C	-5.133506	-0.696459	-0.047474
C	-4.076955	-2.378420	0.852564
C	-5.798396	1.176401	-0.938569
H	1.234789	2.478911	0.122346

H	0.409528	4.700105	0.205665
H	1.014509	5.009216	-0.664758
H	-0.522431	5.282461	0.219539
H	0.993643	4.932399	1.113401
H	-6.494120	-1.409705	-0.061059
H	6.431557	-1.470578	-0.084058
H	6.408452	-2.551580	-1.195791
H	7.383856	-3.068937	-1.232154
H	5.630106	-3.313223	-1.017708
H	6.223766	-2.097423	-2.185319
H	6.694657	-2.148217	1.286056
H	7.669968	-2.666496	1.263873
H	6.721139	-1.400666	2.098449
H	5.921605	-2.895671	1.532932
H	7.591223	-0.497494	-0.376782
H	7.477664	-0.002800	-1.357736
H	7.683206	0.283072	0.399298
H	8.541384	-1.058921	-0.396445
H	-6.381422	-2.708372	-0.901001
H	-5.631341	-3.404720	-0.489126
H	-7.354983	-3.230202	-0.911112
H	-6.102619	-2.481230	-1.945099
H	-6.887820	-1.773301	1.394647
H	-6.975559	-0.866949	2.019440
H	-7.864892	-2.288894	1.398809
H	-6.150612	-2.445098	1.866607
H	-7.611891	-0.535747	-0.664208
H	-7.768308	0.392604	-0.086683
H	-7.401768	-0.262695	-1.713628
H	-8.561201	-1.098777	-0.651148

Sum of electronic and zero-point energies = -1083.12729426 Hartree

Table S39. Atom coordinates for the optimized geometry of compound **4** in DCM based on BPE0 method.

Atom	X	Y	Z
C	-0.031340	2.885382	-0.130598
C	1.181903	2.241352	-0.124382
O	1.248709	0.814722	-0.076301
C	0.016022	0.125326	-0.031081
C	-1.196873	0.808230	-0.044380
C	2.083977	2.851787	-0.188823
C	-0.003747	-0.960307	0.063528
C	-2.531362	0.233610	0.006262
C	-3.675152	1.060083	0.187266
C	-2.729755	-1.162948	-0.128500
C	-4.949170	0.511252	0.240047
C	-3.554990	2.140893	0.296039
C	-4.005799	-1.723990	-0.079125
C	-1.881826	-1.833453	-0.292683
C	-5.130264	-0.887496	0.109117
C	-5.828252	1.145616	0.386738
C	-4.118319	-2.804019	-0.194424
C	2.527800	0.107504	-0.065749
C	2.624523	-1.252521	-0.475345
O	3.718518	0.752288	0.355438
C	3.839921	-1.922925	-0.468053
O	1.741789	-1.782631	-0.844593
C	4.944708	0.086708	0.383852
H	3.689783	1.786994	0.709116
H	5.015344	-1.262039	-0.033753
H	3.911665	-2.961359	-0.804667
H	5.832582	0.615724	0.736890

H	-1.191426	2.172706	-0.094330
H	-0.266760	4.354094	-0.191641
H	-0.840816	4.689618	0.690003
H	0.689302	4.895729	-0.222356
H	-0.856276	4.614415	-1.088266
H	6.148480	-2.003609	-0.057917
H	-6.411029	-1.322928	0.175424
H	7.384134	-1.389397	0.360214
H	7.326133	-1.071594	1.415457
H	8.146816	-2.171102	0.248219
H	7.631604	-0.529072	-0.285052
H	-6.665591	-2.737020	0.056727
H	-7.754841	-2.842166	0.144581
H	-6.331189	-3.114161	-0.925022
H	-6.168689	-3.293559	0.869828

Sum of electronic and zero-point energies = -997.868399449 Hartree

Table S40. Atom coordinates for the optimized geometry of compound **4** in ACN based on BPE0 method.

Atom	X	Y	Z
C	-0.031367	2.884977	-0.132359
C	1.182075	2.240694	-0.125880
O	1.248264	0.814646	-0.076454
C	0.015815	0.124857	-0.030238
C	-1.196421	0.808339	-0.044293
C	2.084121	2.851072	-0.190469
C	-0.004205	-0.960664	0.065250
C	-2.531497	0.233820	0.006738
C	-3.674358	1.060159	0.192245
C	-2.730282	-1.162039	-0.132295
C	-4.948716	0.511347	0.245334
C	-3.553504	2.140552	0.304489

C	-4.006668	-1.722905	-0.082679
C	-1.882828	-1.832125	-0.300237
C	-5.130277	-0.886747	0.110155
C	-5.827017	1.146026	0.395688
C	-4.119401	-2.802509	-0.201481
C	2.527645	0.106954	-0.065420
C	2.624063	-1.252971	-0.474695
O	3.718104	0.751912	0.355628
C	3.839815	-1.923377	-0.467208
O	1.741283	-1.783428	-0.843205
C	4.944517	0.086292	0.383987
H	3.689520	1.786820	0.708563
H	5.015028	-1.262321	-0.033309
H	3.910770	-2.962057	-0.803383
H	5.832259	0.615767	0.736608
H	-1.190995	2.172224	-0.095466
H	-0.266526	4.353474	-0.194222
H	-0.840166	4.689160	0.687588
H	0.689707	4.894628	-0.225748
H	-0.856558	4.612837	-1.090738
H	6.149271	-2.003929	-0.057319
H	-6.411810	-1.322810	0.177172
H	7.384057	-1.387636	0.360771
H	7.325427	-1.069120	1.415722
H	8.148068	-2.168175	0.249388
H	7.630352	-0.527143	-0.284659
H	-6.664755	-2.737005	0.054484
H	-7.753727	-2.844069	0.143859
H	-6.331357	-3.110771	-0.928849
H	-6.165555	-3.295501	0.864773

Sum of electronic and zero-point energies = -997.873558620 Hartree

Table S41. Atom coordinates for the optimized geometry of compound **5** in DCM based on BPE0 method.

Atom	X	Y	Z
C	0.114011	2.867537	0.160406
C	-1.131907	2.278972	0.130967
O	-1.258227	0.863862	0.065277
C	-0.063508	0.110656	0.029735
C	1.176146	0.738796	0.064600
C	-2.008110	2.926867	0.190736
C	-0.098067	0.973530	-0.080008
C	2.489013	0.101113	0.017951
C	3.655009	0.871296	0.216894
C	2.618757	-1.296459	0.209592
C	4.911003	0.264843	-0.269783
C	3.578766	1.950401	-0.371513
C	3.871520	-1.909693	0.161895
C	1.745149	-1.919085	0.419267
C	5.011483	-1.124133	-0.080421
C	5.806177	0.862509	-0.459927
C	3.965474	-2.987348	0.317963
C	-2.574604	0.213884	0.023941
C	-2.750456	-1.101400	0.521463
Cl	-3.698562	0.888525	-0.514140
Cl	-4.001382	-1.720867	0.491927
H	-1.913268	-1.638819	0.976509
H	-4.950814	0.272771	-0.565913
H	-3.593740	1.891842	-0.937063
H	-5.094507	-1.029201	-0.057252
H	-4.131315	-2.728003	0.896532
H	-5.807422	0.793796	-1.001409

H	1.232293	2.096670	0.129758
H	0.417532	4.320710	0.241949
H	1.015282	4.637844	-0.630704
H	-0.511802	4.906583	0.271802
H	1.011762	4.539883	1.146389
H	6.580031	-1.887098	-0.144286
H	-6.660047	-1.801348	-0.106798

Sum of electronic and zero-point energies = -1687.86179677 Hartree

Table S42. Atom coordinates for the optimized geometry of compound **5** in ACN based on BPE0 method.

Atom	X	Y	Z
C	0.114491	2.867086	0.162400
C	-1.131932	2.278600	0.132606
O	-1.257696	0.864272	0.065750
C	-0.063622	0.110168	0.029611
C	1.175421	0.738695	0.065199
C	-2.007984	2.926618	0.192408
C	-0.098344	-0.973925	-0.080604
C	2.488909	0.100914	0.018245
C	3.653731	0.870782	-0.221737
C	2.618964	-1.295643	0.214671
C	4.910083	0.264454	-0.275105
C	3.576644	1.949271	-0.380135
C	3.872033	-1.908921	0.166506
C	1.745839	-1.917446	0.428451
C	5.010521	-1.123516	-0.080983
C	5.804441	0.862023	-0.469296
C	3.966092	-2.986009	0.326289
C	-2.574630	0.213963	0.023790
C	-2.750942	-1.099720	0.524492
Cl	-3.697086	0.887513	-0.517965

Cl	-4.002153	-1.719320	0.494574
H	-1.914270	-1.636227	0.981417
H	-4.949697	0.271834	-0.569901
H	-3.591305	1.889888	-0.942730
H	-5.093576	-1.028443	-0.057970
H	-4.132261	-2.725571	0.901287
H	-5.805347	0.792350	-1.007860
H	1.231875	2.095831	0.131322
H	0.418165	4.319898	0.244558
H	1.015818	4.636687	-0.628225
H	-0.511191	4.905558	0.274927
H	1.012817	4.537944	1.148932
H	6.580955	-1.887137	-0.145545
H	-6.661064	-1.801305	-0.107860

Sum of electronic and zero-point energies = -1687.86773813 Hartree

Table S43. Atom coordinates for the optimized geometry of compound **6** in DCM based on BPE0 method.

Atom	X	Y	Z
C	0.115138	2.641947	0.177160
C	-1.131580	2.056482	0.141514
O	-1.261447	0.642069	0.058314
C	-0.067830	-0.112324	0.011522
C	1.173417	0.512514	0.054049
C	-2.006083	2.705705	0.210574
C	-0.104069	-1.194707	-0.113968
C	2.484619	-0.127242	-0.001736
C	3.650395	0.644000	-0.241230
C	2.610153	-1.526900	0.185855
C	4.905712	0.036767	-0.302601
C	3.572146	1.723330	-0.392403
C	3.860707	-2.144129	0.129677

C	1.734624	-2.145352	0.399278
C	4.984909	-1.347800	-0.116084
C	5.811011	0.618239	-0.495152
C	3.971235	-3.220962	0.280588
C	-2.578821	-0.004446	0.010336
C	-2.753598	-1.327991	0.489591
F	-3.702784	0.682868	-0.514862
F	-4.005019	-1.946344	0.454504
H	-1.914482	-1.871206	0.933687
H	-4.957130	0.071782	-0.572516
H	-3.594516	1.692105	-0.922069
H	-5.082453	-1.232345	-0.081537
H	-4.153119	-2.958374	0.840178
H	-5.824358	0.586593	-0.994095
H	1.232448	1.869481	0.136657
H	0.421904	4.093549	0.276221
H	1.017731	4.420577	-0.594120
H	-0.506164	4.680882	0.315977
H	1.019044	4.300369	1.181623
H	-6.301840	-1.830410	-0.125878
H	6.204024	-1.943789	-0.173279

Sum of electronic and zero-point energies = -967.373978608 Hartree

Table S44. Atom coordinates for the optimized geometry of compound **6** in ACN based on BPE0 method.

Atom	X	Y	Z
C	0.115612	2.641609	0.178808
C	-1.131563	2.056290	0.142794
O	-1.260982	0.642568	0.058682
C	-0.067969	-0.112644	0.011444
C	1.172737	0.512497	0.054586

C	-2.005877	2.705702	0.211719
C	-0.104366	-1.194949	-0.114269
C	2.484450	0.127401	-0.001539
C	3.649232	0.643583	-0.245142
C	2.610249	-1.526246	0.189729
C	4.904838	0.036367	-0.307001
C	3.570289	1.722445	-0.399225
C	3.861110	-2.143475	0.133042
C	1.735128	-2.144071	0.406319
C	4.984157	-1.347384	-0.116804
C	5.809370	0.617966	-0.502771
C	3.971502	-3.219924	0.286766
C	-2.578832	-0.004260	0.010152
C	-2.753857	-1.326679	0.491612
F	-3.701677	0.682276	-0.517686
F	-4.005539	-1.945165	0.456121
H	-1.915062	-1.869347	0.936845
H	-4.956296	0.071117	-0.575494
H	-3.592802	1.690944	-0.925989
H	-5.081766	-1.231813	-0.082292
H	-4.153440	-2.956694	0.843192
H	-5.822749	0.585823	-0.998802
H	1.232125	1.868793	0.138021
H	0.422584	4.092882	0.278332
H	1.018414	4.419464	-0.592114
H	-0.505493	4.680040	0.318422
H	1.020030	4.298707	1.183700
H	-6.302758	-1.830611	-0.126989
H	6.204883	-1.943965	-0.174569

Sum of electronic and zero-point energies = -967.379939610 Hartree

Table S45. Atom coordinates for the optimized geometry of compound **7** in DCM based on BPE0 method.

Atom	X	Y	Z
C	0.119159	3.209707	0.162518
C	-1.130151	2.620568	0.142144
O	-1.253787	1.208765	0.089823
C	-0.062592	0.449870	0.058001
C	1.175558	1.079040	0.081845
C	-2.007811	3.267338	0.196516
C	-0.101376	-0.635608	-0.039078
C	2.492137	0.438875	0.033364
C	3.649474	1.202901	-0.248712
C	2.620367	-0.951010	0.266445
C	4.902523	0.588739	-0.306969
C	3.568105	2.275927	-0.437472
C	3.874199	-1.562662	0.210464
C	1.749149	-1.563323	0.512068
C	5.015506	-0.794325	-0.080966
C	5.788645	1.186184	-0.536628
C	3.961277	-2.636743	0.394571
C	-2.574460	0.556519	0.055206
C	-2.760661	-0.724766	0.628202
F	-3.676522	1.201599	-0.552682
C	-4.014205	-1.338803	0.599574
F	-1.934420	-1.230459	1.136209
F	-4.928126	0.580408	-0.598857
F	-3.553270	2.178763	-1.028305
C	-5.097960	-0.687581	-0.018282
F	-4.149540	-2.319580	1.064201
F	-5.767122	1.083180	-1.086408
H	1.231979	2.434778	0.134232

H	0.424210	4.662063	0.228723
H	1.020480	4.968793	-0.648676
H	-0.504193	5.249270	0.255438
H	1.021855	4.888479	1.129173
H	-6.434626	-1.389650	-0.081204
H	6.375100	-1.454411	-0.099856
H	6.315855	-2.745366	-0.541137
H	7.262276	-0.794511	-0.899218
H	6.929121	-1.493305	1.155743
H	-6.428580	-2.393659	-1.017220
H	-6.759952	-1.975240	1.111610
H	-7.456326	-0.549643	-0.409573

Sum of electronic and zero-point energies = -1442.55429343 Hartree

Table S46. Atom coordinates for the optimized geometry of compound **7** in ACN based on BPE0 method.

Atom	X	Y	Z
C	0.119672	3.208983	0.164063
C	-1.130132	2.619920	0.143295
O	-1.253237	1.208855	0.089794
C	-0.062611	0.449157	0.057398
C	1.174885	1.078765	0.082016
C	-2.007567	3.266885	0.197669
C	-0.101412	-0.636233	-0.040021
C	2.492027	0.438621	0.033415
C	3.648266	1.202356	-0.252810
C	2.620837	-0.950249	0.270675
C	4.901630	0.588607	-0.311180
C	3.565886	2.274725	-0.444738
C	3.874842	-1.561740	0.214522
C	1.750067	-1.561773	0.519512
C	5.015390	-0.793787	-0.081191

C	5.786773	1.186270	-0.543931
C	3.961915	-2.635222	0.402053
C	-2.574398	0.556353	0.054664
C	-2.760978	-0.723867	0.629349
F	-3.675447	1.200830	-0.555143
C	-4.014654	-1.337879	0.600555
F	-1.934963	-1.229310	1.137805
F	-4.927371	0.580075	-0.601164
F	-3.551475	2.177531	-1.031346
C	-5.097868	-0.687083	-0.018806
F	-4.149693	-2.318243	1.066128
F	-5.765500	1.083029	-1.089976
H	1.231664	2.433850	0.135306
H	0.424707	4.661005	0.231091
H	1.022856	4.967122	-0.645153
H	-0.503787	5.247974	0.256191
H	1.020739	4.886493	1.132797
H	-6.433824	-1.388362	-0.081378
H	6.374142	-1.453305	-0.100294
H	6.316851	-2.744968	-0.542064
H	7.263254	-0.794042	-0.899108
H	6.930783	-1.494249	1.155252
H	-6.429846	-2.395977	-1.015063
H	-6.762448	-1.972338	1.112293
H	-7.456640	-0.549935	-0.412719

Sum of electronic and zero-point energies = -1442.56112353 Hartree

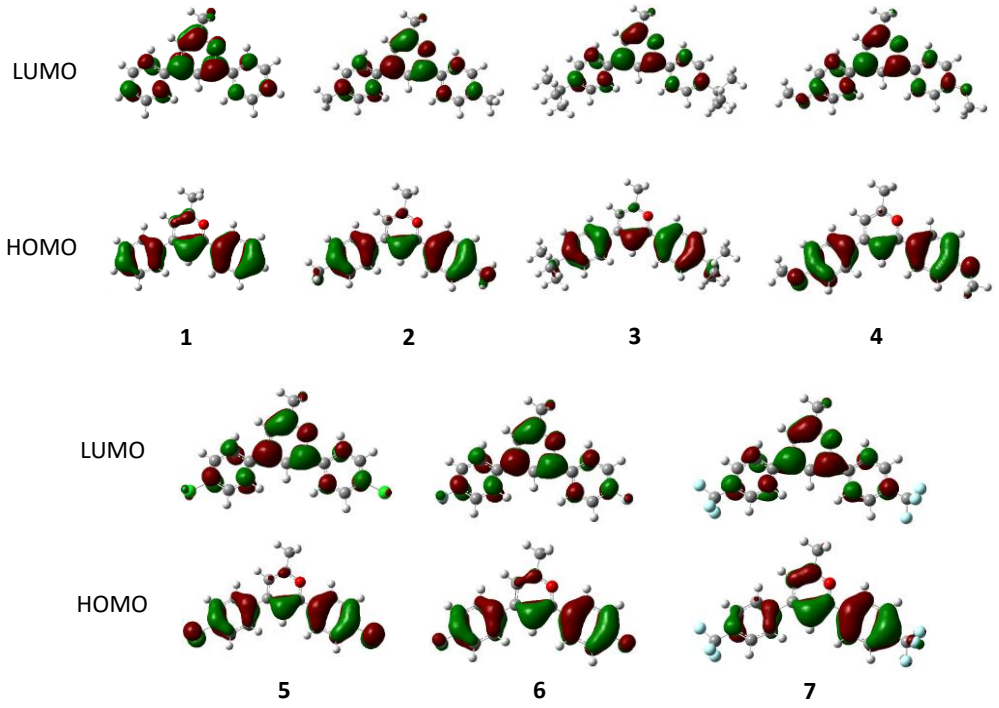


Figure S11. The HOMO and LUMO orbitals of compounds **1-7** in DCM based on B3LYP method.

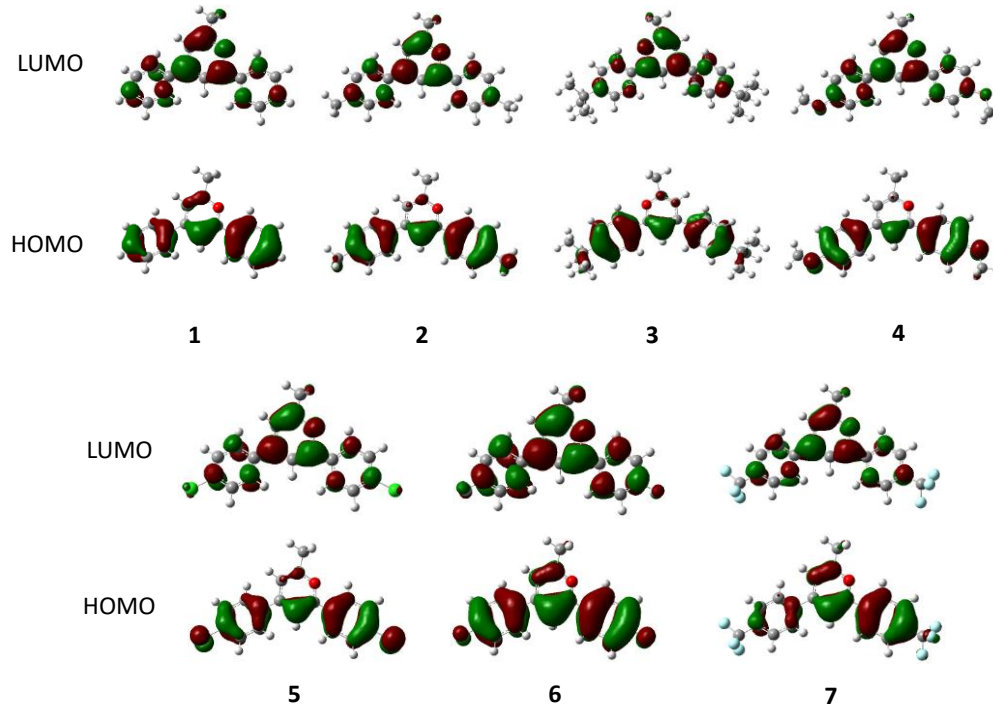


Figure S12. The HOMO and LUMO orbitals of compounds **1-7** in ACN based on B3LYP method.

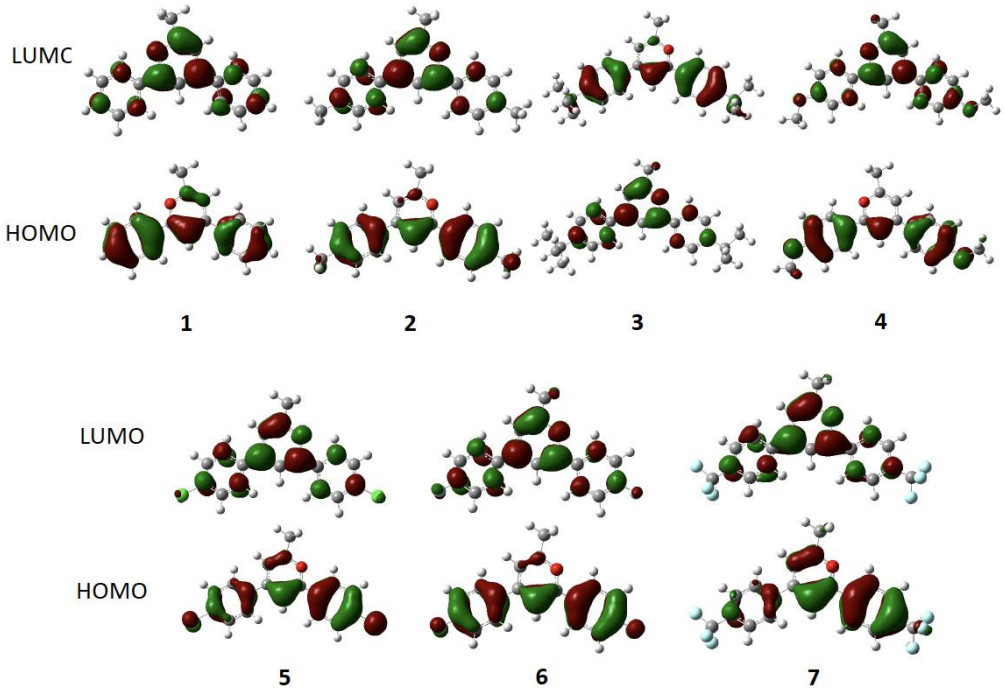


Figure S13. The HOMO and LUMO orbitals of compounds **1**-**7** in DCM based on CAM-B3LYP method.

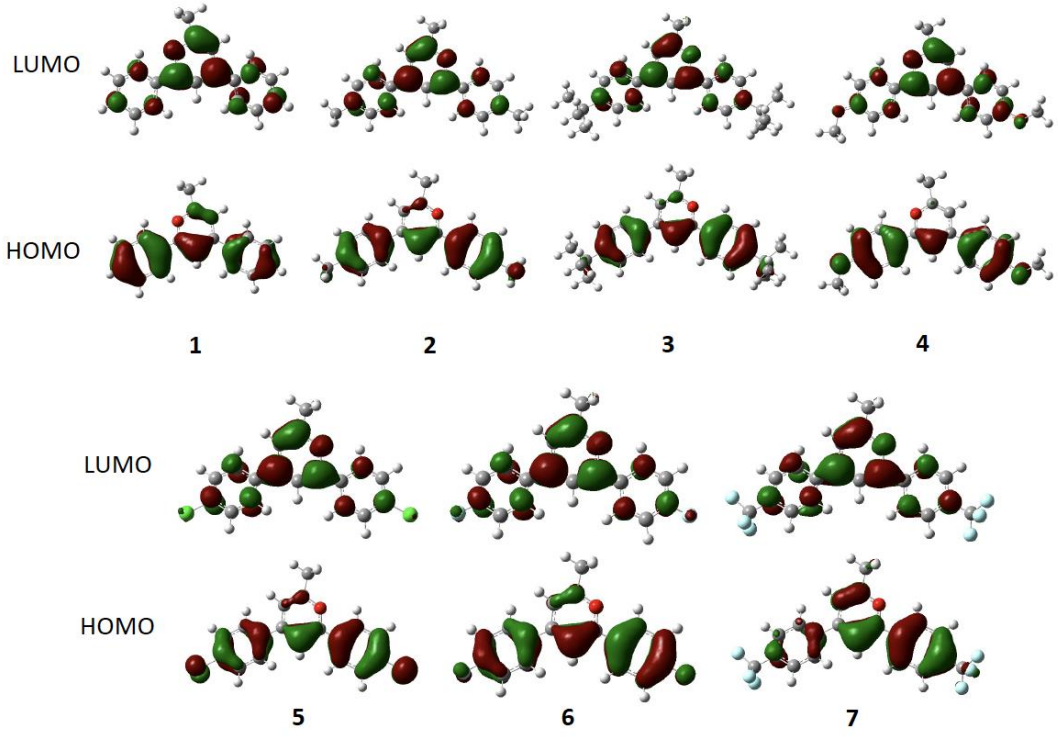


Figure S14. The HOMO and LUMO orbitals of compounds **1**-**7** in ACN based on CAM-B3LYP method.

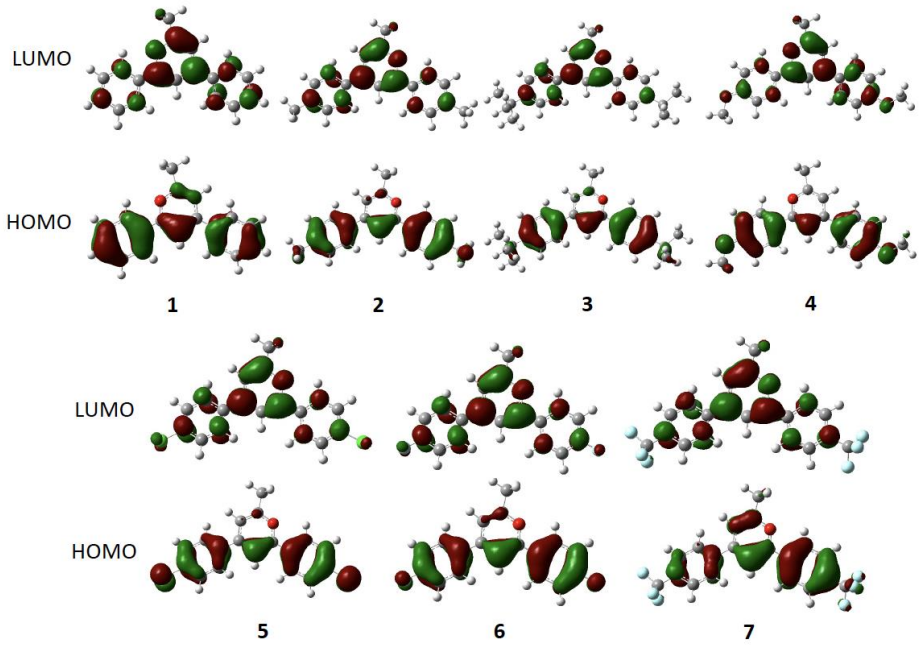


Figure S15. The HOMO and LUMO orbitals of compounds **1**-**7** in DCM based on BPE0 method.

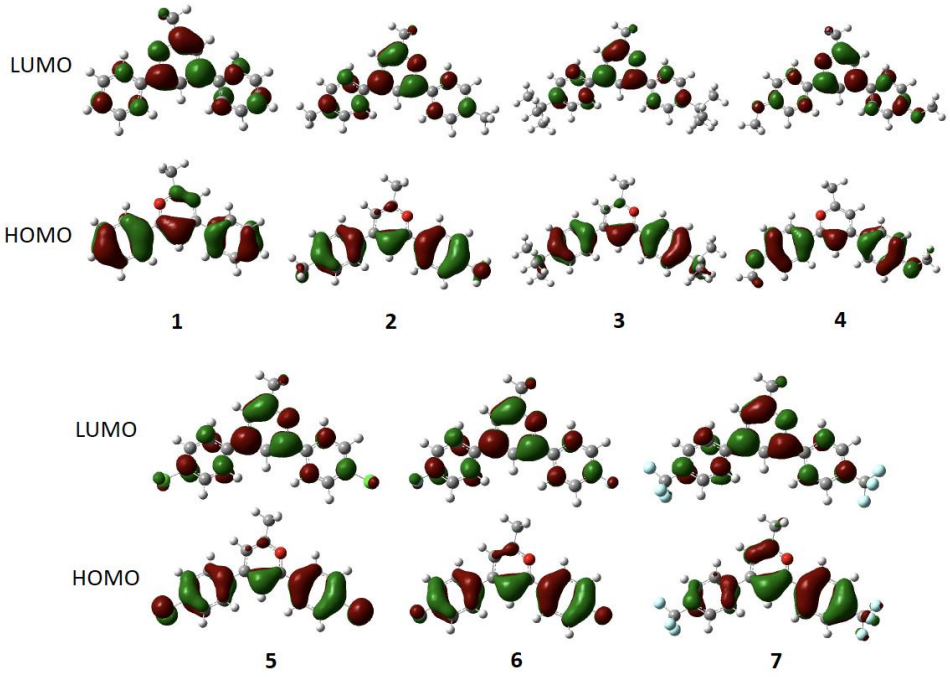


Figure S16. The HOMO and LUMO orbitals of compounds **1**-**7** in ACN based on BPE0 method.

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