Supporting Information for:

Anthracene-Naphthalenediimide Compact Electron Donor/Acceptor Dyads: Electronic Coupling, Electron Transfer and Intersystem Crossing

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Index

1. NMR and HRMS spectra.

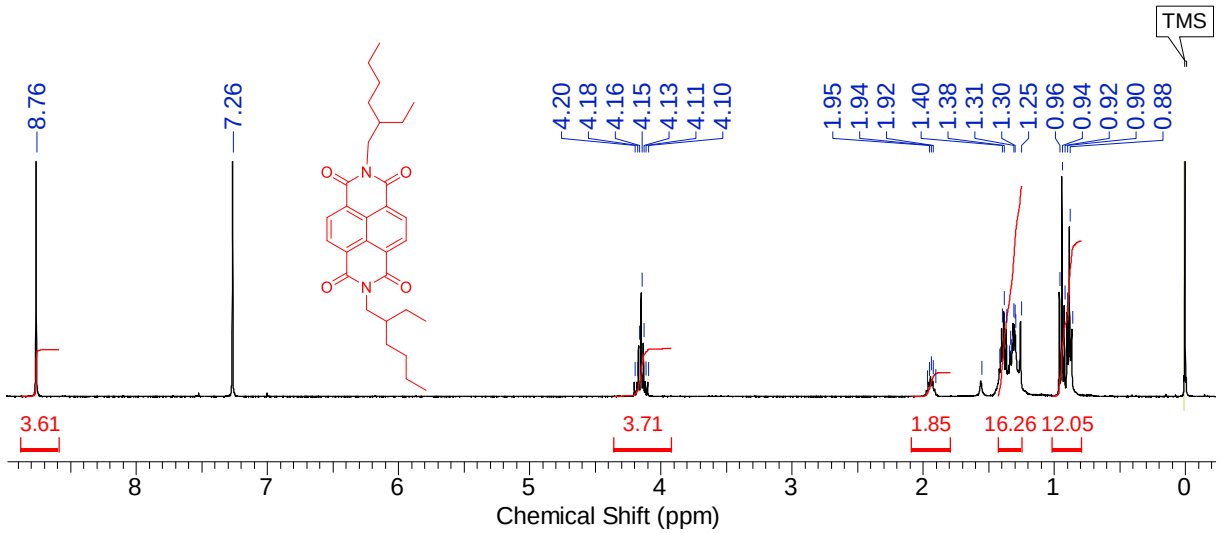


Figure S1. ^{1}H NMR spectrum of **NDI** (400 MHz, $CDCl_3$), 25 °C.

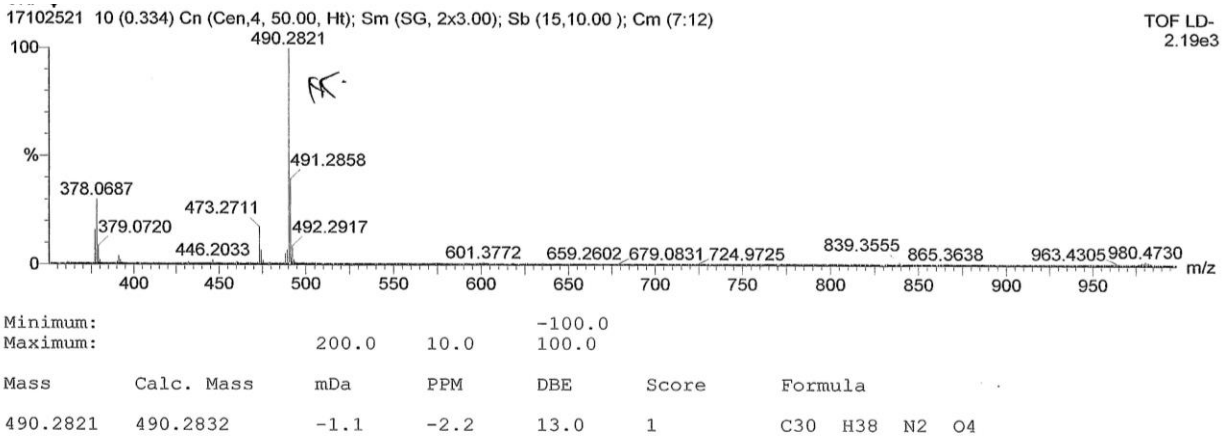


Figure S2. MALDI–TOF–HRMS spectrum of compound of **NDI**.

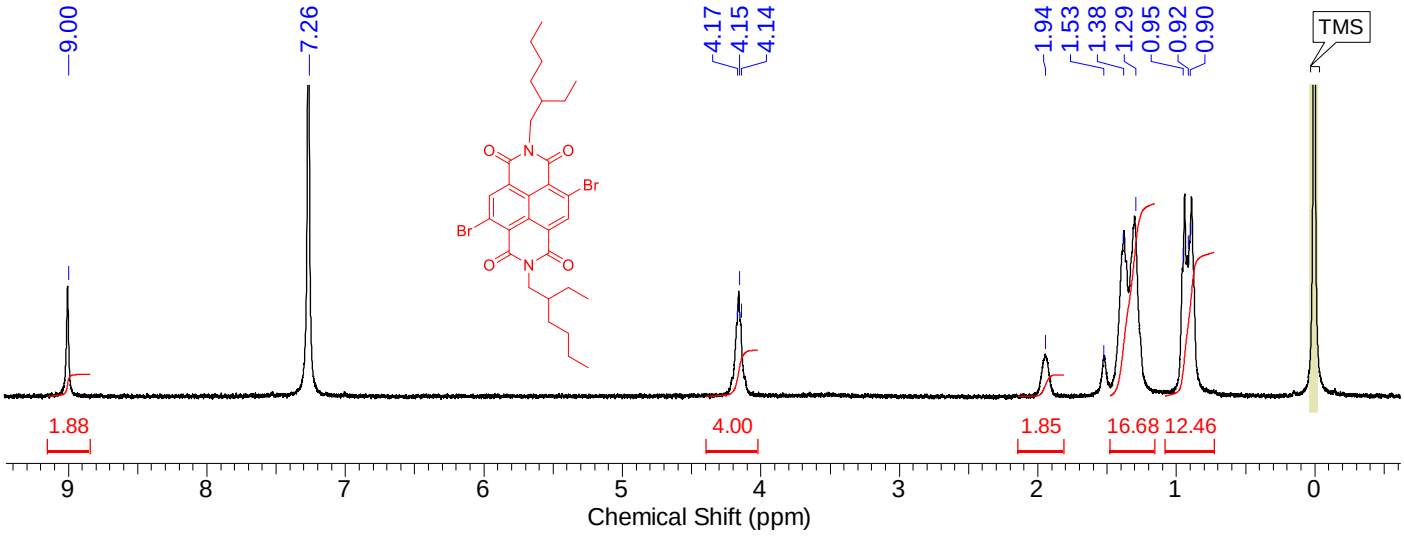


Figure S3. ^{1}H NMR spectrum of **2Br-NDI** (400 MHz, $CDCl_3$), 25 °C.

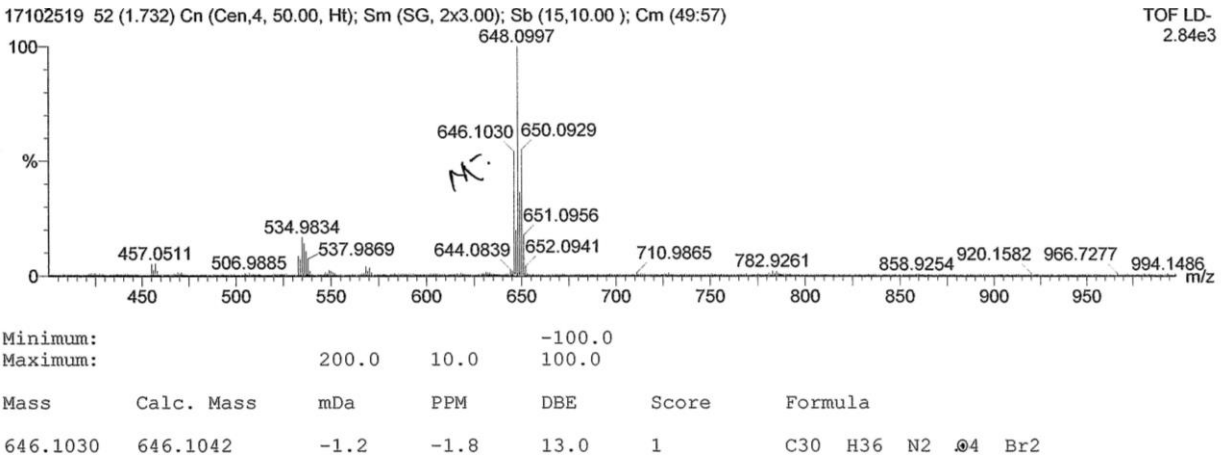


Figure S4. MALDI–TOF–HRMS spectrum of compound of **2Br-NDI**.

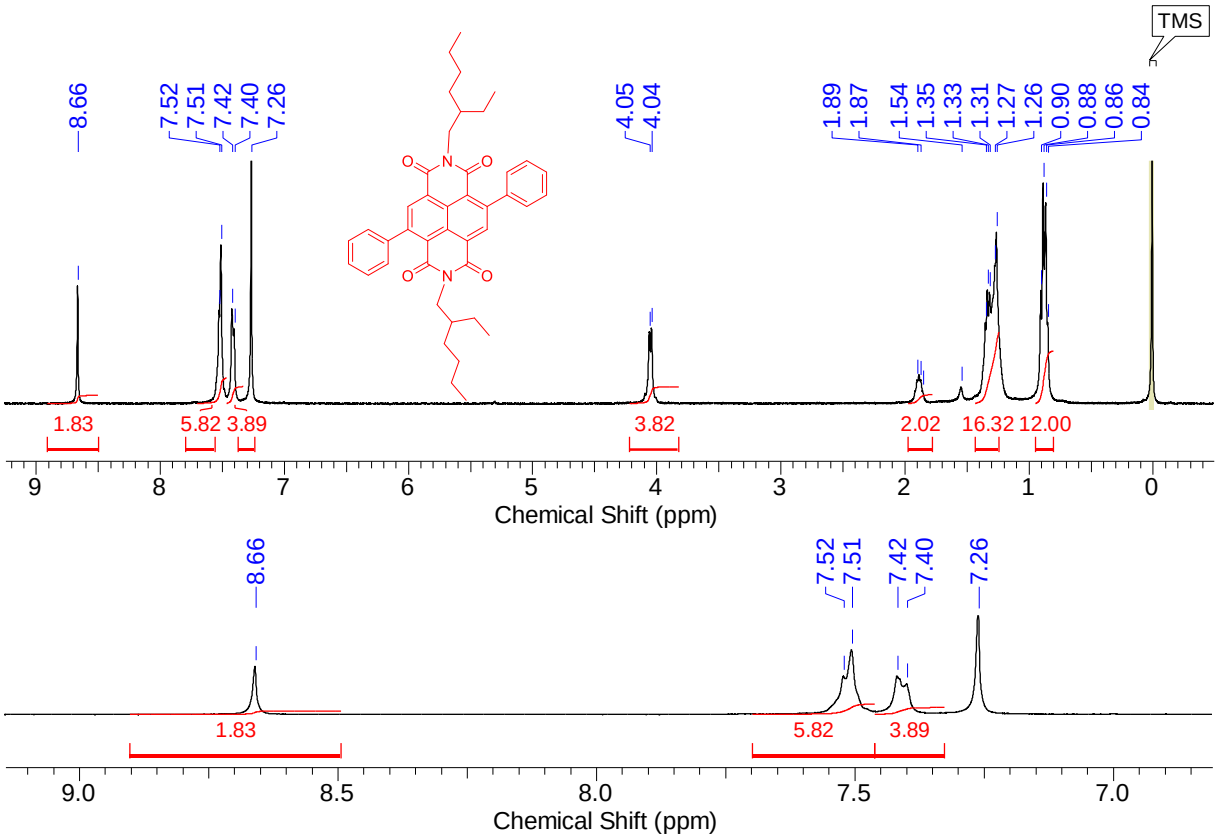


Figure S5. ^{1}H NMR spectrum of **Bis-Ph-NDI** (400 MHz, $CDCl_3$), 25 °C.

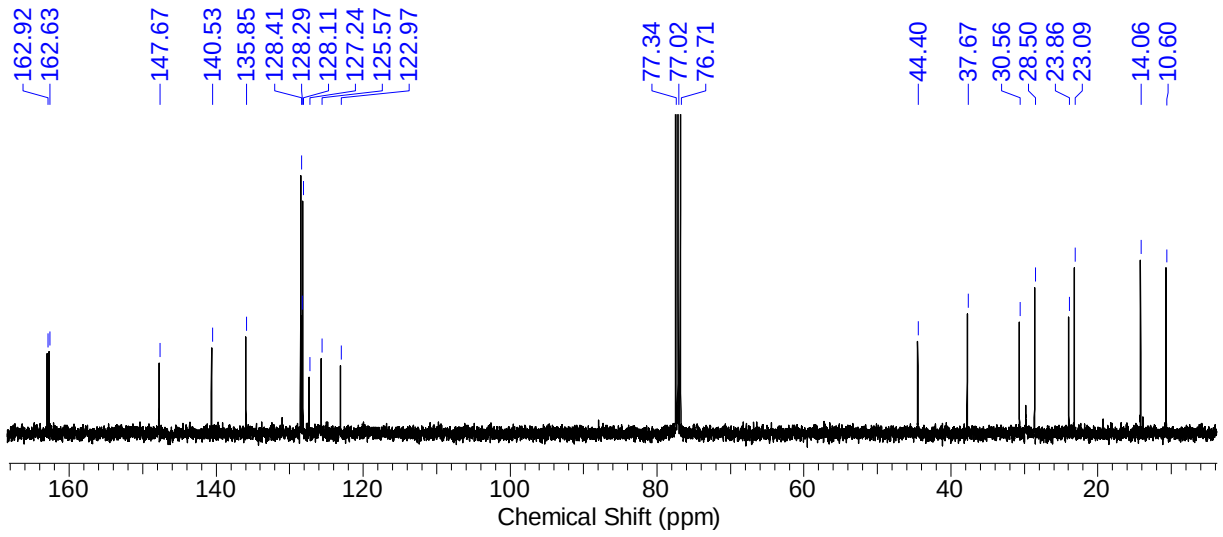
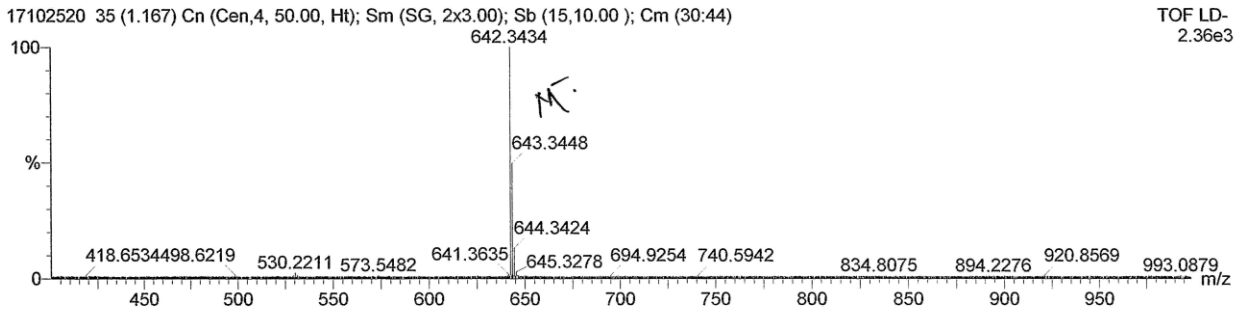


Figure S6. ^{13}C NMR spectrum of **Bis-Ph-NDI** (100 MHz, $CDCl_3$), 25 °C.



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Maximum:		200.0	10.0	100.0		
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642.3434	642.3458	-2.4	-3.7	21.0	1	C42 H46 N2 O4

Figure S7. MALDI–TOF–HRMS spectrum of compound of **Bis-Ph-NDI**.

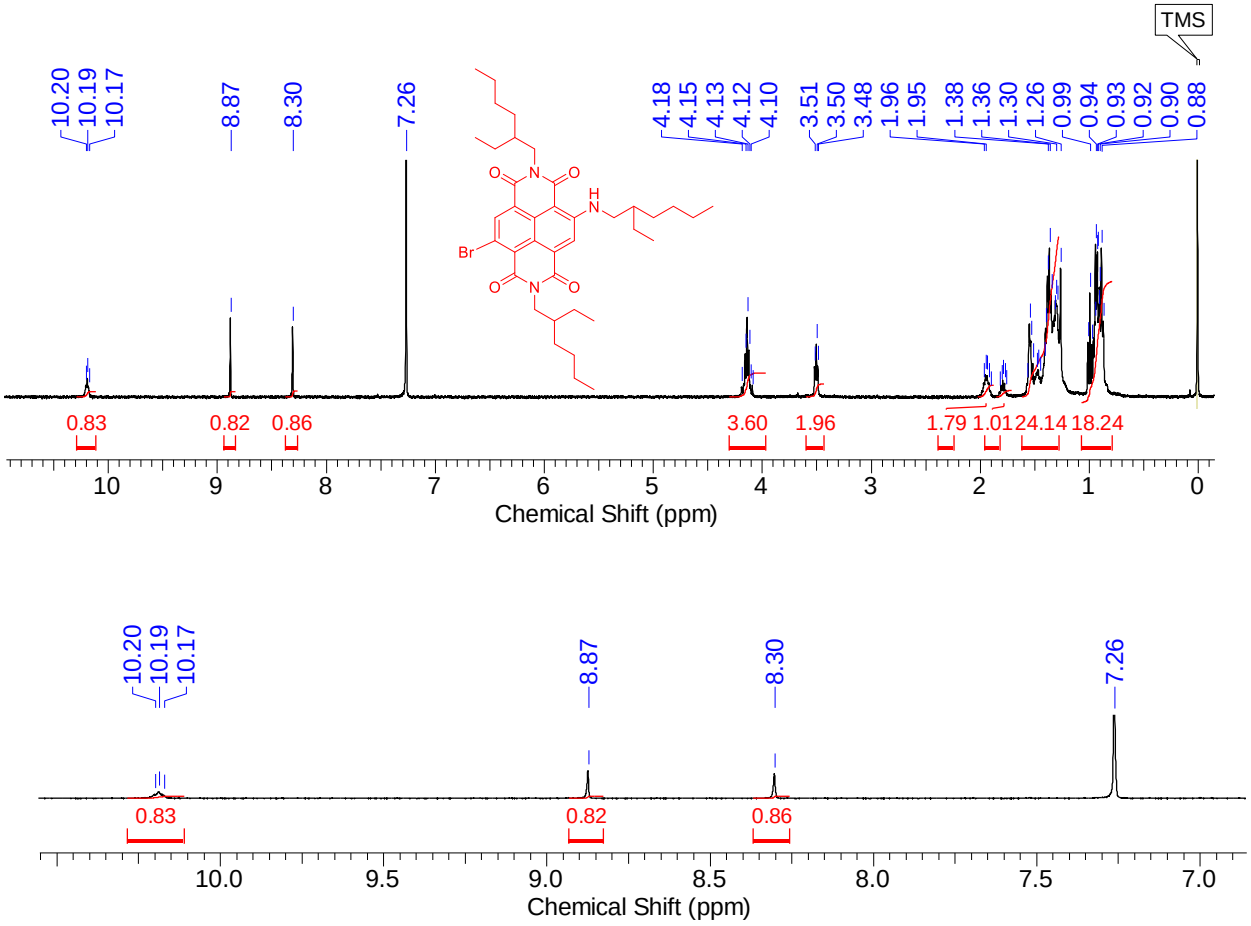
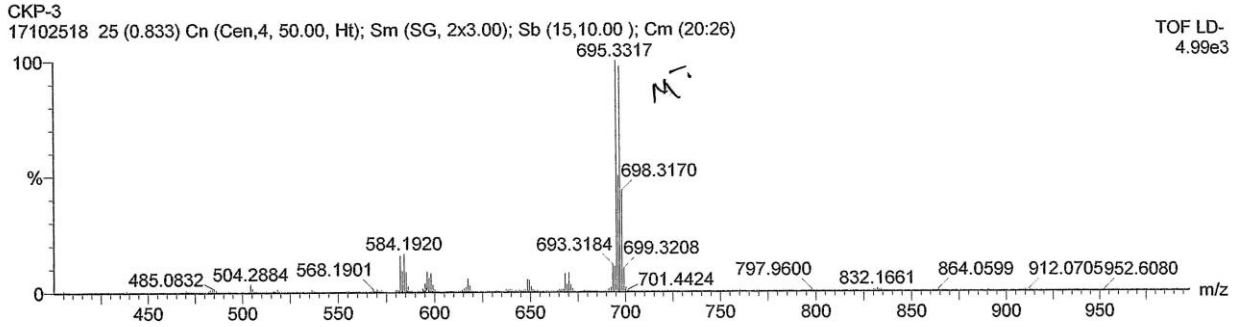


Figure S8. ^{1}H NMR spectrum of **Br-NDI-NH** (400 MHz, $CDCl_3$), 25 °C.



Minimum:				-100.0		
Maximum:		200.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
695.3317	695.3298	1.9	2.8	13.0	1	C38 H54 N3 O4 Br

Figure S9. MALDI–TOF–HRMS spectrum of compound of **Br-NDI-NH**.

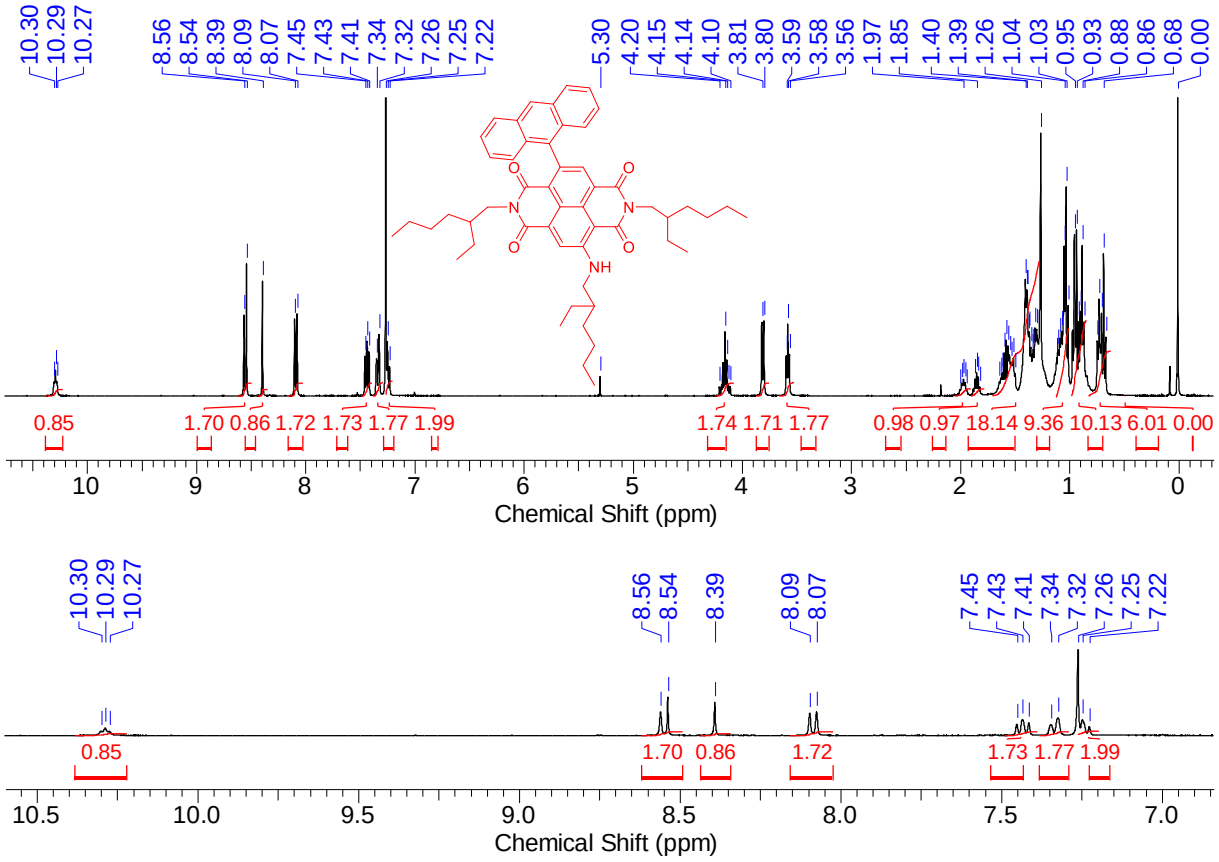


Figure S10. ^{1}H NMR spectrum of **9-An-NDI-NH** (400 MHz, $CDCl_3$), 25 °C.

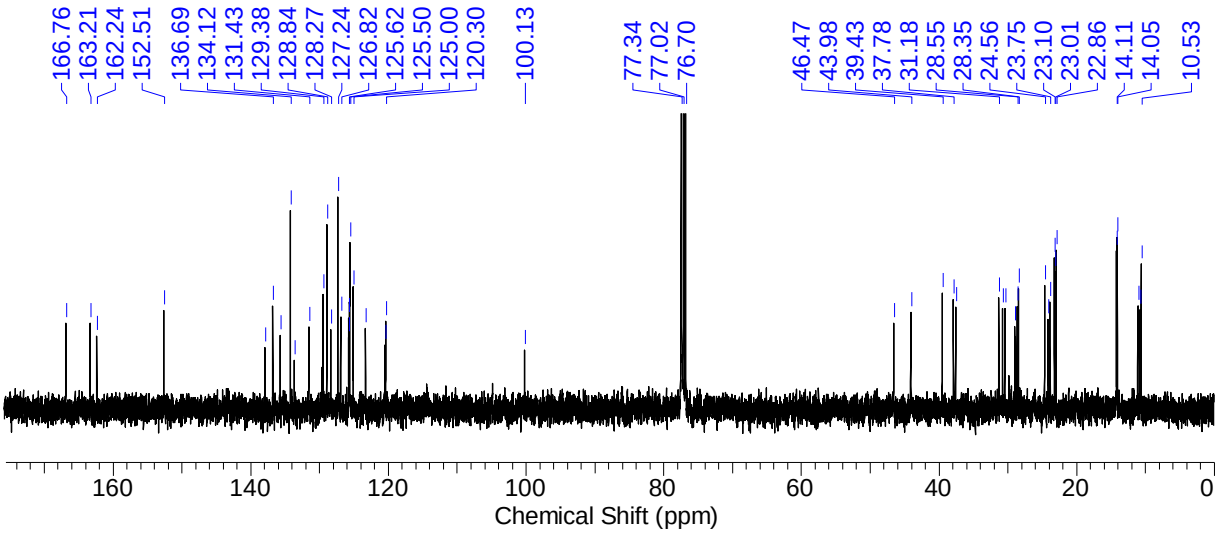


Figure S11. ^{13}C NMR spectrum of **9-An-NDI-NH** (100 MHz, $CDCl_3$), 25 °C.

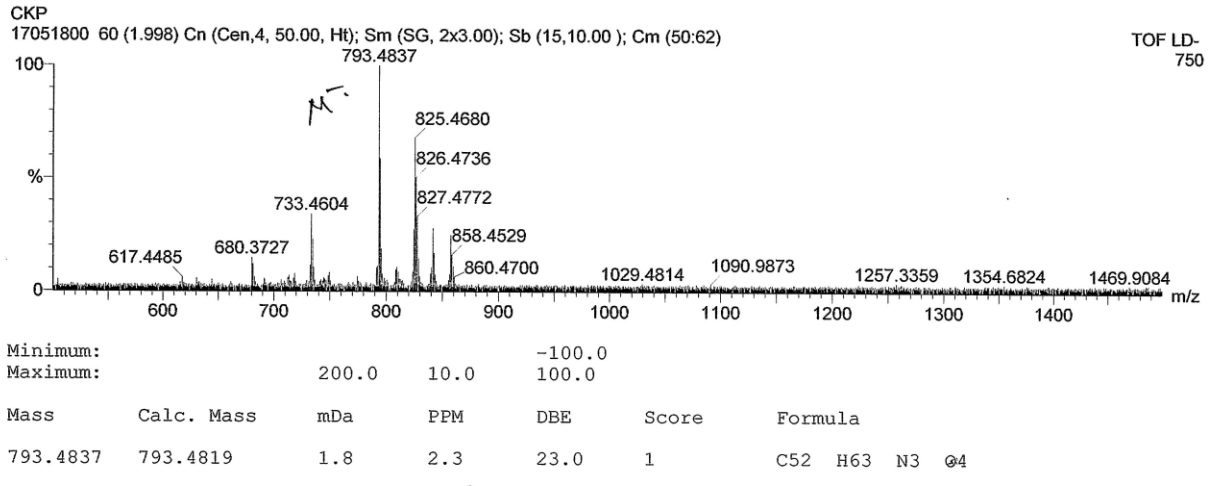


Figure S12. MALDI–TOF–HRMS spectrum of compound of **9-An-NDI-NH**.

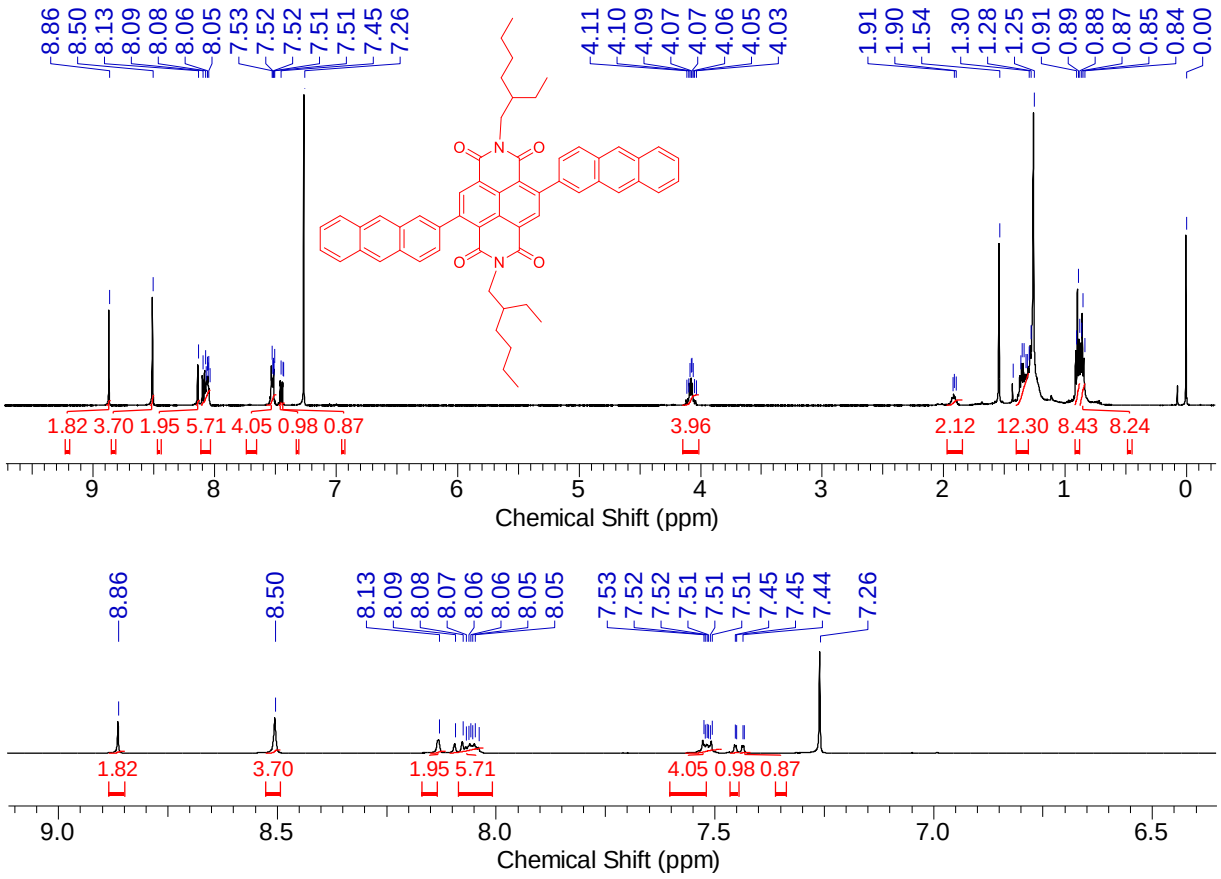


Figure S13. ^{1}H NMR spectrum of **Bis-2-An-NDI** (400 MHz, $CDCl_3$), 25 °C.

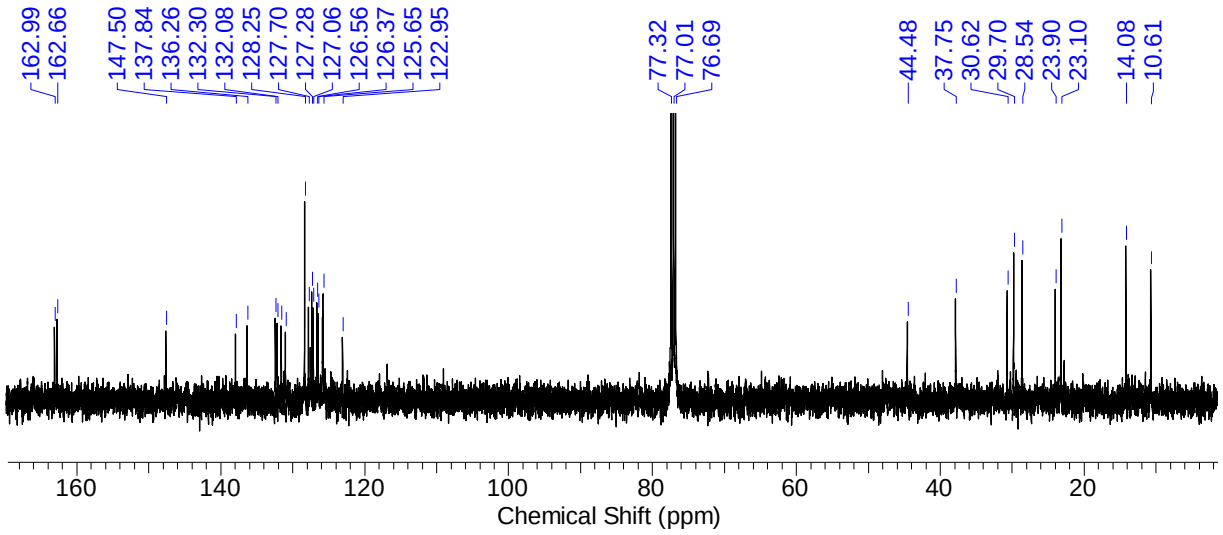


Figure S14. ^{13}C NMR spectrum of **Bis-2-An-NDI** (100 MHz, $CDCl_3$), 25 °C.

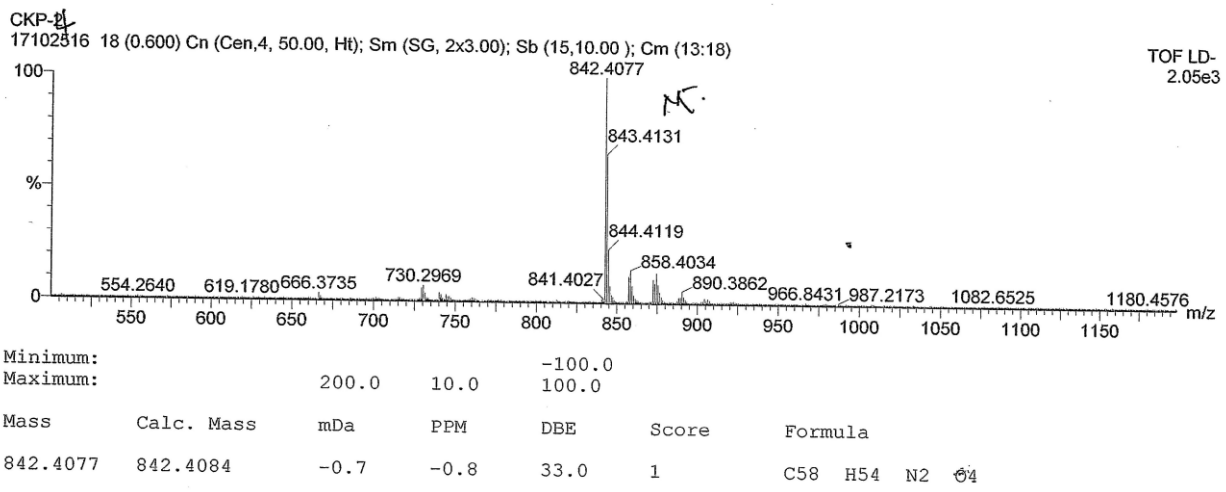


Figure S15. MALDI–TOF–HRMS spectrum of compound of **Bis-2-An-NDI**.

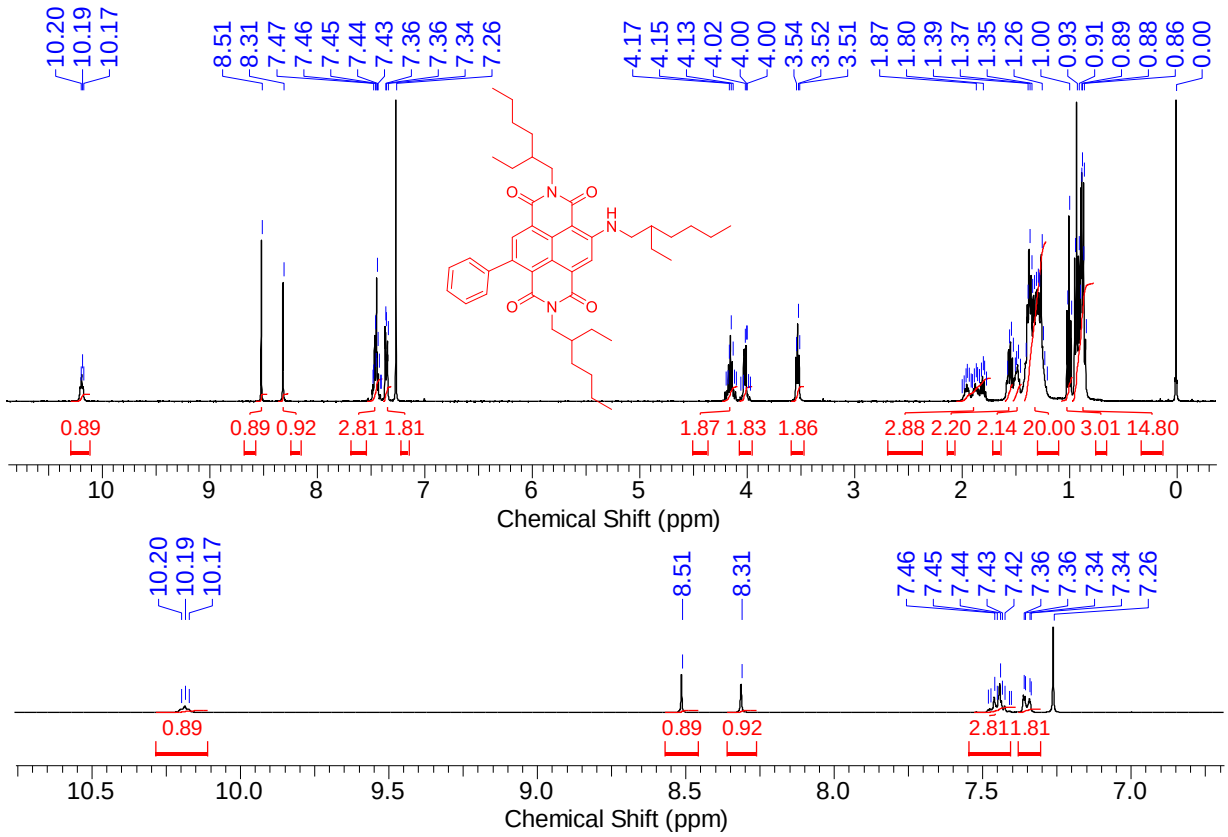


Figure S16. ^{1}H NMR spectrum of **Ph-NDI-NH** (400 MHz, $CDCl_3$), 25 °C.

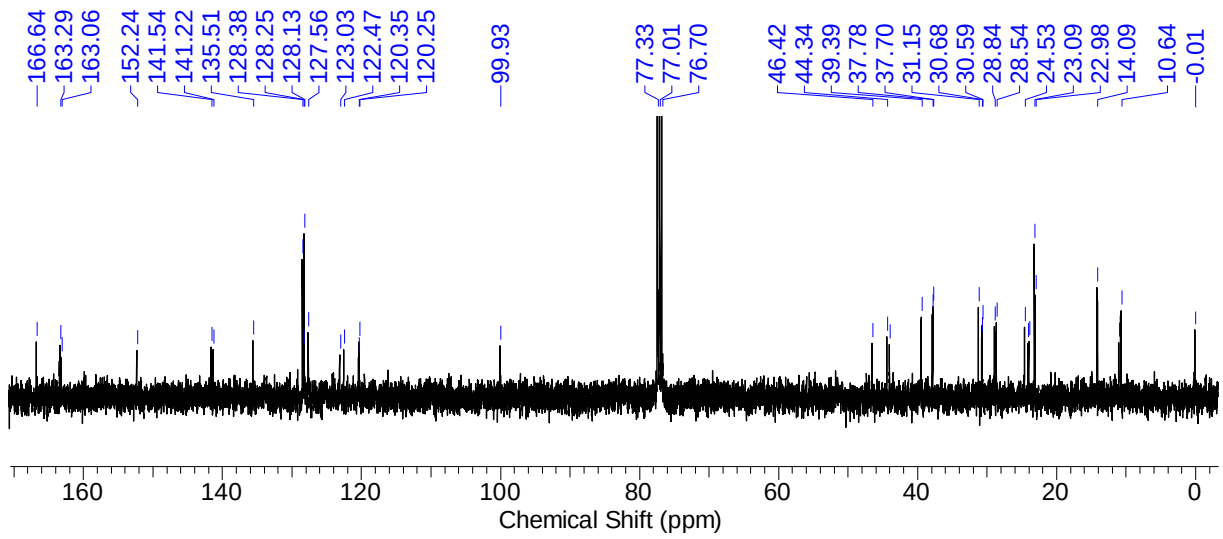
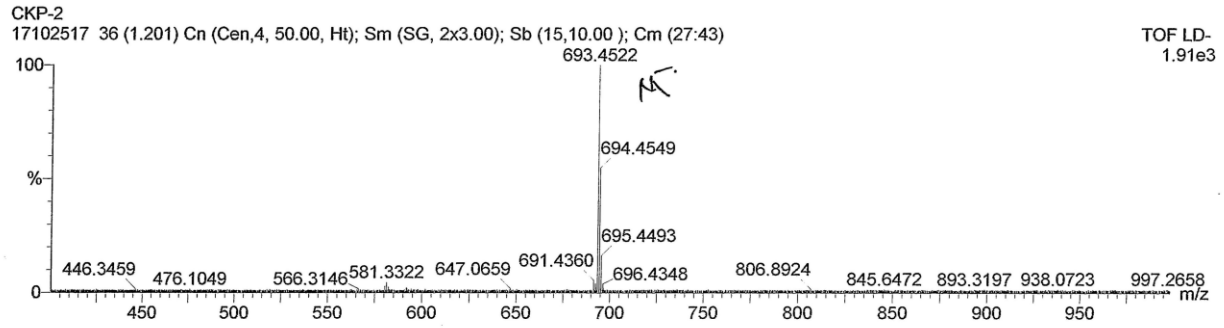


Figure S17. ^{13}C NMR spectrum of **Ph-NDI-NH** (100 MHz, $CDCl_3$), 25 °C.



Minimum:				-100.0		
Maximum:		200.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
693.4522	693.4506	1.6	2.4	17.0	1	C44 H59 N3 O4

Figure S18. MALDI–TOF–HRMS spectrum of compound of **Ph-NDI-NH**.

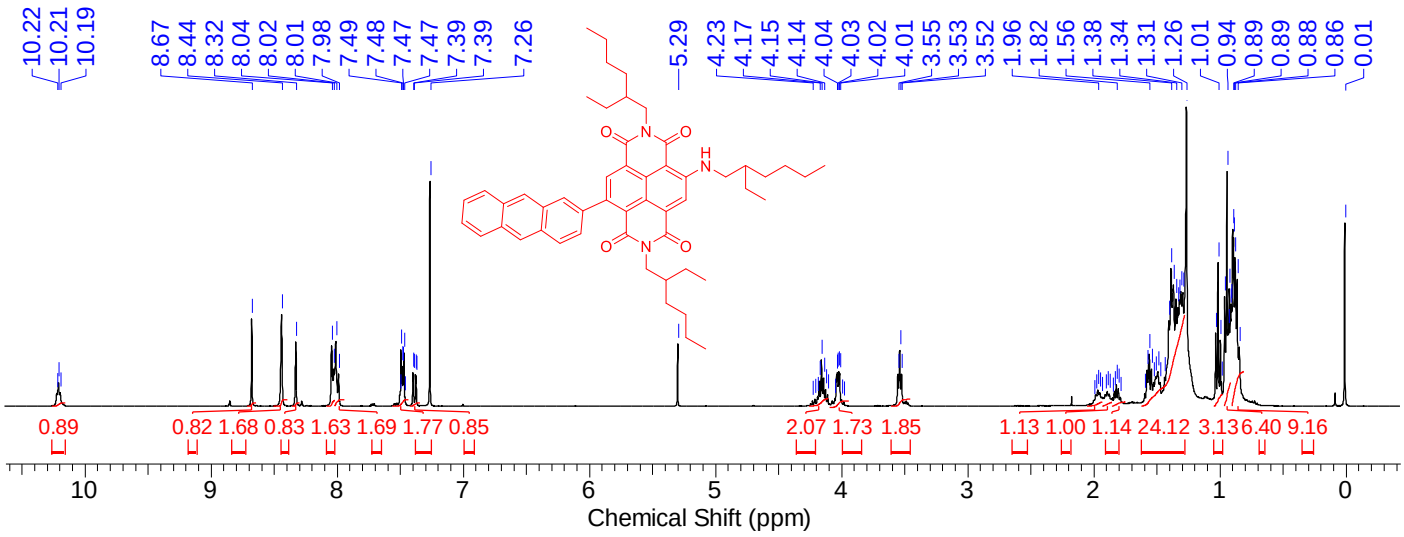


Figure S19. ^{1}H NMR spectrum of **2-An-NDI-NH** (400 MHz, $CDCl_3$), 25 °C.

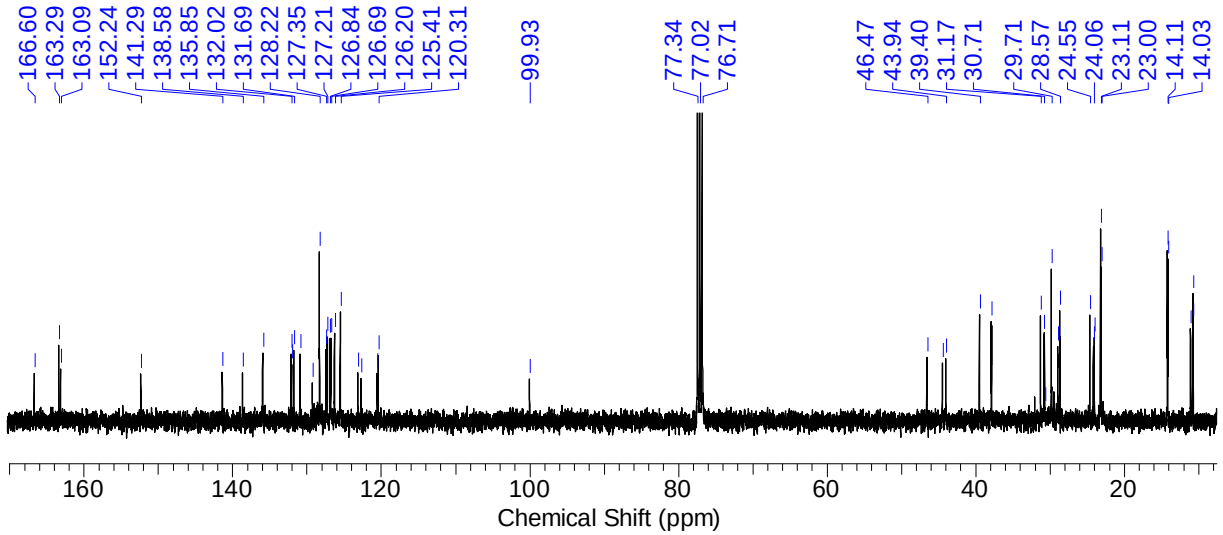
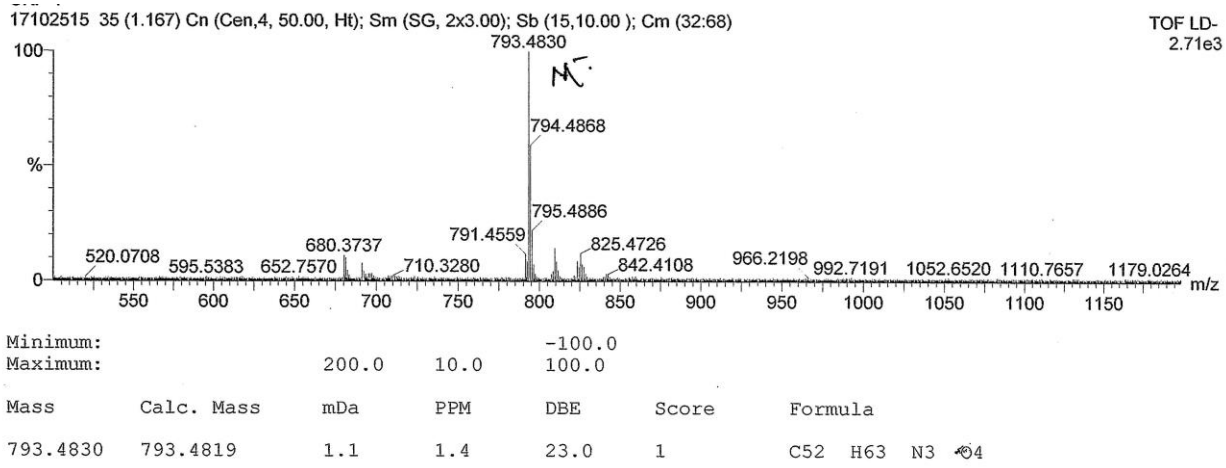


Figure S20. ^{13}C NMR spectrum of **2-An-NDI-NH** (100 MHz, $CDCl_3$), 25 °C.



Minimum:				-100.0		
Maximum:		200.0	10.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
793.4830	793.4819	1.1	1.4	23.0	1	C52 H63 N3 O4

Figure S21. MALDI–TOF–HRMS spectrum of compound of **2-An-NDI-NH**.

2. Steady State UV–Vis Absorption and Luminescence Spectra.

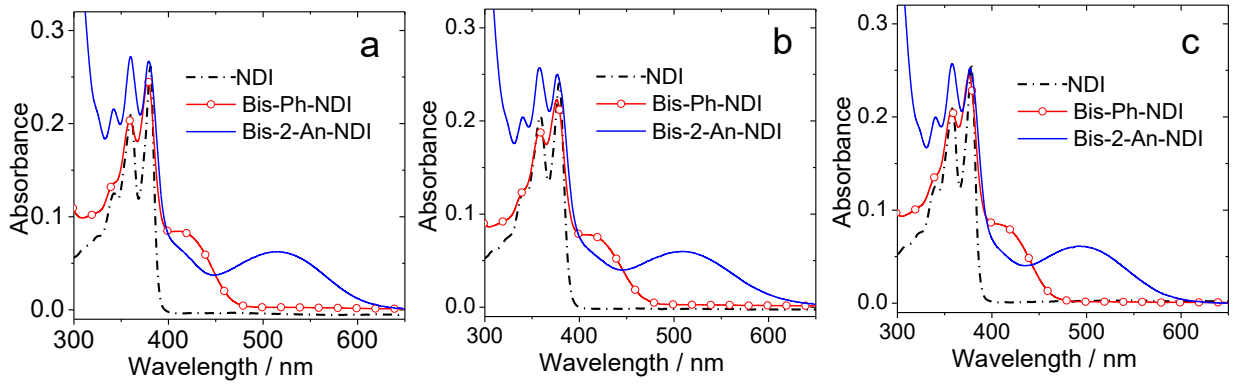


Figure S22. UV-Vis absorption spectra of **NDI**, **Bis-Ph-NDI** and **Bis-2-An-NDI** in (a) DCM, (b) MeOH, (c) CH_3CN; $c = 1.0 \times 10^{-5}$ M, 20 °C.

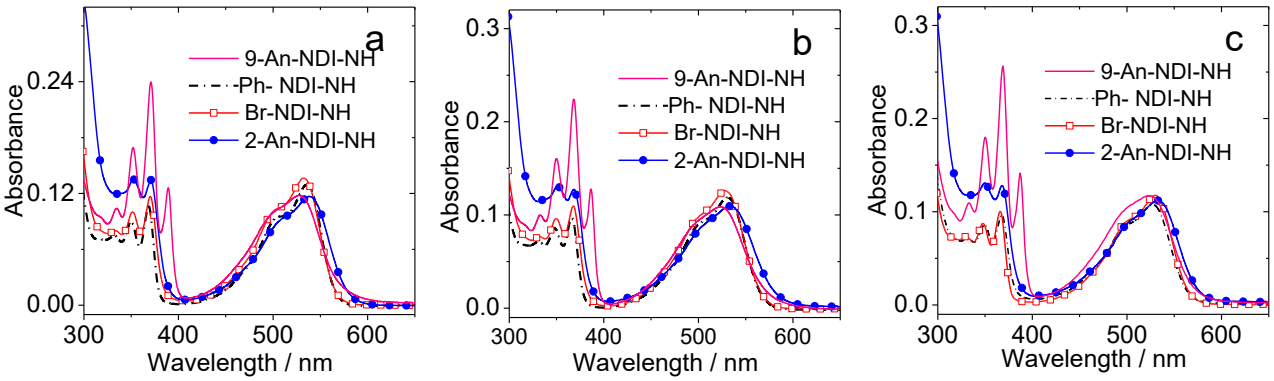


Figure S23. UV-Vis absorption spectra of **Br-NDI-NH**, **Ph-NDI-NH**, **2-An-NDI-NH** and **9-An-NDI-NH** in (a) DCM, (b) MeOH, (c) CH_3CN; $c = 1.0 \times 10^{-5}$ M, 20 °C.

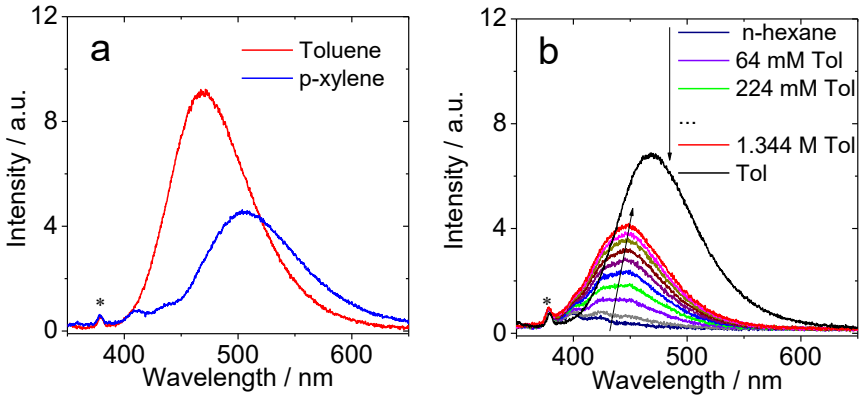


Figure S24. (a) Fluorescence emission spectra of **NDI** in different aromatic solutions, Optically matched solutions were used (A = 0.126). (b) Changes of the emission spectrum of **NDI** in *n*-hexane in presence of different eq. toluene. λ_{ex} = 340 nm, $c = 1.0 \times 10^{-5}$ M, 20 °C.

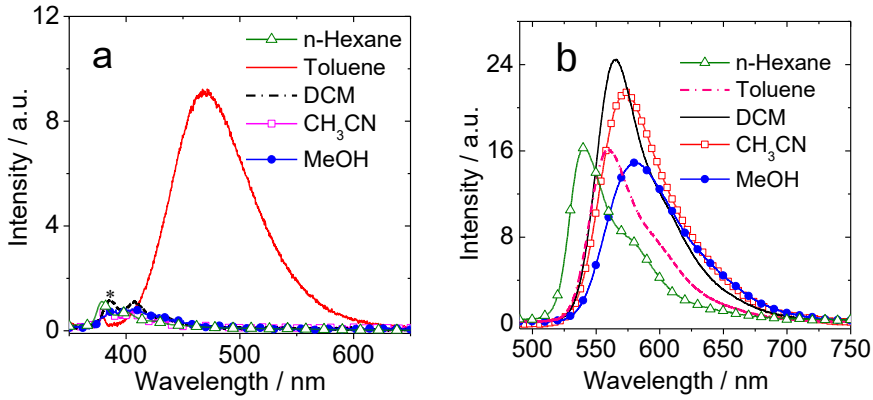


Figure S25. Fluorescence emission spectra of (a) **NDI** (A = 0.126, λ_{ex} = 340 nm), the asterisk designates the Raman scattering peak of the solvent molecules; (b) **Br-NDI-NH** (A = 0.035, λ_{ex} = 470 nm) in different solvents; Optically matched solutions were used, 20 °C.

3. Fluorescence lifetimes of the compounds.

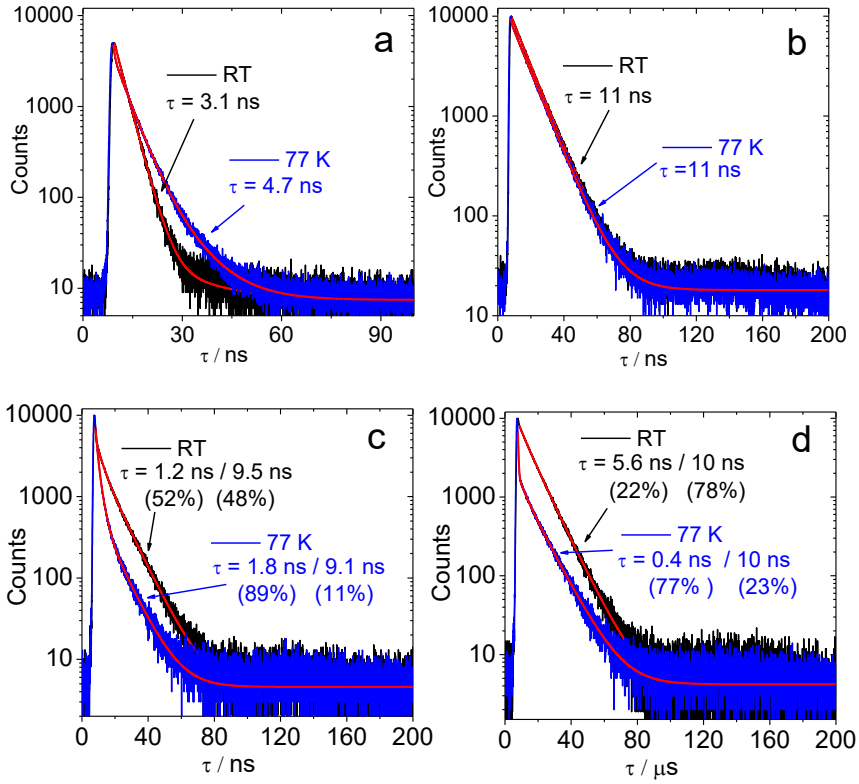


Figure S26. Decay traces of the fluorescence of (a) **Br-NDI-NH**, (b) **Ph-NDI-NH**, (c) **2-An-NDI-NH,** (d) **9-An-NDI-NH** at 570 nm**.** Excited with picoseconds pulsed laser, $c = 1.0 \times 10^{-5}$ M in toluene, $\lambda_{ex} = 445$ nm, 20 °C.

Table S1. Fluorescence Lifetimes of the Compounds [a]

	τ_F /ns [b]	τ_F /ns [c]	τ_F/ns [d]	τ_F /ns [e]	τ_F/ns [f]	τ_F /ns [g]	τ_F /ns [h]
NDI	0.65	_ [i]	_ [i]	_ [i]	_ [i]	_ [i]	_ [i]
Br-NDI-NH	3.1	4.7	3.7	4.5	4.5	4.6	5.4
Ph-NDI-NH	11	11	8.5	11	11	8.7	11
2-An-NDI-NH	1.2 (52%)	1.8 (89%)	1.7 (46%)	2.2 (85%)	4.8 (35%)	2.8 (50%)	5.9 (59%)
	9.5 (48%)	9.1 (11%)	7.7 (54%)	9.3 (15%)	11 (65%)	7.7 (50%)	11 (41%)
9-An-NDI-NH	5.6 (22%)	0.4 (77%)	0.58(24%)	1.7 (30%)	8.9 (72%)	6.6 (53%)	9.7 (95%)
	10 (78%)	10 (23%)	7.6 (76%)	11 (70%)	12 (28%)	8.9 (47%)	14 (5%)

[a] $c = 1.0 \times 10^{-5}$ M. For **NDI**, $\lambda_{ex} = 340$ nm. For other compounds, $\lambda_{ex} = 445$ nm and biexponential fitting was used for PET. [b] In toluene, RT. [c] In toluene, 77 K. [d] In MeTHF, RT. [e] In MeTHF, 77 K. [f] In DCM, RT. [g] In MeOH, RT. [h] In CH_3CN, RT. [i] Not applicable.

4. Nanosecond Transient Absorption Spectra.

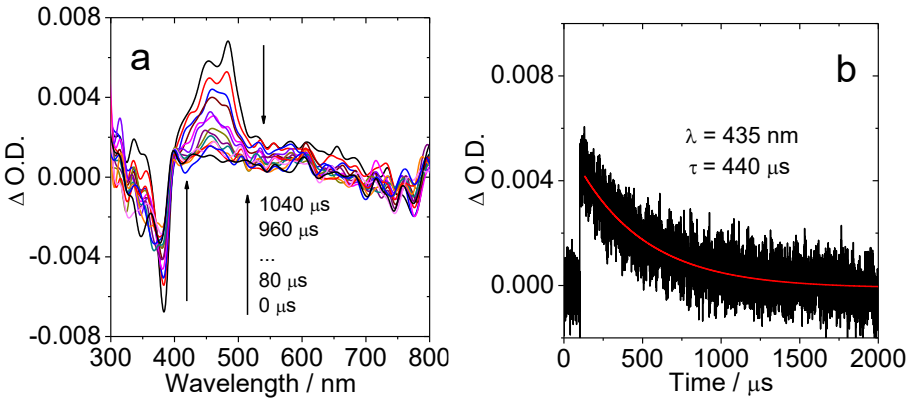


Figure S27. Nanosecond time-resolved transient absorption spectra of (a) **NDI** with different delay time in toluene. Decay trace of (b) **NDI** (λ_{ex} = 355 nm, c = 2.0 × 10^{-5} M in toluene) at 435 nm, 25 °C.

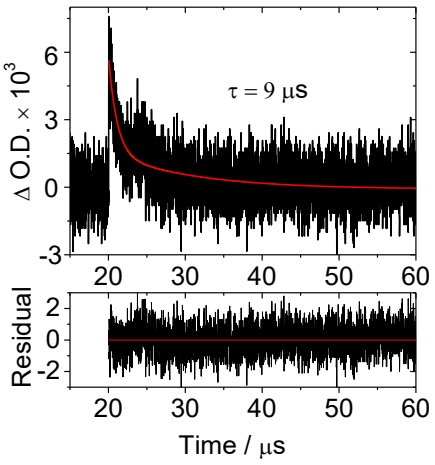


Figure S28. Decay trace of **Bis-2-An-NDI** at 440 nm (λ_{ex} = 532 nm) in DCM. c (**Bis-2-An-NDI**) = 4.0 × 10^{-5} M, 25 °C.

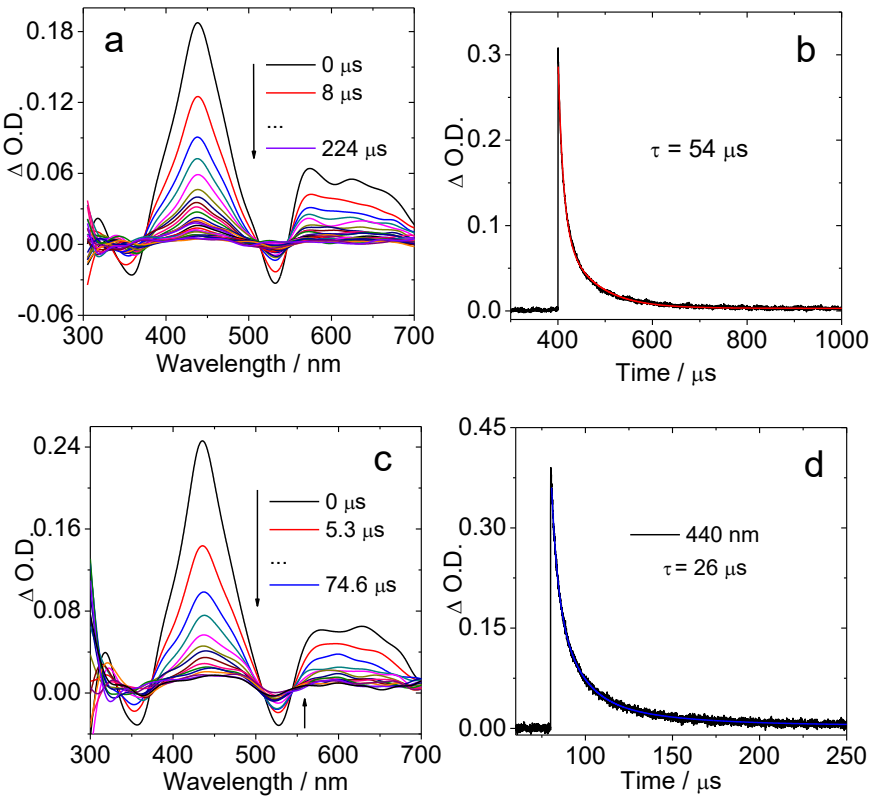


Figure S29. Nanosecond time-resolved transient absorption spectra of compound **Br-NDI-NH**. Transient absorption with different delay time in (a) DCM, (c) CH_3CN. Decay trace of **Br-NDI-NH** at 440 (λ_{ex} = 532 nm) in (b) DCM, (d) CH_3CN. *c* (**Br-NDI-NH**) = 4.0×10^{-5} M, 25 °C.

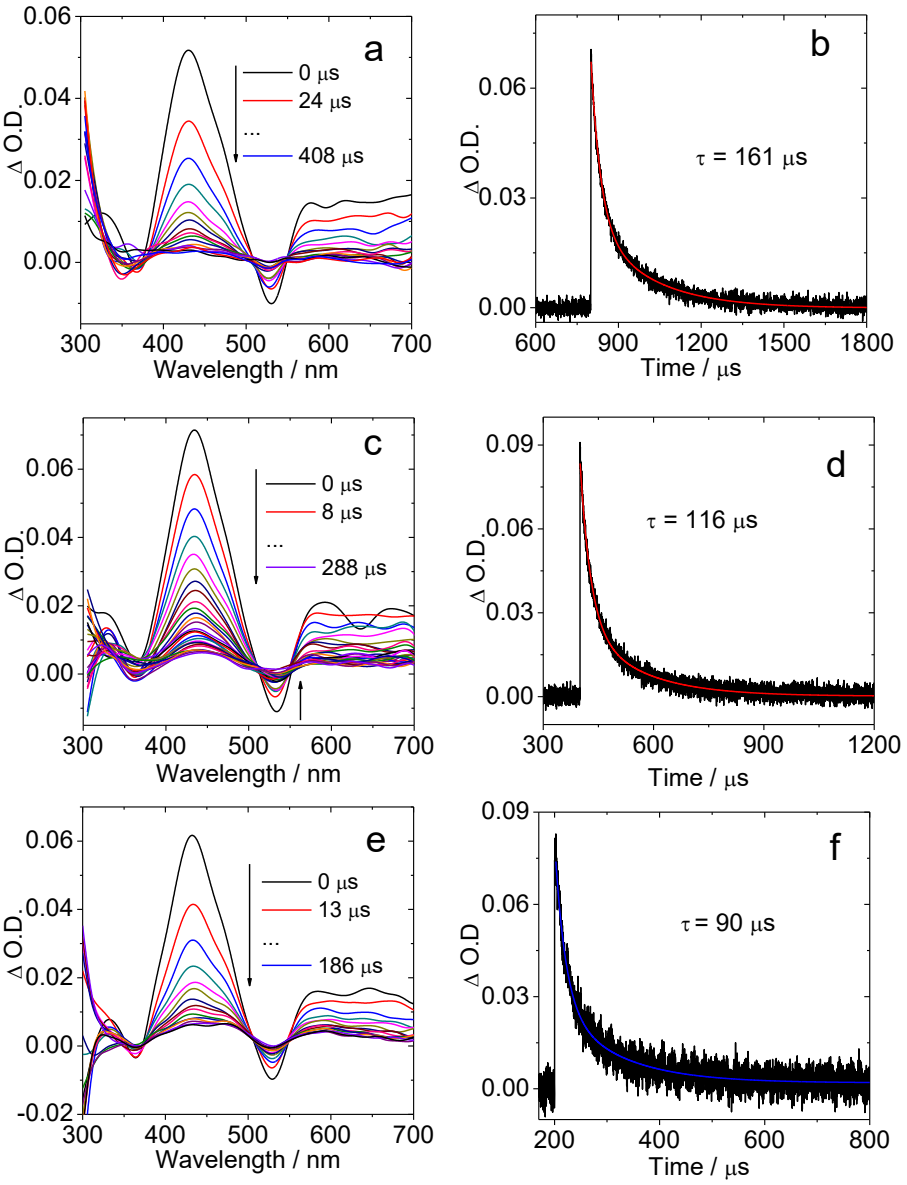


Figure S30. Nanosecond time-resolved transient absorption spectra of compound **Ph-NDI-NH**. Transient absorption with different delay time in (a) toluene, (c) DCM and (e) CH_3CN. Decay trace of **Ph-NDI-NH** at 440 nm (λ_{ex} = 532 nm) in (b) toluene, (d) DCM and (f) CH_3CN. *c* (**Ph-NDI-NH**) = 4.0×10^{-5} M, 25 °C.

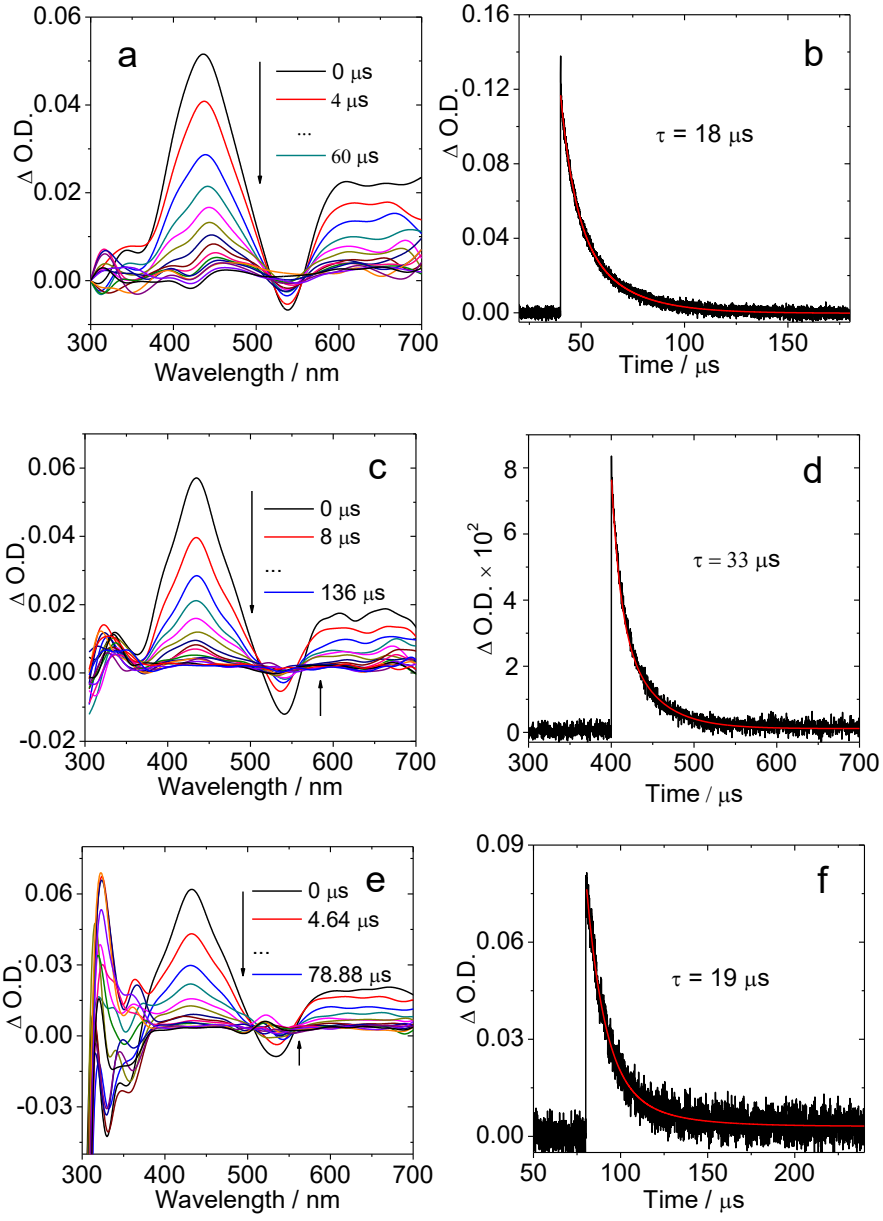


Figure S31. Nanosecond time-resolved transient absorption spectra of compound **2-An-NDI-NH**. Transient absorption with different delay time in (a) DCM, (c) CH_3CN. Decay trace of **2-An-NDI-NH** at 440 nm (λ_{ex} = 532 nm) in (b) DCM, (d) CH_3CN. *c* (**2-An-NDI-NH**) = 4.0×10^{-5} M, 25 °C.

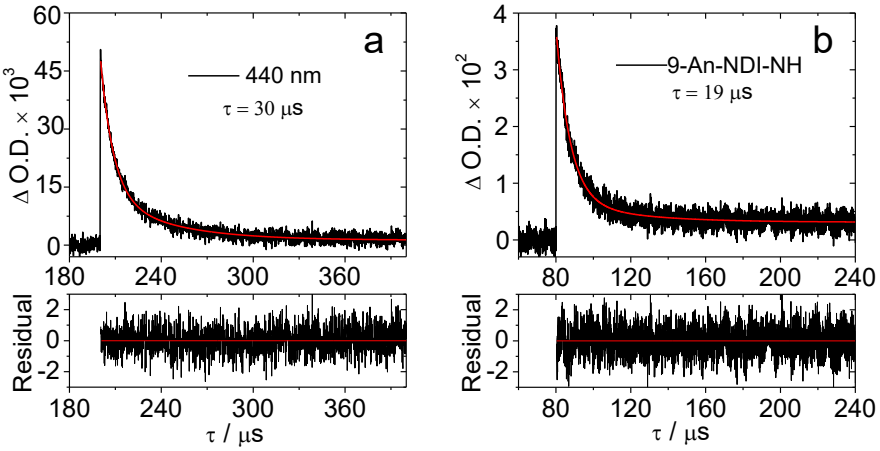


Figure S32. Nanosecond time-resolved transient absorption spectra of compound **9-An-NDI-NH**. Decay trace of **9-An-NDI-NH** at 440 nm (λ_{ex} = 532 nm) in (a) DCM and (b) CH_3CN. *c* (**9-An-NDI-NH**) = 4.0×10^{-5} M, 25 °C.

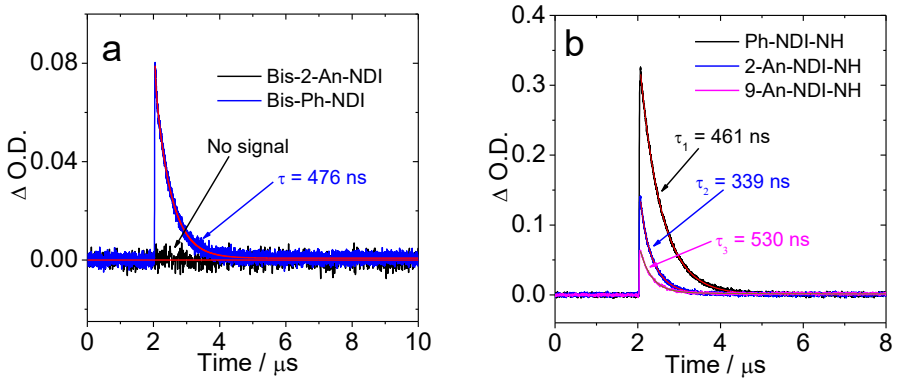


Figure S33. Nanosecond time-resolved transient absorption with different delay time. (a) Decay trace of **Bis-2-An-NDI** and **Bis-Ph-NDI**; (b) Decay trace of **Ph-NDI-NH**, **2-An-NDI-NH** and **9-An-NDI-NH**. $c = 4.0 \times 10^{-5}$ M in aerated toluene, 25 °C.

5. Femtosecond Transient Absorption Spectra.

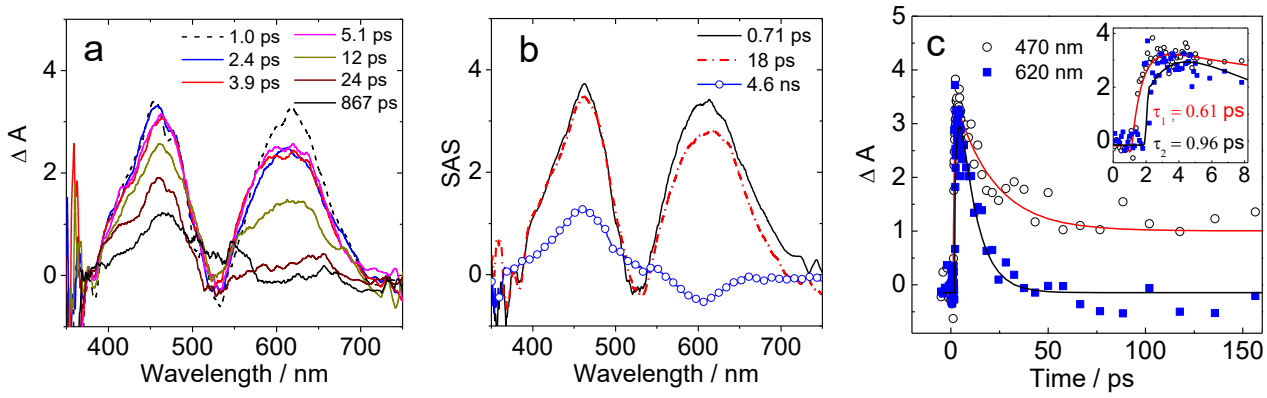


Figure S34. (a) fs TA spectra **9-An-NDI-NH** in CH_3CN; (b) Corresponding SADS obtained from target analysis and (c) Kinetic traces at selected wavelengths with their fitting lines; λ_{ex} = 340 nm, 20 °C.

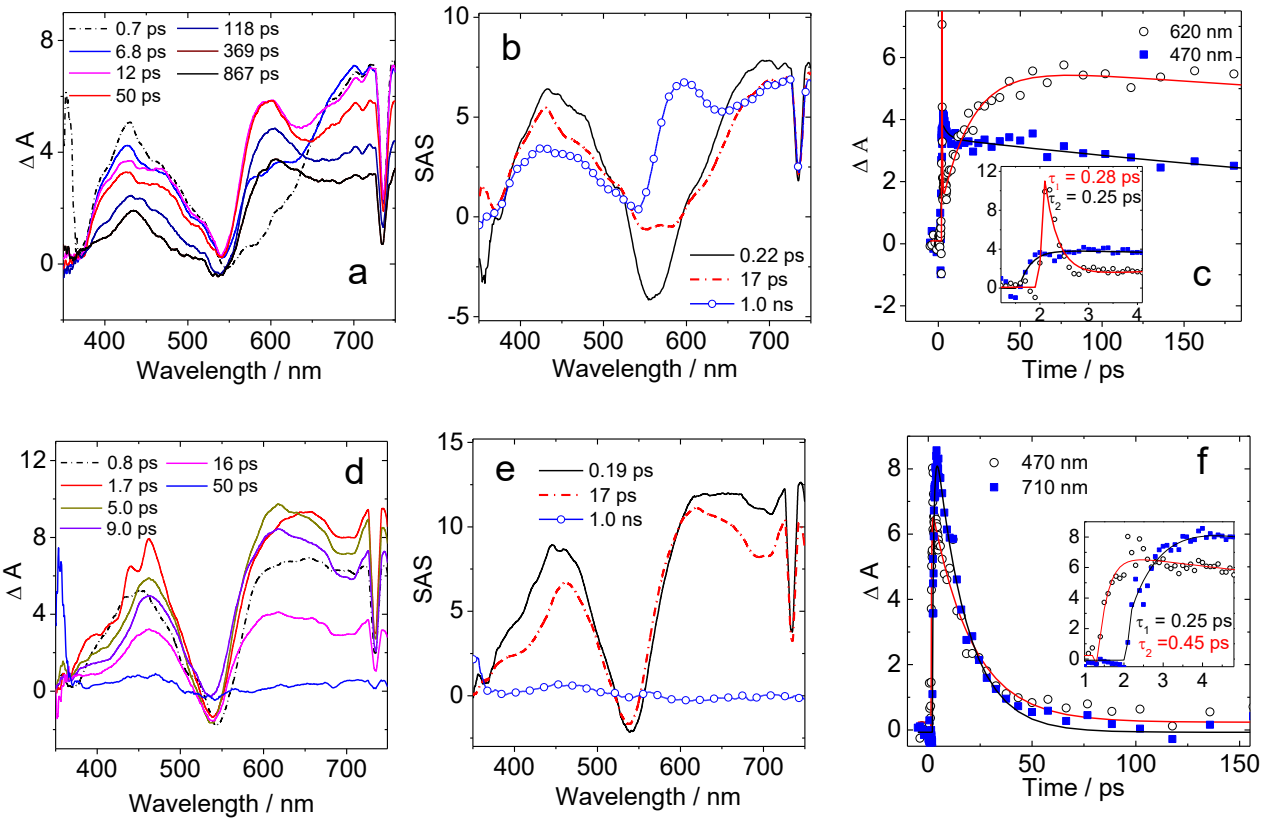


Figure S35. (a) Femtosecond transient absorption spectra of **2-An-NDI-NH** in toluene, (b) Corresponding species-associated difference spectra (SADS) obtained from target analysis and (c) Kinetic traces at selected wavelengths; (d) fs TA spectra **2-An-NDI-NH** in CH_3CN, (e) Corresponding SADS obtained from target analysis and (f) Kinetic traces at selected wavelengths with their fitting lines; λ_{ex} = 340 nm, 20 °C.

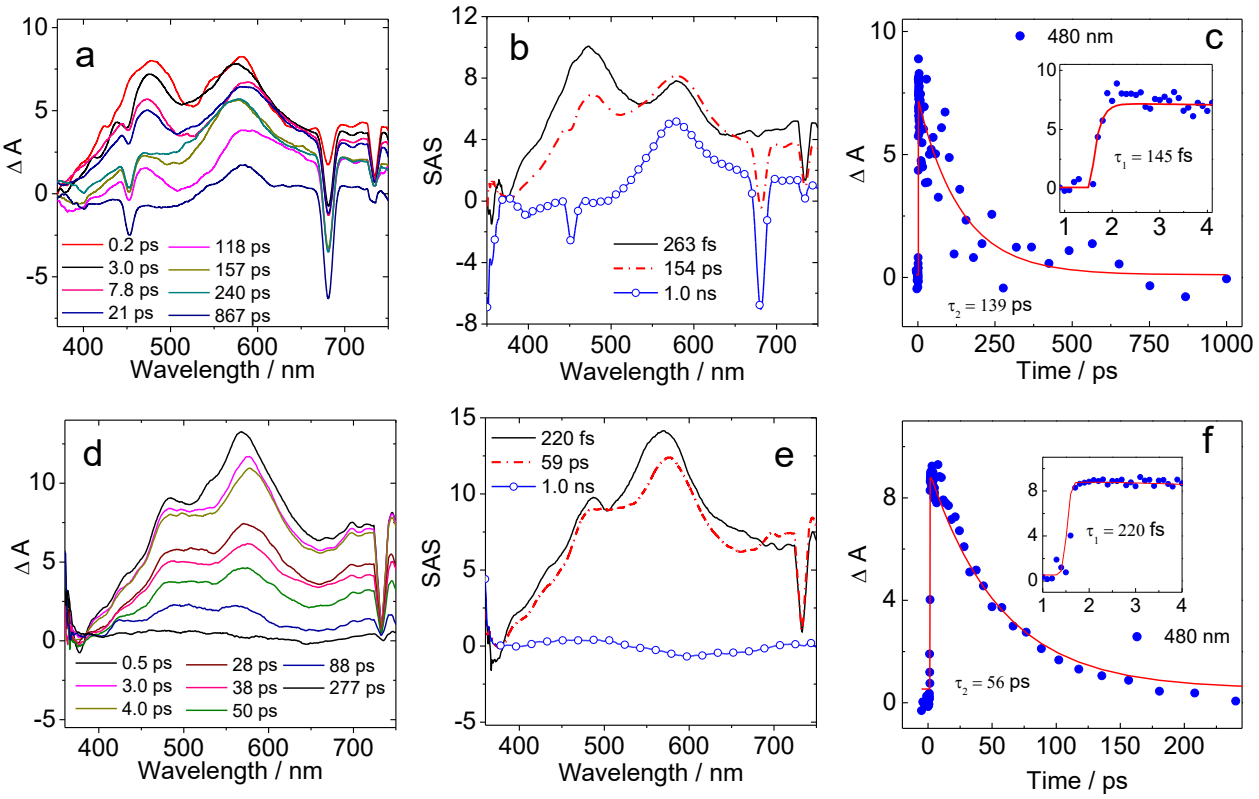


Figure S36. (a) Femtosecond transient absorption spectra of **Bis-2-An-NDI** in toluene, (b) Corresponding species-associated difference spectra (SADS) obtained from target analysis and (c) Kinetic traces at selected wavelengths; (d) fs TA spectra **Bis-2-An-NDI** in CH_3CN, (e) Corresponding SADS obtained from target analysis and (f) Kinetic traces at selected wavelengths with their fitting lines; λ_{ex} = 340 nm, 20 °C.

6. Fluorescence Up-conversion Spectra

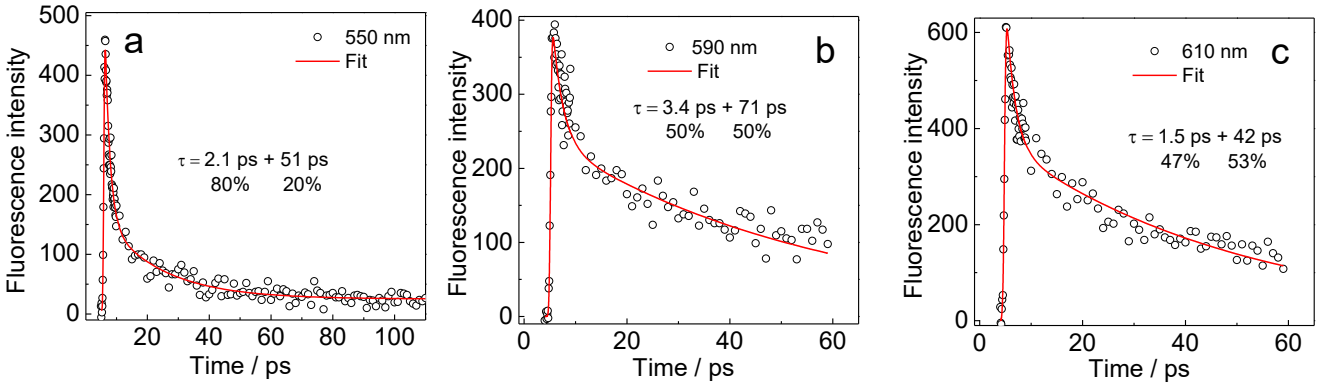
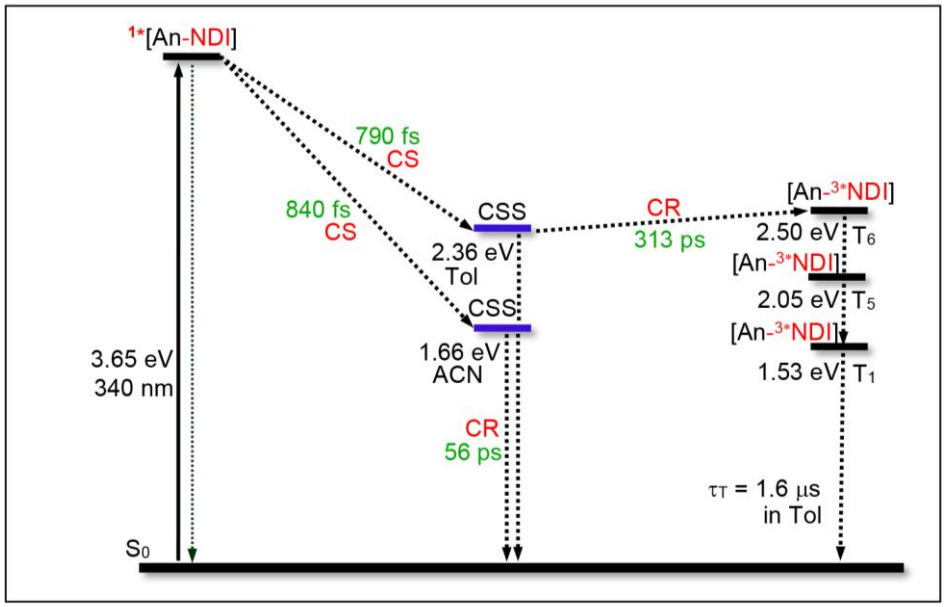


Figure S37. Fluorescence decay kinetics of **9-An-NDI-NH** in toluene (a) at 550 nm, (b) at 590 nm, (c) at 610 nm. λ_{ex} = 400 nm, 20 °C.

7. Photophysical Processes of Bis-2-An-NDI.

Scheme S1. Simplified Jablonski Diagram Illustrating the Photophysical Processes of Bis-2-An-NDI.[a]



[a] Key words: The energy levels of singlet state origin from CT state absorption, the energy level of charge separated state comes from electrochemical parameters and that of triplet state were obtained by DFT calculation. 'Tol' stands for toluene and "ACN" stands for CH_3CN. An stands for "Anthracene"; NDI stands for "Naphthalenediimide".

8. DFT/TDDFT Calculations.

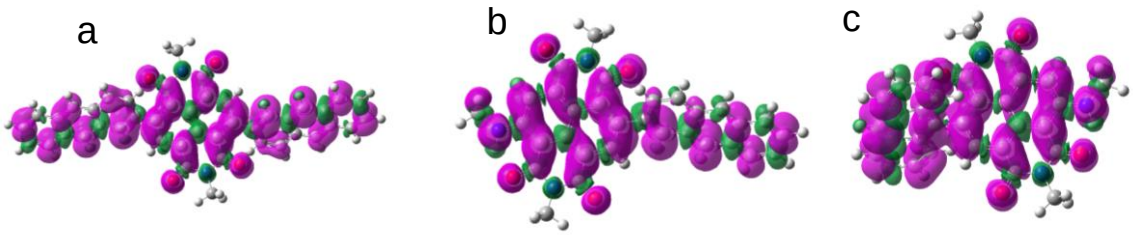


Figure S38. Spin density surfaces of (a) **Bis-2-An-NDI**, (b) **2-An-NDI-NH**, (c) **9-An-NDI-NH** at the optimized triplet state geometry; calculated at B3LYP/6-311G(d,p) level with Gaussian 09W.

Table S2. Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations, and CI Coefficients of the Low-Lying Electronic Excited States of **Bis-2-An-NDI**. The electronic transitions were calculated by TDDFT//B3LYP/6-311G(d, p), based on the DFT//B3LYP/6-311G(d)-optimized ground state and excited geometries [a]

	Transitions [b]	Excitation Energy	*f* [c]	CI [d]	MOs [e]
Excitation	$S_0 \rightarrow S_1$	1.67 eV/744 nm	0.106	0.705	H → L
	$S_0 \rightarrow S_2$	1.70 eV/729 nm	0.000	0.705	H–1 → L
	$S_0 \rightarrow S_3$	2.60 eV/477 nm	0.153	0.694	H–2 → L
	$S_0 \rightarrow S_9$	3.27 eV/379 nm	0.119	0.635	H–4 → L
	$S_0 \rightarrow S_{13}$	3.42 eV/363 nm	0.191	0.384	H–6 → L
Emission	$S_0 \rightarrow S_1$	1.10 eV/1125 nm	0.000	0.704	H → L
	$S_0 \rightarrow S_2$	1.42 eV/871 nm	0.041	0.705	H–1 → L
	$S_0 \rightarrow S_8$	3.01 eV/412 nm	0.041	0.596	H → L + 2
Triplet	$T_0 \rightarrow T_1$	1.53 eV/813 nm	0.000 [f]	0.653	H → L
	$T_0 \rightarrow T_2$	1.58 eV/784 nm	0.000 [f]	0.655	H–1 → L
	$T_0 \rightarrow T_3$	1.93 eV/643 nm	0.000 [f]	0.458	H → L+2
	$T_0 \rightarrow T_4$	1.93 eV/641 nm	0.000 [f]	0.441	H–1 → L+2
	$T_0 \rightarrow T_8$	2.98 eV/415 nm	0.000 [f]	0.612	H–8 → L

[a] TDDFT//B3LYP/6-311G(d, p), based on the DFT//B3LYP/6-311G(d, p)-optimized ground state geometries. [b] Only the selected low lying excited states are presented. [c] Oscillator strengths. [d] CI coefficients are in absolute values. [e] Molecular orbits involved in the transitions. Calculations were TDDFT// B3LYP/6-311G(d, p)-optimized excited state geometries. [f] No spin−orbital coupling effect was considered; thus, the *f* values are zero.

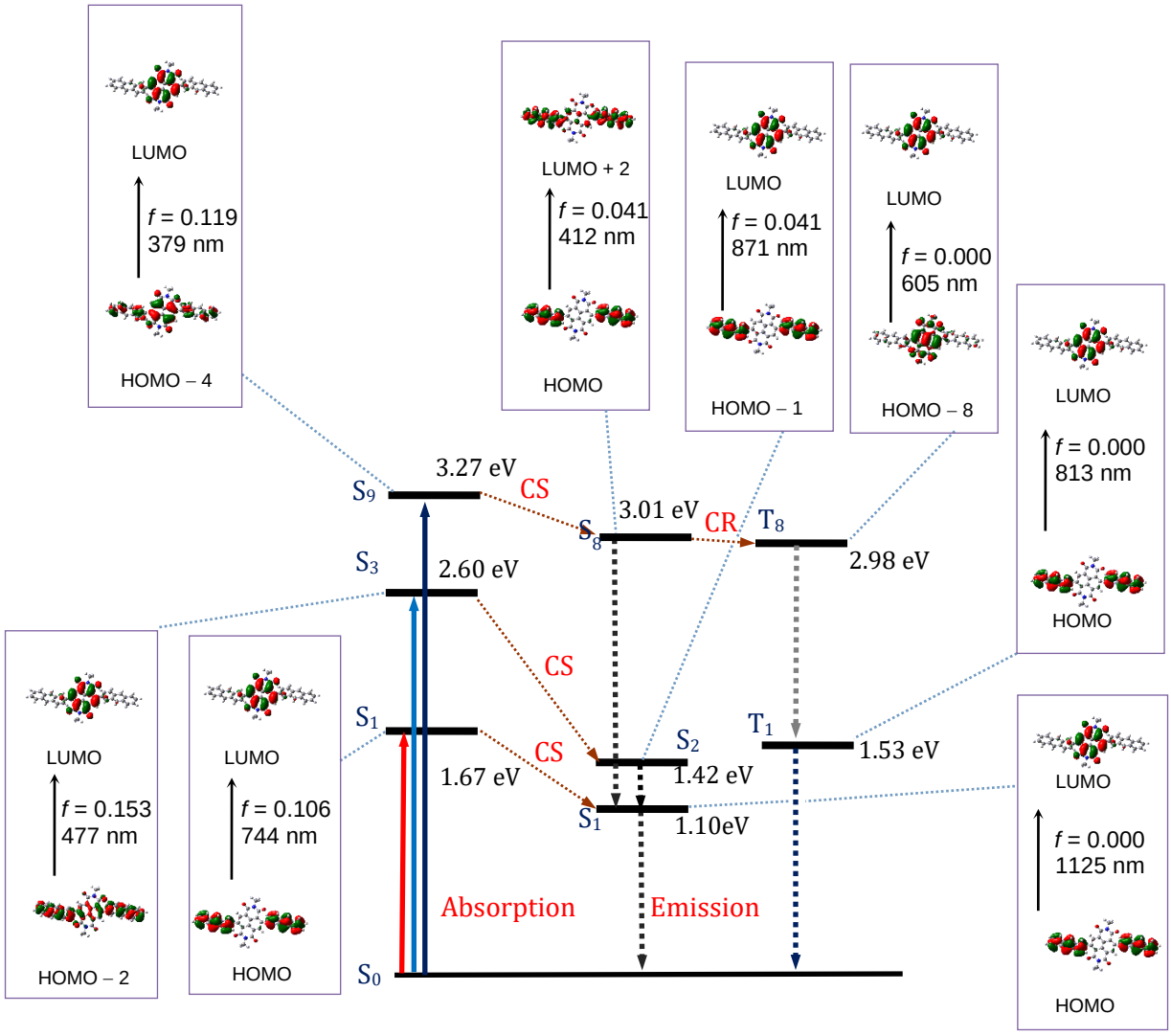


Figure S39. Selected frontier molecular orbitals involved in the excitation and triplet excited states of **Bis-2-An-NDI**. The butyl group was simplified as methylamine in the calculation. The UV−Vis absorption and the fluorescence emission were calculated by DFT and TDDFT// B3LYP/6-311G(d, p) level with Gaussian 09W, based on the optimized ground state and the excited state geometries, respectively. CS = charge separation, CR = charge recombination.

Table S3. Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations, and CI Coefficients of the Low-Lying Electronic Excited States of **2-An-NDI-NH**. The electronic transitions were calculated by TDDFT//B3LYP/6-311G(d, p), based on the DFT//B3LYP/6-311G(d, p)-optimized ground state and excited geometries.

	Transitions [b]	Excitation Energy	*f* [c]	CI [d]	MOs [e]
Excitation	$S_0 \rightarrow S_1$	1.80 eV/688 nm	0.036	0.705	H → L
	$S_0 \rightarrow S_2$	2.55 eV/486 nm	0.164	0.695	H–1 → L
	$S_0 \rightarrow S_3$	2.88 eV/432 nm	0.022	0.682	H–2 → L
	$S_0 \rightarrow S_8$	3.52 eV/352 nm	0.116	0.650	H–4 → L
Emission	$S_0 \rightarrow S_1$	1.47 eV/844 nm	0.052	0.704	H → L
	$S_0 \rightarrow S_7$	3.24 eV/382 nm	0.000	0.675	H–6 → L
Triplet	$T_0 \rightarrow T_1$	1.60 eV/773 nm	0.000 [f]	0.545	H → L
	$T_0 \rightarrow T_2$	1.81 eV/685 nm	0.000 [f]	0.518	H–1 → L
	$T_0 \rightarrow T_3$	1.95 eV/635 nm	0.000 [f]	0.500	H → L+1
	$T_0 \rightarrow T_4$	2.44 eV/509 nm	0.000 [f]	0.674	H–4 → L
	$T_0 \rightarrow T_5$	2.71 eV/458 nm	0.000 [f]	0.631	H–2 → L
	$T_0 \rightarrow T_7$	3.21 eV/386 nm	0.000 [f]	0.509	H–5 → L
	$T_0 \rightarrow T_8$	3.28 eV/378 nm	0.000 [f]	0.339	H–5 → L

[a] TDDFT//B3LYP/6-311G(d, p), based on the DFT//B3LYP/6-311G(d, p)-optimized ground state geometries. [b] Only the selected low lying excited states are presented. [c] Oscillator strengths. [d] CI coefficients are in absolute values. [e] TDDFT// B3LYP/6-311G(d, p)-optimized excited state geometries. [f] No spin−orbital coupling effect was considered; thus, the f values are zero.

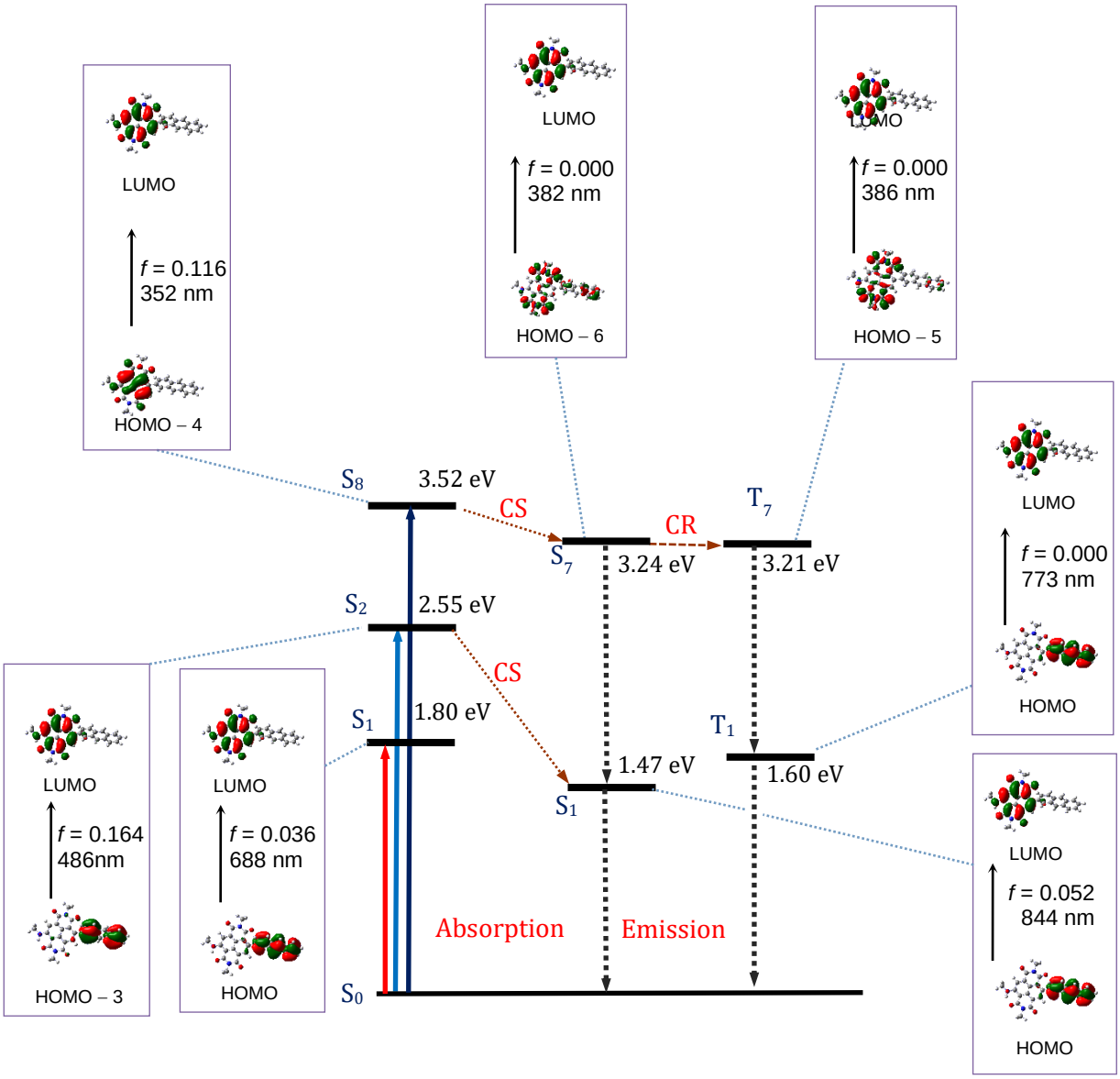


Figure S40. Selected frontier molecular orbitals involved in the excitation and triplet excited states of **2-An-NDI-NH**. The butyl group was simplified as methylamine in the calculation. The UV−Vis absorption and the fluorescence emission were calculated by DFT and TDDFT// B3LYP/6-311G(d, p) level with Gaussian 09W, based on the optimized ground state and the excited state geometries, respectively. CS = charge separation, CR = charge recombination.

Table S4. Electronic Excitation Energies (eV) and Corresponding Oscillator Strengths (*f*), Main Configurations, and CI Coefficients of the Low-Lying Electronic Excited States of **9-An-NDI-NH**. The electronic transitions were calculated by TDDFT//B3LYP/6-311G(d, p), based on the DFT//B3LYP/6-311G(d, p)-optimized ground state and excited geometries.

	Transitions [b]	Excitation Energy	*f* [c]	CI [d]	MOs [e]
Excitation	$S_0 \rightarrow S_1$	1.60 eV/773 nm	0.000	0.704	H → L
	$S_0 \rightarrow S_2$	2.64 eV/470 nm	0.156	0.700	H–1 → L
	$S_0 \rightarrow S_3$	2.92 eV/425 nm	0.002	0.705	H–2 → L
	$S_0 \rightarrow S_4$	3.15 eV/394 nm	0.140	0.697	H→ L+1
	$S_0 \rightarrow S_9$	3.59 eV/345 nm	0.107	0.664	H–4 → L
Emission	$S_0 \rightarrow S_1$	1.41 eV/879 nm	0.000	0.705	H → L
	$S_0 \rightarrow S_3$	2.73 eV/455 nm	0.002	0.705	H–2 → L+1
	$S_0 \rightarrow S_8$	3.37 eV/368 nm	0.000	0.695	H–6 → L
Triplet	$T_0 \rightarrow T_1$	1.59 eV/780 nm	0.000 [f]	0.703	H → L
	$T_0 \rightarrow T_2$	1.76 eV/702 nm	0.000 [f]	0.672	H–1 → L
	$T_0 \rightarrow T_3$	1.77 eV/699 nm	0.000 [f]	0.671	H–1 → L
	$T_0 \rightarrow T_4$	2.45 eV/506 nm	0.000 [f]	0.589	H–4 → L
	$T_0 \rightarrow T_5$	2.91 eV/426 nm	0.000 [f]	0.697	H–2 → L
	$T_0 \rightarrow T_8$	3.25 eV/382 nm	0.000 [f]	0.520	H–1 → L+2

[a] TDDFT//B3LYP/6-311G(d, p), based on the DFT//B3LYP/6-311G(d, p)-optimized ground state geometries. [b] Only the selected low lying excited states are presented. [c] Oscillator strengths. [d] CI coefficients are in absolute values. [e] TDDFT// B3LYP/6-311G(d, p)-optimized excited state geometries. [f] No spin−orbital coupling effect was considered; thus, the *f* values are zero.

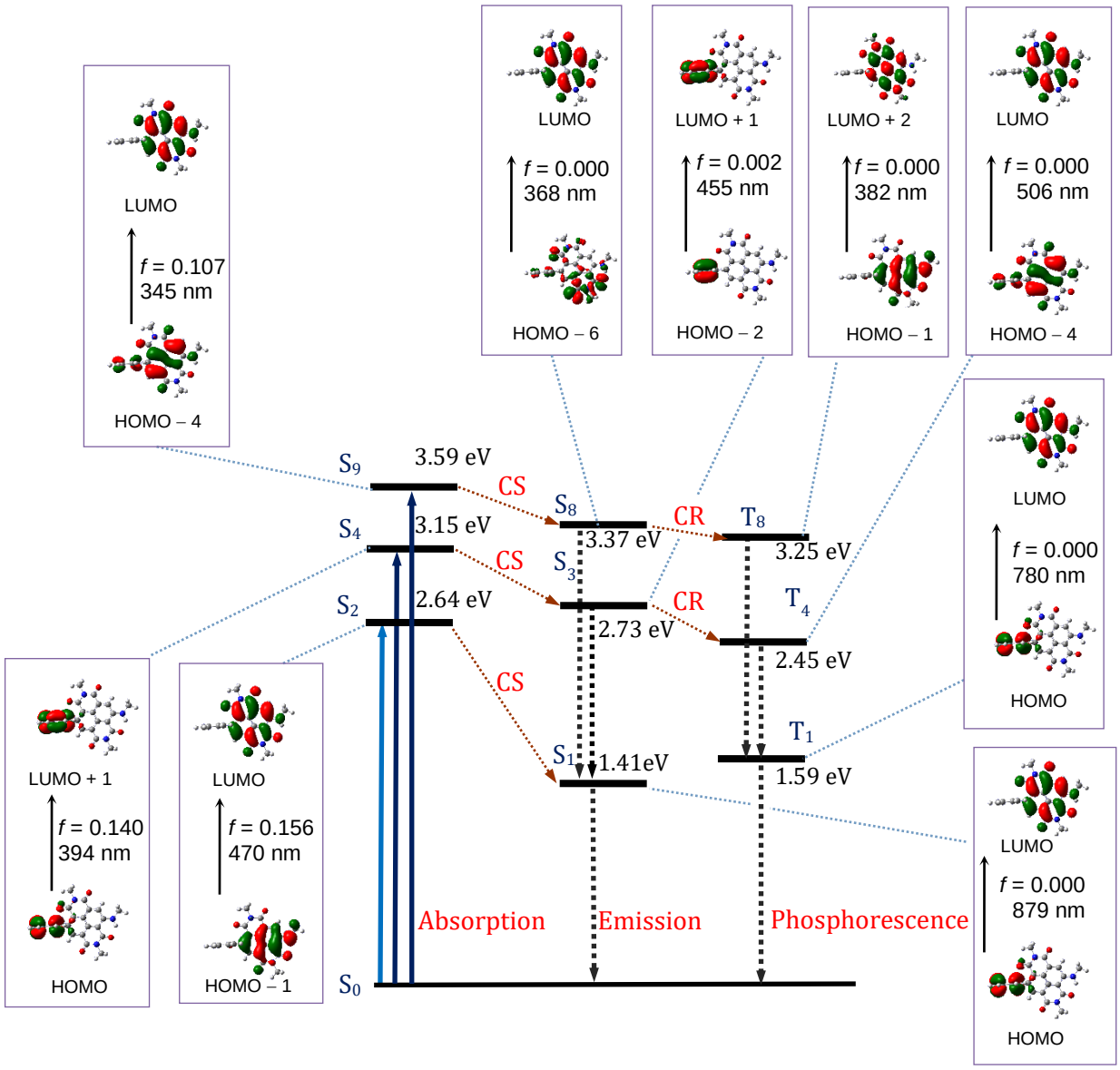


Figure S41. Selected frontier molecular orbitals involved in the excitation and triplet excited states of **9-An-NDI-NH**. The butyl group was simplified as methylamine in the calculation. The UV−Vis absorption and the fluorescence emission were calculated by DFT and TDDFT// B3LYP/6-311G(d, p) level with Gaussian 09W, based on the optimized ground state and the excited state geometries, respectively. CS = charge separation, CR = charge recombination.

9. Optimized Molecular Geometries of NDI compounds.

Optimized S0 state geometry of 2-An-NDI-NH.gjf

2-An-NDI-NH.gjf

Redundant internal coordinates taken from checkpoint file:
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Spin = Singlet
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Imaginary Freq = 0
Dipole Moment = 2.9007 Debye
Point Group = C1

Optimized S0 state geometry of 9-An-NDI-NH.gjf

9-An-NDI-NH.gjf

Redundant internal coordinates taken from checkpoint file:

9-An-NDI-NH.chk
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Spin = Singlet
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RMS Gradient Norm = 0.00003213 a.u.
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Dipole Moment = 3.0458 Debye
Point Group = C1

Optimized S0 state geometry of Bis-2-An-NDI-NH.gjf

Bis-2-An-NDI.gjf

Redundant internal coordinates taken from checkpoint file:
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C,0,4.4611917148,-1.1676362607,-1.5215960173
C,0,6.3259861762,0.1975904597,0.0946309203
H,0,4.591239342,1.0092727084,1.1002699991
C,0,5.7913939754,-1.3233804576,-1.7673964817
H,0,3.7323848839,-1.6818420992,-2.1357541934
C,0,7.2711934887,0.8551284256,0.8869172963
C,0,6.7766999602,-0.6615620018,-0.9704182113
H,0,6.1236567423,-1.9632794154,-2.5779138163
C,0,8.645058277,0.7011153085,0.6717519974
H,0,6.9315105452,1.5017988916,1.6902230571
C,0,8.1470468041,-0.8145534627,-1.1882193118
C,0,9.6219626175,1.3658239771,1.4739130183
C,0,9.0959710445,-0.1576940025,-0.3956543574
H,0,8.4863103559,-1.4610663287,-1.9918164899
C,0,10.9578586658,1.1954214022,1.2395951562
H,0,9.2816553268,2.01158071,2.2766693849
C,0,10.5003231561,-0.306969994,-0.6052832678

C,0,11.4029103263,0.3476822318,0.1859223762
H,0,11.6886443897,1.7062331715,1.8563335414
H,0,10.838984031,-0.9532391773,-1.4083086804
H,0,12.4664682675,0.2248783505,0.0151336194
C,0,-1.9560399692,2.4536396699,-0.2934971385
O,0,-3.1059648176,2.8338405265,-0.3811158887
C,0,-2.5472315069,0.0647628178,0.2679880628
C,0,-4.0026717488,0.3146697394,0.4656651676
C,0,-4.9224577453,-0.3552250373,-0.300244331
C,0,-4.4612006546,1.16763245,1.5216251963
C,0,-6.3259839182,-0.1976033654,-0.0946072347
H,0,-4.5912298655,-1.0092948503,-1.1002266396
C,0,-5.7914048237,1.3233809579,1.7674130604
H,0,-3.7323978467,1.6818431347,2.1357841926
C,0,-7.2711856939,-0.8551457469,-0.8868965201
C,0,-6.7767051853,0.6615576297,0.9704318818
H,0,-6.1236733886,1.9632873829,2.5779221269
C,0,-8.6450520146,-0.7011289315,-0.6717436831
H,0,-6.9314971335,-1.5018227058,-1.6901946867
C,0,-8.1470536396,0.8145531339,1.188220276
C,0,-9.6219507253,-1.365842204,-1.4739077384
C,0,-9.0959723205,0.1576892249,0.3956523802
H,0,-8.4863228766,1.4610727891,1.9918096055
C,0,-10.9578484537,-1.1954357433,-1.2396022923
H,0,-9.2816377688,-2.0116056211,-2.276656329
C,0,-10.5003259597,0.3069691545,0.6052683681
C,0,-11.4029075667,-0.3476877305,-0.1859397707
H,0,-11.6886298387,-1.7062510993,-1.8563428507
H,0,-10.8389925142,0.9532450715,1.4082859793
H,0,-12.4664667359,-0.2248808168,-0.0151608394

Calculation Type = FREQ
Calculation Method = RB3LYP
Basis Set = 6-311G(d,p)
Charge = 0
Spin = Singlet
E(RB3LYP) = -2103.37016681 a.u.
RMS Gradient Norm = 0.00000358 a.u.
Imaginary Freq = 0
Dipole Moment = 0.0000 Debye
Point Group = C1