Supporting Information for

Photophysical and Photochemical Features of Lysine Derivatives Bearing Two Triphenylaminocinnamic-Based Fuorophores

Mario Saletti,[a] Marco Paolino,[a] Jacopo Venditti,[a] Gianluca Giorgi,[a] Claudia Bonechi,[a] Alessandro Donati,[a] Claudio Rossi,[a] Germano Giuliani,[a] Antonella Caterina Boccia,[b] Chiara Botta,[b] Lluís Blancafort,[c] Andrea Cappelli.[,a]*

[a]Dipartimento di Biotecnologie, Chimica e Farmacia, Università degli Studi di Siena, Via Aldo Moro 2, 53100 Siena, Italy

[b]Istituto di Scienze e Tecnologie Chimiche "G. Natta" - SCITEC (CNR), Via A. Corti 12, 20133 Milano, Italy

[c]Institute of Computational Chemistry and Catalysis and Department of Chemistry, University of Girona, C/ M. A. Capmany 69, 17003 Girona, Spain

*Corresponding author. Tel: +39 0577 232416. E-mail: andrea.cappelli@unisi.it.

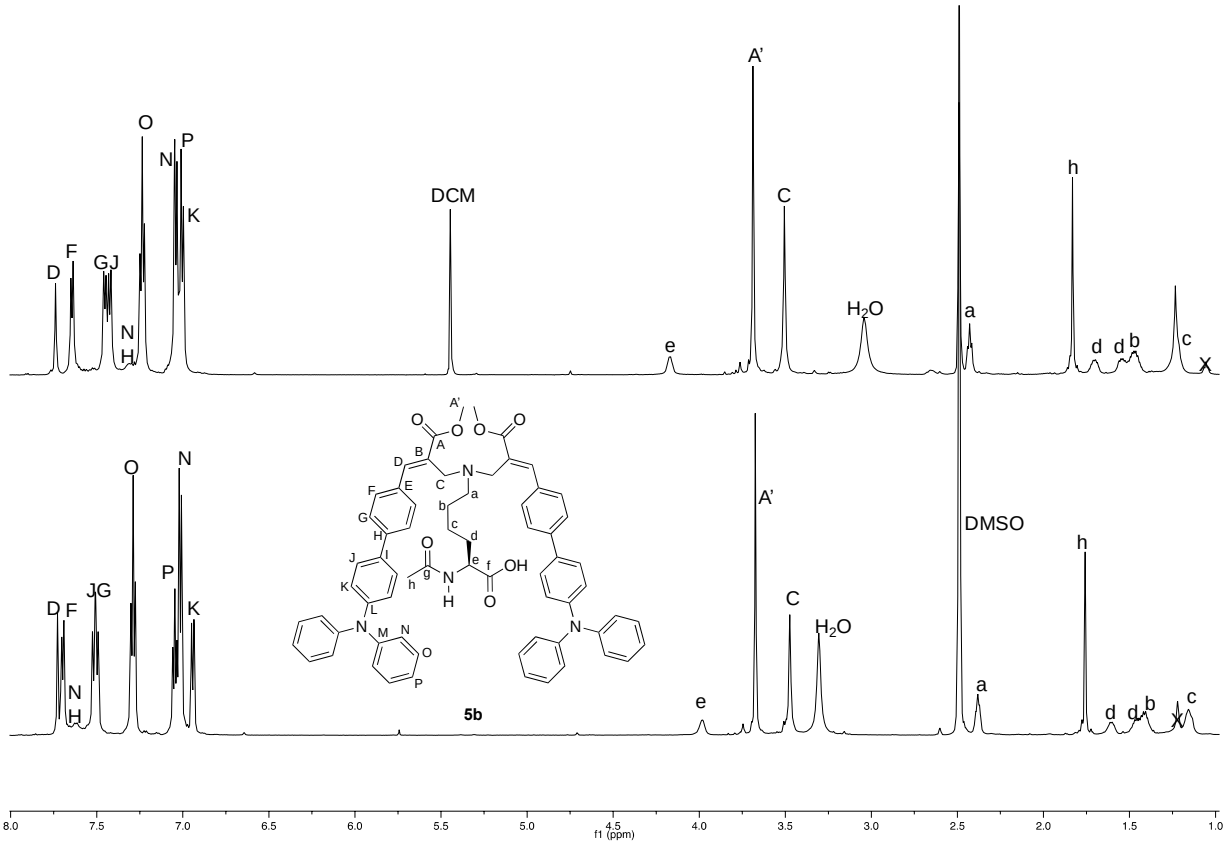

Figure S1. Comparison of the ^{1}H NMR spectra of diadduct **5b** recorded in DMSO-d_6 (bottom) or CD_2Cl_2-DMSO-d_6 (2:1) (top) at 600 MHz.

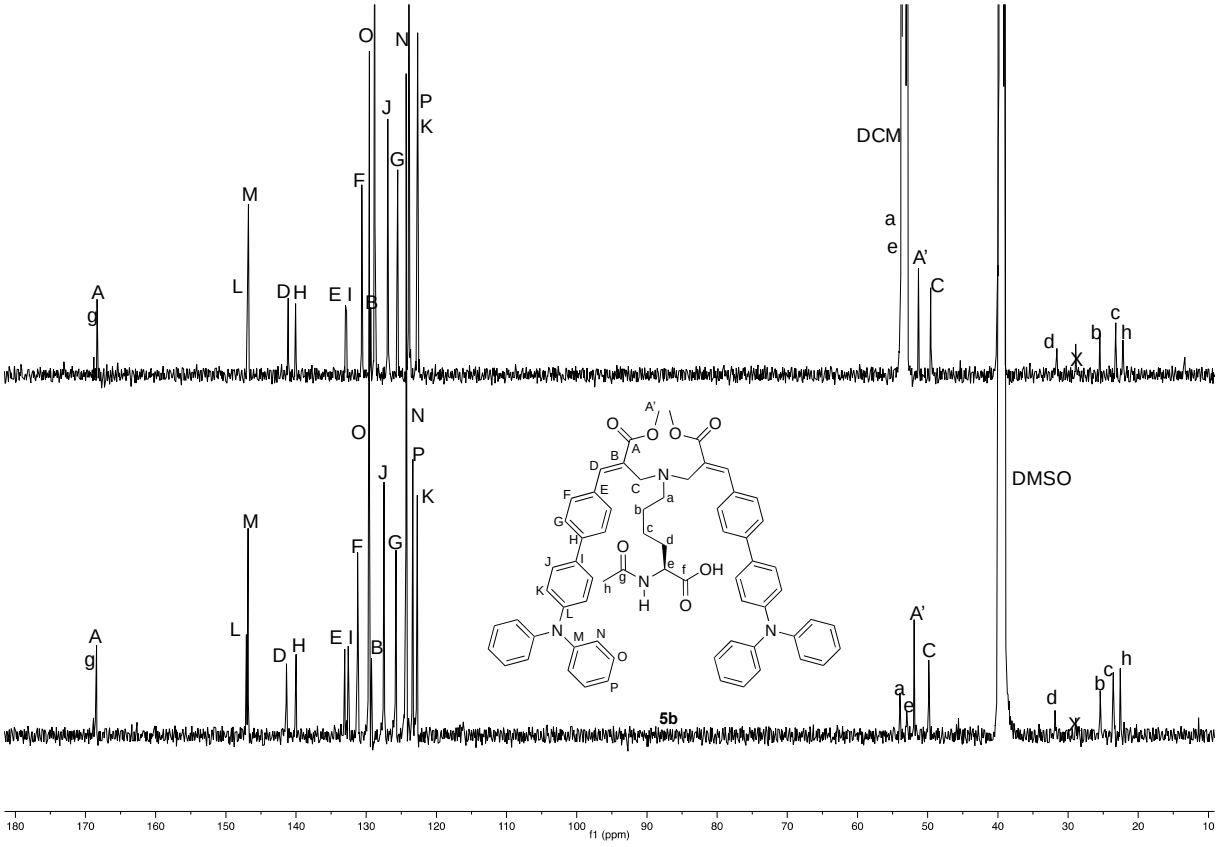

Figure S2. Comparison of the ^{13}C NMR spectra of diadduct **5b** recorded in DMSO-d_6 (bottom) or CD_2Cl_2-DMSO-d_6 (2:1) (top) at 150 MHz.

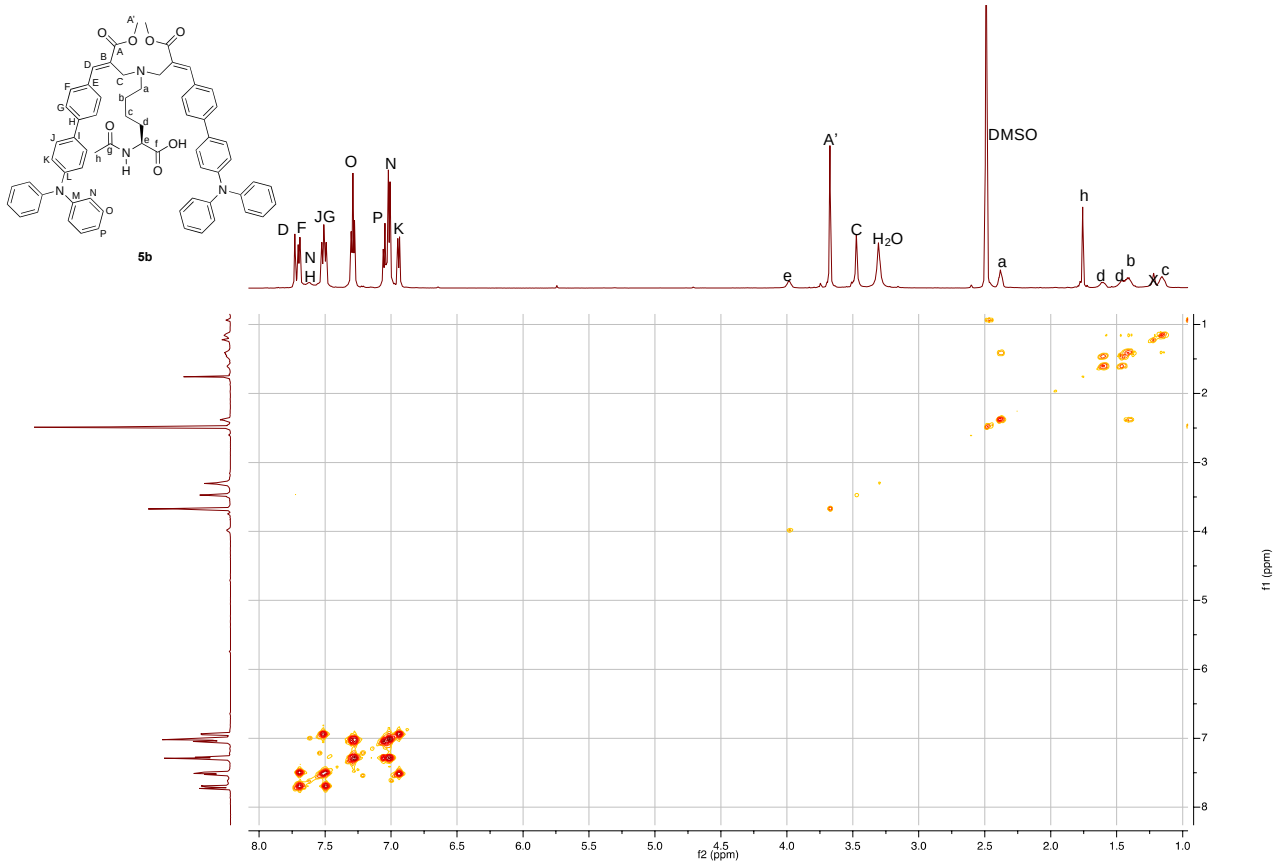

Figure S3. ^{1}H-^{1}H COSY full spectrum of diadduct **5b** in DMSO-d_6 at 600 MHz.

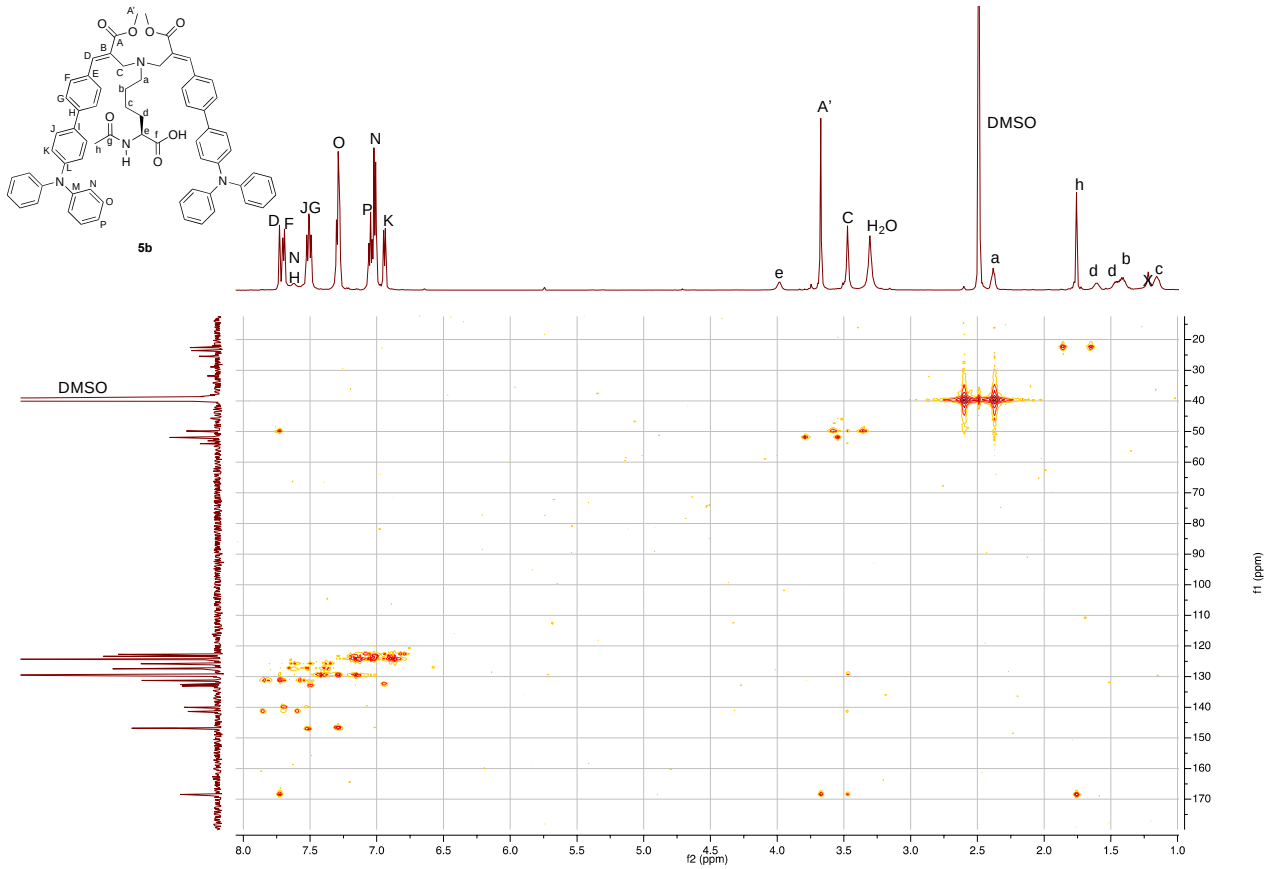

Figure S4. ^{1}H-^{13}C HMBC full spectrum of diadduct **5b** in DMSO-d_6 at 600 MHz.

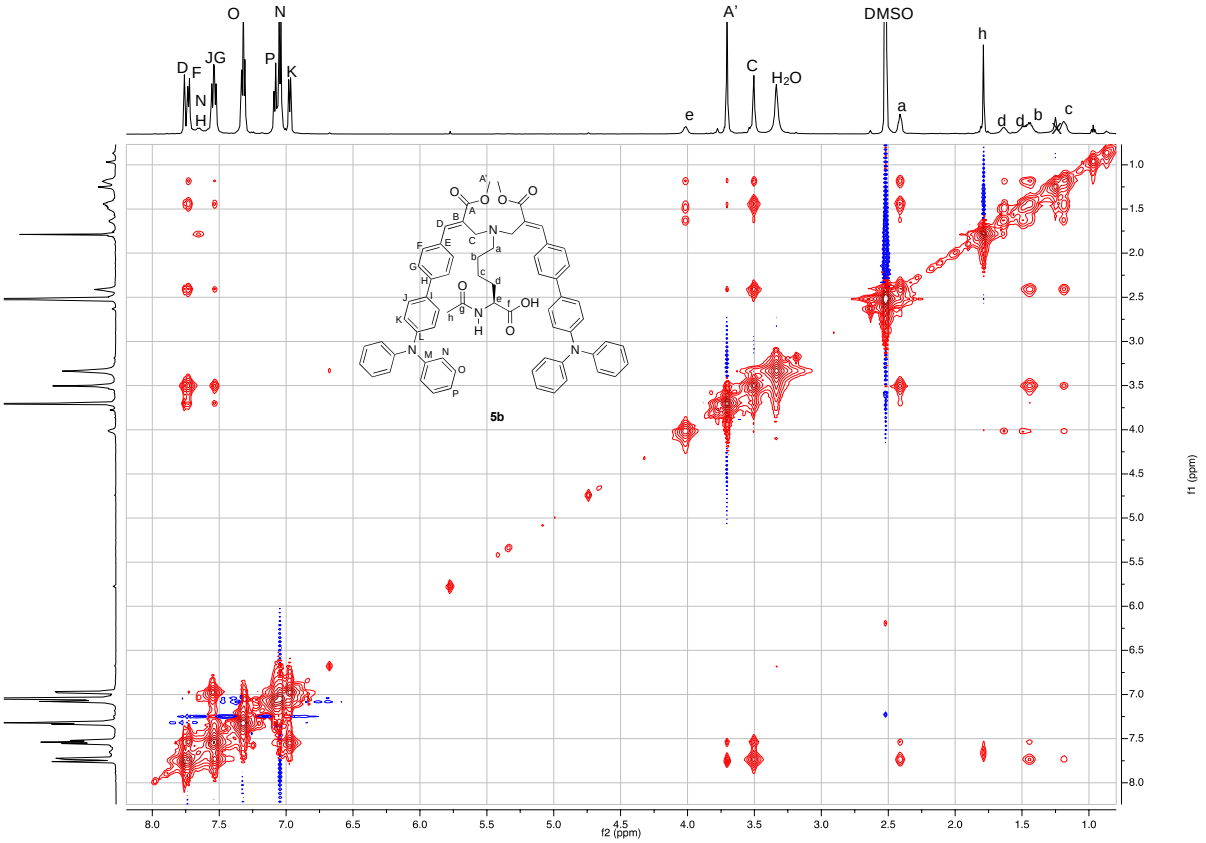

Figure S5. ^{1}H-^{1}H NOESY full spectrum of diadduct **5b** in DMSO-d_6 at 600 MHz.

Experimental procedures

Synthesis. Merck silica gel 60 (230-400 mesh) was used for column chromatography. Merck TLC plates, silica gel 60 F_{254} were used for TLC. NMR spectra were recorded with a Bruker DRX-400 AVANCE III or with a Bruker DRX-600 AVANCE spectrometer in the indicated solvents (TMS as internal standard): the values of the chemical shifts are expressed in ppm and the coupling constants (*J*) in Hz. The HR-MS measurements were performed by the direct infusion (5 μL/min) of sample solutions [methanol-water (9:1) filtered at 0.45 μm] in heated electrospray ionization (ESI) source and a Q-Exactive 240 Orbitrap High-Resolution mass spectrometer (ESI-HRMS-Orbitap, Thermo Fisher Scientific, Waltham, MA, USA). The Orbitrap analyzer was operated in positive mode. The following ion source parameters were used for detection: electrospray voltage, 3.4 kV; capillary temperature, 320 °C; Vaporizer temperature, 200 °C; sheath gas flow-rate (N_2), 7 arbitrary units (AU); auxiliary gas flow-rate (N_2), 5 AU and sweep gas flow rate 0 AU. The MS parameters were: full mass m/z range from 150 to 1500; mass resolution, 240,000 (at m/z 200); AGC target, standard; maximum injection time, auto; RF lens (%), 70; microscans, 1.

Reaction of MBHA derivative 3 with Nα-acetyl-*L*-lysine

A mixture of MBH acetate **3** (139 mg, 0.29 mmol) in acetonitrile (25 mL) containing Nα-acetyl-*L*-lysine (82 mg, 0.436 mmol), water (7.0 mL), and solid PBS (Aldrich, 50 mg) was refluxed for 24 h. The reaction mixture was concentrated under reduced pressure and the resulting residue partitioned between dichloromethane and brine. The organic layer was dried over sodium sulfate and concentrated under reduced pressure. The final residue was purified by flash chromatography with the appropriate eluent to obtain the amino acid derivatives reported below (i. e. **4b** and **5b**).

N^2-Acetyl-N^6-(3-(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)-2-(methoxycarbonyl)allyl)lysine (4b).

Compound **4b** was obtained as a yellow glassy solid (30 mg, yield 17%) by using dichloromethane-methanol (8:2) as the eluent in the above flash chromatography purification. ^{1}H NMR (400 MHz, DMSO-d_6) 1.34 (m, 2H), 1.45 (m, 2H), 1.55 (m, 1H), 1.66 (m, 1H), 1.81 (s, 3H), 2.55 (t, J = 7.0, 2H), 3.50 (s, 2H), 3.75 (s, 3H), 4.10 (m, 1H), 7.02 (m, 2H), 7.05 (m, 6H), 7.34 (m, 4H), 7.65 (m, 2H), 7.70 (m, 4H), 7.76 (s, 1H), 7.95 (d, J = 7.4, 1H). ^{13}C NMR (150 MHz, DMSO-d_6): 22.4, 23.1, 31.1, 45.0, 48.6, 52.0, 52.2, 122.8, 123.4, 124.3, 126.0, 127.6, 129.6, 130.5, 132.7, 133.0, 140.1, 141.1, 146.9, 147.1, 167.7, 169.0, 174.1. HR-MS (ESI) m/z: $[M + H]^+$ Calcd for $C_{37}H_{40}N_3O_5$ 606.2963; Found 606.2972.

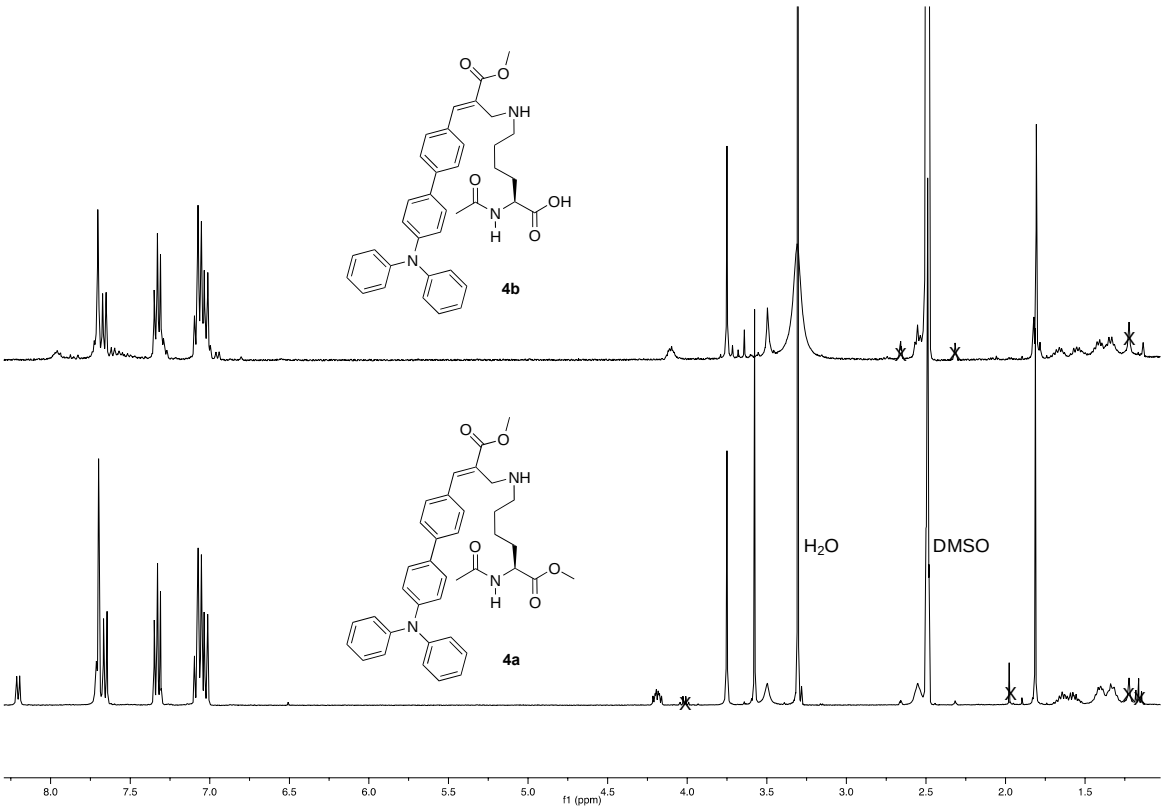

Figure S6. Comparison of ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of monoadduct **4b** with the one (DMSO-d_6, 400 MHz) of the corresponding methyl ester **4a**.

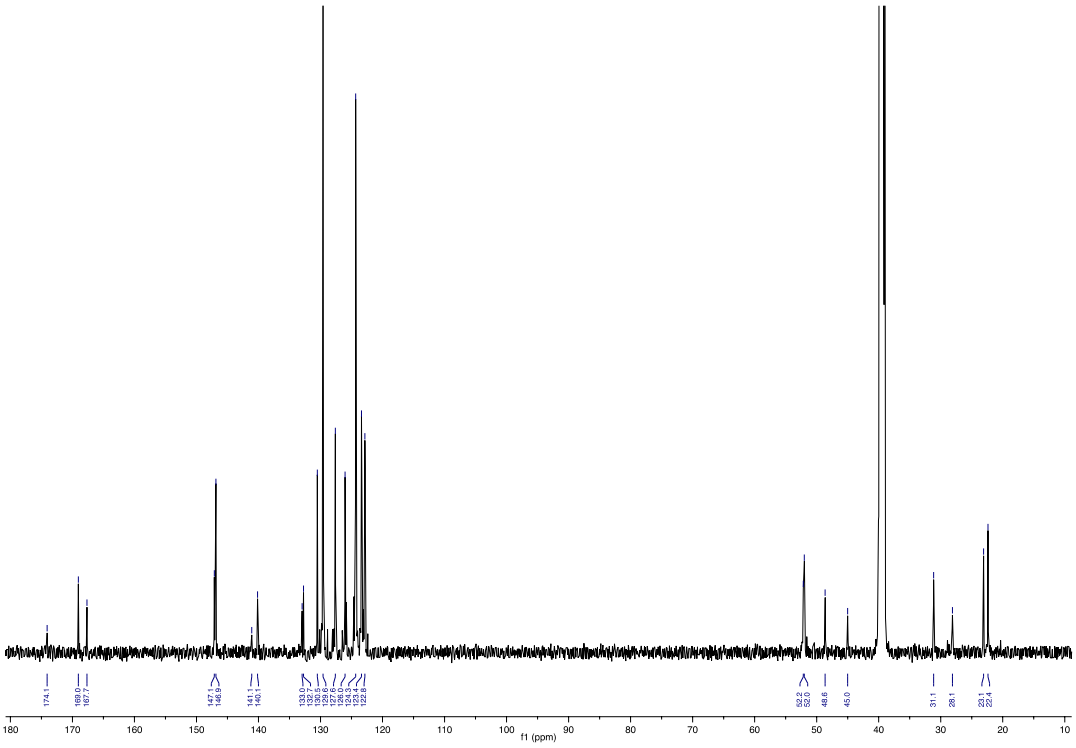

Figure S7. ^{13}C NMR spectrum (DMSO-d$_6$, 150 MHz) of monoadduct **4b**.

N^2-Acetyl-*N*^{6},*N*^{6}-bis(3-(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)-2-(methoxycarbonyl)allyl)lysine (5b).

Compound **5b** was obtained as a yellow-brown glassy solid (74 mg, yield 50%) by using dichloromethane-methanol (96:4) as the eluent in the above flash chromatography purification. ^{1}H NMR (600 MHz, DMSO-d$_6$): 1.15 (m, 2H), 1.41 (m, 2H), 1.46 (m, 1H), 1.60 (m, 1H), 1.76 (s, 3H), 2.38 (t, *J* = 7.3, 2H), 3.47 (s, 4H), 3.67 (s, 6H), 3.98 (q, *J* = 6.8, 1H), 6.94 (d, *J* = 8.2, 4H), 7.01 (d, *J* = 8.0, 8H), 7.05 (t, *J* = 7.4, 4H), 7.29 (t, *J* = 7.7, 8H), 7.50 (d, *J* = 8.1, 4H), 7.52 (d, *J* = 8.2, 4H), 7.62 (br s, 1H), 7.70 (d, *J* = 8.0, 4H), 7.73 (s, 2H). HR-MS (ESI) *m*/*z*: $[M + H]^+$ Calcd for $C_{66}H_{63}N_4O_7$ 1023.4691; Found 1023.4728.

Photochemical features

Procedure A: Solutions contained into quartz cuvettes were irradiated with a UV-A lamp (365 nm, irradiance 6 μw/cm^2/nm).

Procedure B: Samples of **5b** (1.0 mg) were dissolved in deuterated DCM or DMSO-d_6 (0.75 mL), placed into a 5 mm NMR tubes and ^{1}H NMR spectra (Bruker DRX 600 MHz) were recorded at regular time (up to 48 h) to evaluate the stability of the sample over time at room temperature. Subsequntly, the samples were irradiated with with a UV-A lamp (365 nm, irradiance 6 μw/cm^2/nm), and ^{1}H NMR spectra were recorded at regular time intervals (i. e. 0, 0.25, 0.50, 1, 2, 4, and 8 h).

Procedure C: The solutions of compounds **5a**,**b** (5.0 mg) in the suitable deuterated solvent (CD_2Cl_2 for **5a**) or solvent mixture [CD_2Cl_2-DMSO-d_6 (2:1) for **5b**] contained into 5 mm NMR Pyrex tubes were irradiated with a monochromatic light centered at 420 nm, and ^{1}H NMR spectra were recorded at regular time intervals. A tunable light source Zolix (TLS2-X300PU-G, 300W UV Xenon Light Source with monochromator Omni-λ2047i) was used for the irradiation of the solutions.

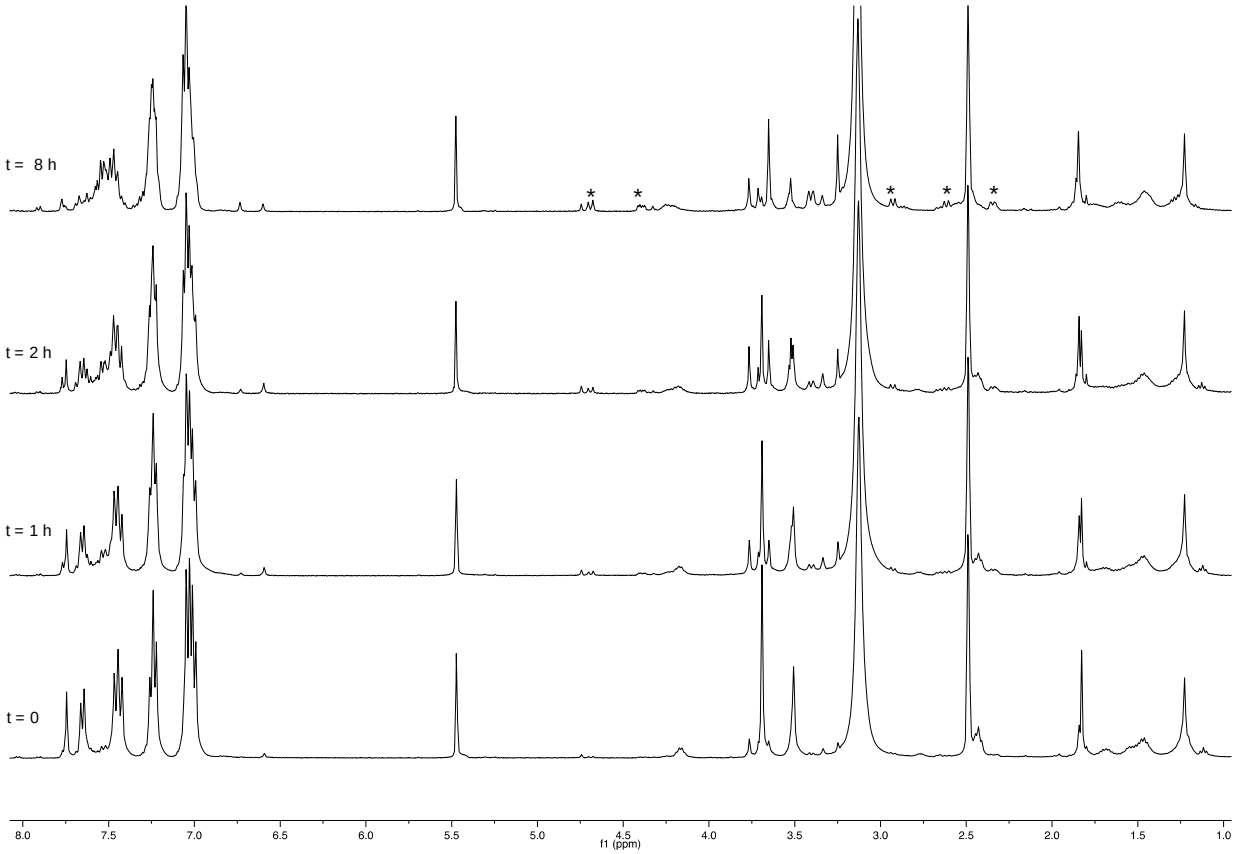

Figure S8. Comparison of the ^{1}H NMR (400 MHz) spectra of the reaction mixtures obtained with diadduct **5b** (5.0 mg, 4.9 micromol) in CD_2Cl_2-DMSO-d_6 (2:1) (0.75 mL) when irradiated with monochromatic light at 420 nm. The reaction mixtures contained into a 5 mm NMR tube were irradiated at room temperature and ^{1}H NMR spectra were recorded at regular time intervals. The peaks marked by an asterisk were attributed to the major product of the [2+2] photocycloaddition reaction.

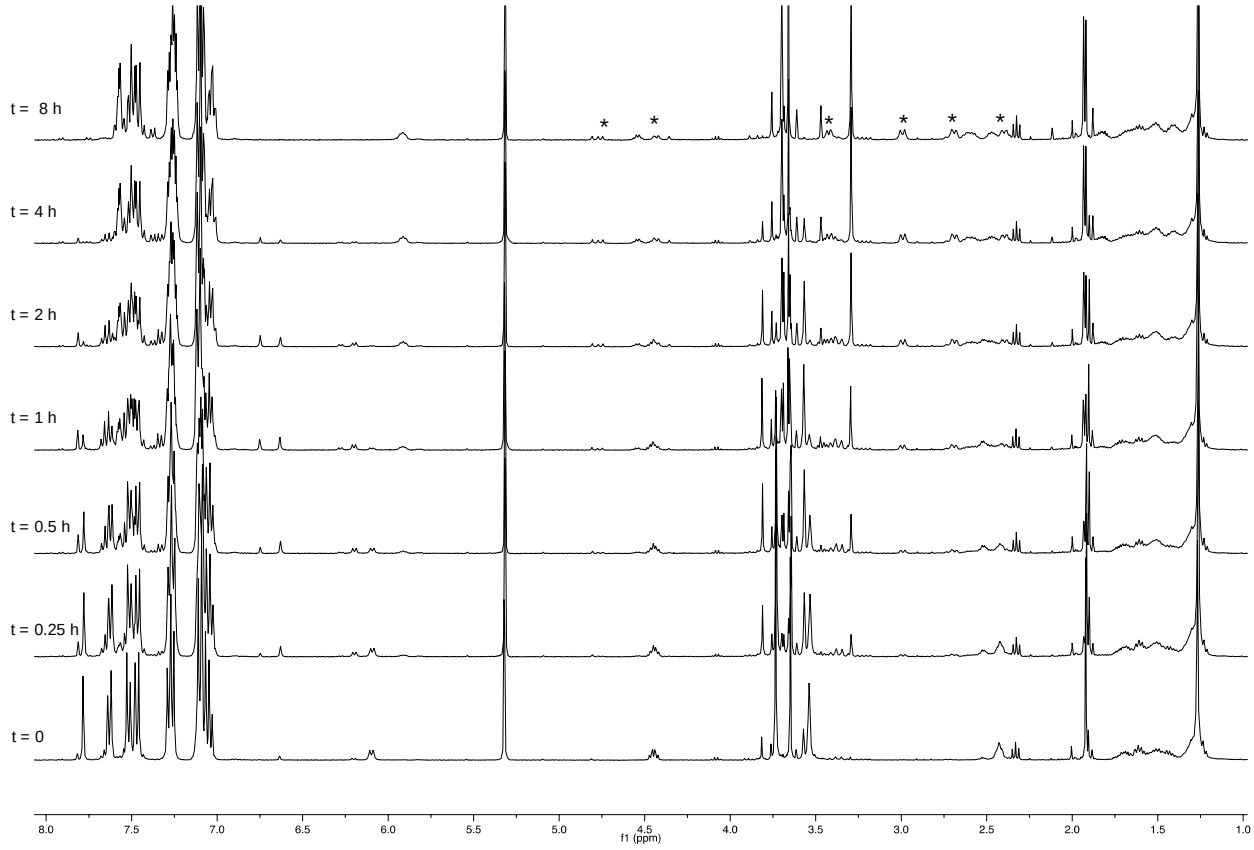

Figure S9. Comparison of the ^{1}H NMR (400 MHz) spectra of the reaction mixtures obtained with diadduct **5a** (5.0 mg, 4.8 micromol) in CD_2Cl_2 (0.75 mL) when irradiated with monochromatic light at 420 nm. The reaction mixtures contained into a 5 mm NMR tube were irradiated at room temperature and ^{1}H NMR spectra were recorded at regular time intervals. The peaks marked by an asterisk were attributed to the major product of the [2+2] photocycloaddition reaction.

Dimethyl 3-(5-acetamido-6-methoxy-6-oxohexyl)-6,7-bis(4'-(diphenylamino)-[1,1'-biphenyl]-4-yl)-3-azabicyclo[3.2.0]heptane-1,5-dicarboxylate (7a).

A solution of compound **5a** (5.0 mg, 0.0048 mmol) in dichloromethane (0.75 mL) contained into a 5 mm NMR Pyrex tube was irradiated with a monochromatic light centered at 420 nm by mean of a tunable light source Zolix (TLS2-X300PU-G, 300W UV Xenon Light Source with monochromator Omni-λ2047i) at room temperature for 24 h. The reaction mixture was then concentrated under reduced pressure and the resulting residue was purified by flash chromatography with petroleum

ether-ethyl acetate (1:1) as the eluent to obtain compound **7a** (2.0 mg, yield 40%) as a pale-yellow glassy solid. The ^{1}H NMR spectrum (Figure SI-9) of the solid showed that compound **7a** was composed by a mixture of diastereomers. HR-MS (ESI) *m*/*z*: $[M + H]^+$ Calcd for $C_{67}H_{65}N_4O_7$ 1037.4848; Found 1037.4855.

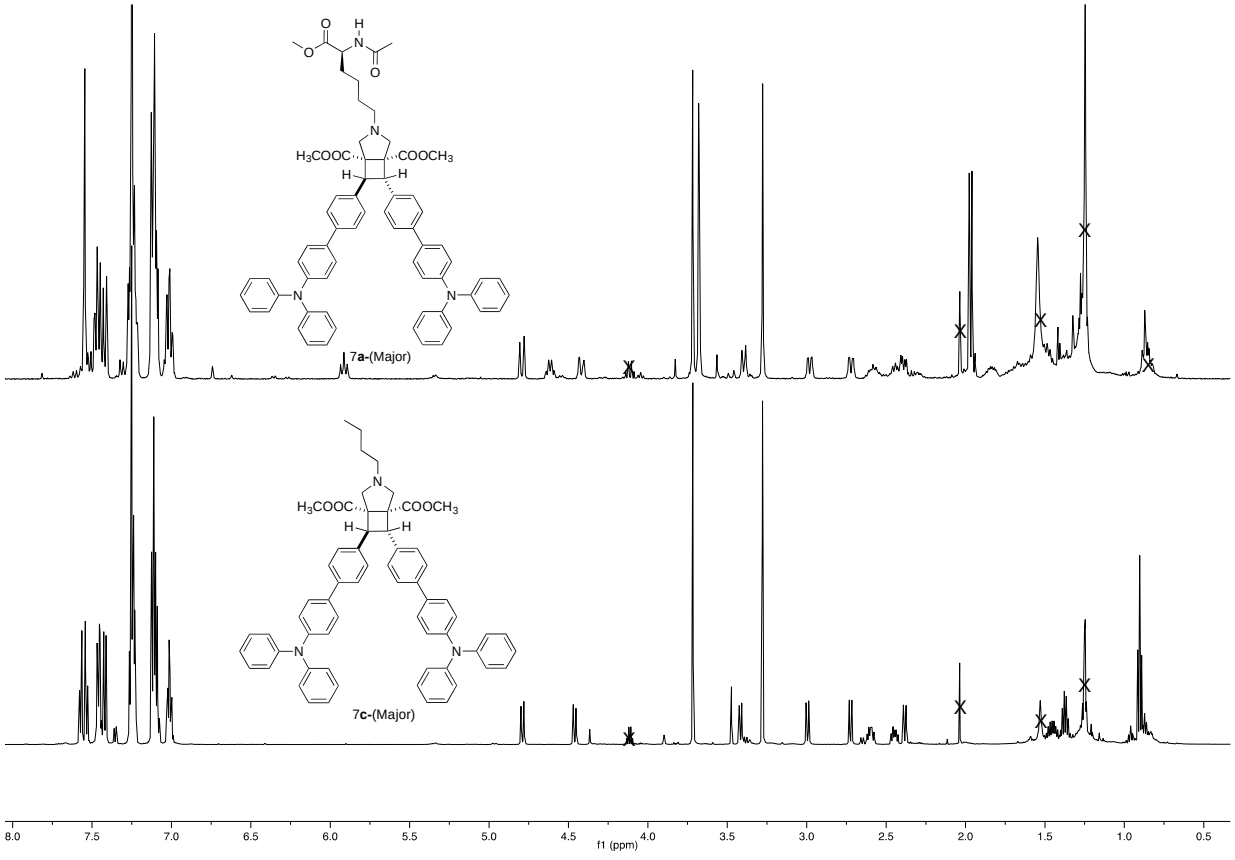

Figure S10. Comparison of ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **7a** with the one ($CDCl_3$, 600 MHz) of the previously published[1] analogue **7c**.

(*E*)-4',4'''-(Ethene-1,2-diyl)bis(*N*,*N*-diphenyl-[1,1'-biphenyl]-4-amine) (6).

A solution of diadduct derivative **5b** (50 mg, 0.049 mmol) in ethanol (9.0 mL) was irradiated with UV-A light for 8 h into a Multyrays chamber equipped with two G15T8 Hg UV-A tubes (2 x 15 Watt) in continuous rotation. The formed crystals were separated from the reaction mixture, washed with a small amount of ethanol, and dissolved in dichloromethane. The resulting solution was then

concentrated under reduced pressure. Purification of the residue by flash chromatography with petroleum ether-ethyl acetate (9:1) as the eluent afforded compound **6** (6.0 mg, yield 18%) as an off-white solid melting at 240-242 °C (lit. mp 242 °C).[2]

^{1}H NMR (600 MHz, $CDCl_3$): 7.03 (t, *J* = 7.4, 4H), 7.14 (m, 14H), 7.26 (m, 8H), 7.50 (d, *J* = 8.1, 2H), 7.57 (s, 8H). ^{13}C NMR (150 MHz, $CDCl_3$): 123.4, 124.2, 124.9, 127.2, 127.3, 127.9, 128.4, 129.7, 134.9, 136.4, 140.1, 147.7, 148.0.

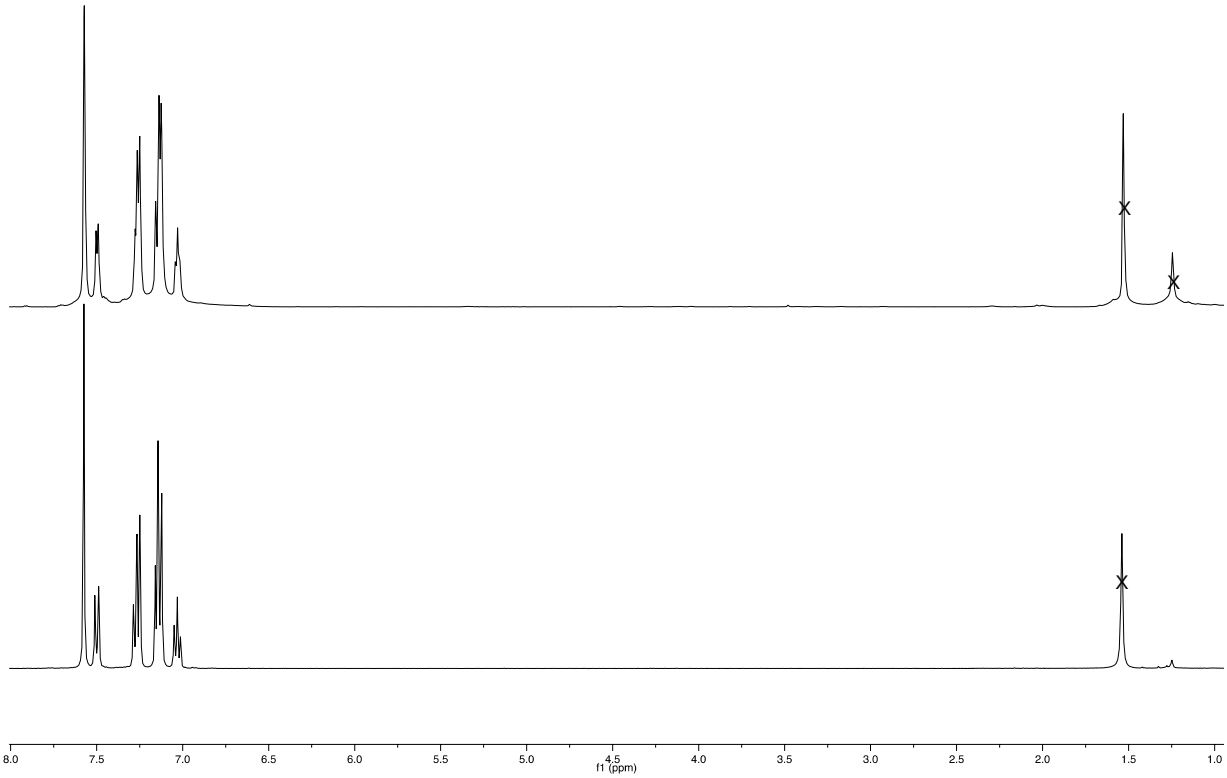

Figure S11. Comparison of ^{1}H NMR spectrum ($CDCl_3$, 600 MHz, top trace) of compound **6** with the one ($CDCl_3$, 400 MHz, bottom trace) of a sample prepared by following a synthetic procedure described in the literature.[2]

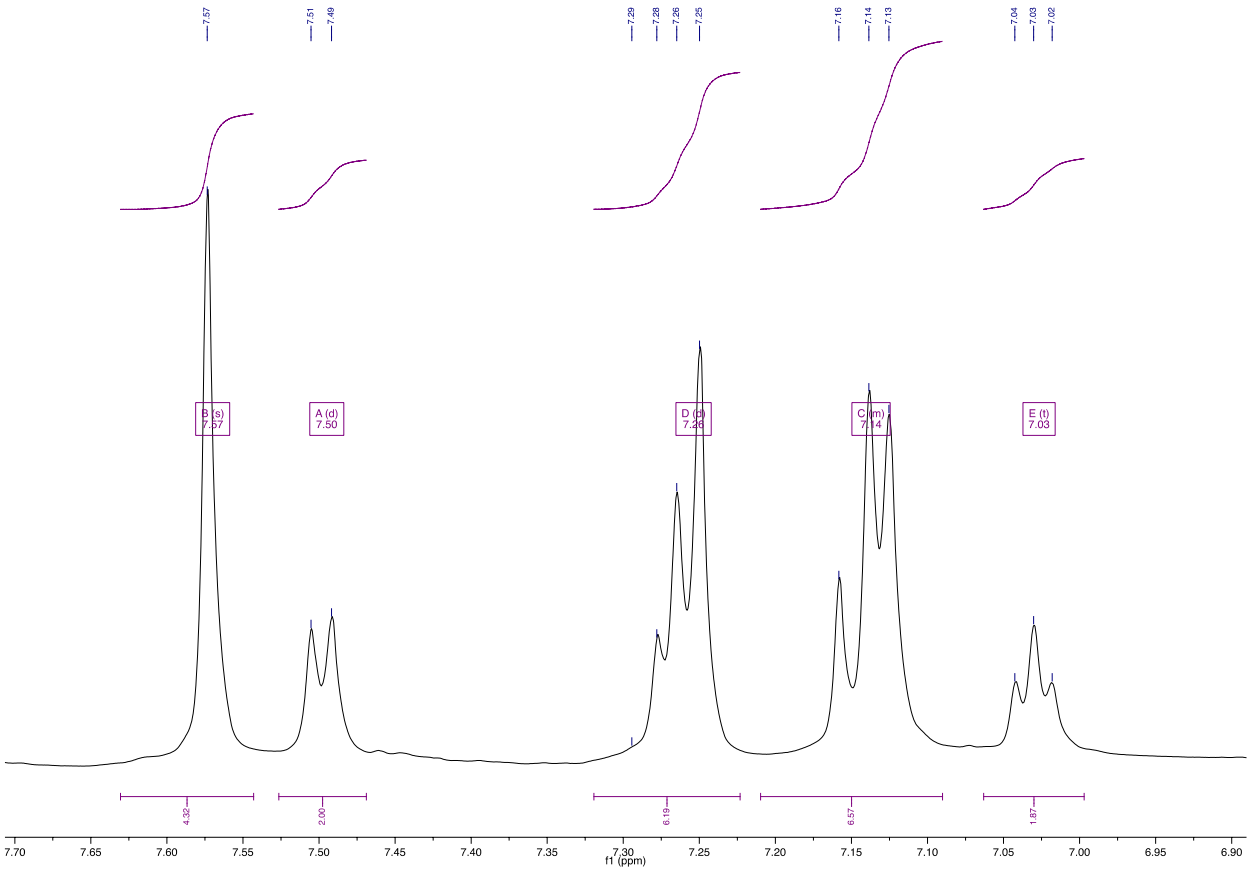

Figure S12. Aromatic region of ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of compound **6**.

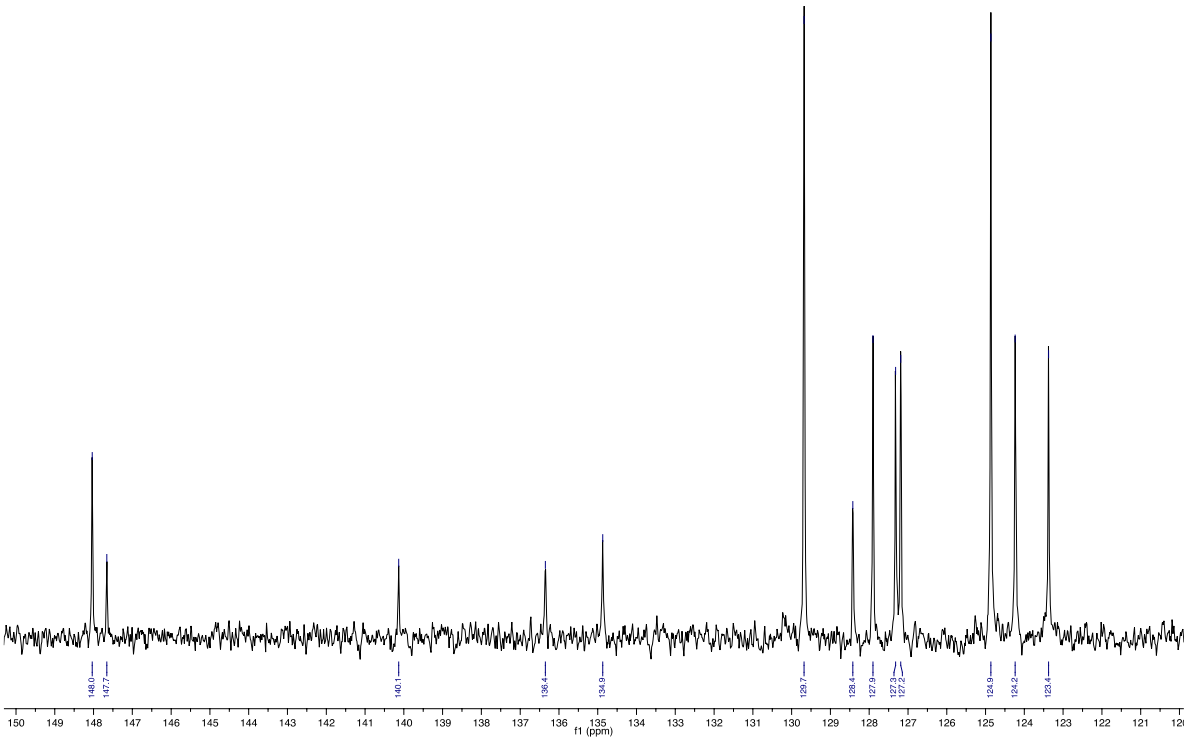

Figure S13. Aromatic region of ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of compound **6**.

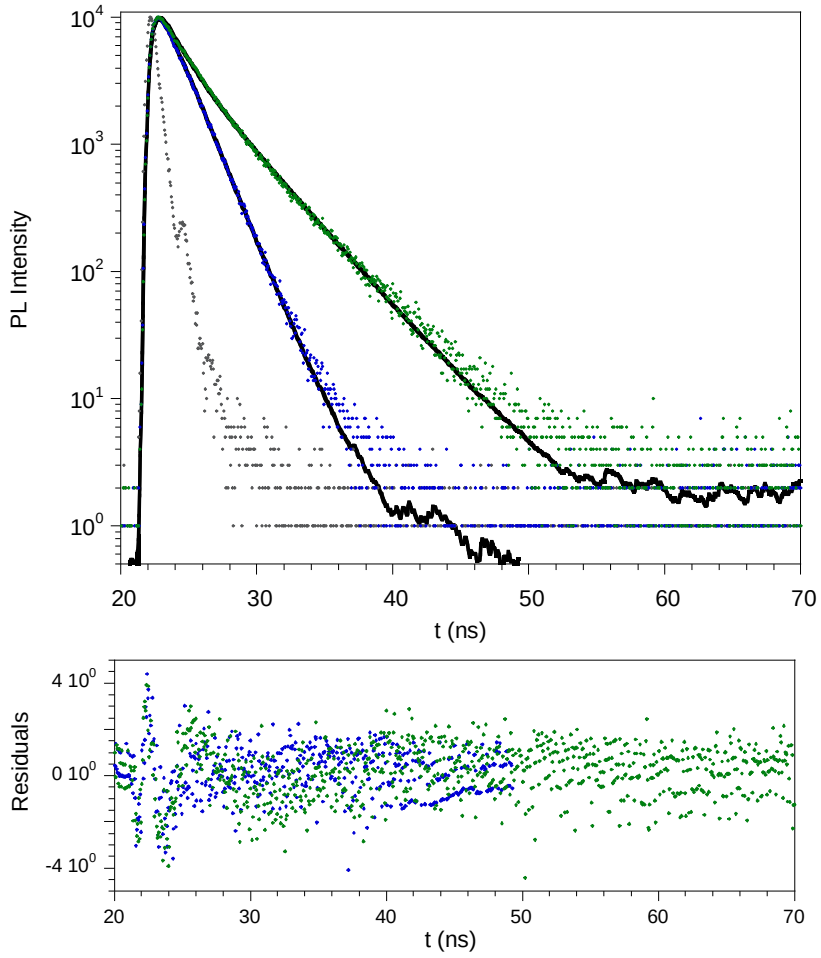

Figure S14. PL decay of **5a** solution (λ_{ex} = 300 nm; blue points, λ_{em} = 406 nm; green points, λ_{em} = 524 nm; prompt, grey points; with monoexponential (λ_{em} = 406 nm, τ = 1.6085 ns, χ^2 = 1.226571) and bi-exponential (λ_{em} = 524 nm; τ_{av} = 1.6085 ns, t_1 = 1.24 ns (0.59), t_2 = 3.60 ns (0.41),χ^2 = 1.393841) fits (solid lines) with residuals (bottom panel).

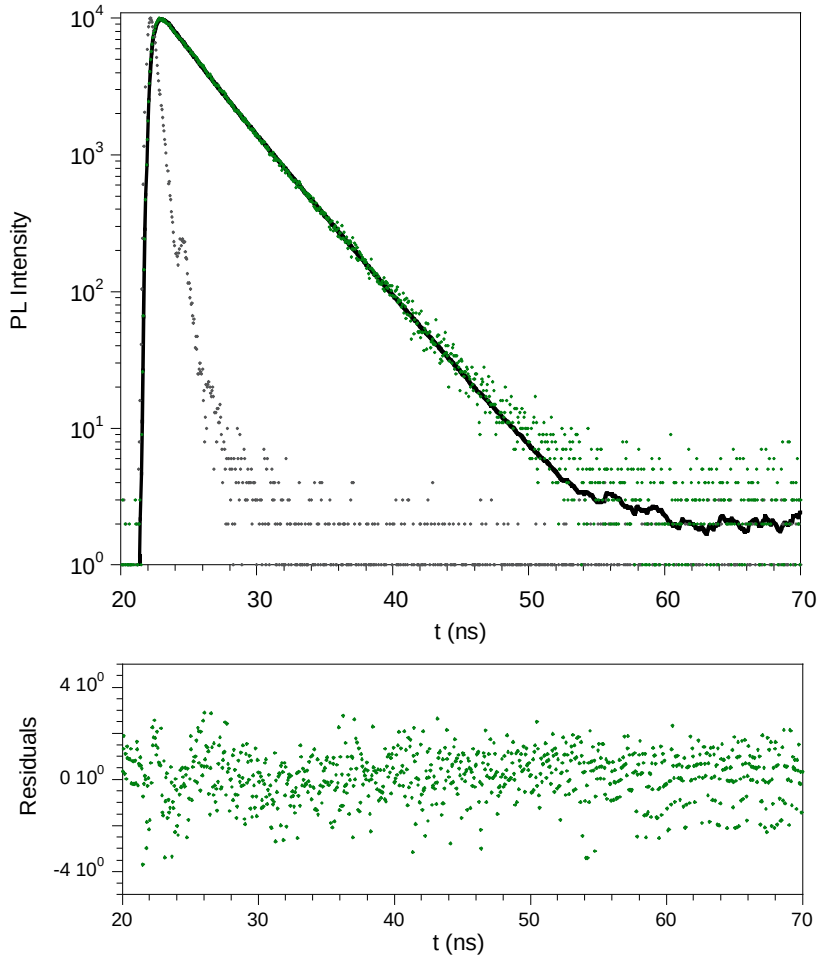

Figure S15. PL decay of **4a** solution (blue points λ_{em} = 535 nm, λ_{ex} = 300 nm), prompt (grey points), with bi-exponential fit (λ_{em} = 535 nm; τ_{av} =3 .38 ns, t_1 = 1.33 ns (0.29), t_2 = 3.68 ns (0.71) χ^2 = 1.251437) (solid lines) with residuals (bottom panel).

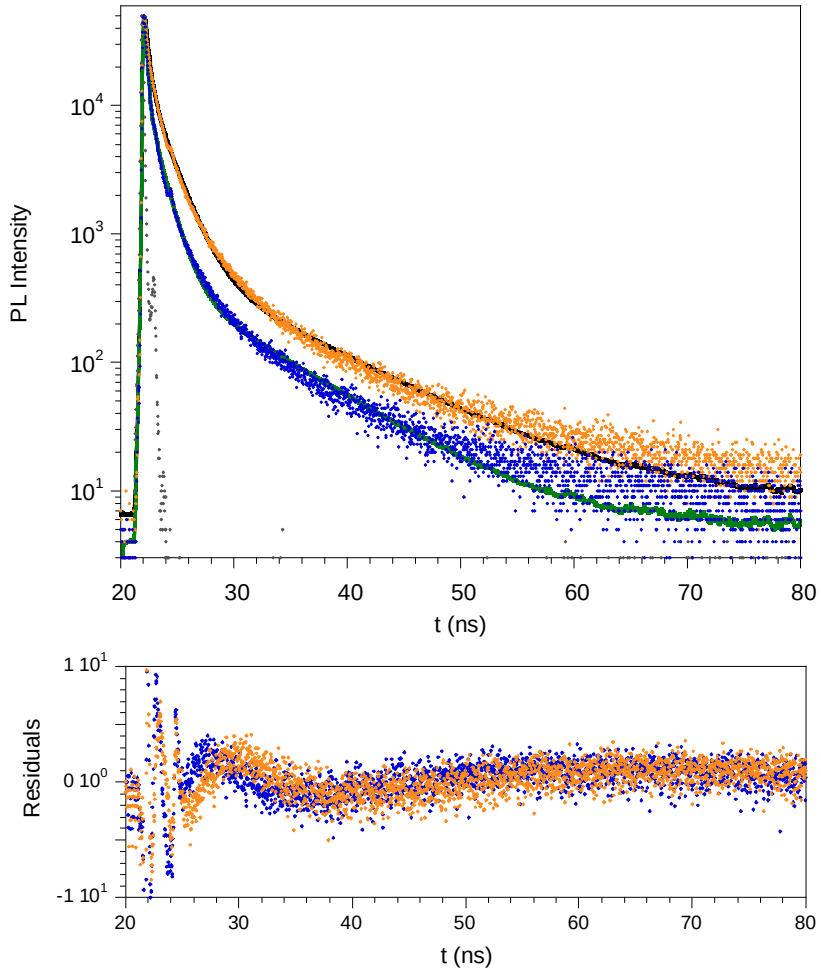

Figure S16. PL decay of **4a** (blue points λ_{em} = 530 nm) and **5a** (orange points λ_{em} = 520 nm) films, prompt (grey points), (λ_{ex} = 407 nm) with three exponential fits (solid lines) with fitting parameters **4a** (τ_{av} = 1.44 ns, t_1 = 1.195 ns (0.10), t_2 = 7.80 ns (0.01), t_3 = 0.18 ns (0.89) χ^2 = 4.604504) and **5a** (τ_{av} = 2.11 ns, t_1 = 1.65 ns (0.20), t_2 = 9.63 ns (0.01), t_3 = 0.30 ns (0.80) χ^2 = 3.894135). with residuals (bottom panel).

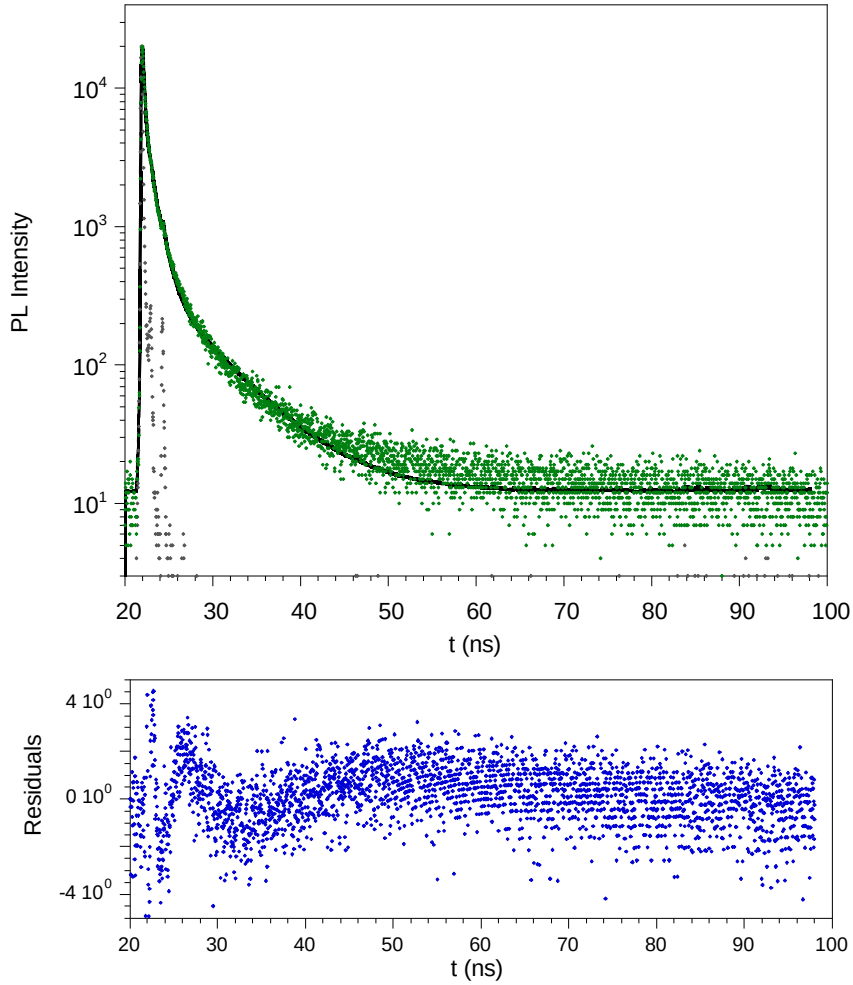

Figure S17. PL decay of **5b** (blue points λ_{em} = 550 nm) powders, prompt (grey points), (λ_{ex} = 407 nm) with three exponential fits (solid lines) with fitting parameters (τ_{av} = 1.57 ns, t_1 = 0.98 ns (0.13), t_2 = 6.11 ns (0.01), t_3 = 0.15 ns (0.86), χ^2 = 1.212054) with residuals (bottom panel).

References

(1) Venditti, J.; Saletti, M.; Paolino, M.; Contena, S.; Bonechi, C.; Giuliani, G.; Giorgi, G.; Boccia, A. C.; Botta, C.; Blancafort, L. et al. Reactivity of a Morita-Baylis-Hillman Adduct Derivative Bearing a Triphenylamine Moiety with Lysine Models. *Chem. Asian J.* **2024**, e202400617.

(2) Hsu, H. L.; Leung, M. K.; Wang, S. S. Organic Electroluminescent Material and Electroluminescent Device by Using the Same. US 2004/0146742 A1, Jul. 29, **2004**.

1) Cartesian coordinates of the Frank-Condon geometry of neutral 5b in CH_2Cl_2.

N	4.328	-0.021	0.080
C	5.388	-0.180	1.078
H	6.356	-0.343	0.607
H	5.477	0.764	1.625
C	4.143	1.356	-0.380
H	4.143	1.999	0.507
H	3.137	1.431	-0.813
C	4.385	-0.958	-1.045
H	3.575	-0.681	-1.727
H	5.319	-0.857	-1.614
C	5.429	-3.247	-0.475
O	6.560	-2.525	-0.558
O	5.442	-4.442	-0.257
C	7.782	-3.249	-0.390
H	8.566	-2.494	-0.392
H	7.765	-3.800	0.552
H	7.918	-3.954	-1.214
C	6.454	-2.028	2.485
O	6.505	-3.106	3.043
O	7.564	-1.313	2.212
C	8.800	-1.867	2.676
H	9.577	-1.201	2.305
H	8.810	-1.903	3.768
H	8.946	-2.873	2.283
C	4.213	-2.411	-0.679
C	3.048	-3.073	-0.569
H	3.155	-4.134	-0.356
C	1.658	-2.646	-0.715
C	0.705	-3.669	-0.831
C	1.193	-1.323	-0.704
C	-0.644	-3.390	-0.941
H	1.037	-4.704	-0.834
C	-0.160	-1.044	-0.833
H	1.882	-0.514	-0.496
C	-1.106	-2.069	-0.941
H	-1.353	-4.205	-1.043
H	-0.499	-0.014	-0.776
C	-2.561	-1.811	-1.031
C	-3.096	-0.809	-1.845
C	-3.462	-2.625	-0.336
C	-4.467	-0.671	-2.019
H	-2.428	-0.158	-2.401
C	-4.830	-2.478	-0.478
H	-3.083	-3.381	0.345
C	-5.359	-1.526	-1.358
H	-4.848	0.084	-2.697
H	-5.500	-3.122	0.080

N	-6.748	-1.472	-1.578
C	-7.526	-2.660	-1.477
C	-8.696	-2.659	-0.717
C	-7.141	-3.823	-2.145
C	-9.474	-3.807	-0.633
H	-8.991	-1.752	-0.199
C	-7.913	-4.973	-2.042
H	-6.233	-3.819	-2.739
C	-9.085	-4.970	-1.290
H	-10.384	-3.795	-0.040
H	-7.604	-5.873	-2.565
H	-9.690	-5.868	-1.218
C	-7.403	-0.279	-1.973
C	-8.386	-0.313	-2.966
C	-7.091	0.937	-1.365
C	-9.049	0.851	-3.332
H	-8.629	-1.255	-3.445
C	-7.742	2.102	-1.751
H	-6.330	0.963	-0.594
C	-8.729	2.065	-2.730
H	-9.812	0.809	-4.103
H	-7.473	3.041	-1.278
H	-9.242	2.975	-3.025
C	5.212	-1.313	2.072
C	4.081	-1.734	2.661
H	4.165	-2.632	3.270
C	2.750	-1.129	2.592
C	2.575	0.256	2.543
C	1.606	-1.932	2.616
C	1.314	0.812	2.454
H	3.439	0.908	2.595
C	0.341	-1.376	2.485
H	1.712	-3.011	2.679
C	0.169	0.007	2.372
H	1.220	1.892	2.445
H	-0.517	-2.036	2.412
C	-1.156	0.620	2.122
C	-2.357	-0.001	2.483
C	-1.249	1.857	1.473
C	-3.585	0.584	2.215
H	-2.339	-0.960	2.990
C	-2.468	2.467	1.234
H	-0.349	2.362	1.139
C	-3.659	1.837	1.600
H	-4.499	0.074	2.497
H	-2.495	3.436	0.750
N	-4.914	2.451	1.374
C	-5.890	2.415	2.411
C	-7.235	2.204	2.103
C	-5.516	2.595	3.744
C	-8.188	2.175	3.114

H	-7.533	2.063	1.070
C	-6.471	2.547	4.752
H	-4.472	2.766	3.986
C	-7.811	2.340	4.443
H	-9.230	2.010	2.858
H	-6.163	2.685	5.784
H	-8.556	2.308	5.232
C	-5.083	3.341	0.285
C	-5.794	4.535	0.433
C	-4.540	3.028	-0.967
C	-5.967	5.387	-0.653
H	-6.214	4.793	1.398
C	-4.702	3.893	-2.039
H	-4.004	2.094	-1.095
C	-5.421	5.077	-1.893
H	-6.526	6.308	-0.518
H	-4.278	3.628	-3.002
H	-5.555	5.746	-2.736
C	5.148	1.913	-1.409
H	4.922	2.976	-1.558
H	4.995	1.428	-2.380
C	6.603	1.735	-0.988
H	6.735	2.131	0.030
H	6.807	0.665	-0.942
C	7.635	2.373	-1.908
H	7.454	3.449	-2.006
H	7.574	1.945	-2.914
C	9.080	2.193	-1.391
H	9.156	2.616	-0.385
C	9.442	0.707	-1.327
O	9.992	0.135	-2.234
O	9.092	0.024	-0.224
H	8.640	0.576	0.435
N	10.052	2.831	-2.250
H	10.393	2.274	-3.025
C	10.494	4.116	-2.197
O	11.271	4.547	-3.039
C	10.005	4.967	-1.045
H	8.913	5.002	-0.996
H	10.371	4.575	-0.091
H	10.390	5.977	-1.182

2) Cartesian coordinates of the Frank-Condon geometry of neutral 5b in DMSO.

N	4.305	-0.137	0.244
C	5.477	-0.779	0.841
H	6.395	-0.458	0.350
H	5.554	-0.435	1.877
C	4.019	1.193	0.793
H	4.109	1.123	1.882
H	2.966	1.419	0.584

C	4.274	-0.127	-1.221
H	3.427	0.500	-1.511
H	5.173	0.342	-1.642
C	5.298	-2.238	-2.298
O	6.435	-1.567	-2.042
O	5.298	-3.332	-2.828
C	7.650	-2.194	-2.463
H	8.445	-1.534	-2.121
H	7.741	-3.182	-2.010
H	7.668	-2.291	-3.550
C	6.853	-2.923	0.641
O	7.057	-4.097	0.402
O	7.862	-2.047	0.799
C	9.184	-2.591	0.722
H	9.857	-1.741	0.816
H	9.346	-3.304	1.532
H	9.340	-3.092	-0.234
C	4.093	-1.476	-1.874
C	2.910	-2.021	-2.209
H	2.962	-2.957	-2.761
C	1.558	-1.498	-2.004
C	0.563	-1.859	-2.923
C	1.195	-0.663	-0.939
C	-0.725	-1.358	-2.819
H	0.813	-2.523	-3.745
C	-0.098	-0.172	-0.832
H	1.915	-0.461	-0.157
C	-1.080	-0.493	-1.776
H	-1.462	-1.625	-3.569
H	-0.362	0.440	0.025
C	-2.455	0.045	-1.674
C	-2.702	1.352	-1.247
C	-3.567	-0.735	-2.010
C	-3.987	1.873	-1.193
H	-1.868	1.997	-0.987
C	-4.857	-0.241	-1.930
H	-3.425	-1.770	-2.306
C	-5.094	1.089	-1.548
H	-4.130	2.902	-0.888
H	-5.690	-0.892	-2.160
N	-6.398	1.605	-1.505
C	-7.451	1.068	-2.297
C	-8.728	0.975	-1.740
C	-7.255	0.675	-3.622
C	-9.789	0.487	-2.493
H	-8.881	1.288	-0.712
C	-8.316	0.171	-4.365
H	-6.269	0.761	-4.066
C	-9.587	0.074	-3.807
H	-10.776	0.420	-2.046
H	-8.147	-0.135	-5.393

H	-10.413	-0.315	-4.392
C	-6.650	2.889	-0.924
C	-6.986	3.963	-1.748
C	-6.585	3.065	0.456
C	-7.258	5.207	-1.193
H	-7.037	3.811	-2.821
C	-6.844	4.316	1.005
H	-6.327	2.226	1.092
C	-7.185	5.388	0.186
H	-7.522	6.038	-1.839
H	-6.788	4.443	2.081
H	-7.395	6.360	0.620
C	5.511	-2.294	0.827
C	4.501	-3.165	0.986
H	4.767	-4.211	0.848
C	3.094	-2.927	1.302
C	2.656	-1.878	2.117
C	2.139	-3.819	0.804
C	1.308	-1.698	2.375
H	3.377	-1.193	2.546
C	0.788	-3.628	1.047
H	2.462	-4.663	0.202
C	0.345	-2.551	1.820
H	0.992	-0.853	2.978
H	0.067	-4.328	0.635
C	-1.096	-2.275	1.995
C	-1.992	-2.500	0.946
C	-1.602	-1.714	3.173
C	-3.325	-2.137	1.045
H	-1.628	-2.902	0.006
C	-2.937	-1.360	3.286
H	-0.944	-1.563	4.023
C	-3.809	-1.533	2.206
H	-3.987	-2.274	0.200
H	-3.306	-0.923	4.207
N	-5.150	-1.092	2.274
C	-6.153	-1.853	1.612
C	-6.992	-1.265	0.664
C	-6.284	-3.214	1.896
C	-7.955	-2.030	0.017
H	-6.880	-0.212	0.427
C	-7.237	-3.978	1.233
H	-5.628	-3.665	2.633
C	-8.080	-3.389	0.295
H	-8.598	-1.561	-0.721
H	-7.327	-5.035	1.460
H	-8.827	-3.985	-0.218
C	-5.473	0.154	2.852
C	-6.724	0.349	3.448
C	-4.557	1.214	2.845
C	-7.042	1.568	4.033

H	-7.444	-0.462	3.455
C	-4.876	2.420	3.454
H	-3.598	1.091	2.357
C	-6.117	2.608	4.055
H	-8.018	1.698	4.490
H	-4.150	3.227	3.441
H	-6.363	3.553	4.527
C	4.866	2.379	0.290
H	4.583	3.263	0.875
H	4.610	2.605	-0.751
C	6.369	2.139	0.392
H	6.614	1.804	1.410
H	6.622	1.319	-0.282
C	7.245	3.332	0.035
H	7.014	4.187	0.678
H	7.065	3.648	-0.999
C	8.751	3.028	0.194
H	8.947	2.713	1.223
C	9.170	1.904	-0.755
O	9.602	2.117	-1.861
O	9.002	0.637	-0.340
H	8.658	0.580	0.567
N	9.575	4.176	-0.116
H	9.814	4.300	-1.092
C	9.980	5.161	0.729
O	10.618	6.121	0.311
C	9.634	5.002	2.193
H	8.560	4.867	2.347
H	10.145	4.132	2.619
H	9.962	5.897	2.719

3) Cartesian coordinates of the neutral emitting intermediate 5b in CH_2Cl_2.

N	4.441	0.295	-0.208
C	5.067	0.173	1.113
H	6.154	0.246	1.080
H	4.720	1.030	1.704
C	4.476	1.635	-0.791
H	4.272	2.347	0.016
H	3.638	1.714	-1.497
C	4.833	-0.741	-1.168
H	4.143	-0.667	-2.017
H	5.835	-0.570	-1.568
C	6.061	-2.859	-0.432
O	7.138	-2.143	-0.819
O	6.169	-3.999	-0.006
C	8.393	-2.820	-0.762
H	9.141	-2.085	-1.051
H	8.592	-3.184	0.245
H	8.394	-3.669	-1.451
C	5.788	-1.928	2.394

O	5.619	-2.945	3.049
O	7.033	-1.445	2.161
C	8.095	-2.202	2.738
H	9.012	-1.760	2.353
H	8.063	-2.137	3.829
H	8.020	-3.251	2.446
C	4.788	-2.133	-0.606
C	3.641	-2.910	-0.466
H	3.844	-3.928	-0.148
C	2.272	-2.622	-0.697
C	1.348	-3.700	-0.567
C	1.718	-1.358	-1.048
C	0.006	-3.541	-0.794
H	1.732	-4.680	-0.298
C	0.370	-1.212	-1.282
H	2.352	-0.483	-1.056
C	-0.532	-2.288	-1.166
H	-0.649	-4.402	-0.710
H	-0.014	-0.221	-1.499
C	-1.966	-2.108	-1.373
C	-2.479	-1.112	-2.221
C	-2.908	-2.901	-0.696
C	-3.836	-0.905	-2.371
H	-1.796	-0.505	-2.806
C	-4.266	-2.681	-0.808
H	-2.569	-3.671	-0.011
C	-4.767	-1.664	-1.640
H	-4.182	-0.143	-3.059
H	-4.949	-3.288	-0.228
N	-6.138	-1.436	-1.731
C	-7.057	-2.387	-1.187
C	-7.833	-2.030	-0.087
C	-7.184	-3.655	-1.751
C	-8.741	-2.938	0.443
H	-7.725	-1.040	0.342
C	-8.085	-4.564	-1.210
H	-6.570	-3.919	-2.606
C	-8.868	-4.207	-0.114
H	-9.343	-2.650	1.299
H	-8.182	-5.551	-1.650
H	-9.574	-4.918	0.303
C	-6.703	-0.251	-2.278
C	-7.802	-0.361	-3.133
C	-6.218	1.016	-1.947
C	-8.405	0.777	-3.651
H	-8.183	-1.345	-3.383
C	-6.813	2.150	-2.488
H	-5.387	1.109	-1.257
C	-7.909	2.039	-3.337
H	-9.261	0.675	-4.311
H	-6.429	3.129	-2.221

H	-8.375	2.929	-3.747
C	4.713	-1.106	1.815
C	3.428	-1.540	2.143
H	3.412	-2.524	2.602
C	2.151	-0.944	1.994
C	1.895	0.401	1.606
C	1.005	-1.742	2.278
C	0.615	0.894	1.534
H	2.716	1.053	1.357
C	-0.272	-1.250	2.173
H	1.157	-2.773	2.582
C	-0.512	0.091	1.806
H	0.472	1.922	1.218
H	-1.109	-1.899	2.409
C	-1.866	0.641	1.721
C	-2.971	-0.165	1.405
C	-2.118	2.005	1.945
C	-4.244	0.359	1.277
H	-2.827	-1.217	1.196
C	-3.391	2.532	1.853
H	-1.307	2.662	2.240
C	-4.480	1.723	1.497
H	-5.062	-0.292	0.991
H	-3.551	3.584	2.060
N	-5.765	2.276	1.356
C	-6.929	1.536	1.691
C	-8.091	1.673	0.924
C	-6.945	0.687	2.801
C	-9.248	0.991	1.276
H	-8.081	2.313	0.050
C	-8.100	-0.011	3.132
H	-6.051	0.579	3.405
C	-9.261	0.143	2.381
H	-10.140	1.110	0.670
H	-8.093	-0.667	3.997
H	-10.165	-0.393	2.651
C	-5.907	3.627	0.936
C	-6.799	4.480	1.588
C	-5.156	4.114	-0.136
C	-6.948	5.794	1.161
H	-7.379	4.107	2.425
C	-5.297	5.434	-0.547
H	-4.459	3.455	-0.643
C	-6.197	6.279	0.094
H	-7.648	6.444	1.675
H	-4.705	5.797	-1.381
H	-6.312	7.307	-0.233
C	5.754	2.068	-1.533
H	5.643	3.127	-1.798
H	5.834	1.526	-2.483
C	7.044	1.865	-0.741

H	6.956	2.361	0.236
H	7.165	0.796	-0.547
C	8.285	2.376	-1.463
H	8.194	3.449	-1.664
H	8.395	1.879	-2.433
C	9.591	2.164	-0.669
H	9.500	2.634	0.315
C	9.845	0.668	-0.486
O	10.477	0.019	-1.284
O	9.297	0.066	0.577
H	8.794	0.678	1.138
N	10.742	2.710	-1.354
H	11.181	2.104	-2.037
C	11.228	3.979	-1.282
O	12.165	4.333	-1.987
C	10.581	4.909	-0.278
H	9.500	4.985	-0.427
H	10.754	4.557	0.743
H	11.029	5.895	-0.393

4) Cartesian coordinates of the neutral emitting intermediate 5b in DMSO.

N	4.306	-0.005	0.323
C	5.378	-0.747	1.010
H	6.363	-0.363	0.758
H	5.247	-0.536	2.080
C	4.133	1.354	0.846
H	4.208	1.294	1.937
H	3.106	1.671	0.622
C	4.326	0.001	-1.144
H	3.513	0.667	-1.454
H	5.251	0.432	-1.542
C	5.279	-2.097	-2.301
O	6.427	-1.409	-2.185
O	5.241	-3.211	-2.792
C	7.603	-2.078	-2.645
H	8.431	-1.431	-2.364
H	7.689	-3.054	-2.164
H	7.563	-2.212	-3.728
C	6.718	-2.845	0.494
O	6.914	-4.031	0.240
O	7.781	-1.983	0.568
C	9.067	-2.596	0.487
H	9.790	-1.788	0.598
H	9.193	-3.330	1.286
H	9.211	-3.091	-0.474
C	4.103	-1.335	-1.805
C	2.907	-1.890	-2.070
H	2.946	-2.829	-2.616
C	1.551	-1.403	-1.814
C	0.526	-1.911	-2.625

C	1.200	-0.474	-0.824
C	-0.780	-1.469	-2.497
H	0.766	-2.648	-3.385
C	-0.111	-0.035	-0.697
H	1.949	-0.154	-0.111
C	-1.124	-0.508	-1.538
H	-1.542	-1.855	-3.167
H	-0.361	0.664	0.096
C	-2.518	-0.018	-1.450
C	-2.815	1.331	-1.248
C	-3.599	-0.890	-1.623
C	-4.122	1.804	-1.274
H	-2.005	2.043	-1.114
C	-4.906	-0.439	-1.623
H	-3.414	-1.954	-1.736
C	-5.193	0.928	-1.488
H	-4.308	2.863	-1.147
H	-5.715	-1.151	-1.733
N	-6.520	1.389	-1.540
C	-7.523	0.719	-2.295
C	-8.830	0.701	-1.804
C	-7.250	0.120	-3.527
C	-9.844	0.084	-2.527
H	-9.045	1.175	-0.852
C	-8.265	-0.510	-4.237
H	-6.241	0.145	-3.924
C	-9.566	-0.532	-3.744
H	-10.855	0.079	-2.130
H	-8.037	-0.974	-5.191
H	-10.357	-1.020	-4.304
C	-6.821	2.741	-1.172
C	-7.005	3.704	-2.163
C	-6.953	3.087	0.169
C	-7.321	5.010	-1.812
H	-6.903	3.417	-3.205
C	-7.261	4.398	0.517
H	-6.817	2.331	0.932
C	-7.447	5.361	-0.470
H	-7.464	5.757	-2.587
H	-7.360	4.661	1.565
H	-7.693	6.382	-0.195
C	5.428	-2.234	0.779
C	4.346	-3.106	0.825
H	4.553	-4.096	0.424
C	3.022	-2.894	1.256
C	2.597	-1.815	2.097
C	2.005	-3.823	0.862
C	1.288	-1.640	2.429
H	3.331	-1.126	2.488
C	0.689	-3.622	1.151
H	2.299	-4.691	0.278

C	0.253	-2.490	1.919
H	1.028	-0.790	3.047
H	-0.038	-4.347	0.805
C	-1.119	-2.178	2.105
C	-2.150	-2.766	1.305
C	-1.553	-1.200	3.056
C	-3.449	-2.345	1.367
H	-1.890	-3.507	0.559
C	-2.851	-0.785	3.131
H	-0.845	-0.791	3.767
C	-3.834	-1.305	2.250
H	-4.182	-2.763	0.690
H	-3.139	-0.055	3.878
N	-5.116	-0.794	2.238
C	-6.214	-1.609	1.839
C	-7.136	-1.132	0.905
C	-6.363	-2.885	2.384
C	-8.198	-1.938	0.517
H	-7.005	-0.147	0.472
C	-7.426	-3.685	1.986
H	-5.648	-3.239	3.118
C	-8.346	-3.215	1.053
H	-8.902	-1.567	-0.220
H	-7.540	-4.675	2.414
H	-9.176	-3.841	0.743
C	-5.364	0.546	2.636
C	-6.483	0.847	3.418
C	-4.484	1.566	2.259
C	-6.698	2.153	3.839
H	-7.167	0.056	3.705
C	-4.699	2.862	2.703
H	-3.647	1.340	1.610
C	-5.801	3.162	3.499
H	-7.565	2.377	4.452
H	-4.012	3.647	2.404
H	-5.967	4.178	3.843
C	5.083	2.457	0.335
H	4.886	3.364	0.920
H	4.839	2.705	-0.705
C	6.561	2.087	0.420
H	6.793	1.745	1.437
H	6.729	1.243	-0.250
C	7.530	3.198	0.042
H	7.414	4.052	0.717
H	7.333	3.564	-0.972
C	9.006	2.745	0.125
H	9.183	2.274	1.096
C	9.320	1.730	-0.976
O	9.816	2.053	-2.028
O	8.997	0.445	-0.769
H	8.586	0.270	0.095

N	9.927	3.847	-0.046
H	10.198	4.056	-1.000
C	10.419	4.675	0.912
O	11.153	5.612	0.615
C	10.044	4.371	2.346
H	8.961	4.311	2.483
H	10.475	3.416	2.663
H	10.443	5.165	2.977