Supporting Information

Synthesis, photophysical, theoretical and electrochemical evaluation of a new Rhodamine-ChalcogenoAmino-Thymidine (RhoCAT) hybrid derivative

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Chemistry

CHEMISTRY

General Considerations

All Chemicals were of analytical grade and obtained from standard commercial suppliers and some reactions were run under an atmosphere of dry argon. Proton nuclear magnetic resonance spectra (^{1}H NMR) were obtained at 400 MHz in a Bruker DPX400 and at 600 MHz in a Bruker Avance III NMR spectrometer. Spectra were recorded in $CDCl_3$ solution. Chemical shifts are reported in ppm, referenced to the solvent peak of tetramethylsilane (TMS) as the external reference. Data are reported as follows: chemical shift (δ) expressed in ppm, multiplicity (br = broad, s = singlet, d = doublet, dd = doublet of doublets, ddd = doublet of doublet of doublets, dt = doublet of triplets, t = triplet, m = multiplet, q = quartet), and coupling constant (J) in Hertz and integrated intensity. Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra were obtained either at 100 MHz in a Bruker DPX400 and at 150 MHz in a Bruker Avance III NMR spectrometer. Chemical shifts (δ) are reported in ppm, referenced to the solvents peak of $CDCl_3$. High-resolution mass spectra (HRMS) were obtained on a LTQ Orbitrap Discovery mass spectrometer (Thermo Fisher Scientific, Bremen, Germany). This hybrid system combines an LTQ XL linear ion-trap mass spectrometer and an Orbitrap mass analyzer. The experiments were performed via direct infusion of the sample (flow rate 10 mL/min) in positive-ion mode using electrospray ionization (ESI). Elemental composition calculations were executed using the specific tool included in the Qual Browser module of the Xcalibur (Thermo Fisher Scientific, release 2.0.7) software. Thin layer chromatography (TLC) was performed using Merck Silica Gel GF254, 0.25 mm. For visualization, TLC plates were either placed under ultraviolet light, or stained with iodine vapor, or acidic vanillin.

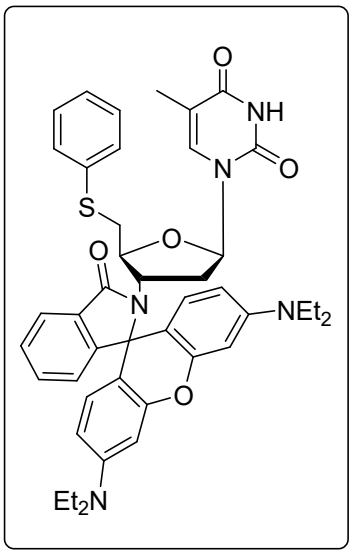
General Methods

Synthetic Procedures

Preparation of 5'-Arylchalcogenyl-3'-N-(E)-Rhodamine-3',5'-dideoxy-aminothymidine (5a-i)

In a two-necked round-bottom flask under argon atmosphere, Rhodamine B (2 eq.), TsCl (3.5 eq.) and dichloromethane (10 mL) were added and the reaction mixture was stirred for 15 min. Then, DMAP (5 eq.) was added and the reaction was left under stirring for 15 min. Next, a solution of compound **3a-i** (1 mmol) in dichloromethane (5 mL) was slowly added to the reaction mixture. Then, the mixture was stirred at reflux temperature until the consumption of compound **3a-i** (3 h; monitored by TLC - DCM:EtOH, 2.5 %). At the end of the reaction time, a saturated aqueous solution of sodium bicarbonate (10 mL) was added and then the mixture was extracted with ethyl acetate (3 x 20 mL). The resulting organic phase was dried over anhydrous $MgSO_4$, filtered and the solvent was evaporated. The crude product was purified by flash chromatography on silica gel with a gradient system until the pure product was obtained (DCM:EtOH 2.5 %).

5'-S-(Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5a)



Physical properties: Pink solid

m.p.: 123-125°C,

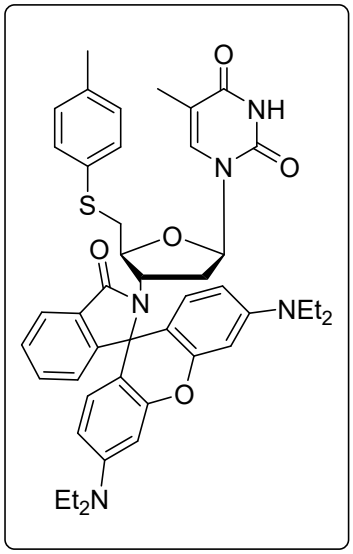
Yield: 60%

HRMS [TOF MS ES+] m/z calculated for $C_{44}H_{47}N_5O_5S$ $[M+H]^+$: 758.3371; found $[M+H]^+$: 758.3379.

^{1}H NMR (600 MHz. $CDCl_3$), δ (ppm): 8.40 (s, 1H), 8.02 – 7.86 (m, 1H), 7.57 – 7.45 (m, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.15 – 7.08 (m, 1H), 7.06 – 7.02 (m, 3H), 6.48 (t, *J* = 6.6 Hz, 1H), 6.44 – 6.38 (m, 4H), 6.32 – 6.23 (m, 2H), 4.82 – 4.69 (m, 1H), 3.55 – 3.48 (m, 1H), 3.33 (h, *J* = 8.4, 7.7 Hz, 8H), 2.92 (dd, *J* = 13.3, 3.5 Hz, 1H), 2.74 (dt, *J* = 13.8, 6.8 Hz, 1H), 2.22 (dd, *J* = 13.2, 4.3 Hz, 1H), 1.70 (s, 3H), 1.61 (ddd, *J* = 14.0, 10.6, 5.9 Hz, 1H), 1.17 (td, *J* = 7.1, 3.1 Hz, 12H).

^{13}C NMR (150 MHz. $CDCl_3$), δ (ppm): 167.4, 163.5, 158.5, 153.5, 152.8, 149.8, 148.9, 136.1, 132.8, 131.9, 131.7, 131.5, 128.7, 128.4, 126.8, 124.0, 122.8, 114.4, 110.4, 108., 98.20, 97.3, 85.3, 79.5, 65., 55.31, 54.2, 44.4, 38.1, 36.5, 12.5.

5'-S-(4-Methyl-Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5b)



Physical properties: Pink solid

m.p.: 115-116°C,

Yield: 70%

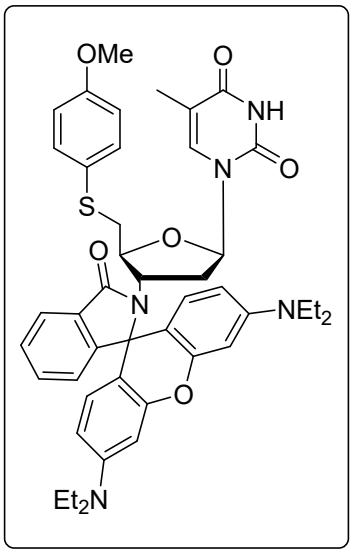
HRMS [TOF MS ES+] m/z calculated for $C_{45}H_{49}N_5O_5S$ $[M+H]^+$: 772.3527; found $[M+H]^+$: 772.3535.

^{1}H NMR (400 MHz. DMSO), δ (ppm): 8.04 (s, 1H), 7.94 – 7.86 (m, 1H), 7.56 – 7.44 (m, 2H), 7.22 – 7.16 (m, 2H), 7.13 – 7.04 (m, 2H), 7.04 – 6.92 (m, 2H), 6.55 (t, *J* = 6.7 Hz, 1H), 6.47 – 6.37 (m, 4H), 6.33 – 6.22 (m, 2H), 4.79 (ddd, *J* = 7.2,

4.3, 3.0 Hz, 1H), 3.69 – 3.60 (m, 1H), 3.33 (p, *J* = 7.1 Hz, 8H), 2.86 (dd, *J* = 13.6, 3.1 Hz, 1H), 2.66 (ddd, *J* = 13.8, 6.9, 5.3 Hz, 1H), 2.26 (s, 3H), 2.14 (dd, *J* = 13.6, 4.3 Hz, 1H), 1.72 – 1.54 (m, 3H), 1.16 (td, *J* = 7.1, 4.7 Hz, 12H).

^{13}C NMR (100 MHz. DMSO), δ (ppm): 167.3, 163.4, 153.5, 153.5, 152.6, 149.7, 136.2, 136.1, 132.7, 131.8, 131.2, 129.7, 128.7, 128.4, 127.0, 124.0, 122.8, 110.3, 108.5, 98.3, 97.8, 84.7, 78.8, 65.8, 55.2, 44.5, 36.2, 30.5, 20.9, 12.5, 12.1.

5'-S-(4-Methoxy-Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5c)



Physical properties: Pink solid

m.p.: 103-107°C,

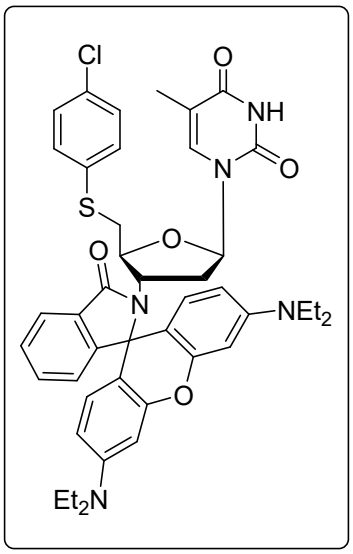
Yield: 65%

HRMS [TOF MS ES+] m/z calculated for $C_{45}H_{49}N_5O_6S$ $[M+H]^+$: 788.3476; found $[M+H]^+$: 788.3482.

^{1}H NMR (600 MHz.$CDCl_3$), δ(ppm): 8.17 (s, 1H), 7.90 (dd, *J* = 5.8, 3.0 Hz, 1H), 7.47 (dd, *J* = 5.8, 3.0 Hz, 2H), 7.16 – 7.11 (m, 3H), 7.10 – 7.05 (m, 1H), 6.78 – 6.72 (m, 2H), 6.61 (t, *J* = 6.8 Hz, 1H), 6.44 – 6.40 (m, 2H), 6.39 – 6.35 (m, 1H), 6.29 – 6.23 (m, 2H), 4.71 (ddd, *J* = 7.5, 4.6, 2.7 Hz, 1H), 3.76 (s, 3H), 3.74 – 3.68 (m, 1H), 3.33 (dq, *J* = 20.5, 7.1 Hz, 8H), 2.79 (dd, *J* = 13.9, 3.0 Hz, 1H), 2.64 (ddd, *J* = 14.0, 6.8, 4.6 Hz, 1H), 2.13 (dd, *J* = 13.9, 4.8 Hz, 1H), 1.72 (s, 3H), 1.71 – 1.65 (m, 1H), 1.16 (dt, *J* = 16.9, 7.0 Hz, 12H).

^{13}C NMR (150 MHz. $CDCl_3$), δ(ppm): 167.4, 163.5, 158.5, 153.4, 152.8, 149.8, 148.9, 136.1, 132.8, 131.9, 131.7, 131.5, 128.7, 128.4, 126.8, 124.0, 122.8, 114.4, 110.4, 108.4, 98.2, 97.3, 85.3, 79.5, 65.8, 55.3, 54.2, 44.4, 38.1, 36.6, 12.5.

5'-S-(4-Chloro-Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5d)



Physical properties: Pink solid

m.p.: 125-129°C,

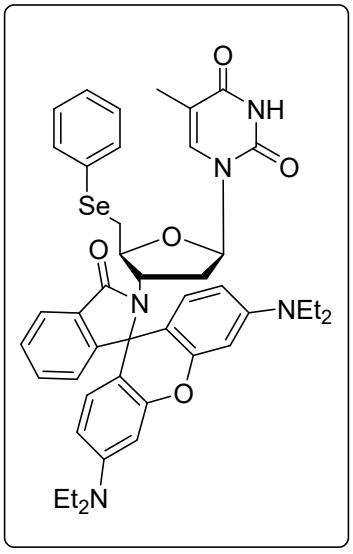
Yield: 76%

HRMS [TOF MS ES+] m/z calculated for $C_{44}H_{46}ClN_5O_5S$ $[M+H]^+$: 792.2981; found $[M+H]^+$: 792.2985.

^{1}H NMR (600 MHz. $CDCl_3$), δ (ppm) 8.31 (s. 1H). 7.91 (q. *J* = 4.2. 3.8 Hz. 1H). 7.48 (q. *J* = 4.0 Hz. 2H). 7.14 (d. *J* = 8.3 Hz. 2H). 7.10 – 7.08 (m. 1H). 7.05 (d. *J* = 8.3 Hz. 2H). 6.99 (s. 1H). 6.64 – 6.53 (m. 1H). 6.40 (dt. *J* = 27.1. 7.2 Hz. 3H). 6.31 – 6.22 (m. 2H). 4.76 (dt. *J* = 7.7. 3.7 Hz. 1H). 3.73 (dt. *J* = 11.5. 5.7 Hz. 1H). 3.33 (dt. *J* = 25.1. 7.3 Hz. 8H). 2.86 (dd. *J* = 13.8. 3.1 Hz. 1H). 2.66 (dt. *J* = 12.9. 6.2 Hz. 1H). 2.16 (dd. *J* = 13.9. 4.6 Hz. 1H). 1.85 (dtt. *J* = 28.1. 22.3. 8.7 Hz. 1H). 1.70 (s. 3H). 1.16 (dt. *J* = 20.1. 7.1 Hz. 12H).

^{13}C NMR (151 MHz. $CDCl_3$), δ (ppm): 167.4, 163.5, 153.4, 149.8, 149.1, 135.9, 135.3, 132.9, 131.6, 129.6, 129.4, 128.8, 128.8, 128.5, 124.0, 122.9, 110.5, 108.4, 107.3, 98.2, 97.8, 85.3, 78.9, 65.8, 54.2, 44.4, 36.1, 14.6, 12.5, 12.3.

5'-Se-(Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5e)



Physical properties: Pink solid

m.p.: 114-115°C,

Yield: 84%

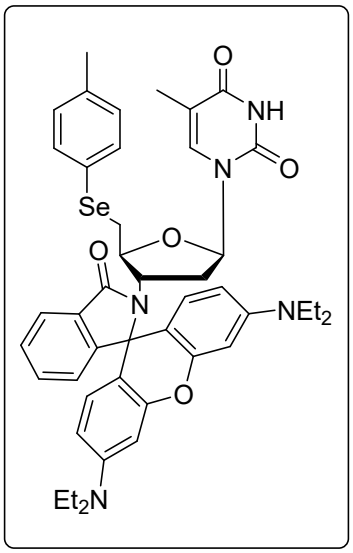
HRMS [TOF MS ES+] m/z calculated for $C_{44}H_{47}N_5O_5Se$ $[M+H]^+$: 806.2820; found $[M+H]^+$: 806.2822.

^{1}H NMR (400 MHz. $CDCl_3$), δ (ppm): 8.02 (s, 1H), 7.95 – 7.86 (m, 1H), 7.55 – 7.40 (m, 2H), 7.33 – 7.27 (m, 2H), 7.18 – 7.08 (m, 4H), 7.04 (d, *J* = 1.3 Hz, 1H), 6.54 (t, *J* = 6.6 Hz, 1H), 6.49 – 6.35 (m, 4H), 6.29 (dt, *J* = 9.1, 3.2 Hz, 2H), 4.88

– 4.76 (m, 1H), 3.72 – 3.60 (m, 1H), 3.33 (dt, *J* = 14.0, 6.9 Hz, 7H), 2.92 (dd, *J* = 13.6, 3.0 Hz, 1H), 2.73 – 2.62 (m, 1H), 2.16 (dd, *J* = 13.6, 4.2 Hz, 1H), 1.69 – 1.62 (m, 1H), 1.61 (d, *J* = 1.2 Hz, 3H), 1.16 (td, *J* = 7.1, 4.0 Hz, 12H).

^{13}C NMR (150 MHz. $CDCl_3$), δ (ppm): 167.2, 163.7, 153.4, 153.3, 152.4, 149.8, 135.9, 132.7, 131.6, 130.8, 130.4, 128.7, 128.7, 128.6, 128.3, 126.1, 123.9, 122.7, 110.2, 98.1, 97.6, 84.5, 78.5, 60.5, 55.0, 44.4, 35.9, 29.9, 12.4, 12.1.

5'-Se-(4-Methyl-Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5f)



Physical properties: Pink solid

m.p.: 95-96°C,

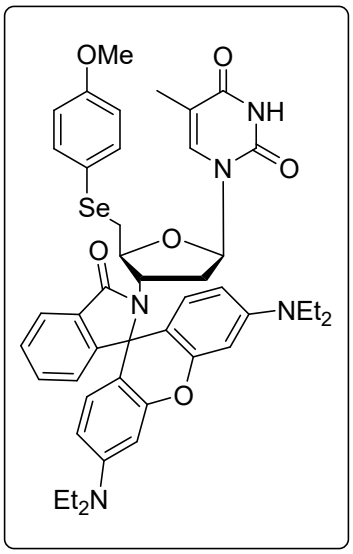
Yield: 96%

HRMS [TOF MS ES+] m/z calculated for $C_{45}H_{49}N_5O_5Se$ $[M+H]^+$: 820.2977; found $[M+H]^+$: 820.2985.

^{1}H NMR (600 MHz. $CDCl_3$), δ (ppm): 8.09 (s, 1H), 7.91 (dd, *J* = 6.0, 2.9 Hz, 1H), 7.48 (dt, *J* = 8.7, 3.9 Hz, 2H), 7.19 (d, *J* = 8.3 Hz, 2H), 7.12 – 7.08 (m, 1H), 7.07 (s, 1H), 6.99 – 6.94 (m, 2H), 6.56 (t, *J* = 6.6 Hz, 1H), 6.45 – 6.41 (m, 2H), 6.39 (d, *J* = 4.0 Hz, 1H), 6.27 (d, *J* = 9.3 Hz, 2H), 4.81 – 4.76 (m, 1H), 3.66 – 3.64 (m, 1H), 3.33 (dd, *J* = 11.3, 7.2 Hz, 8H), 2.87 (dd, *J* = 13.6, 2.6 Hz, 1H), 2.65 (dd, *J* = 13.3, 6.4 Hz, 1H), 2.26 (s, 3H), 2.12 (dd, *J* = 13.4, 4.1 Hz, 1H), 1.74 (t, *J* = 7.5 Hz, 1H), 1.62 (s, 3H), 1.16 (q, *J* = 7.3 Hz, 12H).

^{13}C NMR (151 MHz. $CDCl_3$), δ (ppm): 167.3, 163.4, 153.5, 153.4, 152.6, 149.7, 136.1, 132.7, 131.7, 131.1, 129.7, 128.7, 128.7, 128.4, 126.9, 124.0, 122.8, 110.3, 108.4, 98.2, 97.7, 84.6, 78.8, 65.8, 55.1, 44.4, 36.2, 30.4, 20.9, 12.5, 12.1.

5'-Se-(4-MethoxyPhenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5g)



Physical properties: Pink solid

m.p.: 121-123°C,

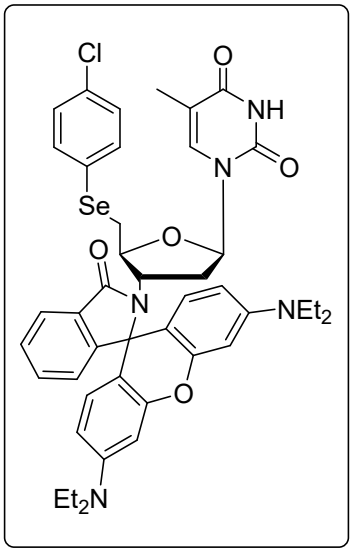
Yield: 82%

HRMS [TOF MS ES+] m/z calculated for $C_{45}H_{49}N_5O_6Se$ $[M+H]^+$: 836.2926; found $[M+H]^+$: 836.2931.

^{1}H NMR (400 MHz. DMSO), δ (ppm): 8.06 (s, 1H), 7.96 – 7.84 (m, 1H), 7.46 (dd, *J* = 5.6, 3.1 Hz, 2H), 7.16 – 7.11 (m, 3H), 7.10 – 7.05 (m, 1H), 6.77 – 6.71 (m, 2H), 6.59 (t, *J* = 6.7 Hz, 1H), 6.46 – 6.36 (m, 3H), 6.33 – 6.24 (m, 2H), 4.72 (ddd, *J* = 6.6, 4.8, 2.9 Hz, 1H), 3.76 (s, 3H), 3.71 (ddd, *J* = 11.1, 6.6, 4.9 Hz, 1H), 3.32 (dq, *J* = 11.3, 7.1 Hz, 8H), 2.78 (dd, *J* = 13.9, 3.0 Hz, 1H), 2.65 (ddd, *J* = 13.8, 6.8, 4.9 Hz, 1H), 2.16 (dd, *J* = 13.9, 4.9 Hz, 1H), 1.75 – 1.62 (m, 4H), 1.15 (dt, *J* = 9.8, 7.1 Hz, 12H).

^{13}C NMR (100 MHz. DMSO), δ (ppm): 167.4, 163.4, 158.6, 153.5, 153.5, 152.8, 149.8, 136.1, 132.8, 131.8, 128.8, 128.8, 128.4, 126.9, 124.0, 122.8, 114.5, 110.4, 108.5, 98.4, 97.9, 85.4, 79.6, 65.8, 55.3, 54.4, 44.5, 38.2, 36.5, 12.6, 12.3.

5'-Se-(4-Chloro-Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5h)



Physical properties: Pink solid

m.p.: 136-139°C,

Yield: 72%

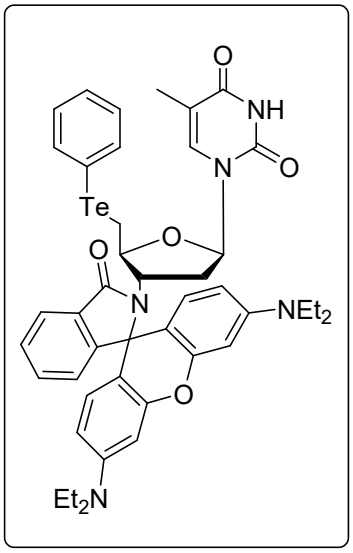
HRMS [TOF MS ES+] m/z calculated for $C_{44}H_{46}ClN_5O_5Se$ $[M+H]^+$: 840.2428; found $[M+H]^+$: 840.2436.

^{1}H NMR (600 MHz. $CDCl_3$), δ (ppm): 8.96 (m, 1H), 7.93 – 7.90 (m, 1H), 7.47 (dd, *J* = 6.1, 2.8 Hz, 2H), 7.22 – 7.19 (m, 2H), 7.12 – 7.07 (m, 3H), 7.01 (d, *J* = 1.4 Hz, 1H), 6.55 (t, *J* = 6.6 Hz, 1H), 6.45 – 6.38 (m, 4H), 6.27 (td, *J* = 8.9, 2.6 Hz, 2H), 4.82 (ddd, *J* = 7.2, 4.3, 3.1 Hz, 1H), 3.68 – 3.64

(m, 1H), 3.33 (dq, *J* = 14.0, 7.1 Hz, 8H), 2.88 (dd, *J* = 13.3, 3.1 Hz, 1H), 2.72 – 2.67 (m, 1H), 2.21 – 2.17 (m, 1H), 1.69 (d, *J* = 1.3 Hz, 3H), 1.68 – 1.63 (m, 1H), 1.16 (q, *J* = 7.3 Hz, 12H).

^{13}C NMR (150 MHz. $CDCl_3$), δ (ppm):167.4, 163.7, 153.5, 152.6, 149.9, 149.0, 135.9, 132.8, 132.4, 132.3, 131.6, 129.1, 128.9, 128.8, 128.7, 128.4, 124.0, 122.8, 110.5, 108.4, 98.2, 97.7, 84.7, 78.5, 65.8, 55.1, 44.5, 35.7, 30.6, 12.5, 12.3.

5'-Te-(Phenyl)-3'-N-Rhodamine-3',5'-dideoxy- aminothymidine (5i)



Physical properties: Pink solid

m.p.: 117-120°C,

Yield: 14%

HRMS [TOF MS ES+] m/z calculated for $C_{44}H_{47}N_5O_5Te$ $[M+H]^+$: 856.2717; found $[M+H]^+$: 856.2724.

^{1}H NMR (600 MHz. $CDCl_3$), δ (ppm): 8.94 (d, *J* = 10.3 Hz, 1H), 7.92 (dd, *J* = 5.7, 3.1 Hz, 1H), 7.47 (dd, *J* = 5.7, 3.0 Hz, 2H), 7.13 (d, *J* = 8.5 Hz, 2H), 7.09 (dd, *J* = 5.6, 3.0 Hz, 1H), 7.06 – 7.03 (m, 2H), 7.00 (s, 1H), 6.57 (t, *J* = 6.7 Hz, 1H), 6.43 (t, *J* = 9.6 Hz, 3H), 6.38 (d, *J* = 2.5 Hz, 1H), 6.31 – 6.24 (m, 2H), 4.80 – 4.75 (m, 1H), 3.73 (ddd, *J* = 11.6, 6.7, 5.1 Hz, 1H), 3.32 (dq, *J* = 22.2, 7.1 Hz, 8H), 2.85 (dd, *J* = 13.8, 3.0 Hz, 1H), 2.72 – 2.64 (m, 1H), 2.20 (ddd, *J* = 13.8, 4.8, 2.7 Hz, 1H), 1.71 (s, 3H), 1.69 (d, *J* = 2.9 Hz, 1H), 1.15 (dt, *J* = 18.0, 7.0 Hz, 12H).

^{13}C NMR (150 MHz. $CDCl_3$), δ (ppm): 167.3, 163.7, 153.4, 152.5, 149.8, 148.9, 135.8, 135.3, 132.7, 131.5, 131.3, 129.2, 128.6, 128.3, 123.9, 122.7, 110.4, 108.3, 105.1, 104.5, 97.9, 97.6, 85.2, 78.8, 65.7, 54.1, 44.3, 35.9, 12.4, 12.2.

Photophysical analysis

The UV-Vis electronic absorption spectroscopy of compounds **5a-i** was recorded using a Shimadzu UV-2600 spectrophotometer (data interval, 1.0 nm) using three solvents (DCM, EtOH and DMSO) according to the distinct dielectric constant (ε_0). All absorption spectra were recorded in the 250–650 nm range at a fixed concentration of 20 μM.

Steady-state fluorescence emission spectra of **5a-i** in the same solvents were measured with a Horiba Yvon-Jobin Fluoromax Plus spectrofluorometer (Em/Exc; slit 1.0 mm) in the 350–650 nm range at a fixed concentration of 2.0 μM. Fluorescence quantum yield values (Φ_f) of the studied compounds were determined by comparing the corrected fluorescence spectra with that of 9,10-diphenylanthracene standard probe in $CHCl_3$ solution (Φ_f = 65%; λ_{exc} = 365 nm) using the appropriate equation according to the literature[1].

Fluorescence lifetime values (τ_f) of **5a-i** were recorded using the Time-Correlated Single Photon Counting (TCSPC) method with a DeltaHub controller and Horiba spectrofluorometer. The data were processed using the DAS6 and OriginPro® 8.5 software, utilizing mono-exponential fitting of the raw data. A NanoLED (Horiba) source (1.0 MHz; pulse width <1.2 ns; 284 nm excitation wavelength) was used as the excitation source.

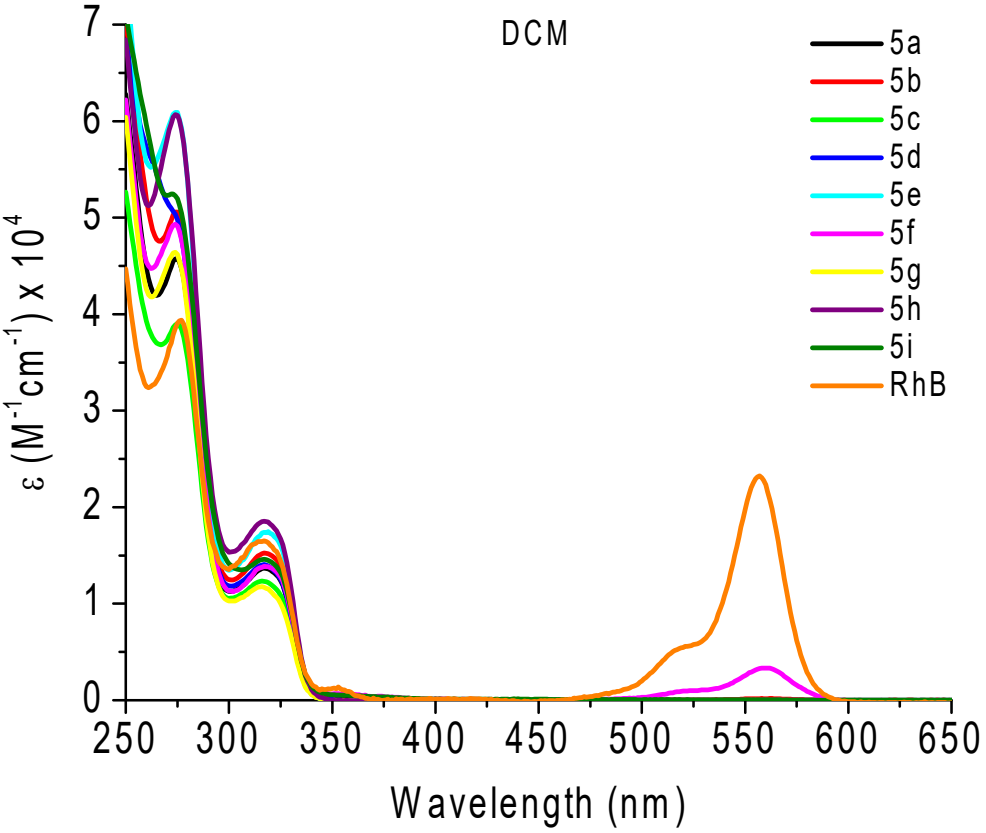


Figure S1. Absorption UV-Vis spectra of studied derivatives in DCM, using fixed concentration at 20 μM.

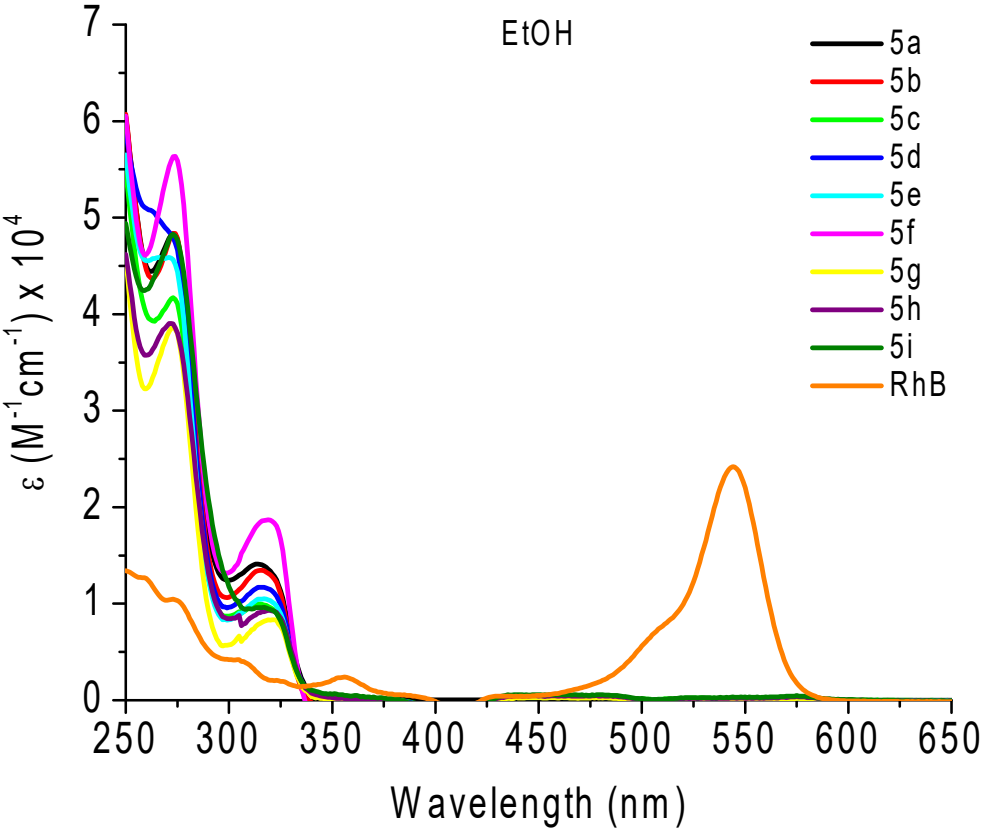


Figure S2. Absorption UV-Vis spectra of studied derivatives in EtOH, using fixed concentration at 20 μM.

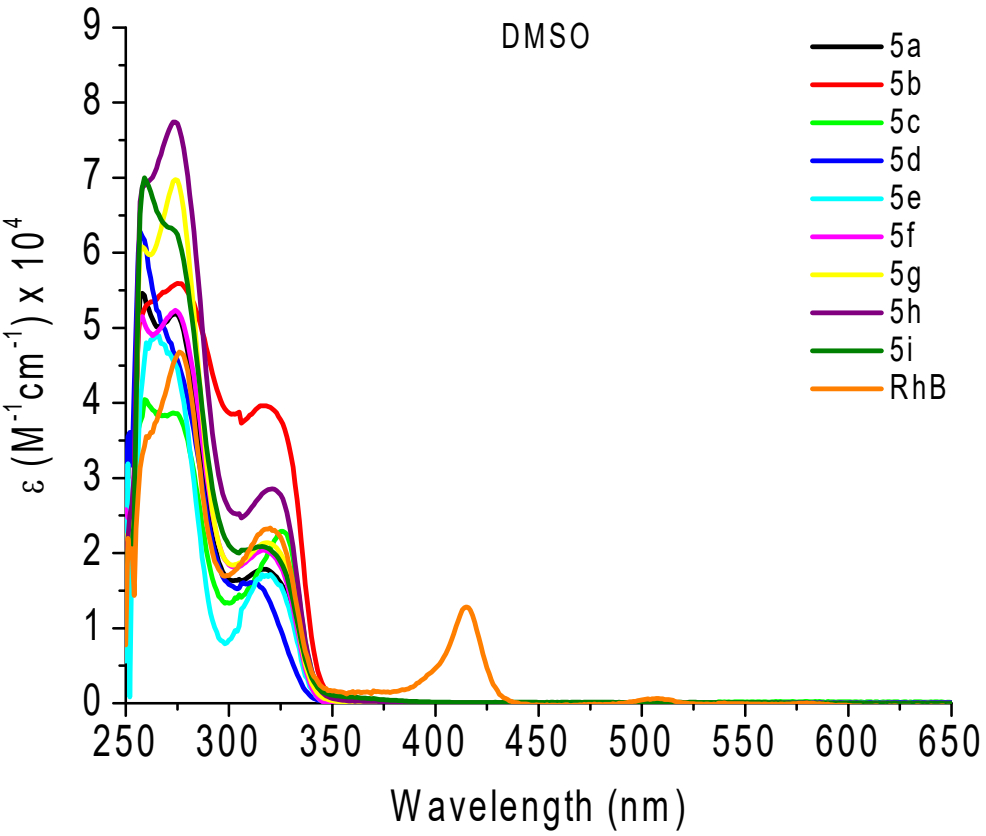


Figure S3. Absorption UV-Vis spectra of studied derivatives in DMSO, using fixed concentration at 20 μM.

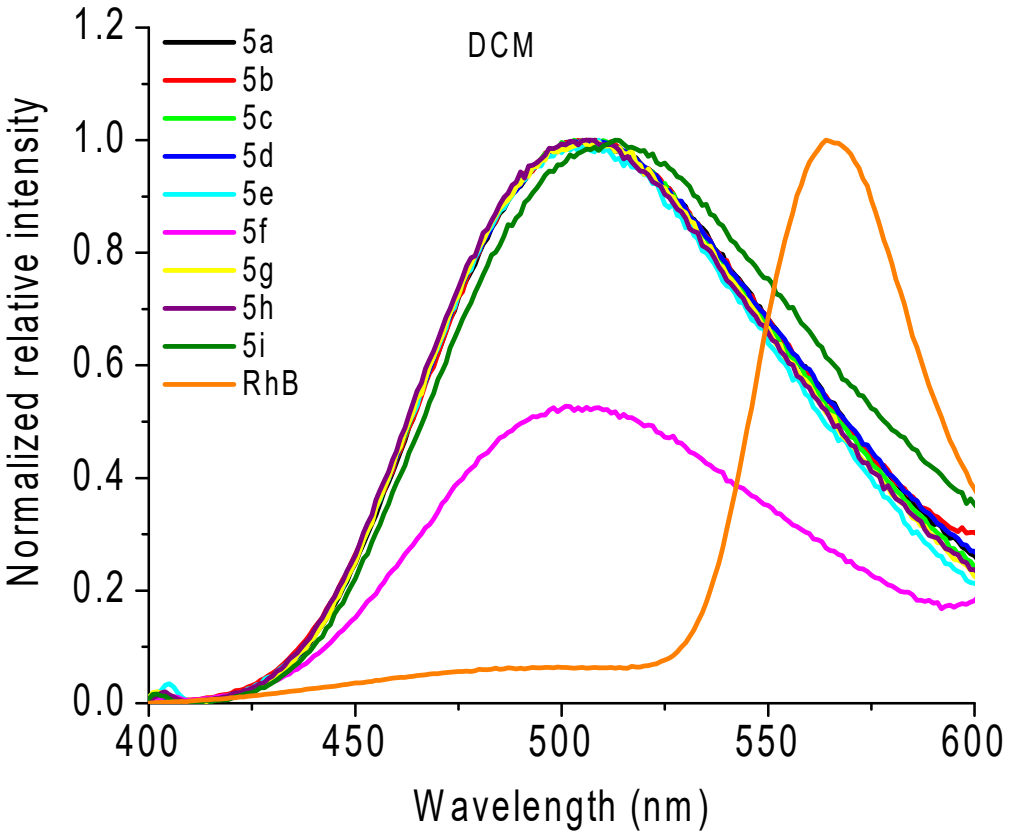


Figure S4. Normalized steady-state fluorescence emission spectra of studied derivatives in DCM, using fixed concentration at 2.0 μM, excited in the less energy transition band.

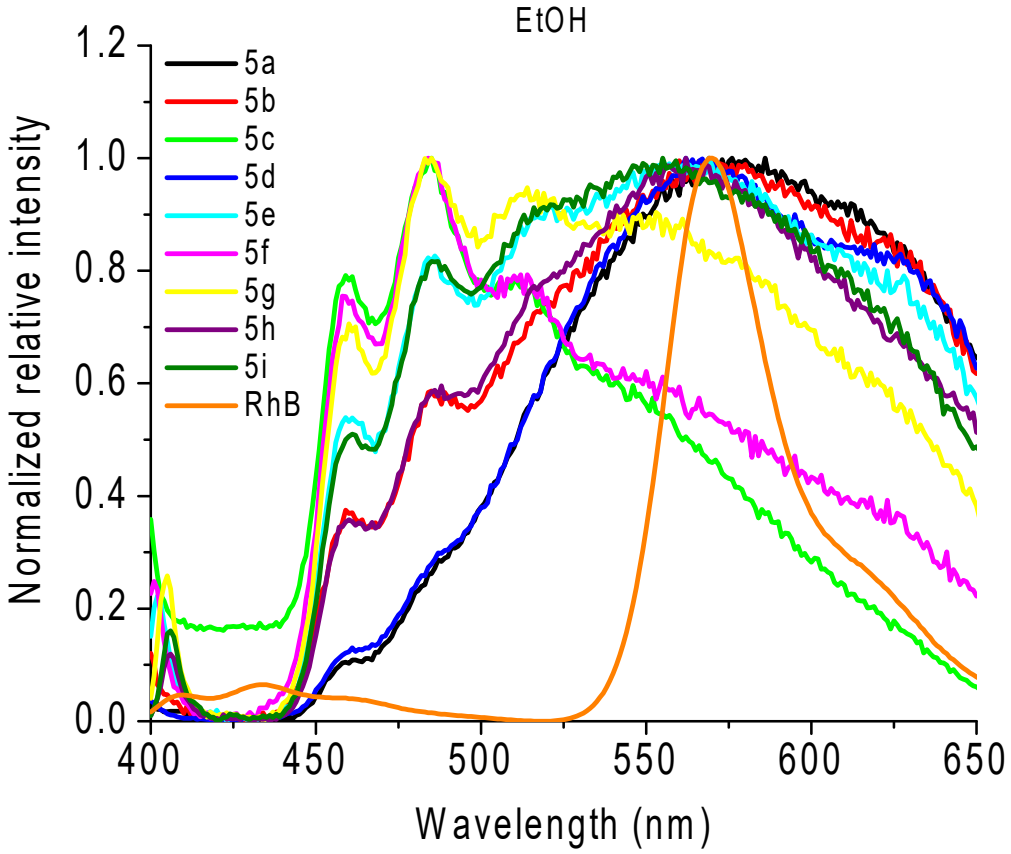


Figure S5. Normalized steady-state fluorescence emission spectra of studied derivatives in EtOH, using fixed concentration at 2.0 μM, excited in the less energy transition band.

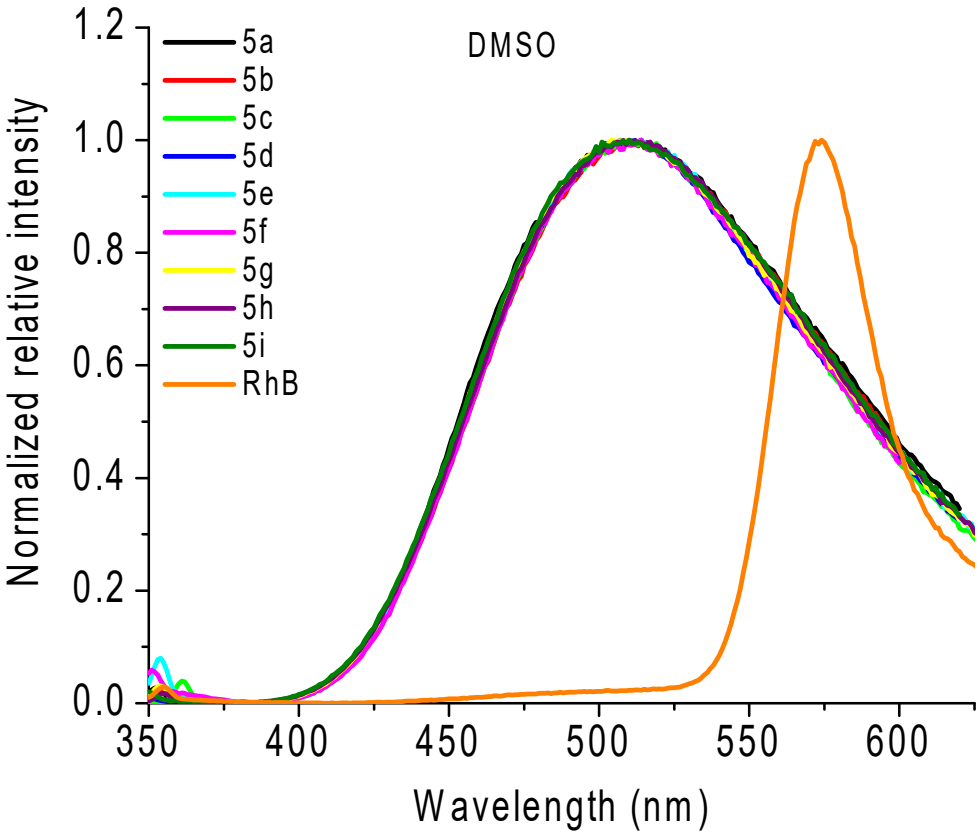


Figure S6. Normalized steady-state fluorescence emission spectra of studied derivatives in DMSO, using fixed concentration at 2.0 μM, excited in the less energy transition band.

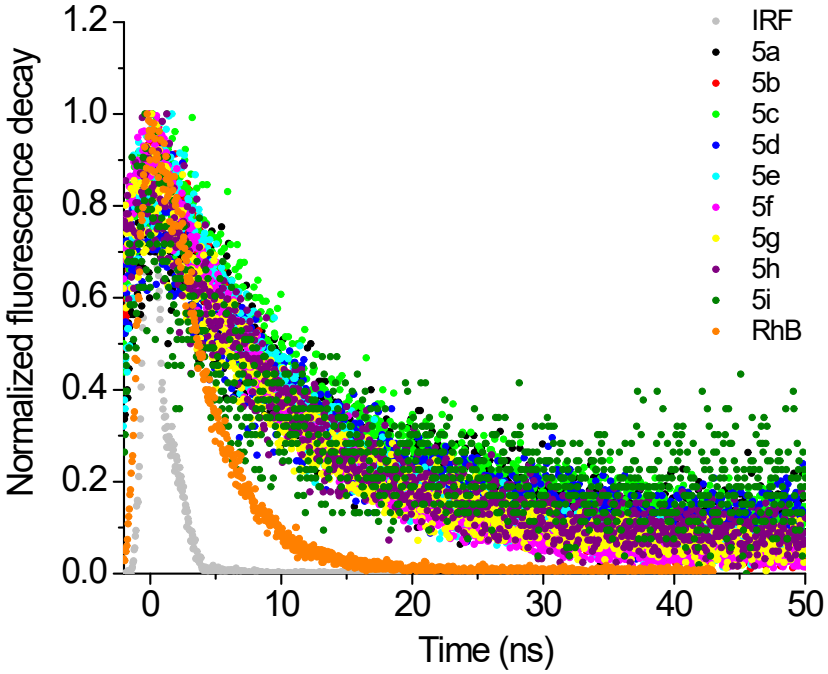


Figure S7. Normalized fluorescence decay plots of studied derivatives in DCM, using fixed concentration at 2.0 μM, excited by NanoLED source at 284 nm.

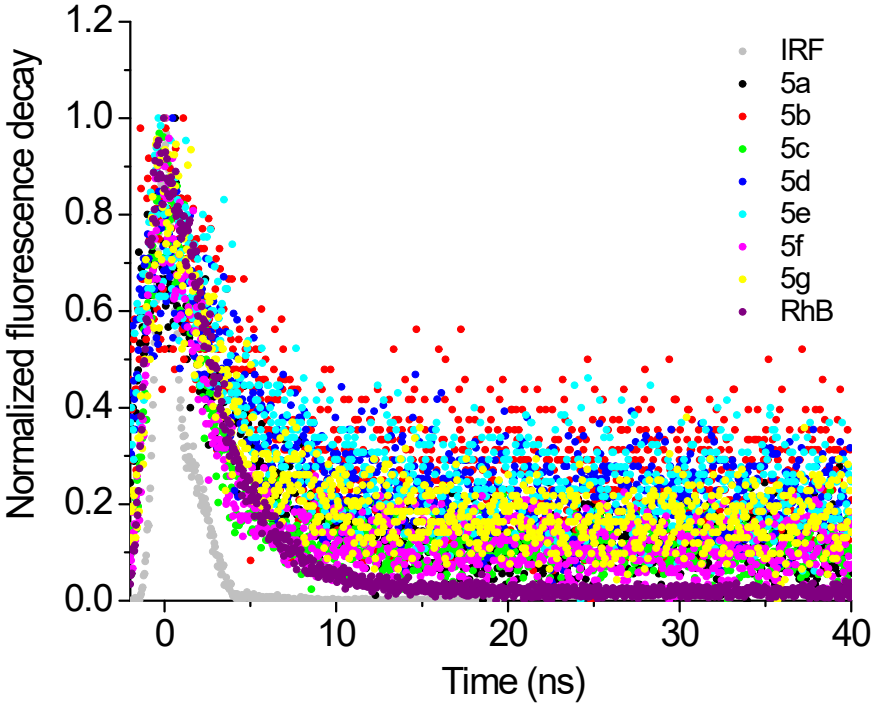


Figure S8. Normalized fluorescence decay plots of studied derivatives in EtOH, using fixed concentration at 2.0 μM, excited by NanoLED source at 284 nm.

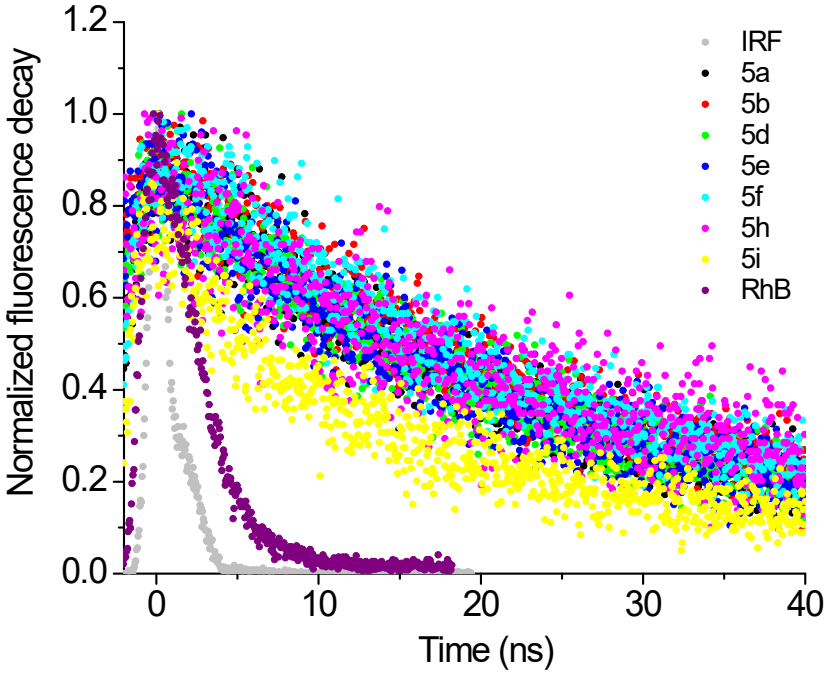


Figure S9. Normalized fluorescence decay plots of studied derivatives in DMSO, using fixed concentration at 2.0 μM, excited by NanoLED source at 284 nm.

Table S1. Photophysical parameters of derivatives in several solvents.

Compound	Solvent*	λ, nm (ε; $M^{-1}cm^{-1}$)[a]	λ_{em}, nm (Φ_f, %)[b,c]	$\Delta\lambda_{SS}$ (nm/cm^{-1})[d]	τ_f, ns (χ^2)[e]	k_r (x10^7 s^{-1})[f]	τ_r (ns)[f]	k_{nr} (x10^7 s^{-1})[f]	τ_{nr} (ns)[f]
	DCM	274 (45680); 317 (14420)	456 (12.0)	139/9615	11.7 (0.92110)	1.02	97.5	7.52	13.3
5a	EtOH	272 (48250); 316 (14020)	525 (1.5)	209/12595	4.20 (0.84629)	0.36	280.0	23.4	4.25
	DMSO	258 (54525); 317 (17970)	510 (14.0)	193/11940	22.2 (0.95500)	0.63	158.5	3.87	25.8
	DCM	275 (50460); 319 (15365)	455 (12.0)	136/9370	10.9 (0.99151)	1.10	90.8	8.07	12.4
5b	EtOH	273 (48460); 317 (13310)	514 (1.5)	197/12090	3.85 (0.85830)	0.39	256.0	25.6	3.90
	DMSO	276 (55665); 319 (39510)	508 (13.0)	189/11660	23.2 (0.95340)	0.56	178.0	3.75	26.5
	DCM	275 (38790); 318 (12190)	455 (11.0)	137/9470	11.6 (0.94616)	0.95	105.4	7.67	13.0
5c	EtOH	273 (41785); 316 (9870)	439 (1.0)	123/8865	2.45 (0.90790)	0.41	245.0	40.4	2.45
	DMSO	274 (38450); 326 (22715)	509 (14.0)	183/11030	23.1 (0.94830)	0.60	165.0	3.70	27.0
	DCM	273 (50565); 318 (13785)	455 (11.0)	137/9470	10.6 (0.92374)	1.04	96.4	8.40	11.9
5d	EtOH	272 (48145); 318 (11790)	513 (1.5)	195/11955	4.00 (0.97165)	0.37	266.0	24.6	4.05
	DMSO	259 (61570); 314 (15910)	510 (14.0)	196/12240	22.6 (0.93550)	0.62	161.0	3.80	26.0
	DCM	274 (60945); 319 (17490)	455 (12.0)	136/9370	10.5 (0.97729)	1.14	87.5	8.40	11.9
5e	EtOH	273 (45520); 319 (10370)	492 (1.5)	173/11020	4.30 (0.97130)	0.35	286.0	22.9	4.35
	DMSO	265 (48880); 319 (16810)	507 (14.0)	188/11625	23.7 (0.94151)	0.59	169.0	3.60	27.5
	DCM	274 (49075); 319 (13875)	453 (11.0)	134/9270	9.75 (0.99110)	1.13	88.6	9.13	10.9
5f	EtOH	274 (56240); 319 (18650)	446 (1.0)	127/8925	2.45 (0.87850)	0.41	245.0	40.4	2.45
	DMSO	274 (52220); 317 (20280)	509 (13.0)	192/11900	23.2 (0.95340)	0.56	178.0	3.75	26.5
	DCM	274 (46320); 318 (11865)	456 (11.0)	138/9515	10.0 (0.98480)	1.10	91.0	8.90	11.2
5g	EtOH	273 (38550); 322 (8350)	461 (2.0)	139/9365	3.30 (0.83150)	0.60	165.0	29.7	3.35
	DMSO	274 (69780); 321 (22080)	507 (14.0)	186/11430	n.d.	n.d.	n.d.	n.d.	n.d.
	DCM	274 (60635); 318 (18650)	453 (11.0)	135/9370	10.3 (0.94025)	1.07	93.6	8.64	11.6

5h	EtOH	272 (39050); 321 (9265)	511 (1.5)	190/11585	n.d.	n.d.	n.d.	n.d.	n.d.
	DMSO	273 (77355); 321 (28490)	510 (14.0)	189/11540	21.1 (0.83330)	0.66	151.0	4.10	24.5
	DCM	273 (52470); 318 (14730)	461 (12.0)	143/9755	7.70 (0.91146)	1.56	64.2	11.4	8.75
5i	EtOH	273 (48355); 321 (9370)	500 (1.5)	179/11150	n.d.	n.d.	n.d.	n.d.	n.d.
	DMSO	259 (69780); 318 (20675)	507 (14.0)	189/11720	13.3 (0.92940)	1.05	95.0	6.45	15.5
	DCM	278 (39425); 317 (16635); 557 (23210)	564 (51.0)	7/220	4.35 (0.98530)	11.8	8.53	11.2	8.90
RhB	EtOH	274 (10440); 543 (24295)	569 (46.0)	26/840	3.30 (0.98645)	13.9	7.17	16.4	6.10
	DMSO	276 (46710); 319 (23485); 415 (12840)	573 (50.0)	158/6645	3.00 (0.98120)	16.6	6.00	16.5	6.00

*Dieletric constant of solventes: DCM ($\varepsilon = 9.10$), EtOH ($\varepsilon = 24.3$), and DMSO ($\varepsilon = 45.0$);

[a]Concentration at 20 μM; [b]Concentration at 2.0 μM;

[c]Using 9,10-diphenylanthracene (DPA) as standard molecule in $CHCl_3$ solution ($\Phi_f = 65\%$) with errors at ±5%;

[d]Stokes Shifts ($\Delta\lambda_{SS}$) = $\lambda_{em} - \lambda_{abs}$ (in nm) and $(1/\lambda_{abs}) - (1/\lambda_{em})$ (in cm^{-1});

[e]Using NanoLED at 284 nm as excitation source, with errors at ±10%;

[f]Using equations $k_r = \Phi_f/\tau_f$ and $k_{nr} = (1 - \Phi_f)/\tau_f$ and $\tau_r = 1/k_r$ and $\tau_{nr} = 1/k_{nr}$, with errors at ±10%.

Theoretical Methodology

The structural and spectroscopic properties of compounds 5a-i, and standard rhodamine (**RhB**) molecule have been studied using the density functional theory (DFT), and its time-dependent version. The polarizable continuum model was used to implicitly simulate the DCM solvent. The exchange and correlation interactions were described by the hybrid PBE0 functional[2]. The molecular orbitals were constructed by linear combinations of the all electron 6-311G (d,p) basis set[3]. For the Te atom in the **5i** compound the effective core potential split valence CEP-31G basis set have been used[4].

The geometrical structures of compounds **5a-i** and **RhB** were optimized without symmetry constraints, and the absorption spectra determined at their ground state conformations. All calculations were performed using the Gaussian 09 code[5].

TDDFT Absorption spectra

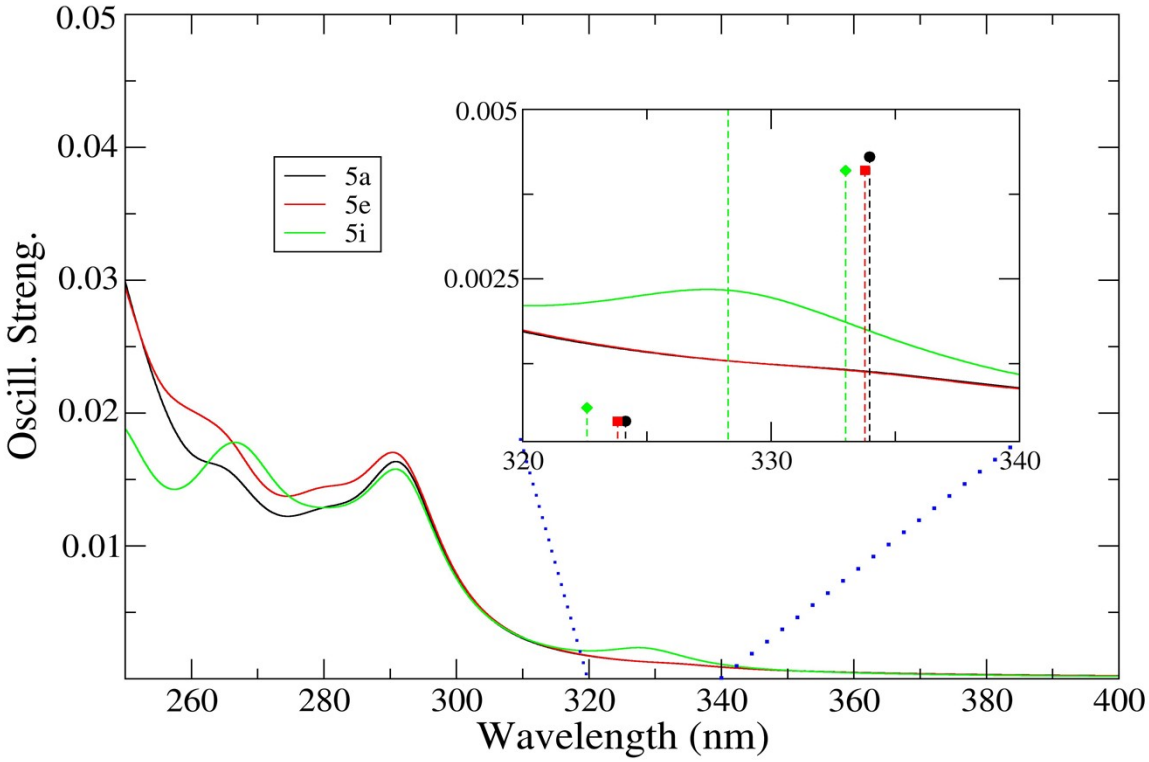


Figure S10. Absorption spectra for compunds 5a, 5e, and 5i in DCM. The inset shows the lowest energy electronic transitions. The vertical lines indicate the precise wavelengths and oscillator strengths of the individual electronic transitions for each compound.

TABLE S2: Coordinates of the optimized structures of compounds 5a, 5e, and 5i

5a

C	-2.336871	5.488499	-0.734613
C	-0.908157	5.972383	-0.477892
N	0.132737	5.164082	-1.098600
C	0.476740	5.456844	-2.484509
C	-0.194115	4.539362	-3.509697
C	0.581631	4.007951	-0.500603
C	0.052709	3.551826	0.734108
C	0.530002	2.397768	1.320091
C	1.535208	1.617277	0.741096
C	2.070302	2.082899	-0.455420
C	1.610640	3.240176	-1.074823
O	3.077858	1.435214	-1.115655
C	3.637472	0.321903	-0.548559
C	3.125431	-0.275254	0.598802
C	3.783272	-1.423837	1.049643
C	4.890063	-1.944268	0.412103
C	5.410152	-1.330734	-0.757265
C	4.753844	-0.174470	-1.213492
N	6.493336	-1.856940	-1.426771
C	7.083875	-1.146550	-2.552988
C	7.225657	-2.992122	-0.880396
C	7.935567	0.066413	-2.169488
C	8.166985	-2.647787	0.276095
H	0.145783	4.791096	-4.519585
H	-1.281971	4.647470	-3.476037
H	0.046371	3.488583	-3.321402
H	-3.048110	6.101279	-0.170671
H	-2.464493	4.444466	-0.431412
H	-2.590427	5.567122	-1.796270
H	8.289321	0.577157	-3.071106
H	8.809001	-0.237978	-1.585545
H	7.361873	0.782400	-1.573343
H	8.635348	-3.557981	0.664872
H	7.627637	-2.163952	1.096320
H	8.959816	-1.970186	-0.053525
H	7.800053	-3.431055	-1.700915
H	6.512556	-3.763346	-0.570934
H	6.288146	-0.845727	-3.243550
H	7.699017	-1.864117	-3.102834
C	1.885410	0.249149	1.282910
N	0.731081	-0.677444	1.067015
C	1.990000	0.224659	2.793995
C	0.996659	-0.578407	3.329869
C	2.894712	0.878790	3.617385

C	2.771064	0.699162	4.994000
C	1.765812	-0.113246	5.532563
C	0.860283	-0.763061	4.699768
C	0.164289	-1.127296	2.229630
O	-0.840221	-1.821423	2.344692
C	0.256834	-0.902795	-0.277530
C	-0.271319	-2.310453	-0.577933
C	-1.184851	-2.075513	-1.790476
C	-0.886784	0.008755	-0.780099
N	-2.513547	-2.727344	-1.620377
O	-1.348116	-0.689067	-1.940347
C	-1.993086	0.225334	0.247157
Cl	-3.206704	1.421005	-0.390544
C	-4.686578	1.012683	0.508257
C	-5.871461	1.600902	0.048420
C	-7.079373	1.326319	0.676909
C	-7.125083	0.457427	1.766248
C	-5.947044	-0.119314	2.228080
C	-4.726990	0.159248	1.612787
C	-3.689086	-2.013023	-1.584639
C	-4.899069	-2.575007	-1.379784
C	-4.972314	-4.019882	-1.216432
N	-3.741363	-4.669587	-1.331041
C	-2.501349	-4.103971	-1.536211
O	-5.991560	-4.664055	-1.011968
O	-1.478391	-4.766064	-1.630588
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H	-0.793387	6.992777	-0.856517
H	1.565983	5.424882	-2.605676
H	0.186521	6.493348	-2.675551
H	-0.748408	4.086048	1.227813
H	0.088368	2.071196	2.258384
H	2.084503	3.519675	-2.006823
H	3.465797	1.199113	5.661932
H	1.693551	-0.233974	6.608745
H	3.673797	1.511110	3.202547
H	0.071604	-1.394694	5.096087
H	3.409012	-1.923601	1.939246
H	5.352766	-2.829695	0.827851
H	5.083937	0.368776	-2.089084
H	1.109738	-0.713759	-0.936870
H	-0.838842	-2.695666	0.268299
H	0.531530	-3.010128	-0.807135
H	-0.760828	-2.468226	-2.716551
H	-1.565768	0.609370	1.174173
H	-2.485781	-0.724631	0.466056
H	-3.823452	-0.288063	2.012407
H	-5.966348	-0.791674	3.080565
H	-8.070497	0.236757	2.251488
H	-7.990309	1.785811	0.305392

H	-3.750171	-5.678849	-1.247785
H	-0.504044	0.970319	-1.133396
H	-5.848012	2.265023	-0.811524
C	-6.170153	-1.783988	-1.311676
H	-6.616628	-1.847907	-0.313297
H	-6.906968	-2.165732	-2.025950
H	-5.984625	-0.729080	-1.525703
H	-3.569131	-0.946625	-1.734832

5e

C	3.169626	-4.730620	-0.534106
C	1.777849	-5.361528	-0.591620
N	0.772356	-4.568065	-1.285201
C	0.718747	-4.663329	-2.738083
C	1.341037	-3.472919	-3.470199
C	0.047868	-3.605386	-0.622496
C	0.342158	-3.242679	0.715571
C	-0.403670	-2.280576	1.363663
C	-1.454210	-1.595640	0.742284
C	-1.766519	-1.987890	-0.554375
C	-1.041235	-2.960223	-1.235096
O	-2.789891	-1.422542	-1.263864
C	-3.603609	-0.511671	-0.646164
C	-3.317285	0.028075	0.604913
C	-4.221118	0.975496	1.096156
C	-5.347667	1.358086	0.396326
C	-5.633681	0.805870	-0.879012
C	-4.731970	-0.152444	-1.373865
N	-6.730441	1.204984	-1.610495
C	-7.073235	0.530674	-2.855366
C	-7.698487	2.141383	-1.055335
C	-7.720194	-0.845029	-2.677235
C	-8.681040	1.528821	-0.054615
H	1.256281	-3.615691	-4.552464
H	2.398268	-3.365807	-3.211529
H	0.838465	-2.536506	-3.209148
H	3.832919	-5.332181	0.096120
H	3.119104	-3.715548	-0.133644
H	3.611393	-4.670186	-1.534547
H	-7.881076	-1.314925	-3.653071
H	-8.688641	-0.758891	-2.176065
H	-7.086551	-1.507034	-2.079210
H	-9.342663	2.304001	0.345940
H	-8.155638	1.060528	0.783482
H	-9.301834	0.766185	-0.533686
H	-8.253158	2.567963	-1.895770
H	-7.164542	2.979925	-0.595724

H	-6.174770	0.448598	-3.477108
H	-7.754740	1.186728	-3.403694
C	-2.055951	-0.339213	1.344399
N	-1.043701	0.769248	1.277795
C	-2.232335	-0.470803	2.841974
C	-1.322132	0.337698	3.501847
C	-3.098418	-1.290101	3.551207
C	-3.026543	-1.264942	4.943034
C	-2.103420	-0.448391	5.607285
C	-1.233204	0.364774	4.887572
C	-0.519090	1.089253	2.503176
O	0.425133	1.833929	2.739256
C	-0.630744	1.278253	-0.010455
C	-0.088482	2.715417	-0.044656
C	0.734564	2.732451	-1.342810
C	0.474224	0.491533	-0.745846
N	2.071334	3.359779	-1.160047
O	0.890342	1.404185	-1.765098
C	1.623362	0.039305	0.143426
Se	2.813459	-1.038219	-0.954518
C	4.316490	-1.150172	0.206256
C	5.533160	-1.534767	-0.365822
C	6.672836	-1.647251	0.422557
C	6.612695	-1.367178	1.786503
C	5.401520	-0.984585	2.355147
C	4.252257	-0.881808	1.573642
C	3.236515	2.630702	-1.170780
C	4.456655	3.159700	-0.945378
C	4.557780	4.591727	-0.711480
N	3.330834	5.260736	-0.753545
C	2.076479	4.723108	-0.952301
O	5.590106	5.211539	-0.497856
O	1.056410	5.396338	-0.942825
H	1.415179	-5.573276	0.418712
H	1.832832	-6.331288	-1.097499
H	-0.319183	-4.805815	-3.064078
H	1.247948	-5.578499	-3.016906
H	1.176475	-3.689399	1.240564
H	-0.128697	-2.011655	2.380609
H	-1.349373	-3.193792	-2.246394
H	-3.695492	-1.892355	5.524066
H	-2.067868	-0.453068	6.692124
H	-3.809368	-1.930186	3.037697
H	-0.507791	1.002835	5.382213
H	-4.029856	1.425780	2.066639
H	-6.008388	2.088143	0.845335
H	-4.872963	-0.639400	-2.329634
H	-1.517712	1.238309	-0.651608
H	0.546040	2.910556	0.818563
H	-0.886014	3.457661	-0.064839

H	0.242596	3.291241	-2.140780
H	1.239913	-0.589061	0.944591
H	2.166547	0.884796	0.571442
H	3.318601	-0.588446	2.041842
H	5.342399	-0.767340	3.417439
H	7.504670	-1.445744	2.400044
H	7.612043	-1.944009	-0.034370
H	3.353546	6.260416	-0.593049
H	0.073704	-0.375672	-1.273767
H	5.591113	-1.735912	-1.432449
C	5.700120	2.321286	-0.924100
H	6.211834	2.409034	0.040220
H	6.408042	2.637623	-1.697475
H	5.451603	1.268087	-1.083326
H	3.117498	1.571541	-1.363118

5i

C	2.859176	-3.967074	-2.754249
C	1.894834	-5.036781	-2.240434
N	0.488609	-4.663305	-2.331330
C	-0.244034	-5.099998	-3.510702
C	-0.063580	-4.229213	-4.758034
C	-0.031659	-3.686161	-1.507438
C	0.602989	-3.330576	-0.288315
C	0.026323	-2.404220	0.555365
C	-1.167395	-1.737836	0.250346
C	-1.775706	-2.082881	-0.950707
C	-1.234195	-3.030786	-1.814583
O	-2.943653	-1.522734	-1.385103
C	-3.562693	-0.585742	-0.607131
C	-3.038155	-0.141728	0.601189
C	-3.778690	0.831963	1.280637
C	-4.973072	1.328015	0.800094
C	-5.507155	0.866899	-0.431649
C	-4.766643	-0.109425	-1.118327
N	-6.684242	1.372011	-0.941728
C	-7.257472	0.820301	-2.161920
C	-7.515626	2.265286	-0.144817
C	-7.956111	-0.530875	-1.987391
C	-8.294982	1.579513	0.980186
H	-0.749055	-4.557729	-5.546470
H	0.956149	-4.303878	-5.147378
H	-0.267572	-3.175805	-4.541850
H	3.892824	-4.313734	-2.652541
H	2.753780	-3.037357	-2.185347
H	2.675115	-3.745613	-3.809190
H	-8.307906	-0.901527	-2.956090

H	-8.820613	-0.440733	-1.323233
H	-7.277911	-1.276854	-1.561756
H	-8.846261	2.323945	1.564385
H	-7.624530	1.041579	1.657568
H	-9.015339	0.861458	0.577014
H	-8.215716	2.750690	-0.830428
H	-6.892668	3.069112	0.262712
H	-6.472002	0.744235	-2.922072
H	-7.972887	1.553835	-2.544601
C	-1.717801	-0.648020	1.144389
N	-0.747208	0.478538	1.261890
C	-1.827921	-1.080513	2.593874
C	-1.051206	-0.262365	3.397625
C	-2.567511	-2.118938	3.141258
C	-2.499737	-2.310361	4.520359
C	-1.713168	-1.481763	5.330852
C	-0.975685	-0.441421	4.773465
C	-0.360077	0.740683	2.549332
O	0.412069	1.614886	2.928155
C	-0.311379	1.162082	0.066972
C	-0.177105	2.681737	0.147972
C	0.644316	2.964635	-1.106684
C	1.072124	0.732612	-0.498636
N	1.487583	4.155594	-1.010864
O	1.472996	1.835427	-1.316530
C	2.093561	0.447643	0.584173
Te	4.056063	-0.152154	-0.149353
C	3.959610	-2.091257	0.783370
C	4.483351	-3.194329	0.107226
C	4.384601	-4.470519	0.659902
C	3.755289	-4.655760	1.888707
C	3.254974	-3.553030	2.578002
C	3.371592	-2.273550	2.037665
C	2.586989	4.151875	-0.178532
C	3.414446	5.201749	-0.015644
C	3.131868	6.419168	-0.768342
N	2.007475	6.335877	-1.590758
C	1.149485	5.269069	-1.761805
O	3.788402	7.448577	-0.723603
O	0.182512	5.321524	-2.503940
H	2.144708	-5.296739	-1.205705
H	2.019472	-5.956369	-2.819575
H	-1.305143	-5.169212	-3.250579
H	0.076517	-6.123265	-3.732614
H	1.536259	-3.791274	0.012482
H	0.521294	-2.187503	1.498698
H	-1.772634	-3.215619	-2.734878
H	-3.064958	-3.117906	4.975693
H	-1.679341	-1.656445	6.401616
H	-3.177476	-2.762886	2.514863

H	-0.357983	0.210343	5.383192
H	-3.398556	1.212901	2.225310
H	-5.492491	2.074546	1.386794
H	-5.097396	-0.529549	-2.059033
H	-1.057355	0.929882	-0.700698
H	0.362193	2.975234	1.050680
H	-1.141396	3.193027	0.129321
H	0.008907	3.126882	-1.978758
H	3.000016	-1.426448	2.607539
H	2.780350	-3.683666	3.545957
H	3.662993	-5.651047	2.312217
H	4.789021	-5.321390	0.119311
H	1.778080	7.163325	-2.127776
H	0.968257	-0.141630	-1.148255
H	4.955013	-3.069039	-0.862344
C	4.609497	5.183812	0.888665
H	4.524438	5.955965	1.660546
H	5.526589	5.389180	0.326752
H	4.713966	4.212516	1.379708
H	2.754340	3.214387	0.336843
H	1.761151	-0.409305	1.169194
H	2.208749	1.287553	1.269120

Electrochemical study

Electrochemical analysis by cyclic voltammetry was recorded with a potentiostat/galvanostat AutoLab Eco Chemie PGSTAT 128 N system at room temperature and under an argon atmosphere in a dry DCM solution. Electrochemical grade tetrabutylammonium hexafluorophosphate (0.1 M $TBAPF_6$) was used as a supporting electrolyte. The electrochemical cell is composed of three components: glassy carbon electrode (working electrode; 5.0 mm, Metrohm®), a Pt auxiliary electrode and a Pt pseudo-reference electrode. To monitor the reference electrode, the Fc/Fc^+ redox couple pair ($E_{1/2}$ = 0.42 V) was used as an internal reference[6], and used SHE (Standard Hydrogen Electrode).

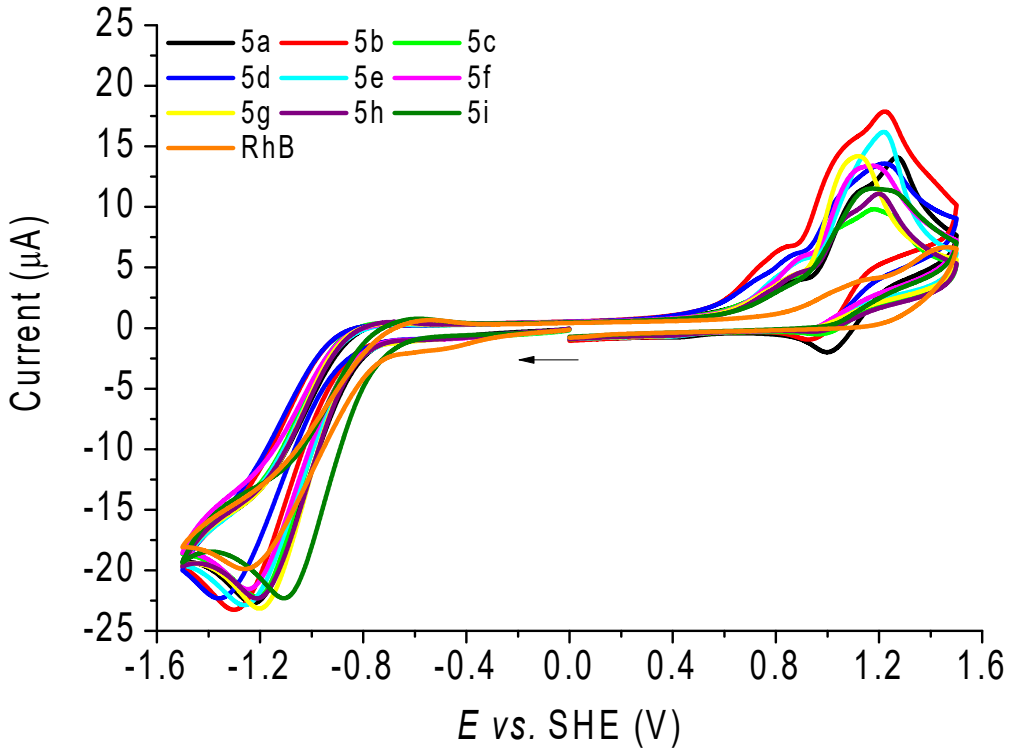


Figure S11. CV plots of derivatives in DCM solution.

ROS Generation

Singlet oxygen production ($^1O_2$) was recorded according to typical 9,10-diphenylanthracene (DPA) photoxidation assays, with compounds **5a-i**, according to the literature[7]. In order to measure singlet oxygen generation, absorption UV–Vis spectra of each solution were recorded at diferente exposure times (0 to 20 min), using red-light diode laser (Thera Laser DMC – São Paulo; potency of 100 mW). The photoxidation constant (k_{po}) and singlet oxygen production quantum yield (Φ_Δ) was calculated by ln A_0/A versus time plots.

For superoxide generation assays, the nitroblue tetrazolium (NBT) experiment was used to detect the formation of superoxide radical species ($O_2^{\bullet-}$) in the presence of compounds **5a-i**. This approach was carried out using at the same conditions in the literature, using NBT and NADH in DMF solution[8]. Control experiments were performed in the absence of compounds. Samples were irradiated under aerobic conditions using red-light diode laser (Thera Laser DMC – São Paulo; potency of 100 mW). The progress of the reaction was monitored by following the increase of the

absorbance close to 530 nm. The superoxide generation constant (k_{SO}) can be obtained from the slope.

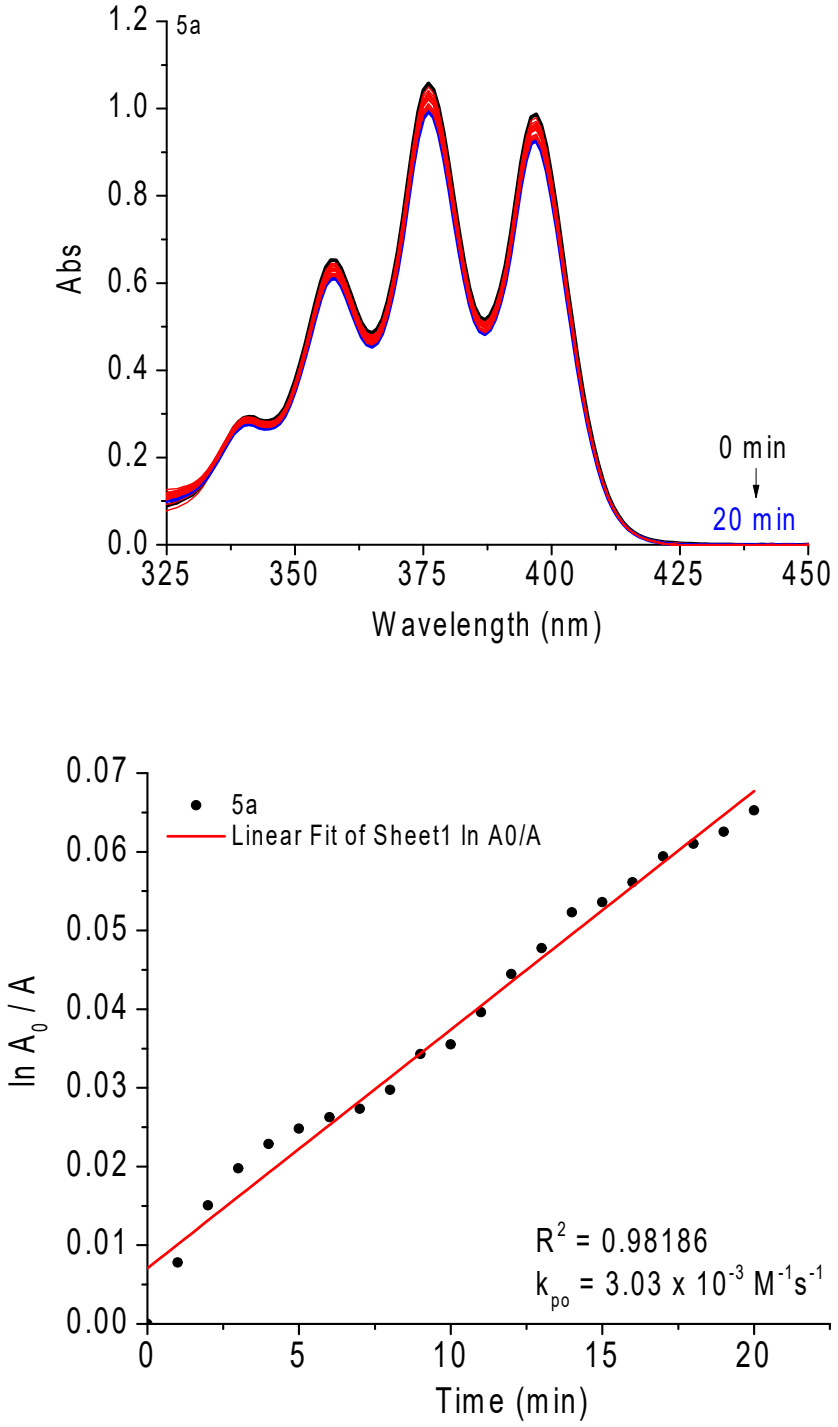


Figure S12. DPA photooxidation assays of compound 5a in DMSO.

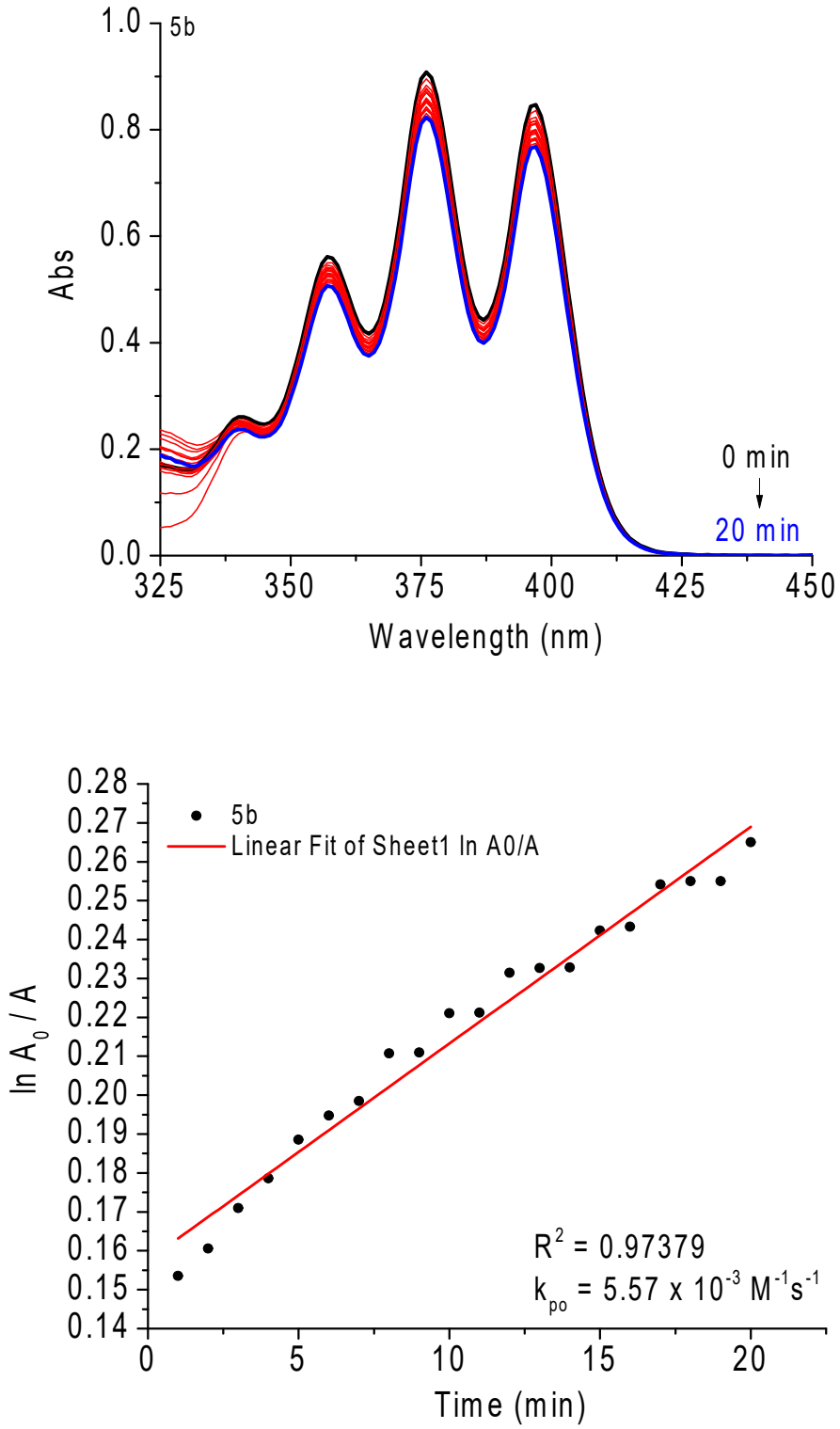


Figure S13. DPA photooxidation assays of compound 5b in DMSO.

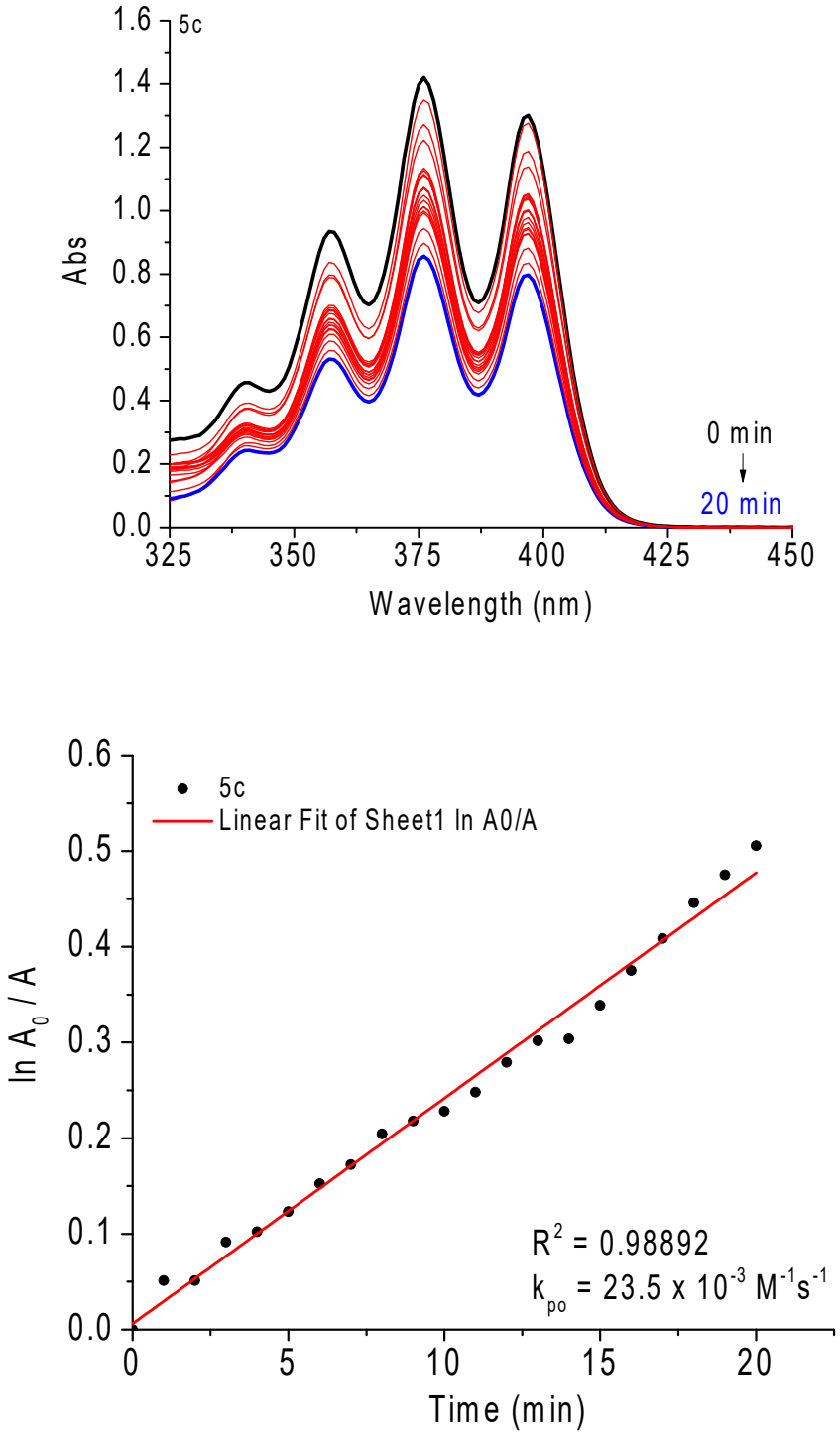


Figure S14. DPA photooxidation assays of compound 5c in DMSO.

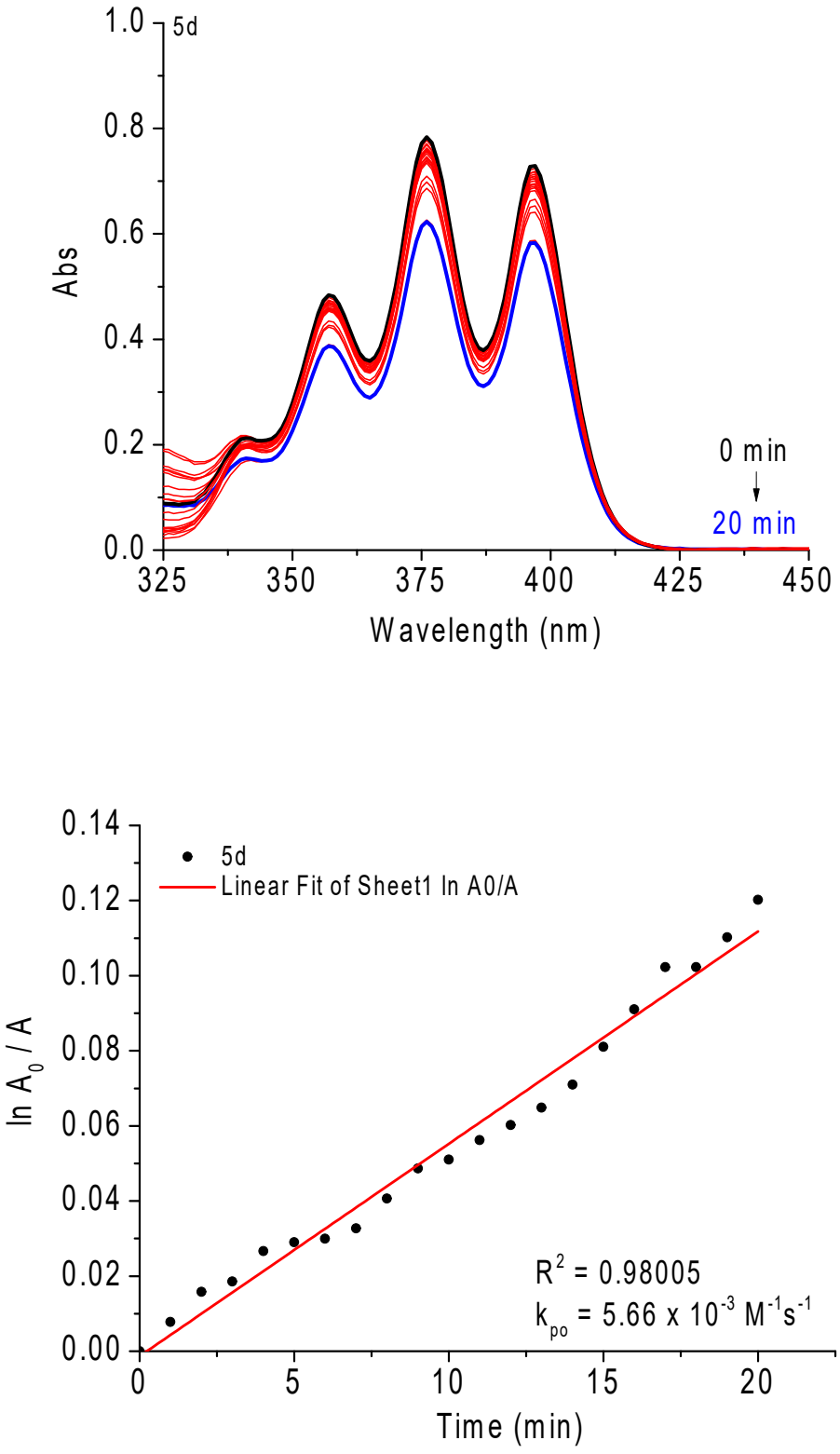


Figure S15. DPA photooxidation assays of compound 5d in DMSO.

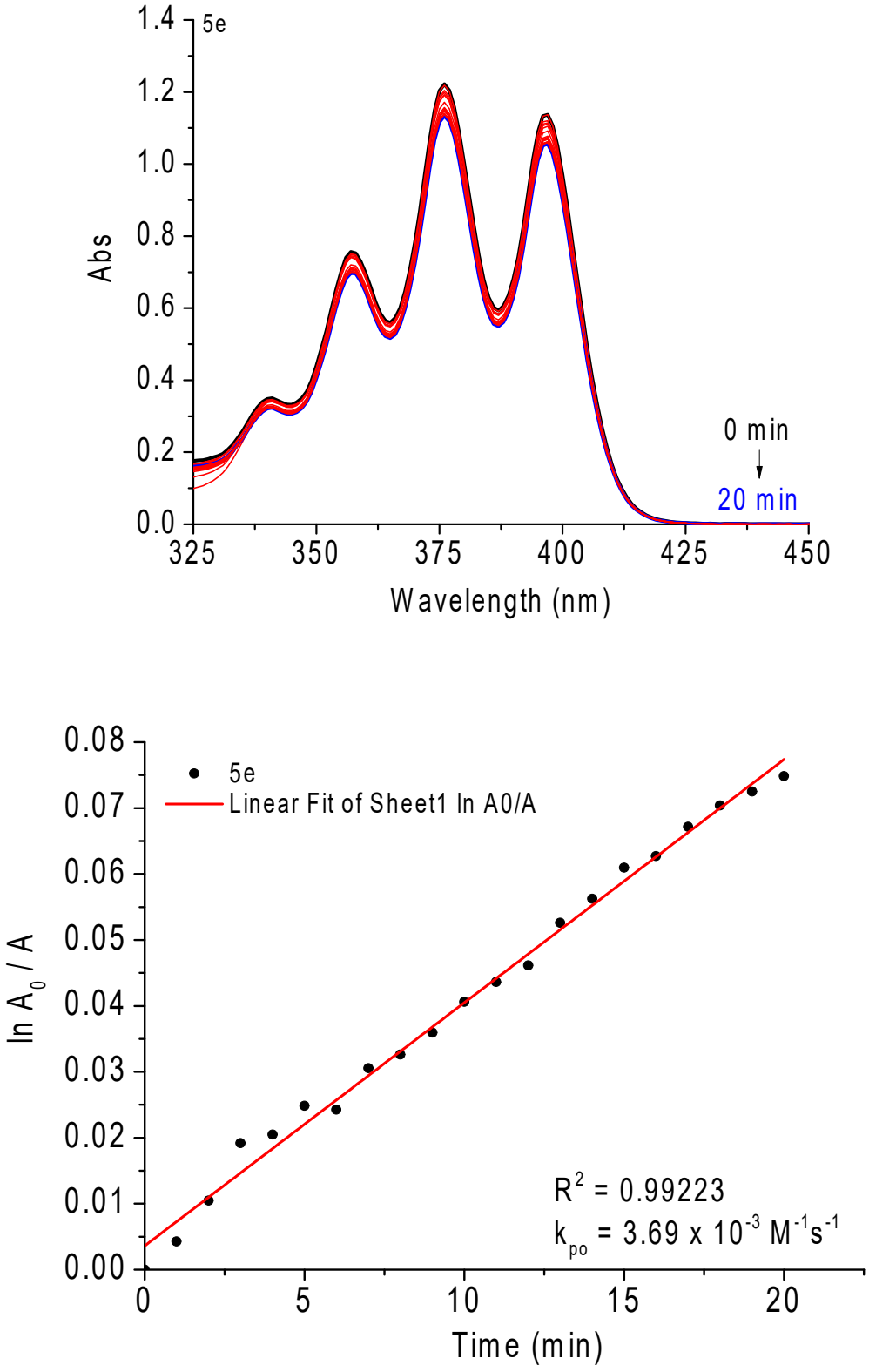


Figure S16. DPA photooxidation assays of compound 5e in DMSO.

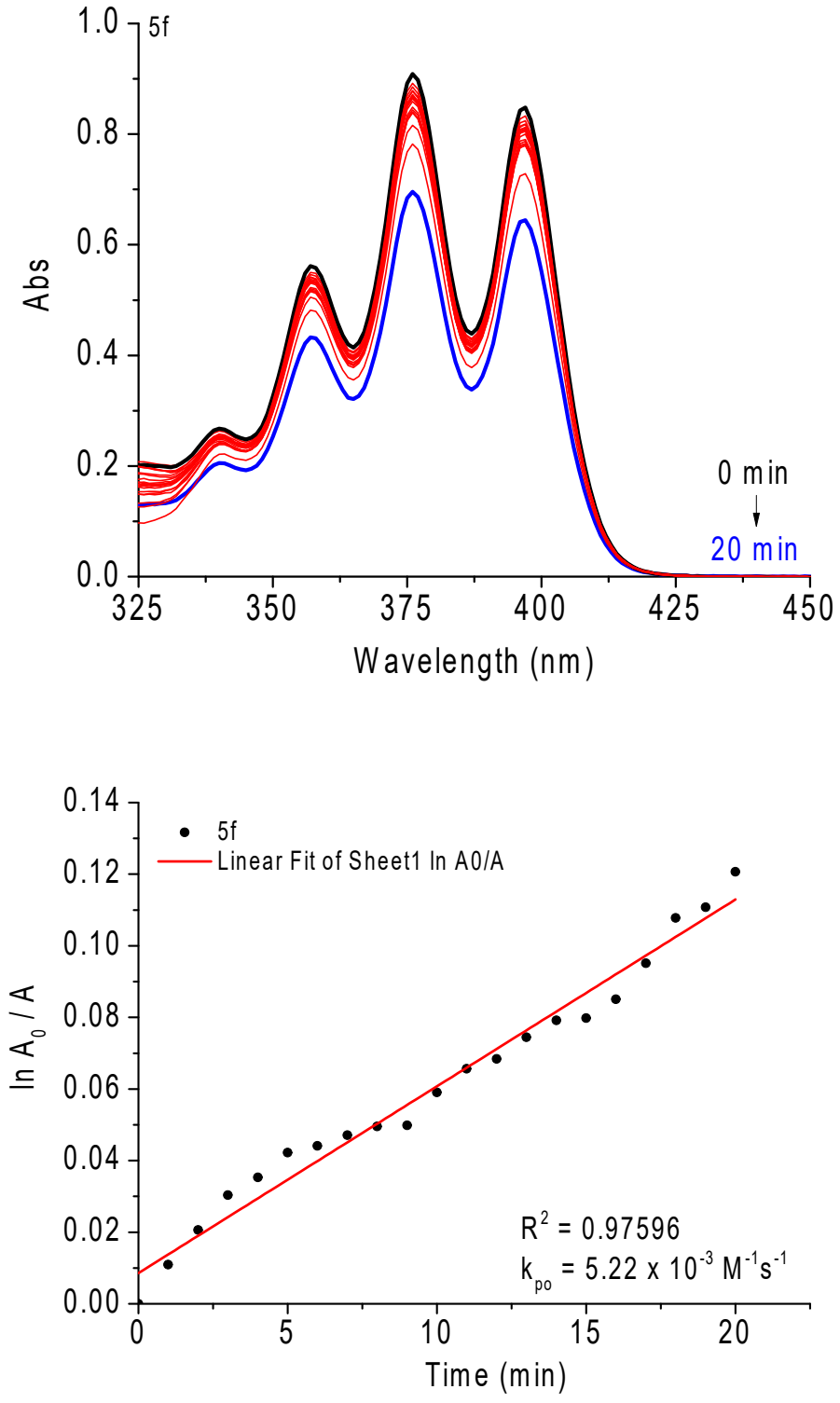


Figure S17. DPA photooxidation assays of compound 5f in DMSO.

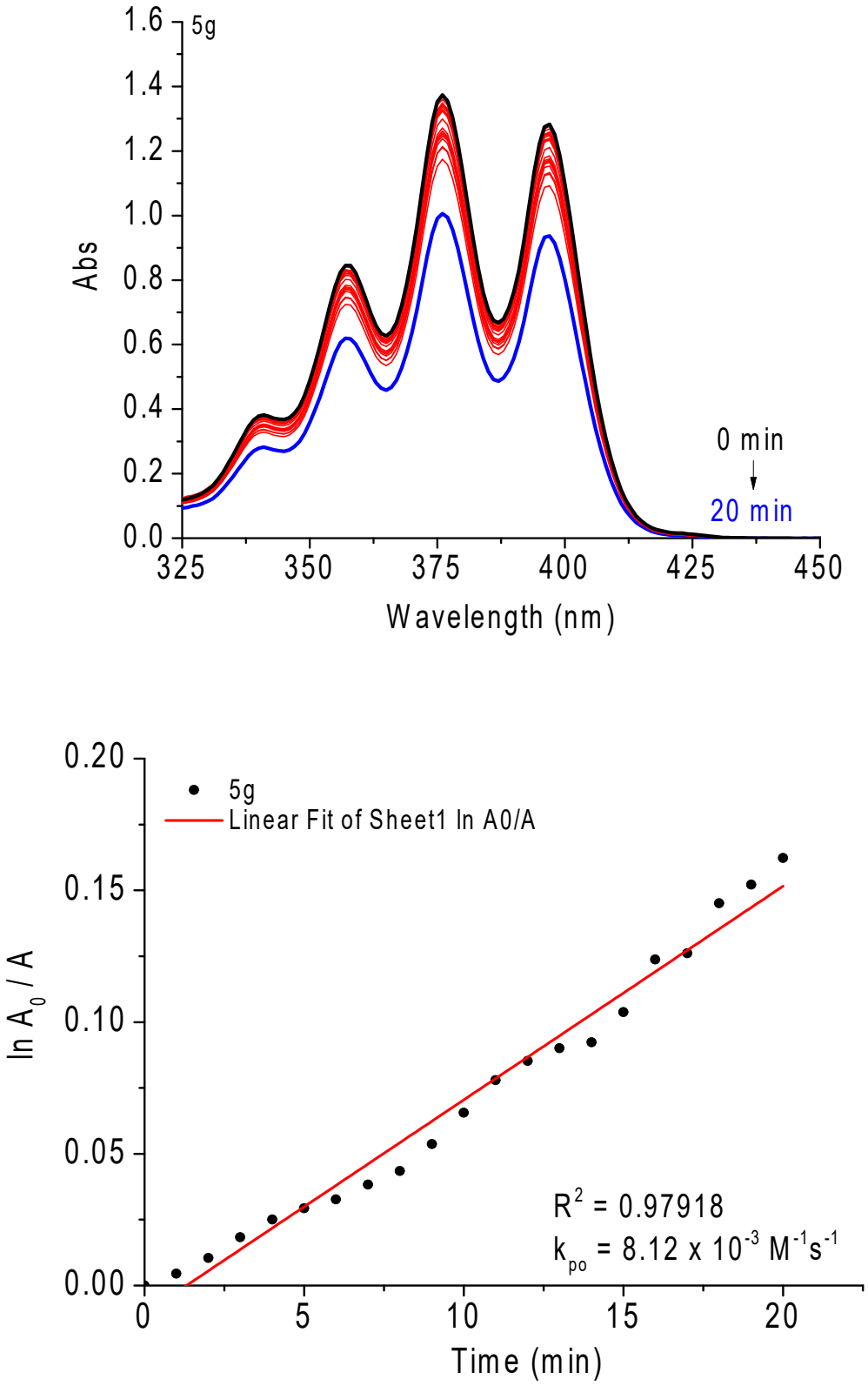
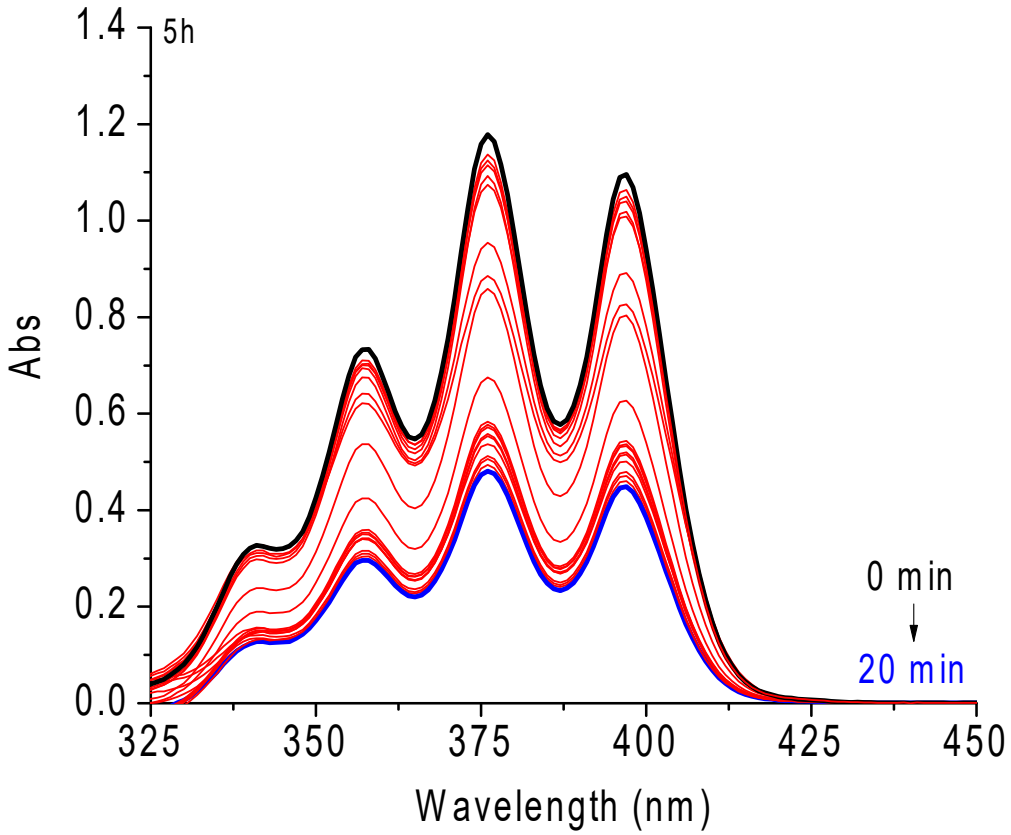


Figure S18. DPA photooxidation assays of compound 5g in DMSO.


1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Abs
5h
0 min
20 min
325
350
375
400
425
450
Wavelength (nm)

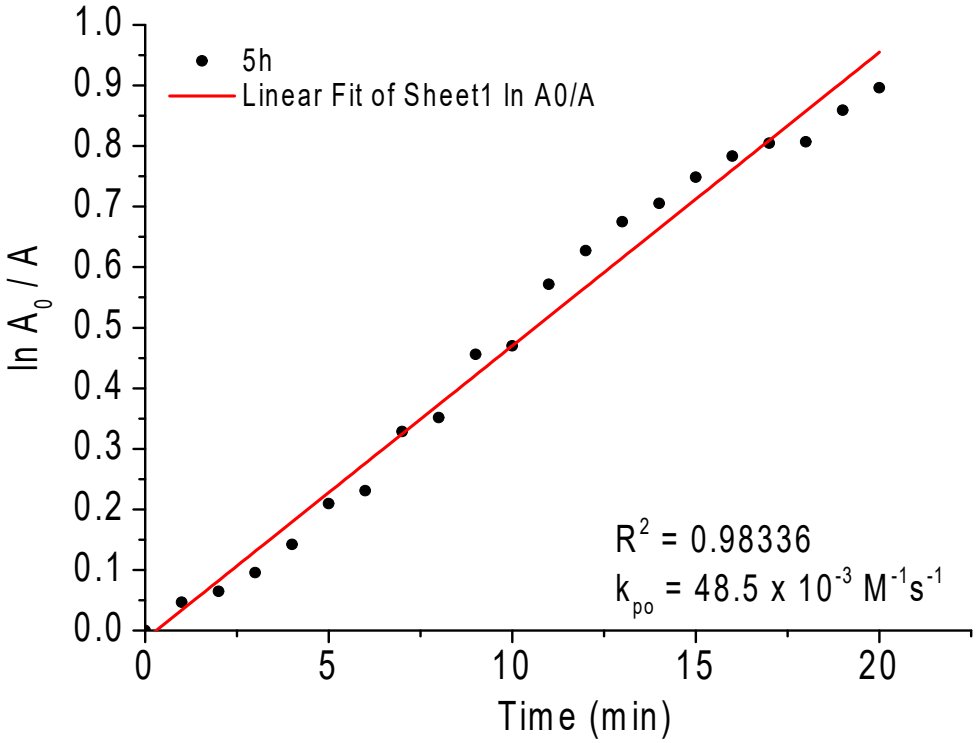
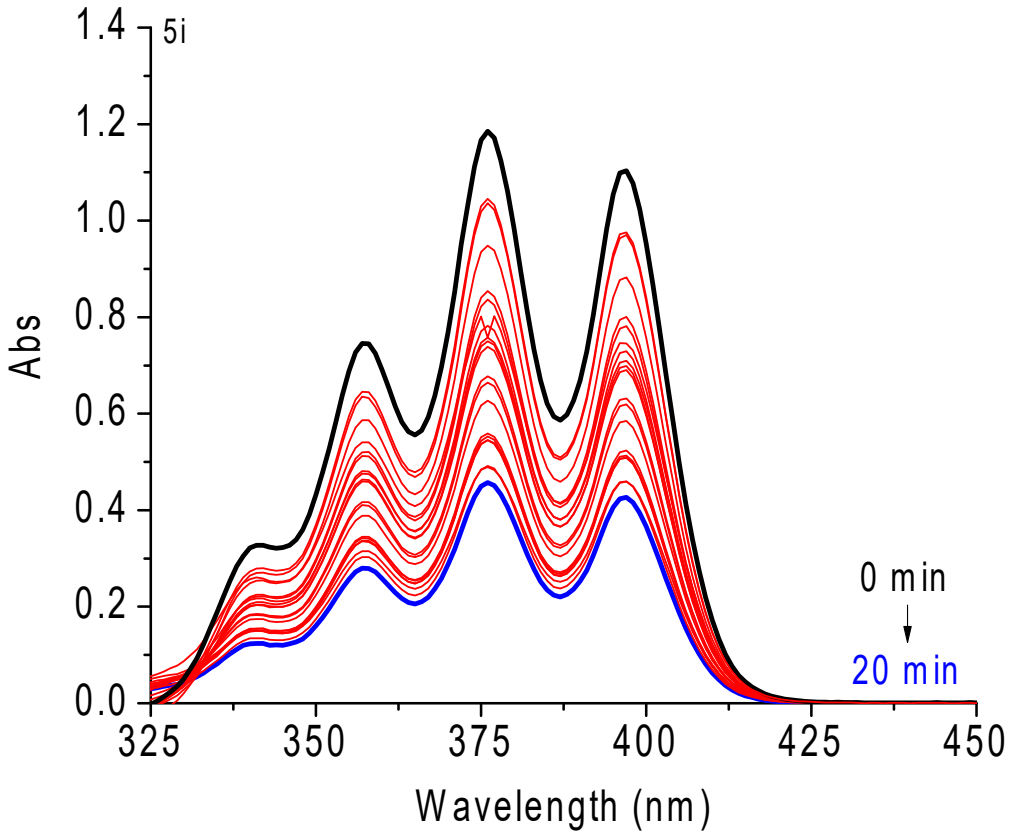


Figure S19. DPA photooxidation assays of compound 5h in DMSO.


5i
Abs
Wavelength (nm)
0 min
20 min
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
325
350
375
400
425
450

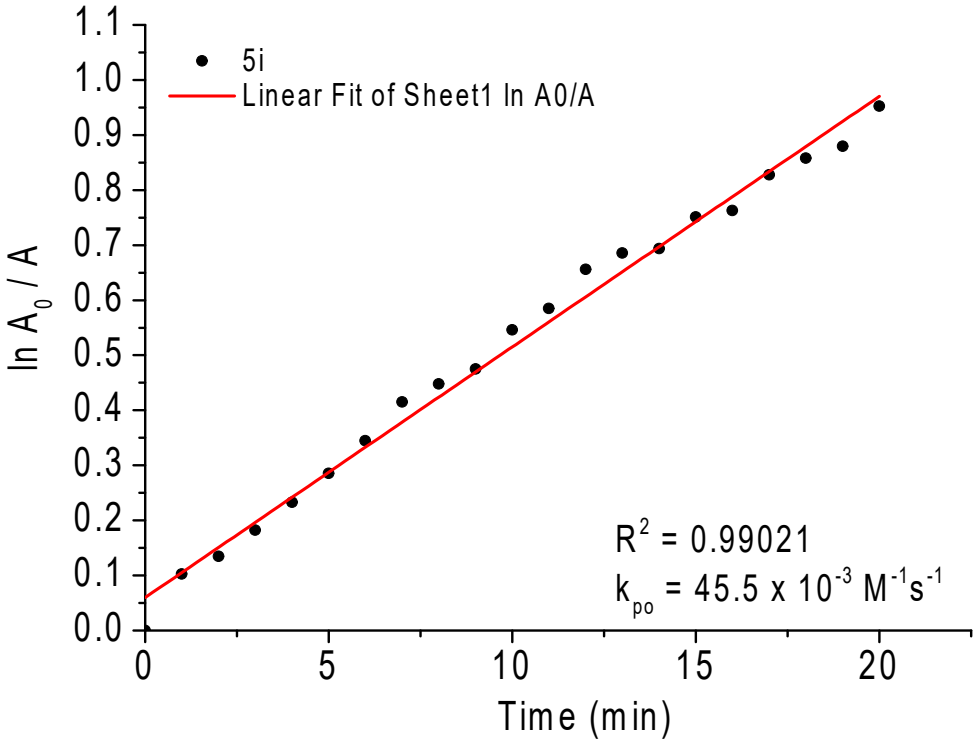
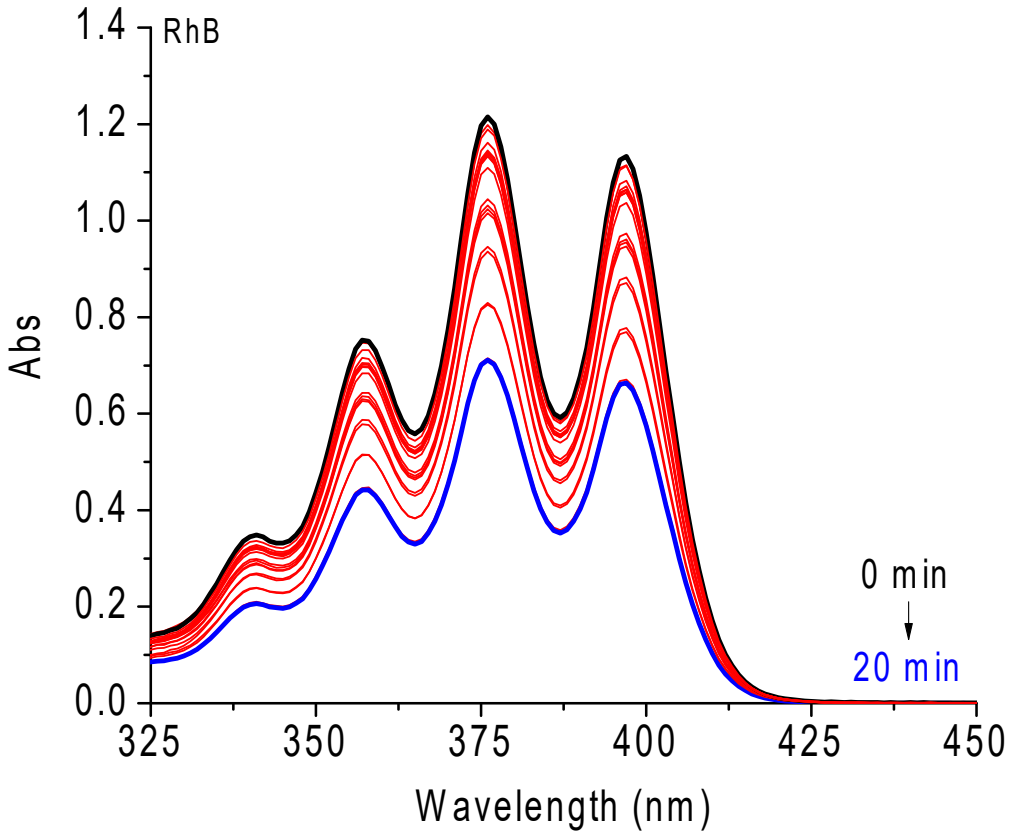


Figure S20. DPA photooxidation assays of compound 5i in DMSO.


RhB
Abs
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
325
350
375
400
425
450
Wavelength (nm)
0 min
20 min

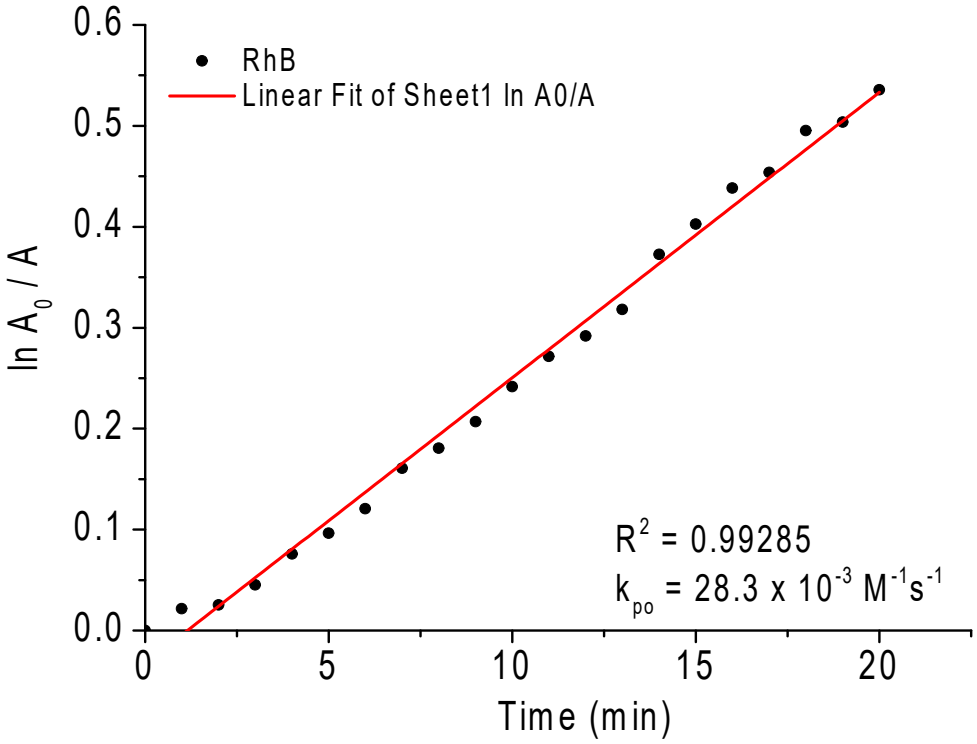


Figure S21. DPA photooxidation assays of compound RhB in DMSO.

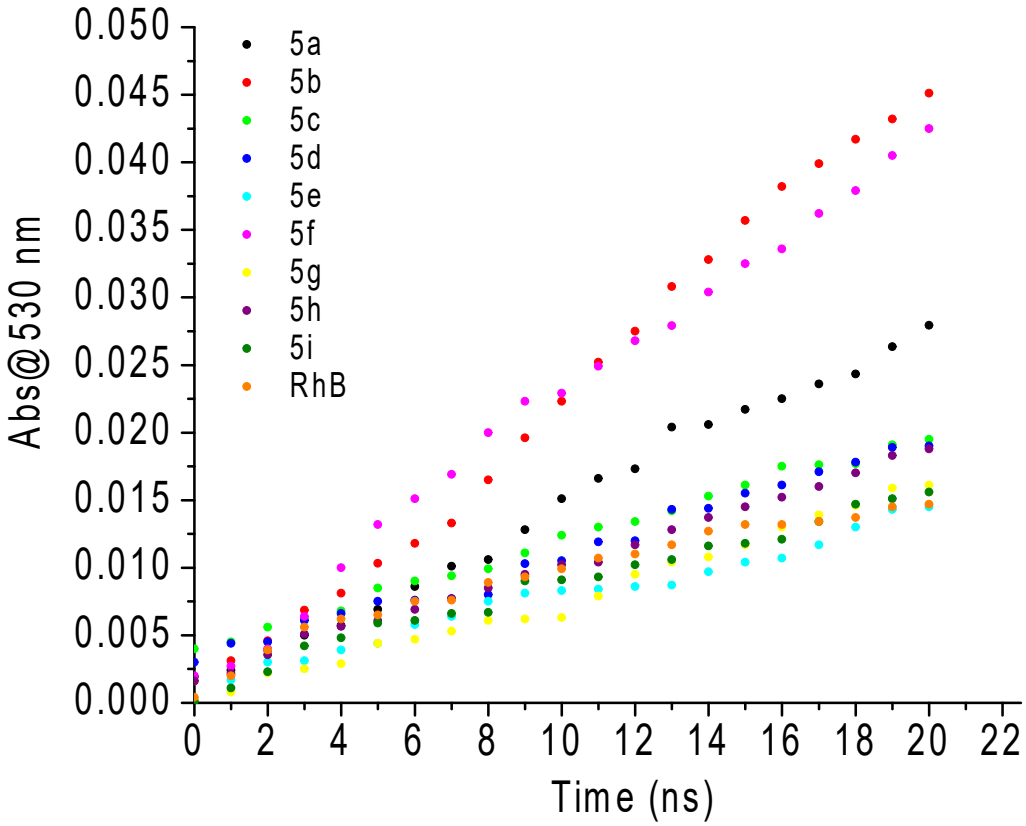


Figure S22. NBT assays of studied compounds in DMF solution.

NMR SPECTRAS

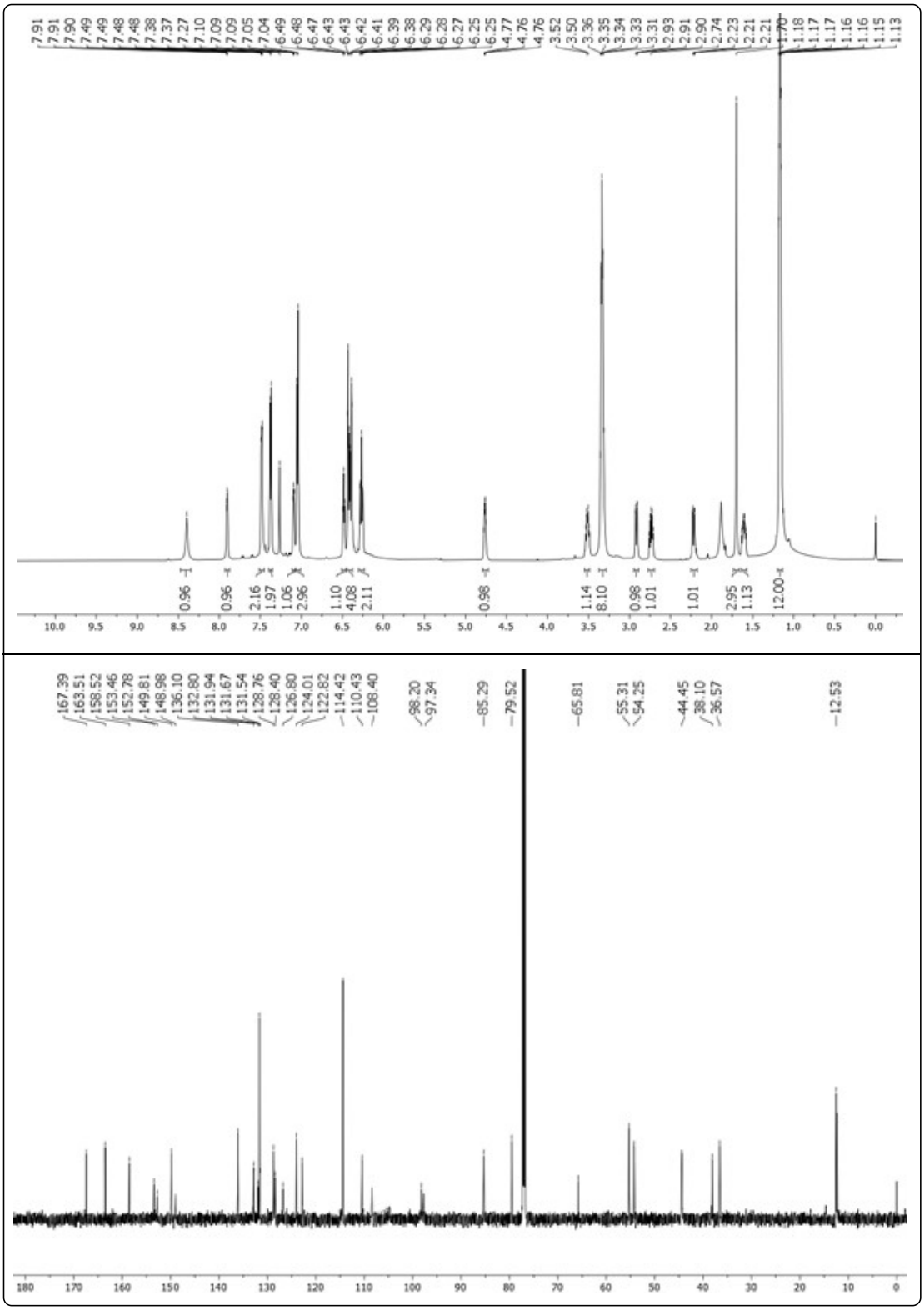


Figure S23. ^{1}H and ^{13}C NMR of the compound **5a** in $CDCl_3$ at 600 MHz and 150 MHz respectively.

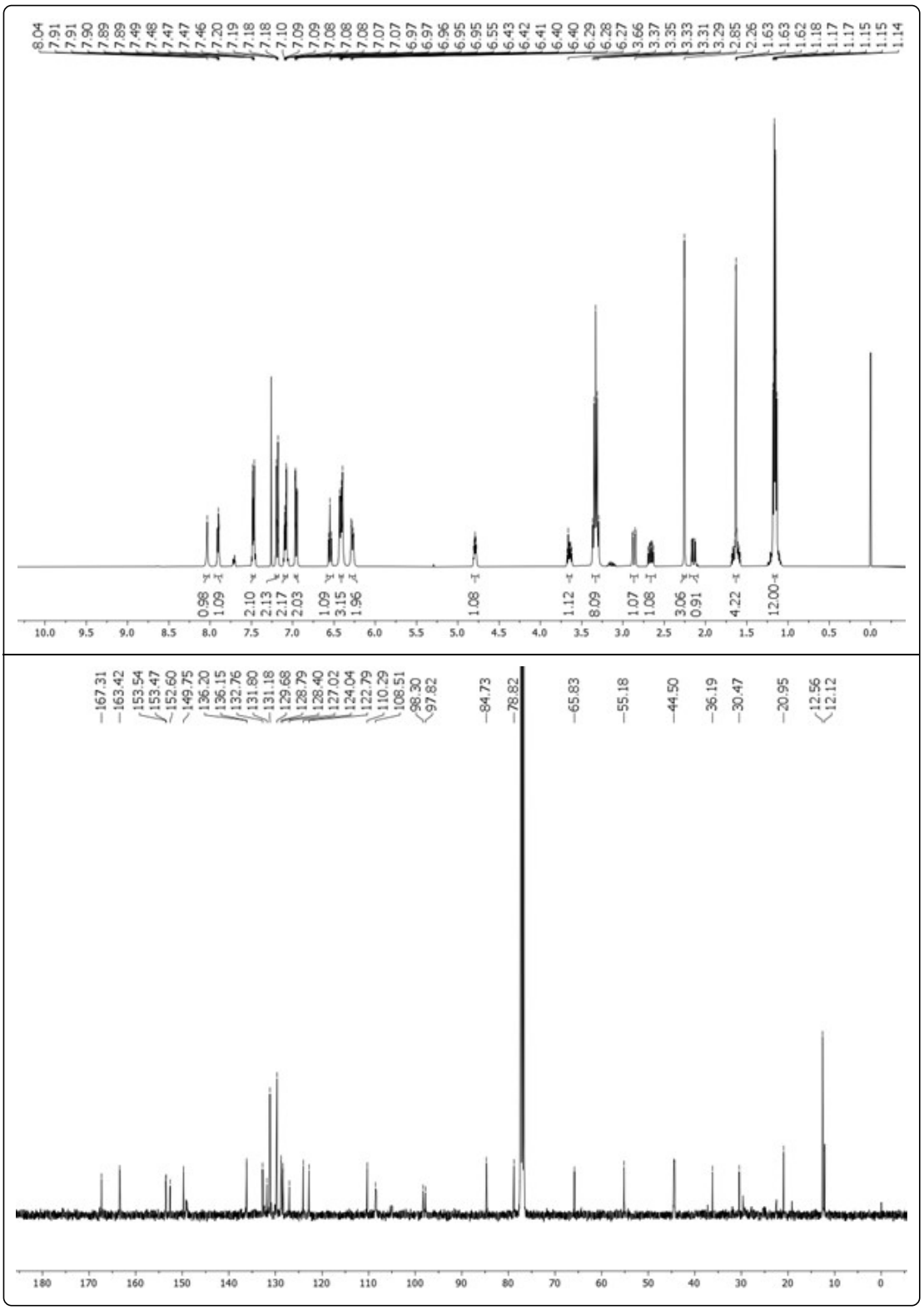


Figure S24. ^{1}H and ^{13}C NMR of the compound **5b** in $CDCl_3$ at 400 MHz and 100 MHz respectively.

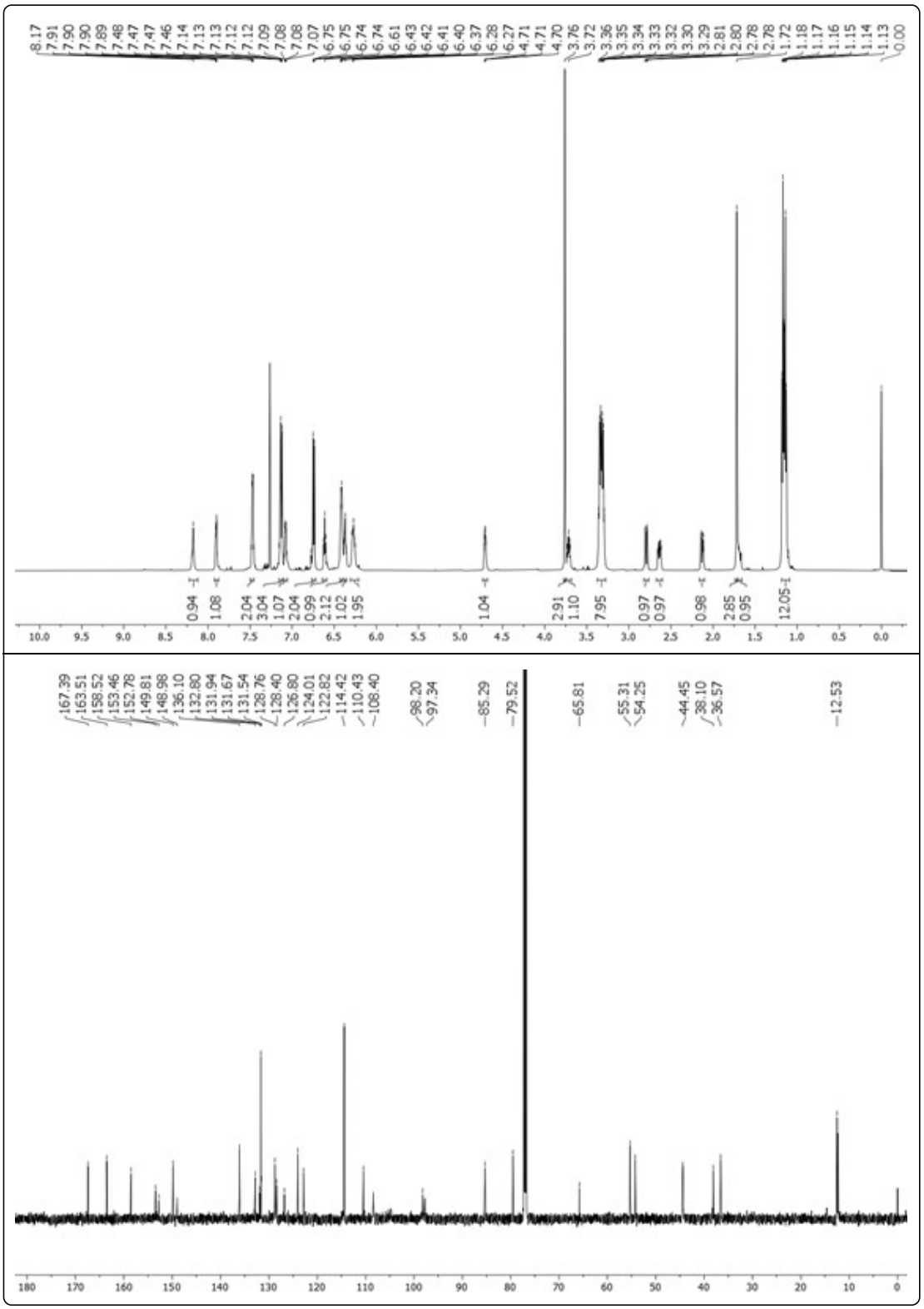


Figure S25. ^{1}H and ^{13}C NMR of the compound **5c** in $CDCl_3$ at 600 MHz and 150 MHz respectively.

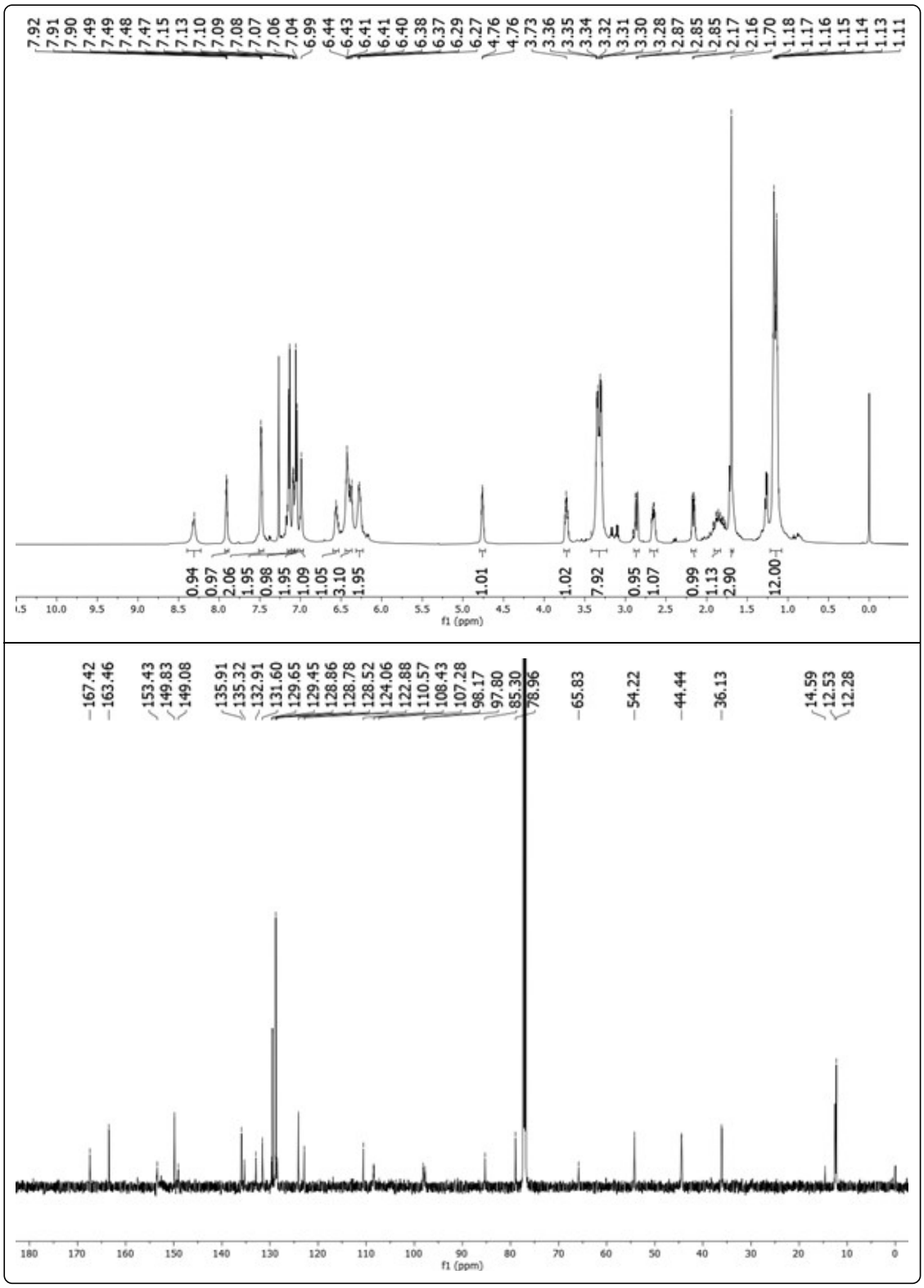


Figure S26. ^{1}H and ^{13}C NMR of the compound **5d** in $CDCl_3$ at 600 MHz and 150 MHz respectively.

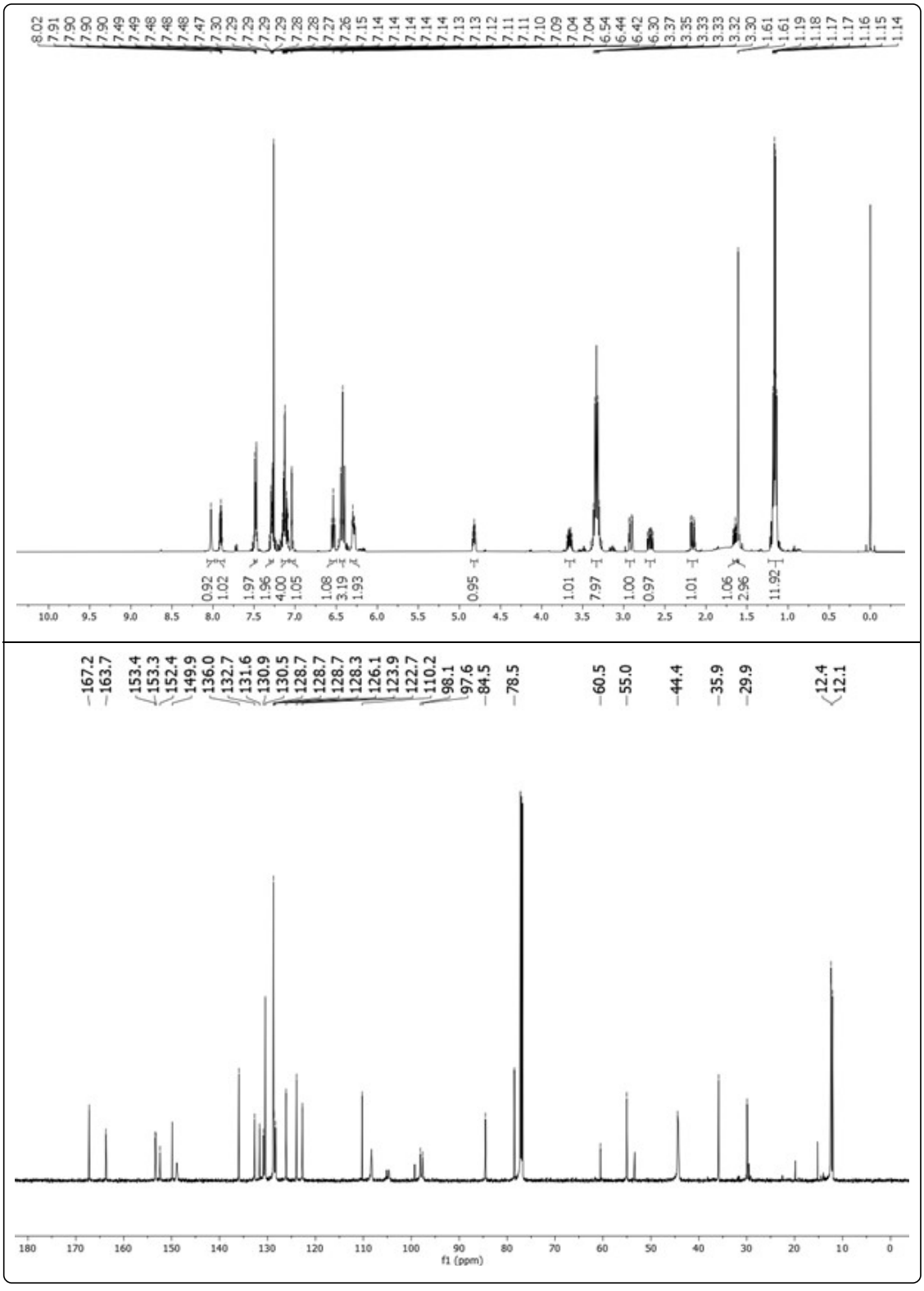


Figure S27. ^{1}H and ^{13}C NMR of the compound **5e** in $CDCl_3$ at 400 MHz and 100 MHz respectively.

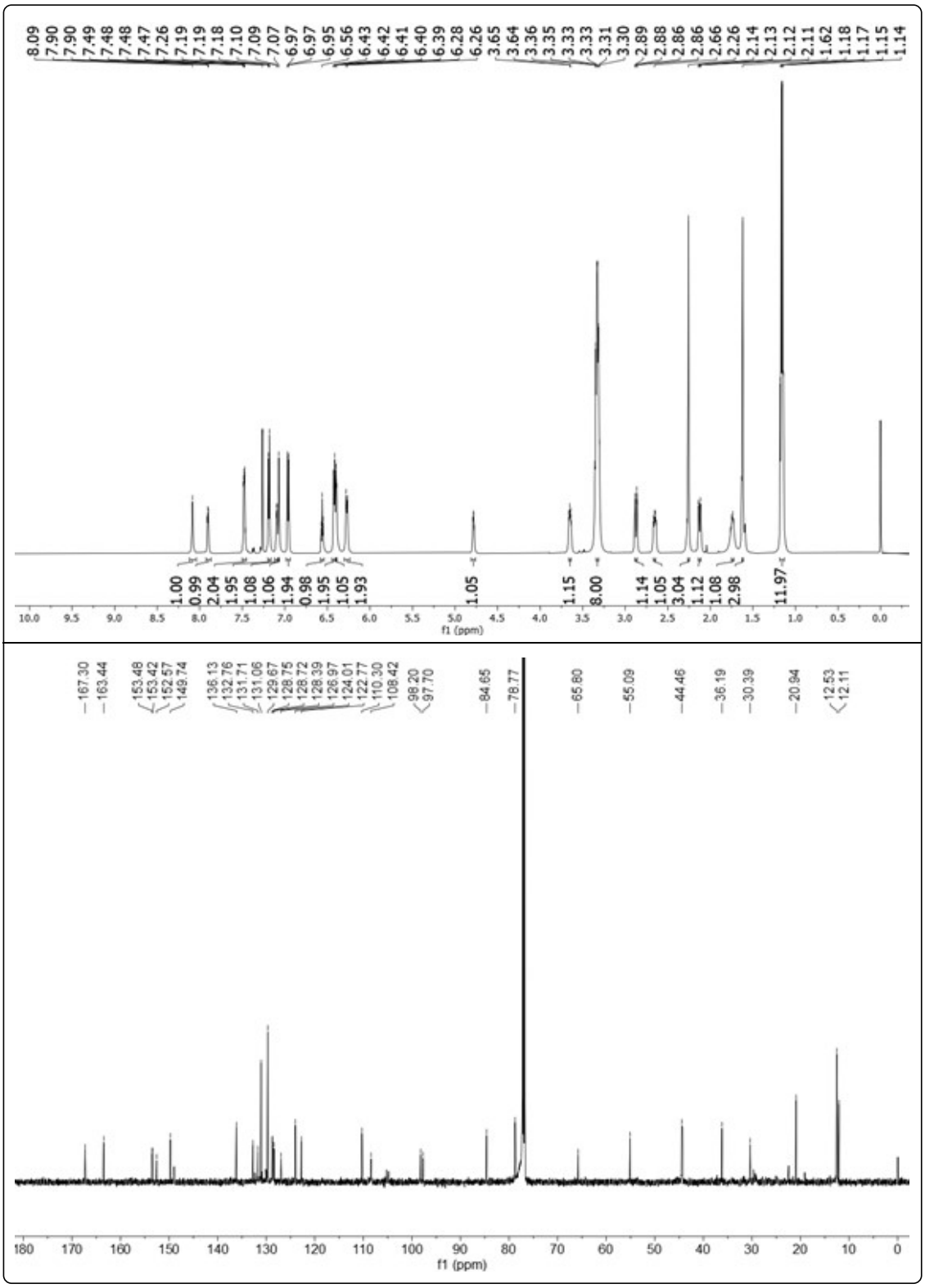


Figure S28. ^{1}H and ^{13}C NMR of the compound **5f** in $CDCl_3$ at 600 MHz and 150 MHz respectively.

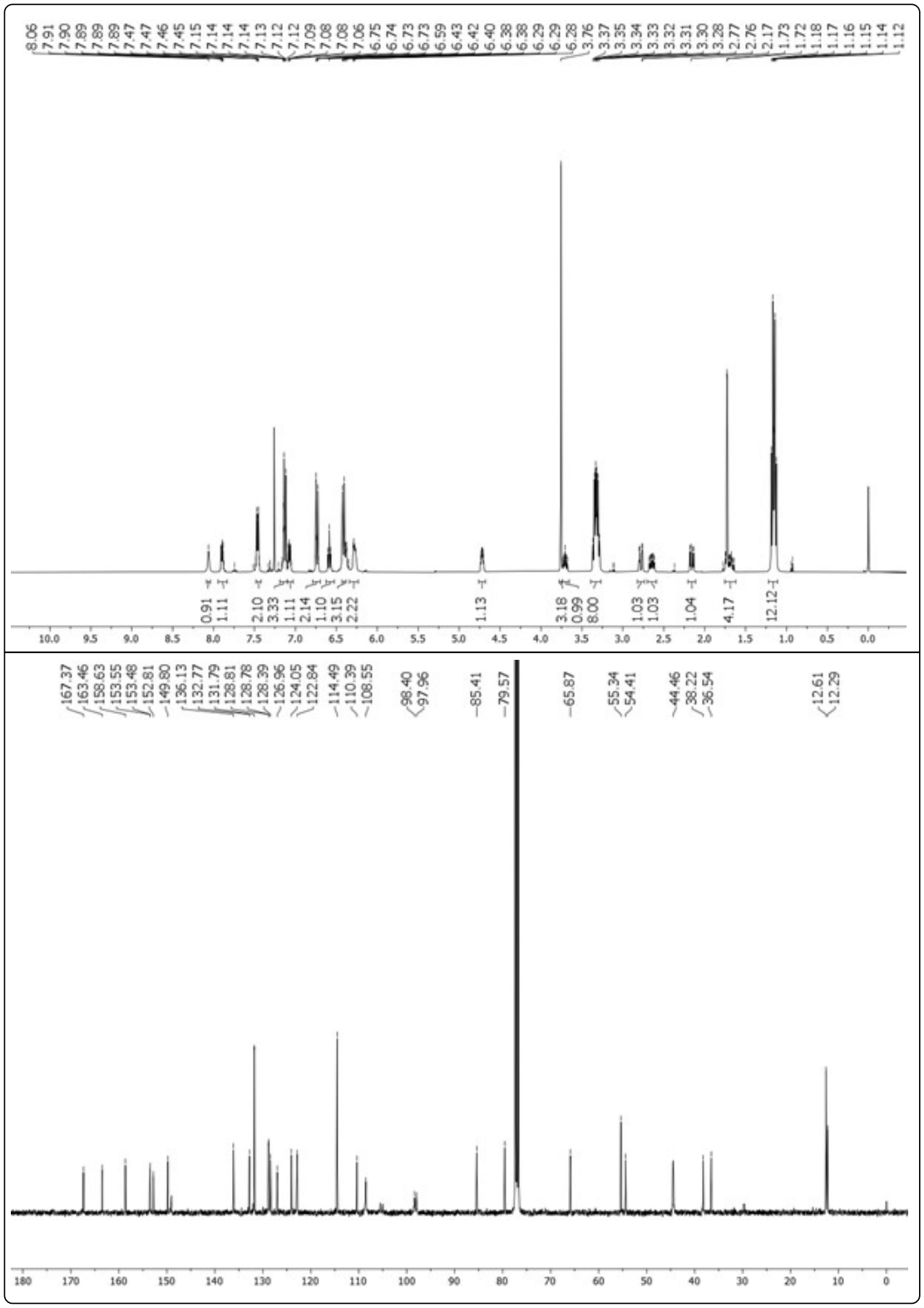


Figure S29. ^{1}H and ^{13}C NMR of the compound **5g** in $CDCl_3$ at 400 MHz and 100 MHz respectively.

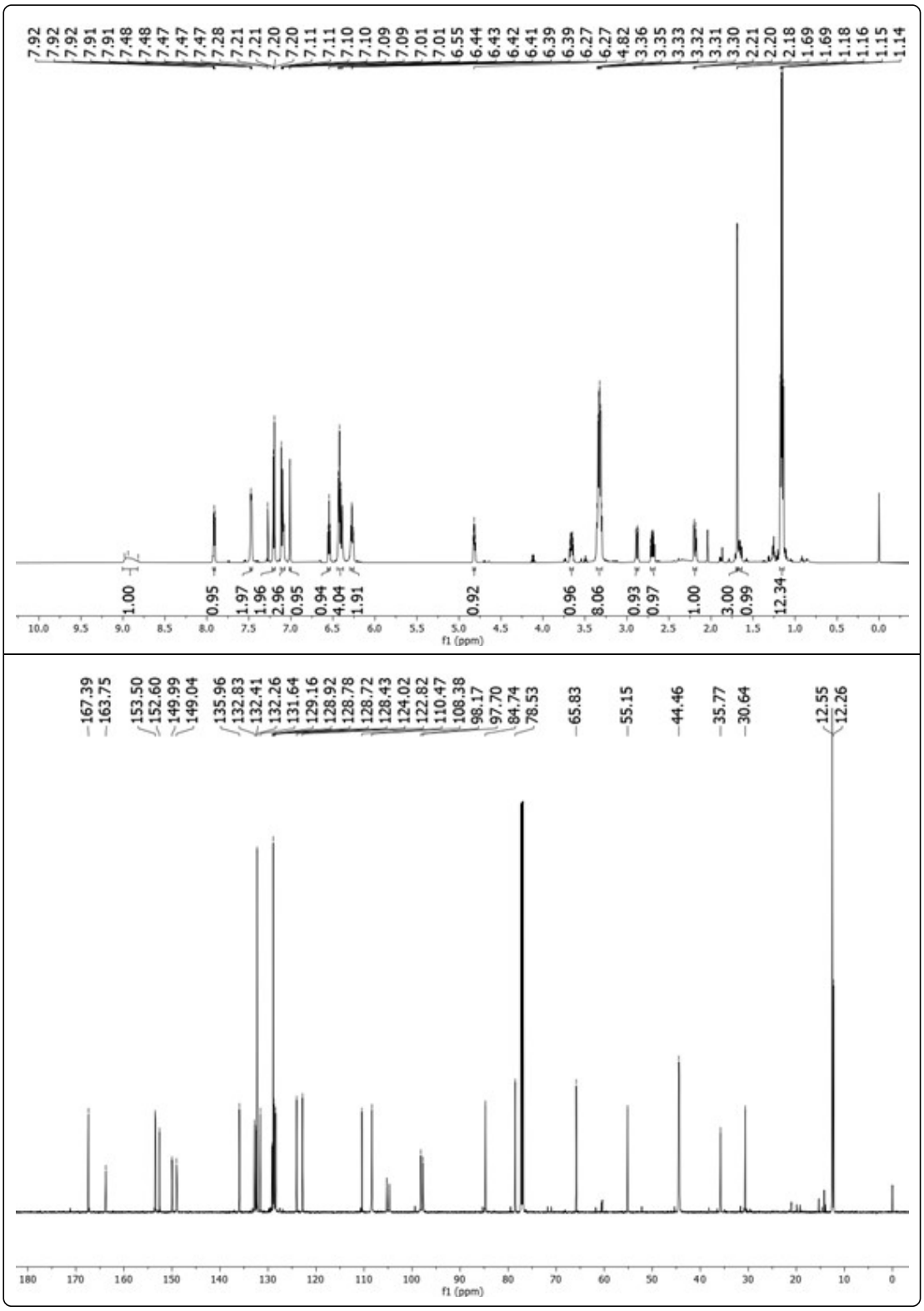


Figure S30. ^{1}H and ^{13}C NMR of the compound **5h** in $CDCl_3$ at 600 MHz and 150 MHz respectively.

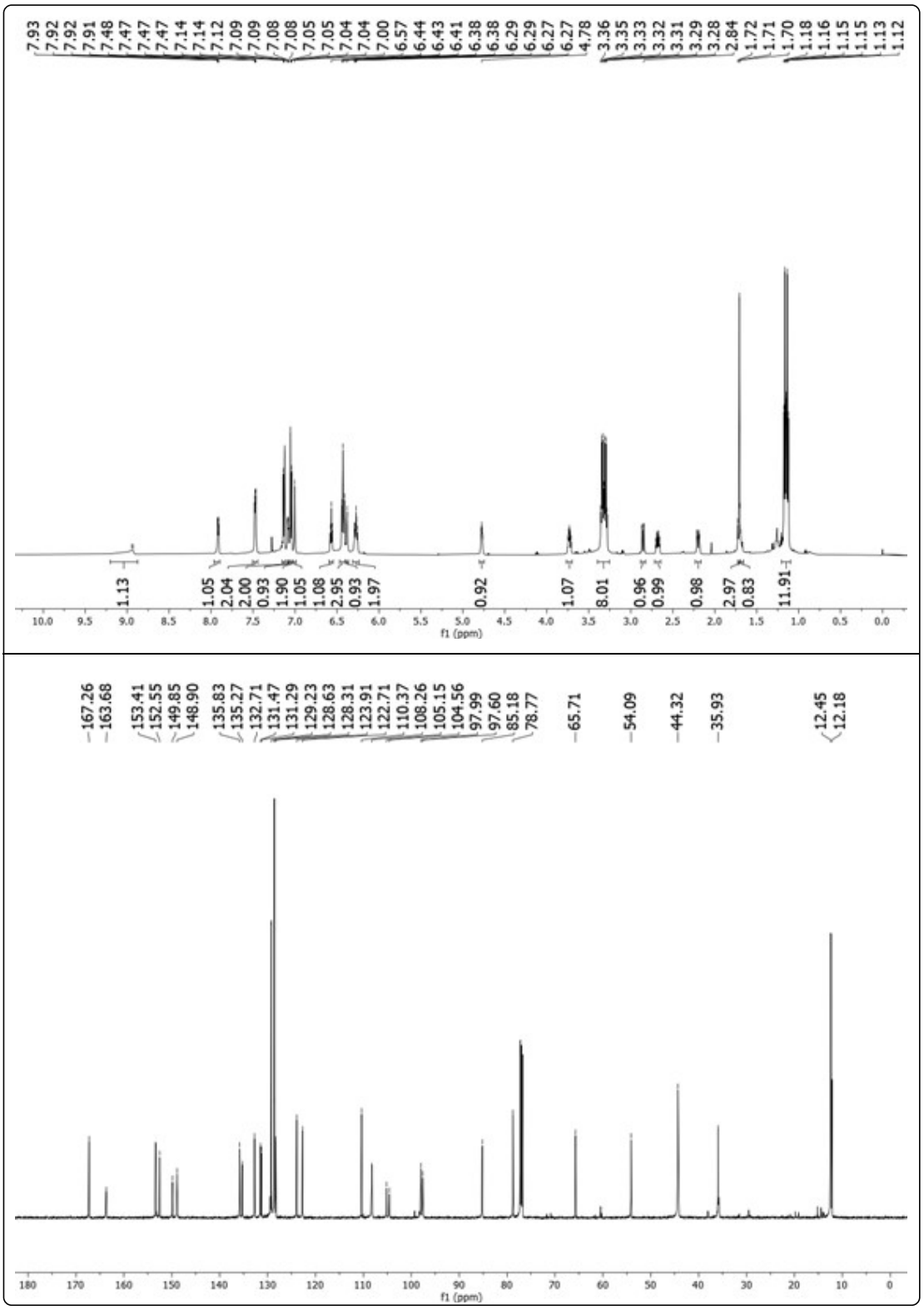


Figure S31. ^{1}H and ^{13}C NMR of the compound **5i** in $CDCl_3$ at 600 MHz and 150 MHz respectively.

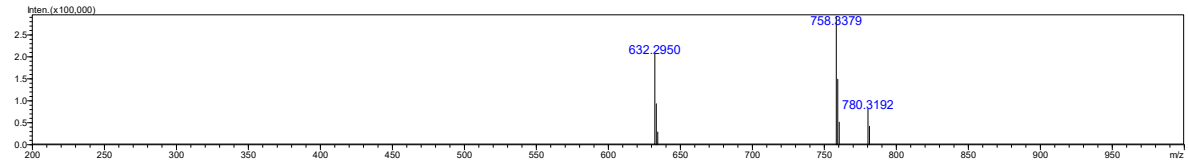


Figure S32. HRMS of **5a** (calculated for M+H$^+$: 758.3371).

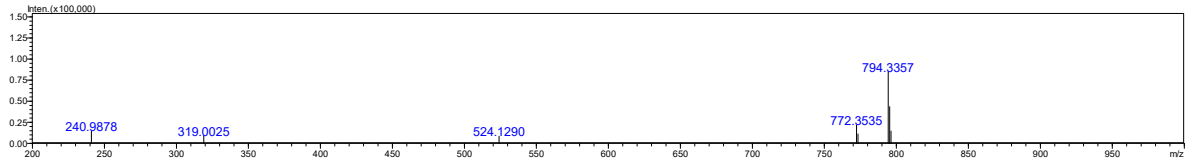


Figure S33. HRMS of **5b** (calculated for M+H$^+$: 772.3527).

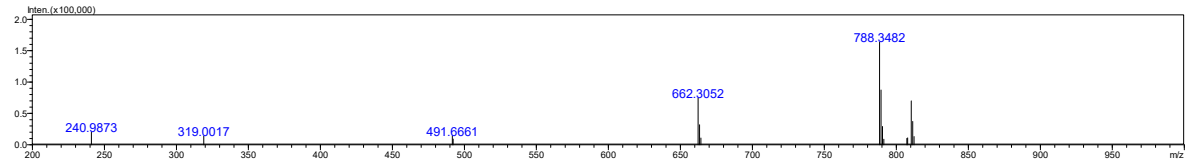


Figure S34. HRMS of **5c** (calculated for M+H$^+$: 788.3476).

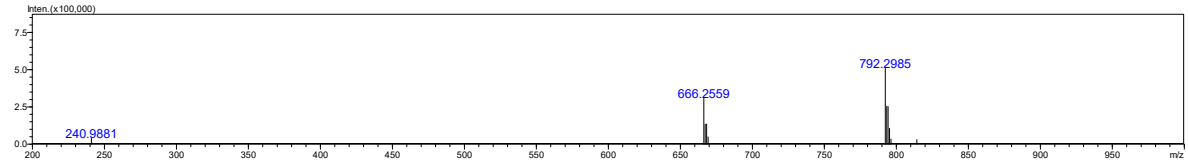


Figure S35. HRMS of **5d** (calculated for M+H$^+$: 792.2981).

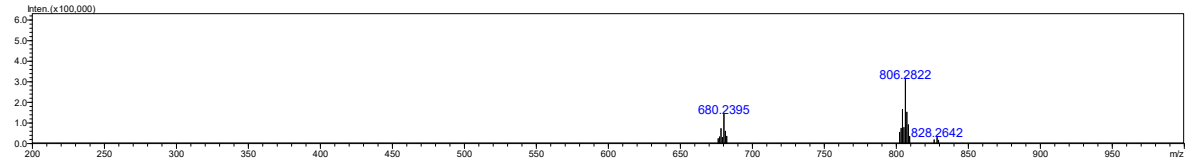


Figure S36. HRMS of **5e** (calculated for M+H$^+$: 806.2820).

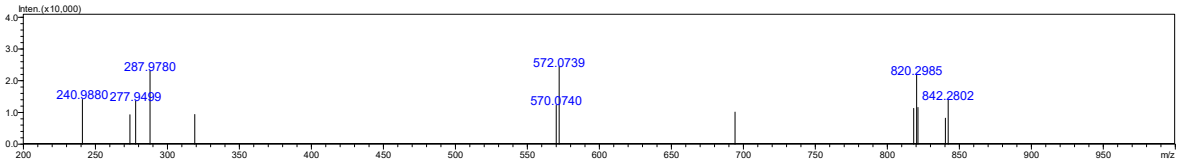


Figure S37. HRMS of **5f** (calculated for M+H$^+$: 820.2977).

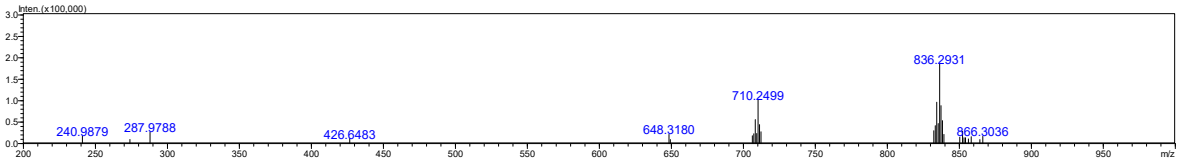


Figure S38. HRMS of **5g** (calculated for M+H$^+$: 836.2926).

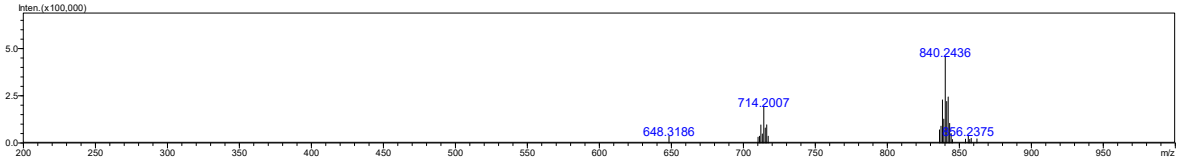


Figure S39. HRMS of **5h** (calculated for M+H$^+$: 840.2428).

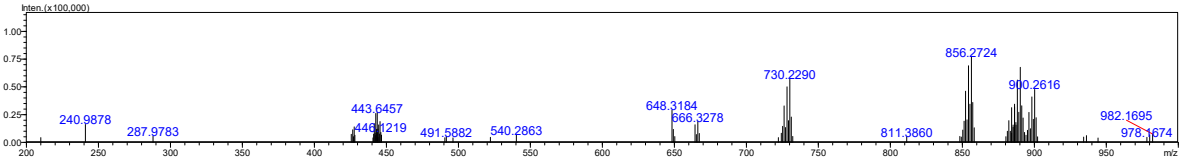


Figure S40. HRMS of **5i** (calculated for M+H$^+$: 856.2717).

References

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