Supplementary information

SYNTHESIS, STRUCTURE, PHOTOPHYSICAL PROPERTIES OF NOVEL THIAZOLO[2,3-b]PTERIDINES

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Content

Spectral data of obtained compounds

7-(4-Fluorobenzylidene)-2,3-dimethyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.1)****.* ^{1}H NMR (400 M*Hz*, DMSO-*d6*) δ 8.05 (s, 1H, 7-=CH-Ar), 7.74 (dd, *J* = 8.1, 5.5 *Hz*, 2H, 7-Ar H-2,6), 7.29 (t, *J* = 8.3 *Hz*, 2H, 7-Ar H-3,5), 2.66 (s, 3H, 2-CH_3), 2.65 (s, 3H, 3-CH_3); ^{13}C NMR (101 M*Hz*, TFA-*d1*) δ 166.8 (d, *J* = 258.4 *Hz*), 165.9, 163.9, 159.67 (C-5a), 157.8, 156.9, 146.8, 143.7, 134.6 (d, *J* = 9.4 *Hz*), 130.6, 128.9, 117.9 (d, *J* = 22.9 *Hz*), 115.2, 21.39-18.42 (m); LC-MS: m/z = 355; Anal. Calcd. For $C_{17}H_{11}FN_4O_2S$: C, 57.62; H, 3.13; N, 15.81; found: C, 57.57; H, 3.19; N, 15.87.

7-(4-(Dimethylamino)benzylidene)-2,3-dimethyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.2)****.* ^{1}H NMR (400 M*Hz*, DMSO-*d6*) δ 7.89 (s, 1H, 7-=CH-Ar), 7.49 (d, *J* = 8.7 *Hz*, 2H, 7-Ar H-2,6), 6.79 (d, *J* = 8.7 *Hz*, 2H, 7-Ar H-3,5), 3.09 (s, 6H, N(CH_3)$_2$), 2.65 (s, 3H, 2-CH_3), 2.64 (s, 3H, 3-CH_3); ^{13}C NMR (101 M*Hz*, TFA-*d1*) δ 164.3, 163.2, 160.3, 158.3, 156.8, 147.1, 144.6, 139.6, 136.0, 133.8, 130.6, 122.2, 120.7, 47.9, 22.6-13.3; LC-MS: m/z = 380; Anal. Calcd. For $C_{19}H_{17}N_5O_2S$: C, 60.14; H, 4.52; N, 18.46; found: C, 60.07; H, 4.50; N, 18.54.

2,3-Dimethyl-7-(3-nitrobenzylidene)-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.3)****.* ^{1}H NMR (400 M*Hz*, DMSO-*d6*) δ 8.57 (s, 1H, 7-Ar H-2), 8.33 (d, *J* = 9.3 *Hz*, 1H, 7-Ar H-4), 8.24 (s, 1H, 7-=CH-Ar), 8.16-7.97 (m, 1H, 7-Ar H-6), 7.96-7.67 (m, 1H, 7-Ar H-5), 2.75-2.69 (m, 6H, 2-CH_3, 3-CH_3); LC-MS: m/z = 382; Anal. Calcd. For $C_{17}H_{11}N_5O_4S$: C, 53.54; H, 2.91; N, 18.36; found: C, 53.49; H, 2.84; N, 18.42.

7-(Furan-2-ylmethylene)-2,3-dimethyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.4)****.* ^{1}H NMR (400 M*Hz*, DMSO-*d6*) δ 7.97 (s, 1H, 7-=CH-Ar), 7.88 (d, *J* = 1.9 *Hz*, 1H, furan H-5), 7.14 (d, *J* = 2.0 *Hz*, 1H, furan H-3), 6.79 – 6.61 (m, 1H, furan H-4), 2.72 – 2.56 (m, 6H, 2-CH_3, 3-CH_3); ^{13}C NMR (101M*Hz*, TFA-*d1*) δ 167.7, 163.8, 159.2, 157.2, 156.8, 151.3, 150.1, 146.5 , 130.5, 128.7, 125.9, 115.5, 112.3, 20.7– 20.1 (m); LC-MS: m/z = 327; Anal. Calcd. For $C_{15}H_{10}N_4O_3S$: C, 55.21; H, 3.09; N, 17.17; found: C, 55.15; H, 3.03; N, 17.25.

2,3-Diphenyl-7-(3-phenylallylidene)-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.5)****.* ^{1}H NMR (400 M*Hz*, DMSO-*d6*) δ 8.84 – 5.83 (m, 18H, =CH-CH=CH-, 2-Ar 2,3,4,5,6, 3-Ar H-2,3,4,5,6, 7-Ar H-2,3,4,5,6); LC-MS: m/z = 487; ^{13}C NMR (101 M*Hz*, TFA-*d1*) δ 166.0, 163.3, 157.7, 156.9, 156.2, 153.8, 146.8, 145.2, 135.3, 135.0, 134.1, 133.0, 132.5, 131.8, 130.8, 130.5, 130.3, 129.9, 129.8, 129.5, 122.0, 116.0. Anal. Calcd. For $C_{29}H_{18}N_4O_2S$: C, 71.59; H, 3.73; N, 11.52; found: C, 71.52; H, 3.79; N, 11.61.

7-(3-Fluorobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.6)****.* ^{1}H NMR (400 M*Hz*, DMSO-*d6*) δ 8.08 (s, 1H, 7-=CH-Ar), 7.64 – 7.43 (m, 7H, 2-Ar H-2,6, 3-Ar H-2,6, 7-Ar H-2,5,6), 7.41 – 7.28 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5), 7.25 (t, 1H, 7-Ar H-4); ^{13}C NMR (101 M*Hz*, TFA-*d1*) δ 165.4, 164.3 (d, *J* = 249.0 *Hz*), 163.8, 157.7, 157.3, 157.2, 147.6, 142.8, 134.6, 134.5 (d, *J* = 7.7 *Hz*), 134.4, 132.4, 132.2 (d, *J* = 8.0 *Hz*), 131.7, 131.2, 130.8, 130.4, 130.2, 129.7, 127.5 (d, *J*

= 2.2 *Hz*), 120.8 (d, *J* = 22.4 *Hz*), 118.1 (d, *J* = 22.9 *Hz*), 117.8; LC-MS: m/z = 479; Anal. Calcd. For $C_{27}H_{15}FN_4O_2S$: C, 67.77; H, 3.16; N, 11.71; found: C, 67.70; H, 3.10; N, 11.79.

7-(2-Chlorobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.7)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.23 (s, 1H, 7-=CH-Ar), 7.71 (d, *J* = 6.9 *Hz*, 1H, 7-Ar H-6), 7.59 (d, *J* = 8.2 *Hz*, 1H, 7-Ar H-3), 7.56 – 7.43 (m, 6H, 2-Ar H-2,6, 3-Ar H-2,6, 7-Ar H-4,5), 7.42 – 7.18 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d_1) δ 166.1, 163.5, 157.3, 157.3, 156.2, 146.9, 140.4/140.3, 138.2, 135.1-134.3 (m), 134.1, 132.5, 132.2, 131.8, 131.5, 130.9, 130.7, 130.4, 130.4-129.4(m), 128.6-128.0 (m), 118.8; LC-MS: m/z = 495; Anal. Calcd. For $C_{27}H_{15}ClN_4O_2S$: C, 65.52; H, 3.05; N, 11.32; found: C, 65.61; H, 3.01; N, 11.40.

7-(3-Chlorobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.8)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.06 (s, 1H, 7-=CH-Ar), 7.71 (s, 1H, 7-Ar H-2), 7.63 (d, *J* = 7.9 *Hz*, 1H, 7-Ar H-6), 7.56 (d, *J* = 8.0 *Hz*, 1H, 7-Ar H-4), 7.53 – 7.42 (m, 5H, 2-Ar H-2,6, 3-Ar H-2,6, 7-Ar H-5), 7.42 – 7.27 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5); LC-MS: m/z = 495; Anal. Calcd. For $C_{27}H_{15}ClN_4O_2S$: C, 65.52; H, 3.05; N, 11.32; found: C, 65.44; H, 3.00; N, 11.38.

7-(4-Bromobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.9)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.05 (s, 1H, 7-=CH-Ar), 7.69 (d, *J* = 8.5 *Hz*, 2H, 7-Ar H-2,6), 7.64 (d, *J* = 8.7 *Hz*, 2H, 7-Ar H-3,5), 7.51 (d, *J* = 7.6 *Hz*, 2H, 2-Ar H-2,6), 7.49 (d, *J* = 7.6 *Hz*, 2H, 3-Ar H-2,6), 7.42 – 7.23 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d_1) δ 157.0, 154.9, 148.6, 148.4, 147.6, 138.1, 134.7, 126.0 , 125.1, 125.0, 124.0, 123.6, 122.9, 122.3, 121.8, 121.6, 121.4-121.2 (m), 120.8, 120.7, 107.8; LC-MS: m/z = 539; Anal. Calcd. For $C_{27}H_{15}BrN_4O_2S$: C, 60.12; H, 2.80; N, 10.39; found: C, 60.10; H, 2.75; N, 10.44.

7-(2-Chloro-6-fluorobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.10)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.02 (s, 1H, 7-=CH-Ar), 7.67 – 7.20 (m, 13H, 2-Ar H-2,3,4,5,6, 3-Ar H-2,3,4,5,6, 7-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d1) δ 166.3/166.2, 163.4, 161.0 (d, *J* = 255.1 *Hz*), 157.2, 157.2, 156.4/156.4, 147.2/147.1, 137.5 (d, *J* = 4.4 *Hz*), 135.7, 135.1 (d, *J* = 10.4 *Hz*), 134.8, 134.2, 132.38, 132.0, 130.8, 130.7-130.5, 130.3, 130.2, 129.7, 127.3 (d, *J* = 2.4 *Hz*), 123.0, 119.6 (d, *J* = 16.1 *Hz*), 115.6 (d, *J* = 23.0 *Hz*); LC-MS: m/z = 513; Anal. Calcd. for $C_{27}H_{14}ClFN_4O_2S$: C, 63.22; H, 2.75; N, 10.92; found: C, 63.26; H, 2.81; N, 10.99.

7-(2,3-Dichlorobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.11)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.19 (s, 1H, 7-=CH-Ar), 7.66 (dd, *J* = 8.2, 2.5 *Hz*, 2H, 7-Ar H-4,6), 7.56 – 7.42 (m, 5H, 2-Ar H-2,6, 3-Ar H-2,6, 7-Ar H-5), 7.42 – 7.13 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d_1) δ 157.0, 154.9, 148.6, 148.4, 147.6, 138.1, 134.7, 126.0, 125.0, 125.0, 124.0, 123.6, 122.9, 122.32, 121.8, 121.6, 121.4-121.2, 120.8, 120.7, 107.8; LC-MS: m/z = 529; Anal. Calcd. For $C_{27}H_{14}Cl_2N_4O_2S$: C, 61.26; H, 2.67; N, 10.58; found: C, 61.31; H, 2.72; N, 10.60.

2,3-Diphenyl-7-(2-(trifluoromethyl)benzylidene)-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.12)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.17 (s, 1H, 7-=CH-Ar), 7.94 – 7.82 (m, 3H, 7-Ar H-3,4,6), 7.79 – 7.63 (m, 1H, 7-Ar H-5), 7.58-7.44 (m, 4H, 2-Ar H-2,6, 3-Ar H-2,6), 7.42 – 7.18 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d_1) δ 165.8, 162.9, 157.3, 157.2, 156.5, 147.1, 139.9, 134.5, 134.2, 133.2, 132.7, 132.3, 131.9, 131.3 (q, *J* = 31.1 *Hz*), 130.9, 130.7, 130.3, 130.1, 129.6, 129.5, 128.0-127.5, 124.2 (q, *J* = 273.2), 121.6; LC-MS: m/z = 529; Anal. Calcd. For $C_{28}H_{15}F_3N_4O_2S$: C, 63.63; H, 2.86; N, 10.60; found: C, 63.70; H, 2.81; N, 10.55.

2,3-Diphenyl-7-(3-(trifluoromethyl)benzylidene)-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.13)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.23 (s, 1H, 7-Ar H-2), 8.05 (s, 1H, 7-=CH-Ar), 8.02 – 7.94 (m, 1H, 7-Ar H-4), 7.85 – 7.75 (m, 2H, 7-Ar H-5,6), 7.63 – 7.46 (m, 4H, 2-Ar H-2,6, 3-Ar H-2,6), 7.46 – 7.26 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d_1) δ 165.2, 163.7, 157.6, 157.4, 157.0, 147.4, 142.2, 134.6, 134.2, 133.9, 133.9 (q, *J* = 33.6 *Hz*), 133.2, 132.4, 131.7, 131.0, 130.9, 130.8, 130.3, 130.1, 130.0-129.9 (m), 129.7, 128.8-128.2 (m), 127.2-121.2 (m), 118.3; LC-MS: m/z = 529; Anal. Calcd. For $C_{28}H_{15}F_3N_4O_2S$: C, 63.63; H, 2.86; N, 10.60; found: C, 63.60; H, 2.50; N, 10.65.

7-(4-(Dimethylamino)benzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.14)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 7.94 (s, 1H, 7-=CH-Ar), 7.60 – 7.46 (m, 6H, 2-Ar H-2,6, 3-Ar H-2,6, 7-Ar 2,6), 7.43 – 7.26 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5), 6.95 (s, 2H, 7-Ar H-3,5), 3.10 (s, 6H, $N(CH_3)_2$); LC-MS: m/z = 504; Anal. Calcd. For $C_{29}H_{21}N_5O_2S$: C, 69.17; H, 4.20; N, 13.91; found: C, 69.12; H, 4.15; N, 13.95.

7-(2-Nitrobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.15)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.35 (s, 1H, 7-=CH-Ar), 8.26 (d, *J* = 8.2 *Hz*, 1H, 7-Ar H-3), 7.94 (t, *J* = 7.3 *Hz*, 1H, 7-Ar H-5), 7.87 (d, *J* = 7.3 *Hz*, 1H, 7-Ar H-6), 7.78 (t, *J* = 7.4 *Hz*, 1H, 7-Ar H-4), 7.61 – 7.49 (m, 4H, 2-Ar H-2,6, 3-Ar H-2,6), 7.45 – 7.25 (m, 6H, 2-Ar H-3,4,5 3-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d_1) δ 165.5, 162.7, 157.3, 157.3, 156.7, 147.9, 147.2, 140.4, 136.1, 134.6, 134.2, 133.2, 132.3, 131.9, 130.9-130.7, 130.3, 130.1, 129.9, 129.6, 129.2, 126.9, 122.5; LC-MS: m/z = 506; Anal. Calcd. For $C_{27}H_{15}N_5O_4S$: C, 64.15; H, 2.99; N, 13.85; found: C, 64.19; H, 2.03; N, 13.89.

7-(3-Nitrobenzylidene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.16)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) ^{1}H NMR (400 M*Hz*, DMSO-d6) δ 8.60 (s, 1H, 7-Ar H-2), 8.45 – 8.22 (m, 2H, 7-=CH-Ar, 7-Ar-H-4), 8.14 (d, *J* = 8.8 *Hz*, 1H, 7-Ar H-6), 7.96 – 7.76 (m, 1H. 7-Ar H-5), 7.65 – 7.50 (m, 4H, 2-Ar H-2,6, 3-Ar H-2,6), 7.46 – 7.27 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5); ^{13}C NMR (101 M*Hz*, TFA-d_1) δ 164.3, 163.5, 158.0-157.3, 149.4, 147.8, 140.0, 137.0, 134.5, 134.5, 134.3, 132.4, 131.8, 131.5, 131.3, 130.8, 130.3, 130.1, 129.7, 127.3, 126.1, 120.4; LC-MS: m/z = 506; Anal. Calcd. For $C_{27}H_{15}N_5O_4S$: C, 64.15; H, 2.99; N, 13.85; found: C, 64.11; H, 3.02; N, 13.89.

7-(Furan-2-ylmethylene)-2,3-diphenyl-10H-thiazolo[2,3-b]pteridine-8,10(7H)-dione ***(3.17)***. ^{1}H NMR (400 M*Hz*, DMSO-d_6) δ 8.00 (d, *J* = 3.2 *Hz*, 1H, furan H-5), 7.93 (s, 1H, 7-=CH-Ar), 7.57 – 7.44

(m, 4H, 2-Ar H-2,6, 3-Ar H-2,6), 7.44 – 7.27 (m, 6H, 2-Ar H-3,4,5, 3-Ar H-3,4,5), 7.24 – 7.16 (m, 1H, furan H-3), 6.86 – 6.23 (m, 1H, furan H-4); ^{13}C NMR (101 M*Hz*, TFA-*d*$_1$) δ 168.1, 163.8, 157.6, 156.8, 155.8, 151.4, 150.2, 146.5, 135.1, 134.0, 132.5, 131.9, 130.8, 130.3, 130.3, 130.1, 129.8, 129.0, 126.1, 115.5, 112.3; LC-MS: m/z = 451; Anal. Calcd. For $C_{25}H_{14}N_4O_3S$: C, 66.66; H, 3.13; N, 12.44; found: C, 66.70; H, 3.17; N, 12.48.

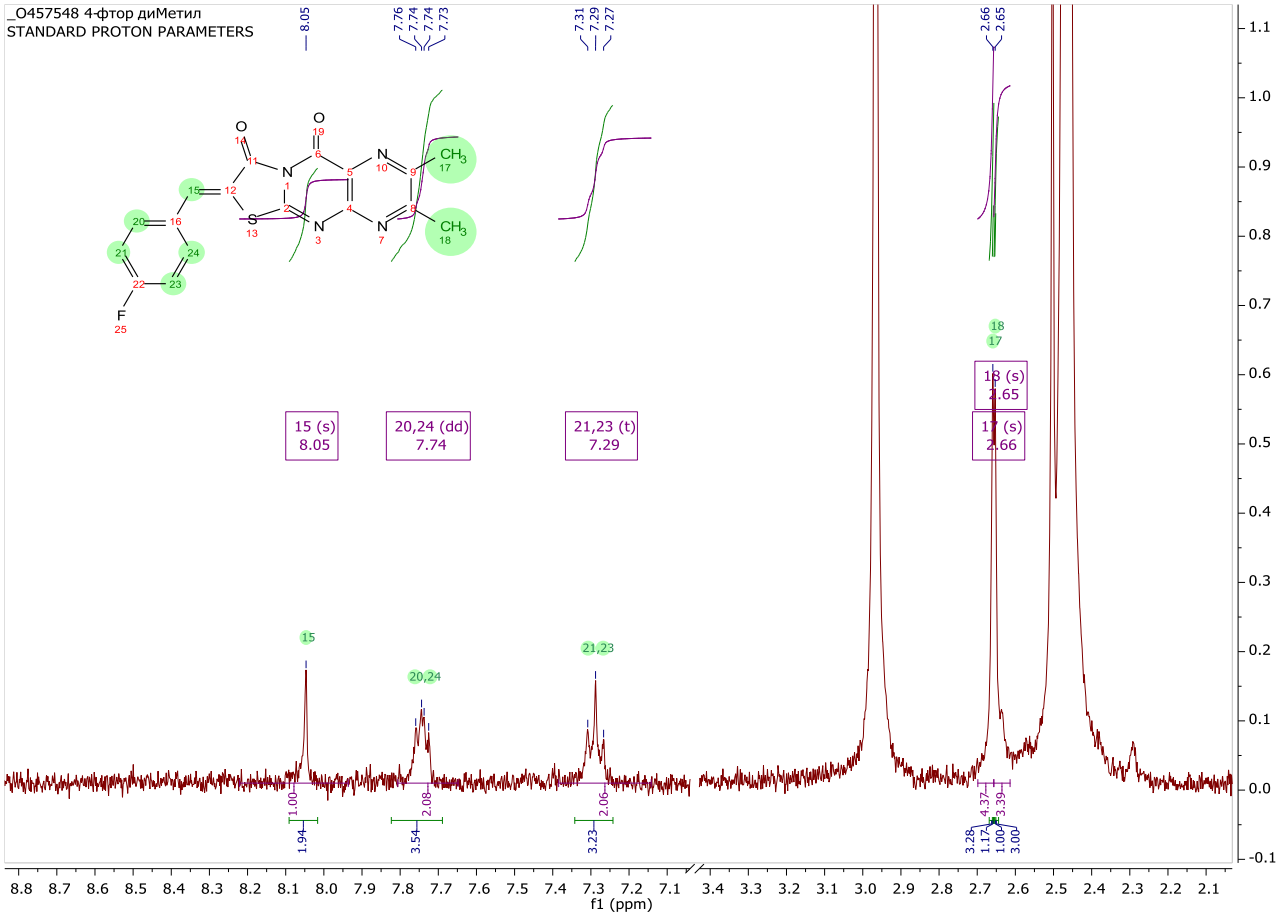


Figure S1 ^{1}H NMR spectra of compound **3.1**

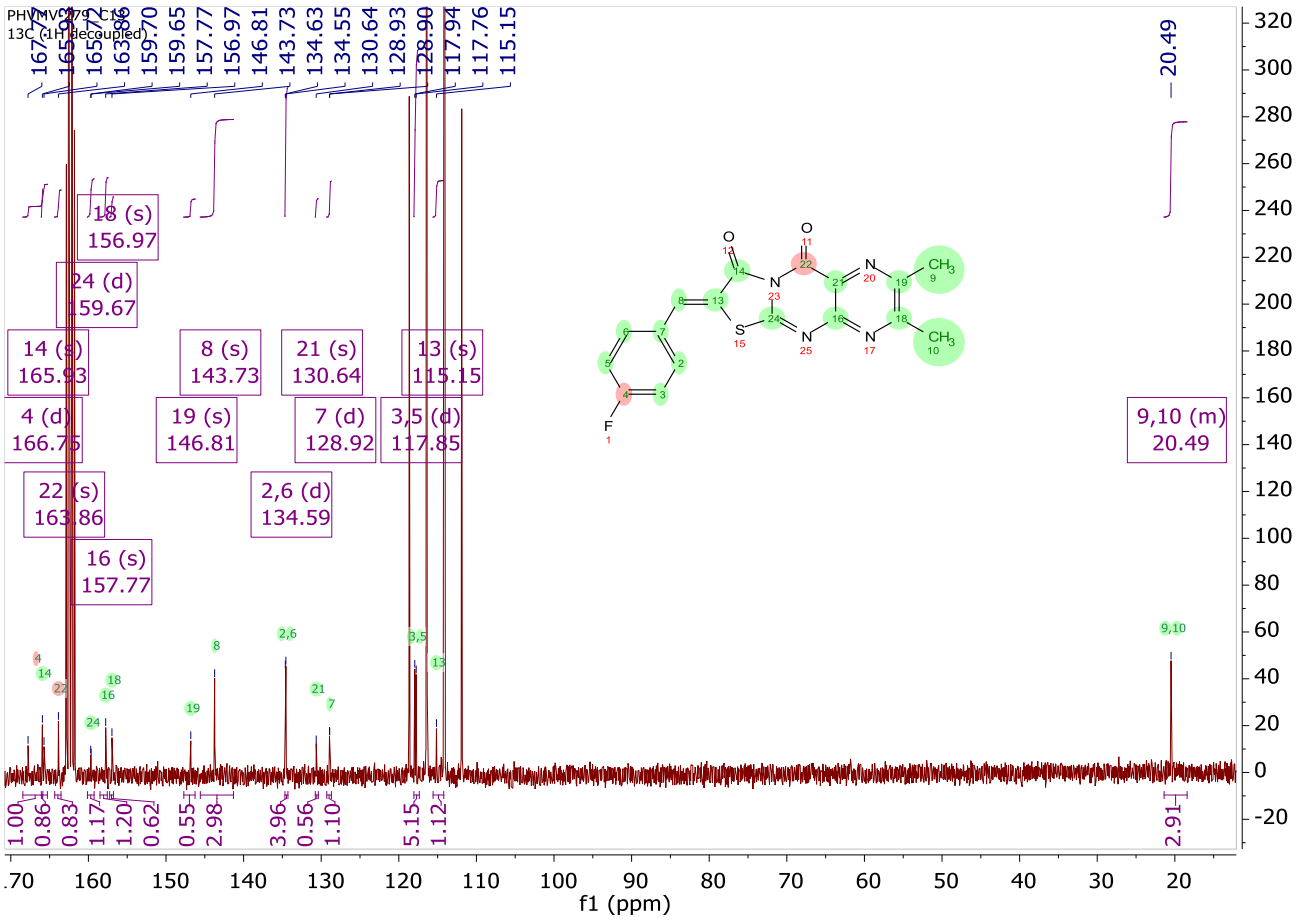


Figure S2 ^{13}C NMR spectra of compound **3.1**

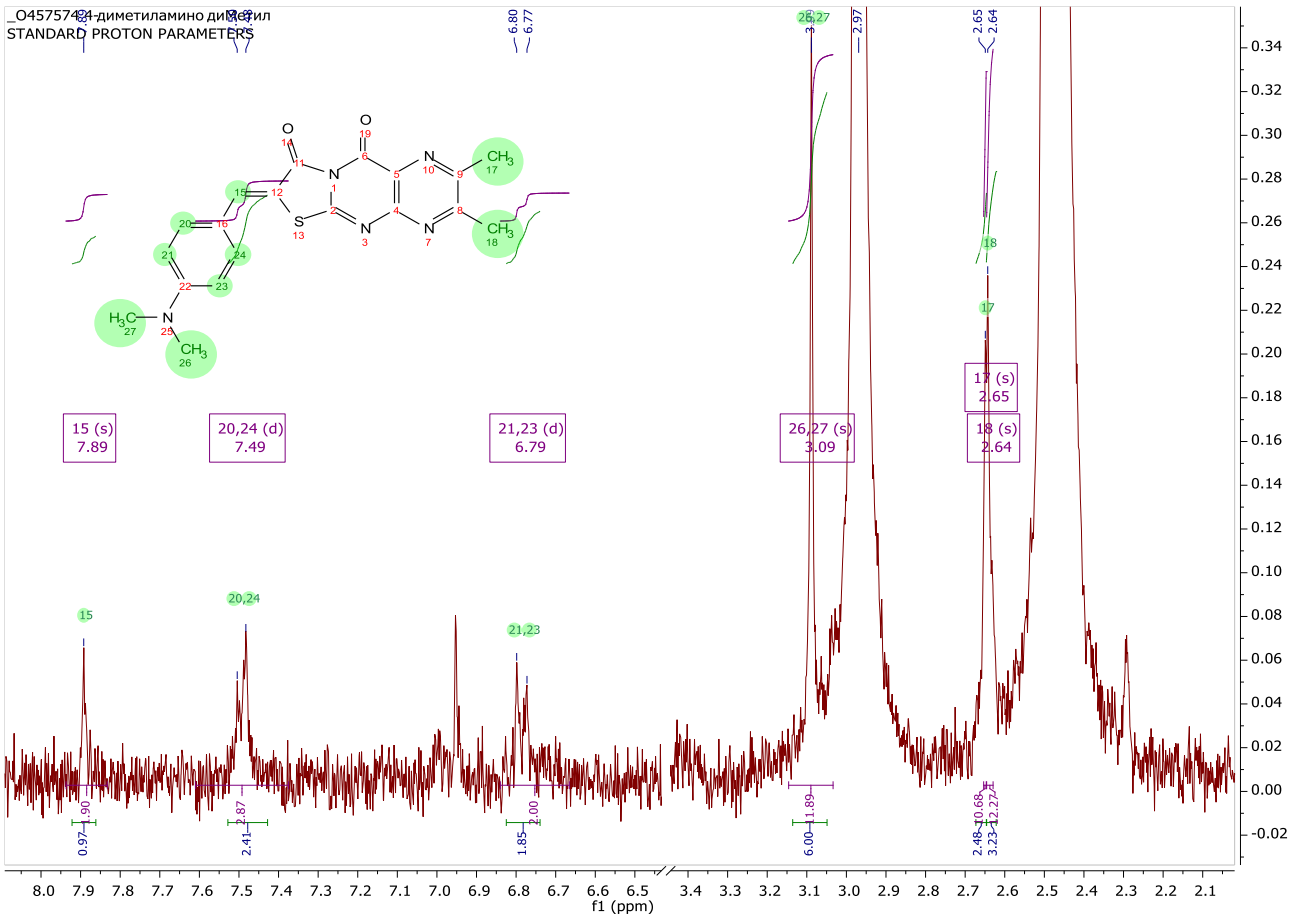


Figure S3 ^{1}H NMR spectra of compound **3.2**

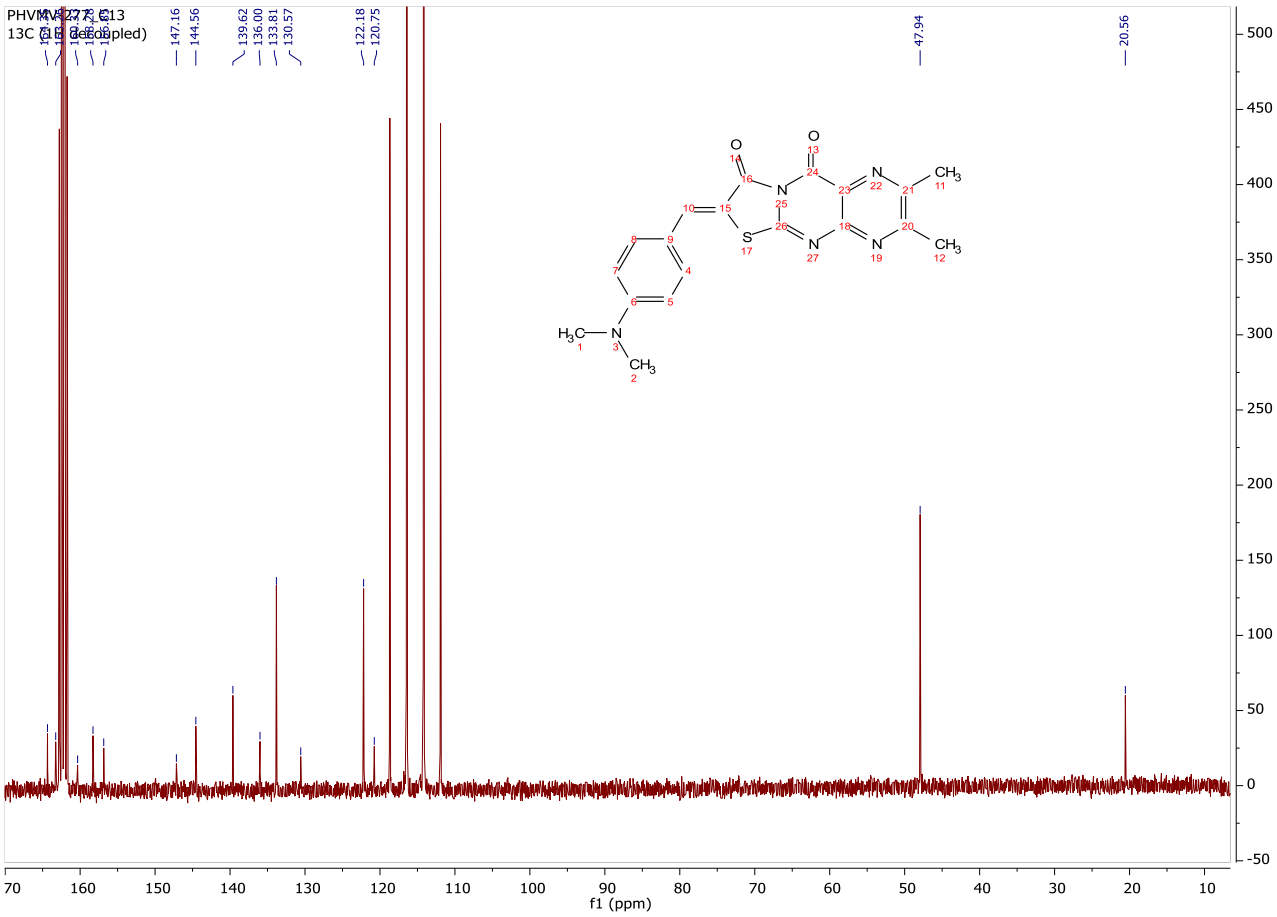


Figure S4 ^{13}C NMR spectra of compound **3.2**

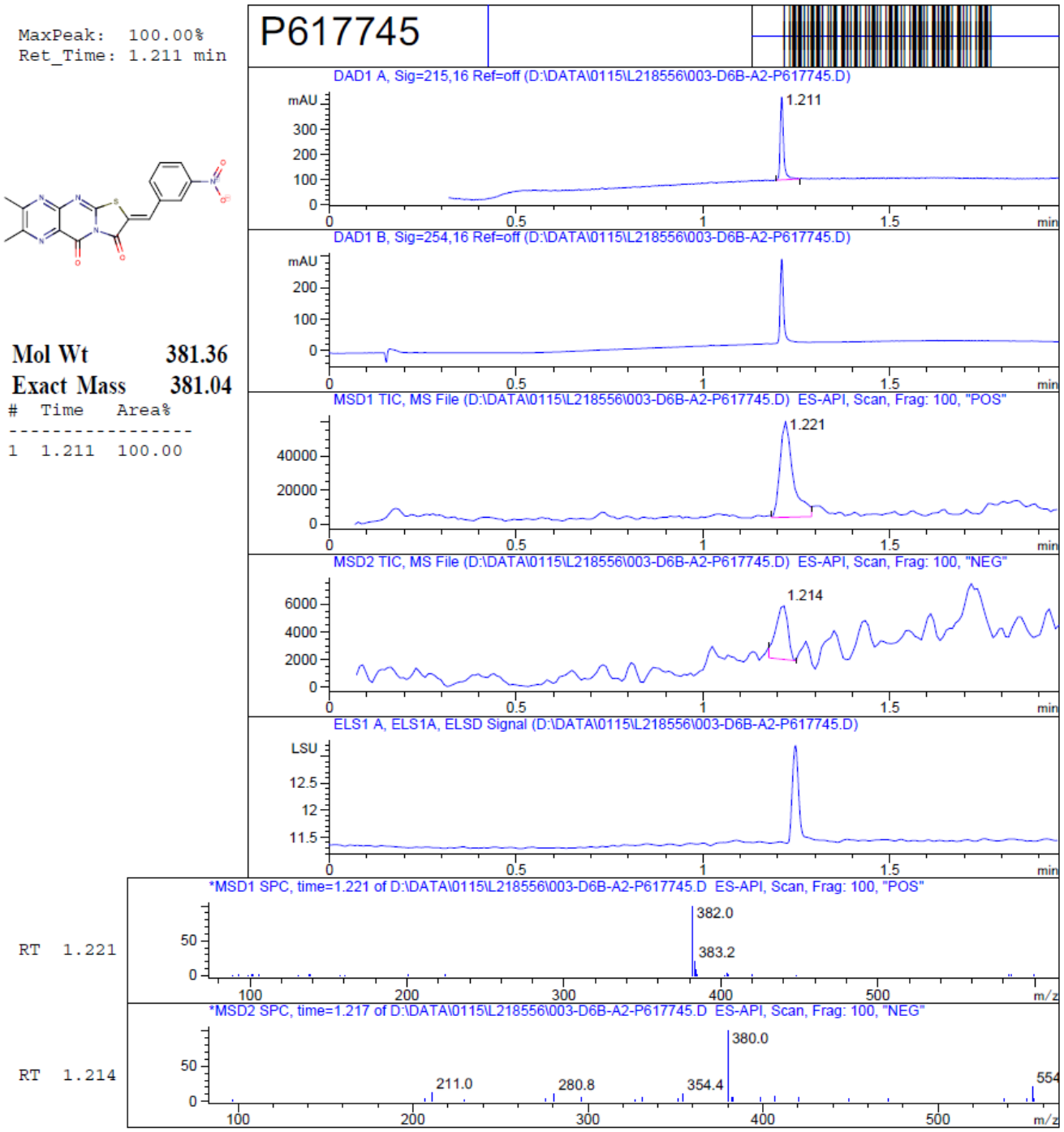


Figure S5 HPLC-MS spectra of compound **3.3**

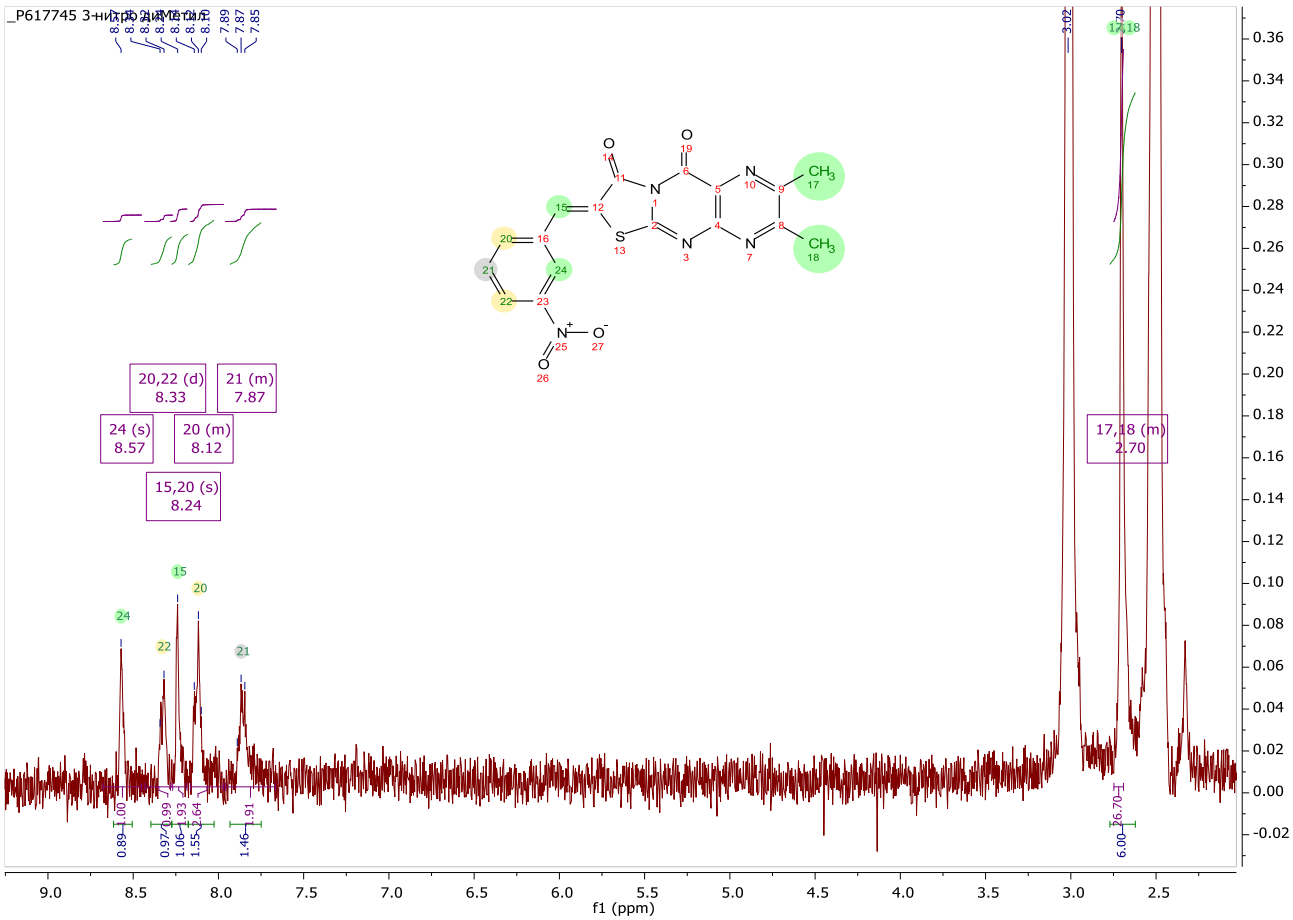


Figure S6 ^{1}H NMR spectra of compound **3.3**

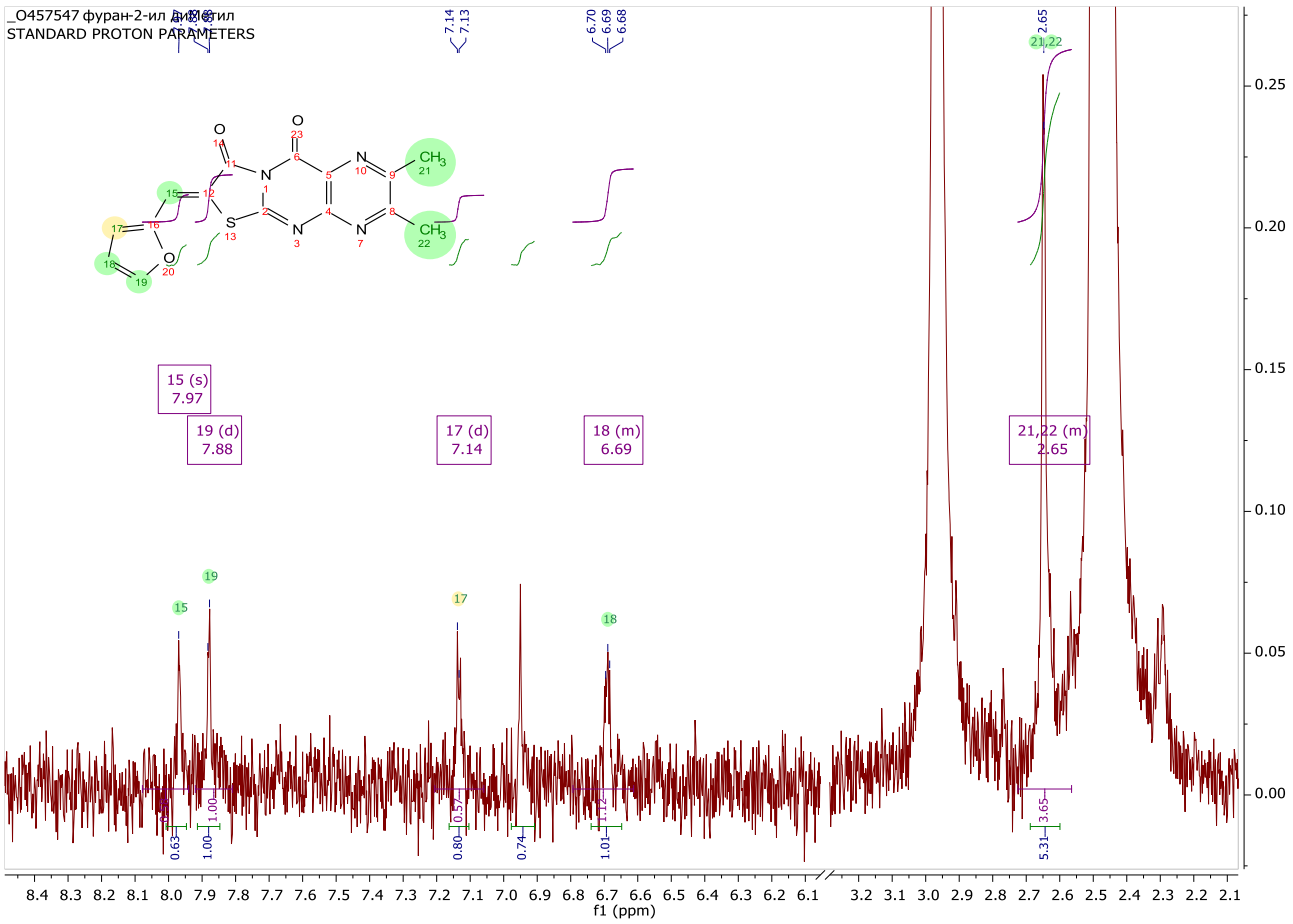


Figure S7 ^{1}H NMR spectra of compound **3.4**

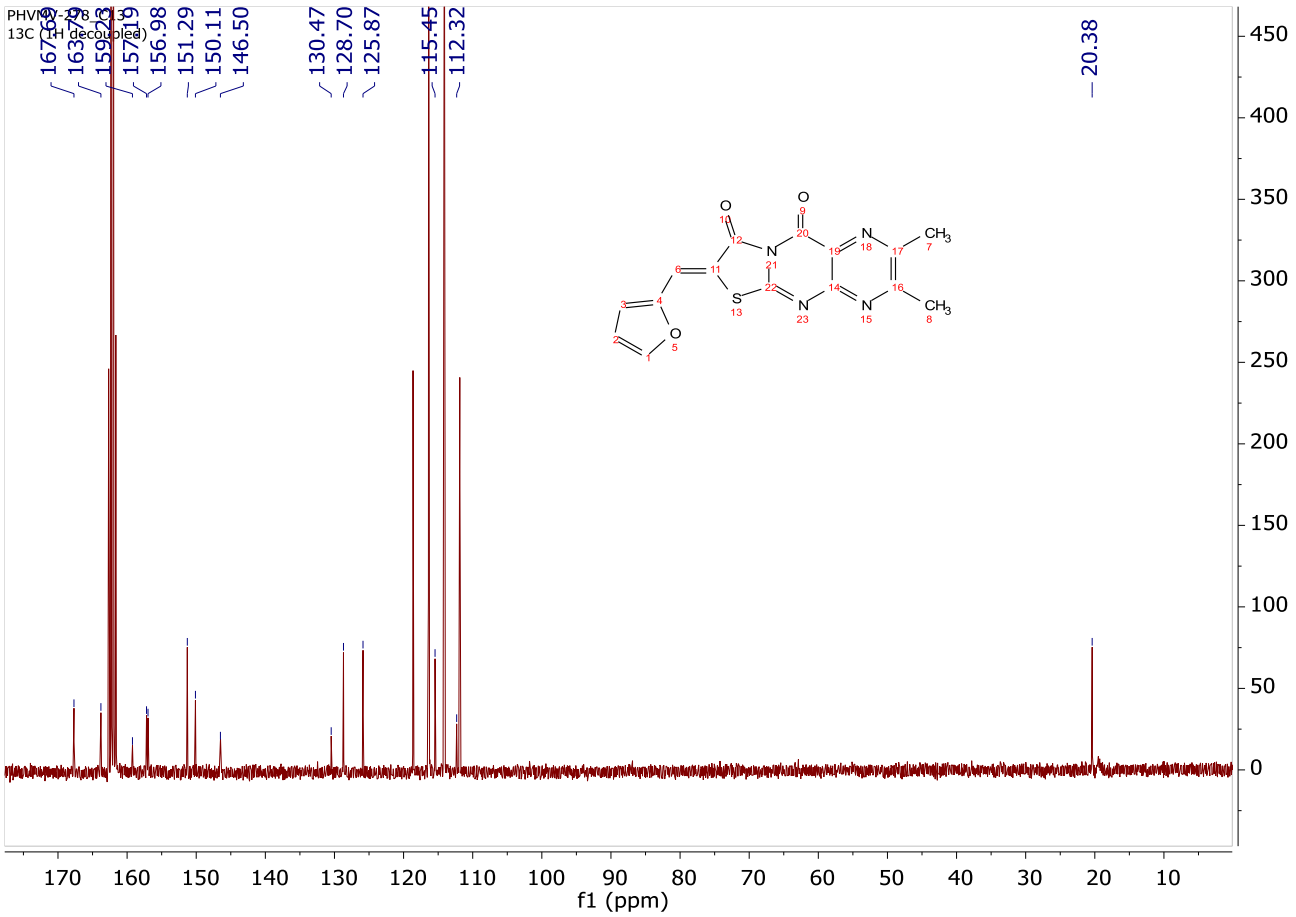


Figure S8 ^{13}C NMR spectra of compound **3.4**

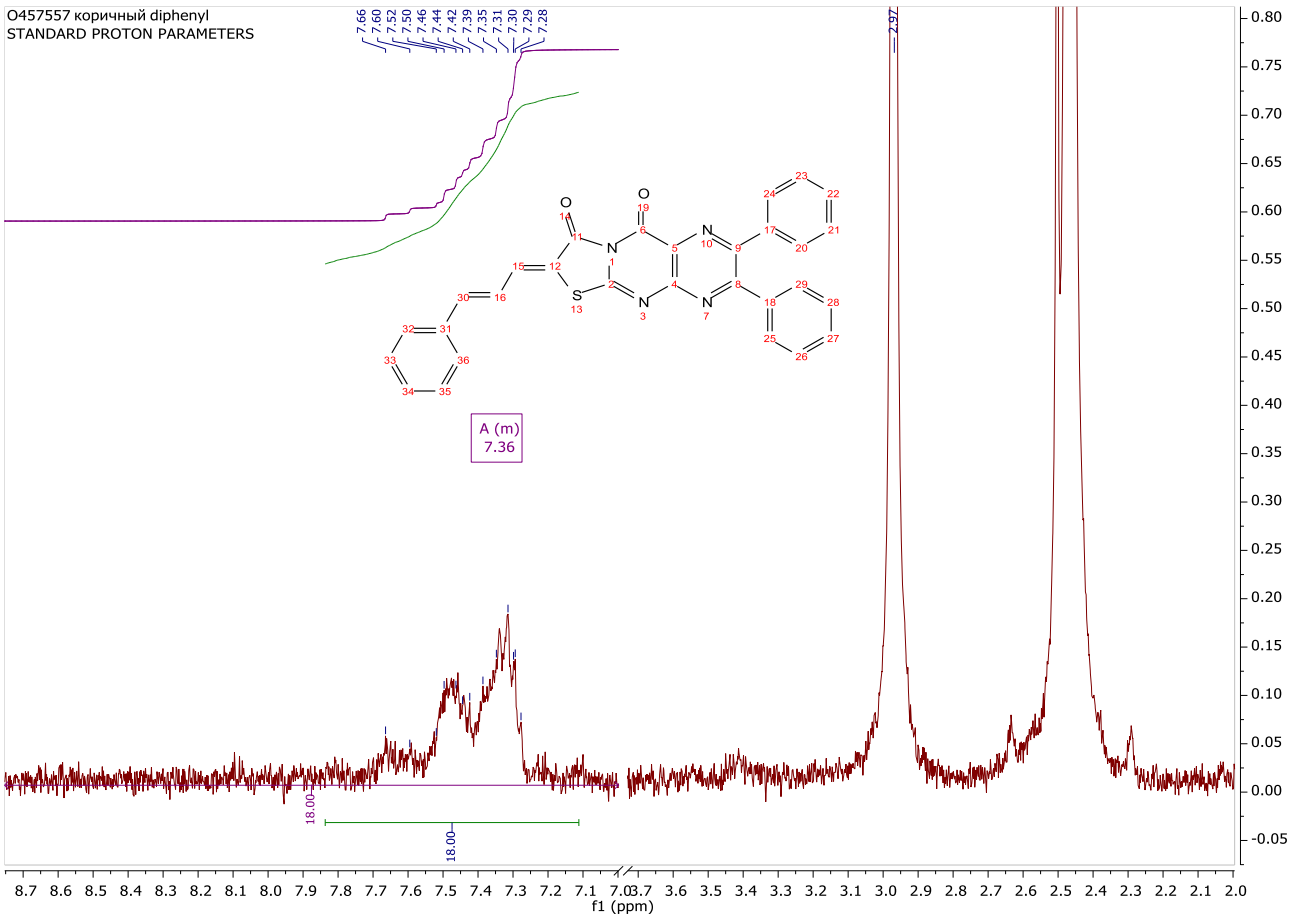


Figure S9 ^{1}H NMR spectra of compound **3.5**

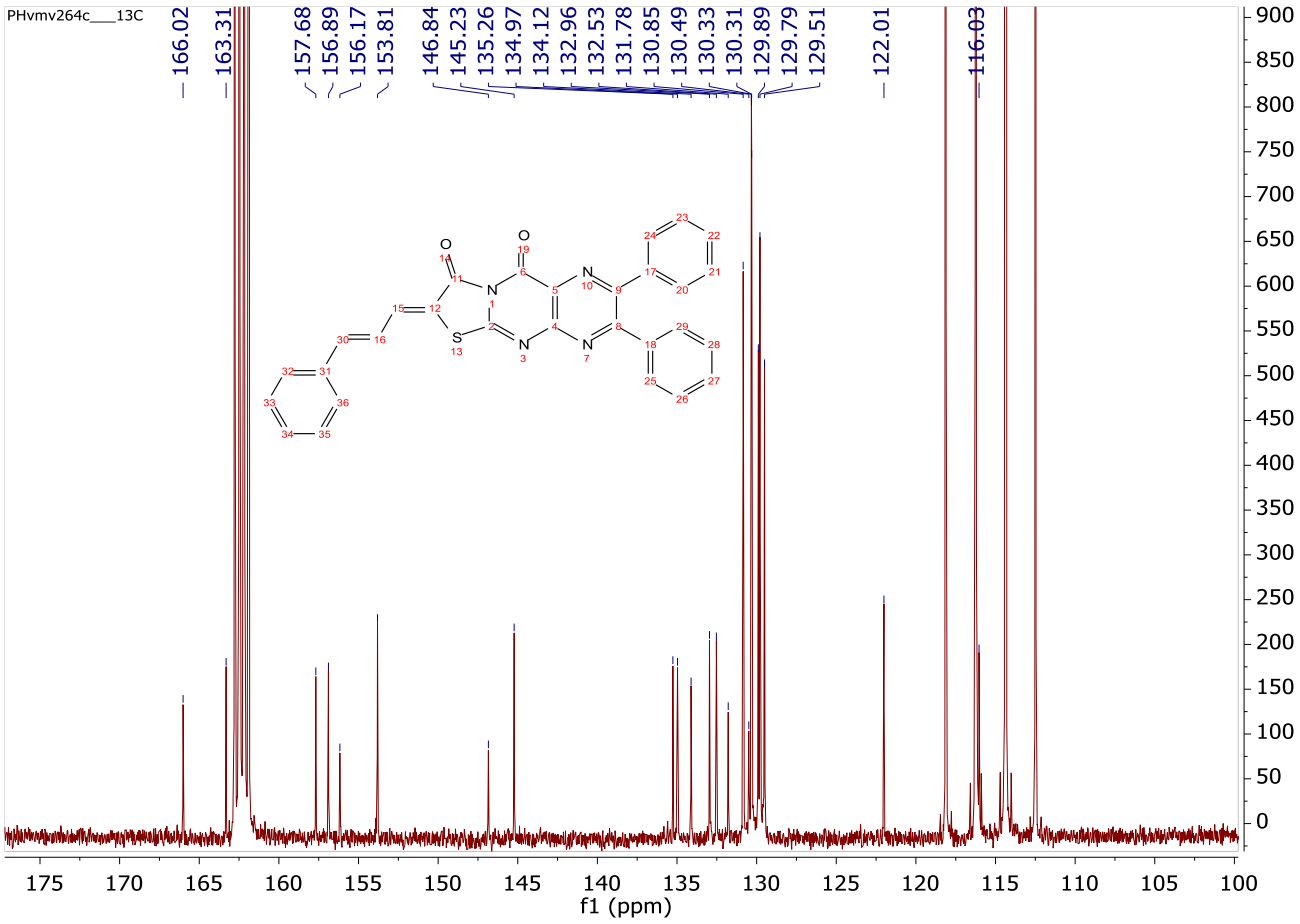


Figure S10 ^{13}C NMR spectra of compound **3.5**

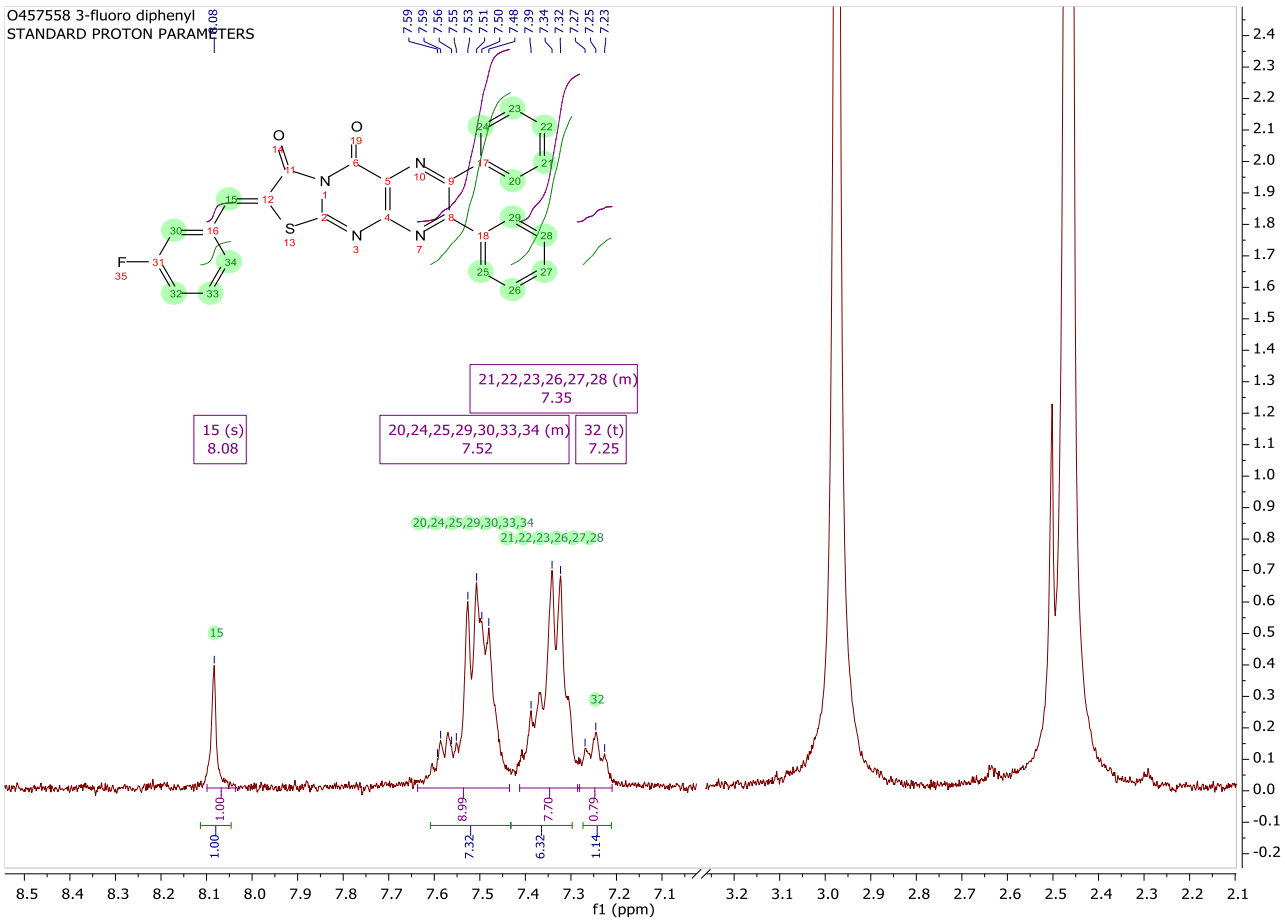


Figure S11 ^{1}H NMR spectra of compound **3.6**

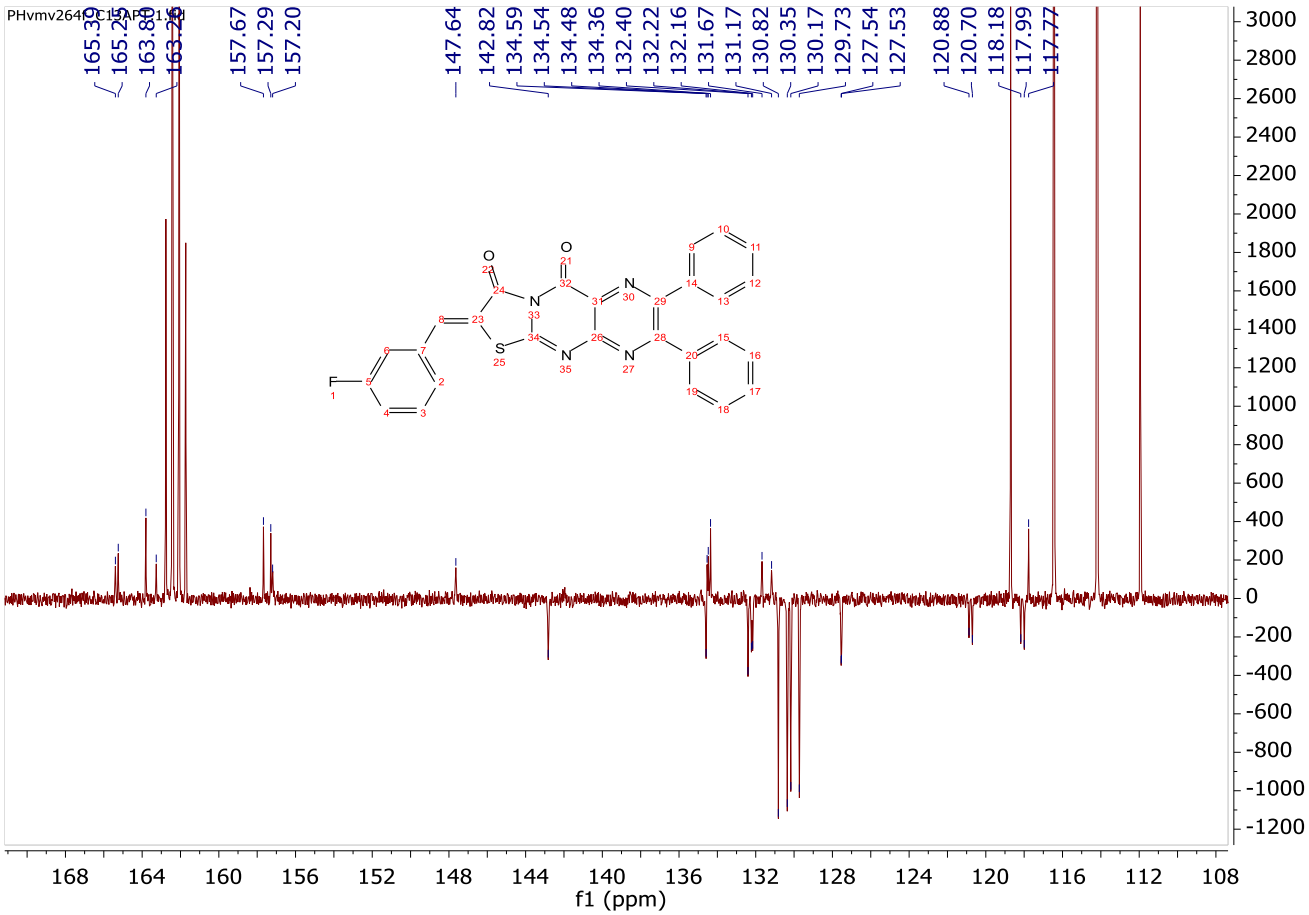


Figure S12 ^{13}C NMR (APT) spectra of compound **3.6**

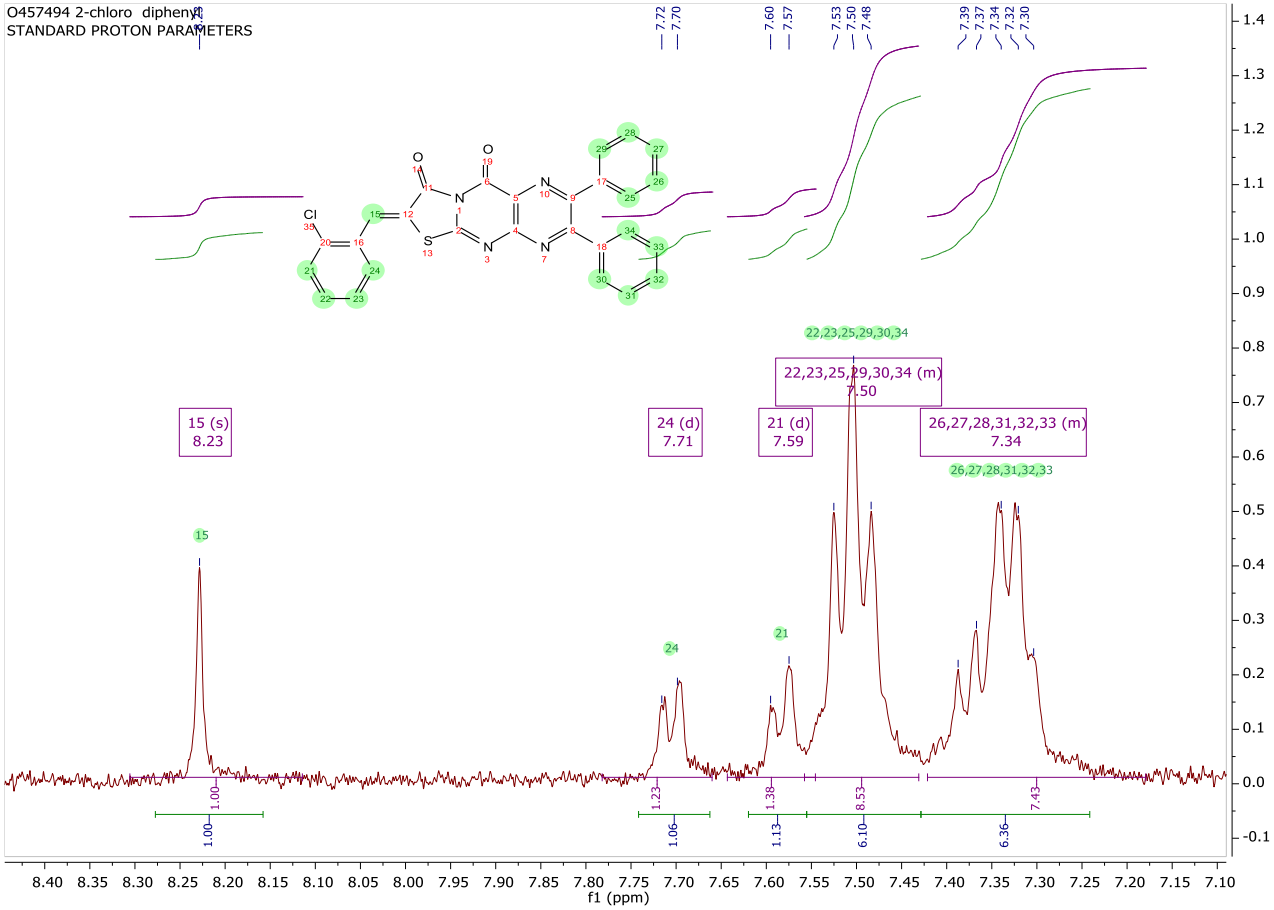


Figure S13 ^{1}H NMR spectra of compound **3.7**

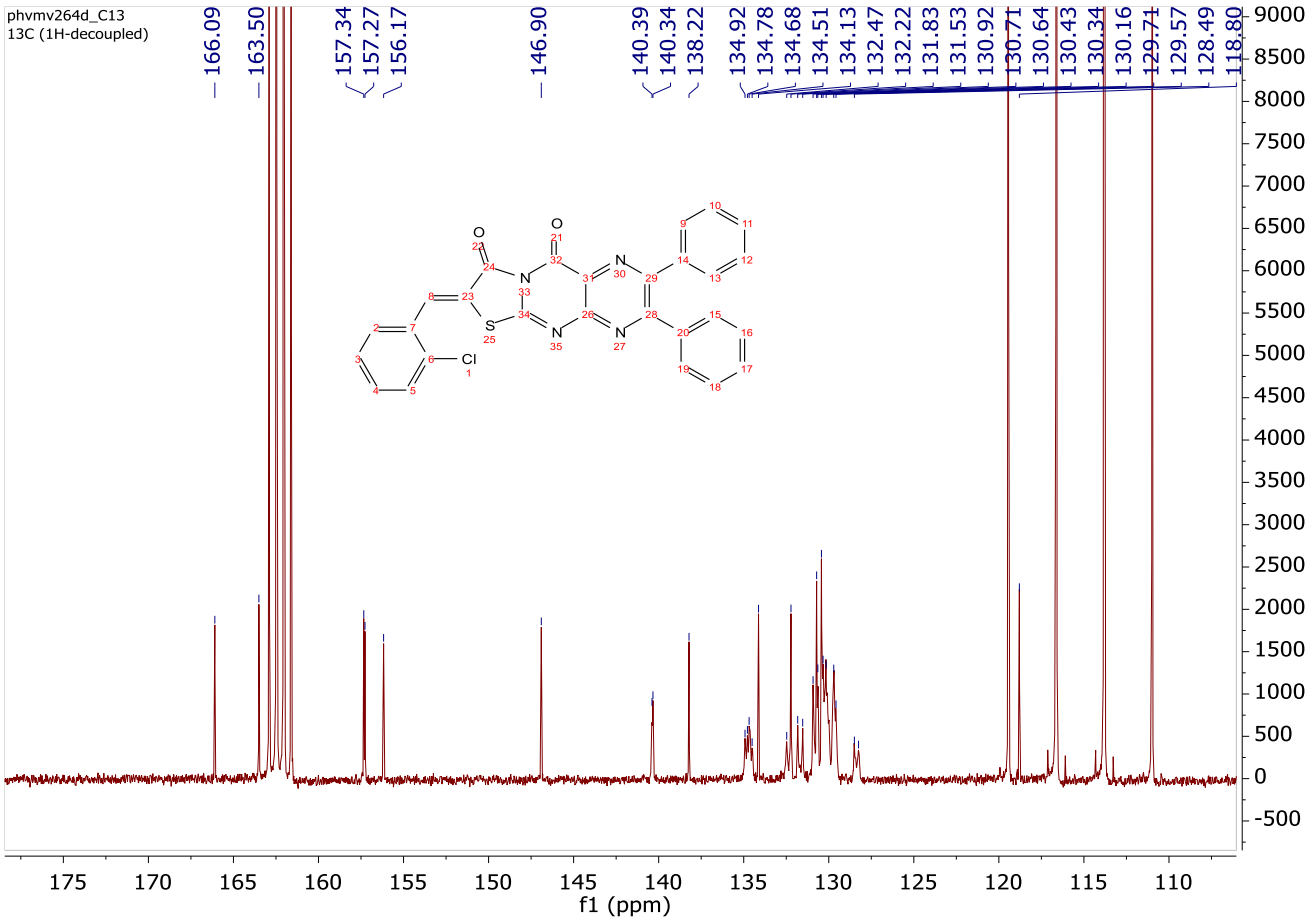


Figure S14 ^{13}C NMR spectra of compound **3.7**

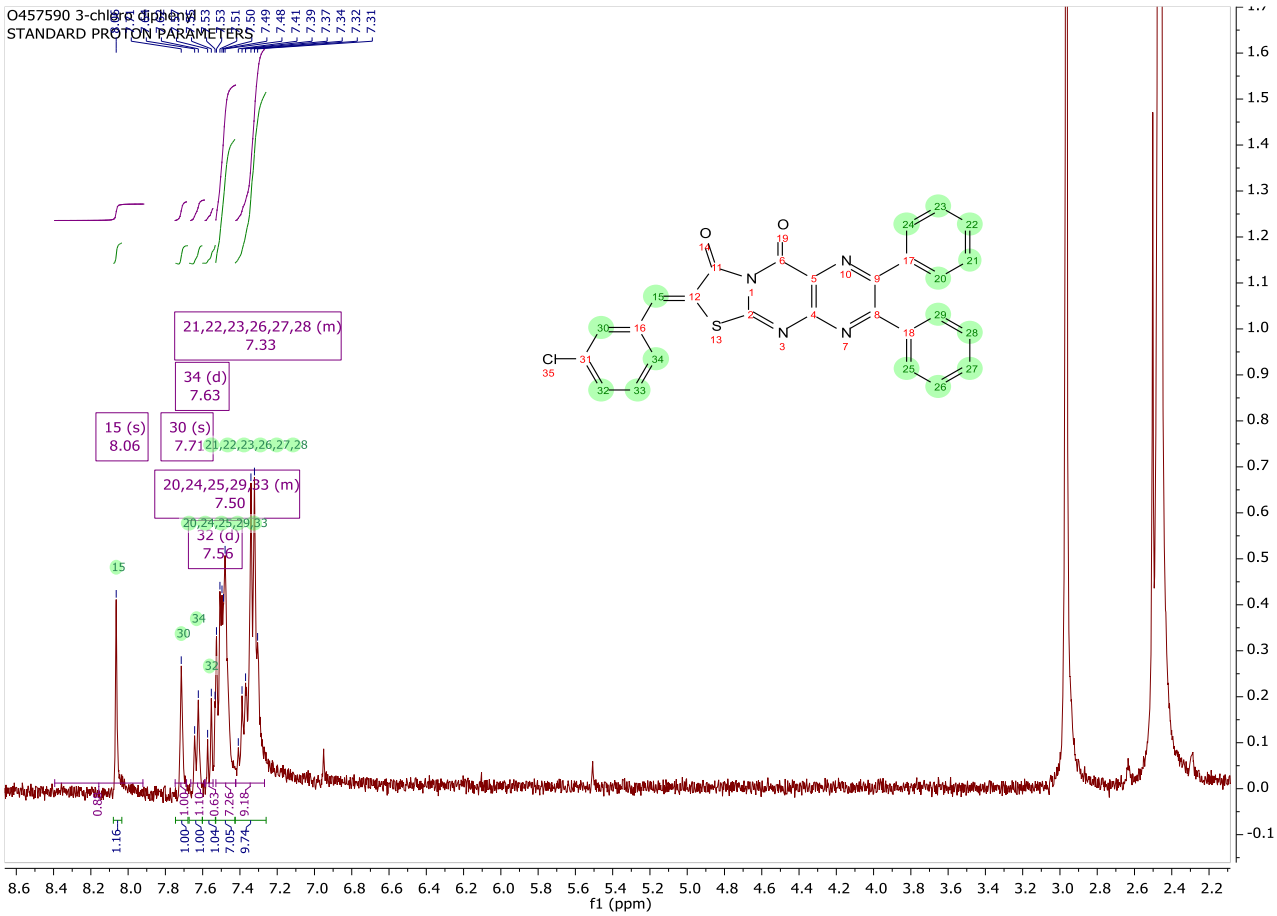


Figure S15 ^{1}H NMR spectra of compound **3.8**

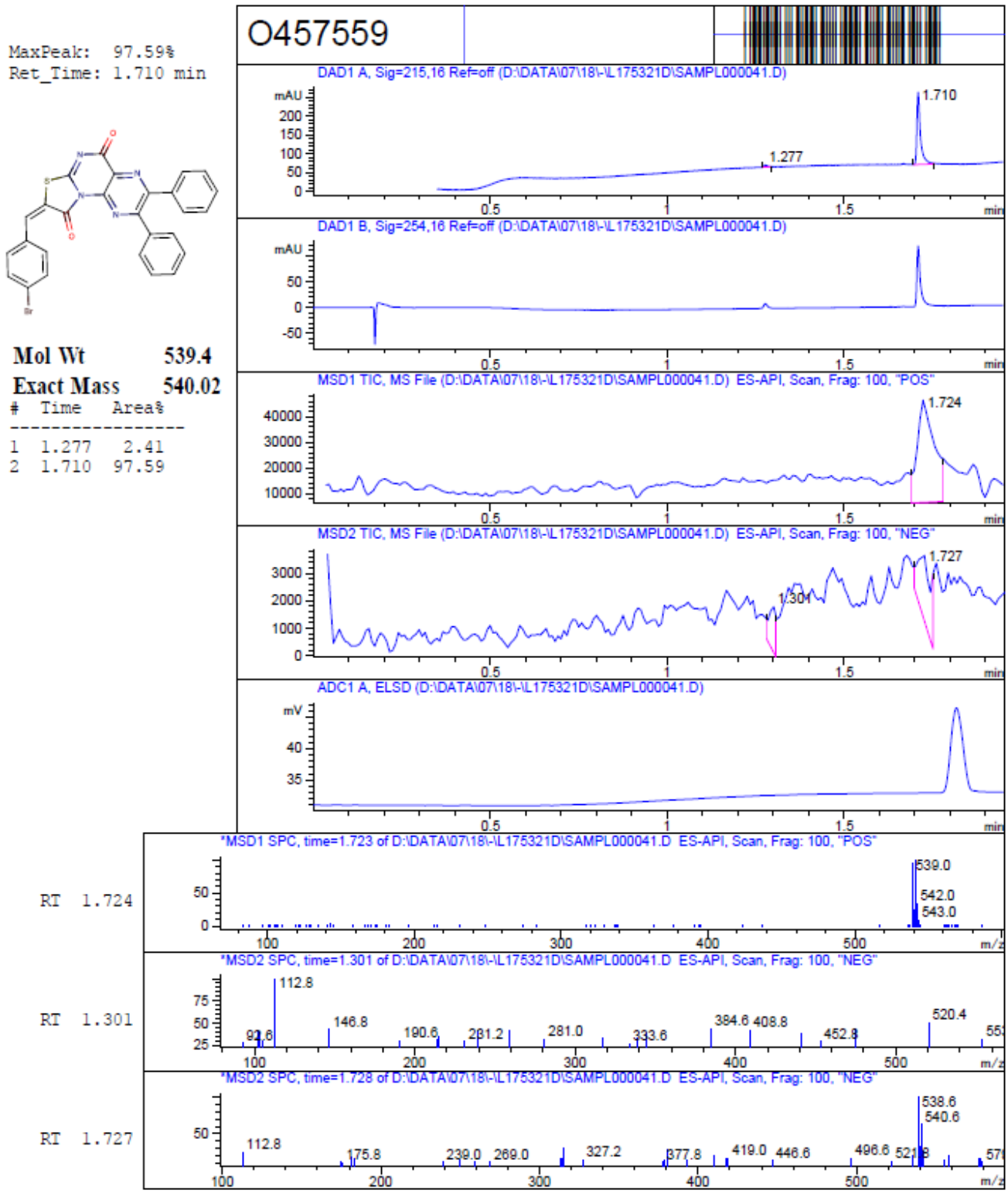


Figure S16 HPLC-MS spectra of compound **3.9**

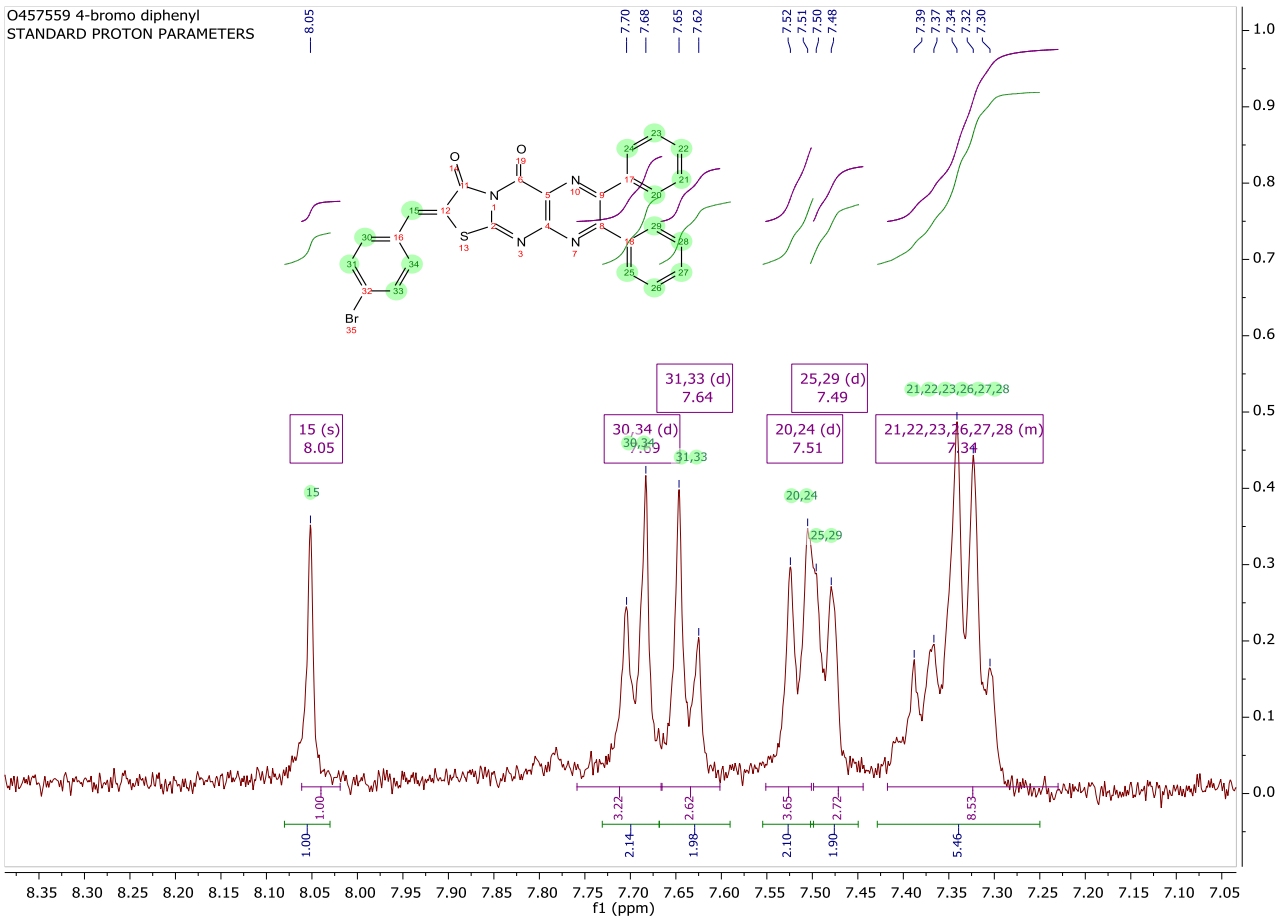


Figure S17 ^{1}H NMR spectra of compound **3.9**

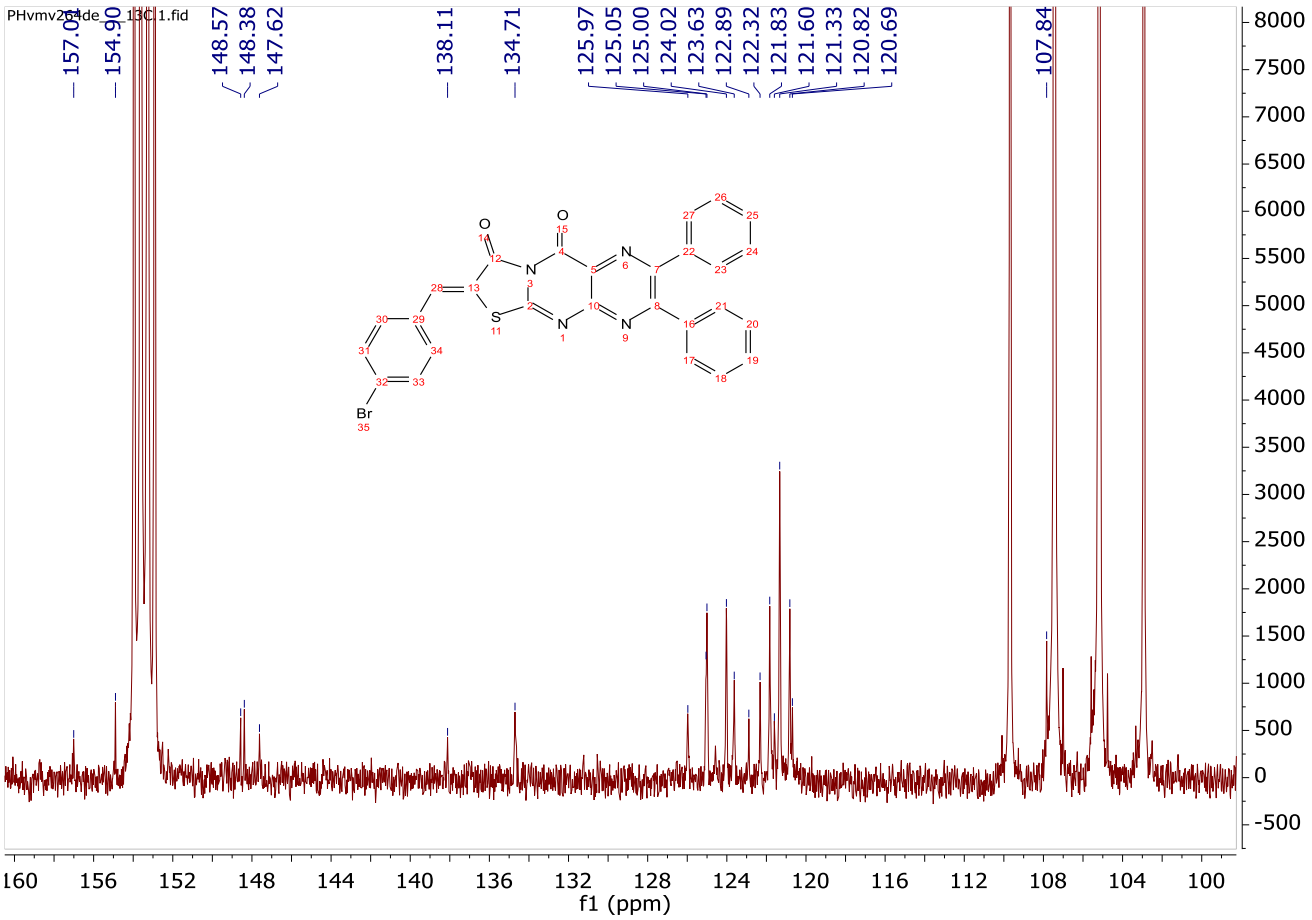


Figure S18 ^{13}C NMR spectra of compound **3.9**

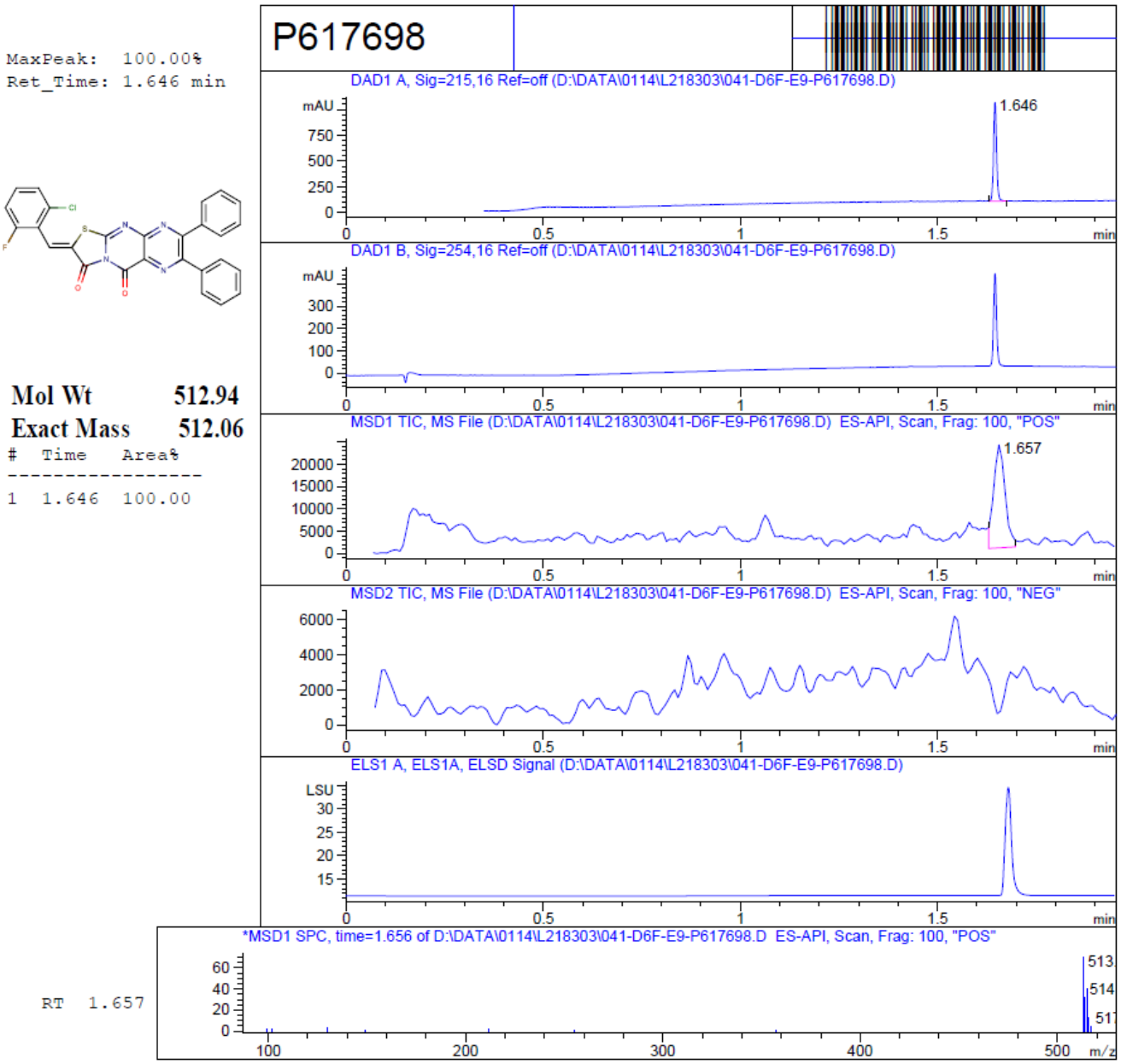


Figure S19 HPLC-MS spectra of compound **3.10**

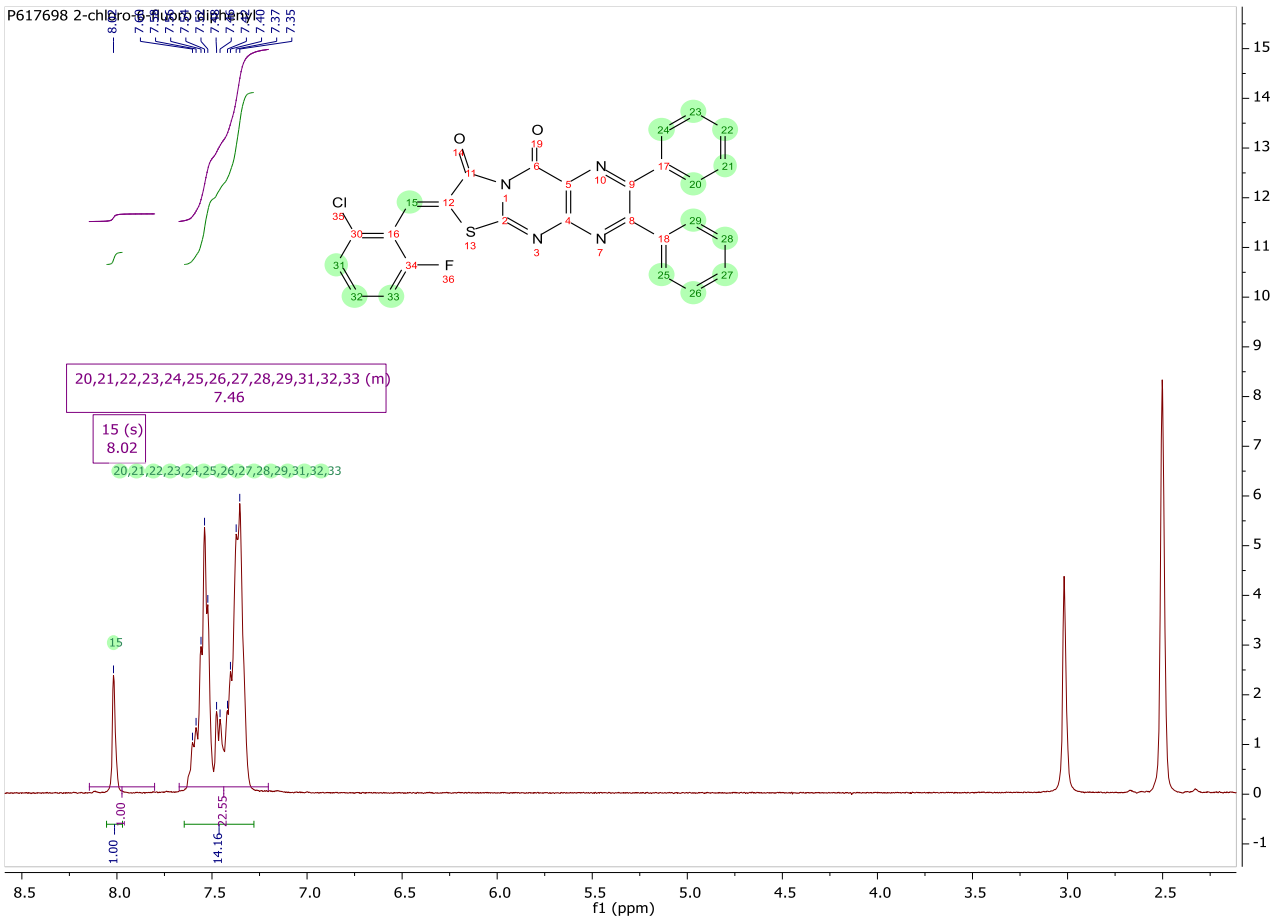


Figure S20 ^{1}H NMR spectra of compound **3.10**

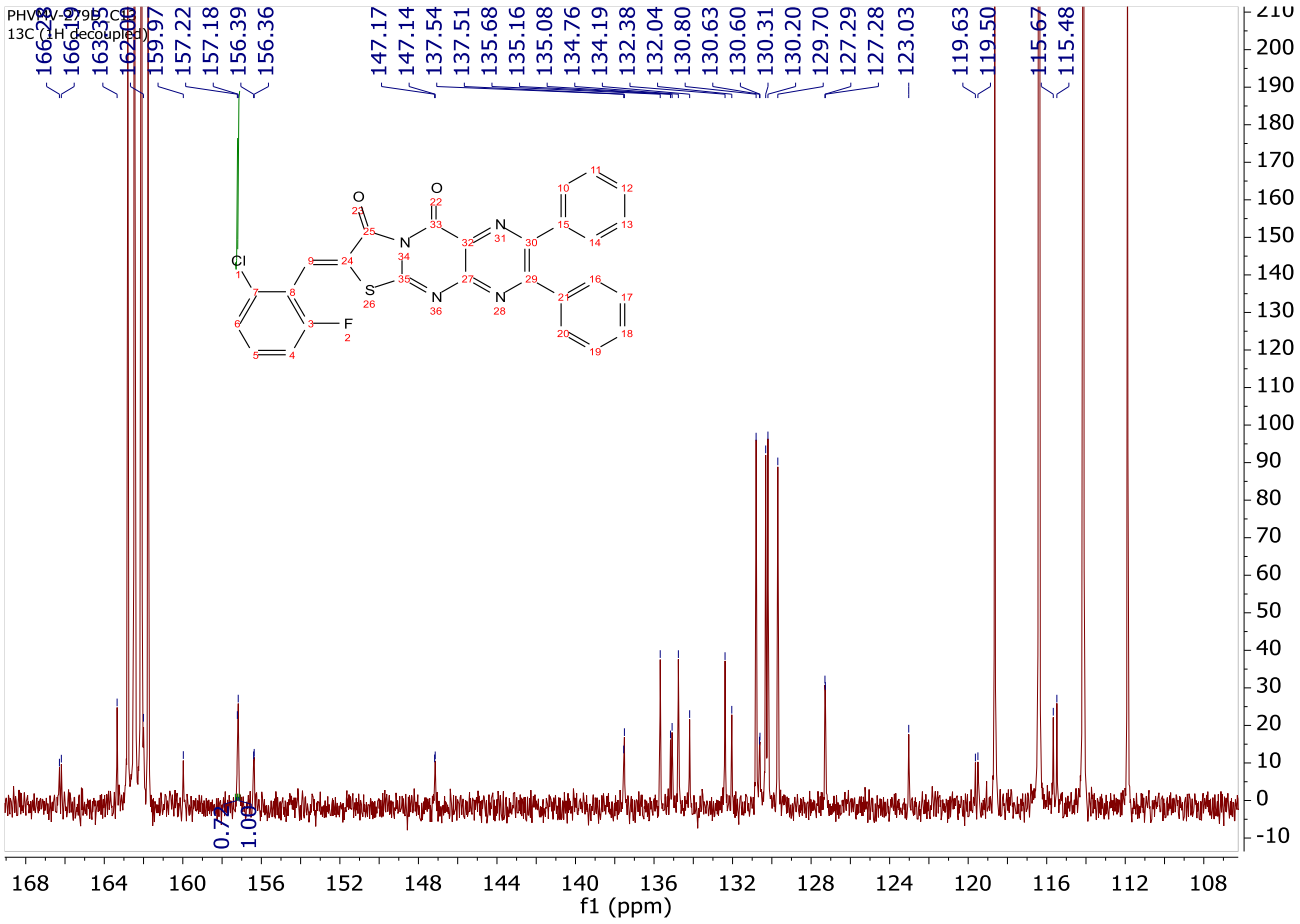


Figure S21 ^{13}C NMR spectra of compound **3.10**

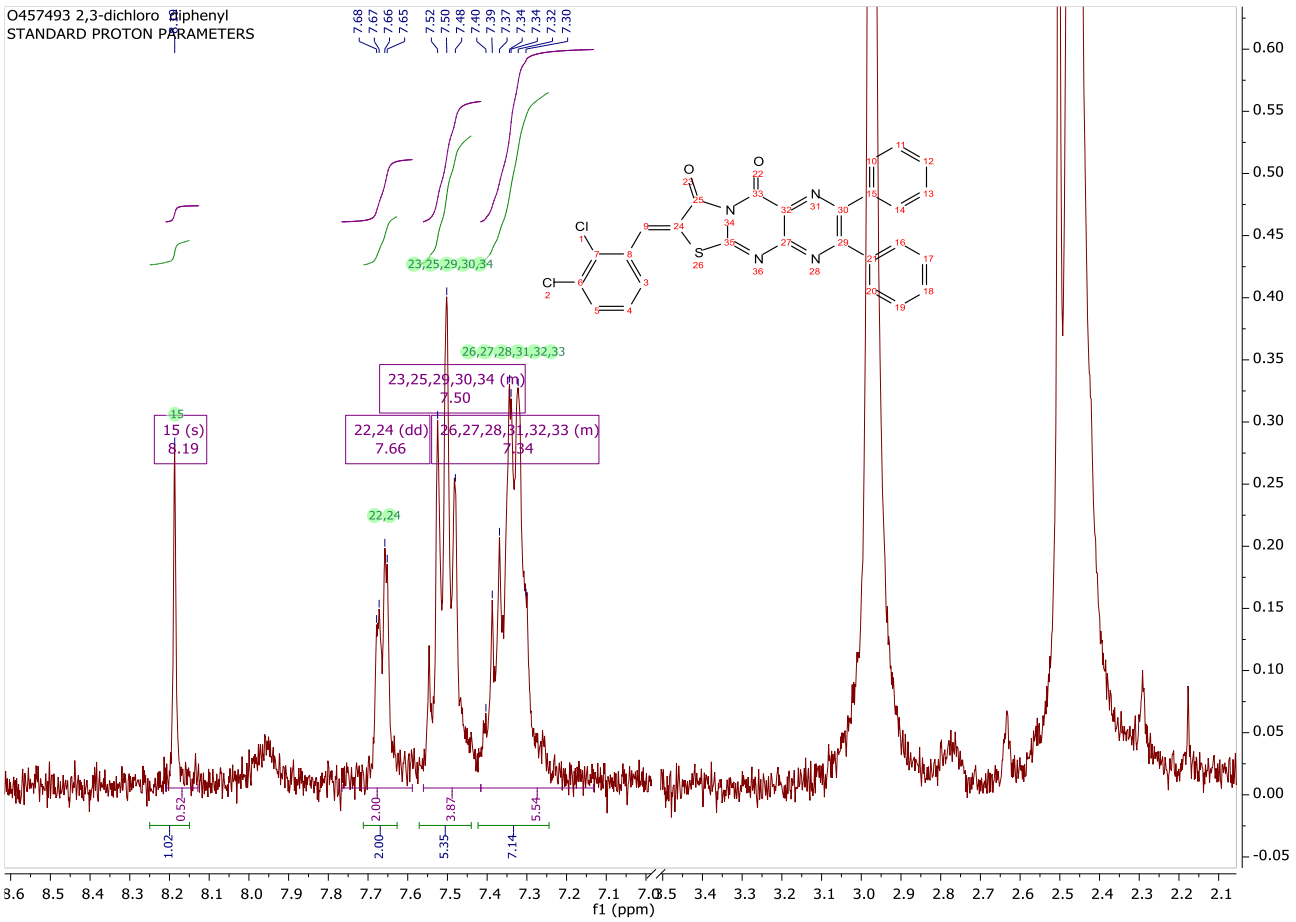


Figure S22 ^{1}H NMR spectra of compound **3.11**

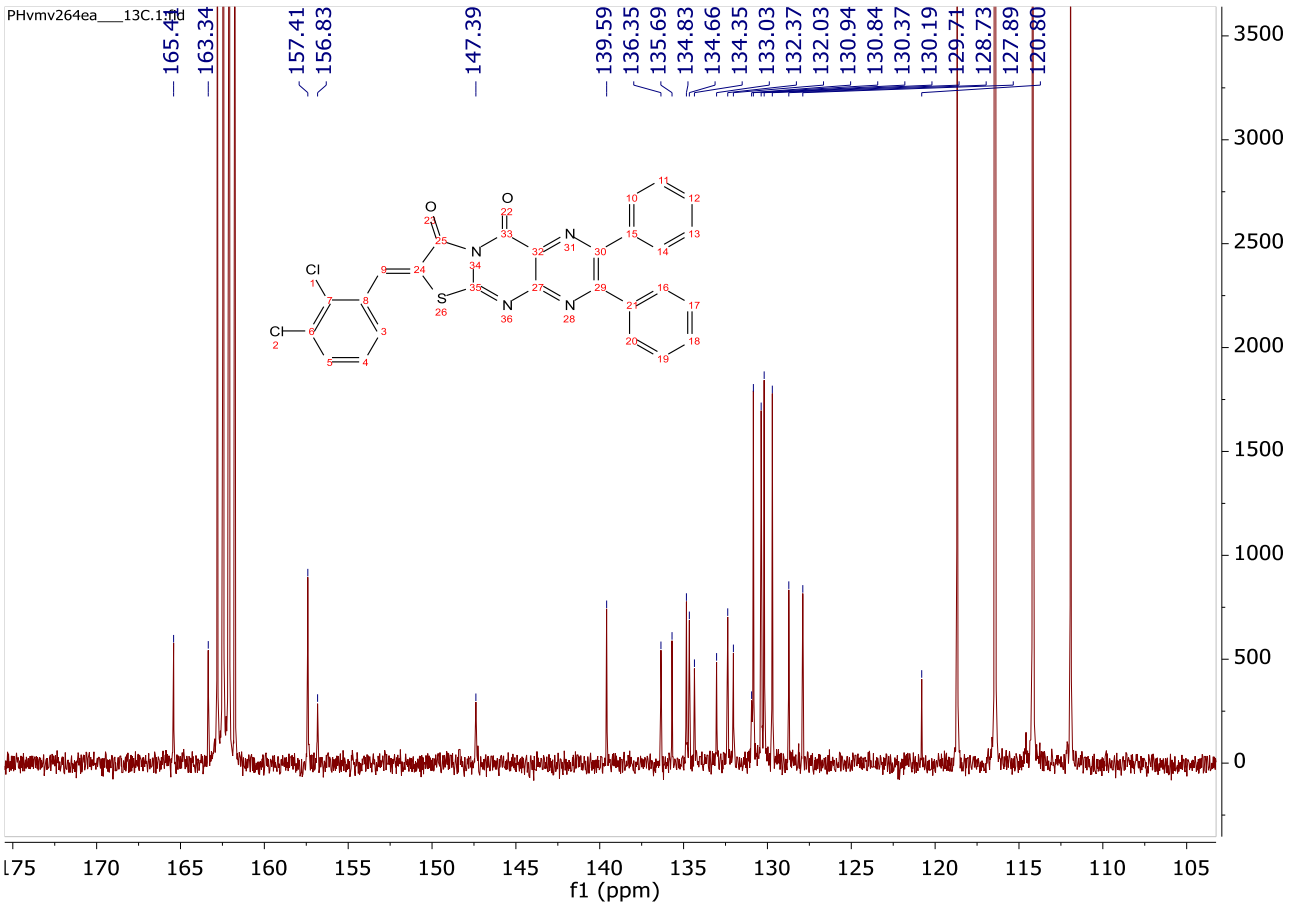


Figure S23 ^{13}C NMR spectra of compound **3.11**

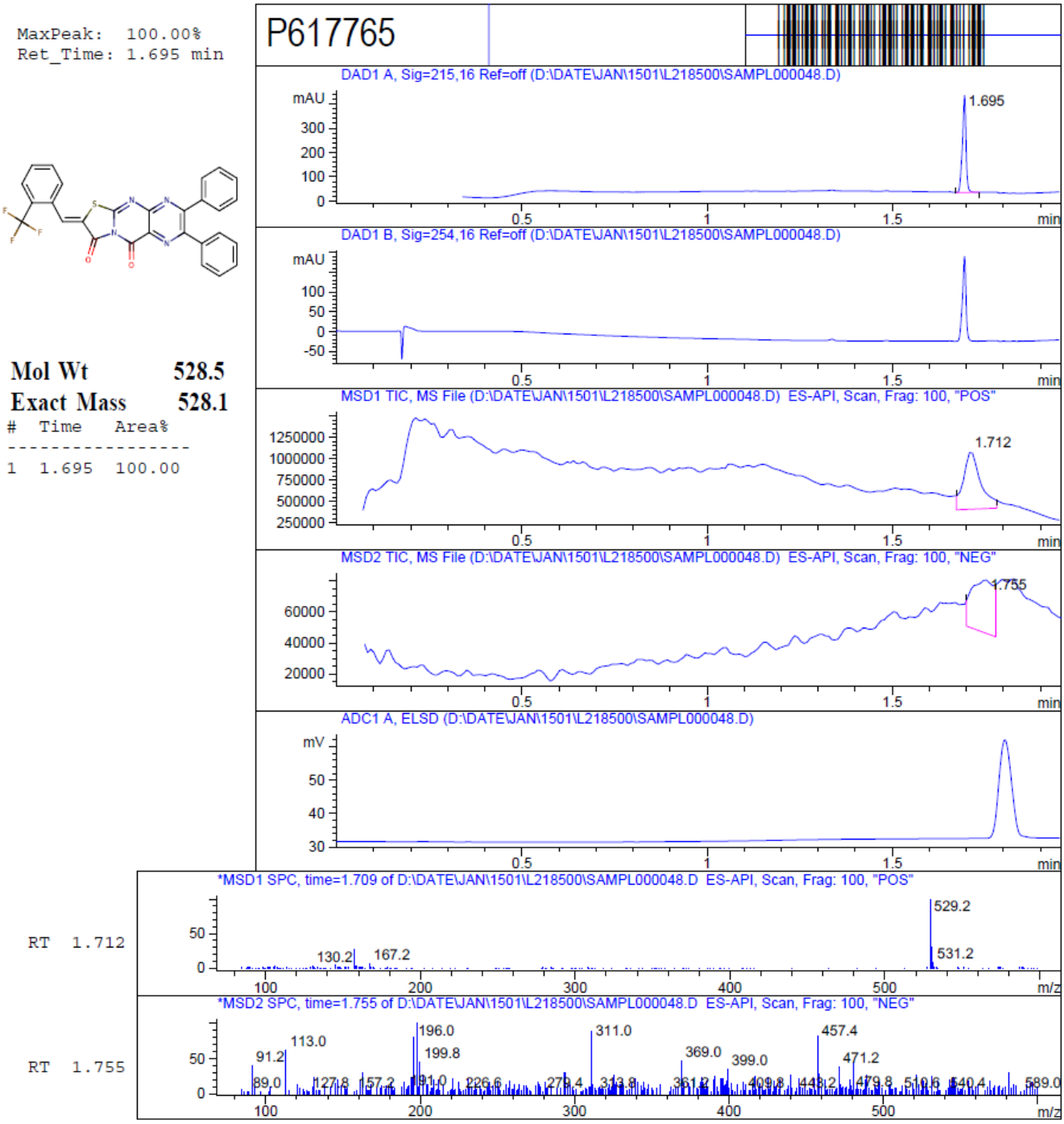


Figure S24 HPLC-MS spectra of compound **3.12**

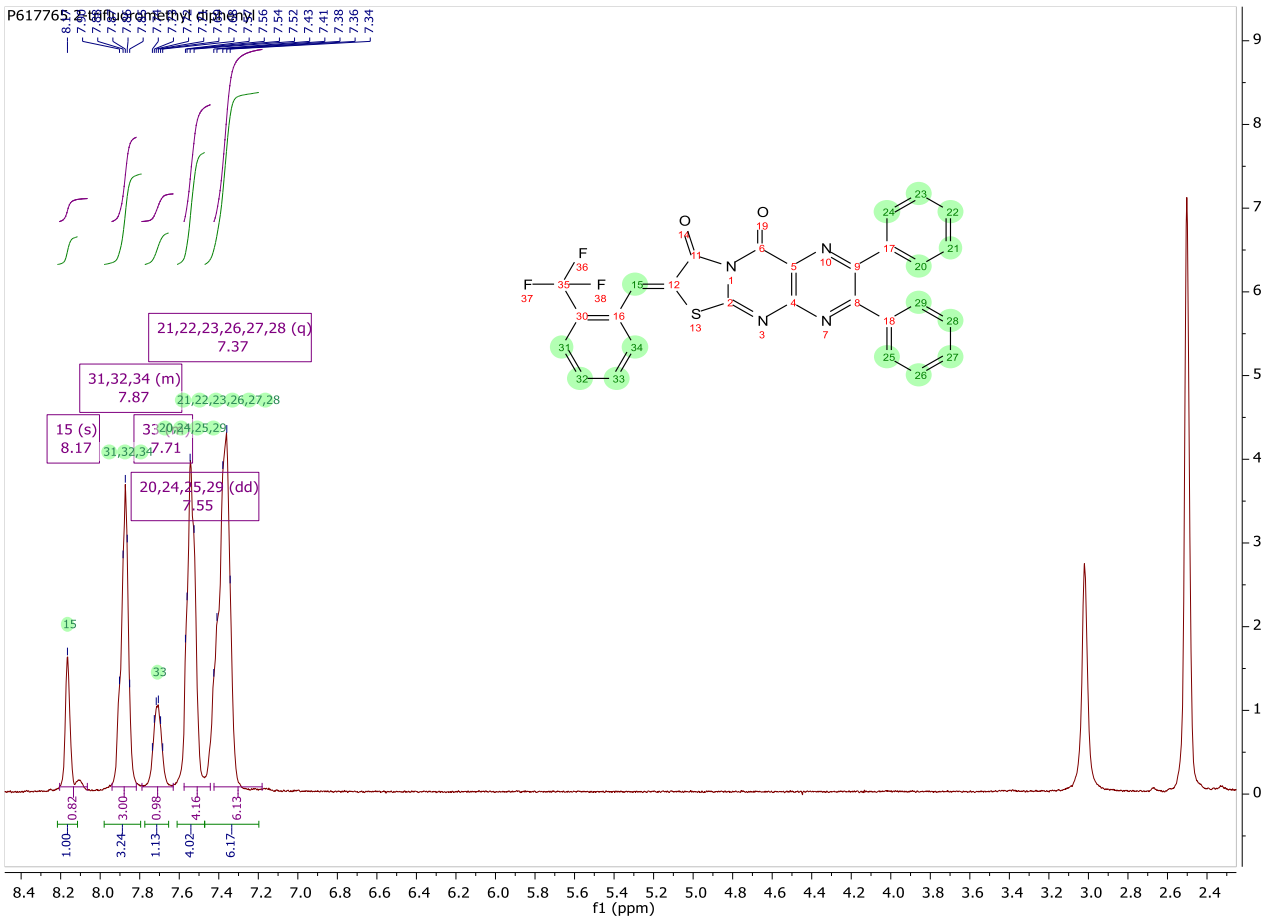


Figure S25 ^{1}H NMR spectra of compound **3.12**

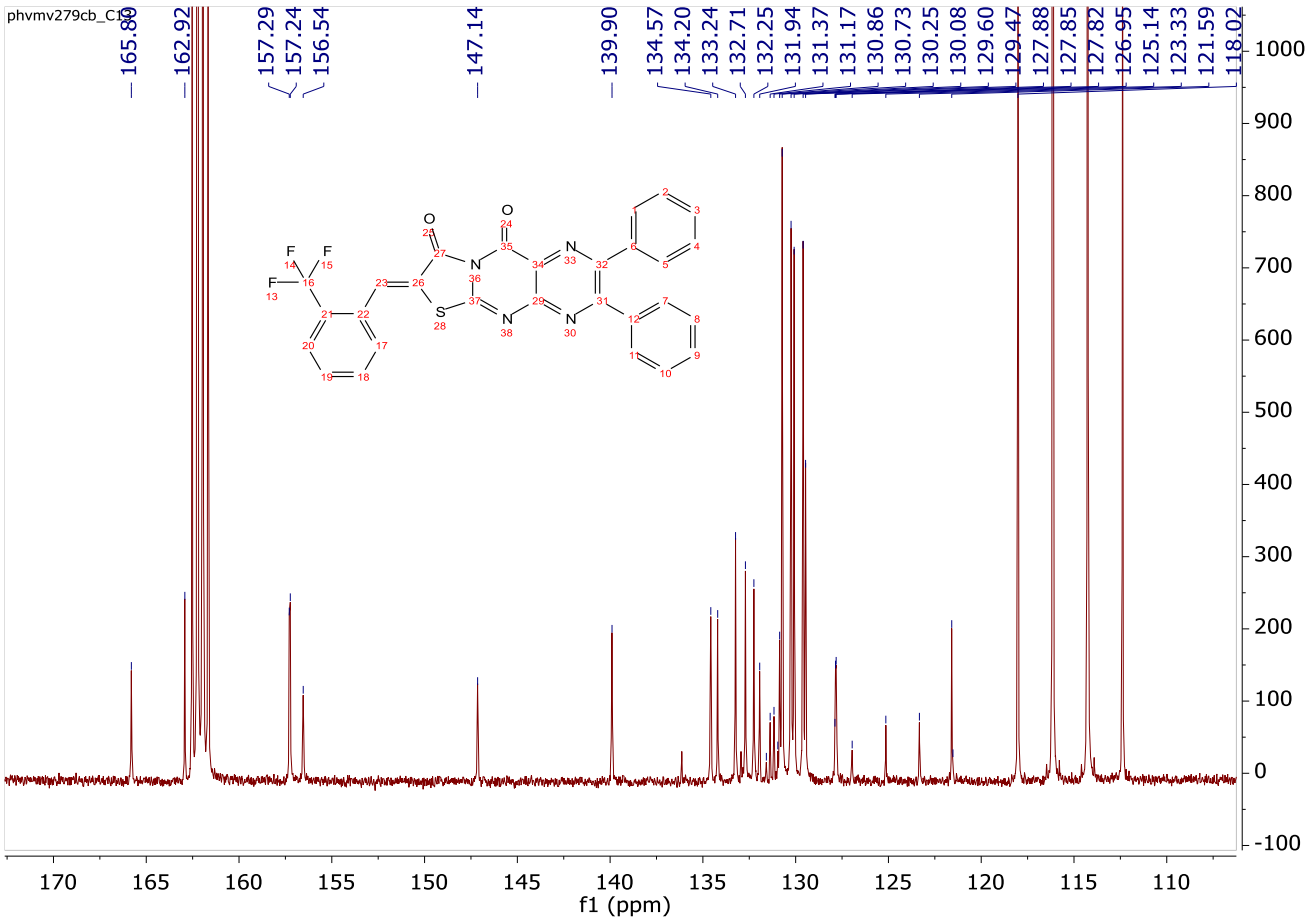


Figure S26 ^{13}C NMR spectra of compound **3.12**

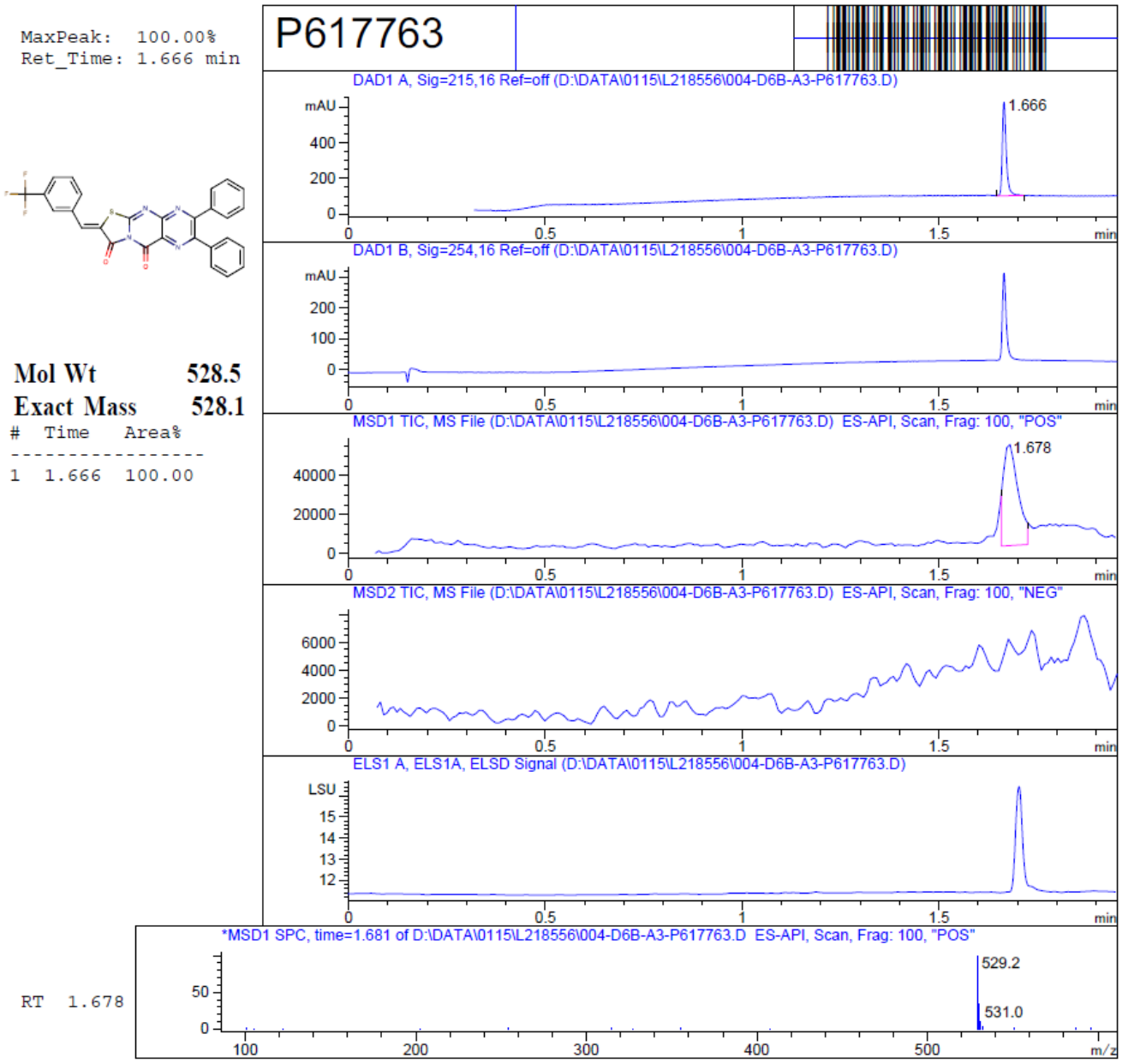


Figure S27 HPLC-MS spectra of compound **3.13**

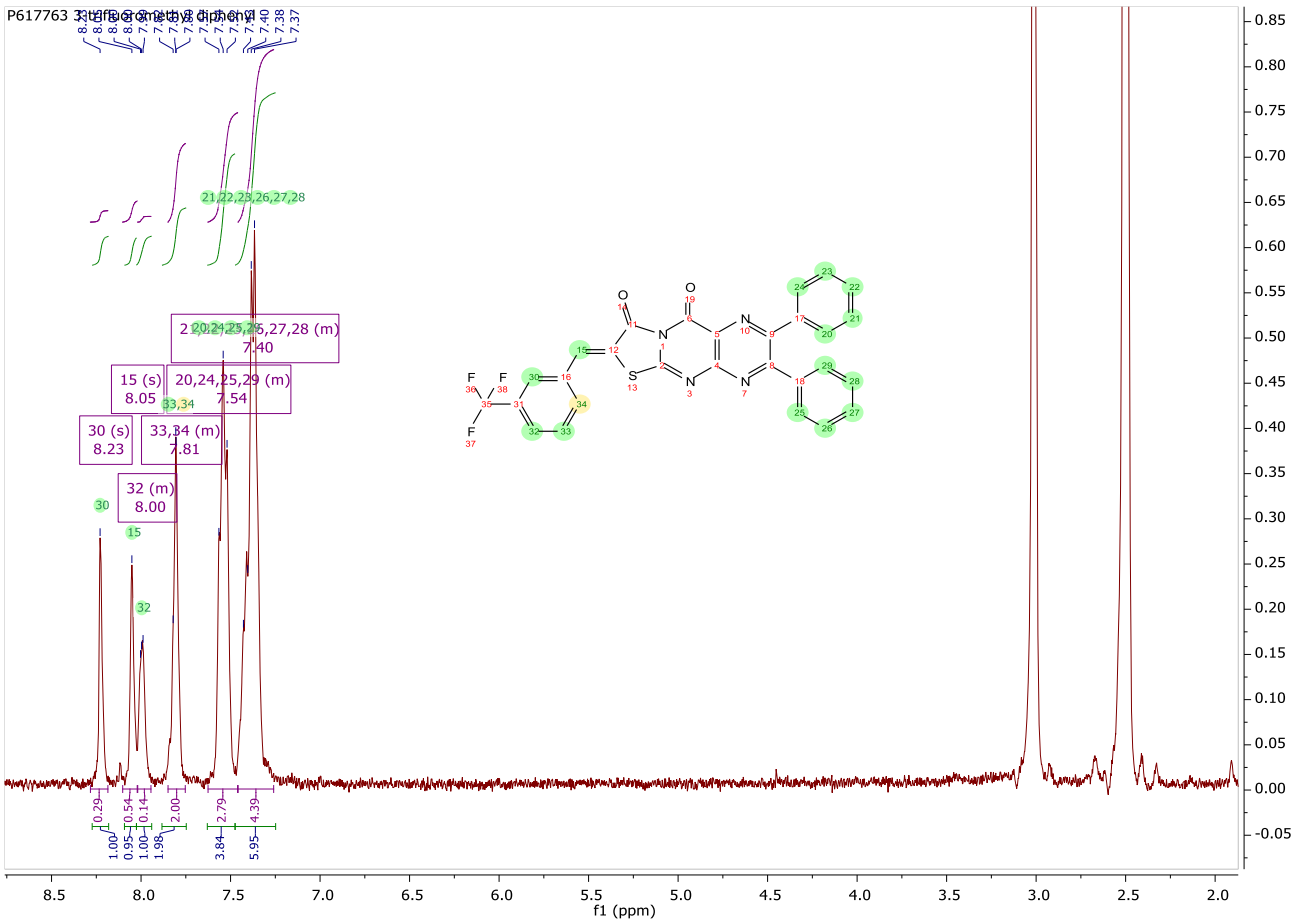


Figure S28 ^{1}H NMR spectra of compound **3.13**

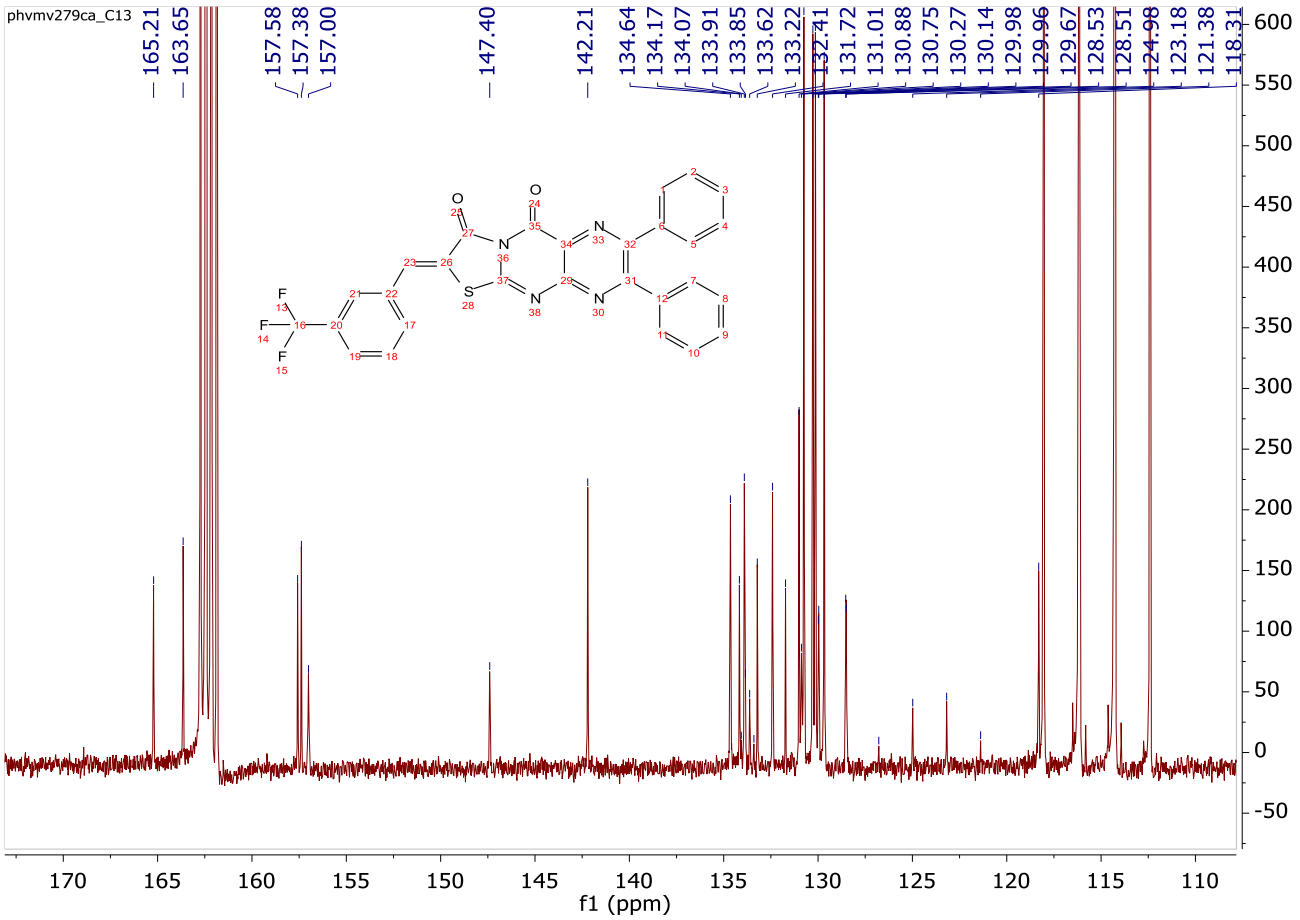


Figure S29 ^{13}C NMR spectra of compound **3.13**

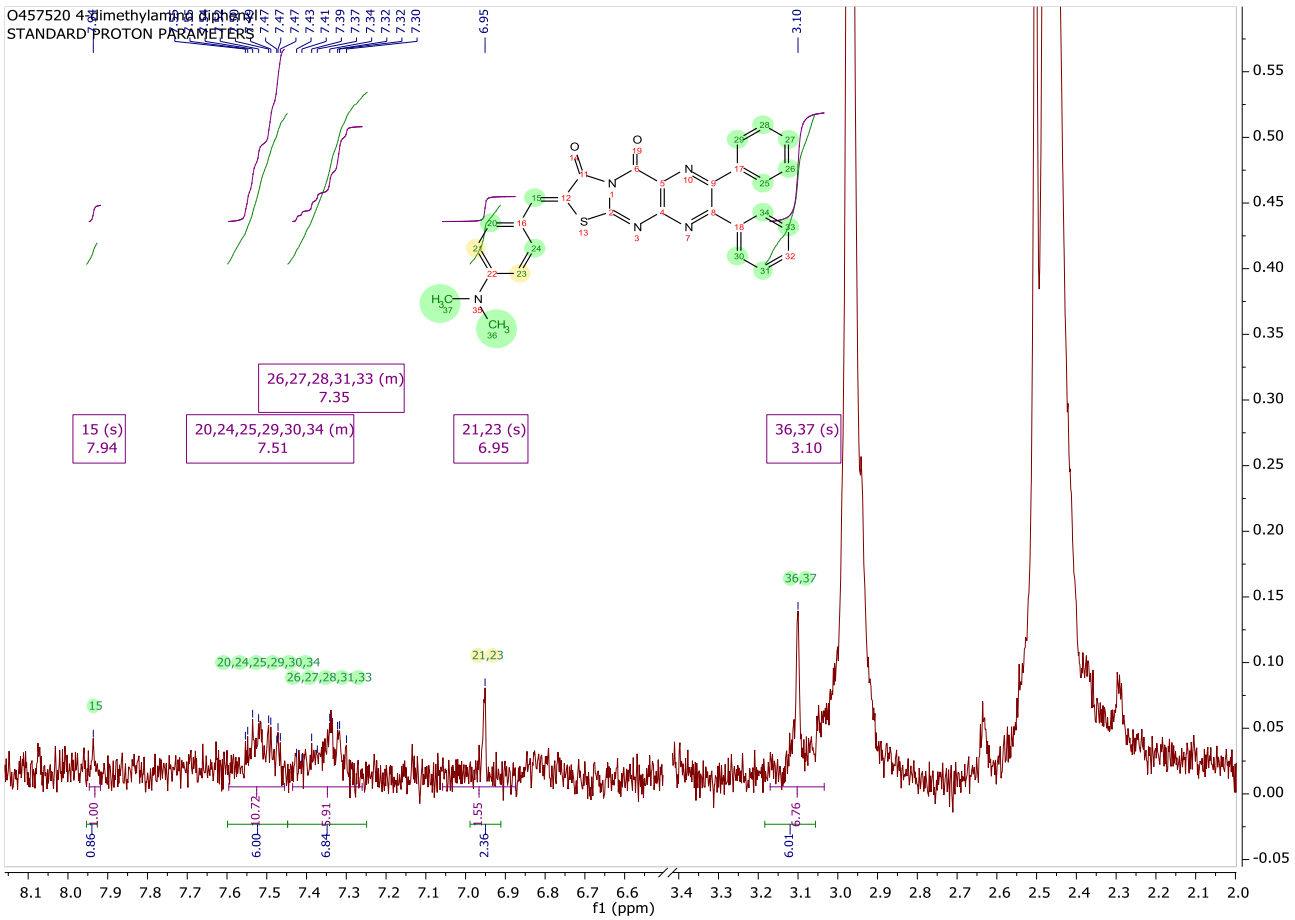


Figure S30 ^{1}H NMR spectra of compound **3.14**

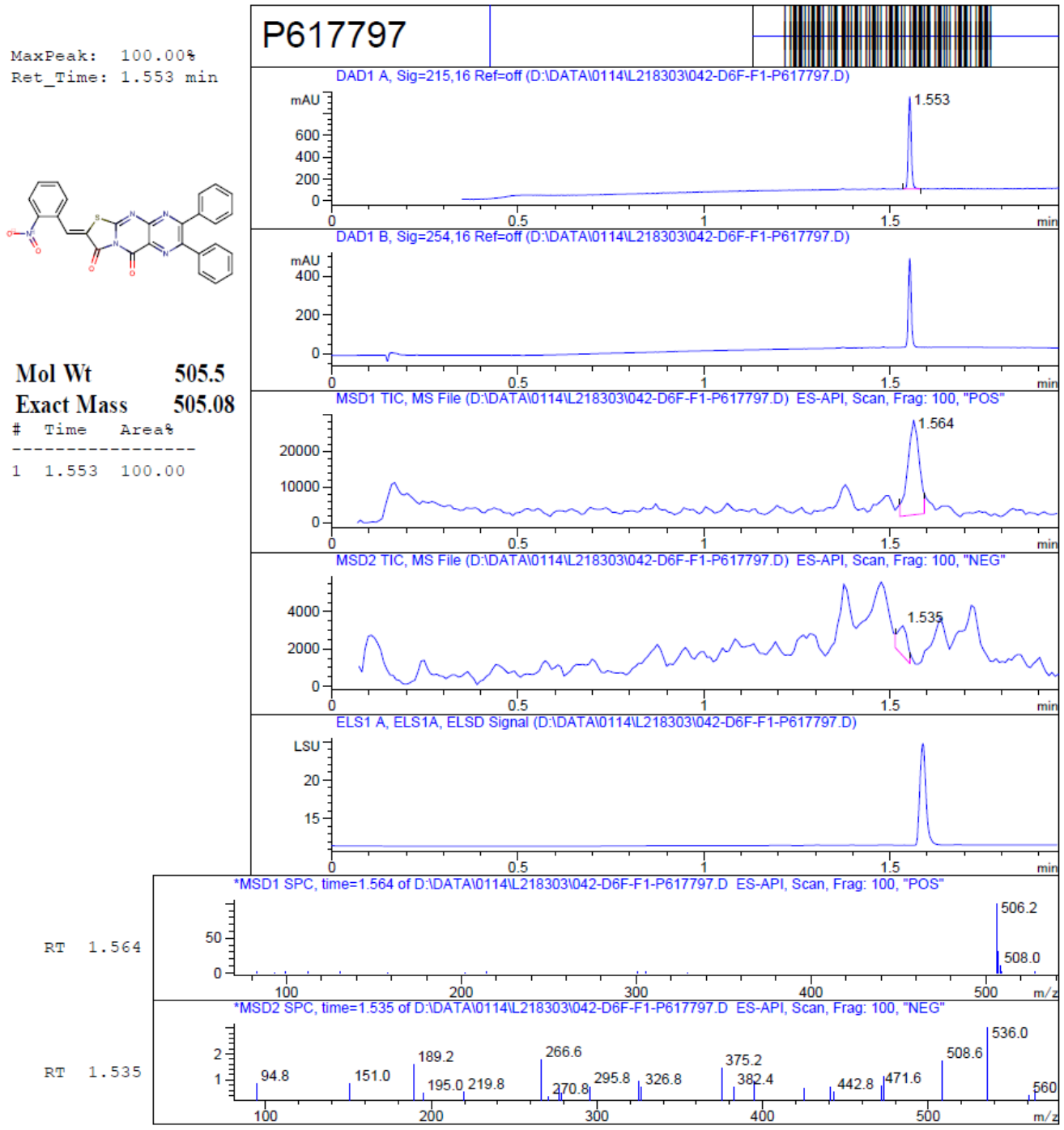


Figure S31 HPLC-MS spectra of compound **3.15**

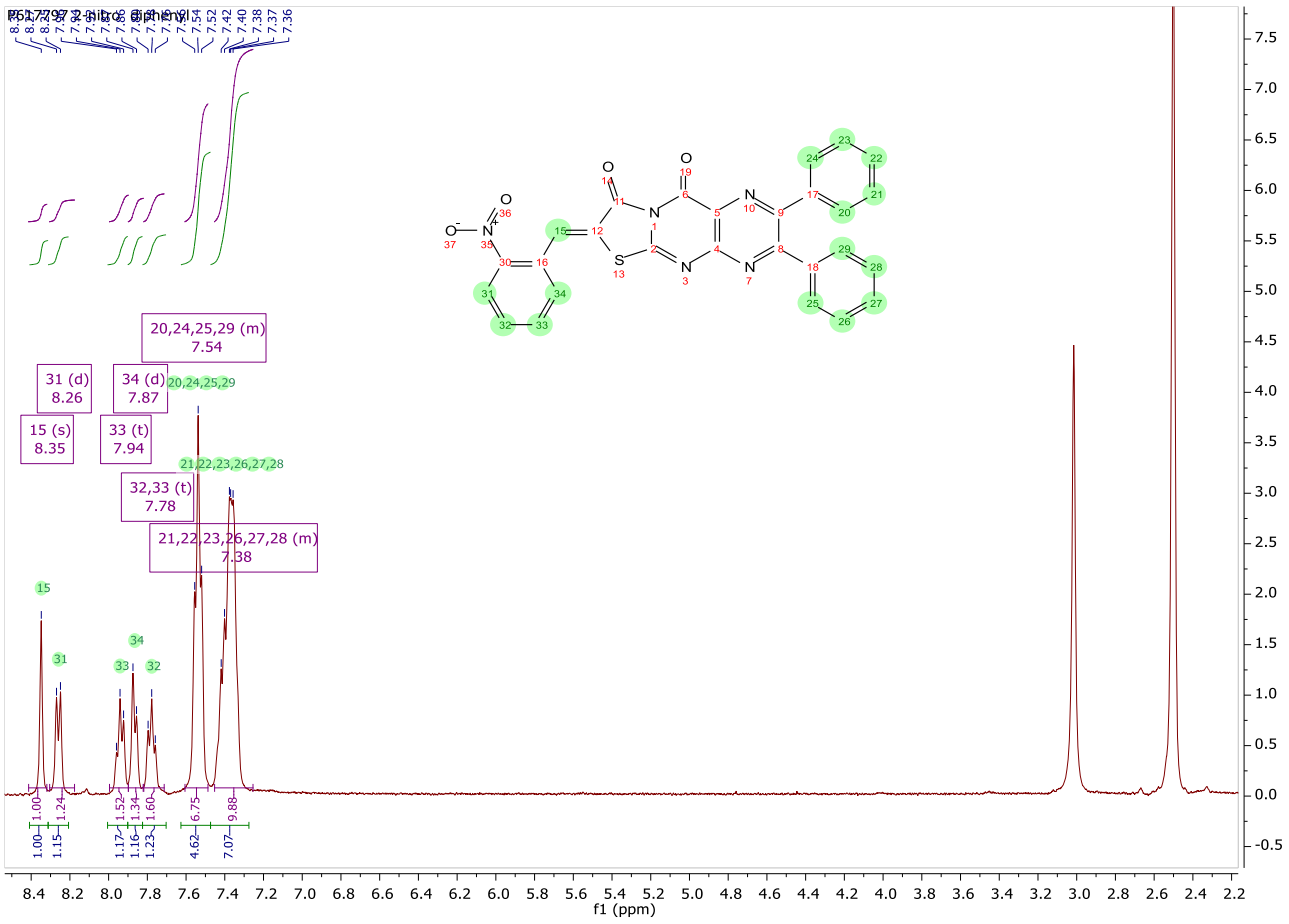


Figure S32 ^{1}H NMR spectra of compound **3.15**

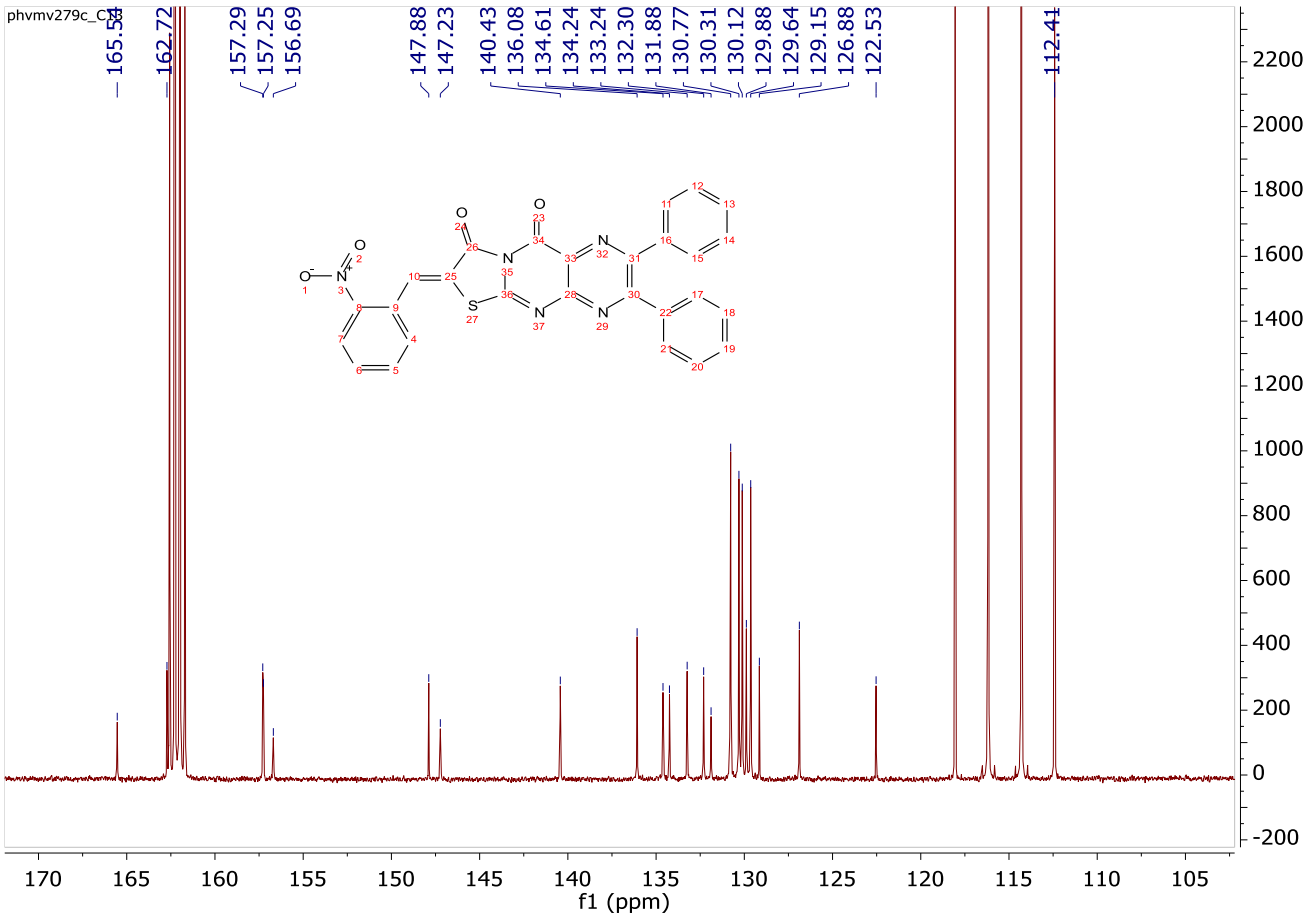


Figure S33 ^{13}C NMR spectra of compound **3.15**

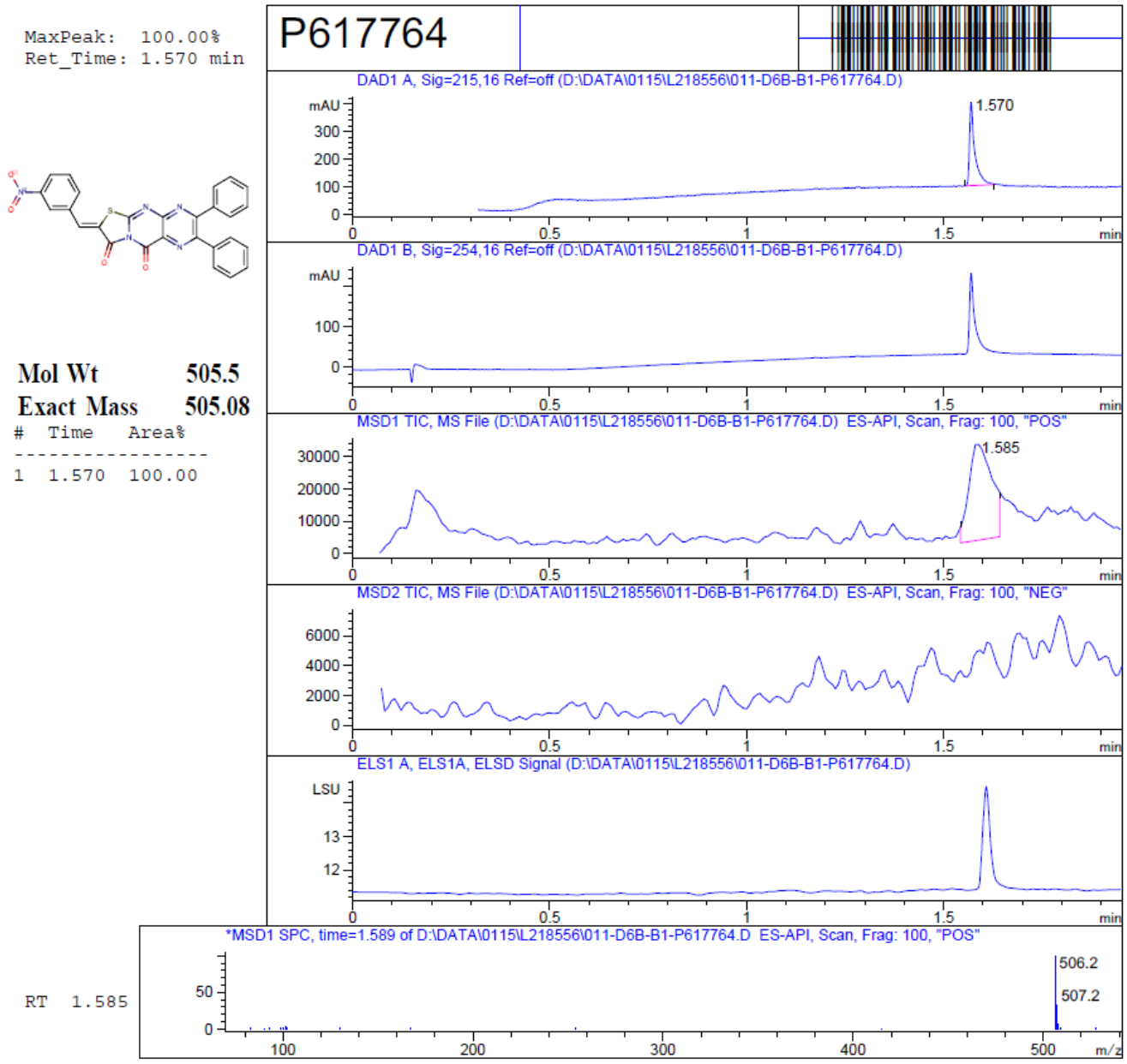


Figure S34 HPLC-MS spectra of compound **3.16**

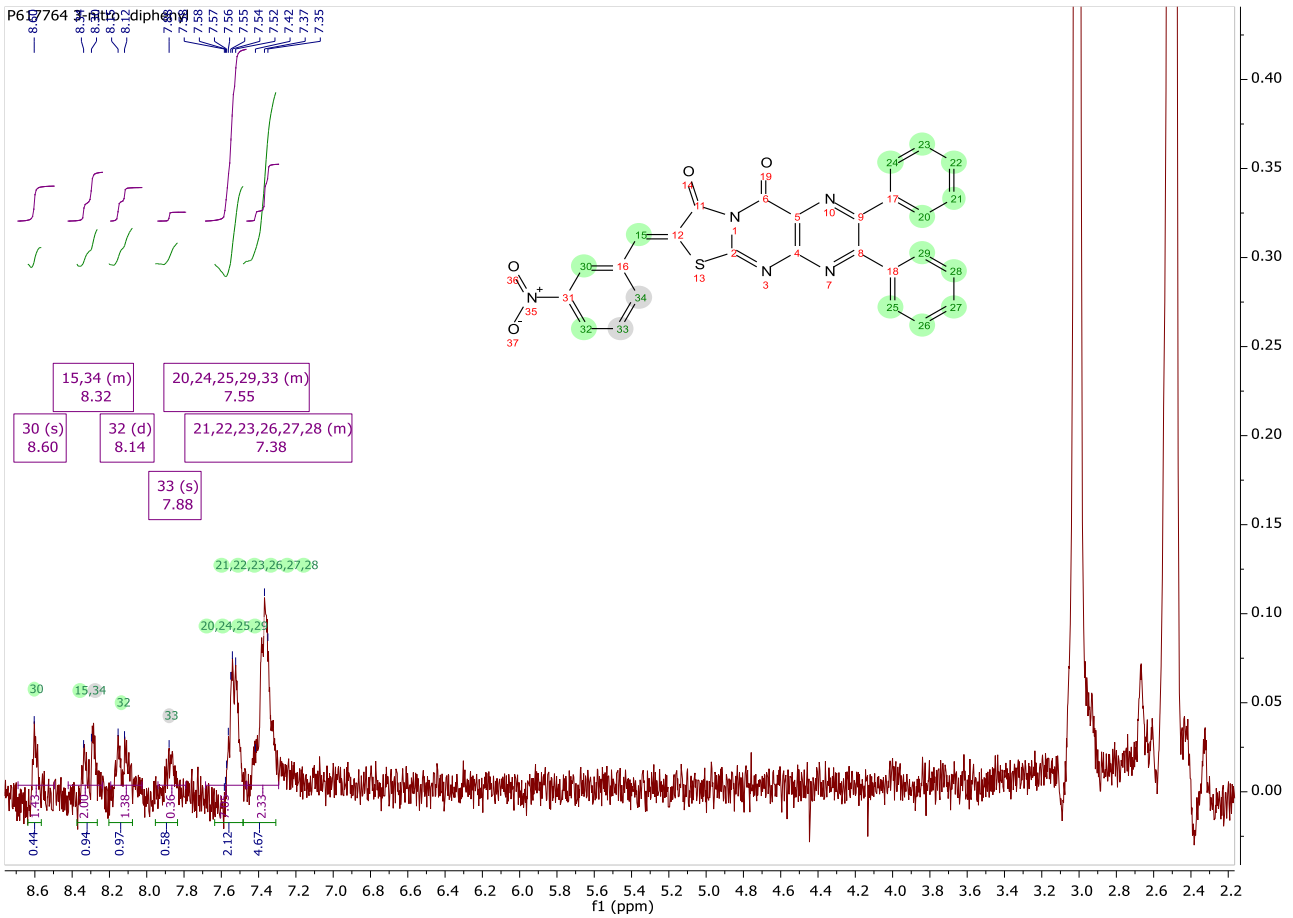


Figure S35 ^{1}H NMR spectra of compound **3.16**

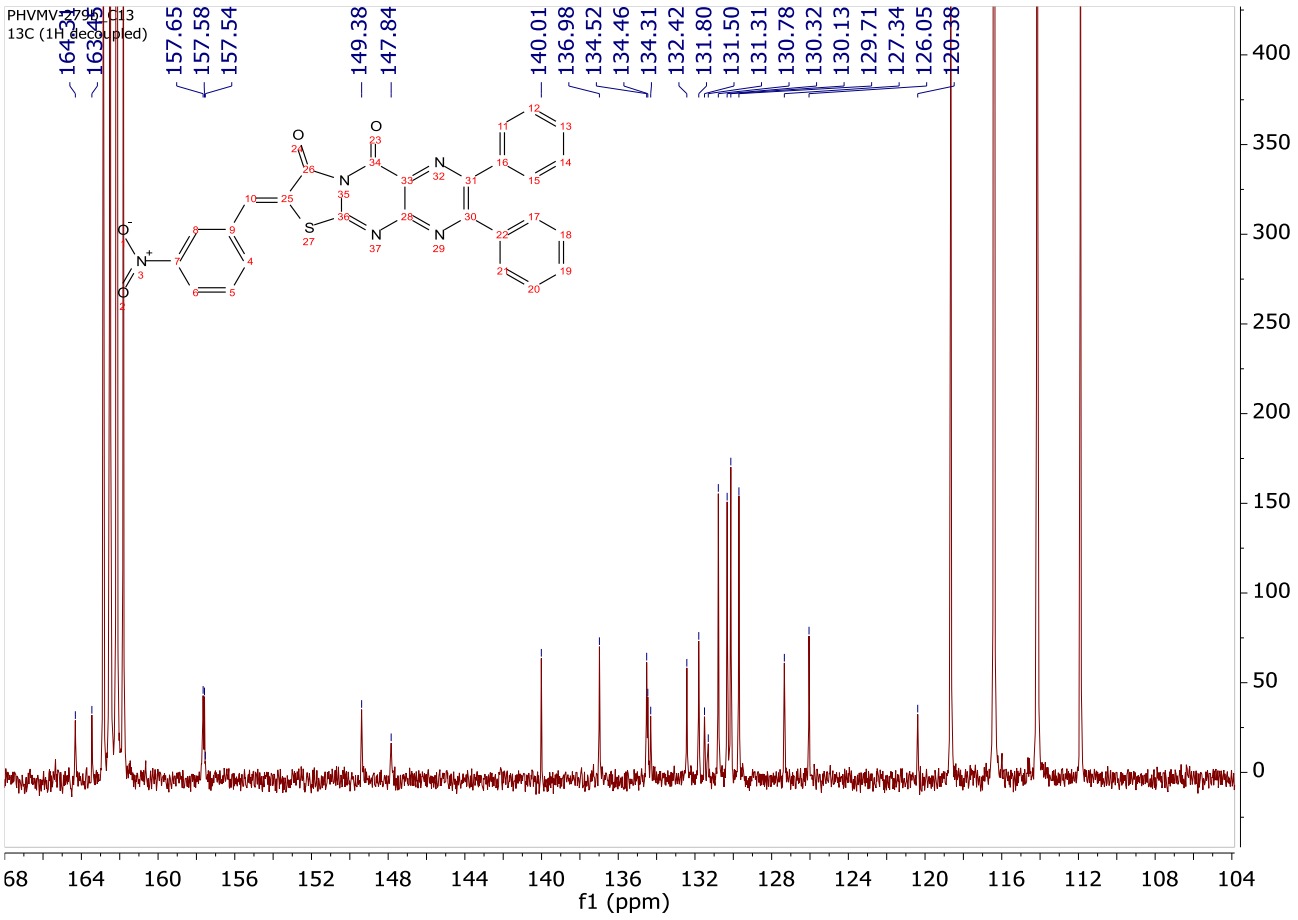


Figure S36 ^{13}C NMR spectra of compound **3.16**

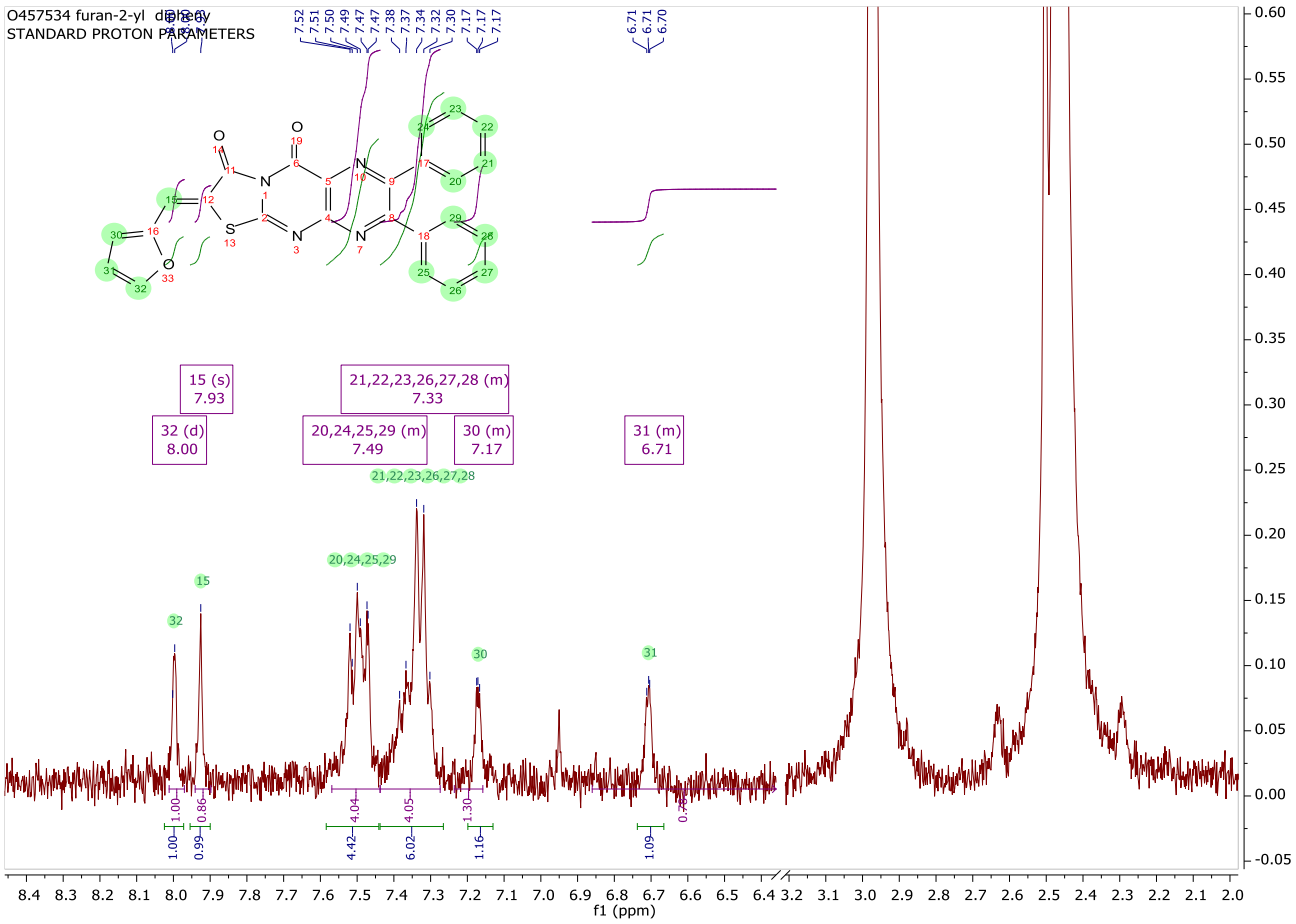


Figure S37 ^{1}H NMR spectra of compound **3.17**

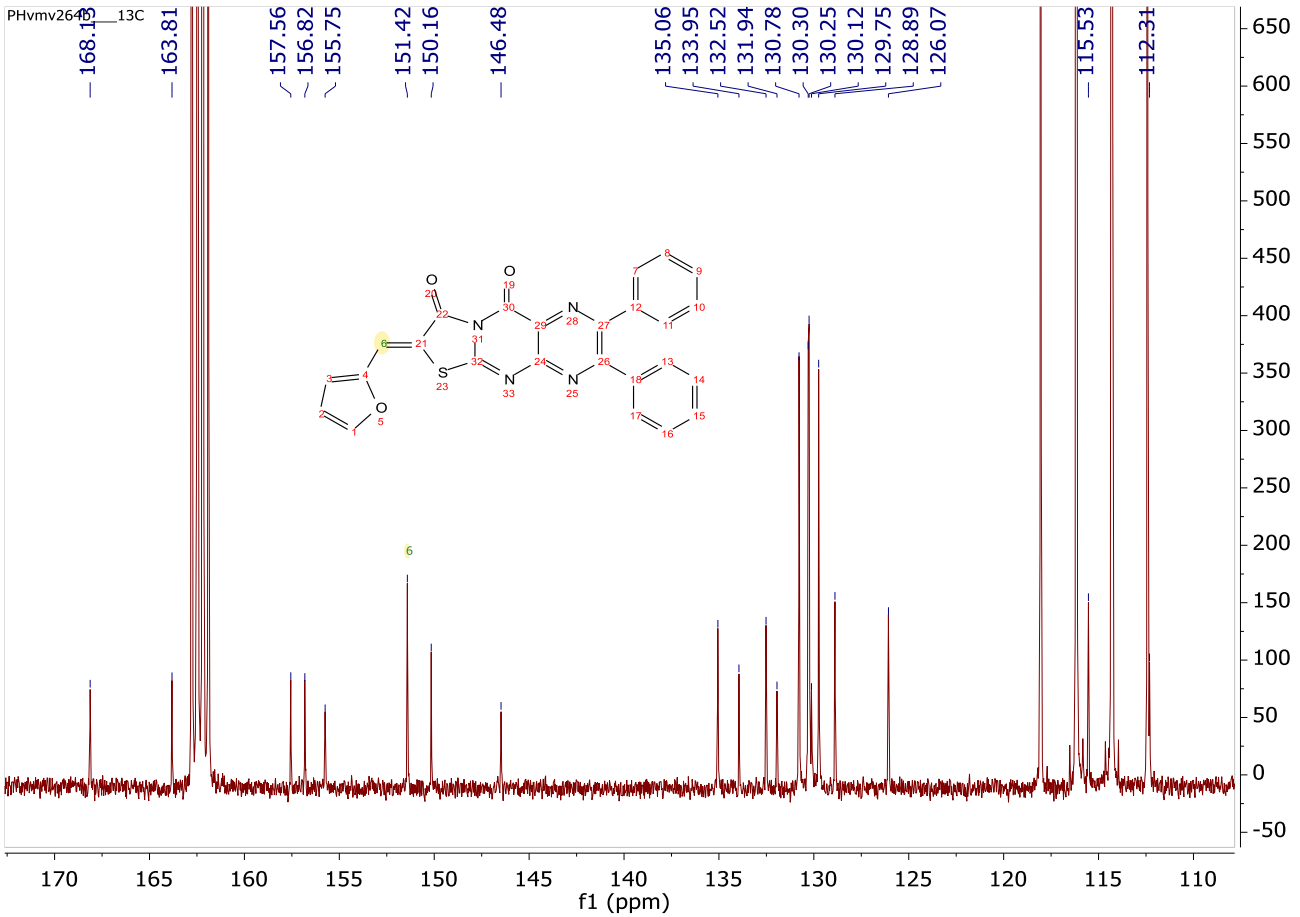


Figure S38 ^{13}C NMR spectra of compound **3.17**

Absorption, fluorescence excitation and emission spectra of compounds 3

Absorption spectra of the compounds were recorded for solutions in acetonitrile. All the absorption spectra were recorded in 1 cm quartz cells at 25 °C using a PerkinElmer Lambda 35 UV/Vis spectrophotometer. Absorption maxima were determined with an accuracy of ±0.5 nm and rounded off.

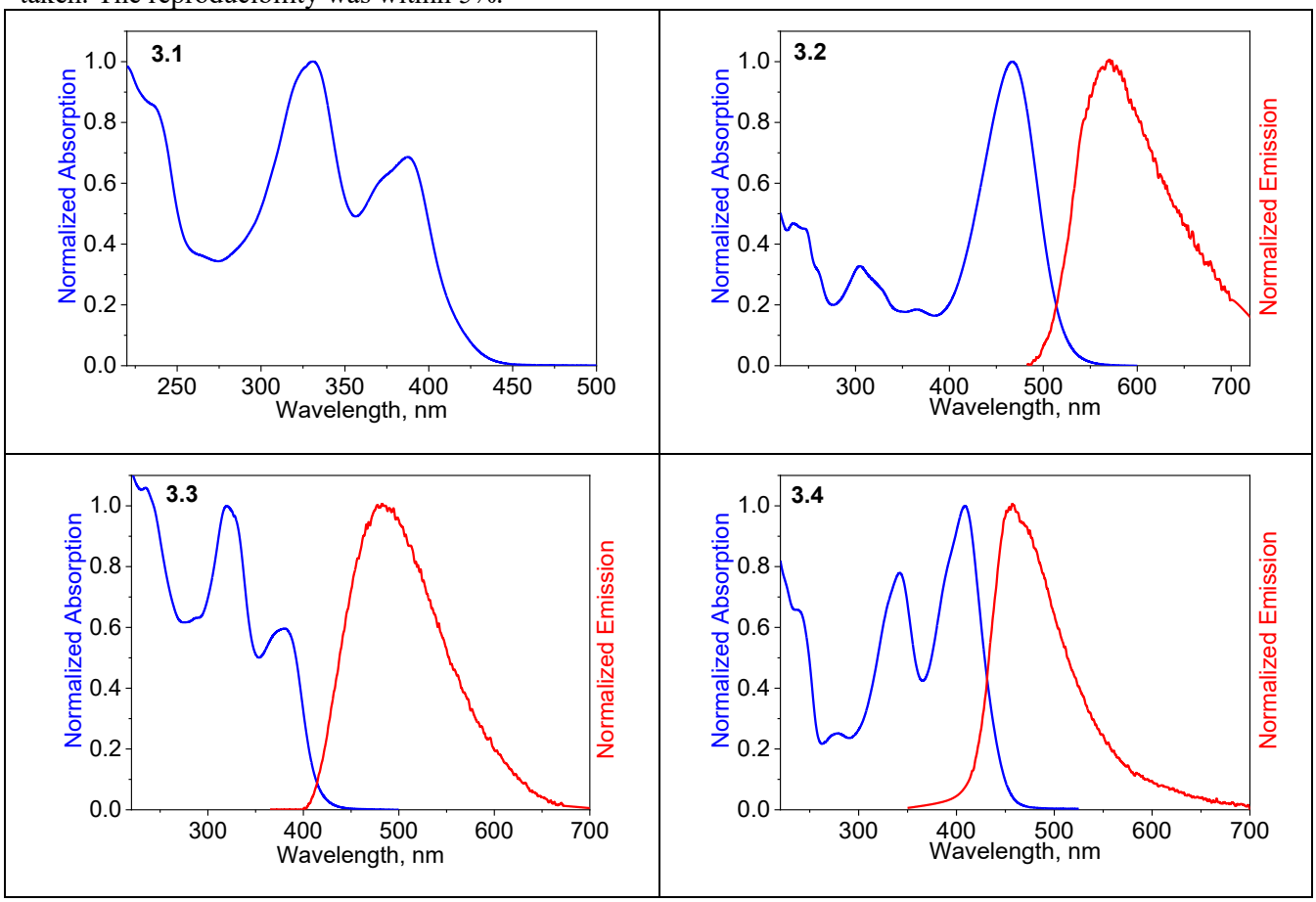
Emission spectra were measured for the dye solution in acetonitrile with absorbance at the excitation wavelength (350 nm) around 0.05. The fluorescence measurements were done in 1 cm standard quartz cells at 25 °C using a Varian Cary Eclipse spectrofluorometer. The emission spectra were corrected for the wavelength-dependent instrument sensitivity. Emission maxima were determined with an accuracy of ±1.0 nm.

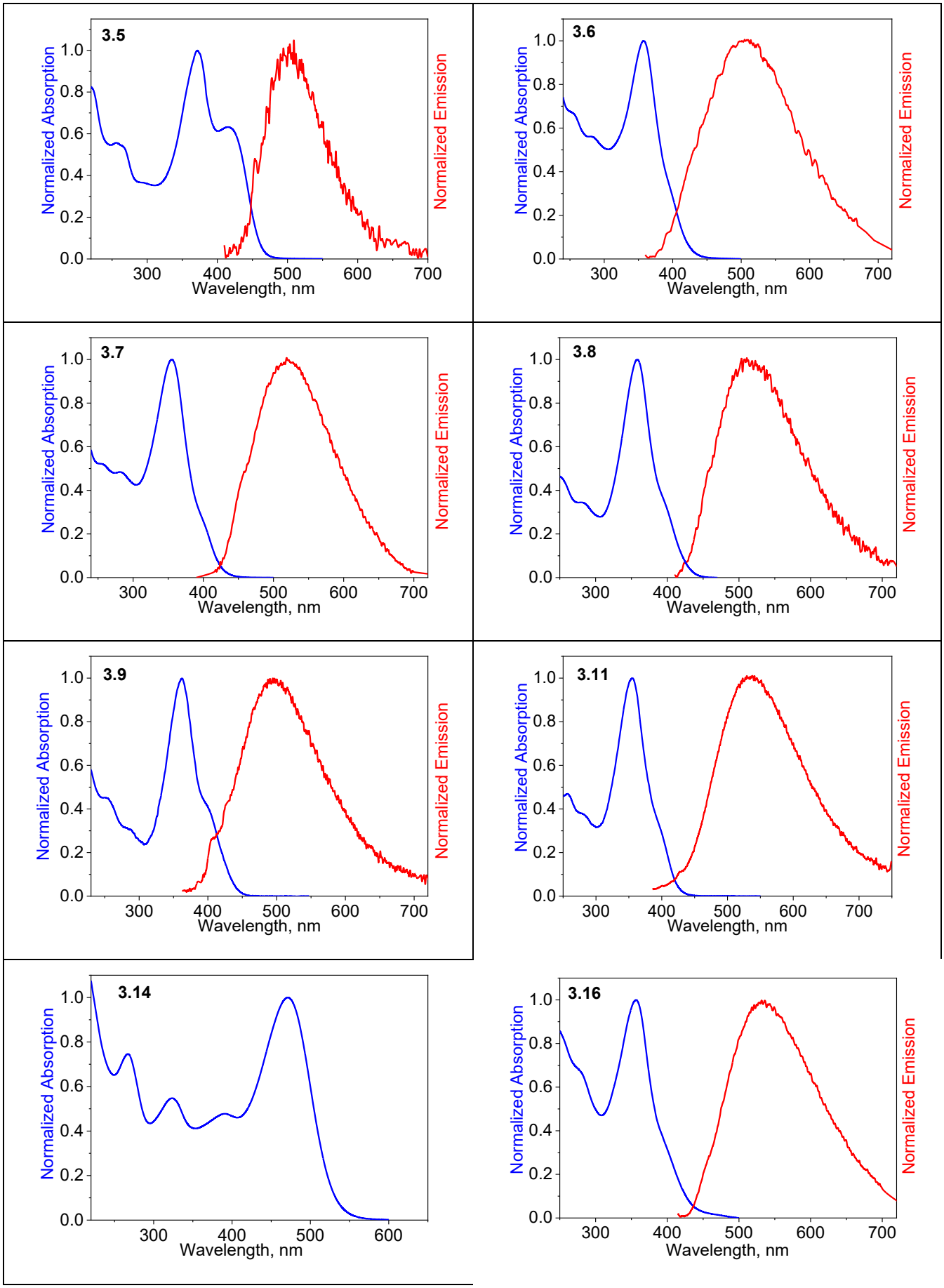
Fluorescence quantum yields (Φ_F). The integrated relative intensities of the dyes were measured in 1 cm cells against Quinine in 0.1 M H_2SO_4 as the reference. The quantum yields were calculated according to Equation S1.

$$\Phi_F = \Phi_{F,ref} \times (F / F_{ref}) \times (A_{ref} / A) \times (n_{D(media)}^2 / n_{D(media,ref)}^2), \qquad \text{(Equation S1)}$$

where $\Phi_{F,ref}$ is the quantum yield of Quinine ($\Phi_{F,ref}$ = 54.6% in 0.1 M H_2SO_4), F_{ref} and F are the areas (integral intensities) of the emission spectra ($F = \int I(\lambda)d(\lambda)$) of Quinine and the dye under examination, respectively; A_{ref} and A are the absorbencies at the excitation wavelength of Quinine and the dye under examination, respectively; $n_{D(media,ref)}$ and $n_{D(media)}$ are the refractive indices of the solvent, where the reference Quinine and the dye under examination are dissolved, respectively.

The quantum yield of each sample was independently measured 3–4 times and the average value was taken. The reproducibility was within 5%.




3.5
3.6
3.7
3.8
3.9
3.11
3.14
3.16
Normalized Absorption
Normalized Emission
Wavelength, nm
0.0
0.2
0.4
0.6
0.8
1.0
300
400
500
600
700

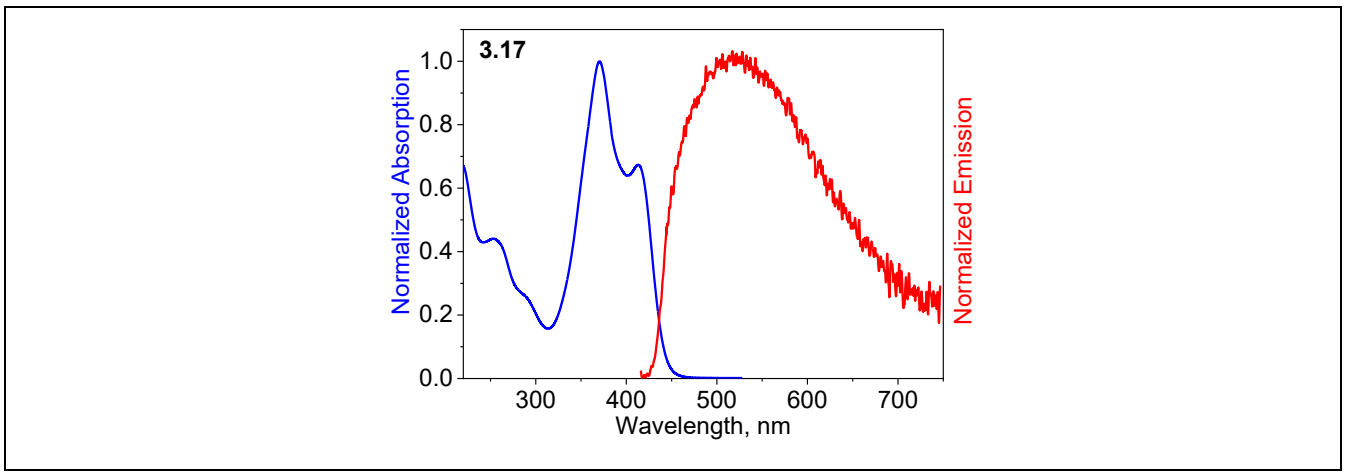
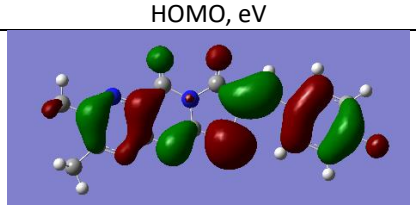
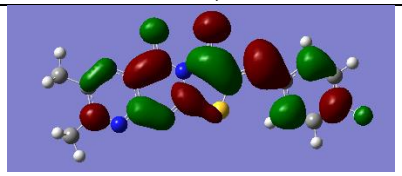
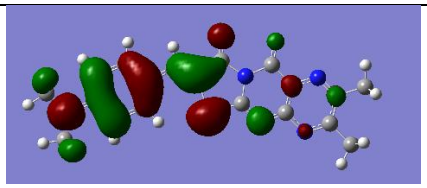
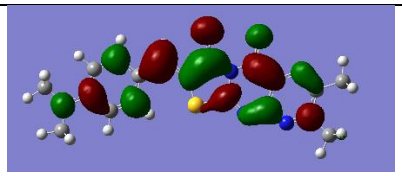
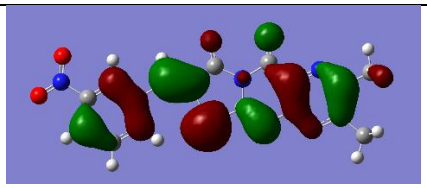
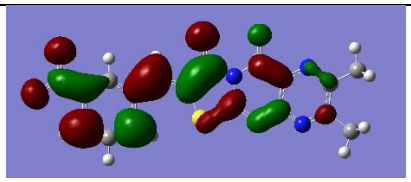
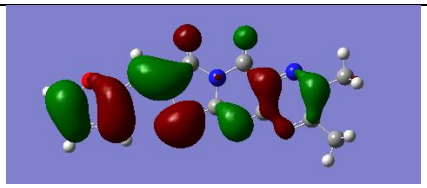
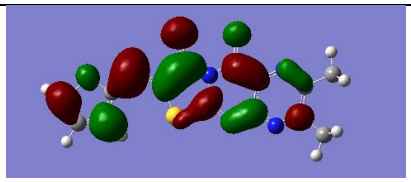
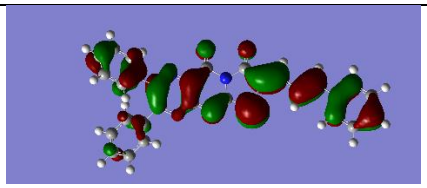
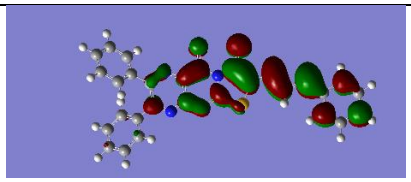
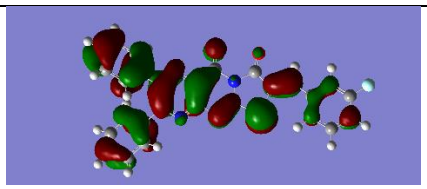
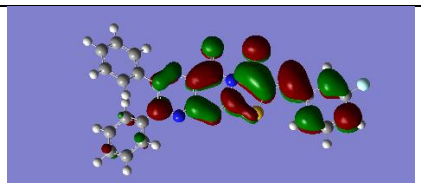
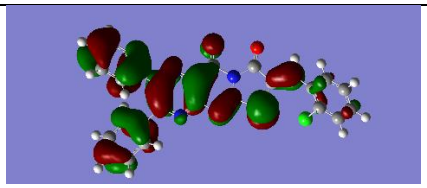
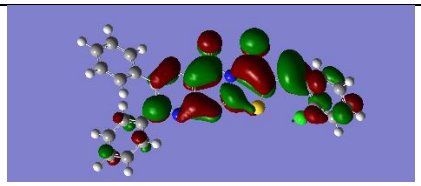
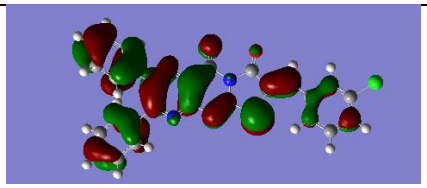
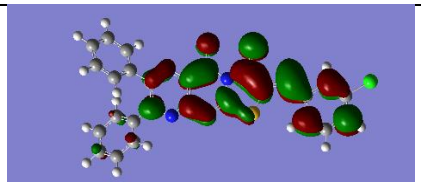


Figure S39. Absorption (blue line) and fluorescence (red line) spectra of 7-aryl-(hetaryl)iden-10*H*-thiazolo[2,3-*b*]pteridine-8,10(7*H*)-diones (**3**) in acetonitrile.

DFT calculations for compounds 3.

The structure of the synthesized compounds was optimized using the Gaussian 16 program, and the results were visualized using GaussView 6.1. In all the structures studied, the geometry was optimized using density functional theory (DFT) using the B3LYP approximation with the standard 6-311G++(d,p) basis set.

Compond.	HOMO, eV	LUMO, eV
3.1	 -6.561	 -3.026
3.2	 -5.680	 -2.564
3.3	 -6.886	 -3.418
3.4	 -6.363	 -2.996
3.5	 -6.180	 -3.103
3.6	 -6.460	 -3.144
3.7	 -6.418	 -2.975
3.8	 -6.463	 -3.151

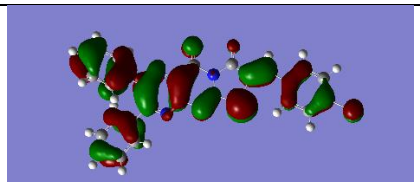
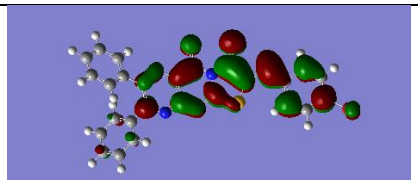
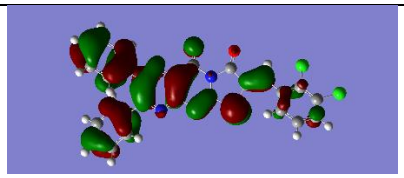
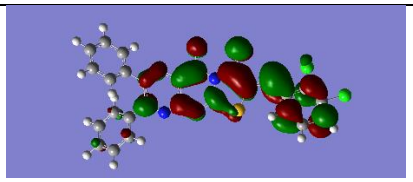
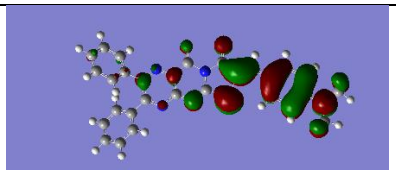
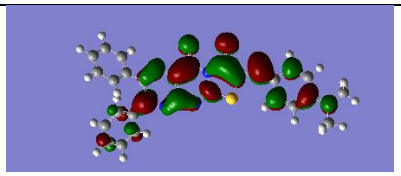
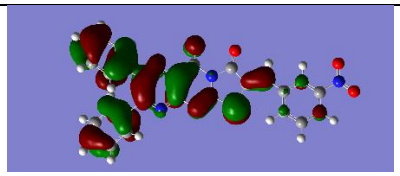
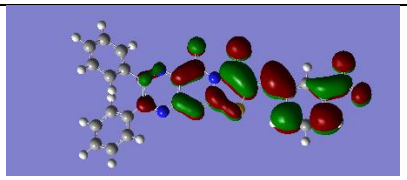
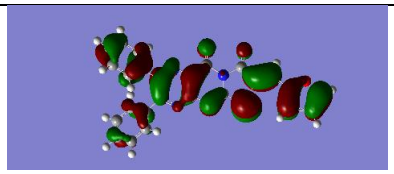
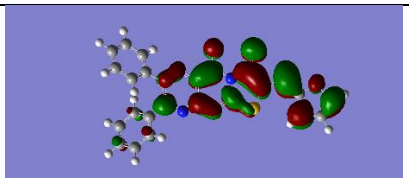
3.9	 -6.423	 -3.127
3.11	 -6.493	 -3.182
3.14[c]	 -5.694	 -2.640
3.16	 -6.589	 -3.427
3.17	 -6.297	 -3.034

Figure S40 DFT calculated HOMO and LUMO orbitals of compounds **3**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3-5

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3-5

Bond precision: C-C = 0.0103 A Wavelength=0.71073

Cell: a=7.4146(16) b=16.862(3) c=23.337(3)
alpha=104.12(2) beta=98.934(14) gamma=93.499(17)

Temperature: 293 K

	Calculated	Reported
Volume	2780.3(9)	2780.2(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C29 H18 N4 O2 S, C2 H6 O S	C29 H18 N4 O2 S, C2 H6 O S
Sum formula	C31 H24 N4 O3 S2	C31 H24 N4 O3 S2
Mr	564.66	564.66
Dx,g cm-3	1.349	1.349
Z	4	4
Mu (mm-1)	0.232	0.232
F000	1176.0	1176.0
F000'	1177.43	
h,k,lmax	8,20,27	8,20,27
Nref	9803	9726
Tmin,Tmax	0.956,0.977	0.175,1.000
Tmin'	0.911	

Correction method= # Reported T Limits: Tmin=0.175 Tmax=1.000
AbsCorr = NONE

Data completeness= 0.992 Theta(max)= 24.998

wR2(reflections)=

R(reflections)= 0.1014(3494)

0.3073(9726)

S = 0.897 Npar= 725

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**. Click on the hyperlinks for more details of the test.

Alert level B

```
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low ..        36% Check
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01027 Ang.
PLAT910_ALERT_3_B Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.94 Note
                  1  0  0,   0  1  0,   0  2  0,   0 -2  1,   0 -1  1,  -1  0  1,
                  0  0  1,   0  1  1,   0  2  1,   0 -2  2,   0 -1  2,   0  0  2,
                  0  1  2,   0 -1  3,   0  0  3,
```

Alert level C

```
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.31 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.11 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C10B     --C11B     .        5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12A     --C17A     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1B      --C2B      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C18B     --C23B     .       0.17 Ang.
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       S1SB Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      S1SA      0.130 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      S1SB      0.226 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     61.124 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.415 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      9.246 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.456 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.119 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         62 Report
                  5  1  0,  -1  2  0,   3 -7  1,  -3  0  1,  -5  1  1,  -4  5  1,
                  1-15  2,  -3-10  2,   4  0  2,   4  4  2,   5  8  2,   7  8  2,
                  6-10  3,  -2 -1  3,  -7  1  3,  -3  2  3,  -1  0  4,   8 -7  5,
                 -2 -1  5,  -3  0  5,   2  0  5,   1 -2  6,   1 -1  6,   1  0  6,
                 -3-16  7,   6 -4  7,  -1  5  7,  -7 10  7,   0 -4  8,  -3 -3  8,
                     (   32 More Missing: see the .ckf listing file)
```

Alert level G

```
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.13 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         20 Note
              S1SA    O1SA    C1SA    H1SA    H1SB    H1SC    C2SA    H2SA
              H2SB    H2SC    S1SB    O1SB    C1SB    H1SD    H1SE    H1SF
              C2SB    H2SD    H2SE    H2SF
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C29 H18 N4 O2 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              C2 H6 O S
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         61 Note
                 -7 -4 12,  -7 -3 13,  -7 -2 20,  -7  1  3,  -7 10  7,  -6 -9 19,
                 -6 -6 20,  -5  1  1,  -5  6 14,  -4  5  1,  -4 14  8,  -3-16  7,
                 -3-10  2,  -3 -3  8,  -3  0  1,  -3  0  5,  -3  2  3,  -2-11 24,
                 -2 -1  3,  -2 -1  5,  -1 -2  8,  -1 -2  9,  -1 -2 13,  -1 -1 10,
```

```
               -1 -1 11,  -1  0  4,  -1  2  0,  -1  5  7,   0-11  9,   0 -4  8,
                0 -2  8,   0 -2  9,   0 -2 10,   0 -2 11,   0 -2 12,   0 -2 13,
0 -2 16,   0  0 11,   0  3 15,   1-15  2,   1 -2  6,   1 -1  6,
1 -1  8,   1  0  6,   2-11 12,   2 -3  8,   2 -2 10,   2  0  5,
               3 -7  1,   3  1 20,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.2 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......    Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     2.228 Note
             Predicted wR2: Based on SigI**2 13.79 or SHELX Weight 34.26
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        0 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
 15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 13 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  7 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
  7 ALERT type 4 Improvement, methodology, query or suggestion
  3 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 04/06/2025; check.def file version of 30/05/2025

Datablock 3-5 - ellipsoid plot

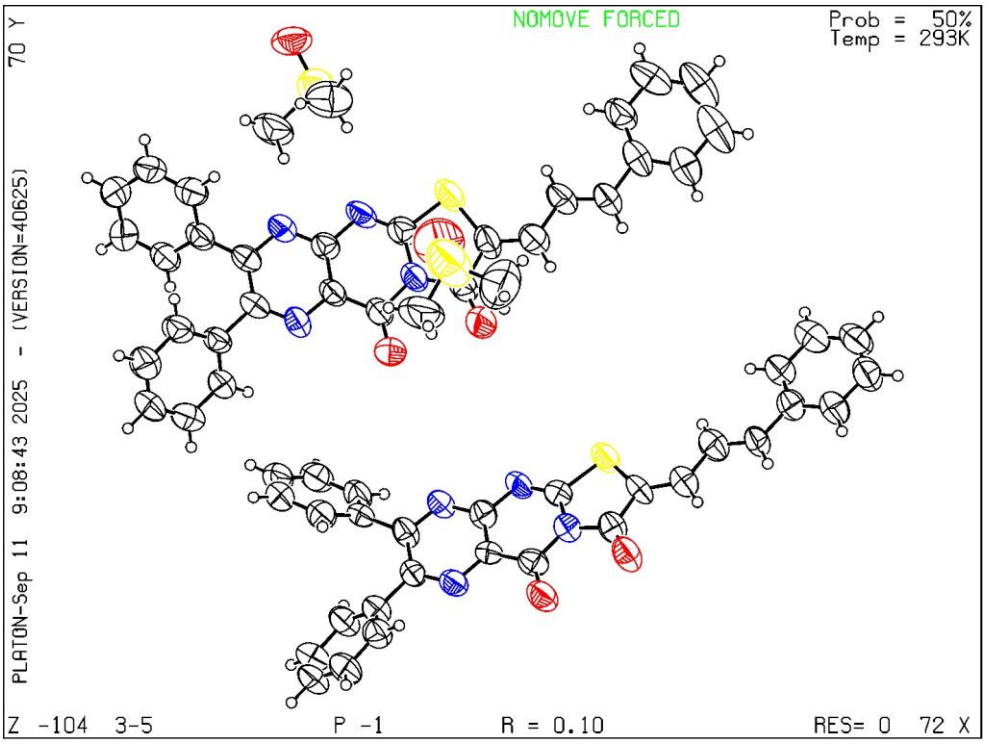


Figure S41 Molecular structure of compound **3.5** DMSO solvate according to X-ray diffraction data.