

Synthesis of new heterylmethylidene derivatives
of isomeric imidazo[4,5-*e*]thiazolo-fused [1,2,4]triazines

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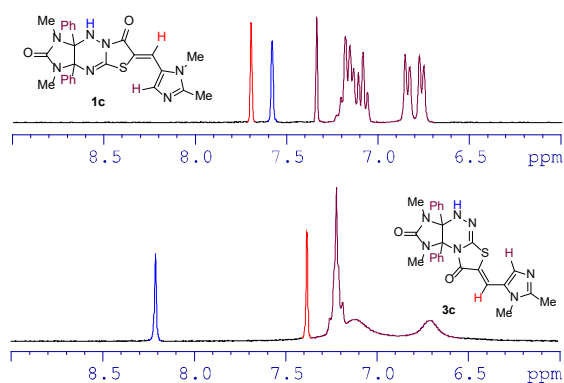


Figure S1 ^1H NMR spectra of compounds **1c** and **3c** in $\text{DMSO}-d_6$ in the region of 6.0–9.0 ppm.

Experimental section

All standard reagents and methanol were purchased from Aldrich or Acros Organics and used without further purification. Melting points were determined on a Stuart SMP20 apparatus. IR spectra were recorded on a Bruker "Alpha" spectrophotometer in the range 400–4000 cm^{-1} (resolution: 2 cm^{-1}). ^1H and ^{13}C NMR spectra were recorded on a Bruker AM-300 (300.13 and 75.47 MHz, respectively), Bruker DRX500 (125.76 MHz, (^{13}C)) and Bruker AV600 (150.90 MHz (^{13}C)) spectrometers and referenced to the residual solvent peak. The chemical shifts are reported in ppm (δ); multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad). Coupling constants, J , are reported in Hertz. High-resolution mass spectra (HRMS) were measured on the Bruker micrOTOF II instrument using electrospray ionization (ESI). The measurements were done in a positive ion mode (interface capillary voltage: 4500 V); mass range from m/z 50 to 3000 Da; external or internal calibration was done with Electrospray Calibrant Solution (Fluka). A syringe injection was used for solutions in MeCN or MeOH (flow rate 3 $\mu\text{L}/\text{min}$). N_2 was applied as a dry gas; interface temperature was set at 180 $^\circ\text{C}$.

5,7-Dimethyl-3-thioxo-4a,7a-diphenyloctahydro-6*H*-imidazo[4,5-*e*][1,2,4]triazin-6-one **2** was prepared according to literature procedure.^{S1}

Synthesis of compounds 1a-g.

General Procedure

Compounds **1a-g** were prepared according to known procedures.^{S2,S3} The corresponding heteroaromatic aldehyde (4 mmol) was added to a suspension of imidazotriazine **2** (1.412 g, 4 mmol), bromoacetic acid (0.556 g, 4 mmol) and anhydrous NaOAc (0.656 g, 8 mmol) in glacial AcOH (30 ml), and the mixture was refluxed with stirring for 8 h. After cooling, the precipitate of compounds **1a-g** was filtered off, washed with AcOH and MeOH and dried at 50 $^\circ\text{C}$. Compounds **1c-e** were recrystallized from methanol.

(Z)-1,3-Dimethyl-3a,9a-diphenyl-6-(pyridin-3-ylmethylene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]-thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1a). Yield 998 mg (52%); light grey solid; mp: 272–274 $^\circ\text{C}$. IR (KBr): ν 3437, 3225 (NH), 3033, 3001 (Ar), 2935 (Alk), 1727, 1685, 1646, 1614 (C=O, C=N) cm^{-1} . ^1H NMR (300 MHz, DMSO- d_6): δ 2.64 (s, 3H, CH₃), 2.65 (s, 3H, CH₃), 6.76 (d, J = 7.2 Hz, 2H, Ph-2,6), 6.75 (d, J = 7.3 Hz, 2H, Ph-2,6), 7.06–7.21 (m, 6H, 2Ph-3,4,5), 7.61 (dd, J = 7.8, 4.8 Hz, 1H, Ar-5), 7.70 (s, 1H, NH), 7.97 (s, 1H, =CH), 8.07 (d, J = 7.9 Hz, 1H, Ar-4), 8.67 (d, J = 4.6, 1H, Ar-6), 8.92 (s, 1H, Ar-2). ^{13}C NMR (75 MHz, DMSO- d_6): δ 25.22, 25.95 (2NCH₃), 79.86, 82.17 (C-3a, C-9a), 121.45, 124.15, 126.10, 127.31, 127.65, 127.86, 127.96, 128.02, 128.20, 129.36, 133.86, 134.72, 135.91 (2Ph, Ar-3,4,5, C-6, =CH), 147.13 (4a-C=N), 150.31, 151.08 (Ar-2,6), 159.03, 159.92 (2-C=O, 7-C=O). HRMS (ESI): m/z [M + H]⁺ calcd for C₂₆H₂₂N₆O₂S: 483.1598; found: 483.1604.

(Z)-1,3-Dimethyl-3a,9a-diphenyl-6-(pyridin-4-ylmethylene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]-thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1b). Yield 405 mg (21%); light grey solid; mp: 288–290 $^\circ\text{C}$. IR (KBr): ν 3434 (NH), 3091, 3064, 3032 (Ar), 2927 (Alk), 1710, 1649, 1613, 1597 (C=O, C=N) cm^{-1} . ^1H NMR (300 MHz, DMSO- d_6): δ 2.64 (s, 3H, CH₃), 2.65 (s, 3H, CH₃), 6.76 (d, J

= 7.0 Hz, 2H, Ph-2,6), 6.85 (d, J = 7.3 Hz, 2H, Ph-2,6), 7.07-7.21 (m, 6H, 2Ph-3,4,5), 7.64 (d, J = 5.7 Hz, 2H, Ar-3,5), 7.73 (s, 1H, NH), 7.90 (s, 1H, =CH), 8.77 (d, J = 5.7 Hz, 2H, Ar-3,5). ^{13}C NMR (150 MHz, DMSO- d_6): δ 25.32, 26.04 (2NCH₃), 79.94, 82.27 (C-3a, C-9a), 123.34, 124.47, 126.18, 127.41, 127.73, 127.98, 128.07, 128.31, 128.45, 133.88, 134.71, 140.32 (2Ph, Ar-3-5, C-6, =CH), 147.02 (4a-C=N), 150.65 (Ar-2,6), 159.09, 159.80 (2-C=O, 7-C=O). HRMS (ESI): m/z [M + H]⁺ calcd for C₂₆H₂₂N₆O₂S: 483.1598; found: 483.1594.

(Z)-6-((1,2-Dimethyl-1H-imidazol-5-yl)methylene)-1,3-dimethyl-3a,9a-diphenyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1H,6H)-dione (1c). Yield 1.46 g (74%); pale yellow solid; mp: >300 °C. IR (KBr): ν 3415 (NH), 3061, 3033 (Ar), 2967, 2931 (Alk), 1714, 1646, 1603 (C=O, C=N) cm⁻¹. ^1H NMR (300 MHz, DMSO- d_6): δ 2.42 (s, 3H, CH₃), 2.62 (s, 3H, CH₃), 2.63 (s, 3H, CH₃), 3.68 (s, 3H, CH₃), 6.76 (d, J = 7.1 Hz, 2H, Ph-2,6), 6.84 (d, J = 7.3 Hz, 2H, Ph-2,6), 7.06-7.20 (m, 6H, 2Ph-3,4,5), 7.34 (s, 1H, Ar-4), 7.58 (s, 1H, NH), 7.70 (s, 1H, =CH). ^{13}C NMR (75 MHz, DMSO- d_6): δ 13.26, 25.14, 25.93, 30.35 (4CH₃), 79.90, 82.00 (C-3a, C-9a), 114.76, 117.32, 126.07, 127.26, 127.69, 127.78, 127.94, 128.14, 132.09, 133.98, 134.91 (2Ph, Ar-4,5, C-6, =CH), 147.49, 149.10 (4a-C=N, Ar-2), 159.07, 160.22 (2-C=O, 7-C=O). HRMS (ESI): m/z [M + H]⁺ calcd for C₂₆H₂₅N₇O₂S: 500.1863; found: 500.1871.

(Z)-6-(Furan-2-ylmethylene)-1,3-dimethyl-3a,9a-diphenyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1H,6H)-dione (1d). Yield 980 mg (52%); beige solid; mp: >300 °C [Lit.^{S2}: yield 48%; beige powder; mp: 280–283 °C]. IR (KBr): ν 3434, 3232 (NH), 3084, 3056, 3022 (Ar), 2918, 2886 (Alk), 1713, 1633 (C=O, C=N) cm⁻¹. ^1H NMR (300 MHz, DMSO- d_6): δ 2.63 (s, 6H, 2CH₃), 6.75-6.85 (m, 5H, 2Ph-2,6, Ar-4), 7.06-7.20 (m, 7H, 2Ph-3,4,5, Ar-3), 7.60 (s, 1H, NH), 7.75 (s, 1H, =CH), 8.09 (s, 1H, Ar-5). ^{13}C NMR (150 MHz, DMSO- d_6): δ 25.26, 25.99 (2NCH₃), 79.87, 81.87 (C-3a, C-9a), 113.51, 116.24, 117.90, 118.09, 126.15, 127.37, 127.74, 127.87, 128.04, 128.23, 134.05, 135.00 (2Ph, Ar-3,4, C-6, =CH), 147.21, 148.20, 149.59 (4a-C=N, Ar-2,5), 159.17, 160.29 (2-C=O, 7-C=O). HRMS (ESI): m/z [M + H]⁺ calcd for C₂₅H₂₁N₅O₃S: 472.1438; found: 472.1441.

(Z)-1,3-Dimethyl-3a,9a-diphenyl-6-(thiophen-2-ylmethylene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1H,6H)-dione (1e). Yield 1.77 g (91%); light beige solid; mp: >300 °C [Lit.^{S2}: yield 44%; beige powder; mp: 278–282 °C]. IR (KBr): ν 3478, 3418, 3258 (NH), 3059, 3034 (Ar), 2972, 2933 (Alk), 1723, 1690, 1645, 1606 (C=O, C=N) cm⁻¹. ^1H NMR (300 MHz, DMSO- d_6): δ 2.63 (s, 6H, 2CH₃), 6.76 (d, J = 6.0 Hz, 2H, Ph-2,6), 6.85 (d, J = 7.1 Hz, 2H, Ph-2,6), 7.06-7.17 (m, 6H, 2Ph-3,4,5), 7.34 (dd, J = 5.0, 3.7 Hz, 1H, Ar-4), 7.63 (s, 1H, NH), 7.73 (d, J = 3.8 Hz, 1H, Ar-3), 8.05 (d, J = 4.9 Hz, 1H, Ar-5), 8.20 (s, 1H, =CH). ^{13}C NMR (75 MHz, DMSO- d_6): δ 25.19, 25.95 (2NCH₃), 79.89, 82.12 (C-3a, C-9a), 116.52, 124.65, 126.06, 127.29, 127.68, 127.82, 127.96, 128.17, 128.89, 132.59, 133.93, 134.02, 134.82, 137.24 (2Ph, Ar, C-6, =CH), 147.38 (4a-C=N), 159.05, 160.16 (2-C=O, 7-C=O). HRMS (ESI): m/z [M + H]⁺ calcd for C₂₅H₂₁N₅O₂S₂: 488.1209; found: 488.1207.

(Z)-6-((1H-Pyrrol-2-yl)methylene)-1,3-dimethyl-3a,9a-diphenyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1H,6H)-dione (1f). Yield 598 mg (32%); dark grey solid; mp: >300 °C. IR (KBr): ν 3397, 3229 (NH), 3060, 3029, 3012 (Ar), 2940 (Alk), 1694, 1630, 1603 (C=O, C=N) cm⁻¹. ^1H NMR (300 MHz, DMSO- d_6): δ 2.61 (s, 6H, 2CH₃), 6.39-6.40 (m, 1H, Ar), 6.56-6.57 (m, 1H, Ar), 6.75 (d, J = 6.9 Hz, 2H, Ph-2,6), 6.82 (d, J = 7.2 Hz, 2H, Ph-2,6), 7.04-7.22 (m, 7H, 2Ph-3,4,5, Ar-5), 7.50 (s, 1H, NH), 7.77 (s, 1H, =CH), 11.70 (s, 1H, NH). ^{13}C NMR (150 MHz, DMSO- d_6): δ

25.21, 26.01 (2NCH₃), 80.00, 82.00 (C-3a, C-9a), 110.97, 111.91, 113.32, 121.70, 123.98, 126.18, 127.03, 127.30, 127.79, 127.98, 128.17, 134.24, 135.24 (2Ph, Ar-3,4,5, C-6, =CH), 148.16 (4a-C=N), 159.20, 160.81 (2-C=O, 7-C=O). HRMS (ESI): m/z [$M + H$]⁺ calcd for C₂₅H₂₂N₆O₂S: 471.1598; found: 471.1595.

(Z)-6-((1*H*-Indol-3-yl)methylene)-1,3-dimethyl-3a,9a-diphenyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]-thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1g). Yield 1.21 g (58%); light yellow solid; mp: >300 °C. IR (KBr): ν 3258, 3229 (NH), 3059, 3036 (Ar), 2964, 2927 (Alk), 1721, 1690, 1632, 1606 (C=O, C=N) cm⁻¹. ¹H NMR (300 MHz, DMSO-*d*₆): δ 2.64 (s, 3H, CH₃), 2.65 (s, 3H, CH₃), 6.78 (d, J = 7.0 Hz, 2H, Ph-2,6), 6.86 (d, J = 7.1 Hz, 2H, Ph-2,6), 7.06-7.29 (m, 8H, 2Ph-3,4,5, Ar-5,6), 7.53-7.55 (m, 2H, Ar-7, NH), 7.86 (d, J = 2.7 Hz, 1H, Ar-2), 7.96 (d, J = 7.6 Hz, 1H, Ar-4), 8.17 (s, 1H, =CH), 12.17 (s, 1H, NH). ¹³C NMR (150 MHz, DMSO-*d*₆): δ 25.24, 26.01 (2NCH₃), 80.03, 82.04 (C-3a, C-9a), 110.60, 111.94, 112.40, 118.47, 121.02, 123.78, 126.17, 126.79, 127.35, 127.79, 127.82, 128.02, 128.20, 128.33, 134.20, 135.23, 136.19 (2Ph, Ar, C-6, =CH), 148.18 (4a-C=N), 159.24, 160.79 (2-C=O, 7-C=O). HRMS (ESI): m/z [$M + H$]⁺ calcd for C₂₉H₂₄N₆O₂S: 521.1754; found: 521.1750.

Synthesis of compounds 3a-e.

General Procedure

To a stirred suspension of compounds **1a-g** (1 mmol) in refluxing methanol (10 mL), NaOMe (as 30% solution in MeOH) was added (0.186 ml, 1 mmol). The resulting mixture was refluxed with stirring for 1 h. After cooling, the precipitate of compounds **3a-g** was filtered off, washed with methanol and dried at 50 °C.

(Z)-1,3-Dimethyl-3a,9a-diphenyl-7-(pyridin-3-ylmethylene)-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]-thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (3a). Yield 365 mg (76%); yellow solid; mp: 237–239 °C. IR (KBr): ν 3470, 3434, 3305 (NH), 3066, 3029 (Ar), 2959, 2908 (Alk), 1723, 1699, 1656, 1606 (C=O, C=N) cm⁻¹. ¹H NMR (300 MHz, DMSO-*d*₆): δ 2.63 (s, 3H, CH₃), 2.91 (s, 3H, CH₃), 6.72 (br.s, 3H, Ph-2,4,6), 7.14-7.25 (m, 7H, Ph-2,4,6, 2Ph-3,5), 7.57-7.61 (m, 2H, =CH, Ar-5), 7.97 (d, J = 7.9, 1H, Ar-4), 8.30 (s, 1H, NH), 8.62 (d, J = 4.2, 1H, Ar-6), 8.82 (s, 1H, Ar-2). ¹³C NMR (150 MHz, DMSO-*d*₆): δ 25.60, 30.85 (2NCH₃), 81.65, 86.94 (C-3a, C-9a), 123.61, 124.20, 125.34, 127.24, 128.04, 128.48, 128.95, 129.70, 131.93, 132.88, 135.62, 135.81 (2Ph, Ar-3,4,5, C-7, =CH, 5a-C=N), 149.82, 150.97 (Ar-2,6), 158.17 (2-C=O), 163.46 (8-C=O). HRMS (ESI): m/z [$M + H$]⁺ calcd for C₂₆H₂₂N₆O₂S: 483.1598; found: 483.1603.

(Z)-1,3-Dimethyl-3a,9a-diphenyl-7-(pyridin-4-ylmethylene)-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]-thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (3b). Yield 259 mg (54%); yellow solid; mp: 219–221 °C. IR (KBr): ν 3434 (NH), 3060, 3034 (Ar), 2959 (Alk), 1719, 1655 (C=O, C=N) cm⁻¹. ¹H NMR (300 MHz, DMSO-*d*₆): δ 2.63 (s, 3H, CH₃), 2.91 (s, 3H, CH₃), 6.71 (br.s, 3H, Ph-2,4,6), 6.95-7.26 (m, 7H, Ph-2,4,6, 2Ph-3,5), 7.52-7.54 (m, 3H, =CH, Ar-3,5), 8.35 (s, 1H, NH), 8.73 (d, J = 5.9 Hz, 2H, Ar-3,5). ¹³C NMR (125 MHz, DMSO-*d*₆): δ 25.65, 30.87 (2NCH₃), 81.66, 87.07 (C-3a, C-9a), 123.13, 125.65, 126.65, 127.29, 127.79, 128.07, 128.53, 128.99, 131.86, 132.88 (2Ph, Ar-3,5, C-7, =CH), 135.65 (5a-C=N), 150.57 (Ar-2,6), 158.17 (2-C=O), 163.31 (8-C=O). HRMS (ESI): m/z [$M + H$]⁺ calcd for C₂₆H₂₂N₆O₂S: 483.1598; found: 483.1593.

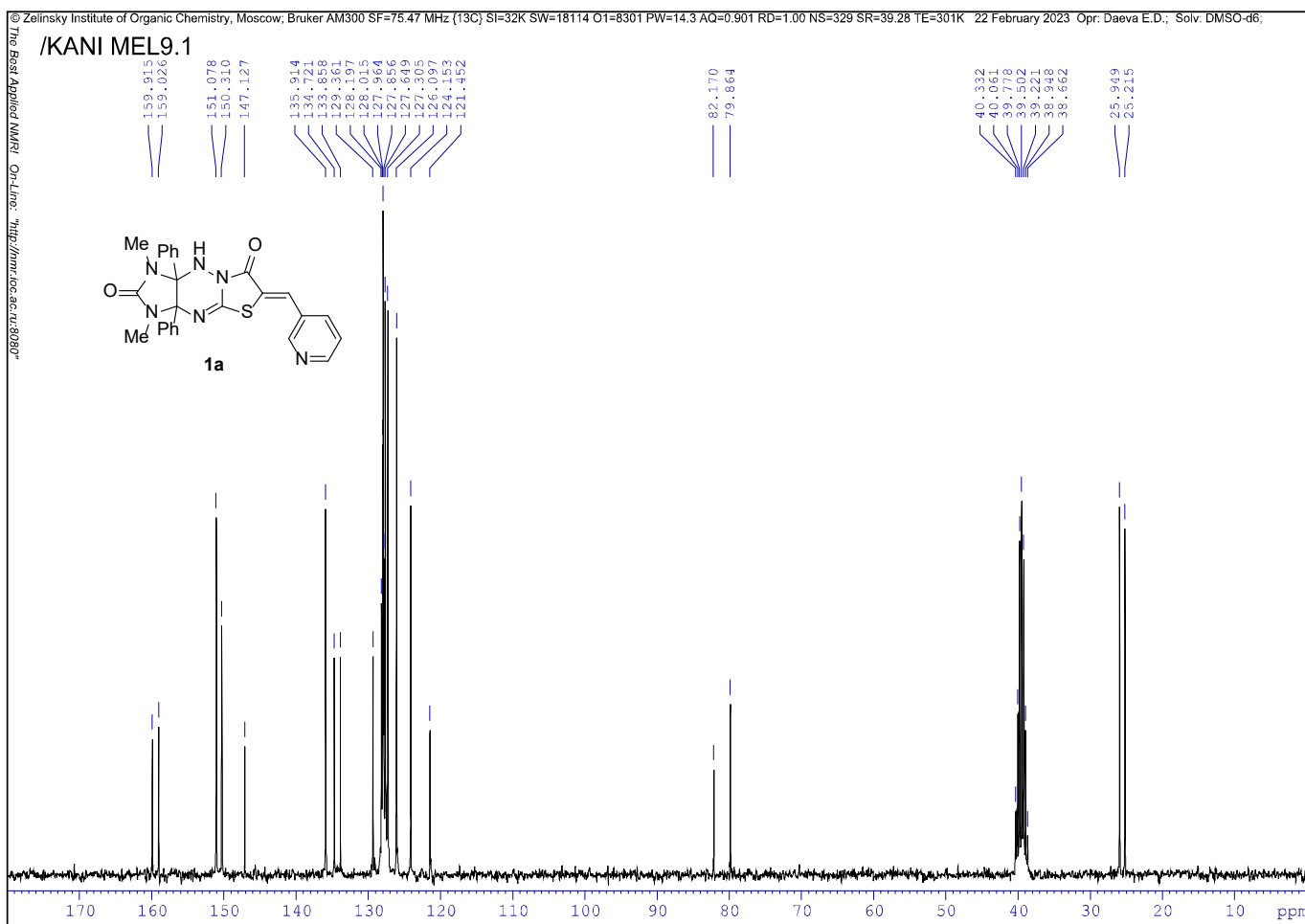
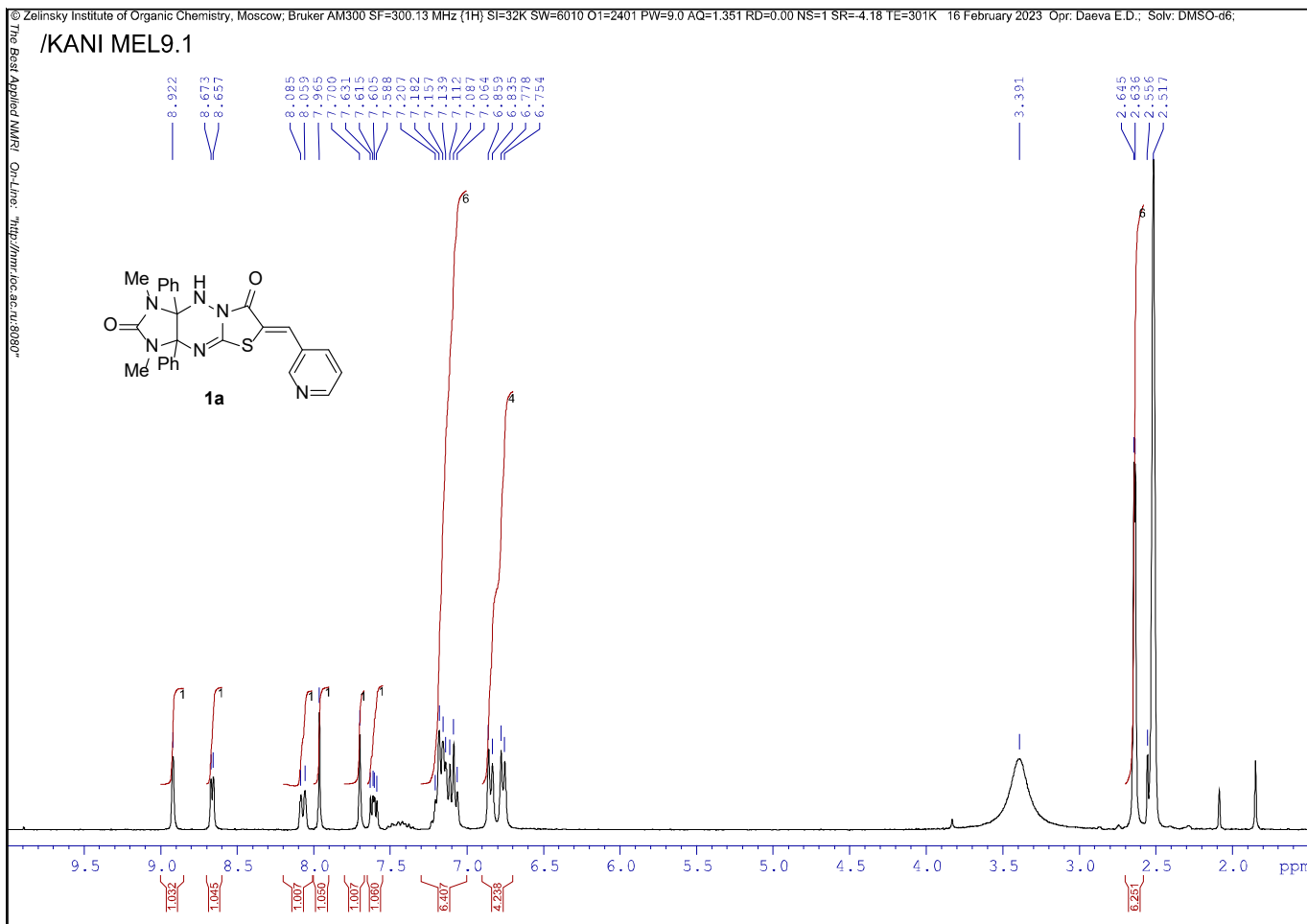
(Z)-7-((1,2-Dimethyl-1H-imidazol-5-yl)methylene)-1,3-dimethyl-1,3a,4,9a-tetrahydroimidazo[4,5-e]-thiazolo[2,3-c][1,2,4]triazine-2,8(3H,7H)-dione (3c). Yield 124 mg (25%); yellow solid; mp: >300 °C. IR (KBr): ν 3302, 3258 (NH), 3061, 3034 (Ar), 2950 (Alk), 1722, 1696, 1650, 1610 (C=O, C=N) cm^{-1} . ^1H NMR (300 MHz, DMSO- d_6): δ 2.39 (s, 3H, CH₃), 2.62 (s, 3H, CH₃), 2.90 (s, 3H, CH₃), 3.59 (s, 3H, CH₃), 6.72 (br.s, 3H, Ph-2,4,6), 7.05-7.23 (m, 8H, Ph-2,4,6, 2Ph-3,5, Ar-4), 7.39 (s, 1H, =CH), 8.21 (s, 1H, NH). ^{13}C NMR (75 MHz, DMSO- d_6): δ 13.77, 26.01, 30.71, 31.30 (4CH₃), 82.10, 87.12 (C-3a, C-9a), 115.40, 117.47, 127.64, 128.12, 128.44, 128.55, 128.80, 129.32, 131.97, 132.69, 133.49 (2Ph, Ar-4,5, C-7, =CH), 136.80 (5a-C=N), 149.18 (Ar-2), 158.65 (2-C=O), 164.13 (8-C=O). HRMS (ESI): m/z [$M + \text{H}$]⁺ calcd for C₂₆H₂₅N₇O₂S: 500.1863; found: 500.1848.

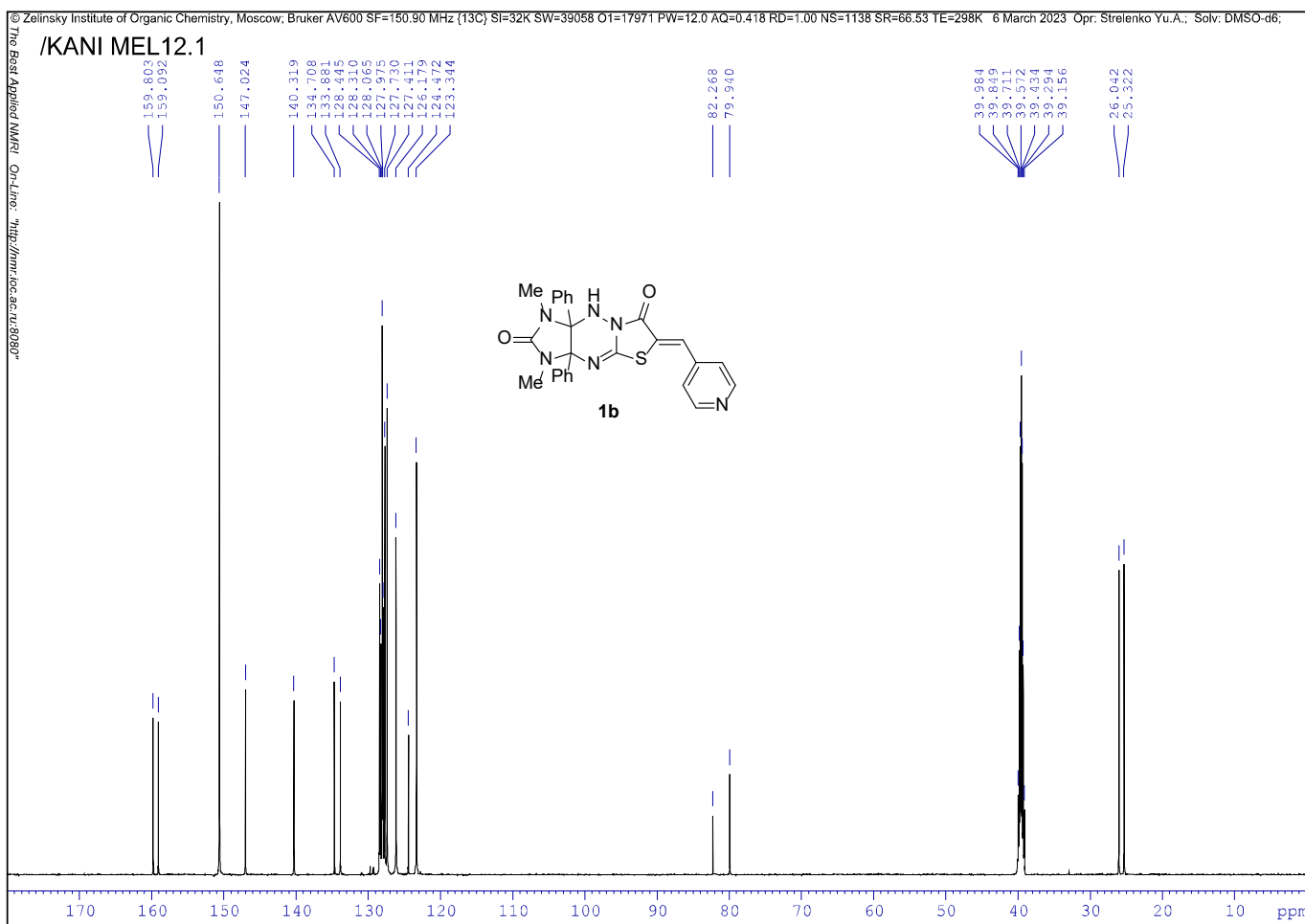
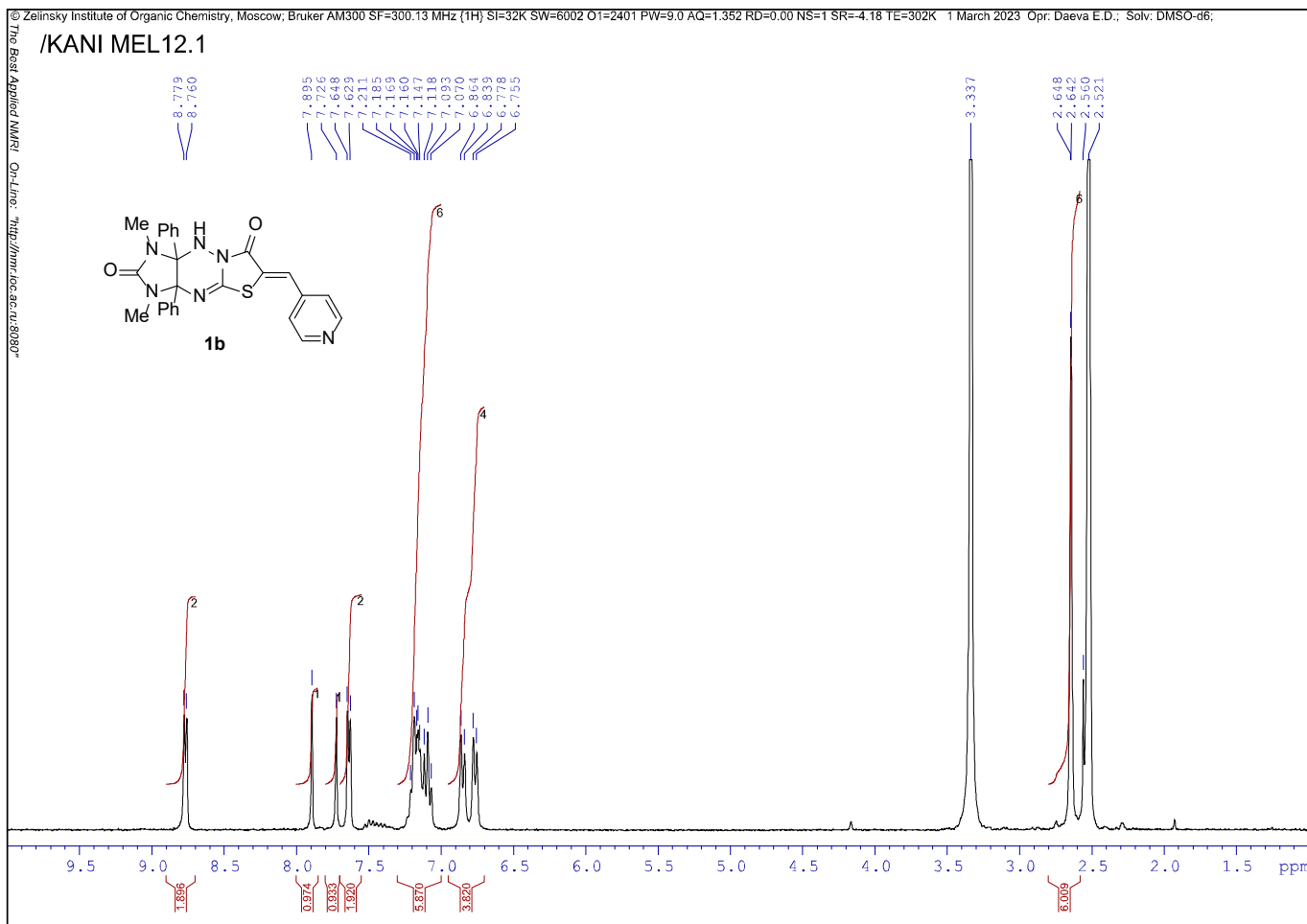
(Z)-7-(Furan-2-ylmethylene)-1,3-dimethyl-3a,9a-diphenyl-1,3a,4,9a-tetrahydroimidazo[4,5-e]-thiazolo[2,3-c][1,2,4]triazine-2,8(3H,7H)-dione (3d). Yield 407 mg (86%); yellow solid; mp: >250–253 °C. IR (KBr): ν 3432, 3301 (NH), 3033 (Ar), 2949, 2907 (Alk), 1722, 1695, 1652, 1614 (C=O, C=N) cm^{-1} . ^1H NMR (300 MHz, DMSO- d_6): δ 2.60 (s, 3H, CH₃), 2.87 (s, 3H, CH₃), 6.68-6.76 (m, 4H, Ph-2,4,6, Ar-4), 6.97 (d, J = 3.5 Hz, 1H, Ar-3), 7.03-7.25 (m, 7H, Ph-2,4,6, 2Ph-3,5), 7.39 (s, 1H, =CH), 8.05 (d, J = 1.6 Hz, 1H, Ar-5), 8.17 (s, 1H, NH). ^{13}C NMR (150 MHz, DMSO- d_6): δ 25.58, 30.80 (2NCH₃), 81.61, 86.68 (C-3a, C-9a), 113.38, 115.77, 116.51, 118.73, 127.21, 127.70, 127.99, 128.38, 128.88, 132.17, 133.07 (2Ph, Ar-3,4, C-7, =CH), 136.90 (5a-C=N), 146.63, 149.85 (Ar-2,5), 158.19 (2-C=O), 163.66 (8-C=O). HRMS (ESI): m/z [$M + \text{H}$]⁺ calcd for C₂₅H₂₁N₅O₃S: 472.1438; found: 472.1436.

(Z)-1,3-Dimethyl-3a,9a-diphenyl-7-(thiophen-2-ylmethylene)-1,3a,4,9a-tetrahydroimidazo[4,5-e]-thiazolo[2,3-c][1,2,4]triazine-2,8(3H,7H)-dione (3e). Yield 324 mg (67%); yellow solid; mp: 260–262 °C. IR (KBr): ν 3432, 3300 (NH), 3029 (Ar), 2955 (Alk), 1723, 1691, 1651, 1595 (C=O, C=N) cm^{-1} . ^1H NMR (300 MHz, DMSO- d_6): δ 2.62 (s, 3H, CH₃), 2.90 (s, 3H, CH₃), 6.72 (br.s, 3H, Ph-2,4,6), 7.05-7.26 (m, 7H, Ph-2,4,6, 2Ph-3,5), 7.34 (dd, J = 4.5, 4.2 Hz, 1H, Ar-4), 7.59 (d, J = 3.6 Hz, 1H, Ar-3), 7.86 (s, 1H, =CH), 8.00 (d, J = 5.1 Hz, 1H, Ar-5), 8.24 (s, 1H, NH). ^{13}C NMR (150 MHz, DMSO- d_6): δ 24.42, 29.65 (2NCH₃), 80.49, 85.69 (C-3a, C-9a), 117.80, 119.28, 121.09, 126.06, 126.82, 127.24, 127.38, 127.73, 128.84, 130.64, 130.92, 131.64, 131.80 (2Ph, Ar-3,5, C-7, =CH), 136.64 (5a-C=N), 157.00 (2-C=O), 162.41 (8-C=O). HRMS (ESI): m/z [$M + \text{H}$]⁺ calcd for C₂₅H₂₁N₅O₂S₂: 488.1209; found: 488.1207.

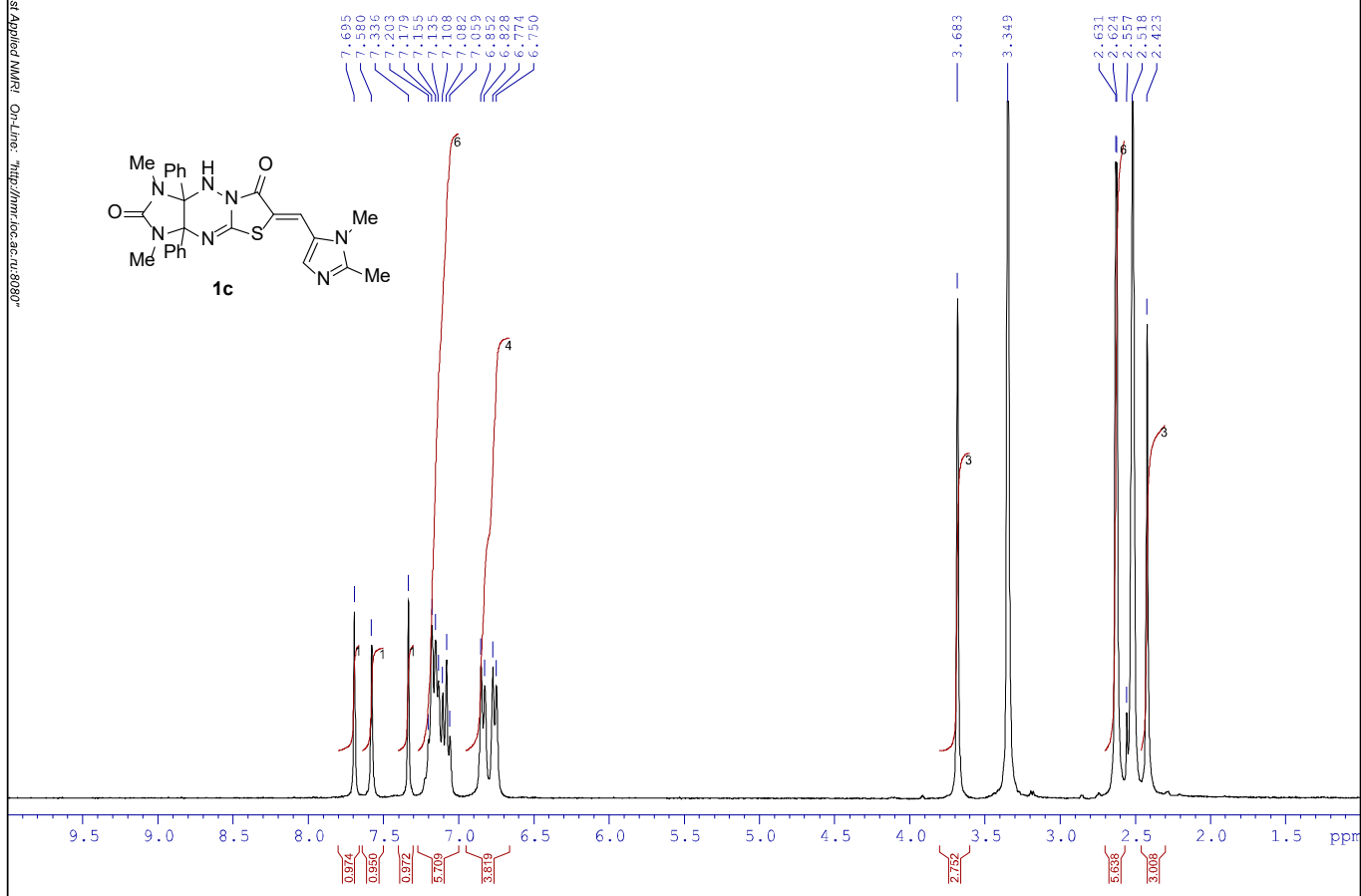
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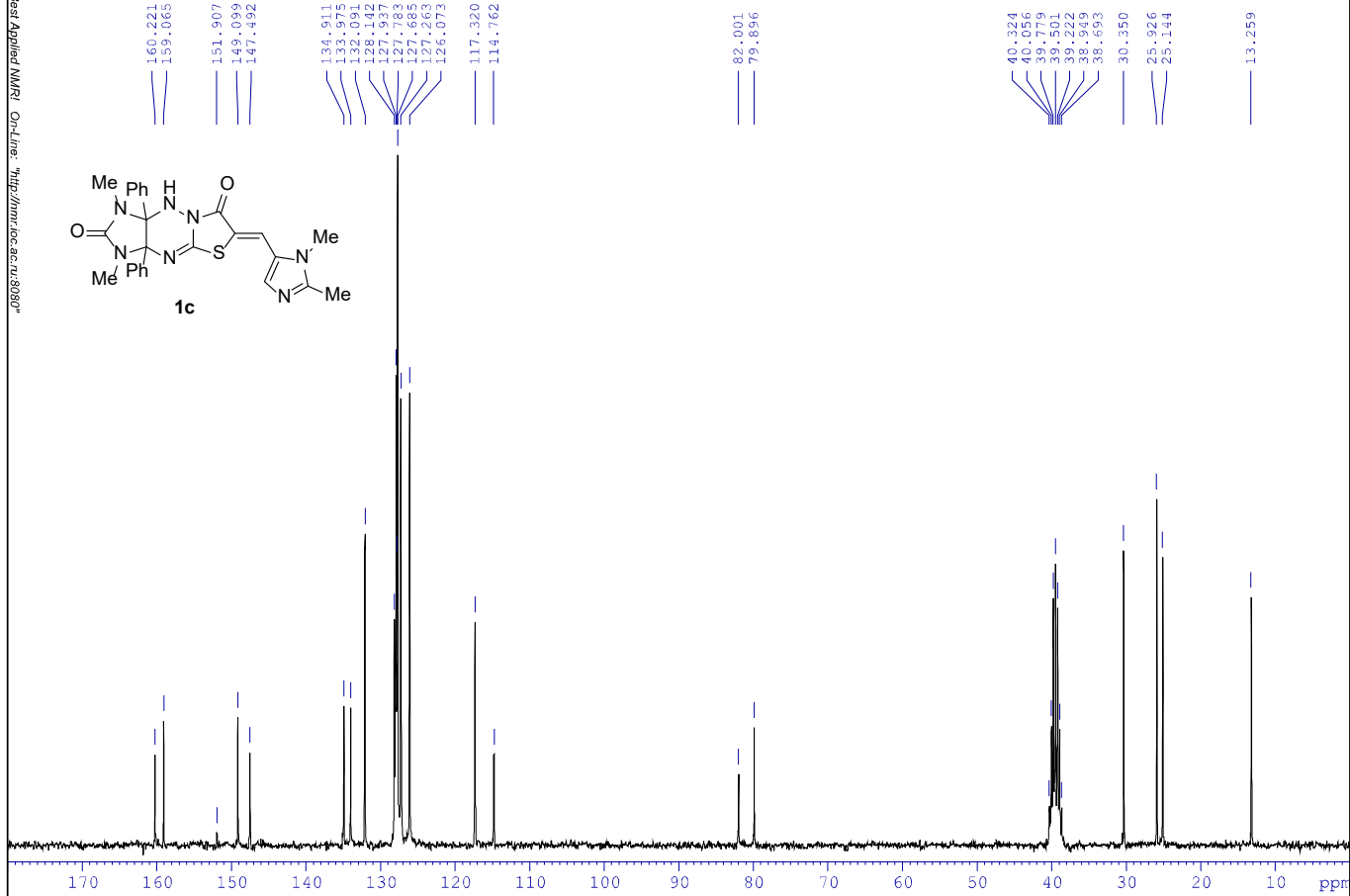




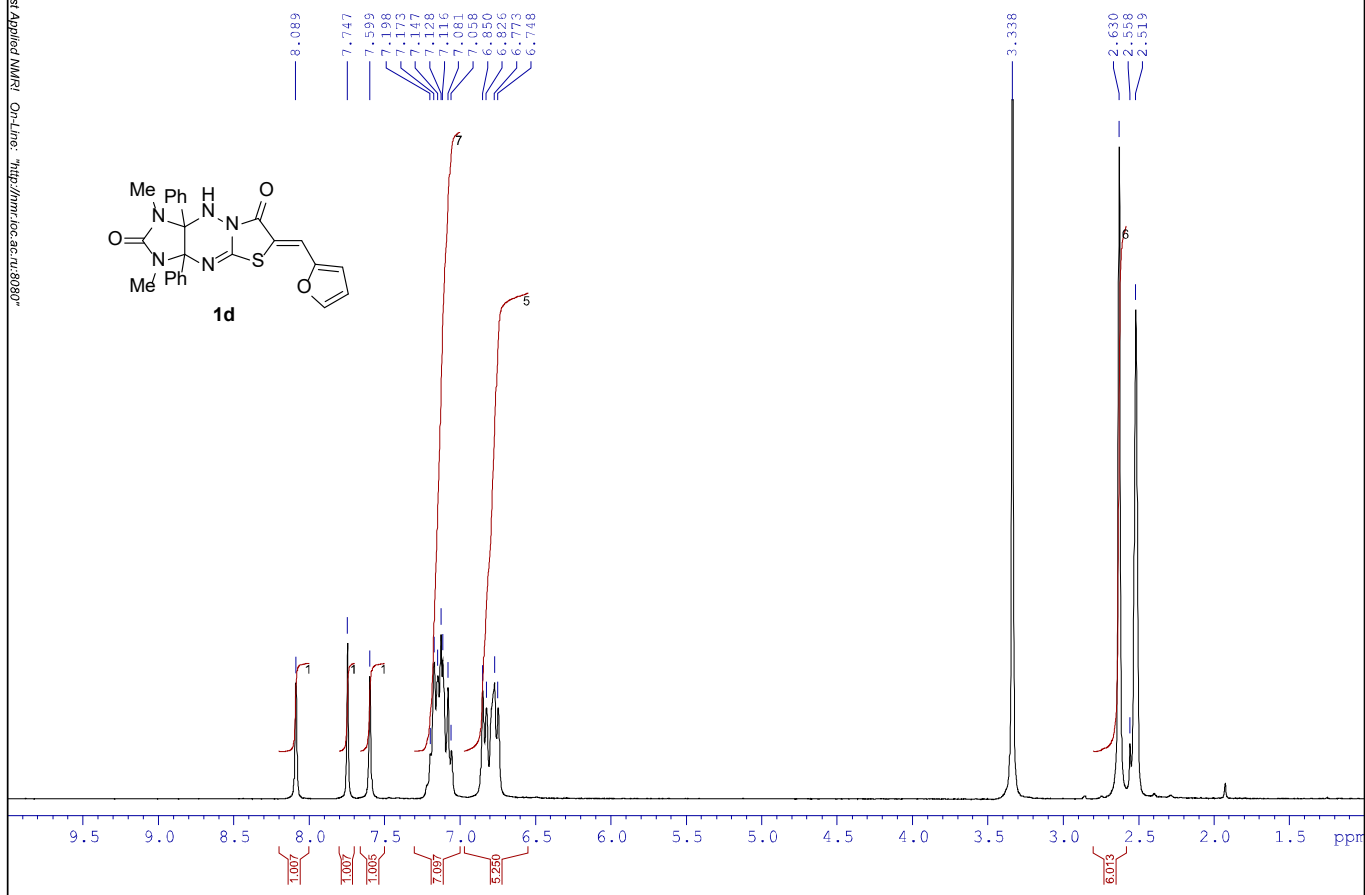
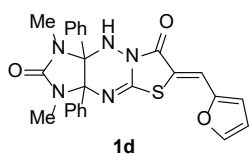
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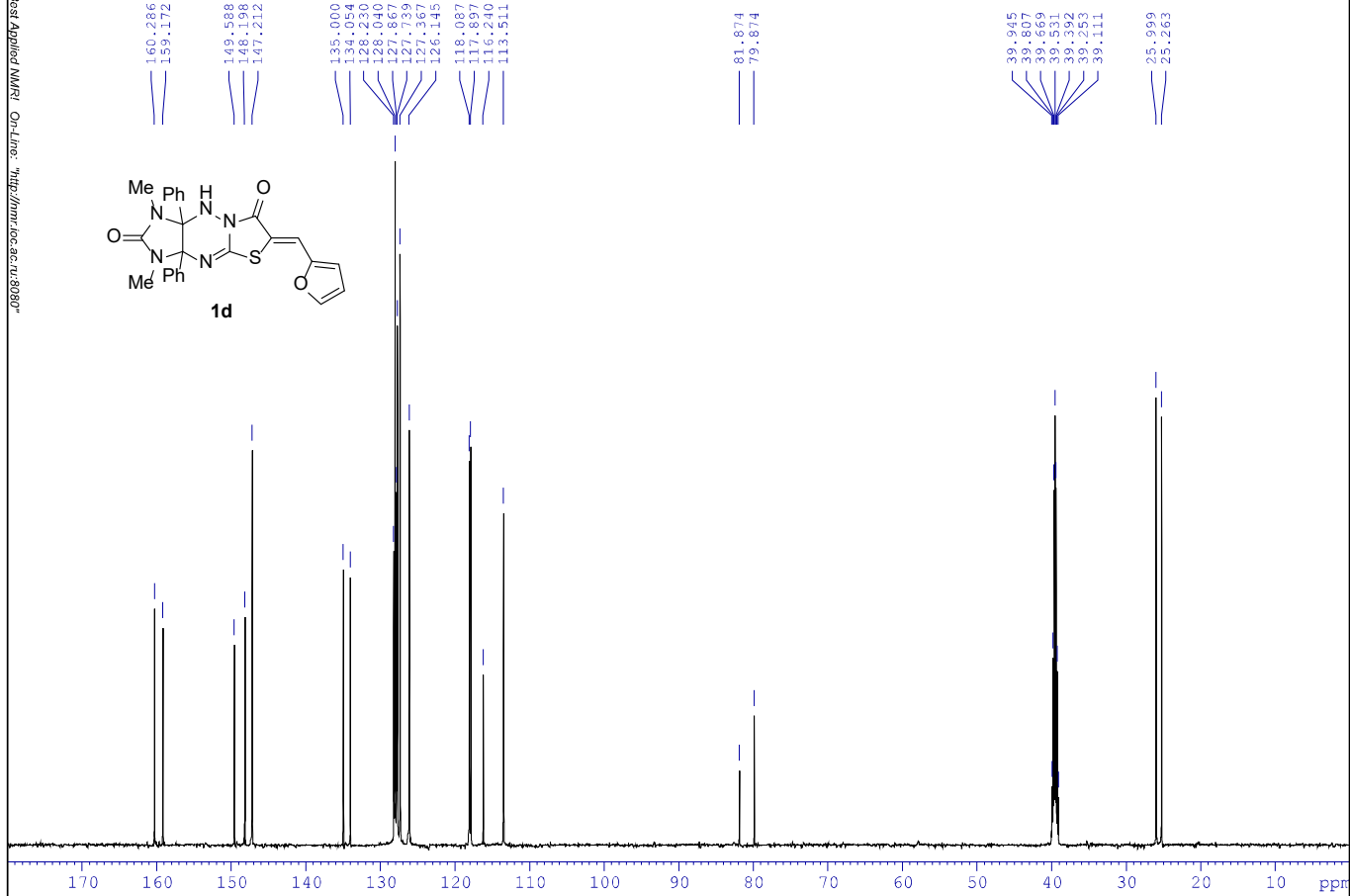
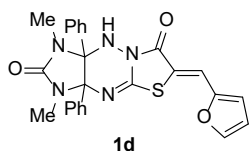
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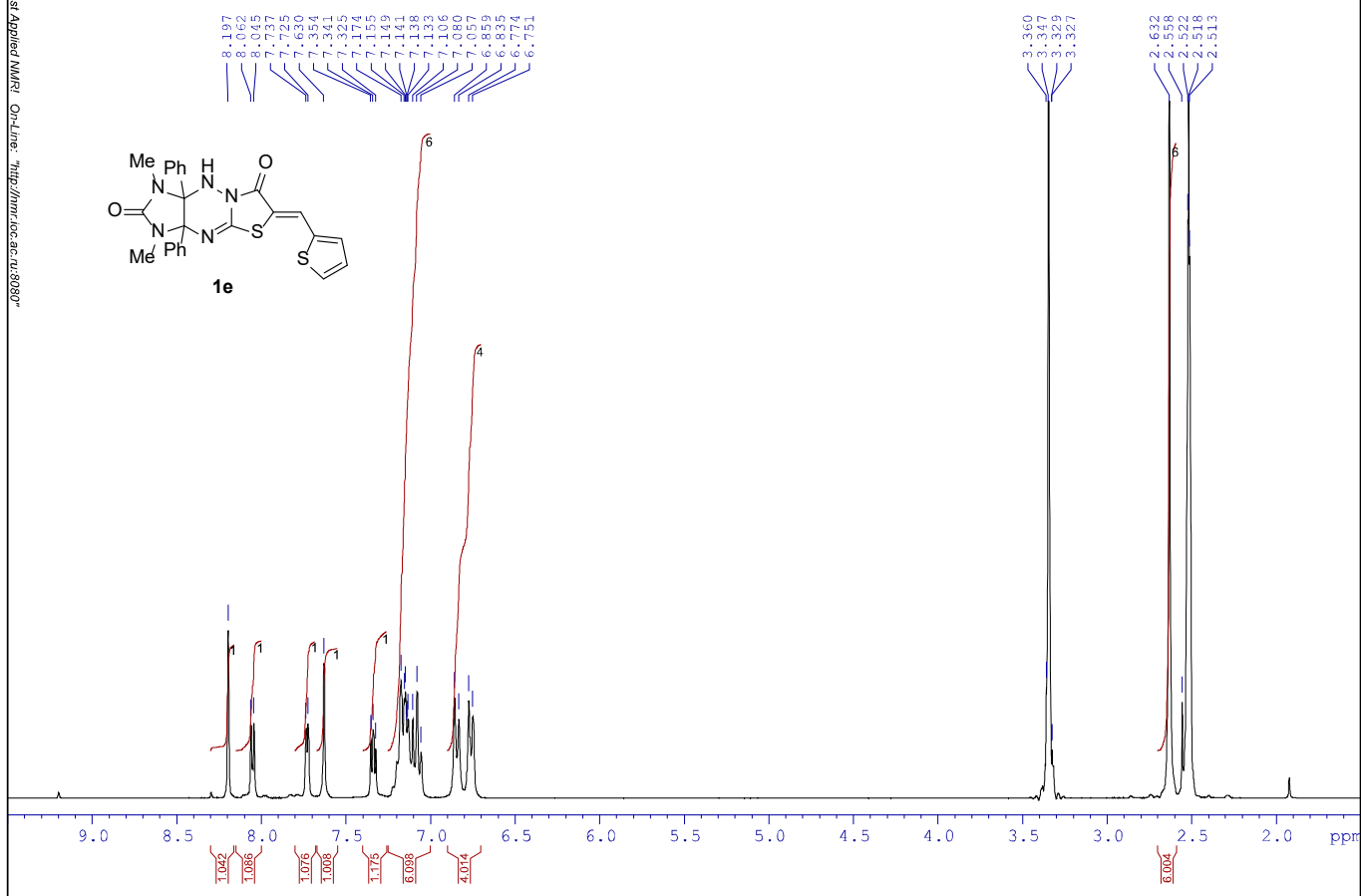
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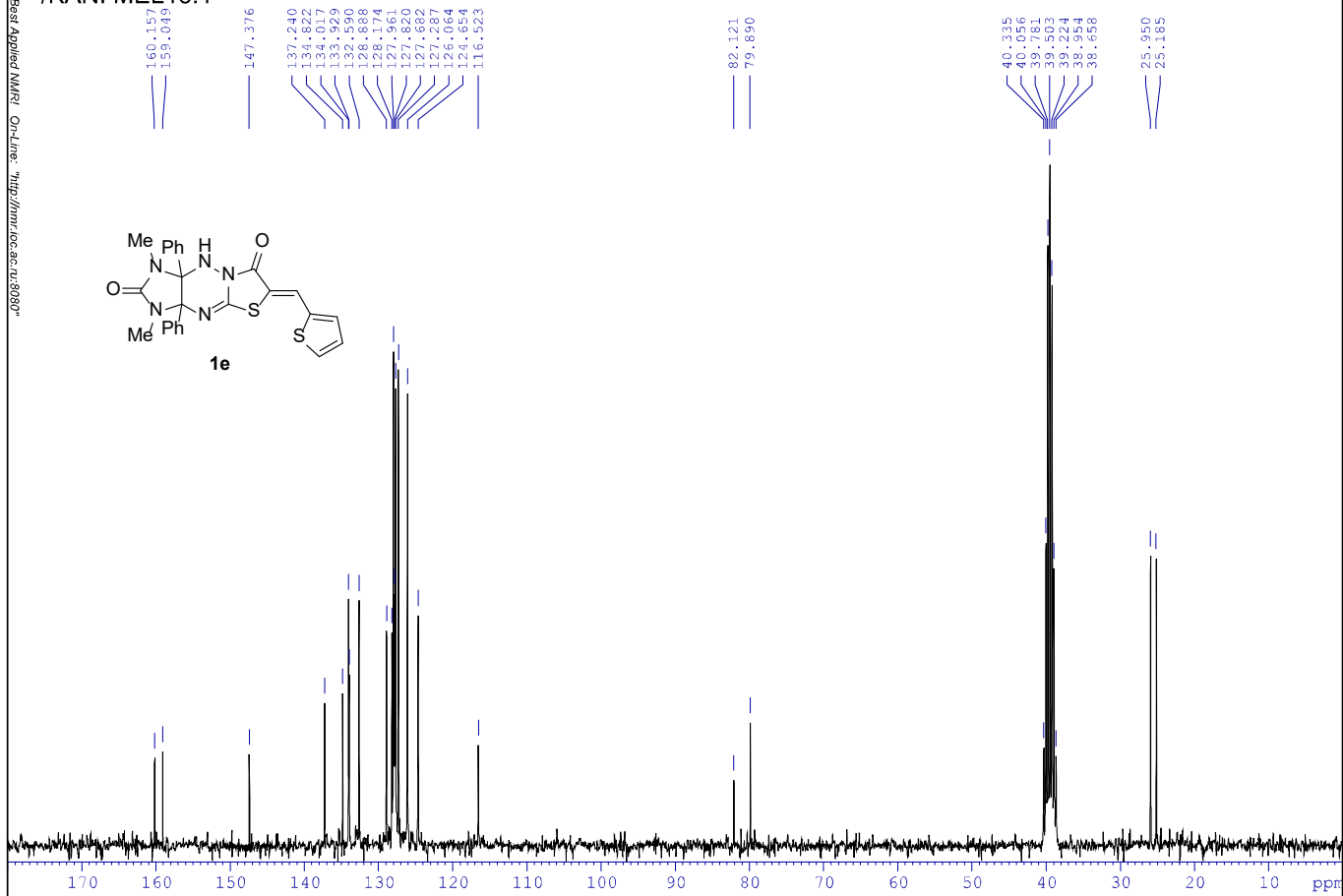
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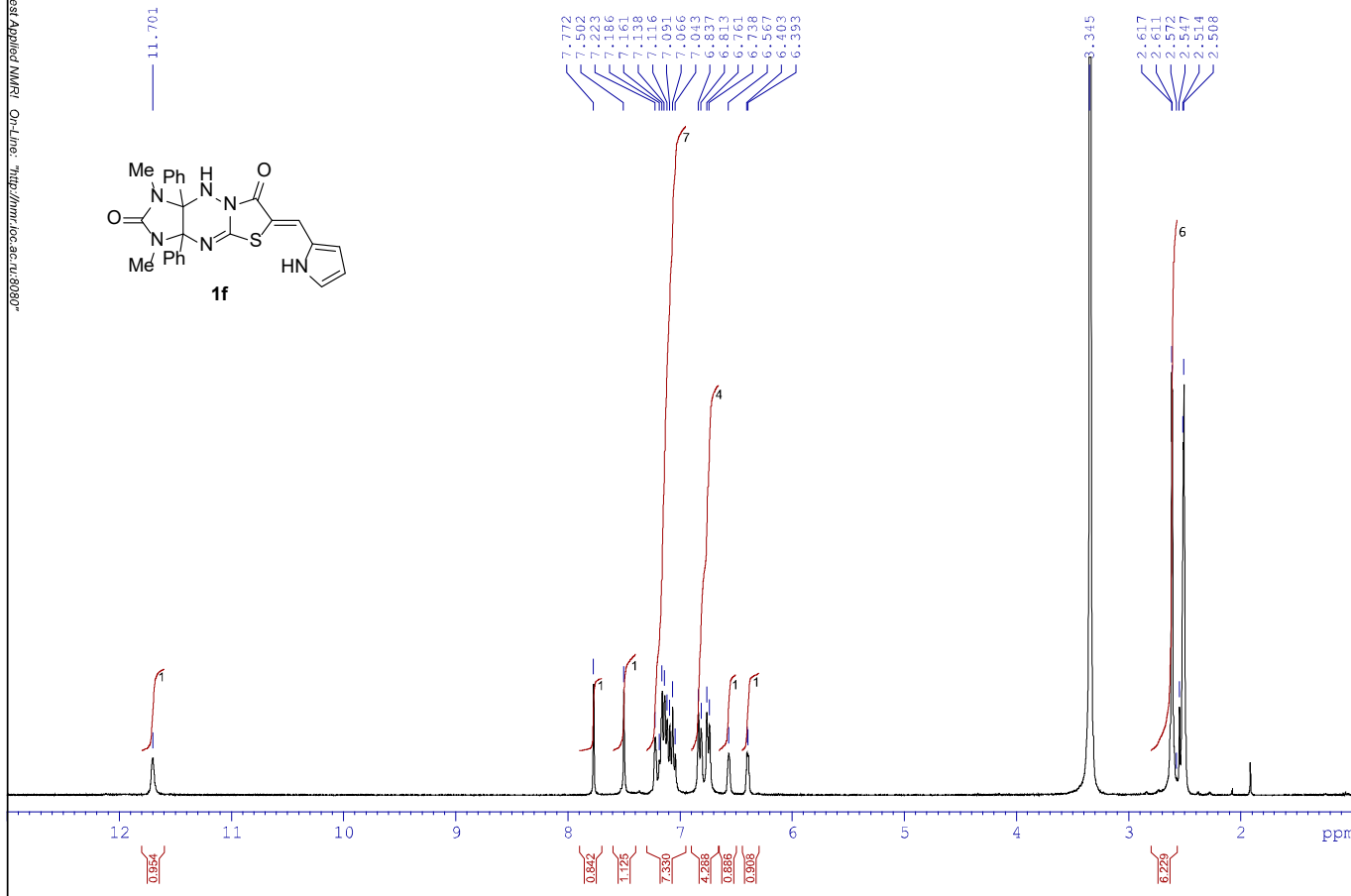
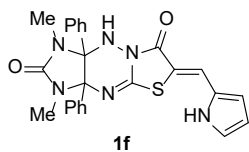
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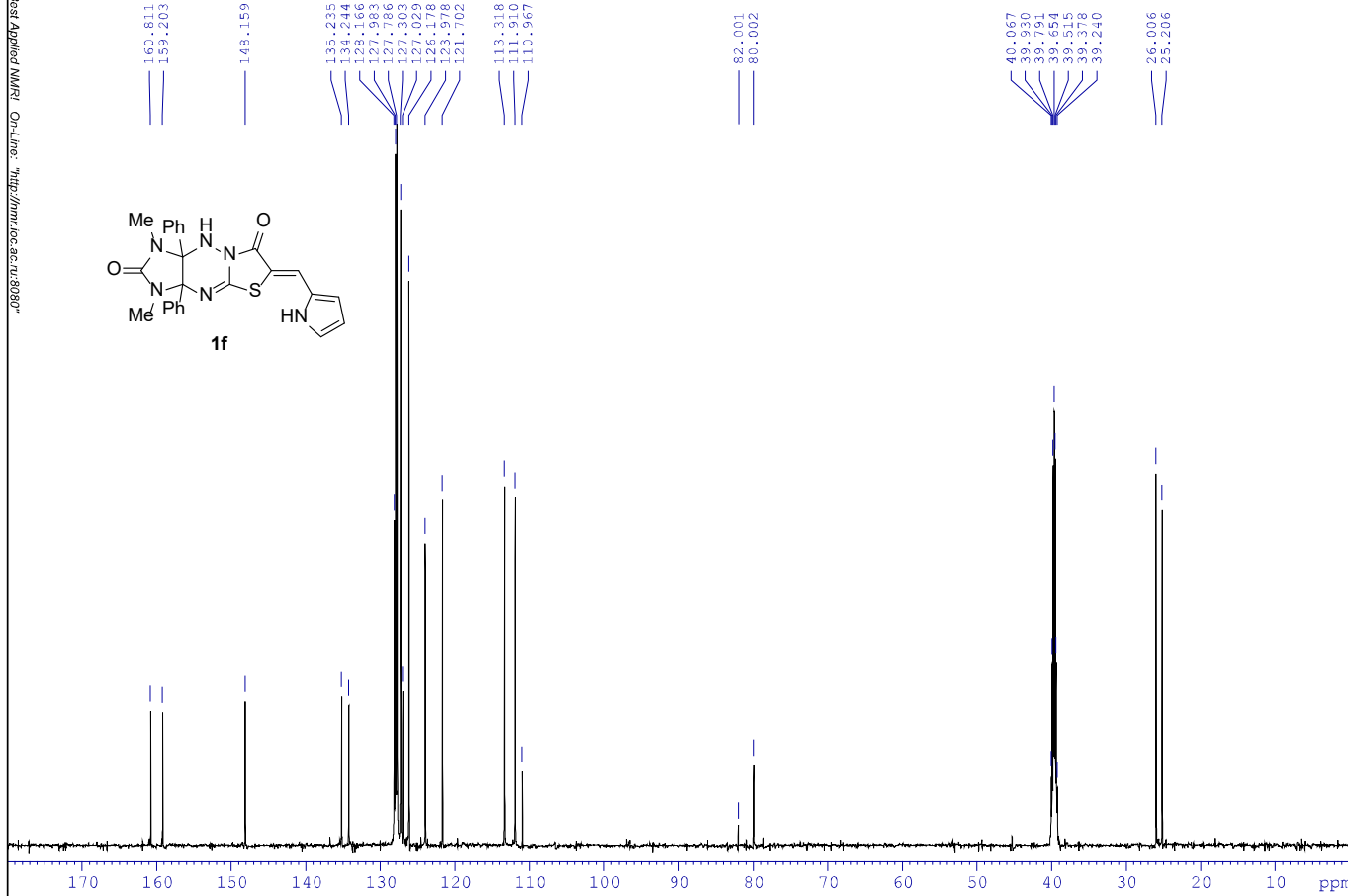
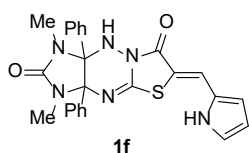
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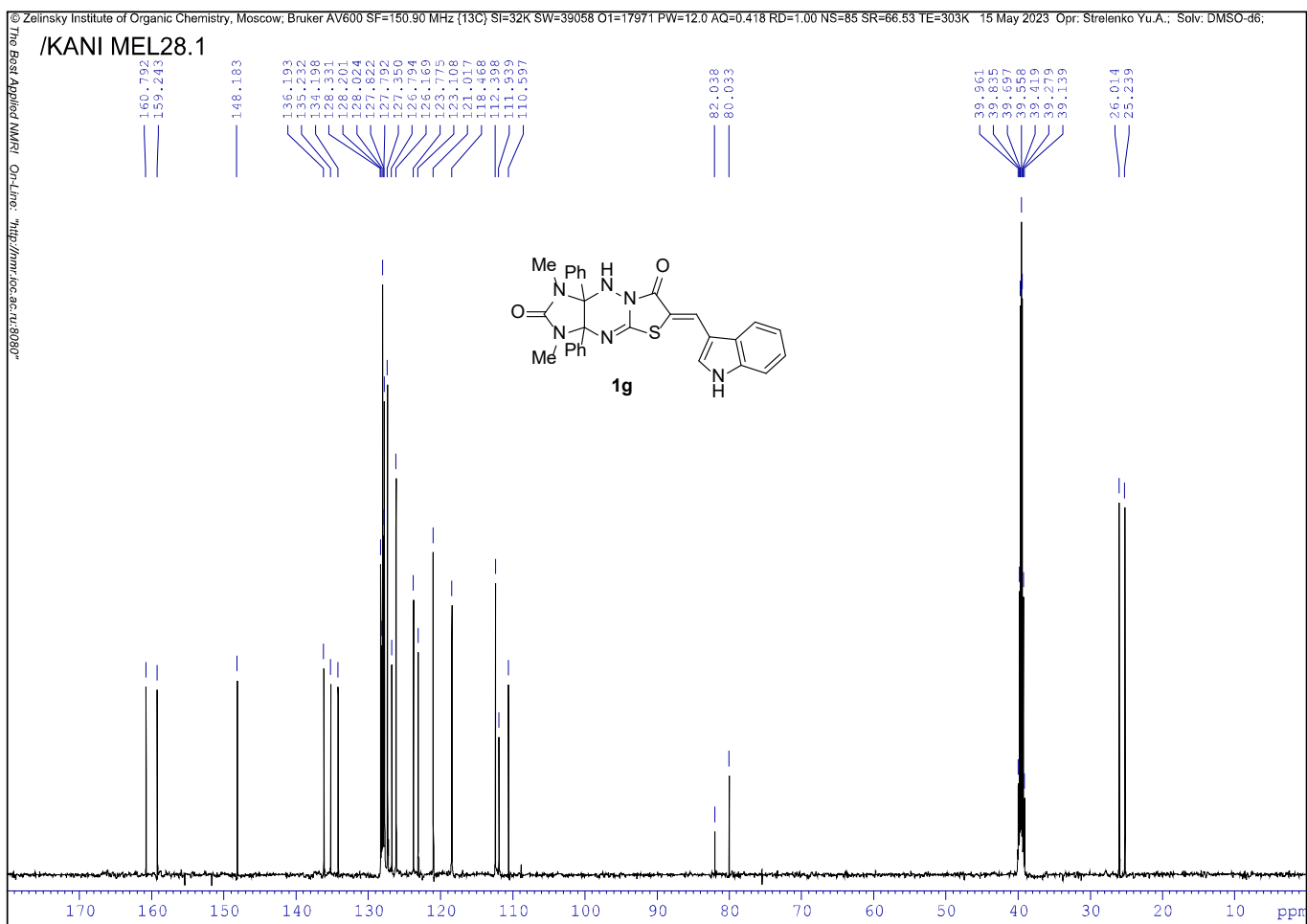
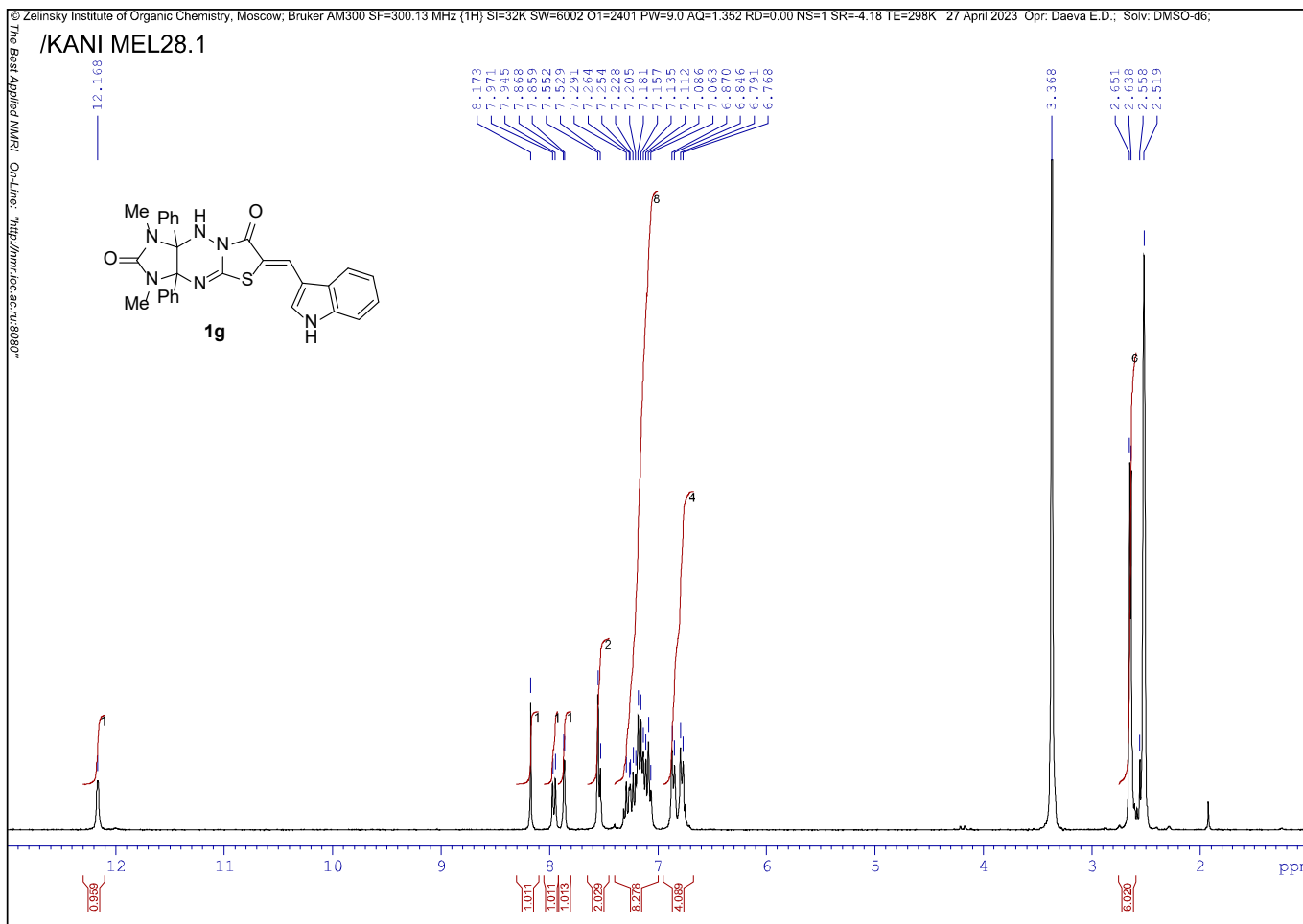


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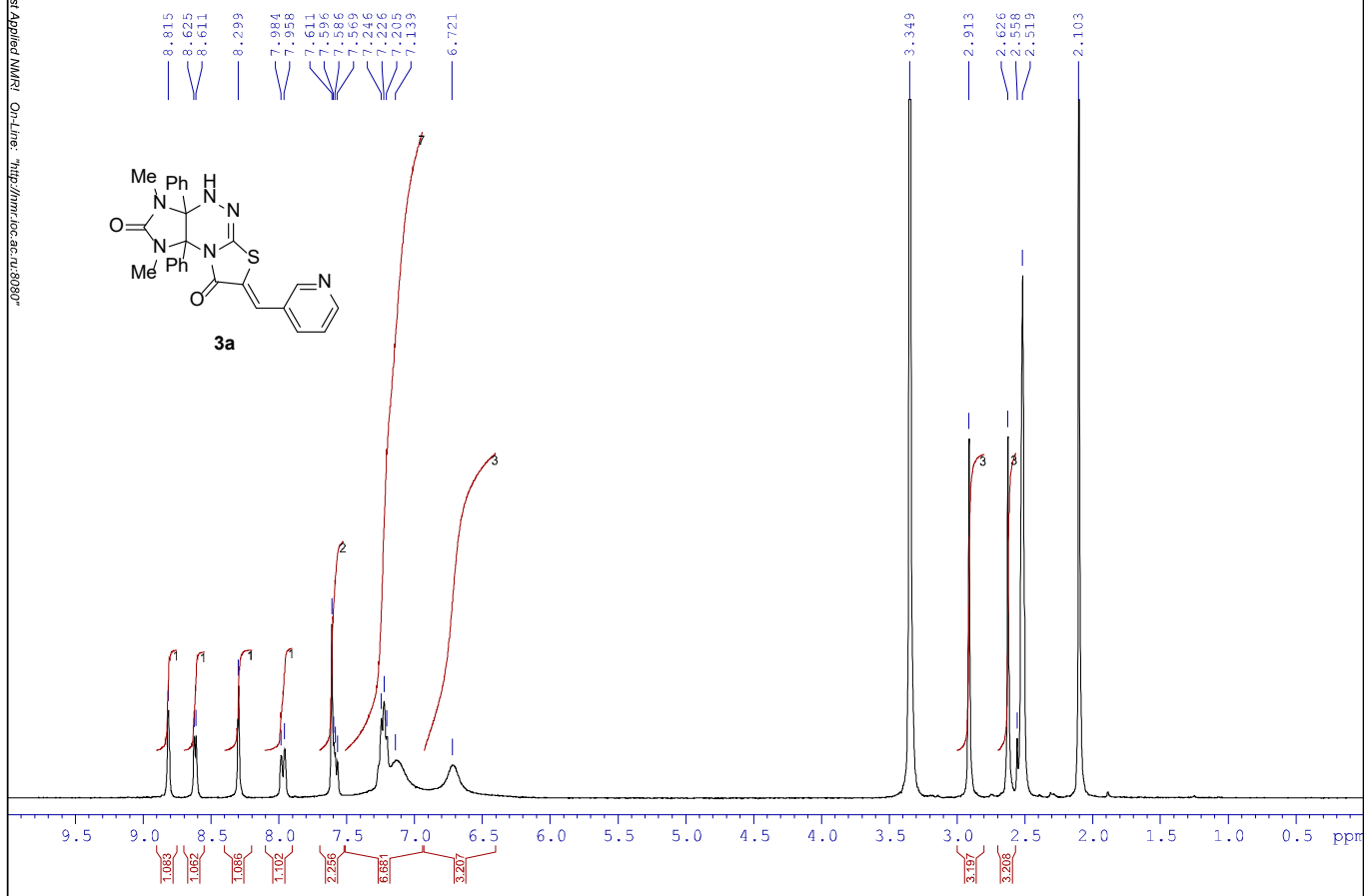


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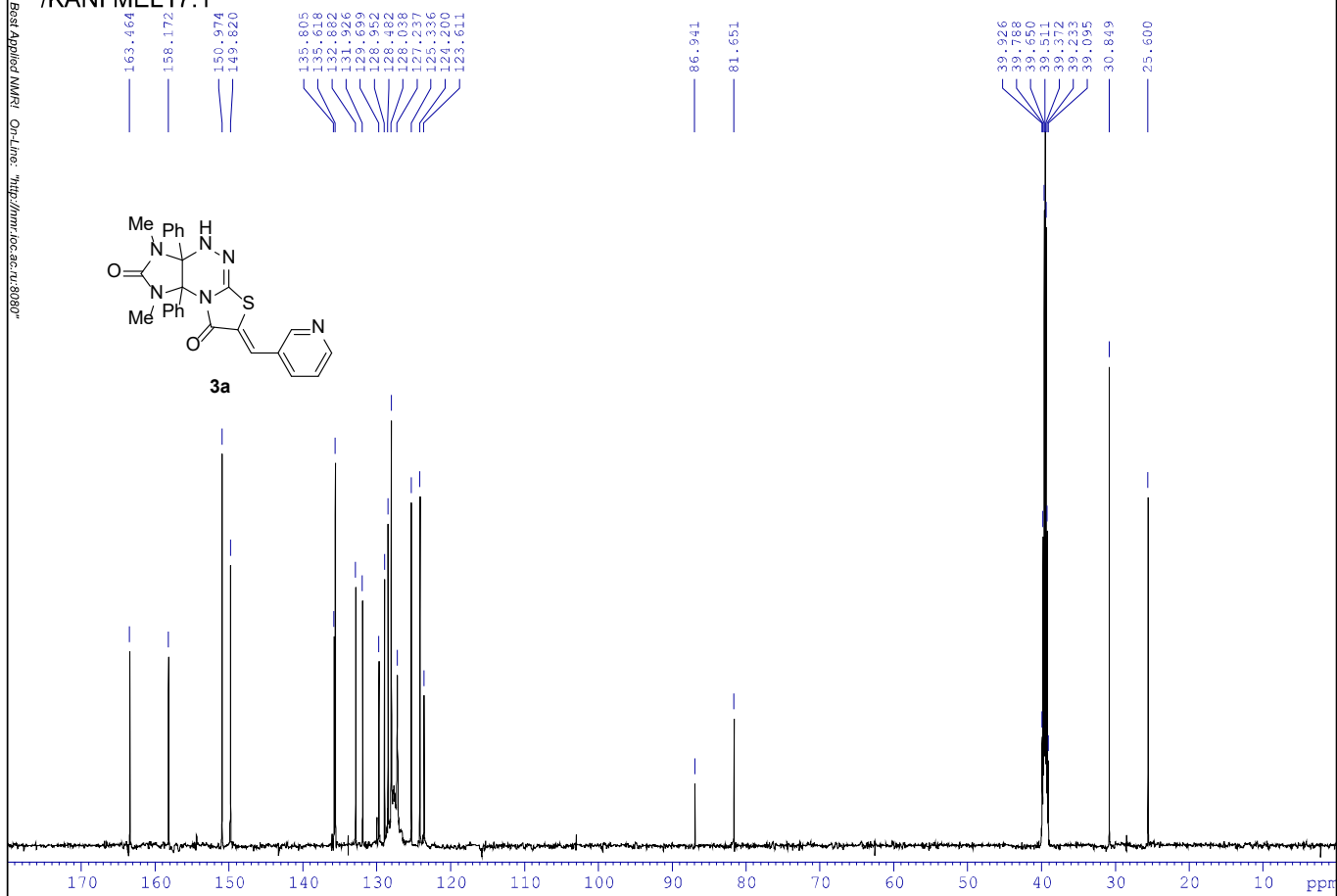


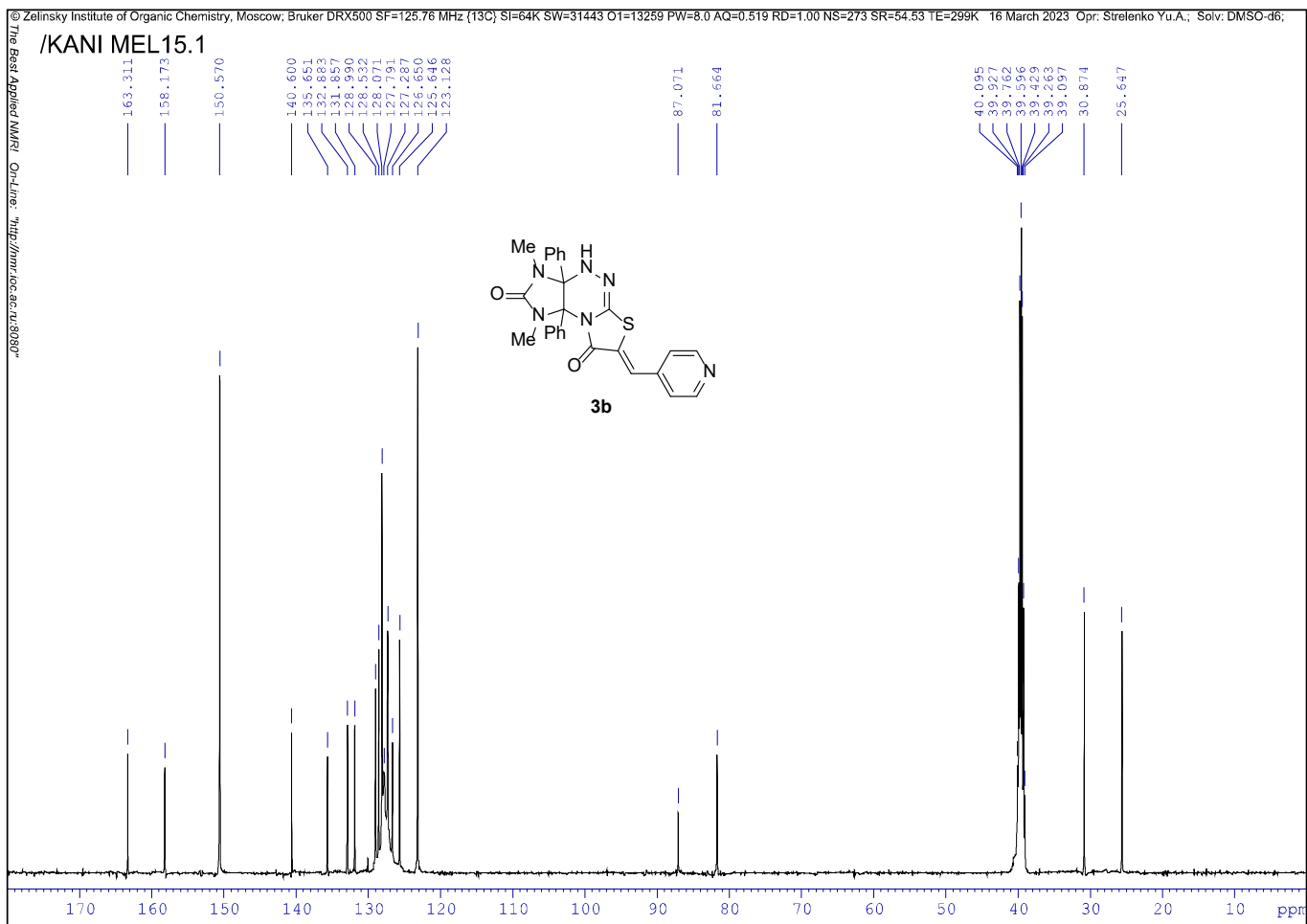
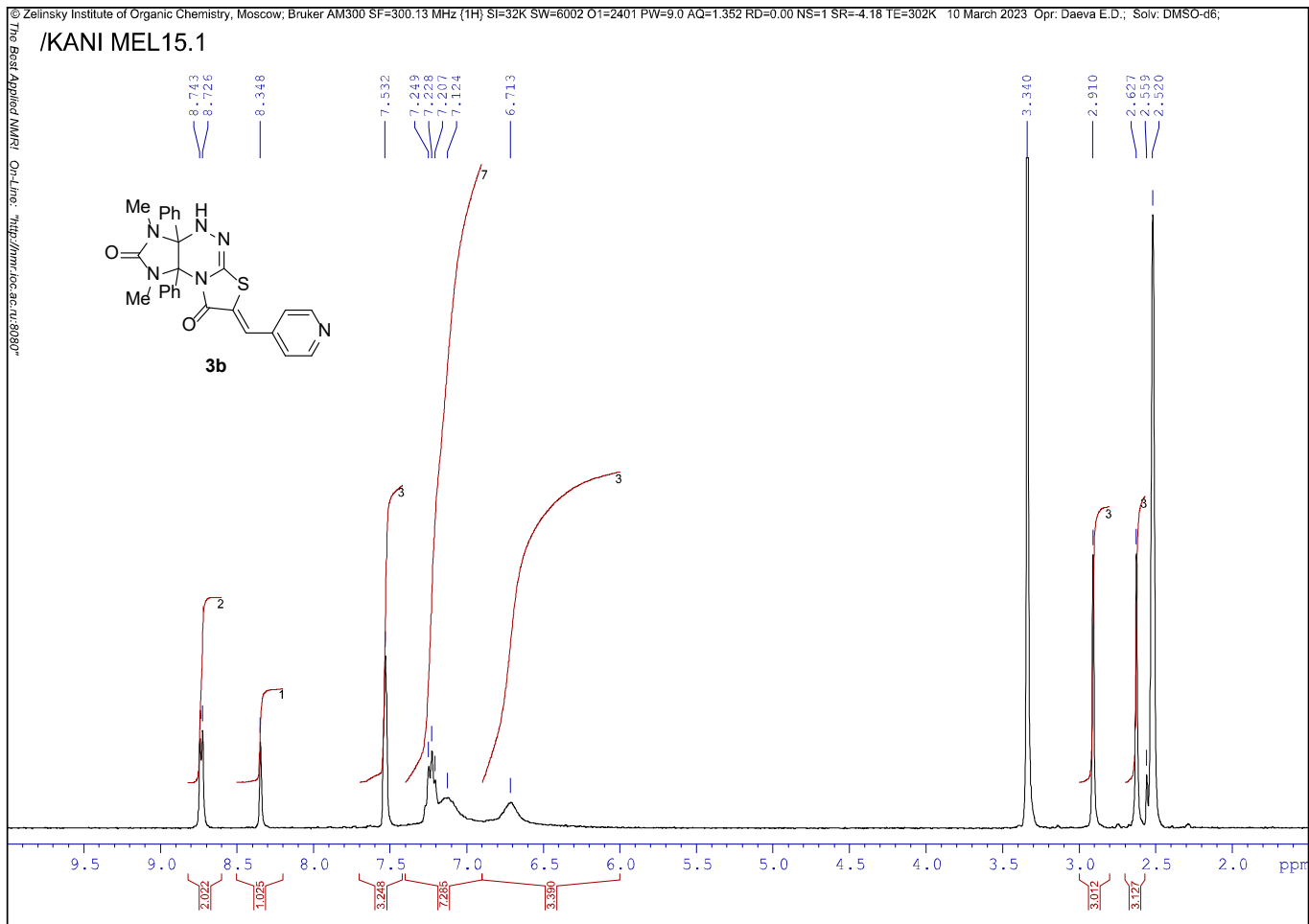


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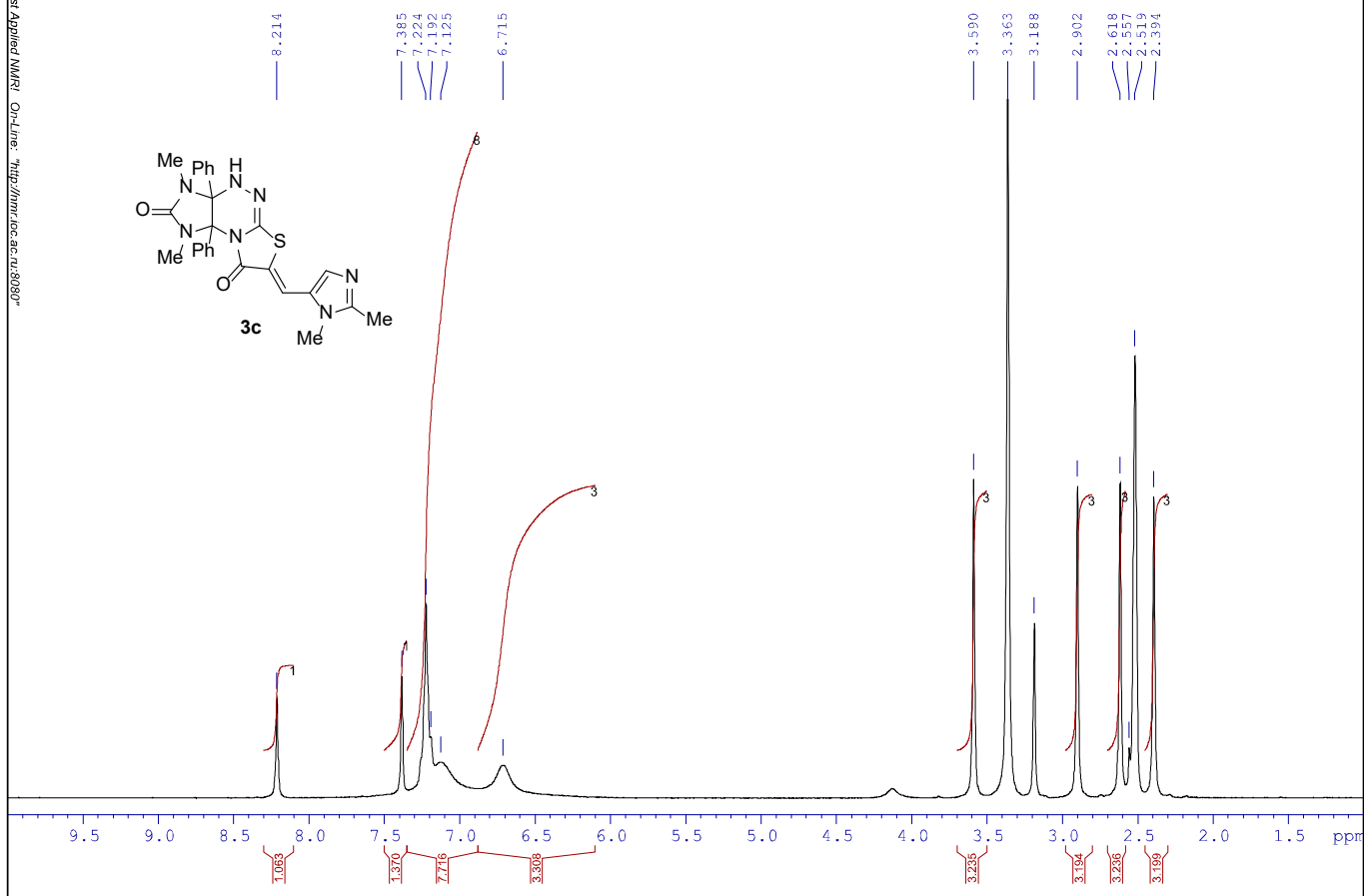


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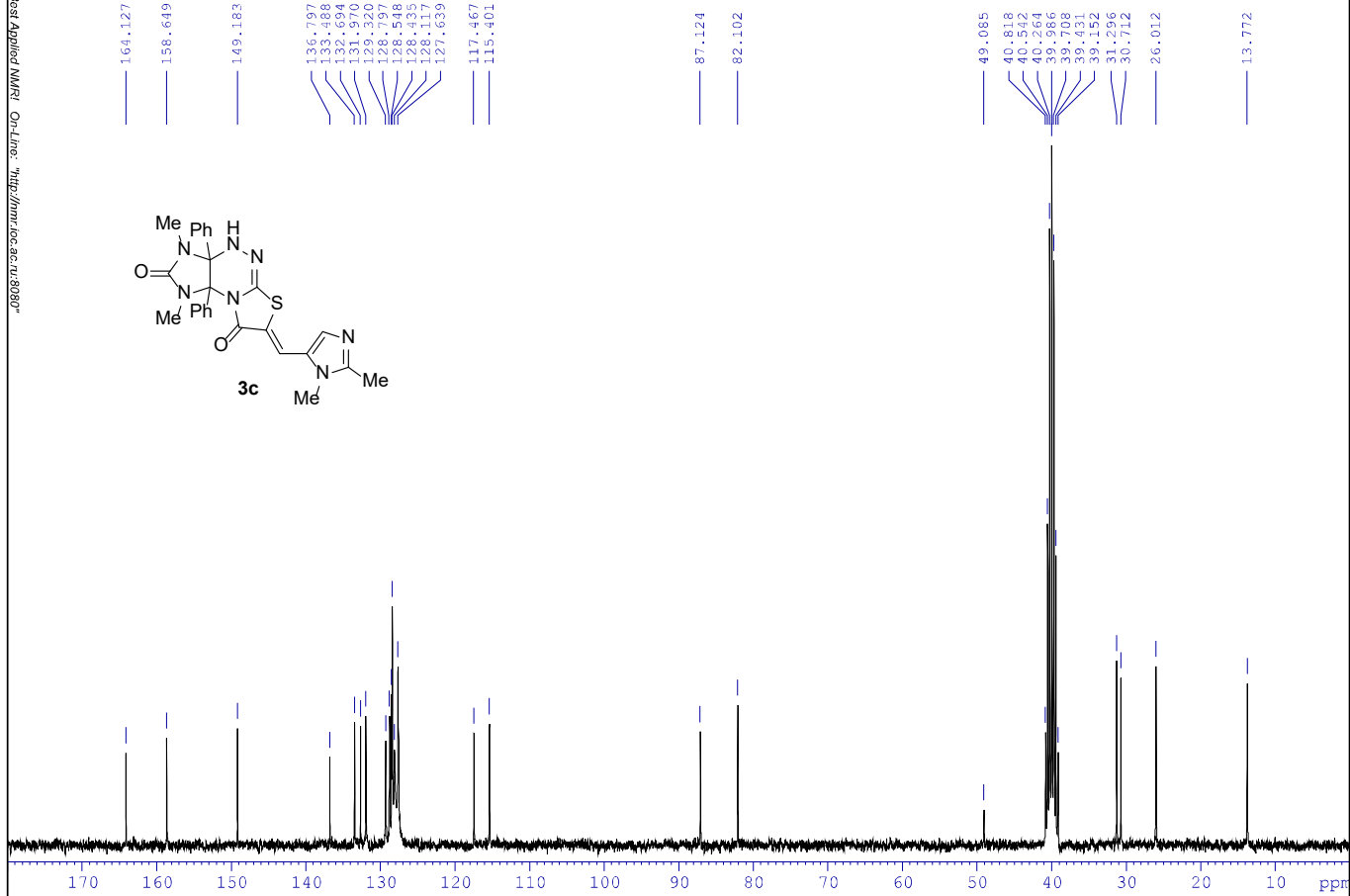


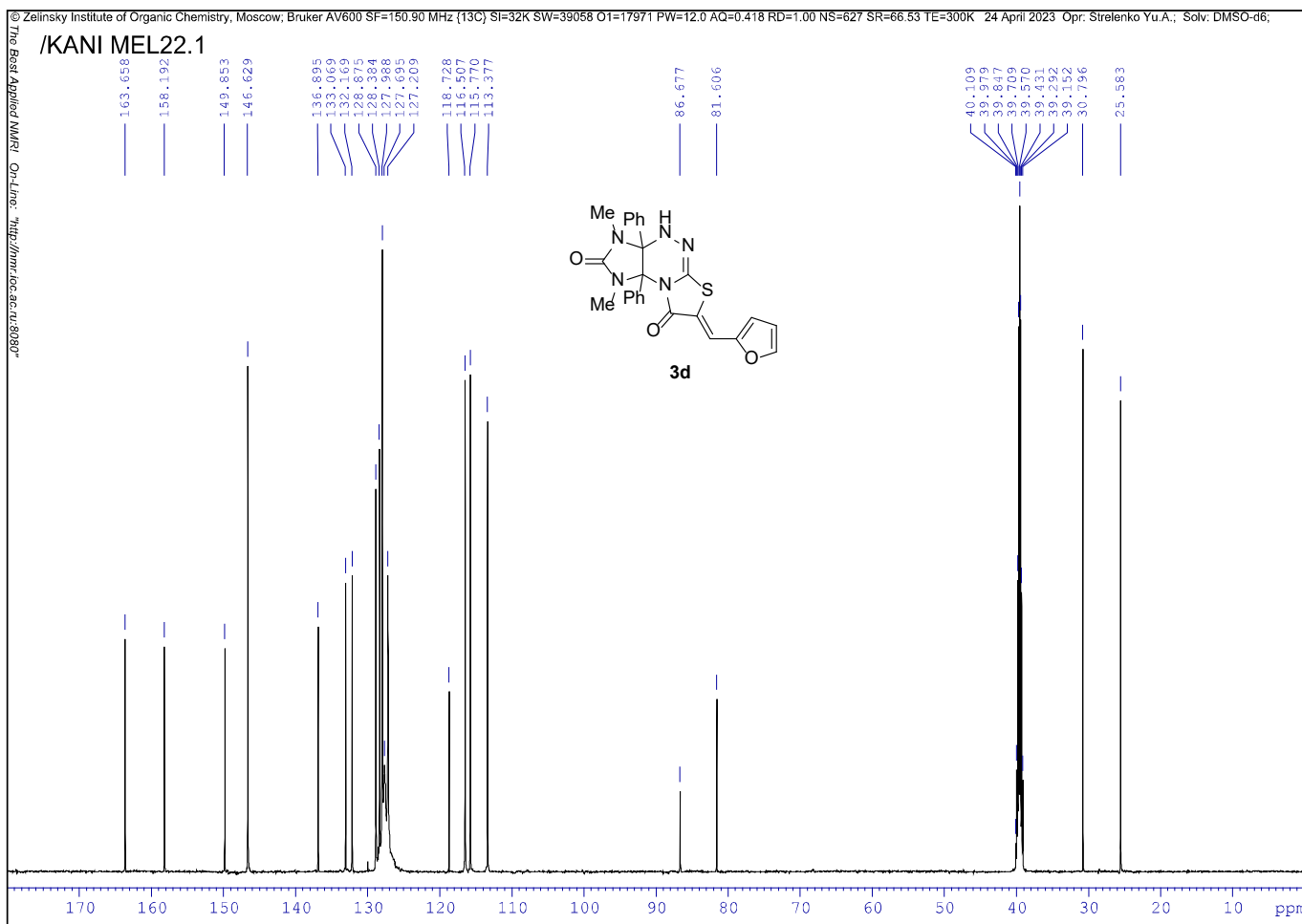
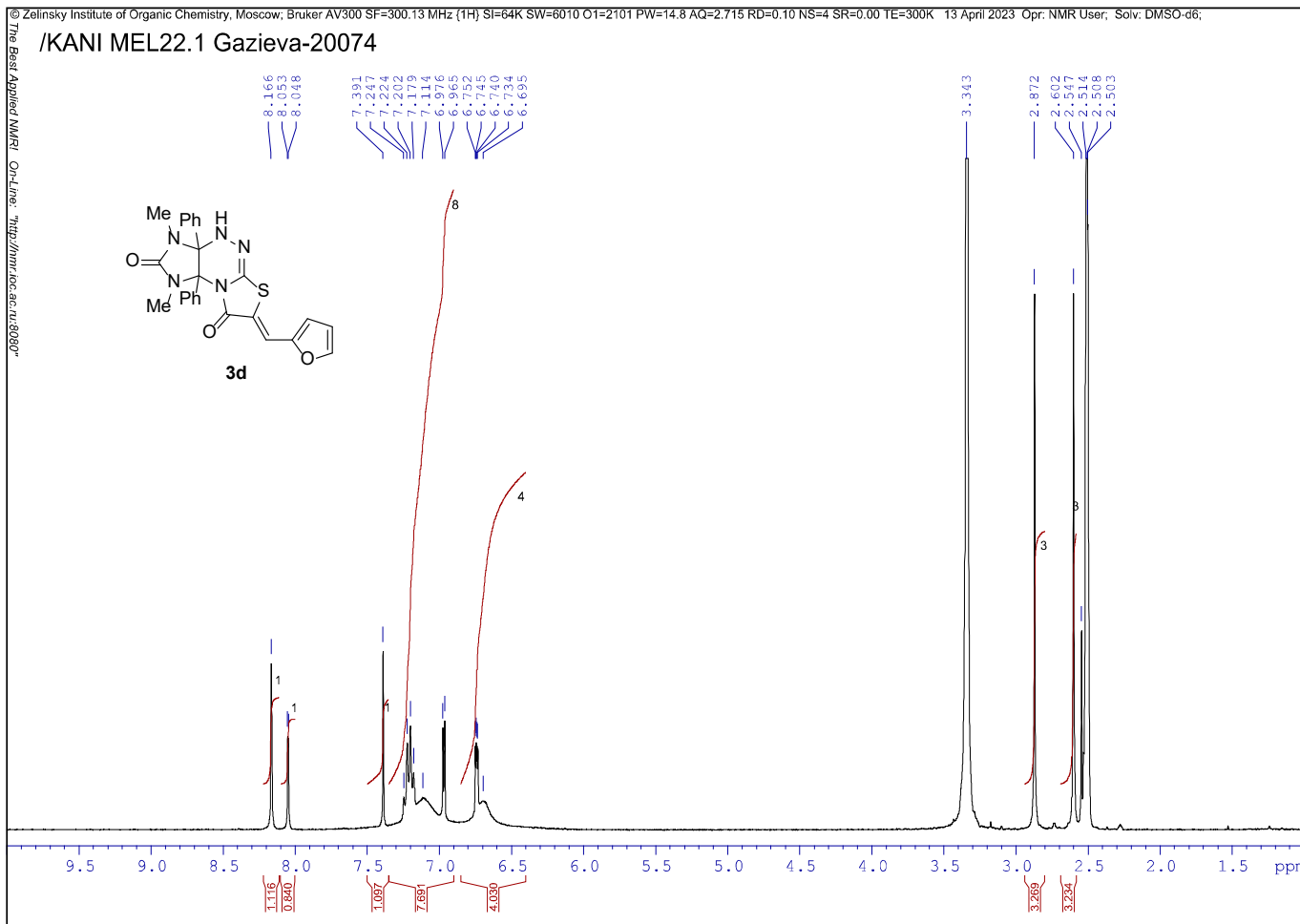


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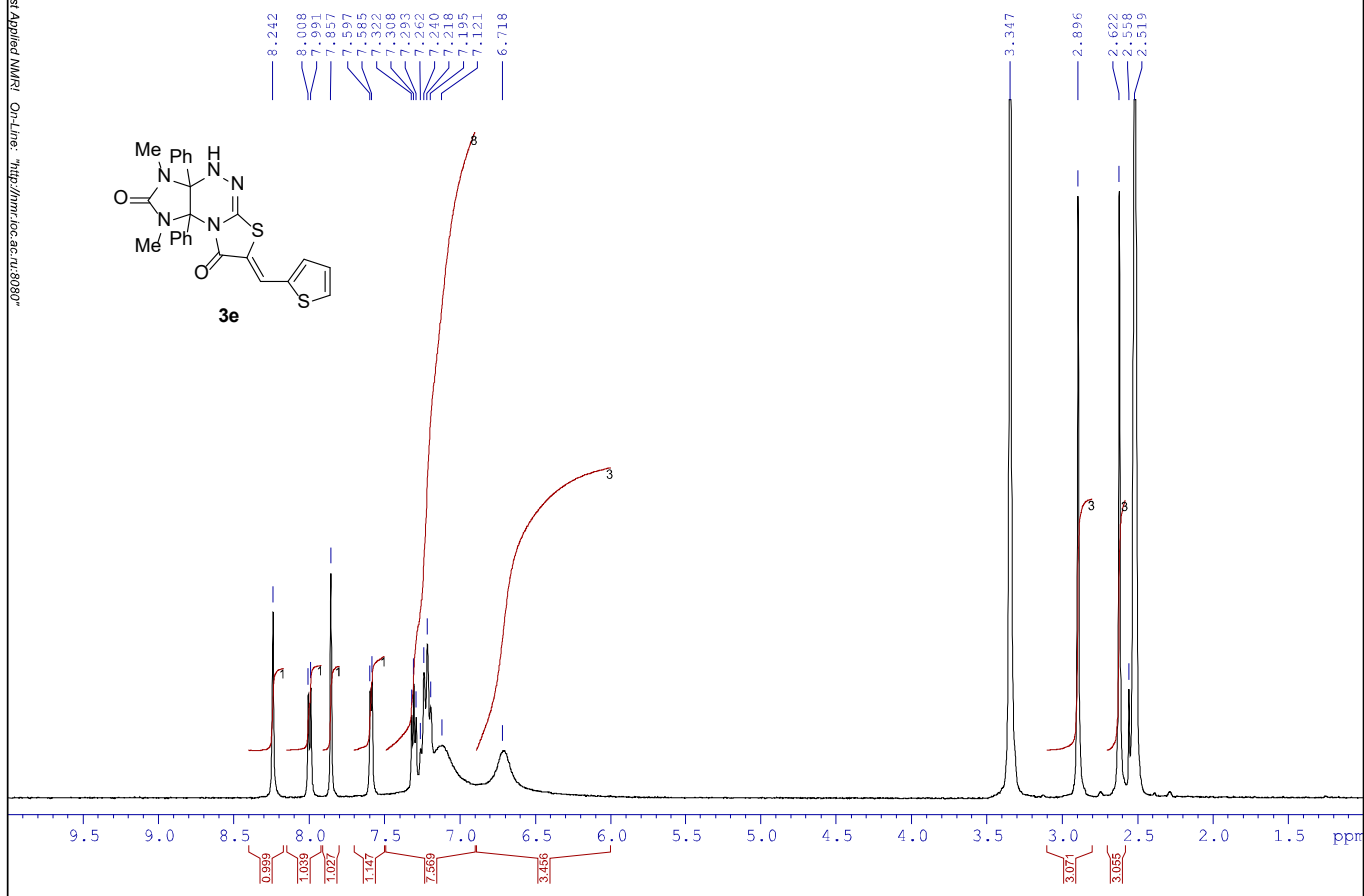
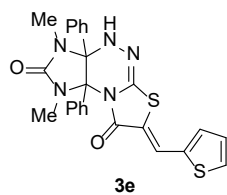


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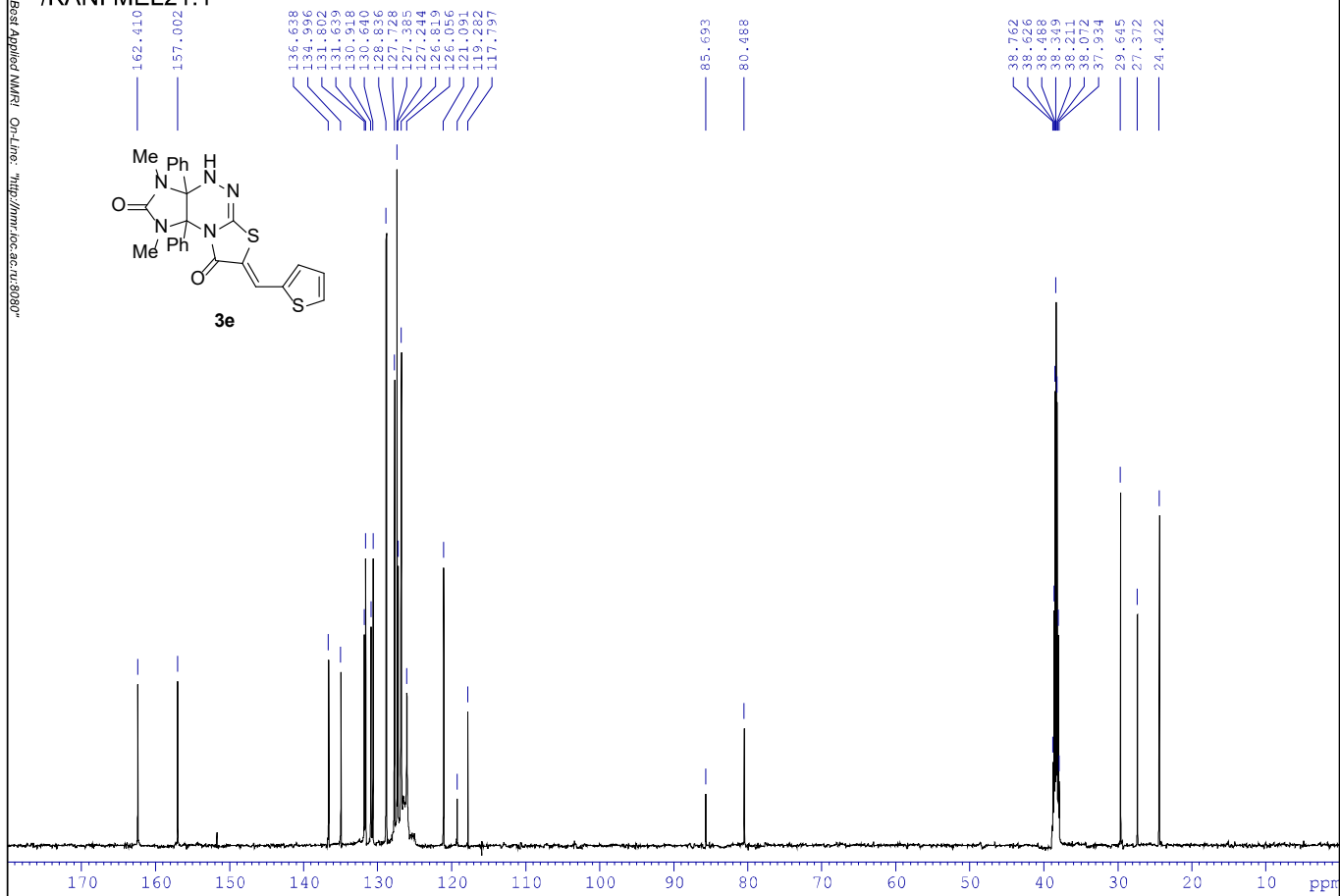
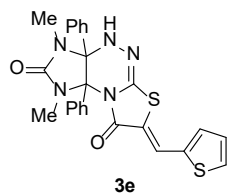


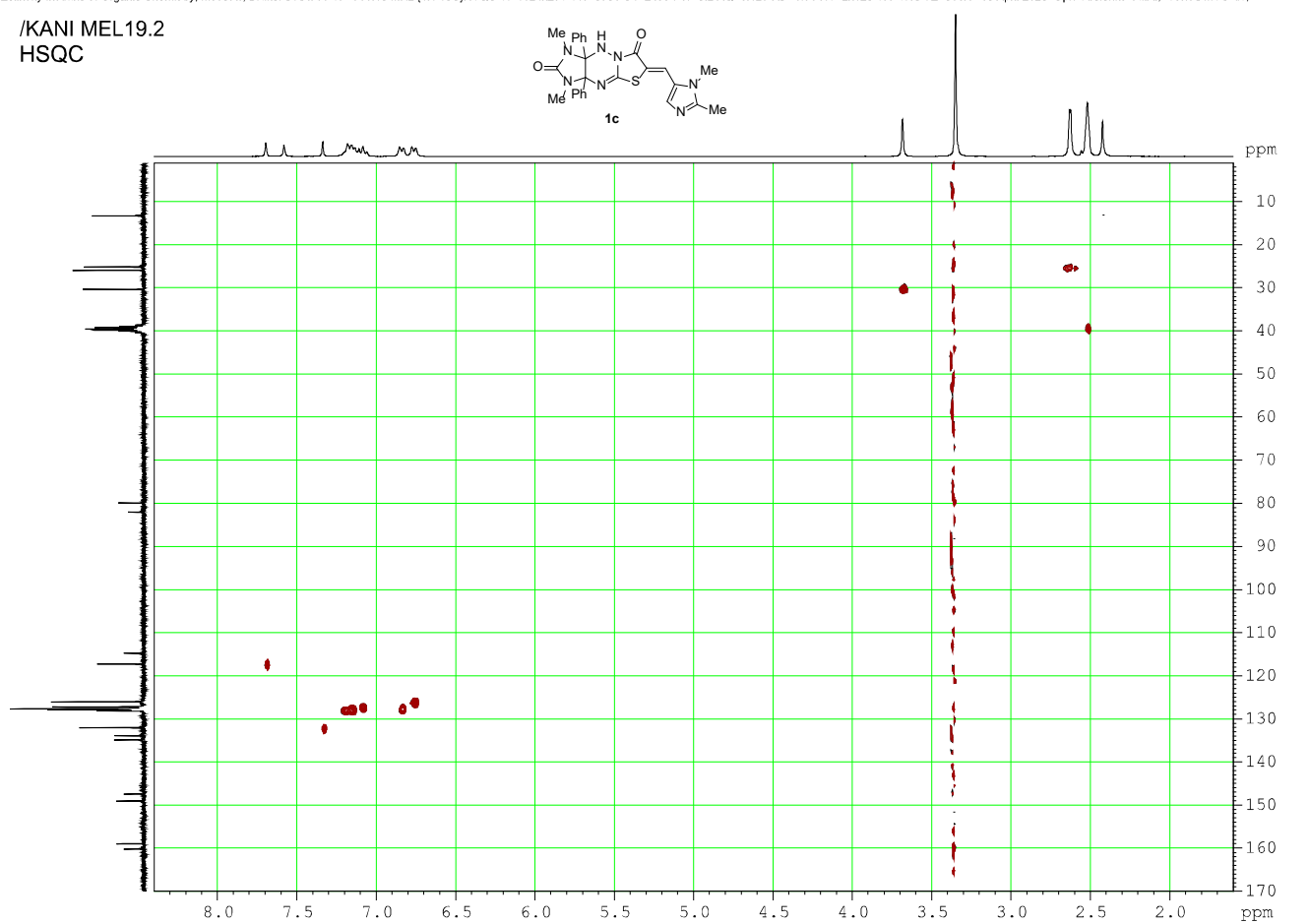


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1H-13C HMBC-qc, DRX500

