Supplementary Information

A new reversible transformation of oxindolylidene derivatives of imidazothiazolotriazine into 3-[(imidazotriazin-3-yl)thio]-2-oxoquinoline-4-carboxylates

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General Methods

Commercially available solvents and reagents were used as purchased.

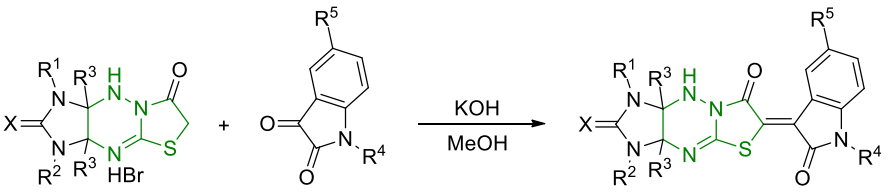
NMR spectroscopy was performed at 298 K using an Bruker AM300 (300.13 MHz, ^{1}H; 75.47 MHz, ^{13}C) or an Bruker DRX500 (500.13 MHz, ^{1}H; 125.76 MHz, ^{13}C). Data is expressed in parts per million (ppm) downfield shift from tetramethylsilane with residual solvent as an internal reference (δ 2.50 ppm for DMSO-d_6 or 4.79 ppm for D_2O) and is reported as position (δ in ppm), multiplicity (s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets), coupling constant (*J* in Hz) and integration (number of protons). ^{13}C NMR spectra were recorded at 298 K with complete proton decoupling. Data is expressed in parts per million (ppm) downfield shift relative to the internal reference (δ 39.51 ppm for DMSO-d_6).

Infrared spectra were obtained on a BrukerALPHA spectrometer using KBr pellets and are reported in wavenumbers (cm^{-1}).

HRMS were performed at the Bruker micrOTOF II 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 μL/min). N_2 was applied as a dry gas.

General procedure for the synthesis of compounds 1a–r

Compounds **1a–r** were prepared according to a known procedure.[1–7] To a stirred suspension of imidazothiazolotriazine **5a–e** (1.0 mmol) and isatin **6a–h** in refluxing methanol (7.5 mL), 0.107 ml of 40% aqueous KOH (1.07 mmol, 1.07 equiv.) was added. The resulting mixture was refluxed with stirring for 2 h. After cooling, the precipitate of compounds **1a–r** was filtered off, washed with methanol and dried in air.



5 **6** **1a-o**

Imidazothiazolo-triazine **5**	X, R^1, R^2, R^3	Isatin **6**	R^4, R^5	Product	Yield
5a	O, Et, Et, H,	**6a**	3-pentyl, H	**1a**	61%
5b	S, Et, Et, H,		3-pentyl, H	**1b**	52%
5c	O, Me, Me, H,		3-pentyl, H	**1c**	72%
5d	O, Me, Ph, H,		3-pentyl, H	**1d**	81%
5e	O, Me, Me, Ph,		3-pentyl, H	**1e**	65%
5a	O, Et, Et, H,	**6b**	cyclopentyl, H	**1f**	67%
5b	S, Et, Et, H,		cyclopentyl, H	**1g**	67%
5c	O, Me, Me, H,		cyclopentyl, H	**1h**	68%
5a	O, Et, Et, H,	**6c**	*i*-Am, H	**1i**	56%
5b	S, Et, Et, H,		*i*-Am, H	**1j**	65%
5c	O, Me, Me, H,		*i*-Am, H	**1k**	65%
5a	O, Et, Et, H,	**6d**	*i*-Bu, H	**1l**	75%
5b	S, Et, Et, H,		*i*-Bu, H	**1m**	70%
5c	O, Me, Me, H,		*i*-Bu, H	**1n**	60%
5a	O, Et, Et, H,	**6e**	3-pentyl, Me	**1o**	65%

(*Z*)-1,3-Diethyl-6-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-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: 284 mg (61%); orange solid; mp 234–236 °C. ^{1}H NMR spectra data are consistent with the literature values.[1]

(*Z*)-1,3-Diethyl-6-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-2-thioxo-1,2,3,3a,9,9a-hexahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazin-7(6*H*)-one (1b). Yield: 348 mg (52%); orange solid; mp 217–219 °C. IR (KBr): 3433, 3247, 3226, 2968, 2931, 2874, 1687, 1636, 1605, 1461, 1414, 1355, 1267, 1250, 1075, 878, 747 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.75 (t, *J* = 7.2 Hz, 6H, 2CH_3), 1.02 (t, *J* = 6.9 Hz, 3H, CH_3), 1.23 (t, *J* = 7.0 Hz, 3H, CH_3), 1.73-1.81 (m, 2H, CH_2), 1.96-2.02 (m, 2H, CH_2), 3.38-3.61 (m, 3H, NCH_2), 3.83-3.95 (m, 1H, NCH_2), 4.11-4.15 (m, 1H, NCH), 5.19-5.26 (m, 2H, 3a-H, 9a-H), 7.08-7.16 (m, 2H, 5'-H, NH), 7.28 (d, *J* = 7.9 Hz, 1H, 7'-H), 7.42 (t, *J* = 7.6 Hz, 1H, 6'-H), 8.89 (d, *J* = 7.8 Hz, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 10.85, 11.95, 13.06 (4CH_3), 24.20 (2CH_2), 38.02, 38.50 (2NCH_2), 56.58 (1'-NCH), 64.91, 66.86 (C-3a, C-9a), 110.08 (C-7'), 119.40 (C-3a'), 122.10, 124.63, 127.68, 129.45, 131.77 (C-3', C-4', C-5', C-6', C-6), 143.48 (C-7a'), 151.42 (C=N), 160.36 (7-C=O), 167.37 (2'-C=O), 181.07 (C=S). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{23}H_{28}N_6O_2S_2$: 485.1788; found: 485.1780.

(*Z*)-1,3-Dimethyl-6-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1c). Yield: 317 mg (72%); bright orange solid; mp 155–157 °C. IR (KBr): 3408, 3204, 2967, 2931, 2879, 1694, 1641, 1607, 1458, 1367, 1255, 1072, 755 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.75 (t, *J* = 7.3, 6H, 2CH_3), 1.73-1.82 (m, 2H, CH_2),

1.96-2.02 (m, 2H, CH_2), 2.61 (s, 3H, CH_3), 2.79 (s, 3H, CH_3), 4.12-4.16 (m, 1H, NCH), 4.80 (d, *J* = 5.7, 1H, 9a-H), 4.92 (d, *J* = 5.8, 1H, 3a-H), 7.04 (s, 1H, NH), 7.13 (t, *J* = 7.7, 1H, 5'-H), 7.28 (d, *J* = 8.0, 1H, 7'-H), 7.42 (t, *J* = 7.8, 1H, 6'-H), 8.19 (d, *J* = 7.8, 1H, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 10.85 ($2CH_3$), 24.21, 26.90, 27.71 ($2CH_2$, $2NCH_3$), 56.58 (1'-NCH), 65.17, 66.08 (C-3a, C-9a), 110.08 (C-7'), 119.43 (C-3a'), 122.07 (C-5'), 124.33, 127.66, 130.06, 131.66 (C-3', C-4', C-6', C-6), 143.46 (C-7a'), 150.09 (C=N), 158.64 (2-C=O), 160.43 (7-C=O), 167.41 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{24}N_6O_3S$: 441.1703; found: 441.1697.

(*Z*)-1-Methyl-6-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-3-phenyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1d). Yield: 407 mg (81%); orange solid; mp 220–200 °C. IR (KBr): 3434, 2964, 2876, 1728, 1687, 1625, 1602, 1501, 1462, 1378, 1358, 1268, 1268, 1143, 1106, 1075, 752 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.74 (t, *J* = 7.1 Hz, 6H, $2CH_3$), 1.72-1.81 (m, 2H, CH_2), 1.94-2.04 (m, 2H, CH_2), 2.75 (s, 3H, NCH_3), 4.12-4.16 (m, 1H, NCH), 5.04 (d, *J* = 6.3 Hz, 1H, 9a-H), 5.66 (d, *J* = 6.0 Hz, 1H, 3a-H), 7.04-7.18 (m, 3H, 5'-H, Ph-4, NH), 7.27-7.45 (m, 4H, 6'-H, 7'-H, Ph-3,5), 7.73 (d, *J* = 8.2 Hz, 2H, Ph-2,6), 8.92 (d, *J* = 7.8 Hz, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 10.83 ($2CH_3$), 24.21, 27.48 ($2CH_2$, 1-NCH_3), 56.60 (1'-NCH), 64.24, 65.19 (C-3a, C-9a), 110.07 (C-7'), 119.25, 119.42 (C-3a', Ph-2,6), 122.08, 122.77, 124.55, 127.70 (C-3', C-4', C-5', Ph-4), 128.54 (Ph-3,5), 129.84 (C-6), 131.72 (C-6'), 138.57 (Ph-1), 143.57 (C-7a'), 150.88 (C=N), 155.63 (2-C=O), 160.34 (7-C=O), 167.38 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{26}H_{26}N_6O_3S$: 503.1860; found: 503.1851.

(*Z*)-1,3-Dimethyl-6-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-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 (1e). Yield: 385 mg (65%); red solid; mp 271–273 °C. IR (KBr): 3433, 3214, 2961, 2934, 2875, 1724, 1711, 1684, 1637, 1605, 1463, 1358, 1077, 1012, 734 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.79 (t, *J* = 7.3 Hz, 6H, $2CH_3$), 1.76-1.85 (m, 2H, CH_2), 1.99-2.10 (m, 2H, CH_2), 2.63 (s, 3H, NCH_3), 2.64 (s, 3H, NCH_3), 4.17-4.21 (m, 1H, NCH), 6.76 (d, *J* = 7.0 Hz, 2H, Ph-2,6), 6.83 (d, *J* = 7.3 Hz, 2H, Ph-2,6), 7.05-7.22 (m, 7H, 5′-H, 2Ph-3-5), 7.32 (d, *J* = 7.9 Hz, 1H, 7'-H), 7.44 (t, *J* = 7.3 Hz, 1H, 6'-H), 7.84 (s, 1H, NH), 8.95 (d, *J* = 7.8 Hz, 1H, 4'-H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 10.99 ($2CH_3$), 24.34, 25.39, 26.11 ($2CH_2$, $2NCH_3$), 56.72 (1'-NCH), 79.91, 81.96 (C-3a, C-9a), 110.31 (C-7'), 119.59 (C-3a'), 122.28, 124.46, 126.38, 127.42, 127.94, 128.05, 128.31, 131.92 (C-3', C-4', C-5', C-6', C-6, 2Ph-2-6), 134.09, 134.88 (2Ph-1), 149.14 (C=N), 159.22, 159.64 (2-C=O, 7-C=O), 167.64 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{33}H_{32}N_6O_3S$: 593.2329; found: 593.2330.

(*Z*)-6-(1-Cyclopentyl-2-oxoindolin-3-ylidene)-1,3-diethyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*] thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1f). Yield: 312 mg (67%); orange solid; mp 231–233 °C. ^{1}H NMR spectra data are consistent with the literature values.[1]

(*Z*)-6-(1-Cyclopentyl-2-oxoindolin-3-ylidene)-1,3-diethyl-2-thioxo-1,2,3,3a,9,9a-hexahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazin-7(6*H*)-one (1g). Yield: 323 mg (67%); brownish orange solid; mp 248–250 °C. IR (KBr): 3269, 2972, 2934, 2873, 1689, 1645, 1604, 1463, 1367, 1247, 1116, 1078, 880, 752 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 1.01 (t, *J* = 7.0 Hz, 3H, CH_3), 1.22 (t, *J* = 7.1 Hz, 3H, CH_3), 1.63-1.66 (m, 2H, Alk), 1.88-2.04 (m, 6H, Alk), 3.39-3.60 (m, 3H, CH_2), 3.85-3.92 (m, 1H, CH_2), 4.67-4.73 (m, 1H, 1′-NCH), 5.18 (d, *J* = 6.9 Hz, 1H, CH), 5.24 (d, *J* = 6.9 Hz, 1H, CH), 7.08-7.22 (m, 2H, 5′-H, 7′-H), 7.45 (t, *J* = 7.9 Hz, 1H, 6′-H), 8.87 (d, *J* = 7.8 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.44, 13.57 ($2CH_3$), 25.09, 28.23 ($4CH_2$), 38.55, 39.01 ($2NCH_2$), 53.12 (1'-NCH), 65.31, 67.22 (C-3a, C-9a), 110.48 (C-7'), 120.05, 122.70, 125.57, 128.16, 129.54, 132.26 (C-3',C-3a', C-4', C-5', C-6', C-6), 143.50 (C-7a'), 151.96 (C=N), 160.88 (7-C=O),

167.29 (2'-C=O), 181.55 (C=S). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{23}H_{26}N_6O_2S_2$: 483.1631; found: 483.1629.

(*Z*)-6-(1-Cyclopentyl-2-oxoindolin-3-ylidene)-1,3-dimethyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1h). Yield: 298 mg (68%); orange solid; mp 243–245 °C. IR (KBr): 3434, 3199, 2951, 2916, 2871, 1686, 1638, 1606, 1463, 1356, 1250, 1077, 1012, 872, 787, 746 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 1.62-1.68 (m, 2H, CH_2), 1.87-2.07 (m, 6H, CH_2), 2.61 (s, 3H, NCH_3), 2.79 (s, 3H, NCH_3), 4.68-4.75 (m, 1H, NCH), 4.80 (d, *J* = 5.6 Hz, 1H, 9a-H), 4.91 (d, *J* = 5.9 Hz, 1H, 3a-H), 6.99 (s, 1H, NH), 7.13 (t, *J* = 7.6 Hz, 1H, 5'-H), 7.20 (d, *J* = 7.9 Hz, 1H, 7'-H), 7.44 (t, *J* = 7.7 Hz, 6'-H), 8.88 (d, *J* = 7.8 Hz, 1H, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 24.54, 26.88, 27.71, 27.78 ($2CH_3$, $4CH_2$), 52.60 (1'-NCH), 65.12, 66.04 (C-3a, C-9a), 109.85 (C-7'), 119.59 (C-3a'), 122.07, 124.68, 127.60, 129.64, 131.51 (C-3', C-4', C-5', C-6, C-6'), 142.88 (C-7a'), 150.06 (C=N), 158.63 (2-C=O), 160.33 (7-C=O), 167.78 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{22}N_6O_3S$: 439.1547; found: 439.1543.

(*Z*)-1,3-Diethyl-6-(1-isopentyl-2-oxoindolin-3-ylidene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*] thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1i). Yield: 262 mg (56%); orange solid; mp 192–194 °C. ^1H NMR spectra data are consistent with the literature values.[1]

(*Z*)-1,3-Diethyl-6-(1-isopentyl-2-oxoindolin-3-ylidene)-2-thioxo-1,2,3,3a,9,9a-hexahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazin-7(6*H*)-one (1j). Yield: 315 mg (65%); brownish orange solid; mp 237–239 °C. IR (KBr): 3435, 3271, 2959, 2932, 2871, 1690, 1642, 1608, 1467, 1370, 1243, 1077, 879, 754 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.92 (d, *J* = 6.1 Hz, 6H, $2CH_3$), 1.02 (t, *J* = 7.1 Hz, 3H, CH_3), 1.23 (t, *J* = 7.2 Hz, 3H, CH_3), 1.46-1.59 (m, 3H, CH_2, CH), 3.38-3.58 (m, 3H, NCH_2), 3.79 (t, *J* = 7.1 Hz, 2H, 1′-NCH_2), 3.86-3.93 (m, 1H, NCH_2), 5.18-5.26 (m, 2H, 3a-H, 9a-H), 7.10-7.16 (m, 3H, 5′-H, 7′-H, NH), 7.46 (t, *J* = 7.8 Hz, 1H, 6′-H), 8.83 (d, *J* = 7.6 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.44, 13.59, 22.71, 22.77, 25.79 (CH, CH_2, $4CH_3$), 36.12, 38.53, 39.00 ($3NCH_2$), 65.36, 67.29 (C-3a, C-9a), 109.73 (C-7'), 119.91, 122.87, 125.24, 128.08, 129.78, 132.35 (C-3', C-3a', C-4', C-5', C-6', C-6), 143.77 (C-7a'), 151.81 (C=N), 150.79 (7-C=O), 167.26 (2'-C=O), 181.55 (C=S). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{23}H_{28}N_6O_2S_2$: 485.1788; found: 485.1780.

(*Z*)-6-(1-Isopentyl-2-oxoindolin-3-ylidene)-1,3-dimethyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1k). Yield: 286 mg (65%); orange solid; mp 238–240 °C. IR (KBr): 3435, 3193, 2963, 2932, 2873, 1697, 1641, 1609, 1469, 1372, 1246, 1075, 743 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.93 (d, *J* = 6.2 Hz, 6H, $2CH_3$), 1.47-1.58 (m, 3H, CH, CH_2), 2.61 (s, 3H, CH_3), 2.80 (s, 3H, CH_3), 3.78 (t, *J* = 6.8 Hz, 2H, 1′-NCH_2), 4.79 (d, *J* = 5.7 Hz, 1H, 9a-H), 4.91 (d, *J* = 5.9 Hz, 1H, 3a-H), 7.10-7.15 (m, 2H, 5′-H, 7′-H), 7.45 (t, *J* = 7.8 Hz, 1H, 6′-H), 8.83 (d, *J* = 7.8 Hz, 1H, 4′-H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 22.87, 22.89 ($2CH_3$), 25.95, 27.57, 28.48 (CH, $2NCH_3$), 36.27, 38.71 ($2CH_2$), 65.72, 66.63 (C-3a, C-9a), 109.79 (C-7'), 120.06, 122.96, 125.06, 128.20, 130.50, 132.36 (C-3', C-3a', C-4', C-5', C-6', C-6), 143.82 (C-7a'), 150.68 (C=N), 159.37, 161.05 (2-C=O, 7-C=O), 167.41 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{24}N_6O_3S$: 441.1703; found: 441.1694.

(*Z*)-1,3-Diethyl-6-(1-isobutyl-2-oxoindolin-3-ylidene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*] thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1l). Yield: 340 mg (75%); orange solid; mp 227–228 °C. ^1H NMR spectra data are consistent with the literature values.[1]

(*Z*)-1,3-Diethyl-6-(1-isobutyl-2-oxoindolin-3-ylidene)-2-thioxo-1,2,3,3a,9,9a-hexahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazin-7(6*H*)-one (1m). Yield: 329 mg (70%); orange solid; mp 236–237 °C. IR (KBr): 3435, 3239, 2965, 2932, 2872, 1694, 1638, 1608, 1467, 1415, 1374, 1270, 1245, 1112, 1074, 876, 749 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.86-0.89 (m, 6H, $2CH_3$), 1.02 (t, *J* = 7.0 Hz, 3H, CH_3), 1.22 (t, *J* = 7.2 Hz, 3H, CH_3), 2.02-2.11 (m, 1H, CH), 3.37-3.60 (m, 5H, NCH2, 1′-NCH_2), 3.83-3.93 (m, 1H, NCH_2), 5.18-5.25 (m, 2H, 3a-H, 9a-H), 7.10-7.19 (m, 3H, 5′-H, 7′-H, NH), 7.44 (t, *J* = 7.7 Hz, 1H, 6′-H), 8.82 (d, *J* = 7.6 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.98, 13.13, 19.89, 19.92 ($4CH_3$), 26.74 (CH), 38.10, 38.57 ($2NCH_3$), 47.05 (1′-NCH_2), 64.88, 66.78 (C-3a, C-9a), 109.63 (C-7'), 119.30, 122.41, 124.75, 127.56, 129.35, 131.86 (C-3', C-3a', C-4', C-5', C-6', C-6), 143.85 (C-7a'), 151.44 (C=N), 160.42 (7-C=O), 167.24 (2'-C=O), 181.12 (2-C=S). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{22}H_{26}N_6O_2S_2$: 471.1631; found: 471.1615.

(*Z*)-6-(1-Isobutyl-2-oxoindolin-3-ylidene)-1,3-dimethyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1n). Yield: 256 mg (60%); orange solid; mp 230–232 °C. IR (KBr): 3434, 3205, 2961, 2928, 2873, 1722, 1692, 1641, 1607, 1466, 1377, 1351, 1247, 1072, 1014, 875, 748 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.87 (d, *J* = 6.6 Hz, 6H, $2CH_3$), 2.02-2.11 (m, 1H, CH), 2.61 (s, 3H, CH_3), 2.79 (s, 3H, CH_3), 3.58 (d, *J* = 7.5 Hz, 2H, NCH_2), 4.79 (d, *J* = 5.9 Hz, 1H, 9a-H), 4.91 (d, *J* = 5.9 Hz, 1H, 3a-H), 7.09-7.18 (m, 2H, 5′-H, 7′-H), 7.43 (t, *J* = 7.6 Hz, 1H, 6′-H), 8.83 (d, *J* = 7.7 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 19.88 ($2CH_3$), 26.73, 26.98, 27.86 (CH, $2NCH_3$), 47.04 (1′-NCH_2), 65.20, 66.07 (C-3a, C-9a), 109.52 (C-7'), 119.34, 122.32, 124.43, 127.53, 129.94, 131.68 (C-3', C-3a', C-4', C-5', C-6', C-6), 143.76 (C-7a'), 150.14 (C=N), 158.75, 160.45 (2-C=O, 7-C=O), 167.24 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{22}N_6O_3S$: 427.1547; found: 427.1547.

(*Z*)-1,3-Diethyl-6-(5-methyl-2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1o). Yield: 313 mg (65%); bright orange solid; mp 174–175 °C. IR (KBr): 3207, 2970, 2941, 2877, 1729, 1685, 1669, 1637, 1472, 1348, 1250, 1073, 770 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.73 (t, *J* = 7.2 Hz, 6H, $2CH_3$), 0.97 (t, *J* = 7.0 Hz, 3H, CH_3), 1.15 (t, *J* = 7.1 Hz, 3H, CH_3), 1.71-1.82 (m, 2H, CH_2), 1.93-1.98 (m, 2H, CH_2), 2.33 (s, 3H, 5′-CH_3), 3.08-3.20 (m, 3H, CH_2), 3.34-3.42 (m, 1H, CH_2), 4.09-4.11 (m, 1H, 1′-NCH), 4.93 (dd, *J* = 6.1, 1.7 Hz, 1H, 9a-H), 4.98 (d, *J* = 5.9 Hz, 1H, 3a-H), 6.98 (s, 1H, NH), 7.16 (d, *J* = 8.1 Hz, 1H), 7.22 (d, *J* = 8.3 Hz, 1H), 8.75 (s, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.37, 13.29, 13.94 ($3CH_3$), 21.28 (5'-CH_3), 24.71 ($2CH_2$), 34.93, 35.52 ($2NCH_2$), 57.06 (1'-NCH), 63.64, 64.79 (C-3a, C-9a), 110.43 (C-7'), 119.99 (C-3a'), 125.10, 128.69, 130.10, 131.46, 132.61 (C-3', C-4', C-5', C-6', C-6), 141.89 (C-7a'), 150.63 (C=N), 158.19 (2-C=O), 160.94 (7-C=O), 167.89 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{24}H_{30}N_6O_3S$: 483.2173; found: 483.2170.

(*Z*)-6-(1-Benzyl-2-oxoindolin-3-ylidene)-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 (1p). Yield: 380 mg (62%); orange solid; mp 218–221 °C. ^1H NMR spectra data are consistent with the literature values.[2,3]

(*Z*)-1,3-Diethyl-6-(5-methyl-2-oxo-1-pentylindolin-3-ylidene)-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1q). Yield: 318 mg (66%); orange solid; mp 230–232 °C. ^1H NMR spectra data are consistent with the literature values.[4]

(*Z*)-6-(5-Chloro-2-oxo-1-pentylindolin-3-ylidene)-1,3-diethyl-3,3a,9,9a-tetrahydroimidazo[4,5-*e*]thiazolo[3,2-*b*][1,2,4]triazine-2,7(1*H*,6*H*)-dione (1r). Yield: 306 mg (61%); orange solid; mp: 233–236 °C. ^1H NMR spectra data are consistent with the literature values.[4]

General procedure for the synthesis of compounds 2a–o

Compounds **2a–d,f–o** were prepared according to a known procedure.[1,4–7] Compound **2e** was prepared according to a known procedure.[8] To a stirred suspension of imidazothiazolotriazine **5a–d** (1.0 mmol) and isatin **6a–e** in refluxing methanol (7.5 mL), 0.160 ml of 40% aqueous KOH (1.6 mmol, 1.6 equiv.) was added. The resulting mixture was refluxed with stirring for 45 min. After cooling, the precipitate of compounds **2a–d,f–o** was filtered off, washed with methanol and dried in air.

For the synthesis of the compound **2e**: To a stirred suspension of compound **1e** (0.5 mmol) in refluxing methanol (7.5 mL), 0.046 ml (0.25 mmol, 0.5 equiv.) of NaOMe (as 30% solution in MeOH) was added. The resulting mixture was refluxed with stirring for 15 min. After cooling, the precipitate of compound **2e** was filtered off, washed with methanol and dried in air.

(*Z*)-1,3-Diethyl-7-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-1,3a,4,9a-tetrahydroimidazo[4,5-*e*] thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2a). Yield: 416 mg (89%); bright orange solid; mp 213–215 °C. ^{1}H NMR spectra data are consistent with the literature values.[1]

(*Z*)-1,3-Diethyl-7-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-2-thioxo-1,2,3,3a,4,9a-hexahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazin-8(7*H*)-one (2b). Yield: 290 mg (60%); red solid; mp 229–232 °C. IR (KBr): 3433, 3291, 2969, 2931, 2874, 1719, 1682, 1636, 1604, 1462, 1402, 1358, 1335, 1266, 1228, 1081, 881, 751 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.74 (t, J = 7.3 Hz, 6H, 2CH_3), 1.09 (t, J = 7.1 Hz, 3H, CH_3), 1.19 (t, J = 6.9 Hz, 3H, CH_3), 1.71-1.82 (m, 2H, CH_2), 1.94-2.06 (m, 2H, CH_2), 3.31-3.42 (m, 1H, NCH_2), 3.51-3.63 (m, 1H, NCH_2), 3.68-3.80 (m, 1H, NCH_2), 3.95-4.07 (m, 1H, NCH_2), 4.13-4.17 (m, 1H, NCH), 5.17 (d, J = 6.2 Hz, 1H, 3a-H), 5.95 (d, J = 6.1 Hz, 1H, 9a-H), 7.13 (t, J = 7.6 Hz, 1H, 5'-H), 7.27 (d, J = 6.8 Hz, 1H, 7'-H), 7.39 (t, J = 7.4 Hz, 1H, 6'-H), 8.19 (s, 1H, NH), 8.24 (d, J = 7.7 Hz, 1H, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.41, 12.61, 12.92 (4CH_3), 24.80 (2CH_2), 38.89, 41.64 (2NCH_2), 57.09 (1'-NCH), 65.15, 65.65 (C-3a, C-9a), 110.52 (C-7'), 120.10 (C-3a'), 122.47, 122.80, 127.77, 131.49, 133.78 (C-3', C-4', C-5', C-6', C-7), 137.78 (C=N), 143.48 (C-7a'), 164.39(8-C=O), 167.97 (2'-C=O), 182.60 (C=S). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{23}H_{28}N_6O_2S_2$: 485.1788; found: 485.1778.

(*Z*)-1,3-Dimethyl-7-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2c). Yield: 304 mg (69%); orange solid; mp 222–223 °C. IR (KBr): 3434, 3282, 2971, 2934, 2875, 1727, 1683, 1643, 1461, 1341, 1341, 1242, 750 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.74 (t, J = 7.3 Hz, 6H, 2CH_3), 1.74-1.83 (m, 2H, CH_2), 1.96-2.02 (m, 2H, CH_2), 2.66 (s, 3H, CH_3), 2.92 (s, 3H, CH_3), 4.13-4.17 (m, 1H, NCH), 4.81 (dd, J = 5.9, 2.0 Hz, 1H, 3a-H), 5.68 (d, J = 5.9 Hz, 1H, 9a-H), 7.12 (t, J = 7.5 Hz, 1H, 5'-H), 7.27 (d, J = 7.7 Hz, 1H, 7'-H), 7.38 (t, J = 7.8 Hz, 1H, 6'-H), 8.02 (d, J = 1.6 Hz, 1H, NH), 8.87 (d, J = 7.9 Hz, 1H, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.42 (2CH_3), 24.80, 28.41, 31.84 (2CH_2, 2NCH_3), 57.04 (1'-NCH), 64.23, 66.23 (C-3a, C-9a), 110.42 (C-7'), 120.20 (C-3a'), 122.39, 127.82, 131.28, 133.77 (C-3', C-4', C-5', C-6', C-7), 143.07 (C-7a'), 137.34 (C=N), 159.49 (2-C=O), 164.59 (8-C=O), 168.01 (2'-C=O). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{24}N_6O_3S$: 441.1703; found: 441.1688.

(*Z*)-3-Methyl-7-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-1-phenyl-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2d). Yield: 387 mg (77%); orange solid; mp 213–218 °C. IR (KBr): 3433, 3246, 2963, 2874, 1721, 1680, 1636, 1601, 1461, 1329, 1329, 1234, 1052, 748 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.72 (t, J = 7.3 Hz, 6H, 2CH_3), 1.71-1.80 (m, 2H, CH_2), 1.93-2.04 (m, 2H, CH_2), 2.71 (s, 3H, NCH_3), 4.10-4.14 (m, 1H, NCH), 5.16 (d, J = 6.2 Hz, 1H, 3a-H), 5.16 (d, J = 5.9 Hz, 1H, 9a-H), 6.93 (t, J = 7.7 Hz, 1H, Ph-4), 7.18-7.23

(m, 2H, 5'-H, 7'-H), 7.28-7.42 (m, 5H, 6'-H, Ph-2,3,5,6), 8.21 (s, 1H, NH), 8.28 (d, *J* = 7.7 Hz, 1H, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 10.90 ($2CH_3$), 24.25, 27.64 ($2CH_2$, 3-NCH_3), 56.50 (1'-NCH), 64.62, 65.00 (C-3a, C-9a), 109.91 (C-7'), 119.45 (C-3a'), 121.70, 121.90 (C-3', C-5'), 125.07 (Ph-2,6), 125.38, 126.91 (C-4', Ph-4), 128.19 (Ph-3,5), 130.77 (C-6'), 132.63 (C-7), 137.28, 138.64 (Ph-1, C=N), 156.84 (2-C=O), 162.80 (8-C=O), 167.40 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{26}H_{26}N_6O_3S$: 503.1860; found: 503.1852.

(*Z*)-1,3-Dimethyl-7-(2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-3a,9a-diphenyl-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2e). Yield: 426 mg (72%); orange solid; mp 232–234 °C. IR (KBr): 3434, 3290, 2964, 2875, 1707, 1679, 1605, 1464, 1330, 1317, 1287, 1235, 1078, 1013, 750 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.74 (t, *J* = 7.3 Hz, 6H, $2CH_3$), 1.73-1.82 (m, 2H, CH_2), 2.00-2.07 (m, 2H, CH_2), 2.61 (s, 3H, NCH_3), 2.94 (s, 3H, NCH_3), 4.14-4.18 (m, 1H, NCH), 6.69 (br.s, 3H, Ph-3-5), 6.97 (t, *J* = 7.7 Hz, 1H, 5′-H), 7.02-7.34 (m, 9H, Ph-2-6, Ph-2,6, 6′-H, 7′-H), 8.38 (s, 1H, NH), 8.57 (d, *J* = 7.8 Hz, 1H, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 10.92 ($2CH_3$), 24.39, 25.59, 30.98 ($2CH_2$, $2NCH_3$), 56.60 (1'-NCH), 81.49, 86.74 (C-3a, C-9a), 109.90 (C-7'), 119.66 (C-3a'), 121.86, 127.26, 127.74, 128.02, 128.49, 128.96, 130.79, 131.73, 132.84, 133.70, (C-3', C-4', C-5', C-6', C-6, 2Ph), 138.88 (C=N), 142.82 (C-7a'), 158.23 (2-C=O), 163.34 (8-C=O), 167.70 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{33}H_{32}N_6O_3S$: 593.2329; found: 593.2318.

(*Z*)-7-(1-Cyclopentyl-2-oxoindolin-3-ylidene)-1,3-diethyl-1,3a,4,9a-tetrahydroimidazo[4,5-*e*] thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2f). Yield: 317 mg (68%); bright orange solid; mp 255–256 °C. ^{1}H NMR spectra data are consistent with the literature values.[1]

(*Z*)-7-(1-Cyclopentyl-2-oxoindolin-3-ylidene)-1,3-diethyl-2-thioxo-1,2,3,3a,4,9a-hexahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazin-8(7*H*)-one (2g). Yield: 324 mg (67%); orange solid; mp 250–252 °C. IR (KBr): 3290, 2974, 2962, 2933, 2871, 1722, 1680, 1639, 1604, 1464, 1401, 1369, 1330, 1265, 1083, 752 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 1.09 (t, *J* = 7.0 Hz, 3H, CH_3), 1.19 (t, *J* = 7.0 Hz, 3H, CH_3), 1.64-1.69 (m, 2H, CH_2), 1.87-2.06 (m, 6H, CH_2), 3.30-3.41 (m, 1H, CH_2), 3.54-3.61 (m, 1H, CH_2), 3.72-3.79 (m, 1H, CH_2), 3.97-4.04 (m, 1H, CH_2), 4.71-4.76 (m, 1H, 1′-NCH), 5.18 (dd, *J* = 6.1, 2.1 Hz, 1H, 3a-H), 5.96 (d, *J* = 6.1 Hz, 1H, 9a-H), 7.12-7.22 (m, 2H, 5′-H, 7′-H), 7.42 (t, *J* = 7.3 Hz, 1H, 6′-H), 8.20 (d, *J* = 2.0 Hz, 1H, NH), 8.83 (d, *J* = 7.7 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.58, 12.97 ($2CH_3$), 25.13, 28.30 ($4CH_2$), 38.86, 41.71 ($2NCH_2$), 53.10 (1'-NCH), 65.26, 65.61 (C-3a, C-9a), 110.33 (C-7'), 120.28, 122.53, 123.14, 127.74, 131.39, 132.77 (C-3',C-3a', C-4', C-5', C-6', C-6), 137.65 (C=N), 142.87 (C-7a'), 164.30 (7-C=O), 167.36 (2'-C=O), 182.58 (C=S). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{23}H_{26}N_6O_2S_2$: 483.1631; found: 483.1620.

(*Z*)-7-(1-Cyclopentyl-2-oxoindolin-3-ylidene)-1,3-dimethyl-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2h). Yield: 364 mg (83%); reddish orange solid; mp 272–274 °C. IR (KBr): 3434, 3277, 2958, 2925, 2872, 1727, 1678, 1647, 1606, 1464, 1338, 1318, 1244, 753 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 1.63-1.69 (m, 2H, CH_2), 1.87-2.07 (m, 6H, CH_2), 2.66 (s, 3H, NCH_3), 2.92 (s, 3H, NCH_3), 4.71-4.83 (m, 2H, NCH, 3a-H), 5.68 (d, *J* = 5.6 Hz, 1H, 9a-H), 7.12 (t, *J* = 7.6 Hz, 1H, 5'-H), 7.19 (d, *J* = 7.9 Hz, 1H, 7'-H), 7.40 (t, *J* = 7.7 Hz, 6'-H), 8.04 (s, 1H, NH), 8.84 (d, *J* = 7.8 Hz, 1H, 4'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 25.12, 28.29, 28.42, 31.87 ($2CH_3$, $4CH_2$), 53.06 (1'-NCH), 64.18, 66.19 (C-3a, C-9a), 110.28 (C-7'), 120.34 (C-3a'), 122.46, 122.77, 127.79, 131.25, 133.42 (C-3', C-4', C-5', C-6', C-7), 137.42 (C=N), 142.73 (C-7a'), 159.53 (2-C=O), 164.53 (8-C=O), 167.39 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{22}N_6O_3S$: 439.1547; found: 439.1537.

(*Z*)-1,3-Diethyl-7-(1-isopentyl-2-oxoindolin-3-ylidene)-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2i). Yield: 356 mg (76%); bright orange solid; mp 236–237 °C. ^{1}H NMR spectra data are consistent with the literature values.[1]

(*Z*)-1,3-Diethyl-7-(1-isopentyl-2-oxoindolin-3-ylidene)-2-thioxo-1,2,3,3a,4,9a-hexahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazin-8(7*H*)-one (2j). Yield: 334 mg (69%); orange solid; mp 236–238 °C. IR (KBr): 3435, 3298, 2957, 2933, 2872, 1719, 1688, 1645, 1607, 1466, 1406, 1371, 1265, 1086, 754 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.92 (d, J = 5.9 Hz, 6H, 2CH$_3$), 1.09 (t, J = 6.8 Hz, 3H, CH$_3$), 1.19 (t, J = 6.8 Hz, 3H, CH$_3$), 1.46-1.59 (m, 3H, CH$_2$, CH), 3.34-3.40 (m, 1H, NCH$_2$), 3.54-3.60 (m, 1H, NCH$_2$), 3.69-3.81 (m, 3H, NCH$_2$), 3.98-4.05 (m, 1H, NCH$_2$), 5.17 (d, J = 6.0 Hz, 1H, 3a-H), 5.95 (d, J = 6.0 Hz, 1H, 9a-H), 7.11-7.21 (m, 2H, 5′-H, 7′-H), 7.41 (t, J = 7.7 Hz, 1H, 6′-H), 8.20 (s, 1H, NH), 8.76 (d, J = 7.9 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.10, 12.52, 22.25, 25.33, 35.75, 38.09, 38.40, 41.28 (CH, 4CH$_2$, 4CH$_3$), 64.85, 65.18 (C-3a, C-9a), 109.05 (C-7'), 122.21, 122.43, 127.19, 131.05, 132.36 (C-3', C-3a', C-4', C-5', C-6', C-7), 137.18 (C=N), 142.68 (C-7a'), 163.76 (7-C=O), 166.84 (2'-C=O), 182.18 (C=S). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{23}H_{28}N_6O_2S_2$: 485.1788; found: 485.1781.

(*Z*)-7-(1-Isopentyl-2-oxoindolin-3-ylidene)-1,3-dimethyl-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2k). Yield: 299 mg (68%); orange solid; mp 232–234 °C. IR (KBr): 3435, 3266, 2960, 2927, 2873, 1732, 1646, 1607, 1467, 1373, 1320, 1193, 1073, 1025, 752 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.92 (d, J = 5.9 Hz, 6H, 2CH$_3$), 1.48-1.59 (m, 3H, CH, CH$_2$), 2.66 (s, 3H, CH$_3$), 2.92 (s, 3H, CH$_3$), 3.81 (t, J = 6.8 Hz, 2H, 1′-NCH$_2$), 4.82 (d, J = 5.4 Hz, 1H, 3a-H), 5.67 (d, J = 5.8 Hz, 1H, 9a-H), 7.10-7.15 (m, 2H, 5′-H, 7′-H), 7.42 (t, J = 7.4 Hz, 1H, 6′-H), 8.04 (s, 1H, NH), 8.80 (d, J = 7.7 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 22.75 (2CH$_3$), 25.81, 28.42, 31.91 (CH, 2NCH$_3$), 36.23, 38.51 (2CH$_2$), 64.31, 66.23 (C-3a, C-9a), 109.45 (C-7'), 120.18, 122.39, 122.58, 127.70, 131.29, 133.56 (C-3', C-3a', C-4', C-5', C-6', C-7), 137.19 (C=N), 143.00 (C-7a'), 159.50 (2-C=O), 164.45 (8-C=O), 167.32 (2'-C=O). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{24}N_6O_3S$: 441.1703; found: 441.1693.

(*Z*)-1,3-Diethyl-7-(1-isobutyl-2-oxoindolin-3-ylidene)-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2l). Yield: 322 mg (71%); bright orange solid; mp 242–243 °C. ^{1}H NMR spectra data are consistent with the literature values.[1]

(*Z*)-1,3-Diethyl-7-(1-isobutyl-2-oxoindolin-3-ylidene)-2-thioxo-1,2,3,3a,4,9a-hexahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazin-8(7*H*)-one (2m). Yield: 272 mg (58%); orange solid; mp 237–239 °C. IR (KBr): 3440, 3302, 2969, 2931, 2872, 1711, 1686, 1646, 1605, 1467, 1405, 1371, 1294, 1260, 1082, 749 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.87 (d, J = 5.7 Hz, 6H, 2CH$_3$), 1.09 (t, J = 7.0 Hz, 3H, CH$_3$), 1.19 (t, J = 6.8 Hz, 3H, CH$_3$), 2.02-2.11 (m, 1H, CH), 3.31-3.43 (m, 1H, NCH$_2$), 3.52-3.58 (m, 3H, NCH$_2$), 3.66-3.80 (m, 1H, NCH$_2$), 3.96-4.07 (m, 1H, NCH$_2$), 5.17 (d, J = 6.2 Hz, 1H, 3a-H), 5.95 (d, J = 6.2 Hz, 1H, 9a-H), 7.10-7.17 (m, 2H, 5′-H, 7′-H), 7.40 (t, J = 7.5 Hz, 1H, 6′-H), 8.20 (d, J = 1.1 Hz, 1H, NH), 8.78 (d, J = 7.8 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.10, 12.48, 19.88 (4CH$_3$), 26.77 (CH), 38.40, 41.23 (2NCH$_3$), 47.04 (1′-NCH$_2$), 64.78, 65.20 (C-3a, C-9a), 109.46 (C-7'), 119.51, 122.21, 122.36, 127.12, 131.01, 132.48 (C-3', C-3a', C-4', C-5', C-6', C-7), 137.17 (C=N), 143.24 (C-7a'), 163.83 (8-C=O), 167.29 (2'-C=O), 182.15 (2-C=S). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{22}H_{26}N_6O_2S_2$: 471.1631; found: 471.1618.

(*Z*)-7-(1-Isobutyl-2-oxoindolin-3-ylidene)-1,3-dimethyl-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2n). Yield: 307 mg (72%); orange solid; mp 240–243 °C. IR (KBr): 3435, 3313, 2961, 2928, 2872, 1700, 1677, 1608, 1465, 1377, 1238, 1222, 1136,

1091, 752 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.89 (d, J = 6.5 Hz, 6H, $2CH_3$), 2.03-2.11 (m, 1H, CH), 2.67 (s, 3H, CH_3), 2.93 (s, 3H, CH_3), 3.11 (d, J = 7.4 Hz, 2H, 1′-NCH_2), 4.82 (d, J = 5.8 Hz, 1H, 3a-H), 5.68 (d, J = 5.9 Hz, 1H, 9a-H), 7.09-7.18 (m, 2H, 5′-H, 7′-H), 7.40 (t, J = 7.4 Hz, 1H, 6′-H), 8.05 (d, J = 1.9 Hz, 1H, NH), 8.80 (d, J = 7.5 Hz, 1H, 4′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 19.85 ($2CH_3$), 26.75, 27.89, 31.39 (CH, $2NCH_3$), 46.98 (1′-NCH_2), 63.76, 65.76 (C-3a, C-9a), 109.26 (C-7'), 119.54, 121.91, 122.04, 127.12, 130.71, 133.01 (C-3', C-3a', C-4', C-5', C-6', C-7), 136.82 (C=N), 143.05 (C-7a'), 159.00 (2-C=O), 163.98 (8-C=O), 167.24 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{22}N_6O_3S$: 427.1547; found: 427.1553.

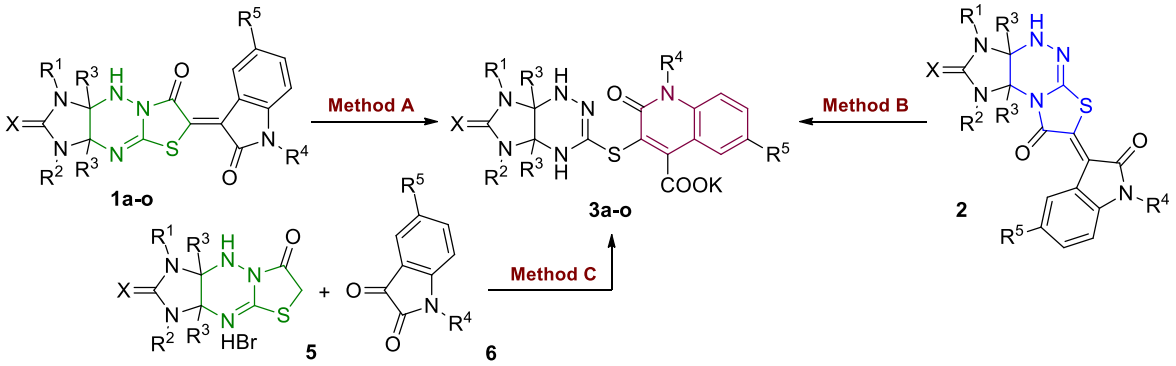
(*Z*)-1,3-Diethyl-7-(5-methyl-2-oxo-1-(pentan-3-yl)indolin-3-ylidene)-1,3a,4,9a-tetrahydroimidazo[4,5-*e*]thiazolo[2,3-*c*][1,2,4]triazine-2,8(3*H*,7*H*)-dione (2o). Yield: 372 mg (77%); reddish orange solid; mp 243–245 °C. IR (KBr): 3295, 2976, 2932, 273, 1724, 1683, 1639, 1472, 1463, 1349, 1213, 1083, 1051, 774 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.73 (t, J = 7.3 Hz, 6H, $2CH_3$), 1.03 (t, J = 7.0 Hz, 3H, CH_3), 1.22 (t, J = 7.1 Hz, 3H, CH_3), 1.71-1.80 (m, 2H, CH_2), 1.93-2.04 (m, 2H, CH_2), 2.32 (s, 3H, 5'-CH_3), 3.04-3.11 (m, 1H, NCH_2), 3.24-3.35 (m, 2H, NCH_2), 3.43-3.50 (m, 1H, NCH_2), 3.68-3.80 (m, 1H, NCH_2), 4.08-4.16 (m, 1H, 1'-NCH), 4.89 (d, J = 5.2 Hz, 1H, 3a-H), 5.75 (d, J = 5.8 Hz, 1H, 9a-H), 7.14-7.21 (m, 2H, 6'-H, 7'-H), 8.01 (s, 1H, NH), 8.68 (s, 1H, 4'-H). ^{13}C NMR (125 MHz, DMSO-d_6): δ 10.97, 12.88, 13.21 ($3CH_3$), 21.02 (5'-CH_3), 24.37 ($2CH_2$), 34.97, 38.05 ($2NCH_2$), 56.55 (1'-NCH), 61.70, 63.72 (C-3a, C-9a), 109.86 (C-7'), 119.81, 122.26, 127.78, 130.70, 131.36, 132.79 (C-3', C-3a', C-4', C-5', C-6', C-7), 136.75 (C=N), 140.38 (C-7a'), 158.09 (2-C=O), 164.11 (8-C=O), 167.59 (2'-C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{24}H_{30}N_6O_3S$: 483.2173; found: 483.2164.

General procedure for the synthesis of compounds 3a–o

Method A (for **3a–o**)**.** To a stirred suspension of compound **1a–o** (0.5 mmol) in refluxing methanol (4 mL), 0.10–0.24 ml of 40% aqueous KOH (1.0–2.4 mmol, 2.0–4.8 equiv.) was added. The resulting mixture was refluxed with stirring for 15 min. After cooling, the precipitate of compounds **3a–o** was filtered off, washed with methanol and dried in air.

Method B (for **3a–d,f–n**)**.** To a stirred suspension of compound **2a–d,f–n** (0.5 mmol) in refluxing methanol (4 mL), 0.10–0.26 ml of 40% aqueous KOH (1.0–2.6 mmol, 2.0–5.2 equiv.) was added. The resulting mixture was refluxed with stirring for 15 min. After cooling, the precipitate of compounds **3a–d,f–n** was filtered off, washed with methanol and dried in air.

Method C (for **3a,d,h,m**)**.** To a stirred suspension of imidazothiazolotriazine **5a–d** (0.5 mmol) and isatin **6a–c** in refluxing methanol (4 mL), 0.080 ml of 40% aqueous KOH (0.8 mmol, 1.6 equiv.) was added. The resulting mixture was refluxed with stirring for 30 min, after which 0.080 ml of 40% aqueous KOH (0.8 mmol, 1.6 equiv.) was additionally added. The resulting mixture was refluxed with stirring for 15 min. After cooling, the precipitate of compounds **3a,d,h,m** was filtered off, washed with methanol and dried in air.



Comp.	X, R^1, R^2, R^3, R^4, R^5	Method A		Method B		Method C
		Equiv. of KOH	Yield	Equiv. of KOH	Yield	Yield
3a	O, Et, Et, H, 3-pentyl, H	2.0	88%	2.0	84%	47%
3b	S, Et, Et, H, 3-pentyl, H	2.0	92%	2.0	94%	
3c	O, Me, Me, H, 3-pentyl, H	2.0	65%	2.2	85%	
3d	O, Me, Ph, H, 3-pentyl, H	2.2	68%	2.2	73%	65%
3e	O, Me, Me, Ph, 3-pentyl, H	4.0	62%			
3f	O, Et, Et, H, cyclopentyl, H	3.2	44%	4.2	23%	
3g	S, Et, Et, H, cyclopentyl, H	4.8	75%	5.2	48%	
3h	O, Me, Me, H, cyclopentyl, H	2.8	82%	2.8	74%	32%
3i	O, Et, Et, H, *i*-Am, H	3.0	84%	3.0	61%	
3j	S, Et, Et, H, *i*-Am, H	2.2	84%	2.2	92%	
3k	O, Me, Me, H, *i*-Am, H	2.5	67%	2.5	51%	
3l	O, Et, Et, H, *i*-Bu, H	3.0	11%	2.5	35%	
3m	S, Et, Et, H, *i*-Bu, H	2.0	79%	2.0	75%	68%
3n	O, Me, Me, H, *i*-Bu, H	2.0	80%	2.0	90%	
3o	O, Et, Et, H, 3-pentyl, Me	2.5	49%			

Potassium 3-((5,7-diethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1-(pentan-3-yl)-1,2-dihydroquinoline-4-carboxylate (3a). Method A: 2.0 equiv. of KOH, yield: 230 mg (88%); Method B: 2.0 equiv. of KOH, yield: 220 mg (84%); Method C: yield: 123 mg (47%); yellow solid; mp 192–196 °C. IR (KBr): 3441, 3273, 2969, 2875, 1699, 1673, 1629, 1467, 1335, 1252, 1215, 1192, 1063, 1047, 749 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.72 (t, *J* = 7.3 Hz, 6H, $2CH_3$), 0.97-1.06 (m, 6H, $2CH_3$), 1.68-1.77 (m, 2H, CH_2), 1.94-2.03 (m, 2H, CH_2), 2.98-

3.11 (m, 2H, CH_2), 3.20-3.34 (m, 2H, CH_2), 4.09 (br.s, 1H, 1-NCH), 4.57 (dd, *J* = 6.4, 2.0 Hz, 1H, CH), 4.85 (dd, *J* = 6.4, 2.4 Hz, 1H, CH), 6.88 (t, *J* = 7.4 Hz, 1H, Ar), 7.03-7.12 (m, 3H, Ar, NH), 7.28 (d, *J* = 2.3 Hz, 1H, NH), 7.64 (d, *J* = 7.6 Hz, 1H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.07, 12.84, 12.94 ($4CH_3$), 24.49 ($2CH_2$), 34.24, 34.29 ($2NCH_2$), 54.98 (1'-NCH), 62.91, 63.56 (C-4a, C-7a), 108.55, 110.95, 120.49, 121.39, 121.68, 126.32 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 139.77, 141.87, 154.45, 157.55, 164.30, 167.46 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{23}H_{29}N_6O_4SK$: 525.1681; found: 525.1671.

Potassium 3-((5,7-diethyl-6-thioxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1-(pentan-3-yl)-1,2-dihydroquinoline-4-carboxylate (3b). Method A: 2.0 equiv. of KOH, yield: 249 mg (92%); Method B: 2.0 equiv. of KOH, yield: 254 mg (94%); light yellow solid; mp 179–181 °C. IR (KBr): 3467, 3285, 2967, 2934, 2874, 1669, 1605, 1464, 1352, 1320, 1276, 1254, 1193, 1106, 1072, 752 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.71 (t, *J* = 7.1 Hz, 6H, $2CH_3$), 1.03-1.11 (m, 6H, $2CH_3$), 1.67-1.76 (m, 2H, CH_2), 1.92-2.02 (m, 2H, CH_2), 3.26-3.41 (m, 2H, CH_2), 3.68-3.86 (m, 2H, CH_2), 4.05-4.13 (m, 1H, 1-NCH), 4.79 (d, *J* = 6.7 Hz, 1H, CH), 5.05 (d, *J* = 6.9 Hz, 1H, CH), 6.88 (t, *J* = 7.3 Hz, 1H, Ar), 7.03-7.13 (m, 2H, Ar), 7.27 (s, 1H, NH), 7.45 (s, 1H, NH), 7.63 (d, *J* = 7.6 Hz, 1H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ 10.99, 12.13, 12.27 ($4CH_3$), 24.41 ($2CH_2$), 37.74 ($2NCH_2$), 54.94 (1'-NCH), 66.15, 66.38 (C-4a, C-7a), 108.63, 110.88, 120.39, 121.27, 121.60, 126.28 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 139.11, 142.12, 154.10, 164.02, 167.37 (C-3', C-4', C=N, 2C=O), 179.73 (2-C=S). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{23}H_{29}N_6O_3S_2K$: 541.1452; found: 541.1454.

Potassium 3-((5,7-dimethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1-(pentan-3-yl)-1,2-dihydroquinoline-4-carboxylate (3c). Method A: 2.0 equiv. of KOH, yield: 162 mg (65%); Method B: 2.2 equiv. of KOH, yield: 211 mg (85%); light yellow solid; mp 197–199 °C. IR (KBr): 3437, 3293, 2965, 2875, 1709, 1678, 1611, 1465, 1353, 1216, 1015, 749 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ ^{1}H NMR (300 MHz, DMSO-d_6) δ 0.72 (t, *J* = 7.3 Hz, 6H, $2CH_3$), 1.68-1.77 (m, 2H, CH_2), 1.94-2.03 (m, 2H, CH_2), 2.60 (s, 3H, CH_3), 2.71 (s, 3H, CH_3), 4.06-4.12 (m, 1H, NCH), 4.47 (dd, *J* = 6.7, 2.1 Hz, 1H, CH), 4.76 (dd, *J* = 6.6, 2.3 Hz, 1H, CH), 6.87 (t, *J* = 7.2 Hz, 1H, 6'-H), 7.02-7.12 (m, 3H, 7'-H, 8'-H, NH), 7.39 (d, *J* = 2.0 Hz, 1H, NH), 7.64 (d, *J* = 7.6 Hz, 1H, 5'-H).^{13}C NMR (75 MHz, DMSO-d_6): δ 11.01 ($2CH_3$), 24.42, 27.06, 27.29 ($2CH_2$, $2NCH_3$), 55.05 (1'-NCH), 65.38, 65.74 (C-4a, C-7a), 108.55, 110.94, 120.45, 121.39, 121.60, 126.27 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 142.08, 154.27, 158.48, 164.23, 167.38 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{25}N_6O_4SK$: 497.1368; found: 497.1363.

Potassium 3-((7-methyl-6-oxo-5-phenyl-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1-(pentan-3-yl)-1,2-dihydroquinoline-4-carboxylate (3d). Method A: 2.2 equiv. of KOH, yield: 190 mg (68%); Method B: 2.2 equiv. of KOH, yield: 204 mg (73%); Method C: yield: 181 mg (65%); light yellow solid; mp 180–182 °C. IR (KBr): 3434, 2965, 2932, 2874, 1711, 1677, 1629, 1604, 1501, 1464, 1399, 1352, 1206, 1138, 1070, 749 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.70 (t, *J* = 7.1 Hz, 6H, $2CH_3$), 1.67-1.78 (m, 2H, CH_2), 1.91-1.99 (m, 2H, CH_2), 2.74 (s, 3H, CH_3), 4.05-4.09 (m, 1H, NCH), 4.64 (dd, *J* = 6.1, 2.3 Hz, 1H, CH), 5.23 (dd, *J* = 6.1, 2.0 Hz, 1H, CH), 6.88 (t, *J* = 7.4 Hz, 1H, 6'-H), 7.01-7.12 (m, 3H, 7'-H, 8'-H, NH), 7.30-7.34 (m, 4H, Ph-3-5, NH), 7.52 (d, *J* = 8.1 Hz, 2H, Ph-2,6), 7.60 (d, *J* = 7.6 Hz, 1H, 5'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.02 ($2CH_3$), 24.43 ($2CH_2$), 27.36 (NCH_3), 54.96 (1'-NCH), 63.98, 64.30 (C-4a, C-7a), 108.68, 111.00, 119.20, 120.53, 121.31, 121.49, 122.76, 126.44, 128.78, 138.06 (C-4a', C-5', C-6', C-7', C-8', C-8a', Ph), 140.01, 141.64, 153.60, 155.69, 164.56, 167.39 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{26}H_{27}N_6O_4SK$: 559.1524; found: 559.1513.

Potassium 3-((5,7-dimethyl-6-oxo-4a,7a-diphenyl-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1-(pentan-3-yl)-1,2-dihydroquinoline-4-carboxylate (3e). Method A: 4.0 equiv. of KOH, yield: 189 mg (62%); light yellow solid; mp 189–191 °C. IR (KBr): 3396, 3219, 2967, 2934, 2875, 1707, 1682, 1637, 1604, 1463, 1352, 1202, 1072, 992, 864, 752, 699 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.72 (t, *J* = 6.1 Hz, 6H, $2CH_3$), 1.68-1.77 (m, 2H, CH_2), 1.93-2.03 (m, 2H, CH_2), 2.52 (s, 3H, CH_3), 2.55 (s, 3H, CH_3), 4.08-4.14 (m, 1H, NCH), 6.79 (d, *J* = 7.6 Hz, 2H, Ph-2,6), 6.86 (t, *J* = 7.4 Hz, 1H, 6'-H), 7.03-7.09 (m, 10H, Ph-2-6, Ph-3-5, 7'-H, 8'-H), 7.28 (s, 1H, NH), 7.64 (d, *J* = 7.6 Hz, 1H, 5'-H), 8.02 (s, 1H, NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.10 ($2CH_3$), 24.90, 25.26, 25.51 ($2CH_2$, $2NCH_3$), 54.98 (1'-NCH), 79.95, 83.38 (C-4a, C-7a), 108.71, 110.86, 120.51, 121.43, 121.66, 126.31, 127.03, 127.22, 127.66, 127.80, 128.13, 128.63 (C-4a', C-5', C-6', C-7', C-8', C-8a', 2Ph-2-6), 135.70, 136.56, 139.41, 141.51, 154.08, 158.50, 164.57, 167.51 (2Ph-1, C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* $[M - K + 2H]^+$ calcd for $C_{33}H_{34}N_6O_4S$: 611.2435; found: 611.2423.

Potassium 1-cyclopentyl-3-((5,7-diethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1,2-dihydroquinoline-4-carboxylate (3f). Method A: 3.2 equiv. of KOH, yield: 115 mg (44%); Method B: 4.2 equiv. of KOH, yield: 60 mg (23%); pale beige solid; mp 239–241 °C. IR (KBr): 3273, 3196, 2972, 2875, 1708, 1674, 1627, 1603, 1565, 15111, 1469, 1344, 1253, 1228, 1190, 1044, 747 cm^{-1}. ^1H NMR (300 MHz, D_2O) δ 1.11 (t, *J* = 6.9 Hz, 6H, $2CH_3$), 1.70-1.81 (m, 4H, CH_2), 1.91-2.03 (m, 4H, CH_2), 3.08-3.21 (m, 2H, NCH_2), 3.31-3.45 (m, 2H, NCH_2), 4.71-4.83 (m, 1H, NCH), 4.92 (d, *J* = 7.1 Hz, 1H, CH), 5.19 (d, *J* = 7.1 Hz, 1H, CH), 7.09-7.17 (m, 2H, 6-H, 8-H), 7.32 (t, *J* = 7.4 Hz, 1H, 7-H), 7.59 (d, *J* = 7.5 Hz, 1H, 5-H). ^{13}C NMR (75 MHz, D_2O): δ 12.22 ($2CH_3$), 24.93, 27.78 ($4CH_2$), 35.03, 35.24 ($2NCH_2$), 52.67 (1'-NCH), 64.17, 64.31 (C-4a, C-7a), 110.35, 115.93, 120.74, 121.09, 122.46, 128.16 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 139.90, 145.21, 148.24 (C-3', C-4', C=N), 159.58, 167.53, 168.60 (3C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{23}H_{27}N_6O_4SK$: 523.1524; found: 523.1509.

Potassium 1-cyclopentyl-3-((5,7-diethyl-6-thioxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1,2-dihydroquinoline-4-carboxylate (3g). Method A: 4.8 equiv. of KOH, yield: 188 mg (75%); Method B: 5.2 equiv. of KOH, yield: 120 mg (48%); yellow solid; mp 190–192 °C. IR (KBr): 3434, 3266, 2964, 2873, 1674, 1630, 1606, 1466, 1356, 1318, 1251, 1078, 989, 748 cm^{-1}. ^1H NMR (300 MHz, D_2O) δ 1.16 (t, *J* = 6.6 Hz, 6H, $2CH_3$), 1.66-1.72 (m, 2H, CH_2), 1.88-2.03 (m, 6H, CH_2), 3.33-3.46 (m, 2H, NCH_2), 3.75-3.90 (m, 2H, NCH_2), 4.70-4.76 (m, 1H, 1′-NCH), 5.13 (d, *J* = 7.5 Hz, 1H, CH), 5.33 (d, *J* = 7.6 Hz, 1H, CH), 7.07-7.15 (m, 2H, 6′-H, 8′-H), 7.30 (t, *J* = 7.8 Hz, 1H, 7′-H), 7.59 (d, *J* = 7.7 Hz, 1H, 5′-H). ^{13}C NMR (75 MHz, D_2O): δ 11.63, 11.75 ($2CH_3$), 24.93, 27.79 ($4CH_2$), 38.60, 38.79 ($2NCH_2$), 52.68 (1'-NCH), 66.89, 67.38 (C-4a, C-7a), 110.36, 116.13, 120.72, 121.14, 122.45, 128.22 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 139.94, 145.62, 147.93 (C-3', C-4', C=N), 167.59, 168.57 (2C=O), 179.16 (C=S). HRMS (ESI): *m/z* $[M - K + 2H]^+$ calcd for $C_{23}H_{28}N_6O_3S_2$: 501.1737; found: 501.1745.

Potassium 1-cyclopentyl-3-((5,7-dimethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-2-oxo-1,2-dihydroquinoline-4-carboxylate (3h). Method A: 2.8 equiv. of KOH, yield: 203 mg (82%); Method B: 2.8 equiv. of KOH, yield: 183 mg (74%); Method C: yield: 79 mg (32%); light beige solid; mp 236–237 °C. IR (KBr): 3281, 3179, 2959, 2875, 1706, 1665, 1623, 1606, 1569, 1514, 1345, 1229, 1019, 748 cm^{-1}. ^1H NMR (300 MHz, D_2O) δ 1.69-1.82 (m, 4H, CH_2), 1.91-2.07 (m, 4H, CH_2), 2.76 (s, 3H, NCH_3), 2.79 (s, 3H, NCH_3), 4.69-4.83 (m, 2H, NCH, CH), 5.05 (d, *J* = 6.1 Hz, 1H, CH), 7.08-7.17 (m, 2H, 6-H, 8-H), 7.32 (t, *J* = 7.4 Hz, 1H, 7-H), 7.59 (d, *J* = 7.5 Hz, 1H, 5-H). ^{13}C NMR (75 MHz, D_2O): δ 24.62, 26.66, 26.71, 27.48 ($4CH_2$, $2NCH_3$), 52.39 (1'-

NCH), 65.91, 66.15 (C-4a, C-7a), 110.03, 115.60, 120.45, 120.80, 122.15, 127.85 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 139.61, 144.87, 147.99 (C-3', C-4', C=N), 160.14, 167.16, 168.30 (3C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{23}N_6O_4SK$: 495.1211; found: 495.1201.

Potassium 3-((5,7-diethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-1-isopentyl-2-oxo-1,2-dihydroquinoline-4-carboxylate (3i). Method A: 3.0 equiv. of KOH, yield: 204 mg (84%); Method B: 3.0 equiv. of KOH, yield: 148 mg (61%); light yellow solid; mp 206–208 °C. IR (KBr): 3435, 3274, 2958, 2871, 1706, 1674, 1625, 1608, 1469, 1357, 1329, 1254, 1189, 1043, 878, 749 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.91-1.06 (m, 12H, $4CH_3$), 1.41-1.56 (m, 3H, CH, CH_2), 2.98-3.13 (m, 2H, CH_2), 3.18-3.34 (m, 2H, CH_2), 3.71 (t, *J* = 7.0 Hz, 2H, 1-NCH_2), 4.59 (dd, *J* = 6.4, 2.2 Hz, 1H, CH), 4.86 (dd, *J* = 6.4, 2.4 Hz, 1H, CH), 6.87-6.93 (m, 2H, Ar), 7.08 (d, *J* = 2.0 Hz, 1H, NH), 7.14 (t, *J* = 7.5 Hz, 1H, Ar), 7.30 (d, *J* = 2.2 Hz, 1H, NH), 7.63 (d, *J* = 7.5 Hz, 1H, Ar). ^{13}C NMR (75 MHz, DMSO-d_6): δ 13.28 ($2CH_3$), 22.85, 25.78 (CH, $2CH_3$), 34.75, 36.59, 37.56, 40.75 ($4CH_2$), 62.96, 64.12 (C-4a, C-7a), 108.02, 111.50, 121.28, 122.93, 126.93 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 140.27, 141.98, 154.84, 157.98, 164.54, 167.11 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* $[M – K + 2H]^+$ calcd for $C_{23}H_{30}N_6O_4S$: 487.2122; found: 487.2118.

Potassium 3-((5,7-diethyl-6-thioxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-1-isopentyl-2-oxo-1,2-dihydroquinoline-4-carboxylate (3j). Method A: 2.2 equiv. of KOH, yield: 227 mg (84%); Method B: 2.2 equiv. of KOH, yield: 248 mg (92%); light yellow solid; mp 184–186 °C. IR (KBr): 3437, 3286, 2957, 2932, 2871, 1668, 1607, 1468, 1355, 1318, 1278, 1255, 1193, 1109, 1059, 754 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6) δ 0.92 (d, *J* = 6.3 Hz, 6H, $2CH_3$), 1.03-1.12 (m, 6H, $2CH_3$), 1.42-1.57 (m, 3H, CH_2, CH), 3.32-3.38 (m, 2H, NCH_2), 3.71-3.84 (m, 4H, NCH_2), 4.88 (d, *J* = 6.9 Hz, 1H, CH), 5.08 (d, *J* = 6.9 Hz, 1H, CH), 6.88-6.94 (m, 2H, 6′-H, 8′-H), 7.15 (t, *J* = 7.6 Hz, 1H, 7′-H), 7.38 (s, 1H, NH), 7.58 (s, 1H, NH), 7.64 (d, *J* = 7.5 Hz, 1H, 5′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.09, 12.29 ($2CH_3$), 22.33, 25.27 (CH, $2CH_3$), 36.08, 37.08, 37.72 ($4CH_2$), 66.26, 66.36 (C-4a, C-7a), 107.51, 111.21, 120.74, 121.29, 121.60, 126.47 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 139.81, 142.11, 154.10, 163.99, 166.62 (C-3', C-4', C=N, 2C=O), 179.72 (C=S). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{23}H_{29}N_6O_3S_2K$: 541.1452; found: 541.1447.

Potassium 3-((5,7-dimethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-1-isopentyl-2-oxo-1,2-dihydroquinoline-4-carboxylate (3k). Method A: 2.5 equiv. of KOH, yield: 164 mg (67%); Method B: 2.5 equiv. of KOH, yield: 126 mg (51%); light yellow solid; mp 206–208 °C. IR (KBr): 3435, 3274, 2958, 2932, 2871, 1711, 1678, 1635, 1607, 1468, 1357, 1257, 1195, 1019, 784, 748 cm^{-1}. ^1H NMR (300 MHz, D_2O) δ 0.88 (d, *J* = 5.9 Hz, 6H, $2CH_3$), 1.43-1.57 (m, 3H, CH, CH_2), 2.73 (s, 3H, CH_3), 2.76 (s, 3H, CH_3), 3.69 (t, *J* = 7.6 Hz, 2H, 1′-NCH_2), 4.77 (d, *J* = 7.2 Hz, 1H, CH), 5.02 (d, *J* = 7.0 Hz, 1H, CH), 6.98 (d, *J* = 7.8 Hz, 1H, 8′-H), 7.06 (t, *J* = 7.5 Hz, 1H, 6′-H), 7.27 (t, *J* = 7.6 Hz, 1H, 7′-H), 7.54 (d, *J* = 7.7 Hz, 1H, 5′-H).^{13}C NMR (75 MHz, DMSO-d_6): δ 22.31, 25.27, 26.99, 27.29 ($4CH_3$, CH), 36.07, 37.04 ($2CH_2$), 65.30, 65.73 (C-4a, C-7a), 107.41, 110.88, 120.70, 121.29, 121.65, 126.30 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 139.76, 141.89, 154.40, 158.39, 163.94, 166.57 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{25}N_6O_4SK$: 497.1368; found: 497.1352.

Potassium 3-((5,7-diethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-1-isobutyl-2-oxo-1,2-dihydroquinoline-4-carboxylate (3l). Method A: 3.0 equiv. of KOH, yield: 28 mg (11%); Method B: 2.5 equiv. of KOH, yield: 89 mg (35%); light yellow solid; mp 239–241 °C. IR (KBr): 3437, 3277, 3167, 2963, 2931, 2873, 1705, 1672, 1624, 1607, 1467, 1355, 1331, 1254, 1191, 1058, 1043, 875, 749 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.86 (d, *J* = 6.5 Hz, 6H,

2CH_3), 0.94-1.06 (m, 6H, 2CH_3), 1.99-2.09 (m, 1H, CH), 2.96-3.13 (m, 2H, NCH_2), 3.18-3.42 (m, 2H, NCH_2), 3.51 (d, *J* = 7.3 Hz, 1H, 1′-NCH), 4.58 (dd, *J* = 6.4, 2.4 Hz, 1H, CH), 4.86 (d, *J* = 6.4, 2.6 Hz, 1H, CH), 6.86-6.96 (m, 2H, 6′-H, 8′-H), 7.07 (d, *J* = 2.4 Hz, 1H, NH), 7.13 (t, *J* = 7.6 Hz, 1H, 7′-H), 7.31 (d, *J* = 2.3 Hz, 1H, NH), 7.62 (d, *J* = 7.5 Hz, 1H, 5′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.73, 12.81, 19.97 (4CH_3), 26.89 (CH), 34.21 (2NCH_2), 46.21 (1′-NCH2), 62.78, 63.51 (C-4a, C-7a), 107.78, 110.82, 120.67, 121.18, 121.50, 126.24 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 140.31, 141.60, 154.54, 157.43, 164.03, 166.97 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{22}H_{27}N_6O_4SK$: 511.1524; found: 511.1501.

Potassium 3-((5,7-diethyl-6-thioxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-1-isobutyl-2-oxo-1,2-dihydroquinoline-4-carboxylate (3m). Method A: 2.0 equiv. of KOH, yield: 208 mg (79%); Method B: 2.0 equiv. of KOH, yield: 197mg (75%); Method C: yield: 179 mg (68%); light yellow solid; mp 182–184 °C. IR (KBr): 3434, 3290, 2964, 2875, 1707, 1679, 1642, 1605, 1464, 1358, 1330, 1317, 1287, 1235, 1078, 1013, 750 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.87 (d, *J* = 6.5 Hz, 6H, 2CH_3), 1.04-1.12 (m, 6H, 2CH_3), 2.00-2.09 (m, 1H, CH), 3.28-3.39 (m, 2H, NCH_2), 3.51 (d, *J* = 7.4 Hz, 1H, 1′-NCH), 3.71-3.84 (m, 2H, NCH_2), 4.83 (dd, *J* = 7.0, 3.1 Hz, 1H, CH), 5.07 (dd, *J* = 7.0, 3.6 Hz, 1H, CH), 6.91 (t, *J* = 7.6 Hz, 1H, 6′-H), 6.96 (d, *J* = 7.8 Hz, 1H, 8′-H), 7.15 (t, *J* = 7.4 Hz, 1H, 7′-H), 7.32 (d, *J* = 2.7 Hz, 1H, NH), 7.51 (d, *J* = 3.3 Hz, 1H, NH), 7.62 (d, *J* = 7.5 Hz, 1H, 5′-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 12.67, 12.72, 20.47 (4CH_3), 27.39 (CH), 38.25, 38.31 (2NCH_2), 46.73 (1′-NCH_2), 66.27, 67.01 (C-4a, C-7a), 108.42, 111.66, 121.27, 121.70, 121.89, 126.96 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 140.86, 142.38, 154.53, 164.48, 167.51 (C-3', C-4', C=N, 2C=O), 180.23 (C=S). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{22}H_{27}N_6O_3S_2K$: 527.1296; found: 527.1293.

Potassium 3-((5,7-dimethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-1-isobutyl-2-oxo-1,2-dihydroquinoline-4-carboxylate (3n). Method A: 2.0 equiv. of KOH, yield: 193 mg (80%); Method B: 2.0 equiv. of KOH, yield: 217 mg (90%); beige solid; mp 222–224 °C. IR (KBr): 3435, 3280, 2962, 2870, 1710, 1670, 1635, 1607, 1466, 1346, 1195, 1017, 783, 750 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6) δ 0.86 (d, *J* = 6.3 Hz, 6H, 2CH_3), 1.97-2.10 (m, 1H, CH), 2.61 (s, 3H, CH_3), 2.70 (s, 3H, CH_3), 3.50 (d, *J* = 7.1 Hz, 2H, 1′-NCH_2), 4.48 (d, *J* = 6.6 Hz, 1H, CH), 4.78 (d, *J* = 6.6 Hz, 1H, CH), 6.87-6.96 (m, 2H, 6′-H, 8′-H), 7.11-7.16 (m, 2H, 7′-H, NH), 7.32 (s, 1H, NH), 7.63 (d, *J* = 7.4 Hz, 1H, 5′-H).^{13}C NMR (75 MHz, DMSO-d_6): δ 20.01 (2CH_3), 26.92, 27.09, 27.34 (CH, 2NCH_3), 46.26 (1′-NCH_2), 65.23, 65.79 (C-4a, C-7a), 107.87, 111.03, 120.78, 121.30, 121.48, 126.38 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 140.39, 141.95, 154.33, 158.50, 164.12, 167.04 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{20}H_{23}N_6O_4SK$: 483.1211; found: 483.1203.

Potassium 3-((5,7-diethyl-6-oxo-4,4a,5,6,7,7a-hexahydro-1*H*-imidazo[4,5-*e*][1,2,4]triazin-3-yl)thio)-6-methyl-2-oxo-1-(pentan-3-yl)-1,2-dihydroquinoline-4-carboxylate (3o). Method A: 2.5 equiv. of KOH, yield: 132 mg (49%); light yellow solid; mp 217–218 °C. IR (KBr): 3466, 3273, 2965, 2933, 2874, 1694, 1668, 1625, 1481, 1344, 1210, 1070, 1043, 802, 675 cm^{-1}. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.71 (t, *J* = 7.2 Hz, 6H, 2CH_3), 0.98-1.07 (m, 6H, 2CH_3), 1.64-1.78 (m, 2H, CH_2), 1.91-1.99 (m, 2H, CH_2), 2.24 (s, 3H, 5'-CH_3), 2.96-3.13 (m, 1H, NCH_2), 3.19-3.40 (m, 2H, NCH_2), 4.03-4.10 (m, 1H, 1'-NCH), 4.54 (dd, *J* = 6.4, 2.6 Hz, 1H, CH), 4.85 (dd, *J* = 6.4, 2.5 Hz, 1H, CH), 6.89-6.95 (m, 2H, 7'-H, 8'-H), 7.06 (s, 1H, NH), 7.26 (d, *J* = 2.9 Hz, 1H, NH), 7.46 (s, 1H, 5'-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 11.48, 13.24, 13.30 (4CH_3), 21.38 (6-CH_3), 24.90 (2CH_2), 34.76 (2NCH_2), 55.47 (1'-NCH), 62.97, 64.14 (C-4a, C-7a), 108.92, 111.35, 122.17, 122.28, 127.20, 129.45 (C-4a', C-5', C-6', C-7', C-8', C-8a'), 138.04, 142.17, 154.18, 157.98, 164.67, 167.91 (C-3', C-4', C=N, 3C=O). HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{24}H_{31}N_6O_4SK$: 539.1837; found: 539.1826.

General procedure for the synthesis of compounds 4a–c

To a stirred suspension of compound **1p–r** (0.5 mmol) in refluxing methanol (5 mL), 40% aqueous KOH was added (0.110 ml (1.1 mmol, 2.2 equiv.) for **4a**; 0.121 ml (1.25 mmol, 2.5 equiv.) for **4b,c**). The resulting mixture was refluxed with stirring for 15 min. After cooling, the precipitate of compounds **4a–c** was filtered off, washed with methanol and dried in air.

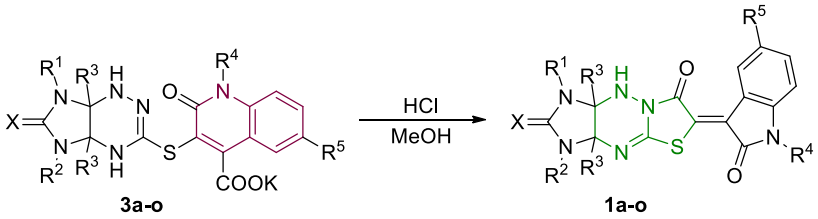
Potassium 3-methoxy-6-methyl-2-oxo-1-pentyl-1,2-dihydroquinoline-4-carboxylate (4a). Yield: 51 mg (30%); light beige solid; mp 226–229 °C. IR (KBr): 3434, 2953, 2930, 2867, 1676, 1611, 1591, 1489, 1457, 1385, 1274, 1096, 798, 689 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.84 (t, *J* = 6.9 Hz, 3H, CH_3), 1.23-1.32 (m, 4H, $2CH_2$), 1.48-1.57 (m, 2H, CH_2), 2.27 (s, 3H, 6-CH_3), 3.60 (t, *J* = 7.1 Hz, 2H, NCH_2), 3.95 (s, 3H, OCH_3), 6.76 (d, *J* = 7.9 Hz, 8-H), 6.87 (d, *J* = 7.7 Hz, 1H, 7-H), 7.35 (s, 1H, 5-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 14.35 (CH_3), 21.47, 22.38, 27.75, 29.03 ($3CH_2$, 6-CH_3), 57.72 (OCH_3), 98.20, 107.26, 122.76, 123.76, 125.67, 129.62, 137.20 (C-4, C-4a, C-5, C-6, C-7, C-8, C-8a), 163.84, 167.57, 170.65 (C-3, 2C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{17}H_{20}NO_4K$: 342.1102; found: 342.1100.

Potassium 6-chloro-3-methoxy-2-oxo-1-pentyl-1,2-dihydroquinoline-4-carboxylate (4b). Yield: 60 mg (33%); light beige solid; mp 238–240 °C. IR (KBr): 3435, 2956, 2931, 2868, 1677, 1610, 1580, 1477, 1380, 1284, 1231, 1101, 801, 664 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 0.84 (t, *J* = 6.9 Hz, 3H, CH_3), 1.22-1.33 (m, 4H, $2CH_2$), 1.51-1.58 (m, 2H, CH_2), 3.63 (t, *J* = 7.1 Hz, 2H, NCH_2), 4.00 (s, 3H, OCH_3), 6.91 (d, *J* = 8.3 Hz, 8-H), 7.10 (dd, *J* = 8.2, 1.9 Hz, 1H, 7-H), 7.48 (d, *J* = 1.9 Hz, 1H, 5-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 13.82 (CH_3), 21.83, 27.16, 28.47 ($3CH_2$), 38.70 (NCH_2), 57.61 (OCH_3), 96.69, 108.20, 120.69, 124.02, 124.59, 125.04, 137.47 (C-4, C-4a, C-5, C-6, C-7, C-8, C-8a), 162.44, 166.58, 172.07 (C-3, 2C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{16}H_{17}ClNO_4K$: 362.0556; found: 362.0557.

Potassium 1-benzyl-3-methoxy-2-oxo-1,2-dihydroquinoline-4-carboxylate (4c). Yield: 49 mg (31%); beige solid; mp >300 °C. IR (KBr): 3450, 3272, 3086, 3031, 2947, 2855, 1640, 1606, 1390, 1363, 1262, 1162, 1002, 750 cm^{-1}. ^1H NMR (300 MHz, DMSO-d_6): δ 4.00 (s, 3H, CH_3), 4.90 (s, 2H, NCH_2), 6.79 (d, *J* = 7.6 Hz, 1H, 8-H), 6.91 (t, *J* = 7.3 Hz, 1H, 7-H), 7.01 (t, *J* = 7.5 Hz, 1H, 6-H), 7.23-7.34 (m, 5H, Ph), 7.56 (d, *J* = 7.2 Hz, 1H, 5-H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 42.00 (NCH_2), 57.28 (OCH_3), 97.92, 107.42, 120.75, 121.47, 123.36, 124.57, 126.96, 127.16, 128.34, 137.58, 138.38 (C-4, C-4a, C-5, C-6, C-7, C-8, C-8a, Ph), 162.77, 167.00, 171.06 (C-3, 2C=O). HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{18}H_{15}NO_4Na$: 332.0902; found: 332.0893.

General procedure for the transformation of compounds 3a–o into 1a–o

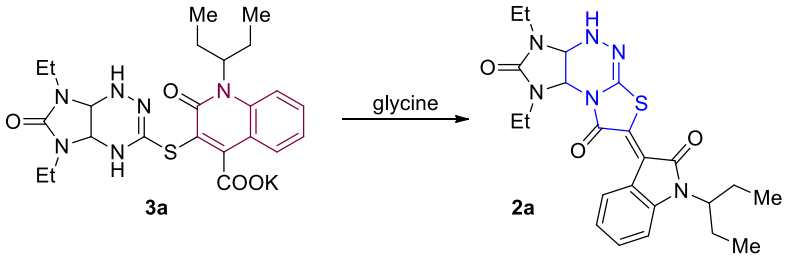
To a stirred suspension of compound **3a–o** (0.25 mmol) in methanol (2 mL), 0.275 ml of 1M HCl (0.275 mmol, 1.1 equiv.) was added. The mixture was stirring for 5 min, the precipitate of compounds **1a–o** was filtered off, washed with methanol and dried in air.



Comp.	X, R^1, R^2, R^3, R^4, R^5	Yield
1a	O, Et, Et, H, 3-pentyl, H	96%
1b	S, Et, Et, H, 3-pentyl, H	83%
1c	O, Me, Me, H, 3-pentyl, H	98%
1d	O, Me, Ph, H, 3-pentyl, H	93%
1e	O, Me, Me, Ph, 3-pentyl, H	95%
1f	O, Et, Et, H, cyclopentyl, H	94%
1g	S, Et, Et, H, cyclopentyl, H	98%
1h	O, Me, Me, H, cyclopentyl, H	95%
1i	O, Et, Et, H, *i*-Am, H	99%
1j	S, Et, Et, H, *i*-Am, H	98%
1k	O, Me, Me, H, *i*-Am, H	96%
1l	O, Et, Et, H, *i*-Bu, H	97%
1m	S, Et, Et, H, *i*-Bu, H	99%
1n	O, Me, Me, H, *i*-Bu, H	91%
1o	O, Et, Et, H, 3-pentyl, Me	94%

Procedure for the transformation of compounds 3a into 2a

To a stirred suspension of compound **3a** (105 mg, 0.25 mmol) in methanol (2.5 mL), 19 mg of glycine (0.25 mmol, 1 equiv.) was added. The mixture was stirring at 37°C for 1.5 h, the precipitate of compound **2a** was filtered off, washed with water and dried in air. Yield of **2a** 75 mg (64%).



NCI-60 Screening Methodology

General Description:

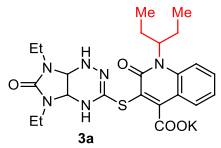
As of early 2007 all compounds submitted to the NCI 60 Cell screen are tested initially at a single high dose (10^{-5} M) in the full NCI 60 cell panel. Only compounds which satisfy pre-determined threshold inhibition criteria in a minimum number of cell lines will progress to the full 5-dose assay. The threshold inhibition criteria for progression to the 5-dose screen was selected to efficiently capture compounds with anti-proliferative activity based on careful analysis of historical DTP screening data. The threshold criteria may be updated as additional data becomes available.

Interpretation of One-Dose Data:

The One-dose data will be reported as a mean graph of the percent growth of treated cells and will be similar in appearance to mean graphs from the 5-dose assay. The number reported for the One-dose assay is growth relative to the no-drug control, and relative to the time zero number of cells. This allows detection of both growth inhibition (values between 0 and 100) and lethality (values less than 0). This is the same as for the 5-dose assay, described below. For example, a value of 100 means no growth inhibition. A value of 40 would mean 60% growth inhibition. A value of 0 means no net growth over the course of the experiment. A value of -40 would mean 40% lethality. A value of -100 means all cells are dead. Information from the One-dose mean graph is available for COMPARE analysis.

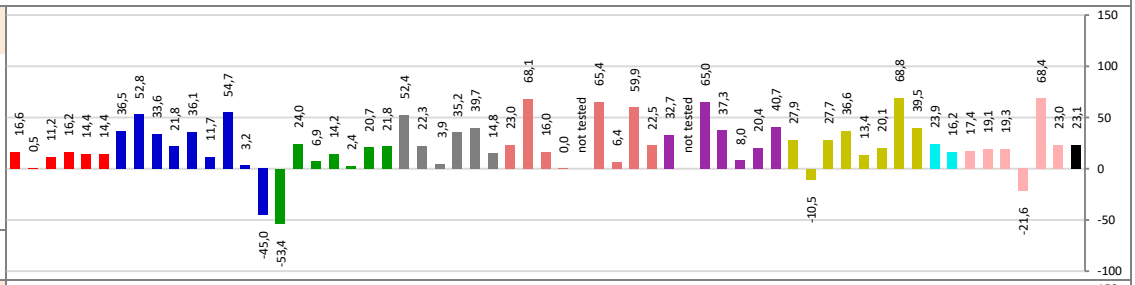
Anticancer Screening Data of 60 Cancer Cell Lines Assay at 10 µmol/L Concentration

Growth Percent, 10 µmol/L

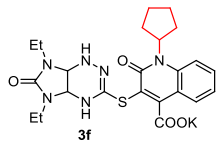


3a

Mean Growth Percent ***23.1***

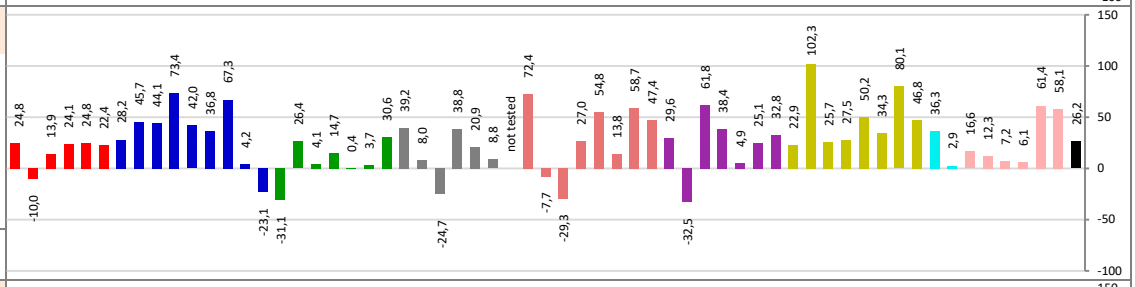


Growth Percent, 10 µmol/L

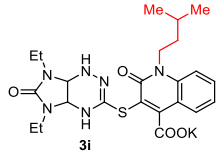


3f

Mean Growth Percent ***26.2***

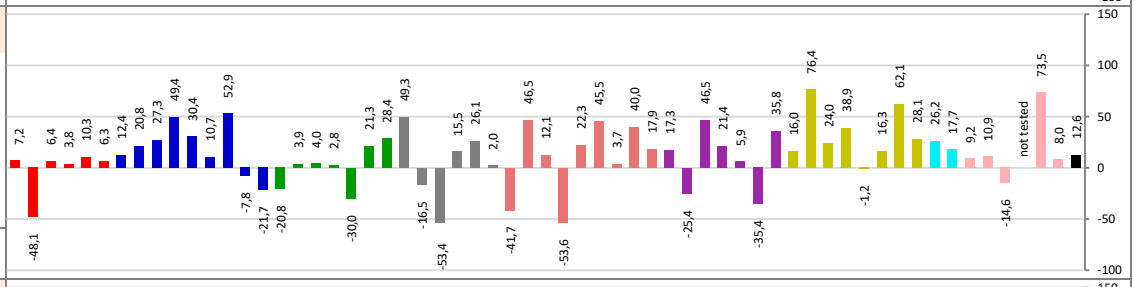


Growth Percent, 10 µmol/L

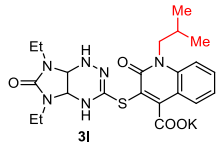


3i

Mean Growth Percent ***12.6***

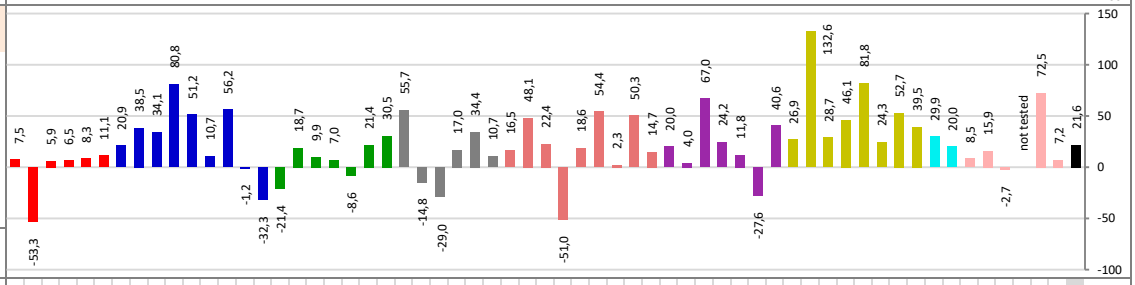


Growth Percent, 10 µmol/L



3l

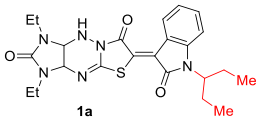
Mean Growth Percent ***21.6***



Cell Line	CCRF-CEM	HL-60(TB)	K-562	MOLT-4	RPMI-8226	SR	A549/ATCC	EKVX	HOP-62	HOP-92	NCI-H226	NCI-H23	NCI-H322M	NCI-H460	NCI-H522	COLO 205	HCC-2998	HCT-116	HCT-15	HT29	KM12	SW-620	SF-268	SF-295	SF-539	SNB-19	SNB-75	U251	LOX IMVI	MALME-3M	M14	MDA-MB-435	SK-MEL-2	SK-MEL-28	SK-MEL-5	UACC-257	UACC-62	IGROV1	OVCAR-3	OVCAR-4	OVCAR-5	OVCAR-8	NCI/ADR-RES	SK-OV-3	786-0	A498	ACHN	CAKI-1	RXF 393	SN12C	TK-10	UO-31	PC-3	DU-145	MCF7	MDA-MB-231/ATCC	HS 578T	BT-549	T-47D	MDA-MB-468	MEAN
Panel	**Leukemia**						**Non-Small Cell Lung Cancer**									**Colon Cancer**							**CNS Cancer**						**Melanoma**									**Ovarian Cancer**							**Renal Cancer**						**Prostate Cancer**			**Breast Cancer**					

Anticancer Screening Data of 60 Cancer Cell Lines Assay at 10 µmol/L Concentration

Growth Percent, 10 µmol/L

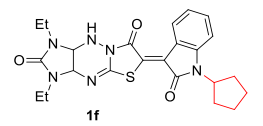


1a

CCRF-CEM	HL-60(TB)	K-562	MOLT-4	RPMI-8226	SR	A549/ATCC	EKVX	HOP-62	HOP-92	NCI-H226	NCI-H23	NCI-H322M	NCI-H460	NCI-H522	COLO 205	HCC-2998	HCT-116	HCT-15	HT29	KM12	SW-620	SF-268	SF-295	SF-539	SNB-19	SNB-75	U251	LOX IMVI	MALME-3M	M14	MDA-MB-435	SK-MEL-2	SK-MEL-28	SK-MEL-5	UACC-257	UACC-62	IGROV1	OVCAR-3	OVCAR-4	OVCAR-5	OVCAR-8	NCI/ADR-RES	SK-OV-3	786-0	A498	ACHN	CAKI-1	RXF 393	SN12C	TK-10	UO-31	PC-3	DU-145	MCF7	MDA-MB-231/ATCC	HS 578T	BT-549	T-47D	MDA-MB-468	MEAN
55,3	26,5	26,0	59,8	64,7	54,5	57,6	59,6	73,2	120,3	79,1	44,1	80,6	27,5	62,7	37,8	65,9	27,9	34,5	44,7	11,2	48,2	63,4	20,3	25,2	71,4	67,9	58,9	39,3	65,2	not tested	9,5	101,4	57,0	55,6	86,1	39,9	44,7	31,5	63,6	57,3	81,6	26,3	95,7	72,7	52,3	50,4	50,8	not tested	56,0	126,5	54,4	43,9	52,0	35,8	53,2	73,1	102,4	86,2	79,9	57,1

Mean Growth Percent ***57.1***

Growth Percent, 10 µmol/L

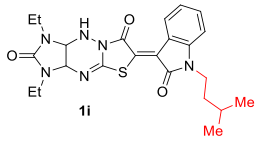


1f

| 29,8 | not tested | 22,0 | 84,4 | 54,1 | 34,8 | 54,4 | 59,7 | 50,0 | 67,4 | 91,8 | 53,9 | 94,8 | 43,9 | 28,0 | 26,2 | 91,8 | 19,8 | 51,2 | 21,3 | 23,8 | 53,9 | 59,5 | 60,6 | 37,0 | 79,2 | 8,3 | 58,9 | 64,5 | 71,0 | 91,9 | -15,9 | 75,9 | 73,4 | 34,8 | not tested | 61,9 | 67,4 | 40,8 | 55,7 | 77,5 | 60,2 | 10,9 | not tested | 63,6 | 30,8 | 59,3 | 32,6 | not tested | 70,6 | 88,1 | 51,7 | 46,5 | 43,6 | 45,7 | 58,2 | 62,0 | not tested | 79,3 | 11,0 | 52,2 |

Mean Growth Percent ***52.2***

Growth Percent, 10 µmol/L

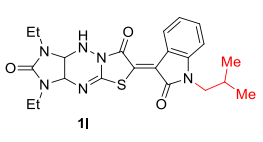


1i

| 57,1 | 83,1 | 26,1 | 85,5 | 73,7 | not tested | 67,1 | 89,2 | 73,2 | 83,9 | 87,8 | 92,4 | 106,2 | 50,4 | not tested | 99,8 | 12,6 | 47,0 | 111,5 | 67,9 | 61,1 | not tested | 98,5 | 86,8 | 88,6 | 59,2 | 87,7 | not tested | 79,9 | 56,6 | 12,5 | 87,7 | 78,6 | 89,5 | 66,3 | 67,1 | not tested | 75,8 | 63,5 | 101,8 | 86,0 | 57,8 | 98,8 | not tested | 72,9 | 67,6 | 51,3 | 84,5 | 89,3 | 38,3 | 54,3 | not tested | 96,3 | not tested | 15,1 | 78,4 | 81,4 | 99,7 | 36,3 | 11,6 | 71,5 |

Mean Growth Percent ***71.5***

Growth Percent, 10 µmol/L

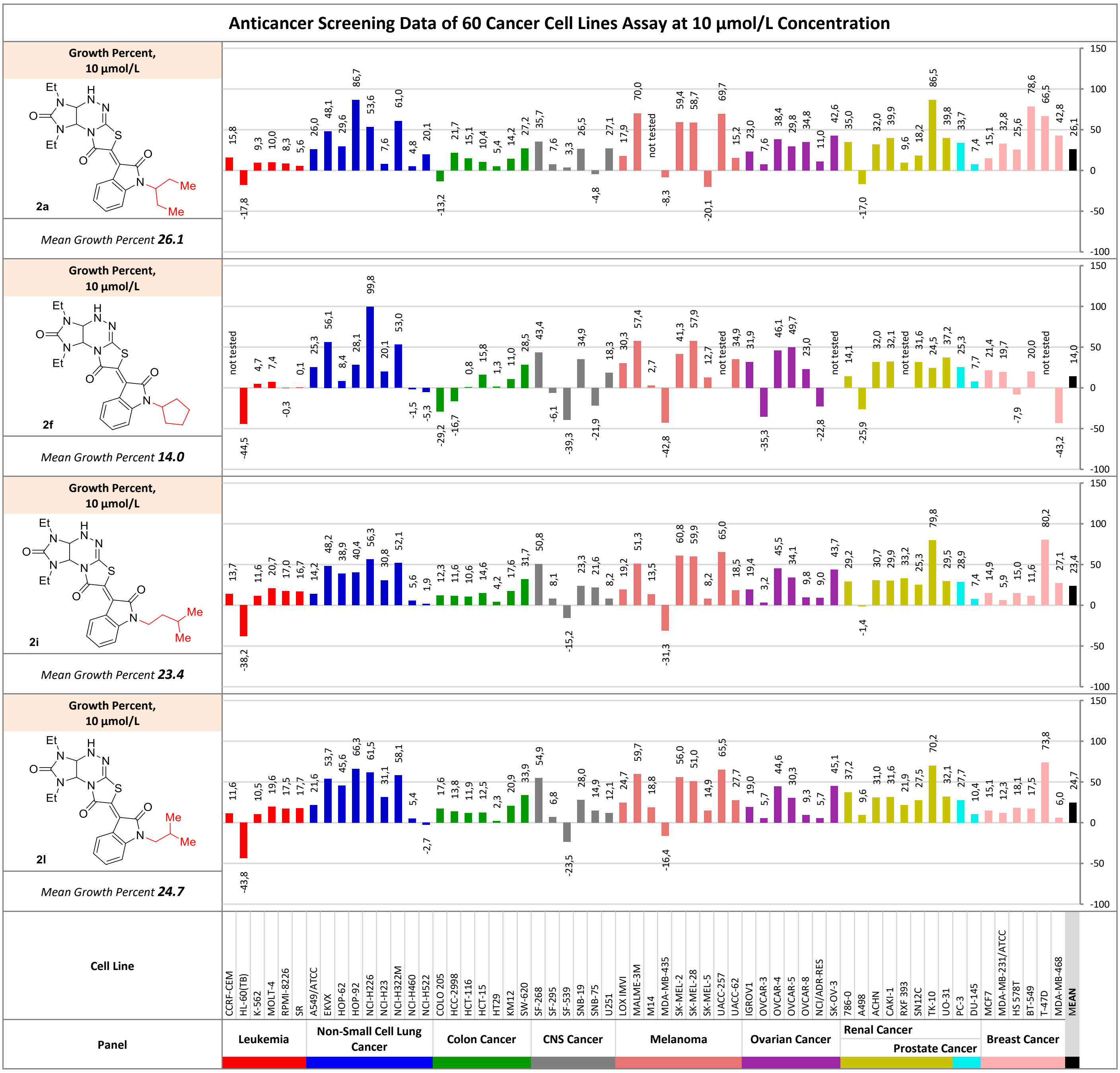


1l

| 42,6 | 18,9 | 15,6 | 48,7 | 50,6 | not tested | 44,6 | 63,8 | 55,2 | 81,2 | 84,1 | 43,1 | 64,9 | 24,5 | 16,0 | 4,6 | 76,5 | 14,4 | 27,3 | 86,4 | 31,9 | 35,7 | 66,1 | 42,4 | 7,6 | 54,7 | 14,1 | 36,3 | 54,2 | 70,0 | 18,9 | -45,9 | 66,4 | 66,0 | 39,9 | 87,5 | 45,4 | 47,9 | 21,5 | 56,5 | 52,5 | 44,7 | 11,3 | 56,2 | 35,3 | -6,4 | 52,5 | 34,1 | -3,7 | 48,9 | 13,1 | 49,8 | 38,1 | 34,5 | 26,1 | 19,6 | 40,5 | 52,7 | 46,0 | 15,8 | 39,7 |

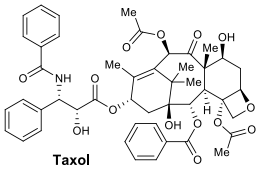
Mean Growth Percent ***39.7***

Panel	Leukemia	Non-Small Cell Lung Cancer	Colon Cancer	CNS Cancer	Melanoma	Ovarian Cancer	Renal Cancer	Prostate Cancer	Breast Cancer


Anticancer Screening Data of 60 Cancer Cell Lines Assay at 10 µmol/L Concentration
Growth Percent, 10 µmol/L
2a
Mean Growth Percent 26.1
15,8 -17,8 9,3 10,0 8,3 5,6 26,0 48,1 29,6 86,7 53,6 7,6 61,0 4,8 20,1 -13,2 21,7 15,1 10,4 5,4 14,2 27,2 35,7 7,6 3,3 26,5 -4,8 27,1 17,9 70,0 not tested -8,3 59,4 58,7 -20,1 69,7 15,2 23,0 7,6 38,4 29,8 34,8 11,0 42,6 35,0 -17,0 32,0 39,9 9,6 18,2 86,5 39,8 33,7 7,4 15,1 32,8 25,6 78,6 66,5 42,8 26,1
Growth Percent, 10 µmol/L
2f
Mean Growth Percent 14.0
not tested -44,5 4,7 7,4 -0,3 0,1 25,3 56,1 8,4 28,1 99,8 20,1 53,0 -1,5 -5,3 -29,2 -16,7 0,8 15,8 1,3 11,0 28,5 43,4 -6,1 -39,3 34,9 -21,9 18,3 30,3 57,4 2,7 -42,8 41,3 57,9 12,7 not tested 34,9 31,9 -35,3 46,1 49,7 23,0 -22,8 not tested 14,1 -25,9 32,0 32,1 not tested 31,6 24,5 37,2 25,3 7,7 21,4 19,7 -7,9 20,0 not tested -43,2 14,0
Growth Percent, 10 µmol/L
2i
Mean Growth Percent 23.4
13,7 -38,2 11,6 20,7 17,0 16,7 14,2 48,2 38,9 40,4 56,3 30,8 52,1 5,6 1,9 12,3 11,6 10,6 14,6 4,2 17,6 31,7 50,8 8,1 -15,2 23,3 21,6 8,2 19,2 51,3 13,5 -31,3 60,8 59,9 8,2 65,0 18,5 19,4 3,2 45,5 34,1 9,8 9,0 43,7 29,2 -1,4 30,7 29,9 33,2 25,3 79,8 29,5 28,9 7,4 14,9 5,9 15,0 11,6 80,2 27,1 23,4
Growth Percent, 10 µmol/L
2l
Mean Growth Percent 24.7
11,6 -43,8 10,5 19,6 17,5 17,7 21,6 53,7 45,6 66,3 61,5 31,1 58,1 5,4 -2,7 17,6 13,8 11,9 12,5 2,3 20,9 33,9 54,9 6,8 -23,5 28,0 14,9 12,1 24,7 59,7 18,8 -16,4 56,0 51,0 14,9 65,5 27,7 19,0 5,7 44,6 30,3 9,3 5,7 45,1 37,2 9,6 31,0 31,6 21,9 27,5 70,2 32,1 27,7 10,4 15,1 12,3 18,1 17,5 73,8 6,0 24,7
150 100 50 0 -50 -100
Cell Line
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522 COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62 IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 PC-3 DU-145 MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 MEAN
Panel
Leukemia
Non-Small Cell Lung Cancer
Colon Cancer
CNS Cancer
Melanoma
Ovarian Cancer
Renal Cancer
Prostate Cancer
Breast Cancer

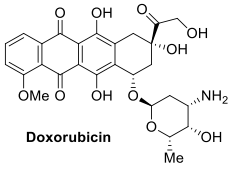
Antinticancer Screening Data of 60 Cancer Cell Lines Assay at 10 µmol/L Concentration

Taxol [NSC 125973]
10 µmol/L



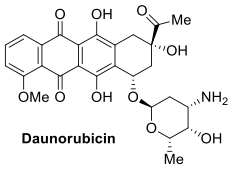
Mean Growth Percent ***14.6***

Doxorubicin [NSC 759155]
10 µmol/L



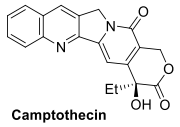
Mean Growth Percent ***-20.4***

Daunorubicin [NSC 82151]
10 µmol/L

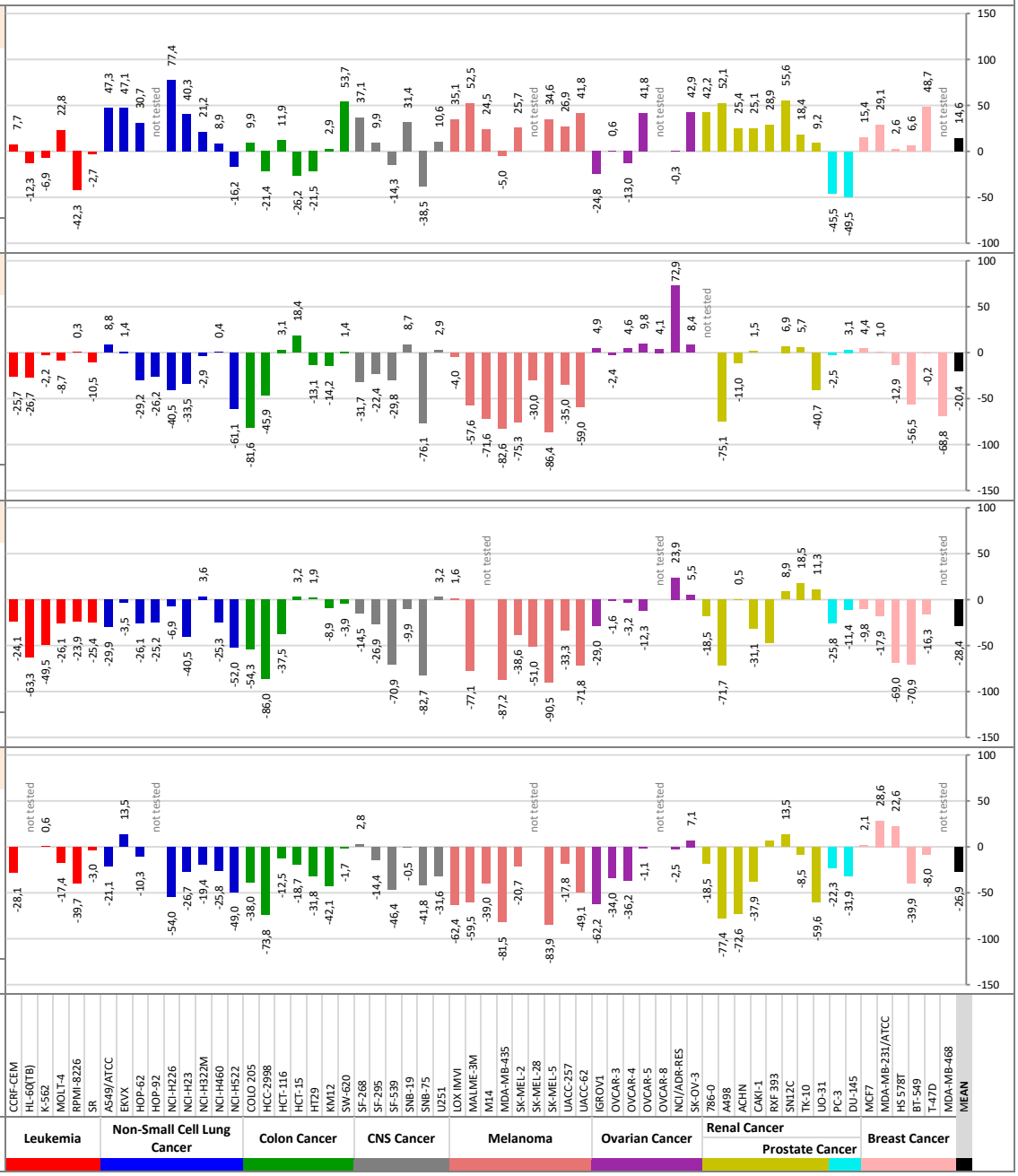


Mean Growth Percent ***-28.4***

Camptothecin [NSC 94600]
10 µmol/L



Mean Growth Percent ***-26.9***

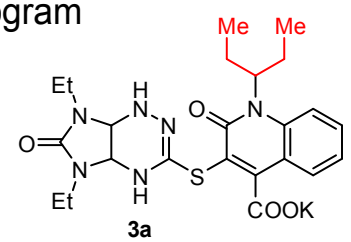


National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 831262 / 1 | Experiment ID : 2110NS03 | Test Type : 08

Report Date : January 14, 2022 | Test Date : October 25, 2021 | QNS :

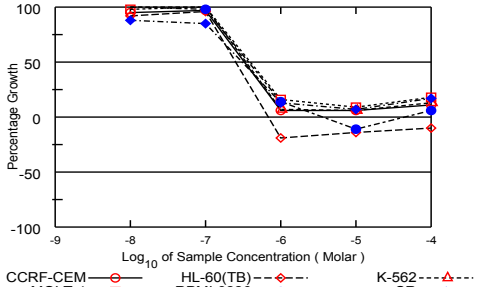
COMI : IA-1119 | Stain Reagent : SRB Dual-Pass Related | SSPL : 1AMN



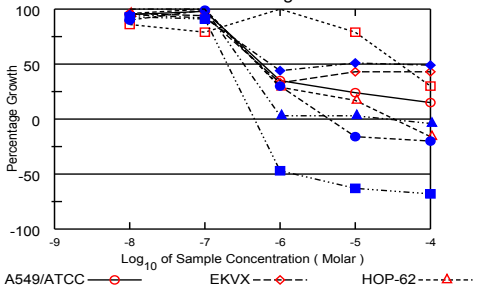
3a

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.499	2.572	2.467	2.502	0.617	0.629	0.737	95	97	6	6	11	3.26E-7	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.561	2.438	2.293	2.359	0.457	0.485	0.507	92	96	-19	-14	-10	2.51E-7	6.87E-7	> 1.00E-4
K-562	0.184	1.982	1.983	2.009	0.314	0.290	0.423	100	101	7	6	13	3.52E-7	> 1.00E-4	> 1.00E-4
MOLT-4	0.573	2.902	2.861	2.925	0.937	0.793	0.981	98	101	16	9	18	3.96E-7	> 1.00E-4	> 1.00E-4
RPMI-8226	0.997	3.055	3.052	3.007	1.278	0.888	1.126	100	98	14	-11	6	3.69E-7	.	> 1.00E-4
SR	0.550	2.618	2.380	2.307	0.827	0.685	0.897	88	85	13	7	17	3.08E-7	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.872	2.956	2.845	2.904	1.602	1.378	1.191	95	98	35	24	15	5.76E-7	> 1.00E-4	> 1.00E-4
EKVX	0.803	2.208	2.148	2.126	1.271	1.407	1.412	96	94	33	43	43	5.32E-7	> 1.00E-4	> 1.00E-4
HOP-62	0.902	2.619	2.550	2.615	1.395	1.191	0.757	96	100	29	17	-16	5.01E-7	3.25E-5	> 1.00E-4
HOP-92	1.688	2.202	2.130	2.093	2.219	2.095	1.842	86	79	103	79	30	3.90E-5	> 1.00E-4	> 1.00E-4
NCI-H226	1.682	2.704	2.599	2.698	1.992	1.410	1.350	90	99	30	-16	-20	5.20E-7	4.49E-6	> 1.00E-4
NCI-H322M	0.792	2.219	2.154	2.110	1.416	1.521	1.493	95	92	44	51	49	.	> 1.00E-4	> 1.00E-4
NCI-H460	0.230	2.410	2.524	2.531	0.293	0.301	0.222	105	106	3	3	-4	3.48E-7	2.93E-5	> 1.00E-4
NCI-H522	1.048	2.788	2.668	2.631	0.558	0.389	0.334	93	91	-47	-63	-68	1.98E-7	4.57E-7	1.58E-6
Colon Cancer															
COLO 205	0.480	1.876	1.852	1.971	0.277	0.082	0.092	98	107	-42	-83	-81	2.40E-7	5.20E-7	1.55E-6
HCC-2998	0.737	2.450	2.464	2.459	0.742	0.685	0.669	101	101	0	-7	-9	3.19E-7	1.09E-6	> 1.00E-4
HCT-116	0.228	2.073	2.065	1.976	0.340	0.253	0.177	100	95	6	1	-22	3.20E-7	1.14E-5	> 1.00E-4
HCT-15	0.382	2.598	2.499	2.431	0.547	0.448	0.402	96	92	7	3	1	3.16E-7	> 1.00E-4	> 1.00E-4
HT29	0.369	2.438	2.427	2.405	0.287	0.235	0.253	99	98	-22	-36	-31	2.52E-7	6.53E-7	> 1.00E-4
KM12	0.696	3.196	3.104	3.105	1.055	0.796	0.765	96	96	14	4	3	3.68E-7	> 1.00E-4	> 1.00E-4
SW-620	0.267	1.966	1.952	2.010	0.628	0.672	0.629	99	103	21	24	21	4.43E-7	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.898	2.624	2.542	2.522	1.681	1.309	1.283	95	94	45	24	22	8.04E-7	> 1.00E-4	> 1.00E-4
SF-295	0.951	2.591	2.613	2.594	1.075	1.144	0.735	101	100	8	12	-23	3.48E-7	2.19E-5	> 1.00E-4
SF-539	0.706	2.391	2.428	2.325	0.617	0.641	0.354	102	96	-13	-9	-50	2.65E-7	7.66E-7	> 1.00E-4
SNB-19	0.553	1.964	1.855	1.875	0.917	0.913	0.676	92	94	26	25	9	4.40E-7	> 1.00E-4	> 1.00E-4
SNB-75	1.689	2.679	2.529	2.492	2.049	1.713	0.893	85	81	36	2	-47	4.95E-7	1.12E-5	> 1.00E-4
U251	0.706	2.793	2.707	2.669	1.001	0.890	0.717	96	94	14	9	1	3.56E-7	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.320	2.101	2.051	1.969	0.764	0.601	0.475	97	93	25	16	9	4.26E-7	> 1.00E-4	> 1.00E-4
MALME-3M	0.621	1.244	1.246	1.205	0.937	0.884	0.719	100	94	51	42	16	1.21E-6	> 1.00E-4	> 1.00E-4
M14	0.560	2.133	2.085	2.044	0.634	0.622	0.537	97	94	5	4	-4	3.12E-7	3.05E-5	> 1.00E-4
MDA-MB-435	0.499	2.470	2.372	2.343	0.209	0.250	0.207	95	94	-58	-50	-59	1.94E-7	4.13E-7	.
SK-MEL-2	1.722	2.674	2.611	2.579	1.850	1.940	1.296	93	90	13	23	-25	3.33E-7	3.03E-5	> 1.00E-4
SK-MEL-28	0.625	1.969	1.996	1.968	1.225	1.149	1.058	102	100	45	39	32	8.00E-7	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.912	3.255	3.228	3.210	1.733	0.699	0.590	99	98	35	-23	-35	5.79E-7	3.98E-6	> 1.00E-4
UACC-257	1.294	2.869	2.789	2.765	2.179	1.911	1.733	95	93	56	39	28	2.31E-6	> 1.00E-4	> 1.00E-4
UACC-62	0.837	2.987	2.841	2.817	1.366	1.216	0.748	93	92	25	18	-11	4.20E-7	4.19E-5	> 1.00E-4
Ovarian Cancer															
IGROV1	0.520	2.308	2.311	2.266	1.082	0.765	0.690	100	98	31	14	10	5.24E-7	> 1.00E-4	> 1.00E-4
OVCAR-3	0.601	2.036	2.048	2.045	0.465	0.478	0.372	101	101	-23	-20	-38	2.57E-7	6.54E-7	> 1.00E-4
OVCAR-4	0.656	1.804	1.839	1.777	1.358	1.189	1.193	103	98	61	46	47	5.69E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.703	1.892	1.806	1.794	1.013	1.025	0.954	93	92	26	27	21	4.32E-7	> 1.00E-4	> 1.00E-4
OVCAR-8	0.308	1.565	1.530	1.528	0.278	0.257	0.240	97	97	-10	-17	-22	2.76E-7	8.11E-7	> 1.00E-4
NCI/ADR-RES	0.581	2.101	2.071	2.061	0.616	0.560	0.513	98	97	2	-4	-12	3.15E-7	2.45E-6	> 1.00E-4
SK-OV-3	1.170	2.150	2.218	2.212	1.383	1.350	1.158	107	106	22	18	-1	4.63E-7	8.85E-5	> 1.00E-4
Renal Cancer															
786-0	0.478	2.263	2.171	2.158	1.045	0.736	0.551	95	94	32	14	4	5.09E-7	> 1.00E-4	> 1.00E-4
A498	1.867	2.637	2.672	2.632	2.612	2.429	1.684	104	99	97	73	-10	1.89E-5	7.61E-5	> 1.00E-4
ACHN	0.260	1.416	1.440	1.443	0.667	0.458	0.407	102	102	35	17	13	6.02E-7	> 1.00E-4	> 1.00E-4
CAKI-1	0.540	2.025	1.880	1.801	0.970	0.627	0.377	90	85	29	6	-30	4.20E-7	1.45E-5	> 1.00E-4
RXF 393	0.825	1.471	1.480	1.443	0.457	0.767	0.240	101	96	-45	-7	-71	2.12E-7	4.81E-7	4.70E-5
SN12C	0.572	2.263	2.223	2.212	0.990	0.741	0.716	98	97	25	10	9	4.47E-7	> 1.00E-4	> 1.00E-4
TK-10	1.383	2.191	2.078	2.056	2.009	1.798	1.310	86	83	77	51	-5	1.05E-5	8.07E-5	> 1.00E-4
UO-31	0.610	1.990	1.801	1.756	1.108	1.012	0.813	86	83	36	29	15	5.05E-7	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.625	2.645	2.492	2.489	1.081	1.006	1.070	92	92	23	19	22	4.04E-7	> 1.00E-4	> 1.00E-4
DU-145	0.442	2.012	2.156	2.070	0.747	0.533	0.461	109	104	19	6	1	4.34E-7	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.461	2.420	2.198	2.250	0.677	0.536	0.544	89	91	11	4	4	3.27E-7	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.540	1.492	1.520	1.436	0.711	0.668	0.511	103	94	18	13	-5	3.79E-7	5.17E-5	> 1.00E-4
HS 578T	1.734	2.782	2.704	2.678	1.915	2.034	1.731	93	90	17	29	0	3.55E-7	9.84E-5	> 1.00E-4
BT-549	1.658	2.888	2.902	2.910	2.264	1.525	1.292	101	102	49	-8	-22	9.69E-7	7.24E-6	> 1.00E-4
T-47D	0.966	2.194	2.122	2.045	1.455	1.538	1.521	94	88	40	47	45	6.14E-7	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.790	1.300	1.276	1.247	0.852	0.858	0.786	95	90	12	13	0	3.25E-7	9.09E-5	> 1.00E-4

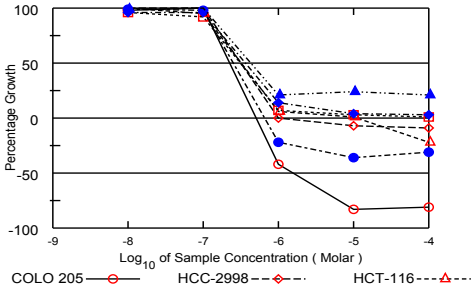
Leukemia



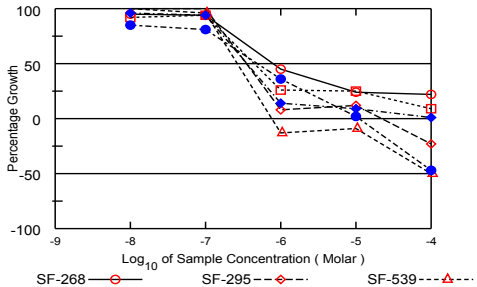
Non-Small Cell Lung Cancer



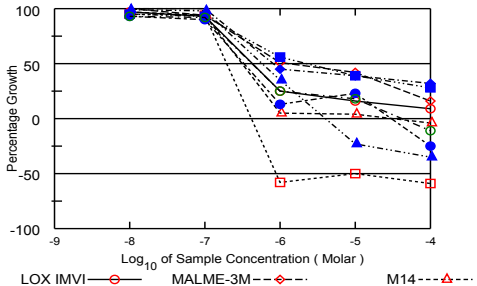
Colon Cancer



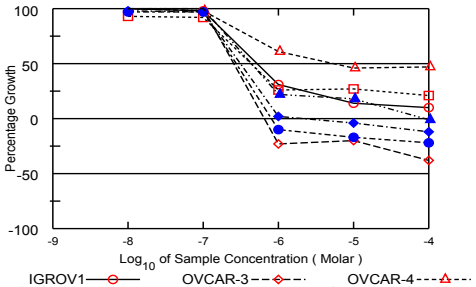
CNS Cancer



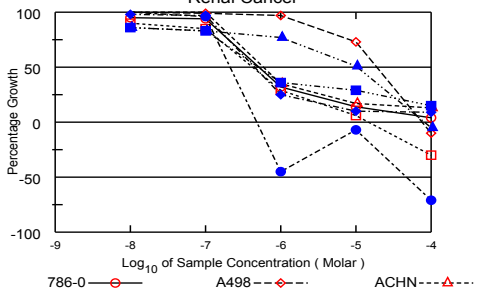
Melanoma



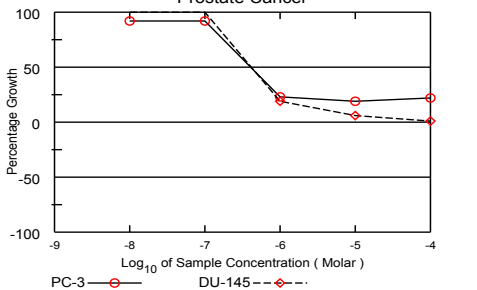
Ovarian Cancer



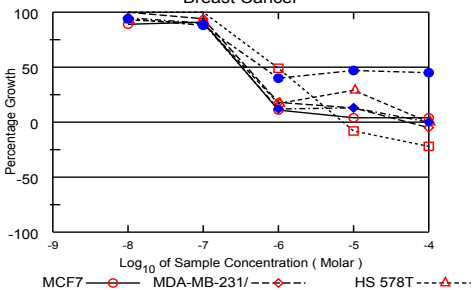
Renal Cancer



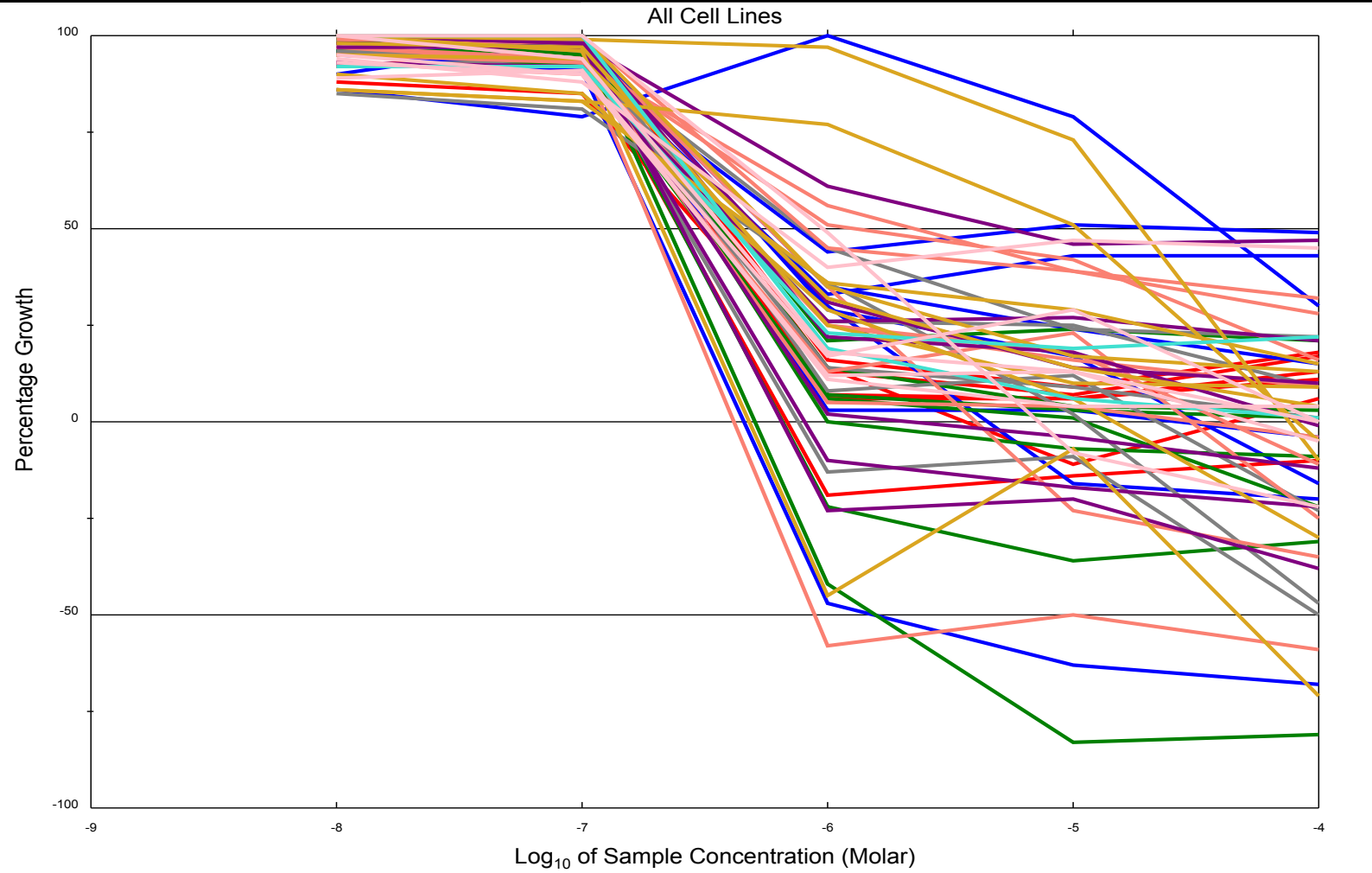
Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 831262/1	SSPL:1AMN	EXP. ID:2110NS03
	Report Date:January 14, 2022	Test Date:October 25, 2021	

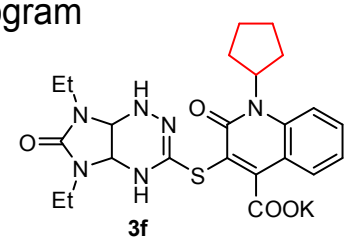


National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 833972 / 1 | Experiment ID : 2203NS93 | Test Type : 08

Report Date : April 29, 2022 | Test Date : March 28, 2022 | QNS :

COMI : IA1301 | Stain Reagent : SRB Dual-Pass Related | SSPL : 1AMN



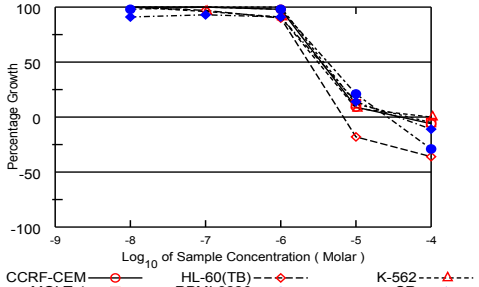
3f

Log10 Concentration

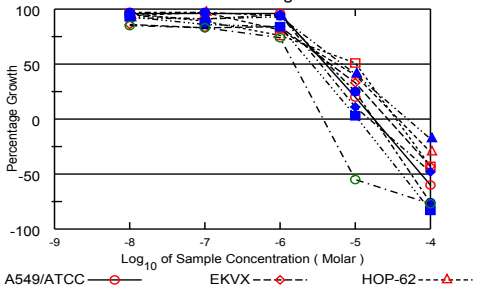
Panel/Cell Line	Time Zero	Mean Optical Densities: Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	Percent Growth: -8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.531	1.847	1.852	1.851	1.817	0.651	0.497	100	100	98	9	-6	3.45E-6	3.83E-5	> 1.00E-4
HL-60(TB)	0.444	1.547	1.571	1.511	1.434	0.366	0.285	102	97	90	-18	-36	2.35E-6	6.86E-6	> 1.00E-4
K-562	0.132	1.322	1.327	1.275	1.214	0.230	0.133	100	96	91	8	0	3.13E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.537	1.915	2.053	1.962	1.965	0.709	0.509	110	103	104	12	-5	3.88E-6	5.03E-5	> 1.00E-4
RPMI-8226	0.739	2.748	2.717	2.744	2.703	1.155	0.521	98	100	98	21	-29	4.17E-6	2.59E-5	> 1.00E-4
SR	0.527	2.297	2.130	2.180	2.142	0.768	0.469	91	93	91	14	-11	3.40E-6	3.57E-5	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.366	1.961	1.890	1.891	1.900	0.685	0.147	96	96	96	20	-60	4.04E-6	1.78E-5	7.50E-5
EKVX	0.777	1.579	1.467	1.444	1.449	1.045	0.445	86	83	84	33	-43	4.69E-6	2.74E-5	> 1.00E-4
HOP-62	0.701	1.549	1.498	1.521	1.388	1.042	0.489	94	97	81	40	-30	5.75E-6	3.72E-5	> 1.00E-4
HOP-92	1.031	1.899	1.867	1.808	1.688	1.476	0.588	96	89	76	51	-43	1.03E-5	3.50E-5	> 1.00E-4
NCI-H226	1.006	2.190	2.161	2.151	2.124	1.300	0.246	97	97	94	25	-76	4.34E-6	1.77E-5	5.56E-5
NCI-H23	0.556	1.651	1.587	1.550	1.597	0.677	0.291	94	91	95	11	-48	3.44E-6	1.54E-5	> 1.00E-4
NCI-H322M	0.779	1.981	1.882	1.869	1.893	1.268	0.640	92	91	93	41	-18	6.61E-6	4.95E-5	> 1.00E-4
NCI-H460	0.198	2.356	2.213	2.047	2.002	0.256	0.034	93	86	84	3	-83	2.60E-6	1.08E-5	4.13E-5
NCI-H522	0.811	2.161	1.960	1.936	1.813	0.362	0.184	85	83	74	-55	-77	1.54E-6	3.74E-6	9.08E-6
Colon Cancer															
COLO 205	0.501	1.585	1.628	1.673	1.587	0.192	0.016	104	108	100	-62	-97	2.04E-6	4.16E-6	8.47E-6
HCC-2998	0.919	2.640	2.558	2.525	2.506	0.912	0.248	95	93	92	0	-73	2.84E-6	9.80E-6	4.80E-5
HCT-116	0.212	1.949	1.910	1.999	1.824	0.306	-0.007	98	103	93	5	-100	3.09E-6	1.12E-5	3.35E-5
HCT-15	0.250	1.495	1.411	1.375	1.354	0.296	0.078	93	90	89	4	-69	2.85E-6	1.12E-5	5.48E-5
HT29	0.287	1.717	1.715	1.589	1.679	0.314	0.024	100	91	97	2	-92	3.13E-6	1.05E-5	3.59E-5
KM12	0.378	2.224	2.223	2.169	2.039	0.618	0.211	100	97	90	13	-44	3.30E-6	1.69E-5	> 1.00E-4
SW-620	0.220	1.673	1.567	1.503	1.419	0.508	0.076	93	88	83	20	-65	3.30E-6	1.71E-5	6.59E-5
CNS Cancer															
SF-268	0.467	2.058	1.955	1.928	1.870	0.936	0.395	94	92	88	29	-15	4.47E-6	4.54E-5	> 1.00E-4
SF-295	0.449	1.393	1.327	1.275	1.272	0.404	0.076	93	87	87	-10	-83	2.41E-6	7.89E-6	3.52E-5
SF-539	0.582	1.913	1.831	1.773	1.780	0.399	0.012	94	90	90	-31	-98	2.13E-6	5.51E-6	1.90E-5
SNB-19	0.690	2.134	2.039	2.017	1.989	1.117	0.625	93	92	90	30	-9	4.59E-6	5.73E-5	> 1.00E-4
SNB-75	0.673	1.632	1.319	1.317	1.248	0.718	0.256	67	67	60	5	-62	1.51E-6	1.18E-5	6.62E-5
U251	0.345	1.825	1.720	1.685	1.719	0.595	0.091	93	91	93	17	-74	3.66E-6	1.53E-5	5.47E-5
Melanoma															
LOX IMVI	0.387	2.412	2.246	2.197	2.077	0.925	-0.007	92	89	83	27	-100	3.87E-6	1.62E-5	4.03E-5
MALME-3M	0.565	1.168	1.111	1.091	1.076	0.835	0.199	90	87	85	45	-65	7.36E-6	2.56E-5	7.32E-5
M14	0.504	1.914	1.835	1.924	1.789	0.666	0.097	94	101	91	11	-81	3.28E-6	1.33E-5	4.63E-5
MDA-MB-435	0.499	2.240	2.125	2.017	1.718	0.252	0.130	93	87	70	-49	-74	1.47E-6	3.85E-6	1.05E-5
SK-MEL-2	1.262	2.719	2.704	2.670	2.578	1.628	0.477	99	97	90	25	-62	4.15E-6	1.94E-5	7.25E-5
SK-MEL-28	0.703	2.246	2.290	2.177	2.043	1.368	0.268	103	96	87	43	-62	6.94E-6	2.57E-5	7.70E-5
SK-MEL-5	0.802	2.844	2.856	2.718	2.723	1.067	0.135	101	94	94	13	-83	3.49E-6	1.36E-5	4.51E-5
UACC-257	0.849	2.138	2.029	2.062	1.934	1.436	0.378	92	94	84	46	-56	7.65E-6	2.82E-5	8.81E-5
UACC-62	0.900	2.722	2.605	2.549	2.416	1.168	0.411	94	90	83	15	-54	3.05E-6	1.63E-5	8.64E-5
Ovarian Cancer															
IGROV1	0.609	2.419	2.339	2.296	2.246	1.110	0.418	96	93	90	28	-31	4.41E-6	2.94E-5	> 1.00E-4
OVCAR-3	0.310	1.412	1.401	1.365	1.340	0.395	0.113	99	96	93	8	-64	3.21E-6	1.28E-5	6.43E-5
OVCAR-4	0.732	2.013	1.917	1.868	1.811	1.256	0.574	92	89	84	41	-22	6.15E-6	4.50E-5	> 1.00E-4
OVCAR-5	0.552	1.771	1.729	1.707	1.665	0.842	0.303	97	95	91	24	-45	4.09E-6	2.21E-5	> 1.00E-4
OVCAR-8	0.356	1.726	1.746	1.699	1.668	0.454	0.133	101	98	96	7	-63	3.28E-6	1.27E-5	6.57E-5
NCI/ADR-RES	0.512	1.623	1.605	1.561	1.505	0.261	0.120	98	94	89	-49	-77	1.92E-6	4.42E-6	1.09E-5
SK-OV-3	0.822	1.546	1.538	1.545	1.455	0.939	0.540	99	100	87	16	-34	3.35E-6	2.08E-5	> 1.00E-4
Renal Cancer															
786-0	0.616	2.365	2.362	2.162	2.064	1.168	0.135	100	88	83	32	-78	4.36E-6	1.94E-5	5.54E-5
A498	1.112	1.875	1.821	1.706	1.666	1.633	0.669	93	78	73	68	-40	1.48E-5	4.28E-5	> 1.00E-4
ACHN	0.455	1.903	1.840	1.827	1.807	0.825	0.025	96	95	93	26	-95	4.36E-6	1.63E-5	4.25E-5
CAKI-1	0.560	2.054	1.951	1.977	1.803	0.975	0.004	93	95	83	28	-99	3.97E-6	1.65E-5	4.09E-5
RXF 393	1.043	1.698	1.741	1.679	1.615	1.078	0.353	107	97	87	5	-66	2.85E-6	1.19E-5	5.94E-5
SN12C	0.429	1.784	1.655	1.663	1.618	0.659	0.148	90	91	88	17	-66	3.41E-6	1.60E-5	6.49E-5
TK-10	0.827	1.698	1.572	1.592	1.655	1.274	0.395	86	88	95	51	-52	1.03E-5	3.13E-5	9.50E-5
UO-31	0.742	2.357	2.010	2.076	1.980	1.309	0.279	79	83	77	35	-62	4.38E-6	2.29E-5	7.46E-5
Prostate Cancer															
PC-3	0.531	2.300	2.207	2.265	2.210	0.903	0.431	95	98	95	21	-19	4.05E-6	3.36E-5	> 1.00E-4
DU-145	0.277	1.536	1.572	1.535	1.537	0.472	0.157	103	100	100	15	-44	3.91E-6	1.83E-5	> 1.00E-4
Breast Cancer															
MCF7	0.208	1.092	0.971	0.969	0.809	0.308	0.043	86	86	68	11	-79	2.07E-6	1.33E-5	4.74E-5
MDA-MB-231/ATCC	0.549	1.480	1.427	1.443	1.402	0.597	0.115	94	96	92	5	-79	3.03E-6	1.15E-5	4.52E-5
HS 578T	0.942	1.953	1.853	1.825	1.737	0.902	0.797	90	87	79	-4	-15	2.21E-6	8.87E-6	> 1.00E-4
BT-549	1.200	2.144	2.073	2.027	1.957	1.667	0.263	92	88	80	49	-78	9.60E-6	2.44E-5	6.02E-5
T-47D	0.926	2.180	2.086	2.050	2.060	1.469	0.862	93	90	90	43	-7	7.20E-6	7.27E-5	> 1.00E-4
MDA-MB-468	0.784	1.262	1.194	1.211	1.177	0.605	0.419	86	89	82	-23	-47	2.02E-6	6.06E-6	> 1.00E-4

National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC: D - 833972 / 1	SSPL: 1AMN	EXP. ID: 2203NS93
	Report Date: April 29, 2022	Test Date: March 28, 2022	

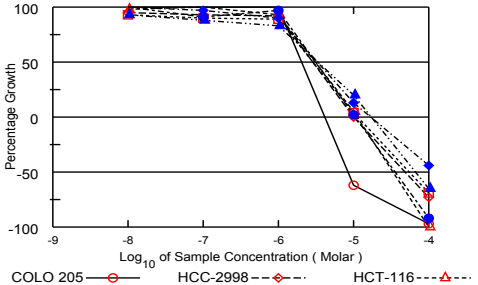
Leukemia



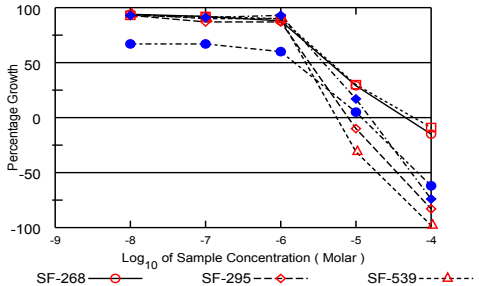
Non-Small Cell Lung Cancer



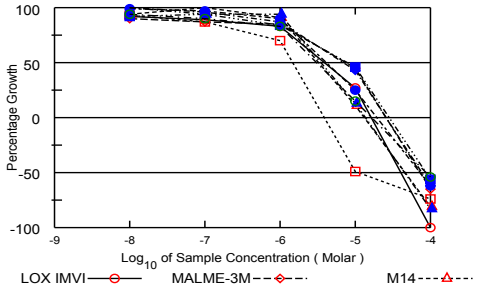
Colon Cancer



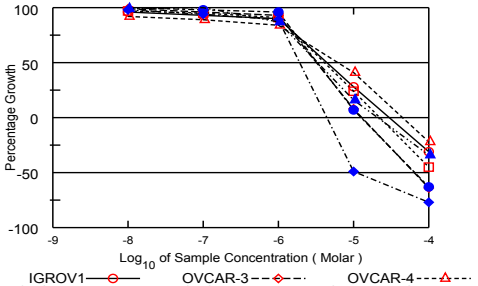
CNS Cancer



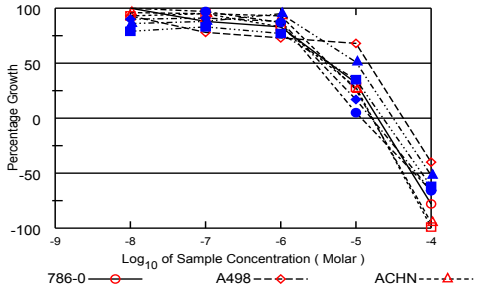
Melanoma



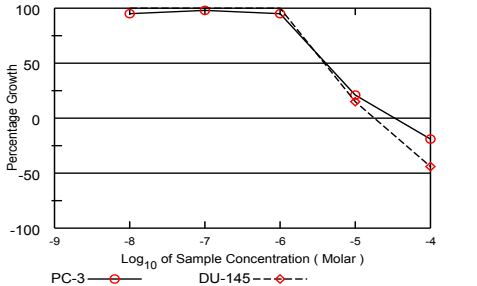
Ovarian Cancer



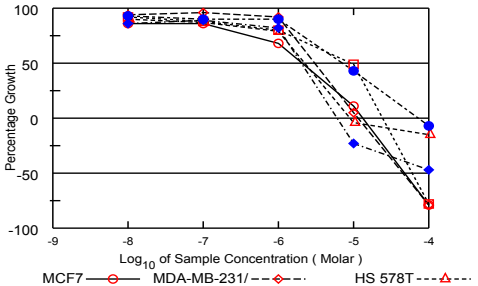
Renal Cancer



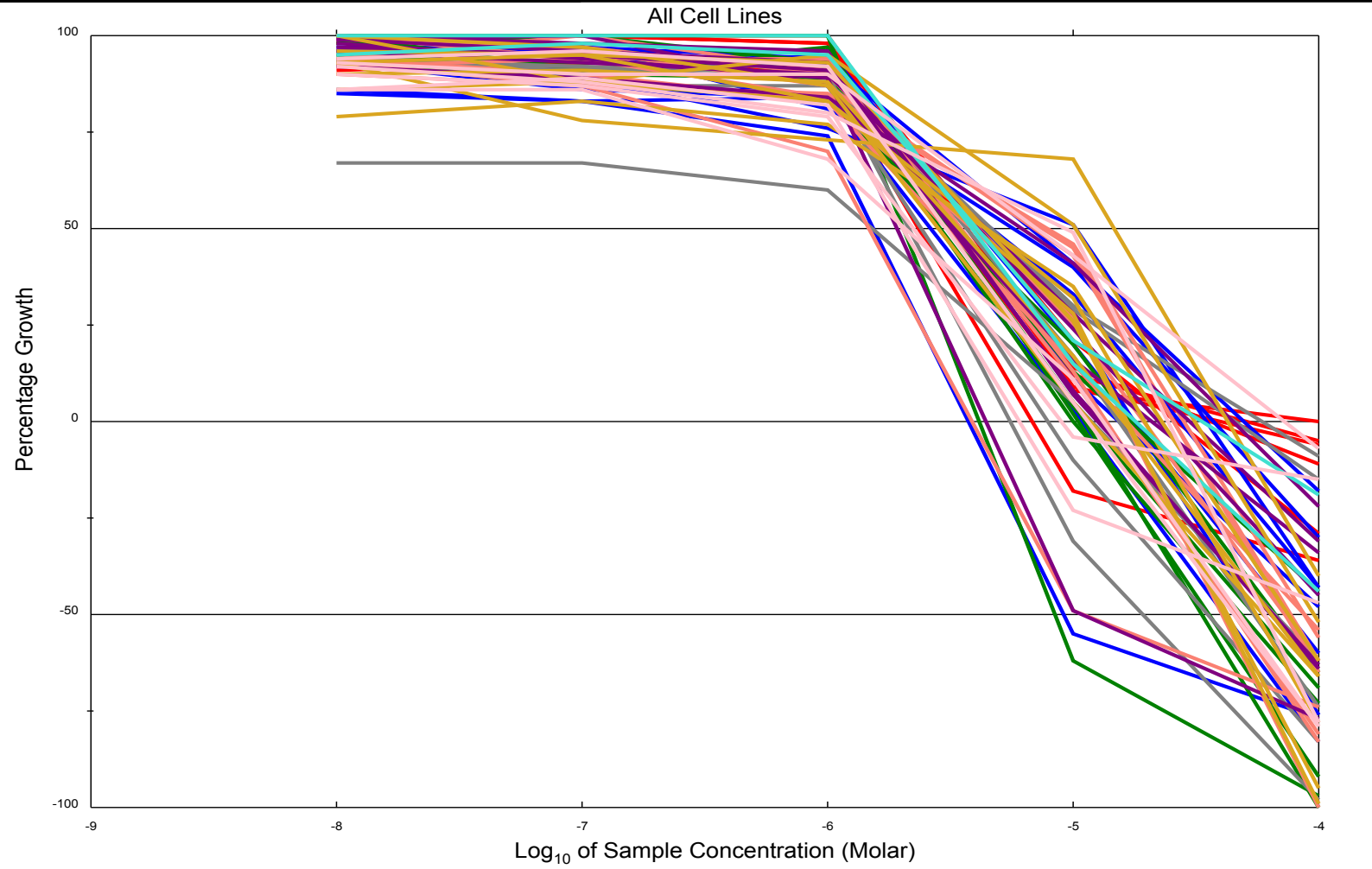
Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 833972/1	SSPL:1AMN	EXP. ID:2203NS93
	Report Date:April 29, 2022	Test Date:March 28, 2022	

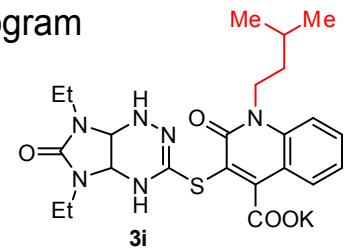


National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 834436 / 1 | Experiment ID : 2204NS06 | Test Type : 08

Report Date : May 26, 2022 | Test Date : April 25, 2022 | QNS :

COMI : IA1351 | Stain Reagent : SRB Dual-Pass Related | SSPL : 1AMN

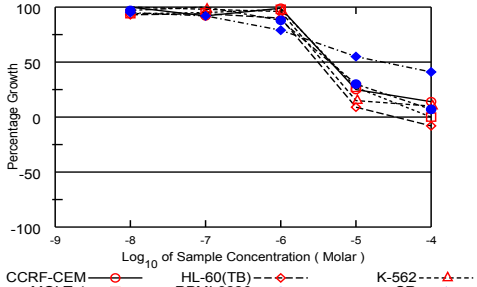


3i

Log10 Concentration

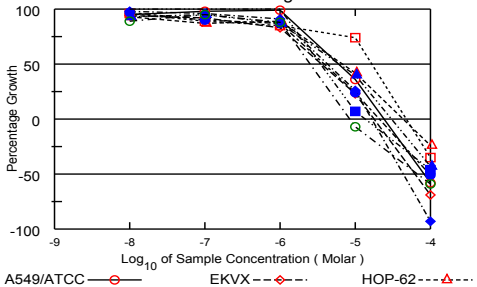
Panel/Cell Line	Time Zero	Mean Optical Densities Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	Percent Growth -8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.438	1.871	1.927	1.762	1.858	0.801	0.636	104	92	99	25	14	4.62E-6	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.630	2.794	2.639	2.671	2.583	0.820	0.582	93	94	90	9	-8	3.12E-6	3.41E-5	> 1.00E-4
K-562	0.212	2.304	2.304	2.257	2.219	0.526	0.419	100	98	96	15	10	3.70E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.668	2.827	2.698	2.714	2.782	1.262	0.668	94	95	98	27	0	4.79E-6	> 1.00E-4	> 1.00E-4
RPMI-8226	0.619	2.660	2.608	2.671	2.425	1.241	0.764	97	101	88	30	7	4.61E-6	> 1.00E-4	> 1.00E-4
SR	0.173	0.748	0.719	0.705	0.625	0.489	0.406	95	92	79	55	41	2.20E-5	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.404	2.340	2.239	2.307	2.316	1.111	0.168	95	98	99	36	-58	6.07E-6	2.42E-5	8.15E-5
EKVX	0.576	1.959	1.872	1.852	1.719	0.890	0.178	94	92	83	23	-69	3.50E-6	1.77E-5	6.18E-5
HOP-62	0.821	2.624	2.495	2.389	2.432	1.572	0.624	93	87	89	42	-24	6.68E-6	4.30E-5	> 1.00E-4
HOP-92	1.108	1.987	1.949	1.888	1.856	1.756	0.716	96	89	85	74	-35	1.65E-5	4.74E-5	> 1.00E-4
NCI-H226	0.719	1.535	1.513	1.455	1.426	0.917	0.353	97	90	87	24	-51	3.87E-6	2.10E-5	9.71E-5
NCI-H23	0.409	1.375	1.359	1.338	1.292	0.665	0.028	98	96	91	26	-93	4.34E-6	1.66E-5	4.35E-5
NCI-H322M	0.761	1.922	1.839	1.858	1.775	1.220	0.434	93	95	87	40	-43	6.03E-6	3.01E-5	> 1.00E-4
NCI-H460	0.290	2.683	2.778	2.826	2.682	0.447	0.158	104	106	100	7	-46	3.43E-6	1.33E-5	> 1.00E-4
NCI-H522	1.172	2.844	2.666	2.761	2.648	1.089	0.478	89	95	88	-7	-59	2.52E-6	8.42E-6	6.64E-5
Colon Cancer															
COLO 205	0.551	2.217	2.367	2.303	2.370	0.617	0.237	109	105	109	4	-57	3.65E-6	1.16E-5	7.66E-5
HCC-2998	0.488	1.924	1.929	1.841	1.736	0.440	0.075	100	94	87	-10	-85	2.41E-6	7.91E-6	3.44E-5
HCT-116	0.239	2.846	2.574	2.706	2.604	0.877	0.325	90	95	91	24	3	4.12E-6	> 1.00E-4	> 1.00E-4
HCT-15	0.337	2.305	2.234	2.259	1.948	0.524	0.135	96	98	82	9	-60	2.75E-6	1.37E-5	7.16E-5
HT29	0.293	1.990	2.020	1.901	1.942	0.408	0.152	102	95	97	7	-48	3.32E-6	1.33E-5	> 1.00E-4
KM12	0.788	3.252	3.270	3.282	2.857	1.498	0.704	101	101	84	29	-11	4.13E-6	5.35E-5	> 1.00E-4
SW-620	0.285	1.883	1.977	1.905	1.794	0.920	0.168	106	101	94	40	-41	6.50E-6	3.10E-5	> 1.00E-4
CNS Cancer															
SF-268	1.015	2.721	2.746	2.674	2.597	1.881	1.201	101	97	93	51	11	1.04E-5	> 1.00E-4	> 1.00E-4
SF-295	0.571	2.168	2.056	1.970	2.037	0.750	0.104	93	88	92	11	-82	3.30E-6	1.32E-5	4.54E-5
SF-539	0.761	2.187	2.099	2.065	2.014	0.539	0.008	94	91	88	-29	-99	2.11E-6	5.63E-6	1.98E-5
SNB-19	0.644	2.057	1.970	1.932	1.901	1.066	0.355	94	91	89	30	-45	4.56E-6	2.51E-5	> 1.00E-4
SNB-75	1.353	2.307	2.284	2.218	2.101	1.313	0.875	98	91	78	-3	-35	2.24E-6	9.19E-6	> 1.00E-4
U251	0.368	1.962	1.878	1.873	1.908	0.741	0.303	95	94	97	23	-18	4.33E-6	3.70E-5	> 1.00E-4
Melanoma															
LOX IMVI	0.264	1.989	1.859	1.829	1.784	0.856	0.017	92	91	88	34	-94	5.11E-6	1.85E-5	4.55E-5
MALME-3M	0.737	1.444	1.386	1.392	1.377	1.132	0.238	92	93	91	56	-68	1.11E-5	2.83E-5	7.19E-5
M14	0.430	2.129	2.231	2.141	2.041	1.221	0.623	106	101	95	47	11	8.47E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.533	2.400	2.366	2.454	2.209	0.365	0.220	98	103	90	-32	-59	2.13E-6	5.50E-6	4.75E-5
SK-MEL-2	1.302	3.047	2.986	2.976	3.000	2.150	0.655	96	96	97	49	-50	9.35E-6	3.12E-5	> 1.00E-4
SK-MEL-28	0.782	2.006	1.951	1.984	1.864	1.388	0.390	95	98	88	49	-50	9.69E-6	3.14E-5	9.97E-5
SK-MEL-5	0.718	3.207	3.151	3.131	3.128	1.307	0.097	98	97	97	24	-87	4.37E-6	1.64E-5	4.66E-5
UACC-257	0.933	2.249	2.219	2.212	2.226	1.933	0.812	98	97	98	76	-13	1.96E-5	7.15E-5	> 1.00E-4
UACC-62	0.894	2.460	2.347	2.347	2.189	1.356	0.271	93	93	83	29	-70	4.11E-6	1.98E-5	6.32E-5
Ovarian Cancer															
IGROV1	0.588	2.090	2.091	2.036	1.703	0.955	0.177	100	96	74	24	-70	3.06E-6	1.81E-5	6.14E-5
OVCAR-3	0.576	1.798	1.842	1.836	1.865	0.896	0.267	104	103	105	26	-54	5.01E-6	2.13E-5	9.00E-5
OVCAR-4	0.876	2.182	2.161	2.054	1.962	1.726	0.947	98	90	83	65	5	1.79E-5	> 1.00E-4	> 1.00E-4
OVCAR-5	0.942	1.710	1.583	1.644	1.595	1.041	0.564	83	91	85	13	-40	3.06E-6	1.75E-5	> 1.00E-4
OVCAR-8	0.550	2.610	2.594	2.632	2.522	1.255	0.475	99	101	96	34	-14	5.54E-6	5.17E-5	> 1.00E-4
NCI/ADR-RES	0.388	1.403	1.403	1.358	1.331	0.277	0.091	100	96	93	-29	-77	2.25E-6	5.80E-6	2.78E-5
SK-OV-3	0.808	2.037	2.048	1.978	2.042	1.338	0.742	101	95	100	43	-8	7.58E-6	6.91E-5	> 1.00E-4
Renal Cancer															
786-0	0.541	2.714	2.459	2.501	2.605	1.900	0.456	88	90	95	63	-16	1.45E-5	6.28E-5	> 1.00E-4
A498	1.641	2.219	2.287	2.137	2.115	2.122	1.148	112	86	82	83	-30	1.96E-5	5.43E-5	> 1.00E-4
ACHN	0.530	2.121	2.133	2.128	2.063	1.092	0.067	101	100	96	35	-87	5.74E-6	1.94E-5	4.96E-5
CAKI-1	0.682	2.306	2.172	2.182	2.037	1.280	0.087	92	92	83	37	-87	5.21E-6	1.98E-5	5.01E-5
RXF 393	0.894	1.518	1.473	1.466	1.371	0.872	0.312	93	92	76	-2	-65	2.16E-6	9.31E-6	5.73E-5
SN12C	0.748	2.557	2.482	2.494	2.391	1.184	0.233	96	97	91	24	-69	4.09E-6	1.82E-5	6.26E-5
TK-10	0.927	2.090	1.974	1.999	2.071	1.758	0.767	90	92	98	71	-17	1.75E-5	6.38E-5	> 1.00E-4
UO-31	0.877	2.600	2.422	2.380	2.284	1.390	0.396	90	87	82	30	-55	4.07E-6	2.25E-5	8.76E-5
Prostate Cancer															
PC-3	0.498	1.883	1.846	1.794	1.713	1.053	0.693	97	94	88	40	14	6.19E-6	> 1.00E-4	> 1.00E-4
DU-145	0.459	1.908	2.024	1.911	1.960	0.927	0.426	108	100	104	32	-7	5.64E-6	6.57E-5	> 1.00E-4
Breast Cancer															
MCF7	0.433	2.257	2.141	2.152	1.297	0.732	0.110	94	94	47	16	-75	8.78E-7	1.51E-5	5.36E-5
MDA-MB-231/ATCC	0.524	1.462	1.413	1.411	1.373	0.703	0.114	95	95	91	19	-78	3.69E-6	1.57E-5	5.12E-5
HS 578T	1.216	2.257	2.220	2.169	2.122	1.391	1.005	96	92	87	17	-17	3.37E-6	3.10E-5	> 1.00E-4
BT-549	1.308	2.298	2.328	2.264	2.445	2.478	1.246	103	97	115	118	-5	3.58E-5	9.14E-5	> 1.00E-4
T-47D	1.636	3.281	3.230	3.181	3.130	2.683	1.963	97	94	91	64	20	2.05E-5	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.701	1.442	1.387	1.425	0.823	0.596	0.214	93	98	16	-15	-69	3.86E-7	3.33E-6	4.39E-5

Leukemia



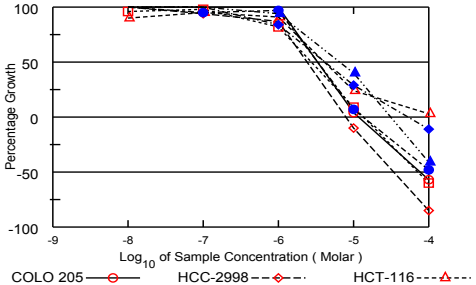
CCRF-CEM, HL-60(TB), K-562, MOLT-4, RPMI-8226, SR

Non-Small Cell Lung Cancer



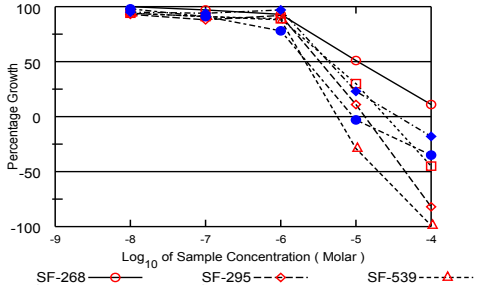
A549/ATCC, EKVX, HOP-62, HOP-92, NCI-H226, NCI-H23, NCI-H322M, NCI-H460, NCI-H522

Colon Cancer



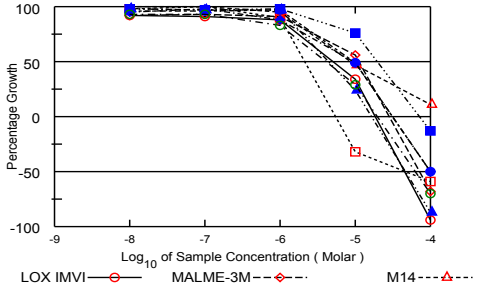
COLO 205, HCC-2998, HCT-116, HCT-15, HT29, KM12, SW-620

CNS Cancer



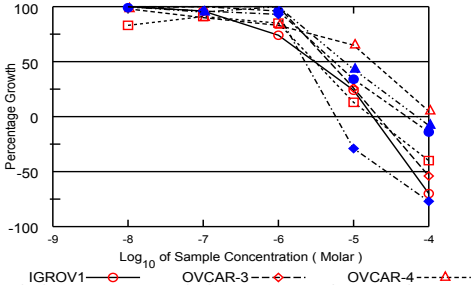
SF-268, SF-295, SF-539, SNB-19, SNB-75, U251

Melanoma



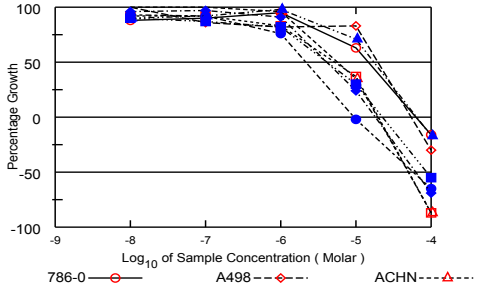
LOX IMVI, MALME-3M, M14, MDA-MB-435, SK-MEL-2, SK-MEL-28, SK-MEL-5, UACC-257, UACC-62

Ovarian Cancer



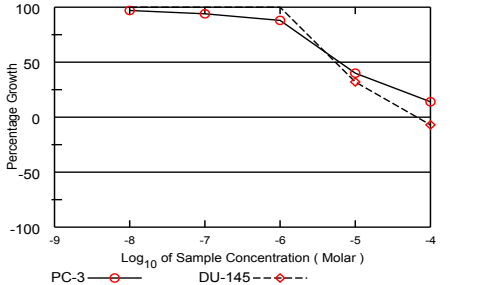
IGROV1, OVCAR-3, OVCAR-4, OVCAR-5, OVCAR-8, NCI/ADR-RES, SK-OV-3

Renal Cancer



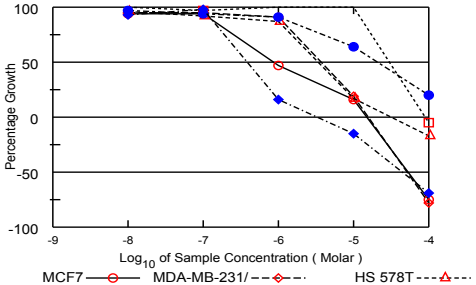
786-0, A498, ACHN, CAKI-1, RXF 393, SN12C, TK-10, UO-31

Prostate Cancer



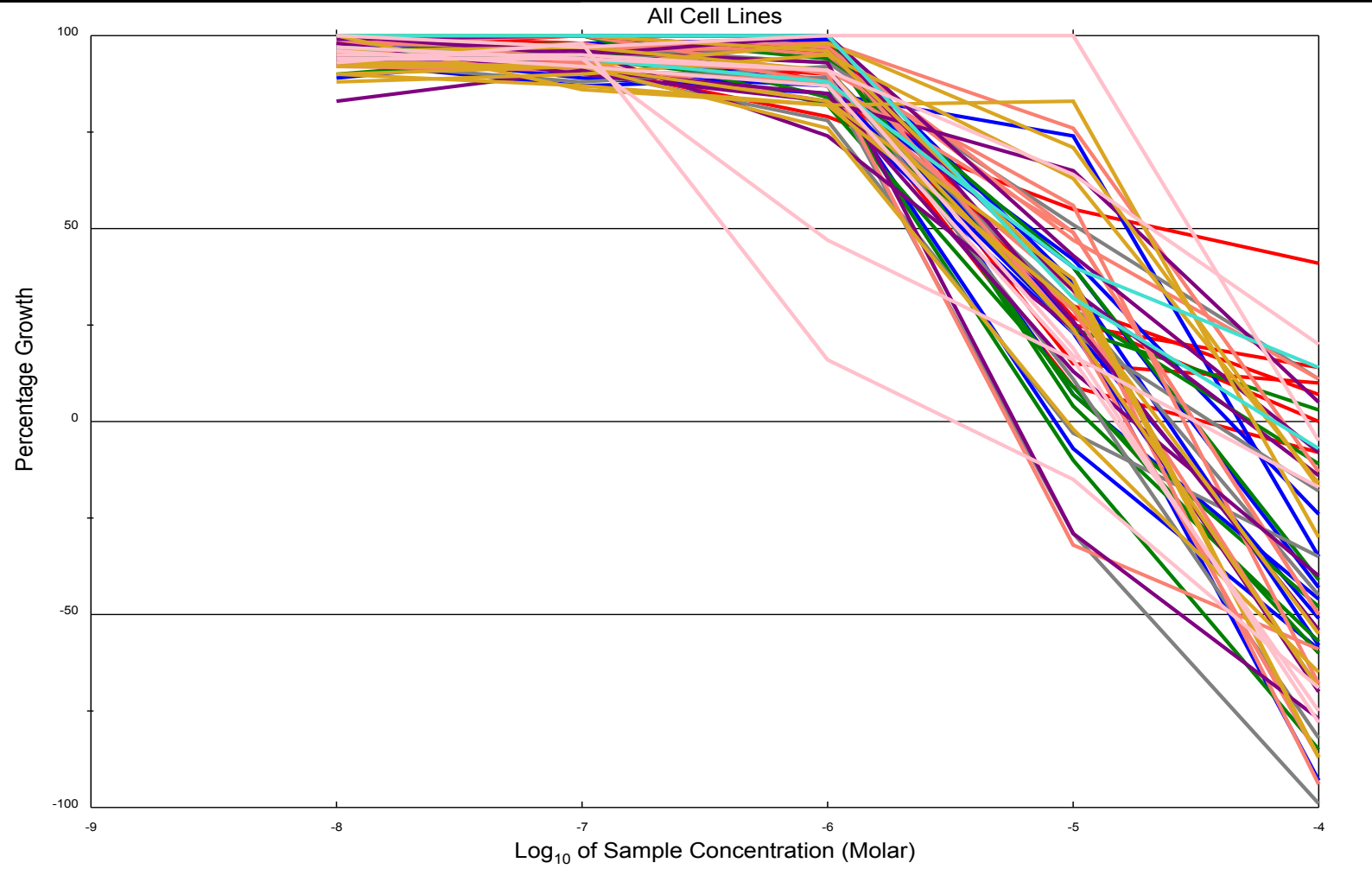
PC-3, DU-145

Breast Cancer



MCF7, MDA-MB-231/, HS 578T, BT-549, T-47D, MDA-MB-468

National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 834436/1	SSPL:1AMN	EXP. ID:2204NS06
	Report Date:May 26, 2022	Test Date:April 25, 2022	

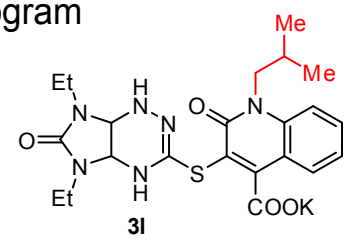


National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 834437 / 1 | Experiment ID : 2204NS06 | Test Type : 08

Report Date : May 26, 2022 | Test Date : April 25, 2022 | QNS :

COMI : IA1354 | Stain Reagent : SRB Dual-Pass Related | SSPL : 1AMN



3l

Log10 Concentration

Panel/Cell Line	Time Zero	Mean Optical Densities Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	Percent Growth -8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.438	1.871	1.854	1.733	1.761	0.657	0.490	99	90	92	15	4	3.54E-6	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.630	2.794	2.547	2.470	2.328	0.687	0.495	89	85	78	3	-22	2.37E-6	1.29E-5	> 1.00E-4
K-562	0.212	2.304	2.330	2.321	1.801	0.573	0.356	101	101	76	17	7	2.77E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.668	2.827	2.949	2.877	2.585	1.099	0.695	106	102	89	20	1	3.66E-6	> 1.00E-4	> 1.00E-4
RPMI-8226	0.619	2.660	2.599	2.477	2.180	0.950	0.720	97	91	76	16	5	2.75E-6	> 1.00E-4	> 1.00E-4
SR	0.173	0.748	0.819	0.779	0.567	0.483	0.301	112	105	68	54	22	1.32E-5	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.404	2.340	2.188	2.237	2.241	0.930	0.487	92	95	95	27	4	4.60E-6	> 1.00E-4	> 1.00E-4
EKVX	0.576	1.959	1.870	1.931	1.649	0.875	0.669	94	98	78	22	7	3.11E-6	> 1.00E-4	> 1.00E-4
HOP-62	0.821	2.624	2.441	2.628	2.412	1.472	1.083	90	100	88	36	15	5.42E-6	> 1.00E-4	> 1.00E-4
HOP-92	1.108	1.987	1.897	1.925	1.805	1.655	0.943	90	93	79	62	-15	1.44E-5	6.41E-5	> 1.00E-4
NCI-H226	0.719	1.535	1.431	1.525	1.488	0.880	0.425	87	99	94	20	-41	3.92E-6	2.11E-5	> 1.00E-4
NCI-H23	0.409	1.375	1.353	1.369	1.253	0.613	0.235	98	99	87	21	-43	3.66E-6	2.14E-5	> 1.00E-4
NCI-H322M	0.761	1.922	1.834	1.911	1.787	1.225	0.977	92	99	88	40	19	6.19E-6	> 1.00E-4	> 1.00E-4
NCI-H460	0.290	2.683	2.649	2.668	2.549	0.375	0.180	99	99	94	4	-38	3.08E-6	1.22E-5	> 1.00E-4
NCI-H522	1.172	2.844	2.699	2.724	2.463	0.911	0.591	91	93	77	-22	-50	1.88E-6	5.97E-6	> 1.00E-4
Colon Cancer															
COLO 205	0.551	2.217	2.277	2.304	2.147	0.452	0.350	104	105	96	-18	-36	2.53E-6	6.95E-6	> 1.00E-4
HCC-2998	0.488	1.924	1.882	1.834	1.793	0.655	0.295	97	94	91	12	-40	3.28E-6	1.69E-5	> 1.00E-4
HCT-116	0.239	2.846	2.735	2.665	2.359	0.734	0.297	96	93	81	19	2	3.18E-6	> 1.00E-4	> 1.00E-4
HCT-15	0.337	2.305	2.253	2.383	1.643	0.483	0.271	97	104	66	7	-20	1.89E-6	1.88E-5	> 1.00E-4
HT29	0.293	1.990	1.863	1.811	1.772	0.379	0.156	92	89	87	5	-47	2.83E-6	1.25E-5	> 1.00E-4
KM12	0.788	3.252	3.310	3.260	2.698	1.248	0.995	102	100	77	19	8	2.93E-6	> 1.00E-4	> 1.00E-4
SW-620	0.285	1.883	1.838	1.843	1.635	0.728	0.450	97	97	84	28	10	4.05E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	1.015	2.721	2.553	2.611	2.501	1.720	1.235	90	94	87	41	13	6.46E-6	> 1.00E-4	> 1.00E-4
SF-295	0.571	2.168	2.011	2.101	1.967	0.718	0.375	90	96	87	9	-34	3.01E-6	1.63E-5	> 1.00E-4
SF-539	0.761	2.187	2.158	2.177	2.014	0.524	0.173	98	99	88	-31	-77	2.08E-6	5.47E-6	2.56E-5
SNB-19	0.644	2.057	1.993	2.029	1.900	0.950	0.612	95	98	89	22	-5	3.78E-6	6.50E-5	> 1.00E-4
SNB-75	1.353	2.307	2.062	2.080	2.003	1.322	0.926	74	76	68	-2	-32	1.81E-6	9.27E-6	> 1.00E-4
U251	0.368	1.962	1.772	1.835	1.834	0.705	0.519	88	92	92	21	9	3.91E-6	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.264	1.989	1.892	1.891	1.752	0.736	0.107	94	94	86	27	-60	4.13E-6	2.06E-5	7.74E-5
MALME-3M	0.737	1.444	1.380	1.459	1.339	0.993	0.611	91	102	85	36	-17	5.23E-6	4.77E-5	> 1.00E-4
M14	0.430	2.129	2.106	2.151	1.832	0.914	0.532	99	101	83	28	6	4.00E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.533	2.400	2.421	2.377	1.457	0.373	0.203	101	99	49	-30	-62	9.76E-7	4.18E-6	4.22E-5
SK-MEL-2	1.302	3.047	2.946	3.000	2.929	1.721	1.356	94	97	93	24	3	4.21E-6	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.782	2.006	1.973	2.069	1.731	1.317	0.783	97	105	77	44	0	6.50E-6	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.718	3.207	3.126	3.188	3.104	1.146	0.266	97	99	96	17	-63	3.83E-6	1.64E-5	6.88E-5
UACC-257	0.933	2.249	2.121	2.178	2.000	1.709	0.998	90	95	81	59	5	1.47E-5	> 1.00E-4	> 1.00E-4
UACC-62	0.894	2.460	2.388	2.328	1.973	1.283	0.693	95	92	69	25	-22	2.68E-6	3.35E-5	> 1.00E-4
Ovarian Cancer															
IGROV1	0.588	2.090	2.095	2.117	1.692	0.822	0.359	100	102	73	16	-39	2.54E-6	1.93E-5	> 1.00E-4
OVCAR-3	0.576	1.798	1.858	1.846	1.591	0.790	0.387	105	104	83	17	-33	3.19E-6	2.23E-5	> 1.00E-4
OVCAR-4	0.876	2.182	2.105	2.143	1.852	1.616	1.119	94	97	75	57	19	1.50E-5	> 1.00E-4	> 1.00E-4
OVCAR-5	0.942	1.710	1.637	1.653	1.622	1.147	0.890	91	93	89	27	-6	4.19E-6	6.71E-5	> 1.00E-4
OVCAR-8	0.550	2.610	2.489	2.637	2.480	0.845	0.464	94	101	94	14	-16	3.55E-6	3.01E-5	> 1.00E-4
NCI/ADR-RES	0.388	1.403	1.383	1.415	1.282	0.234	0.081	98	101	88	-40	-79	1.98E-6	4.89E-6	1.82E-5
SK-OV-3	0.808	2.037	2.077	1.985	1.957	1.273	1.074	103	96	93	38	22	6.05E-6	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.541	2.714	2.411	2.494	2.497	1.500	0.959	86	90	90	44	19	7.45E-6	> 1.00E-4	> 1.00E-4
A498	1.641	2.219	2.174	2.218	2.105	2.174	1.936	92	100	80	92	51	> 1.00E-4	> 1.00E-4	> 1.00E-4
ACHN	0.530	2.121	2.101	2.204	2.020	0.991	0.453	99	105	94	29	-15	4.73E-6	4.62E-5	> 1.00E-4
CAKI-1	0.682	2.306	2.212	2.219	1.709	1.272	0.252	94	95	63	36	-63	3.10E-6	2.32E-5	7.38E-5
RXF 393	0.894	1.518	1.469	1.528	1.403	1.010	0.350	92	102	82	19	-61	3.17E-6	1.71E-5	7.29E-5
SN12C	0.748	2.557	2.448	2.519	2.420	1.045	0.642	94	98	92	16	-14	3.62E-6	3.44E-5	> 1.00E-4
TK-10	0.927	2.090	1.871	1.920	2.286	1.703	0.969	81	85	117	67	4	1.84E-5	> 1.00E-4	> 1.00E-4
UO-31	0.877	2.600	2.400	2.451	2.248	1.418	1.026	88	91	80	31	9	4.11E-6	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.498	1.883	1.829	1.864	1.661	0.898	0.660	96	99	84	29	12	4.14E-6	> 1.00E-4	> 1.00E-4
DU-145	0.459	1.908	1.922	1.990	1.902	0.801	0.591	101	106	100	24	9	4.49E-6	> 1.00E-4	> 1.00E-4
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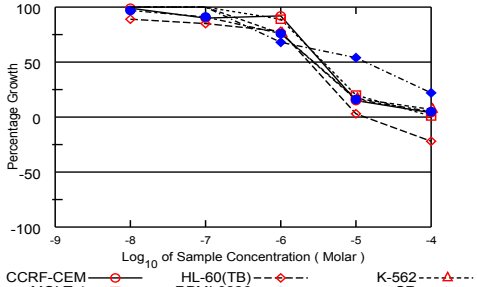
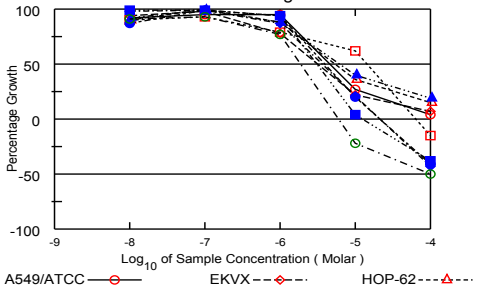
MDA-MB-231/ATCC	0.524	1.462	1.421	1.476	1.213	0.662	0.375	96	102	73	15	-28	2.51E-6	2.19E-5	> 1.00E-4
HS 578T	1.216	2.257	2.178	2.185	2.067	1.360	1.166	92	93	82	14	-4	2.94E-6	5.88E-5	> 1.00E-4
BT-549	1.308	2.298	2.218	2.401	2.239	2.212	1.473	92	110	94	91	17	3.57E-5	> 1.00E-4	> 1.00E-4
T-47D	1.636	3.281	3.161	3.194	3.103	2.604	2.505	93	95	89	59	53	> 1.00E-4	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.701	1.442	1.396	1.456	0.860	0.598	0.351	94	102	21	-15	-50	4.42E-7	3.91E-6	> 1.00E-4

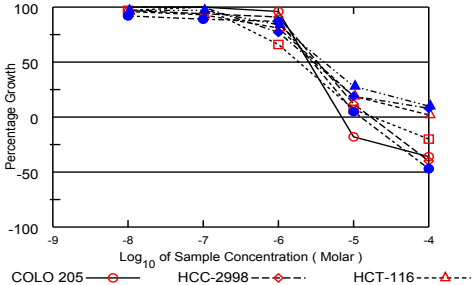
Leukemia



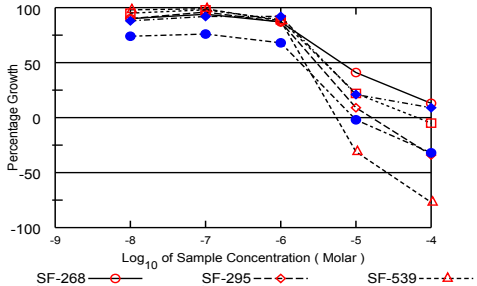
Non-Small Cell Lung Cancer



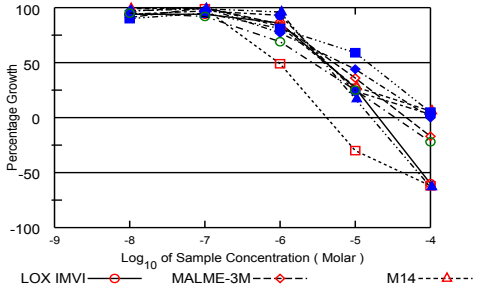
Colon Cancer



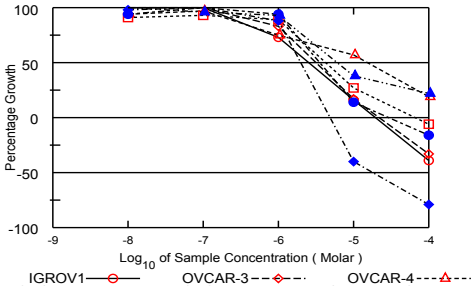
CNS Cancer



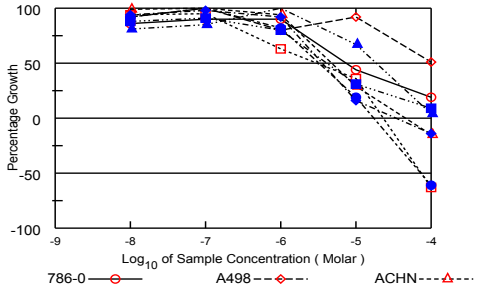
Melanoma



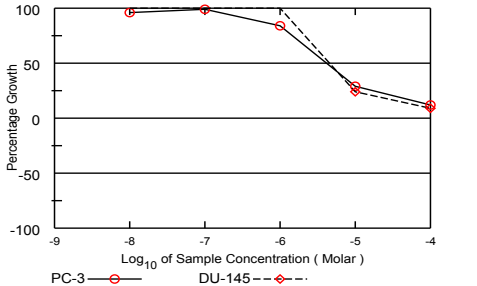
Ovarian Cancer



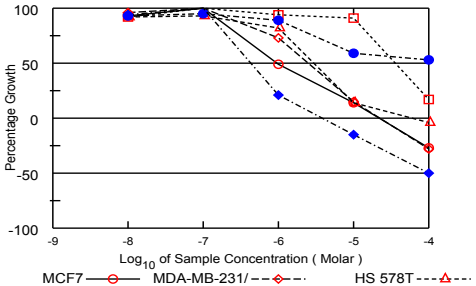
Renal Cancer



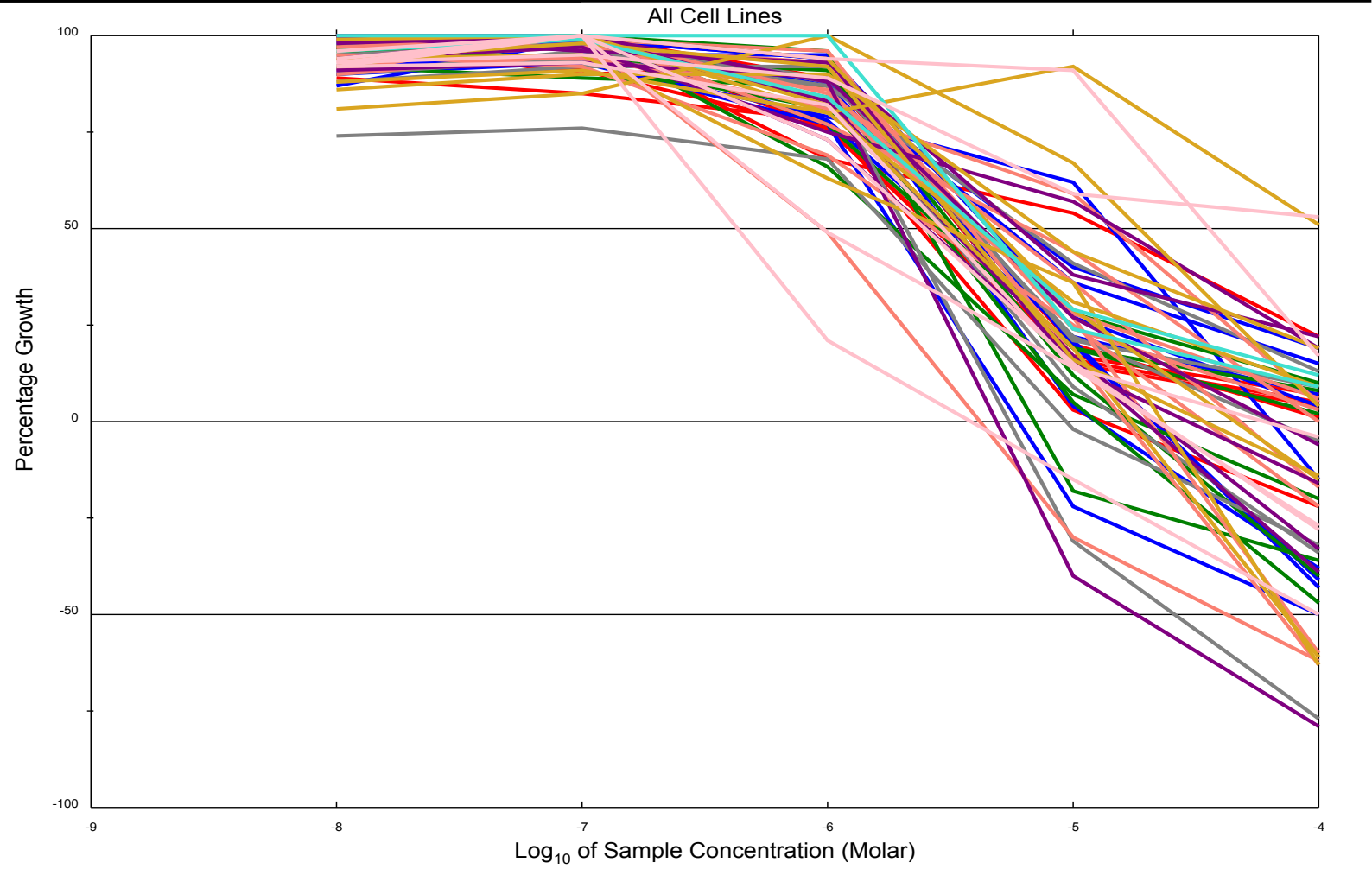
Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 834437/1	SSPL:1AMN	EXP. ID:2204NS06
	Report Date:May 26, 2022	Test Date:April 25, 2022	



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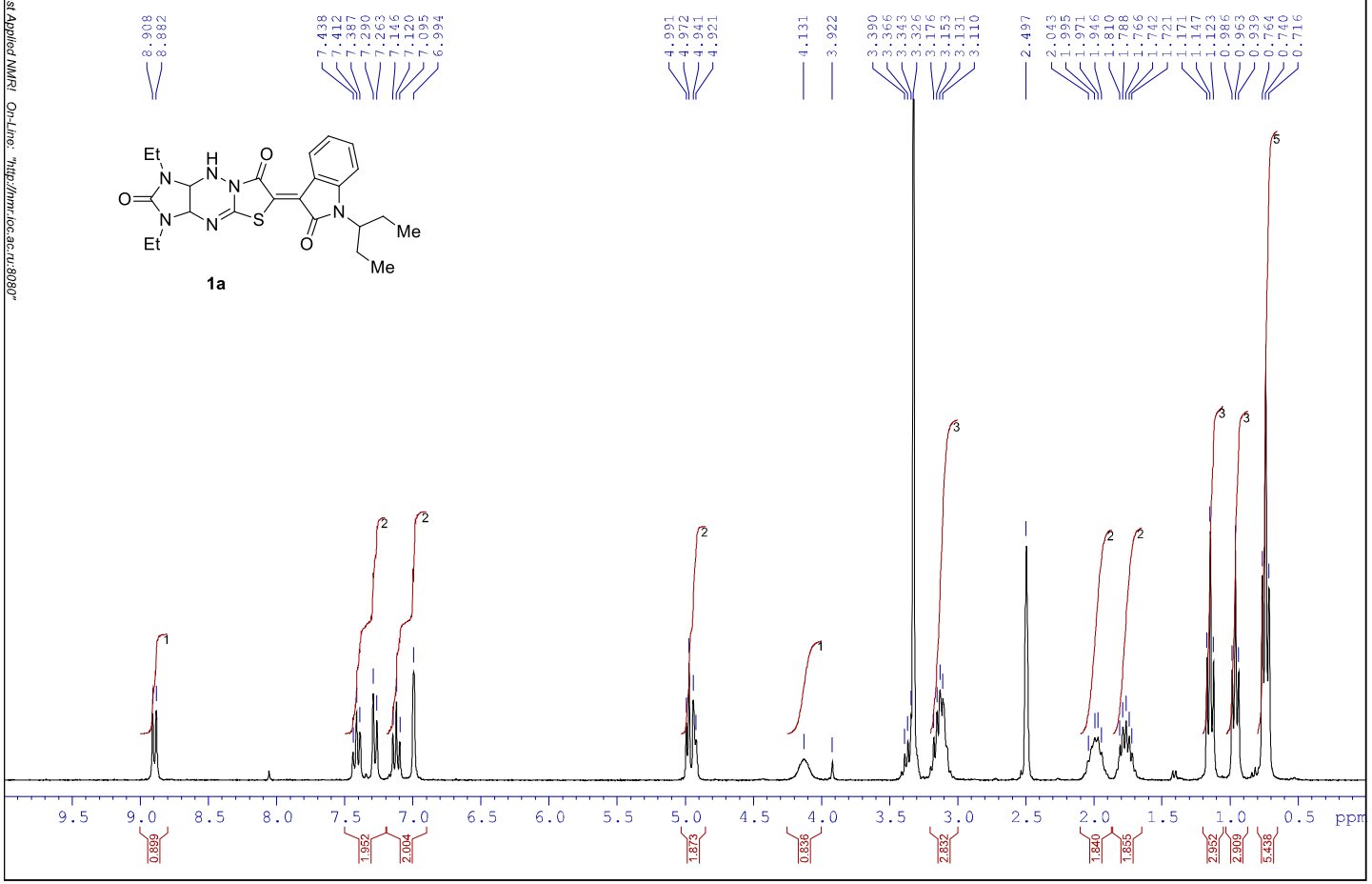

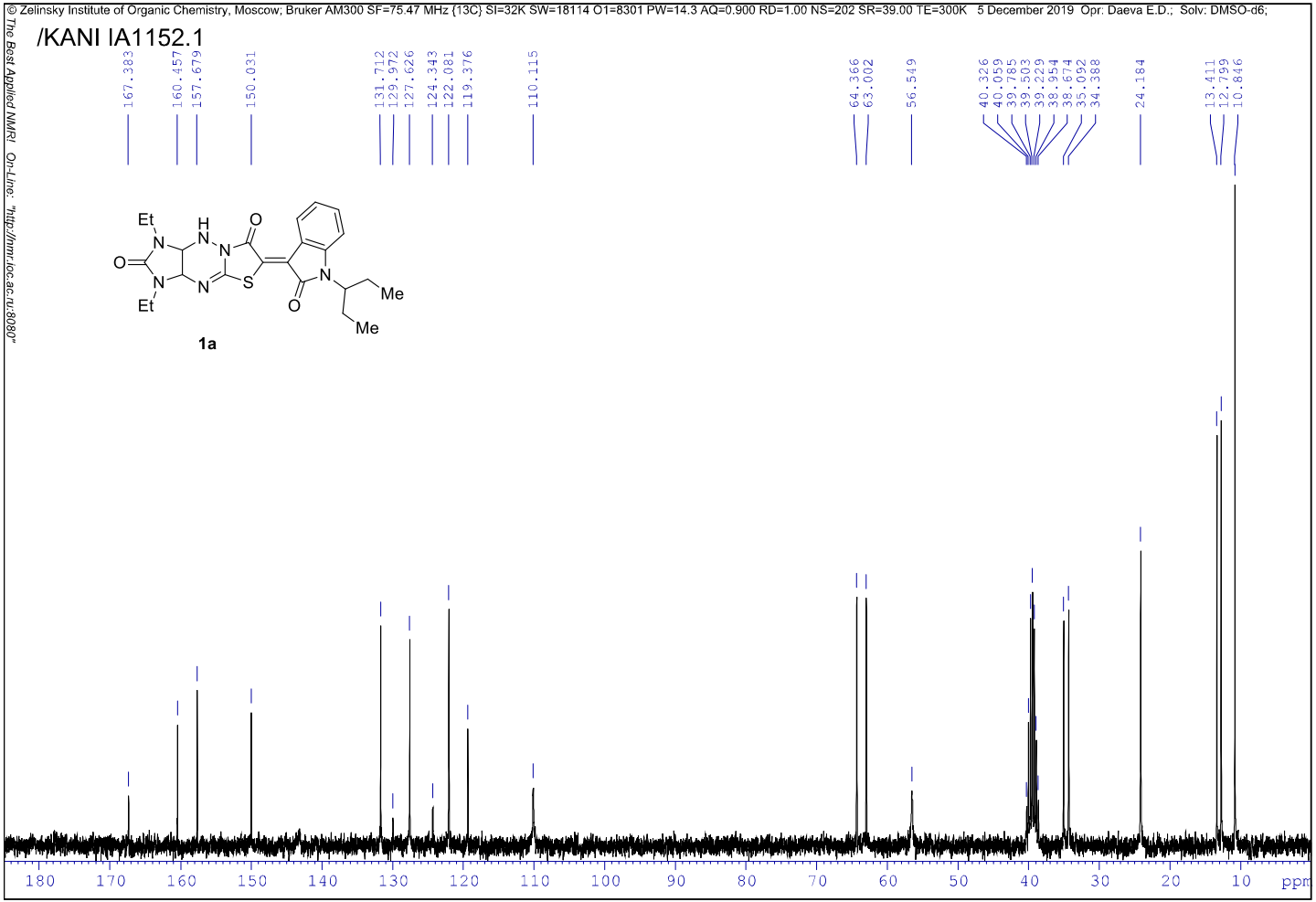
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=202 SR=39.00 TE=300K 5 December 2019 Opr: Daeva E.D.; Solv: DMSO-d6;
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122.081
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63.002
56.549
40.326
40.059
39.785
39.503
39.229
38.954
38.674
35.092
34.388
24.184
13.411
12.799
10.846
Et
N
H
N
O
O
N
N
N
S
N
Et
O
N
Me
Me
1a
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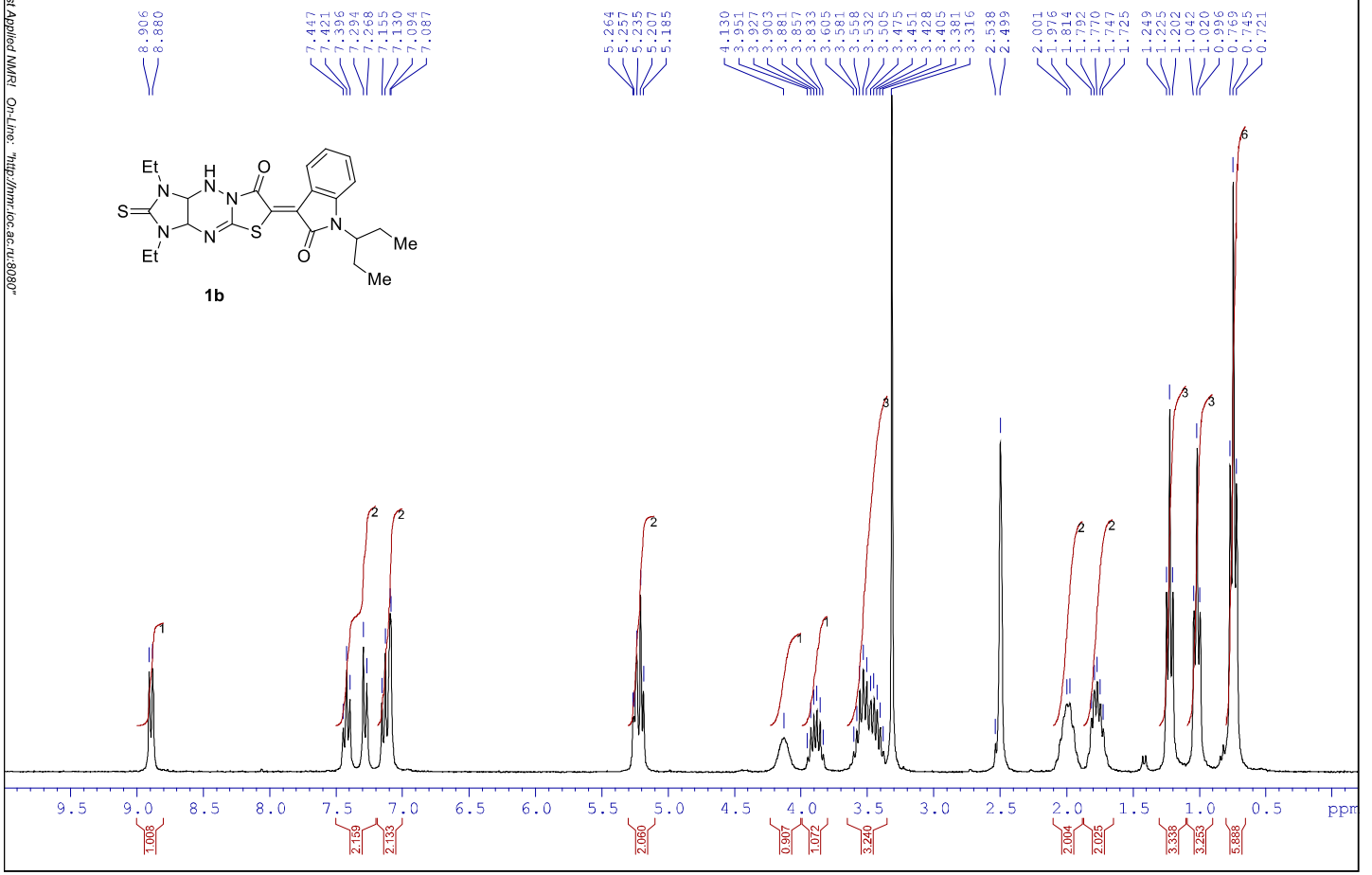
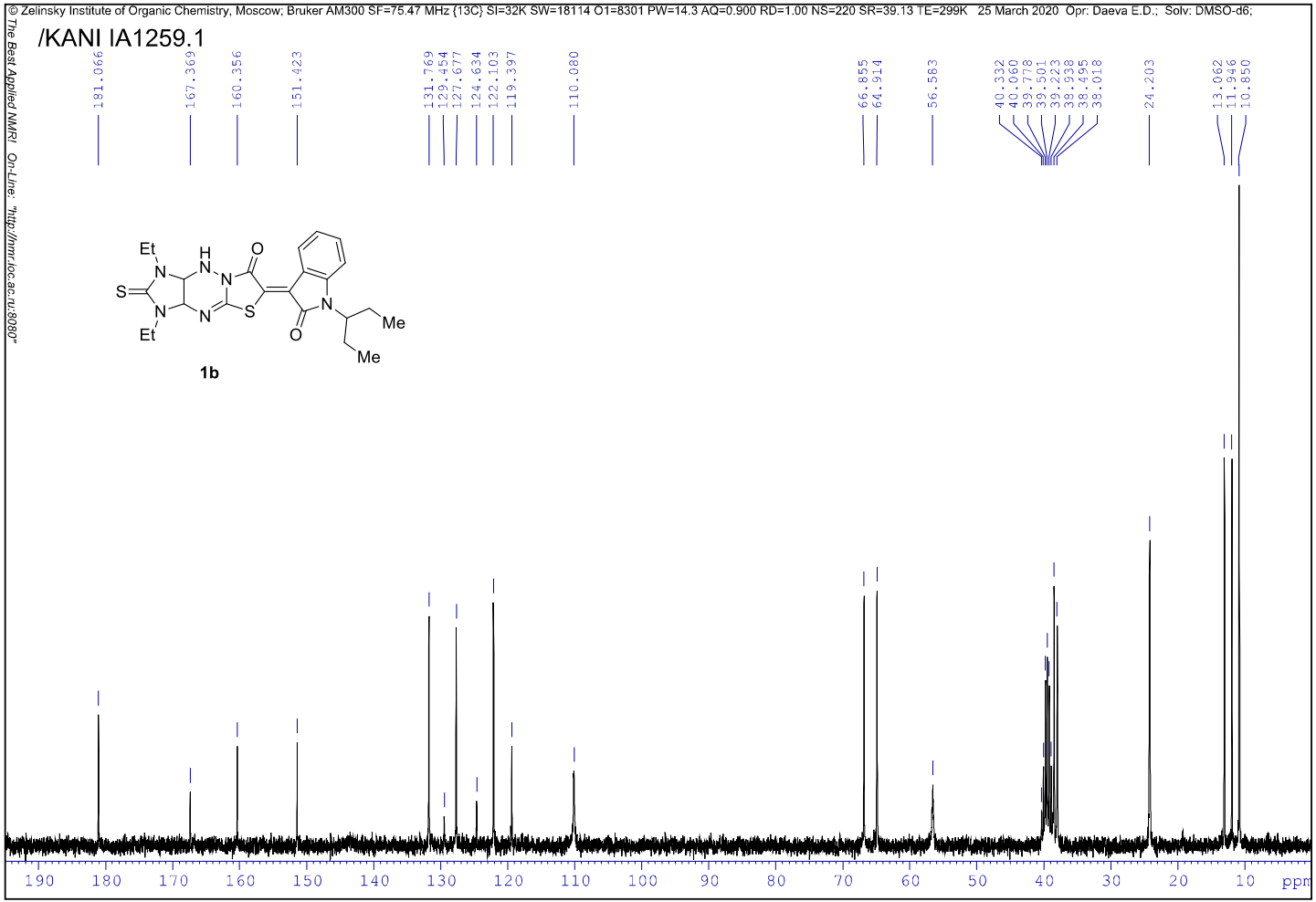
10
ppm

/KANI IA1259.1




© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=220 SR=39.13 TE=299K 25 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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66.855
64.914
56.583
40.332
40.060
39.778
39.501
39.223
38.938
38.495
38.018
24.203
13.062
11.946
10.850
Et
N
H
N
O
S
N
N
N
S
N
Et
O
Me
Me
1b
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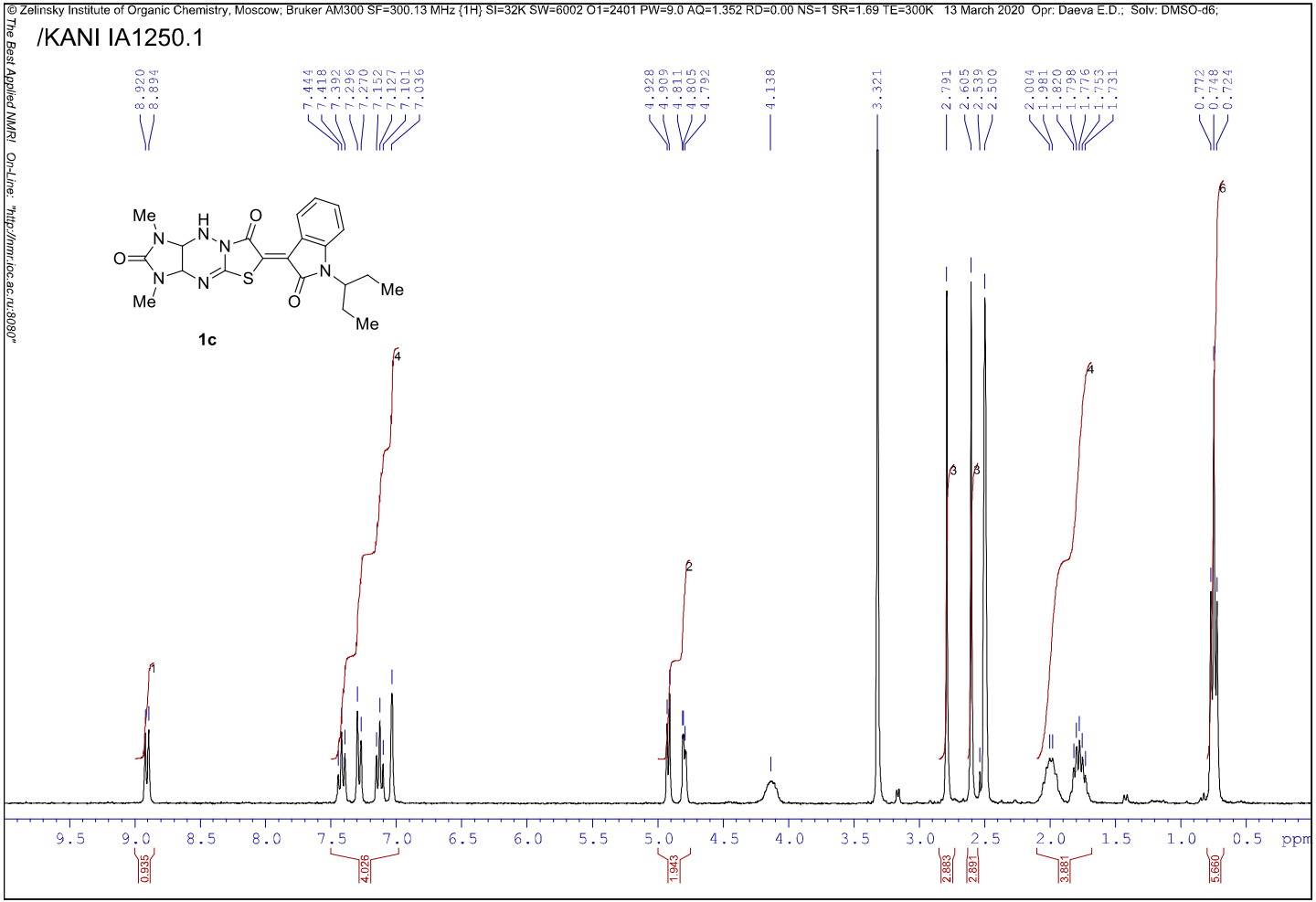
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=300K 13 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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7.296
7.270
7.152
7.127
7.101
7.036
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4.909
4.811
4.805
4.792
4.138
3.321
2.791
2.605
2.539
2.500
2.004
1.981
1.820
1.798
1.776
1.753
1.731
0.772
0.748
0.724
Me
H
N
O
S
1c
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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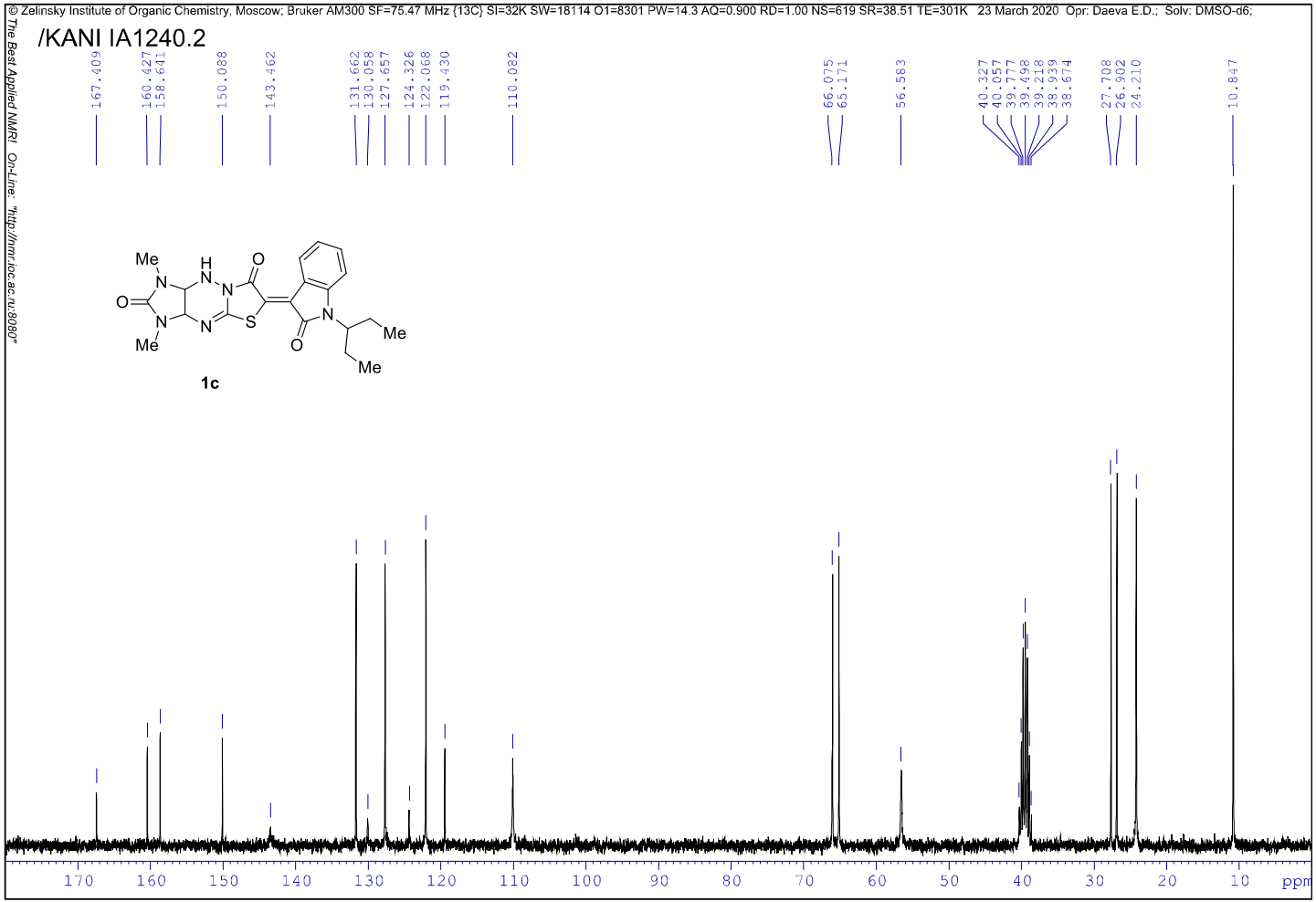
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=619 SR=38.51 TE=301K 23 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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130.058
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124.326
122.068
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110.082
66.075
65.171
56.583
40.327
40.057
39.787
39.498
39.218
38.939
38.674
27.708
26.902
24.210
10.847
Me
H
N
O
N
N
N
N
S
O
N
Me
Me
Me
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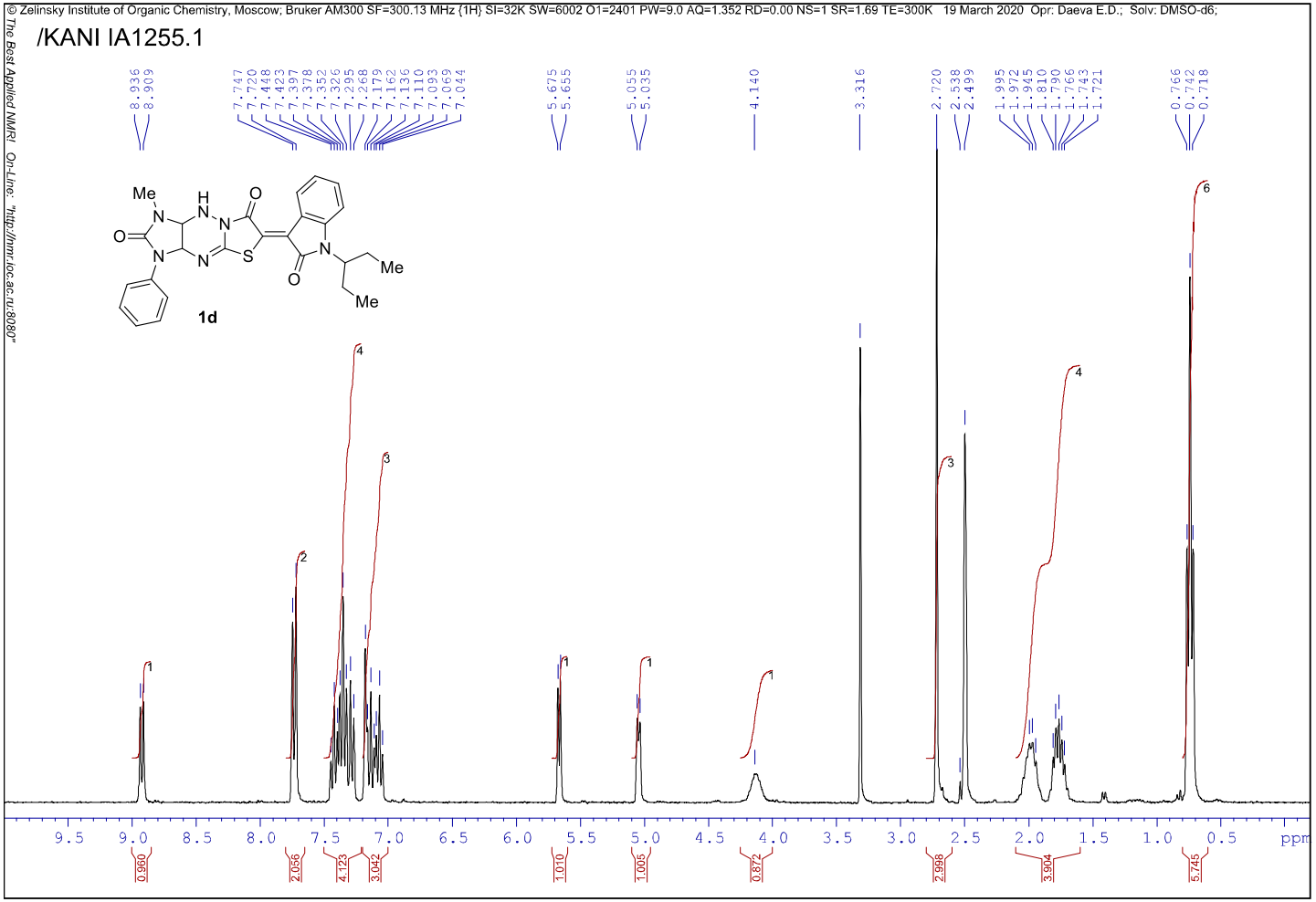
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=300K 19 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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7.378
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7.326
7.295
7.268
7.179
7.162
7.136
7.110
7.093
7.059
7.044
5.675
5.655
5.055
5.035
4.140
3.316
2.720
2.538
2.499
1.995
1.972
1.945
1.810
1.790
1.766
1.743
1.721
0.766
0.742
0.718
1d
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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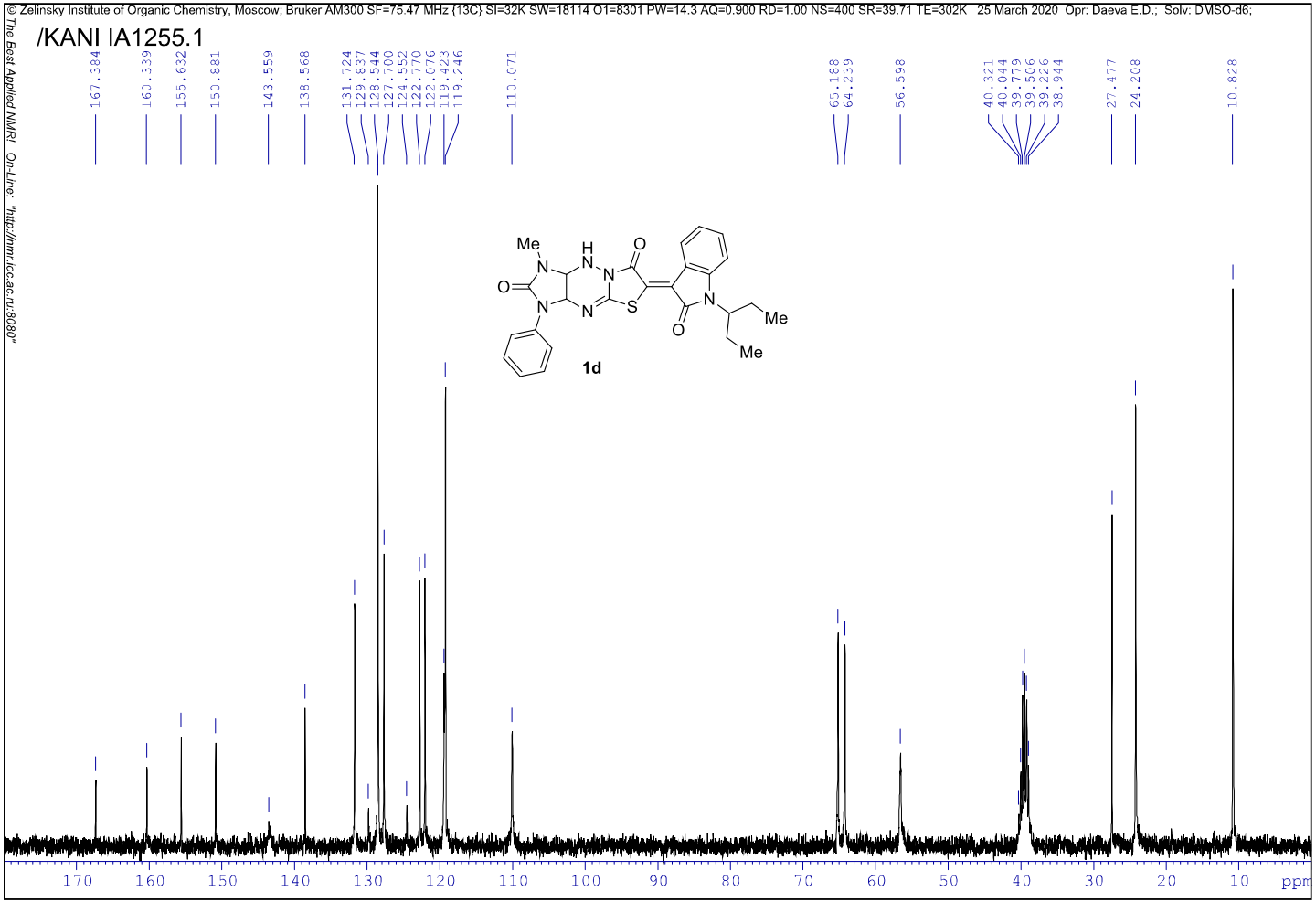
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=400 SR=39.71 TE=302K 25 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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127.700
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122.076
119.423
119.246
110.071
65.188
64.239
56.598
40.321
40.044
39.779
39.506
39.226
38.944
27.477
24.208
10.828
Me
H
O
N
O
N
N
N
S
N
O
Me
Me
1d
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70
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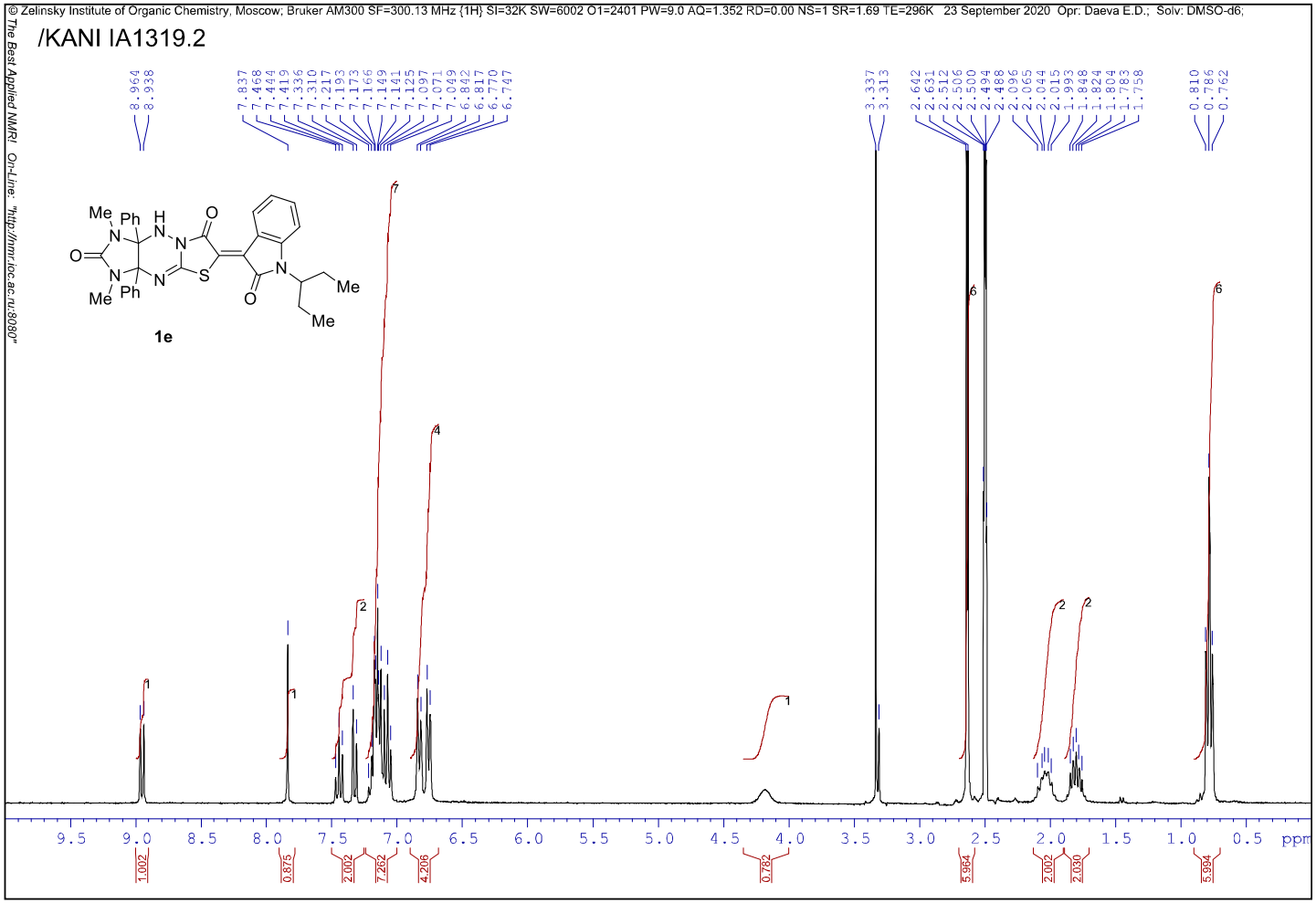
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=296K 23 September 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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7.336
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7.193
7.173
7.166
7.149
7.141
7.125
7.097
7.071
7.049
6.842
6.817
6.770
6.747
3.337
3.313
2.642
2.631
2.512
2.506
2.500
2.494
2.488
2.096
2.065
2.044
2.015
1.993
1.848
1.824
1.804
1.783
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0.786
0.762
Me
Ph
H
N
O
Me
Ph
1e
Me
Me
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8.5
8.0
7.5
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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1.0
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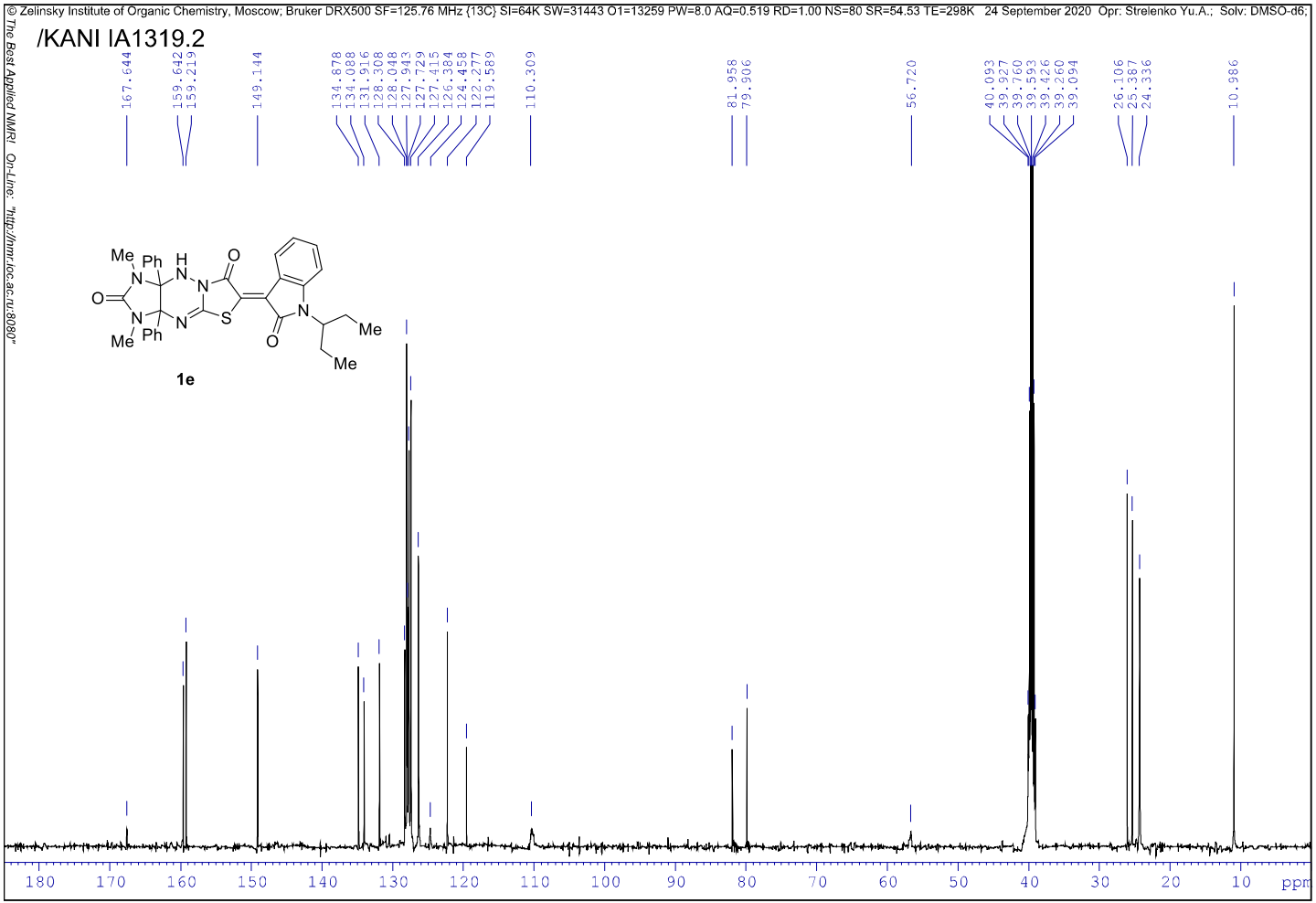
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz {13C} SI=64K SW=31443 O1=13259 PW=8.0 AQ=0.519 RD=1.00 NS=80 SR=54.53 TE=298K 24 September 2020 Opr: Strelenko Yu.A.; Solv: DMSO-d6;
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127.415
126.384
124.458
122.277
119.589
110.309
81.958
79.906
56.720
40.093
39.927
39.760
39.593
39.426
39.260
39.094
26.106
25.387
24.336
10.986
Me
Ph
H
N
O
N
N
S
N
O
N
Me
Ph
Me
Me
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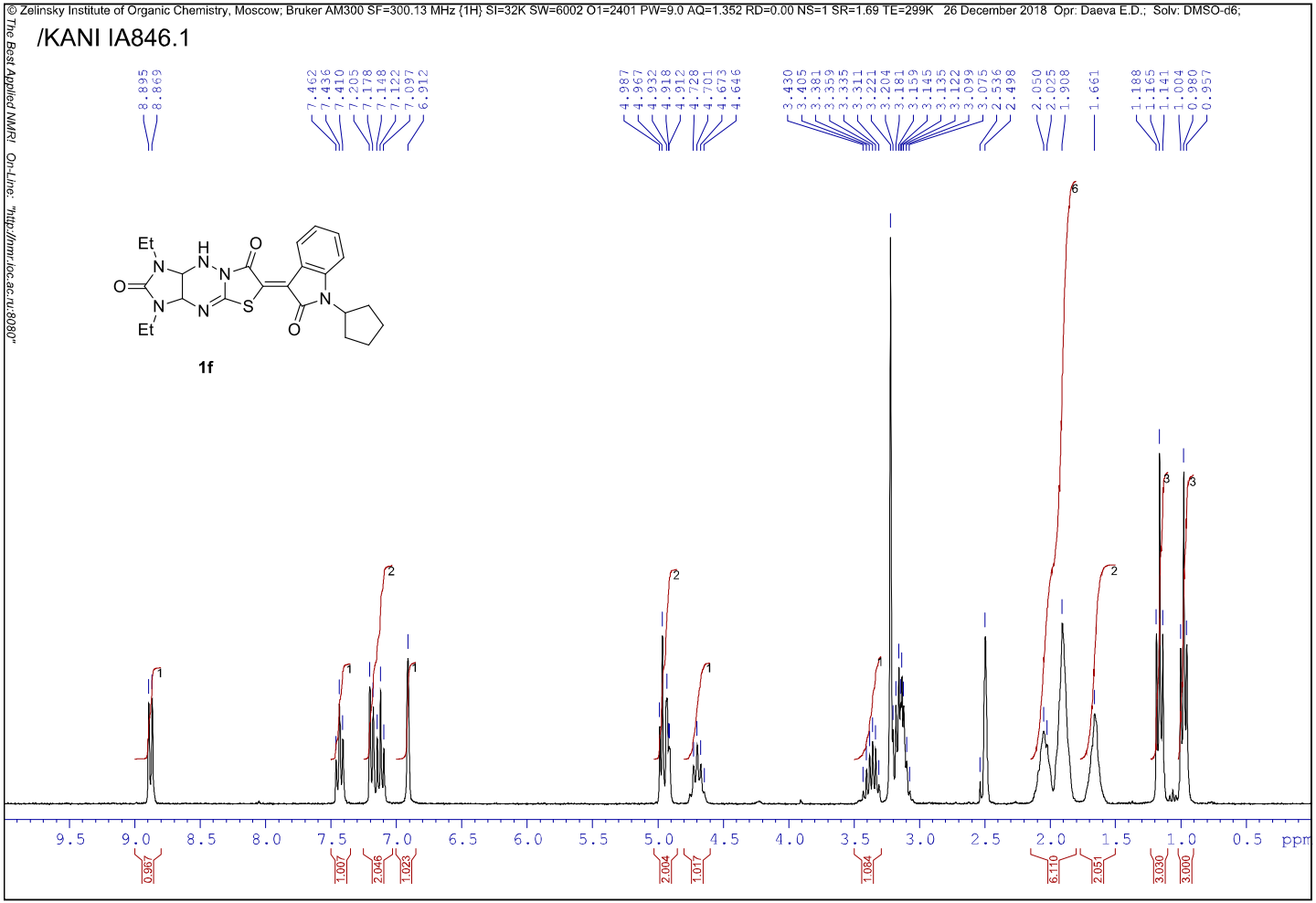
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=299K 26 December 2018 Opr: Daeva E.D.; Solv: DMSO-d6;
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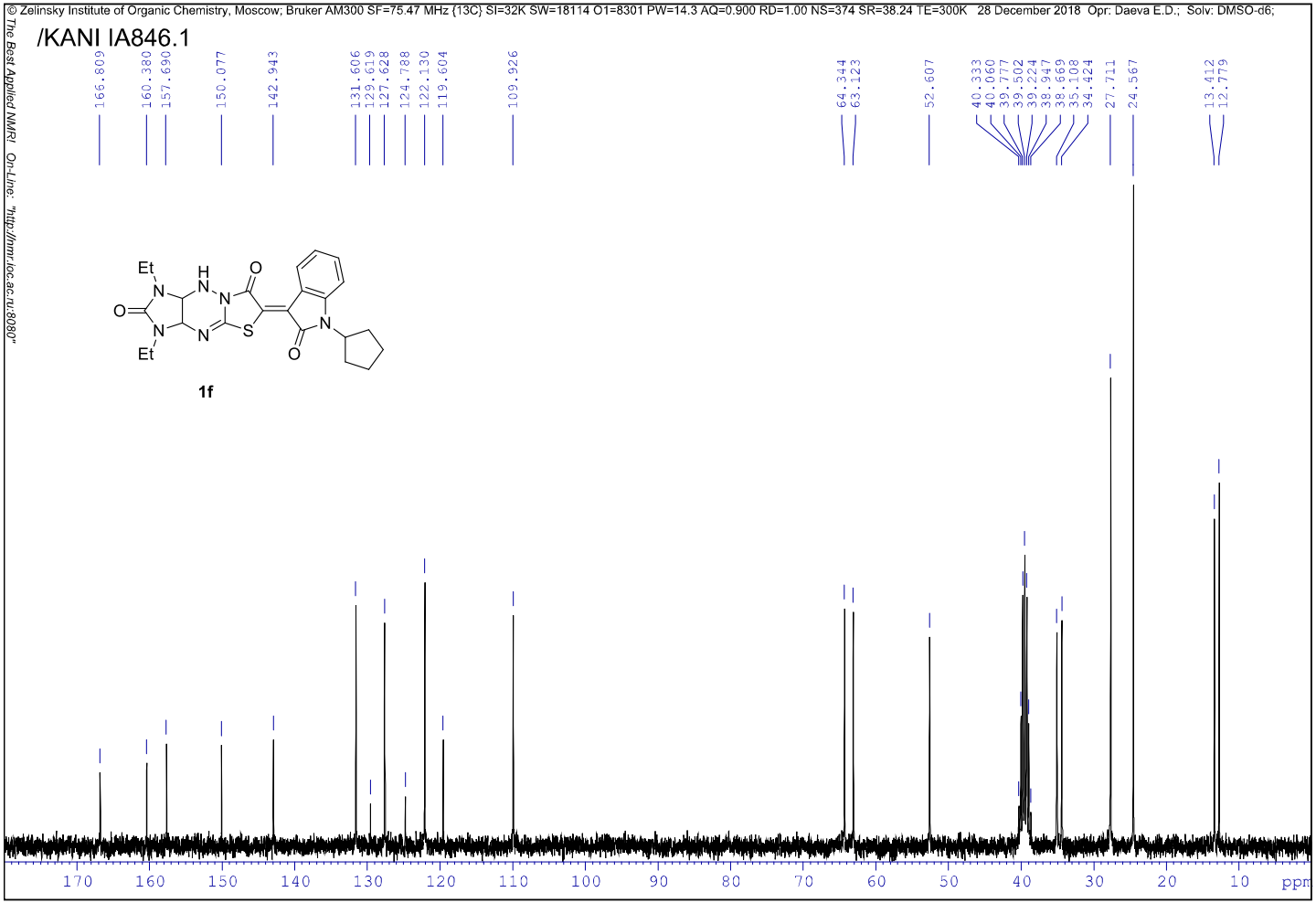
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=374 SR=38.24 TE=300K 28 December 2018 Opr: Daeva E.D.; Solv: DMSO-d6;
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109.926
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63.123
52.607
40.333
40.060
39.777
39.502
39.224
38.947
38.669
35.108
34.424
27.711
24.567
13.412
12.779
Et
H
O
N
O
N
N
N
S
N
O
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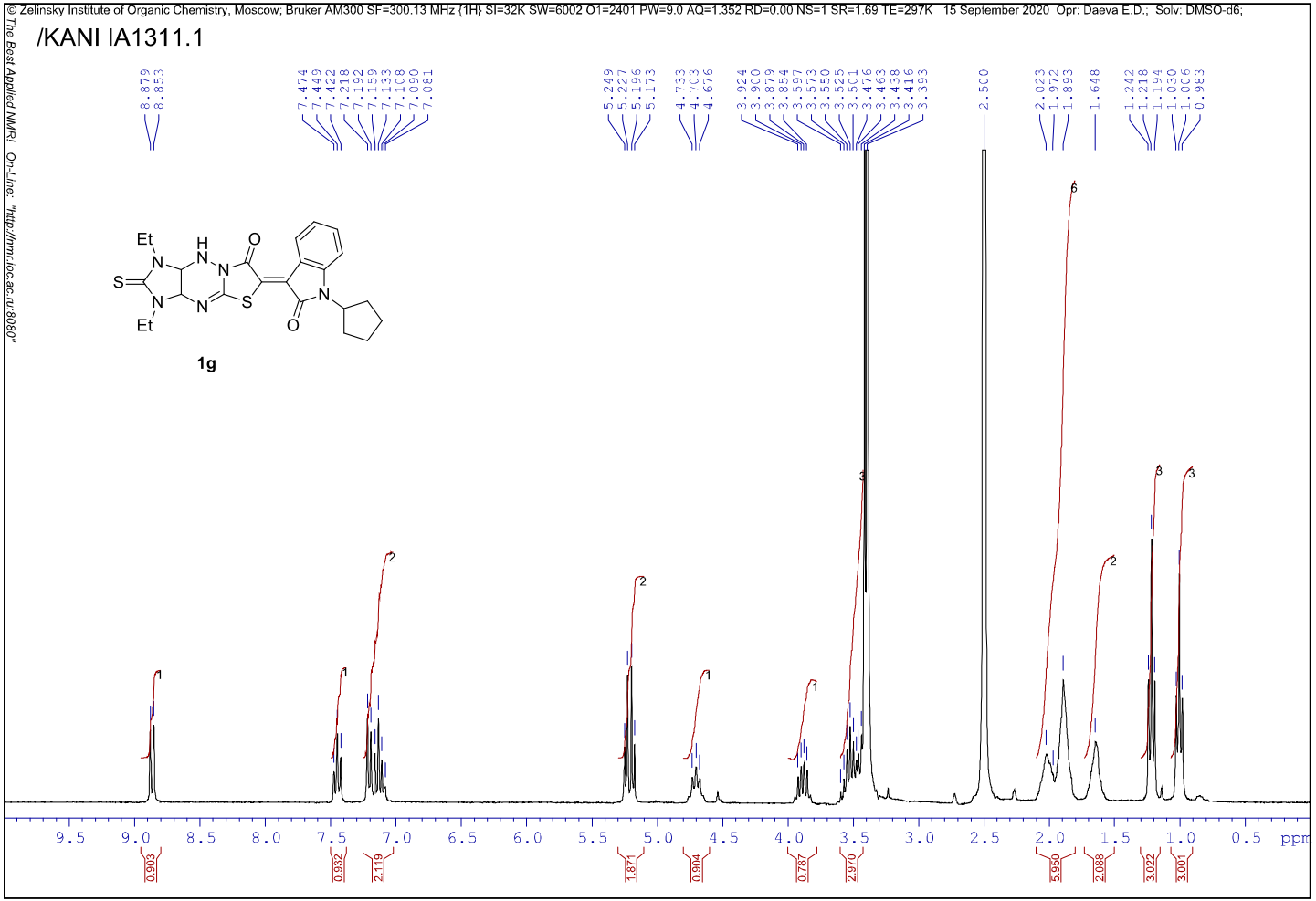
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=297K 15 September 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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5.227
5.196
5.173
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4.703
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3.854
3.597
3.573
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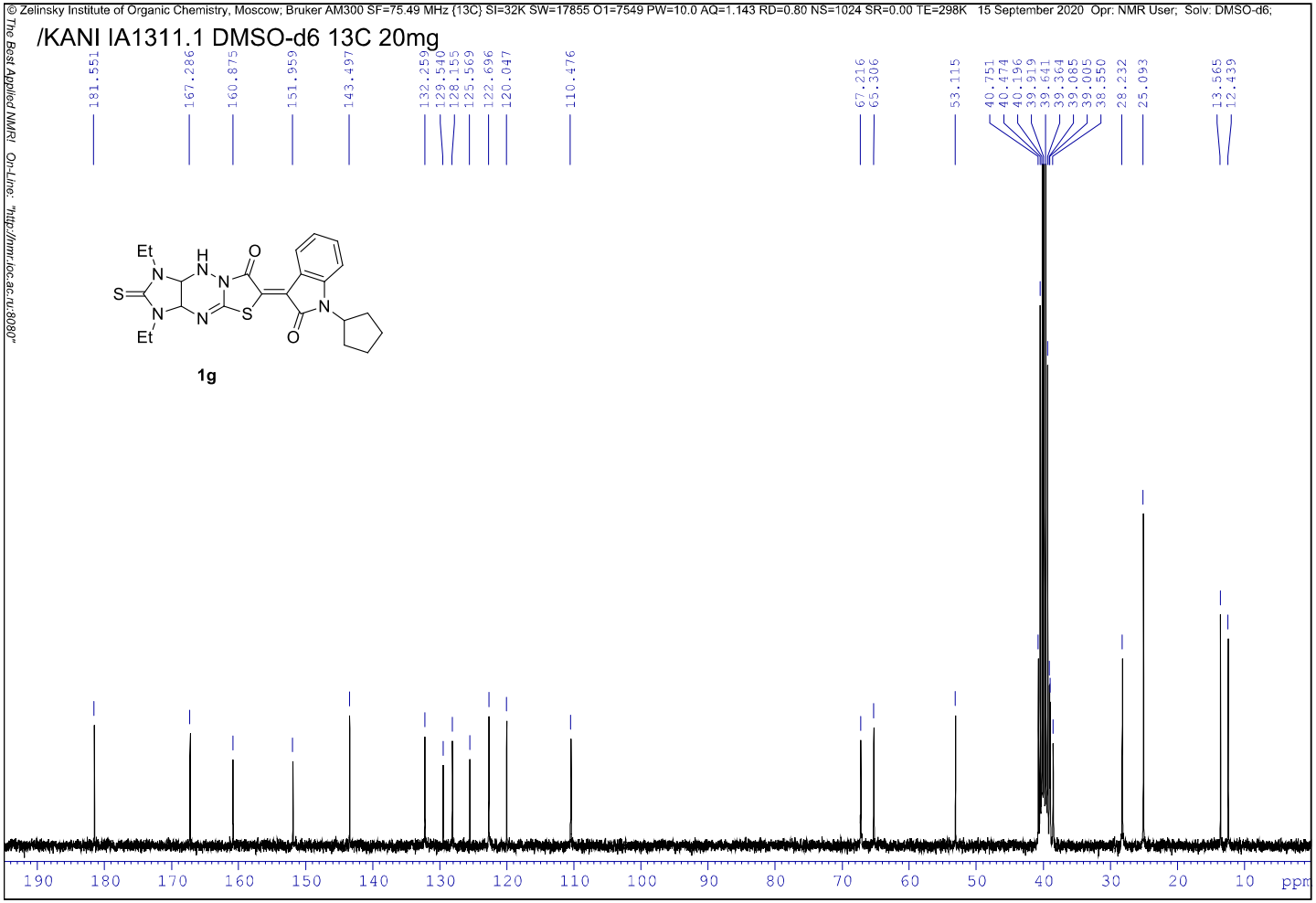
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=1024 SR=0.00 TE=298K 15 September 2020 Opr: NMR User; Solv: DMSO-d6;
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65.306
53.115
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40.196
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25.093
13.565
12.439
1g
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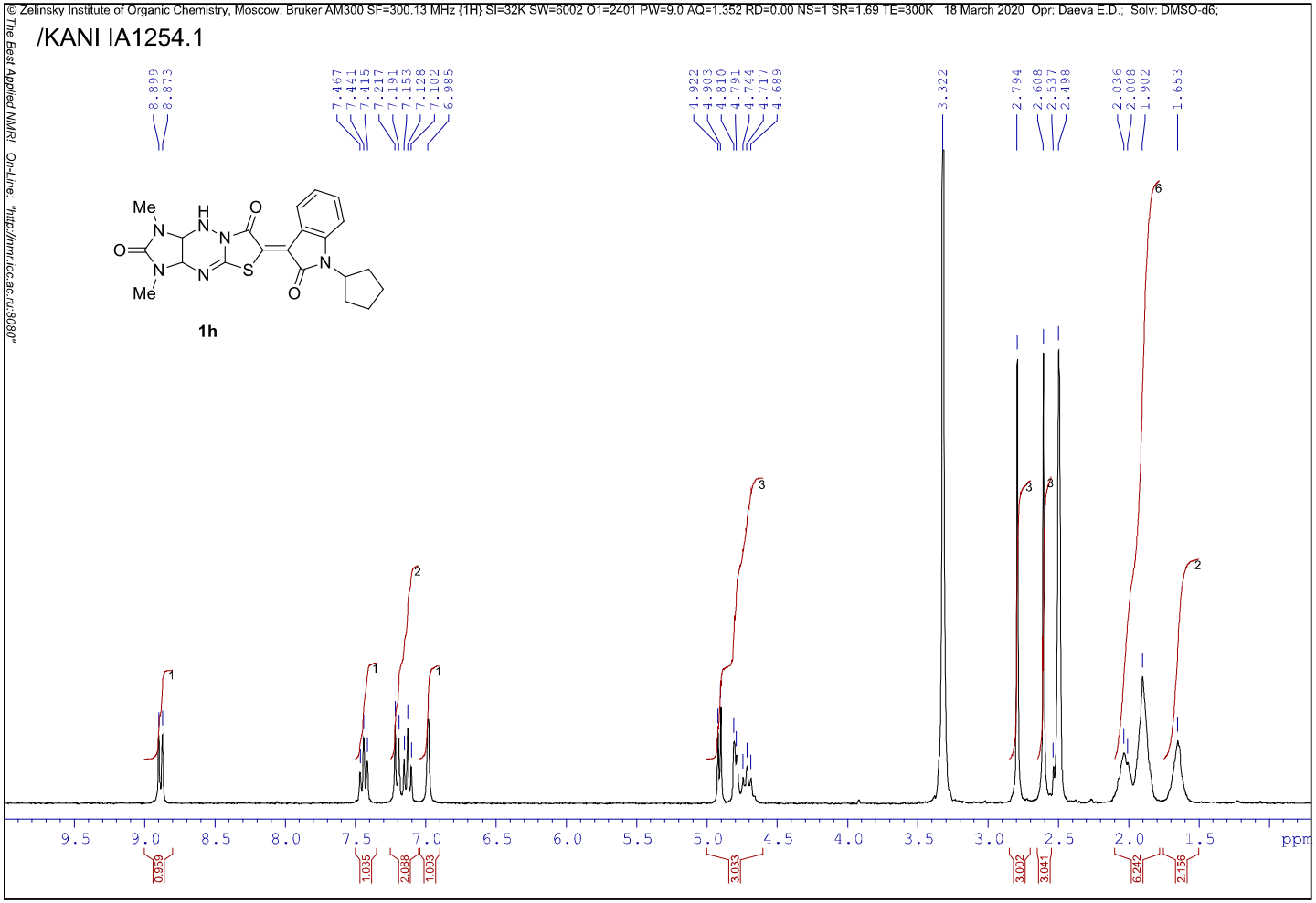
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=300K 18 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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4.689
3.322
2.794
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O
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1h
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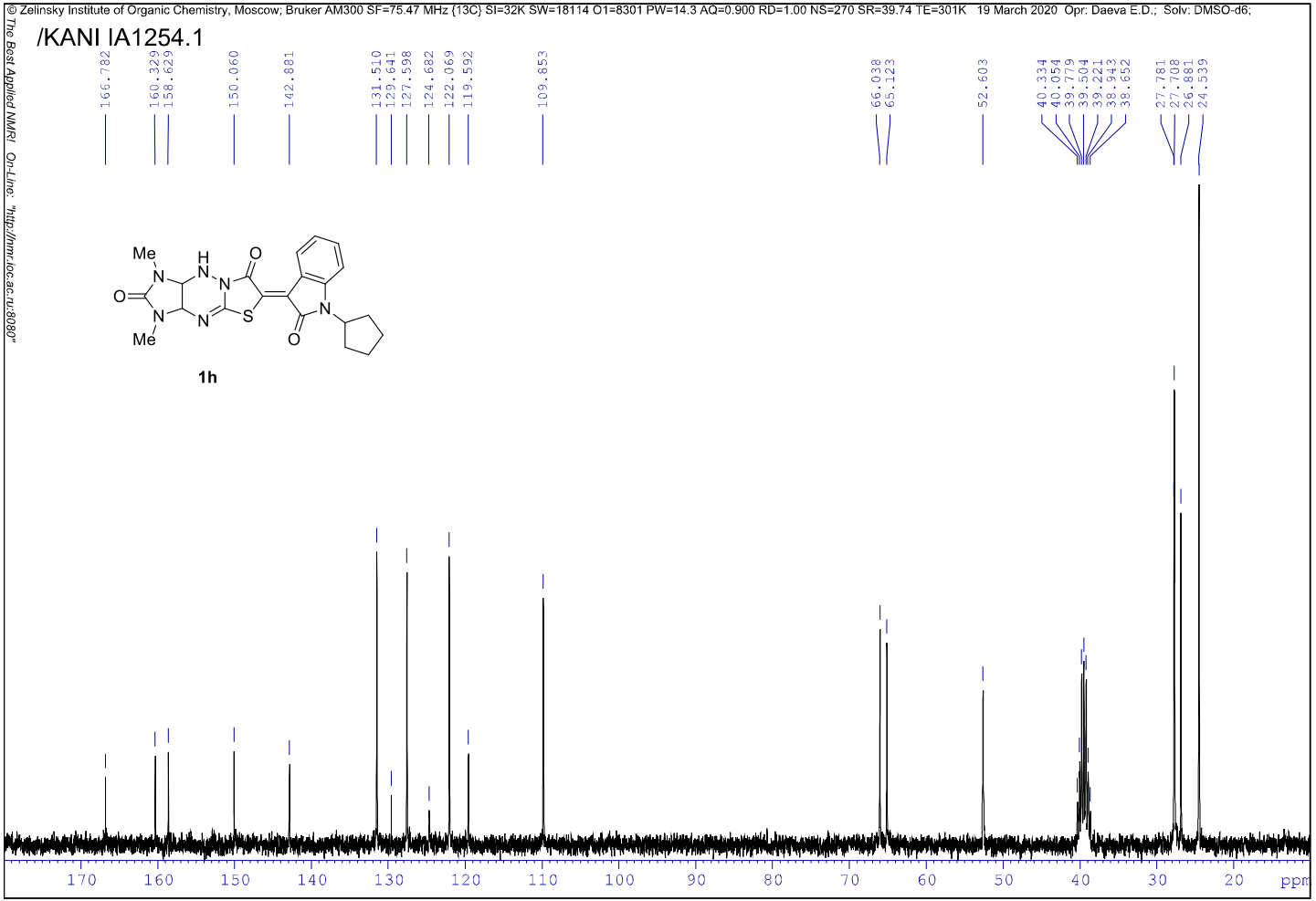
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=270 SR=39.74 TE=301K 19 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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122.069
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109.853
66.038
65.123
52.603
40.334
40.054
39.779
39.504
39.221
38.943
38.652
27.781
27.708
26.881
24.539
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H
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O
N
N
O
N
N
S
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O
1h
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160
150
140
130
120
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70
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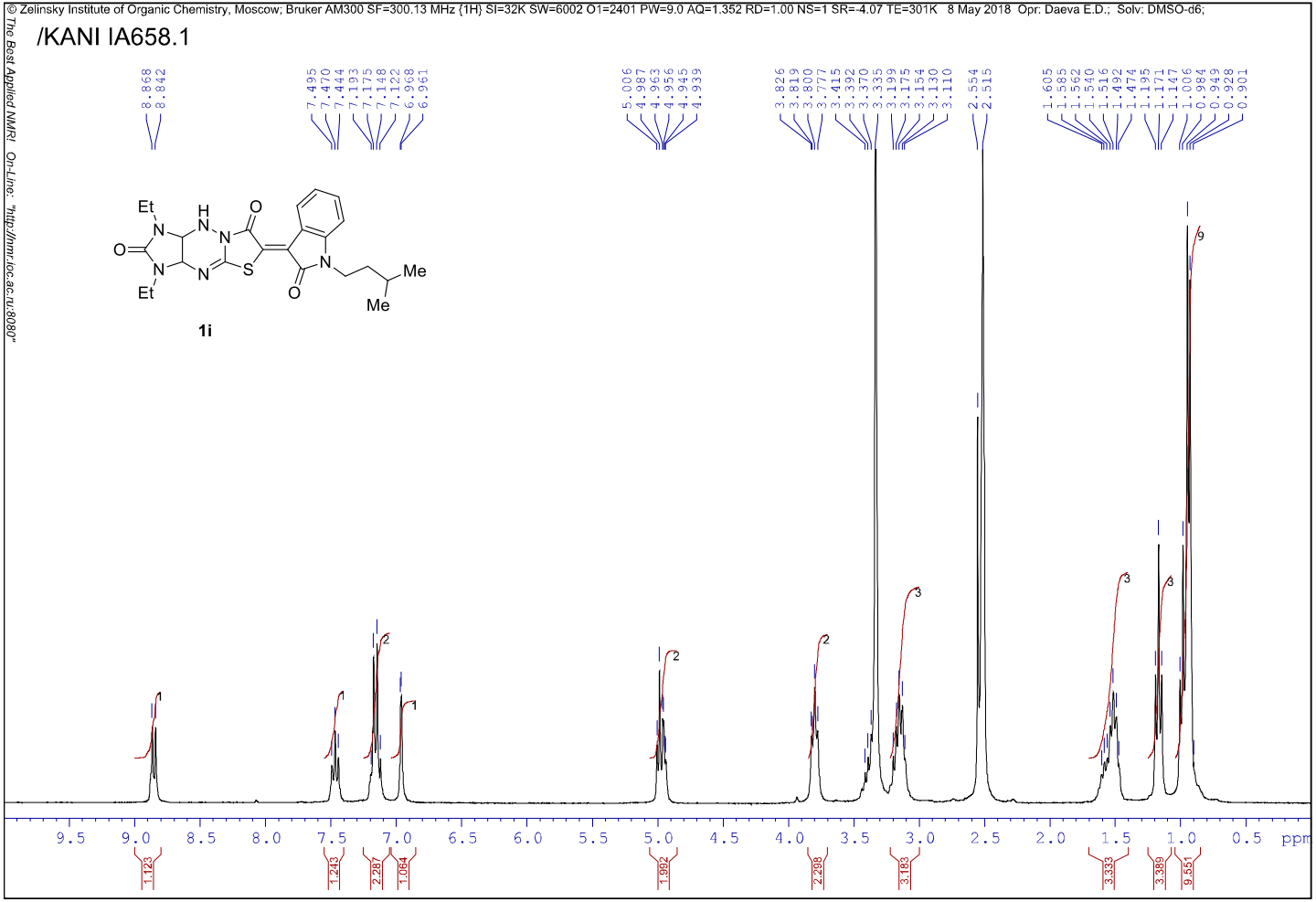
20
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=1.00 NS=1 SR=-4.07 TE=301K 8 May 2018 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line: "http://nmr.ioc.ac.ru:8080/"
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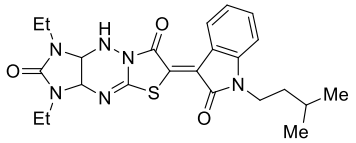
1i
ppm

/KANI IA658.1

166.679 160.239 157.637 149.880 143.130 131.588 129.727 127.481 124.401 122.189 119.373 108.990 64.296 63.111 40.059 39.769 39.504 39.218 38.931 38.023 35.570 35.058 34.410 25.247 22.142 22.102 13.341 12.661



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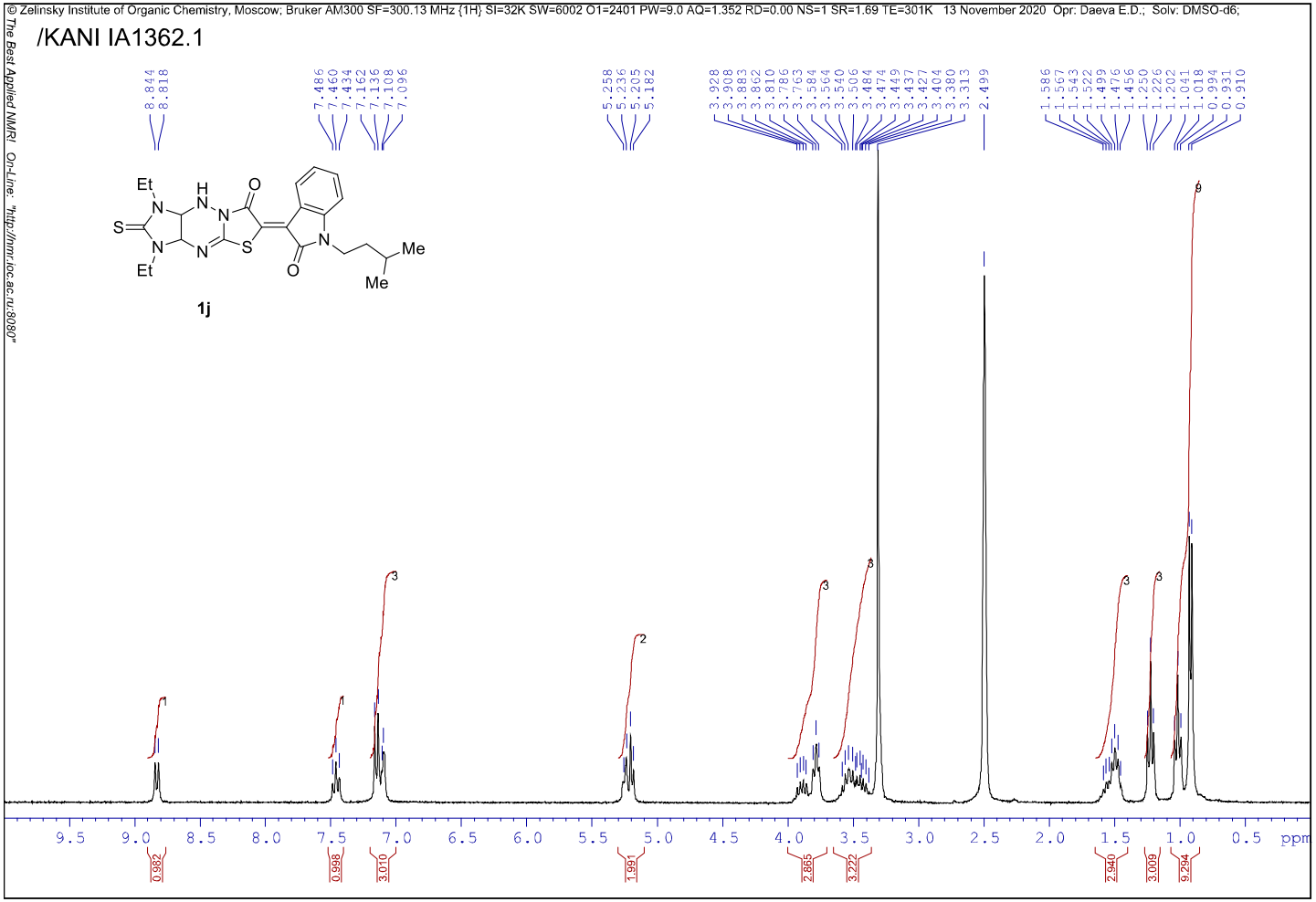
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=301K 13 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
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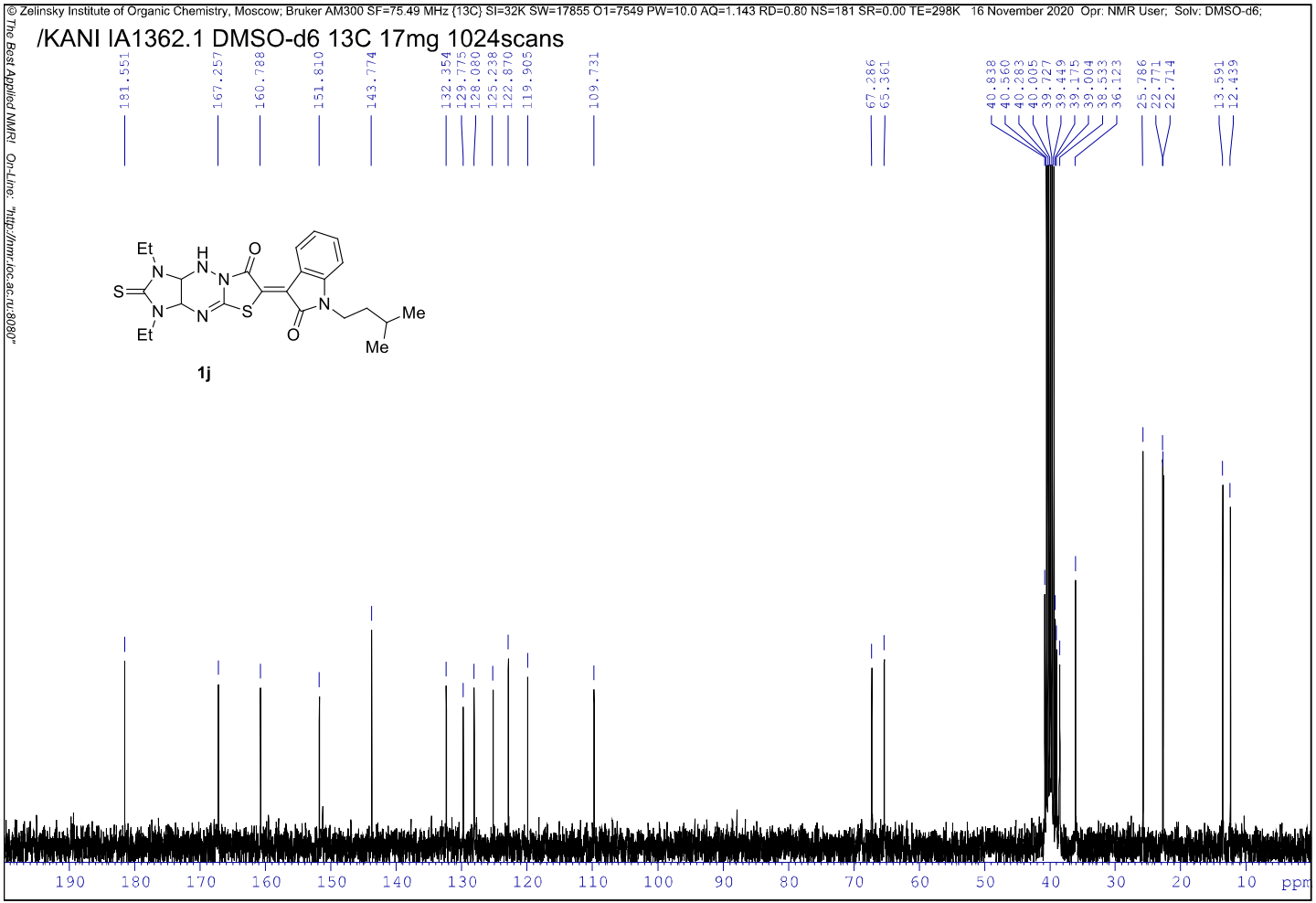
1j
ppm

/KANI IA1362.1 DMSO-d6 13C 17mg 1024scans



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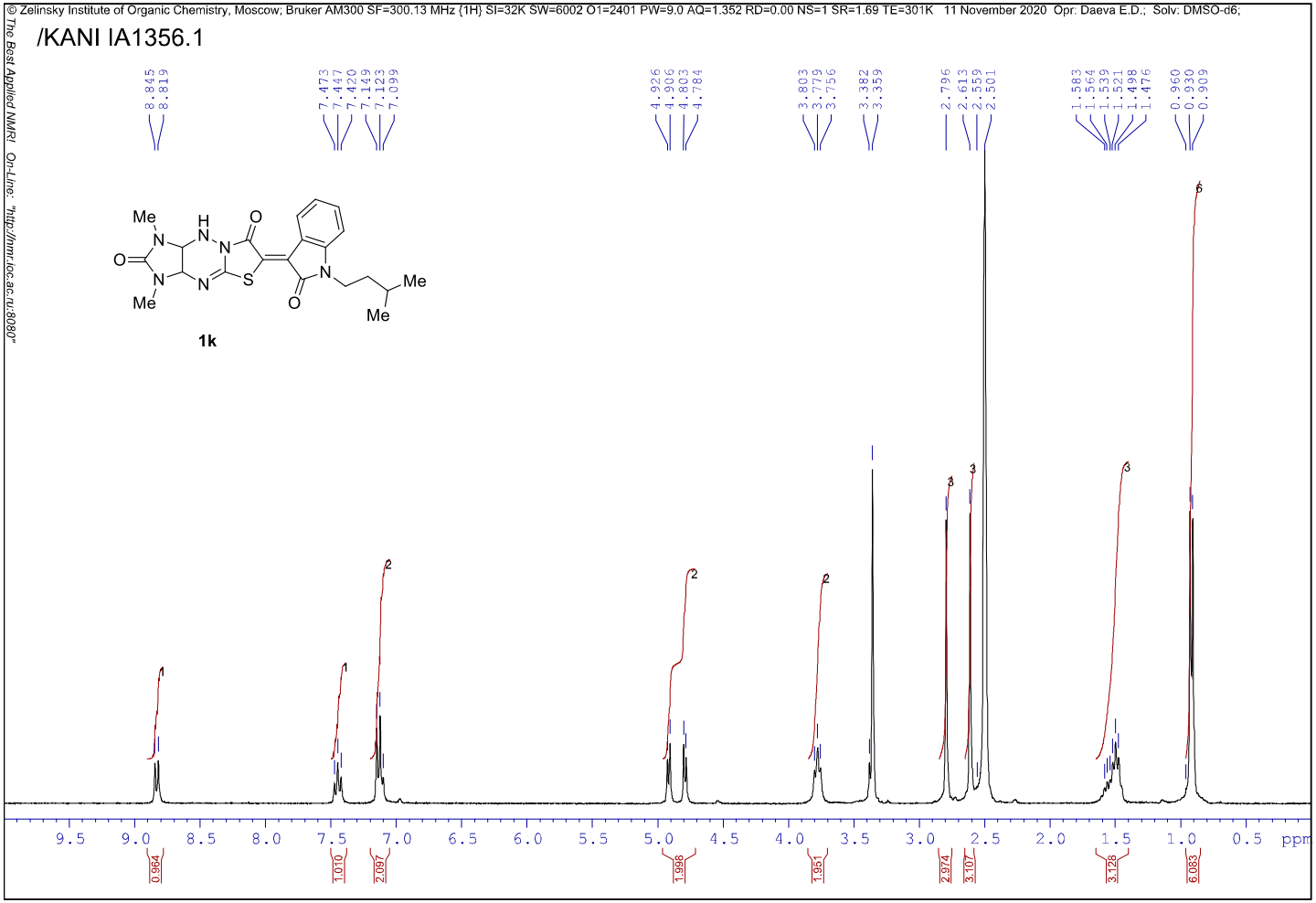
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=301K 11 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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8.819
7.473
7.447
7.420
7.149
7.123
7.099
4.926
4.906
4.803
4.784
3.803
3.779
3.756
3.382
3.359
2.796
2.613
2.559
2.501
1.583
1.564
1.539
1.521
1.498
1.476
0.960
0.930
0.909
Me
H
O
N
N
N
N
S
O
N
Me
O
Me
Me
1k
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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1.998
1.951
2.974
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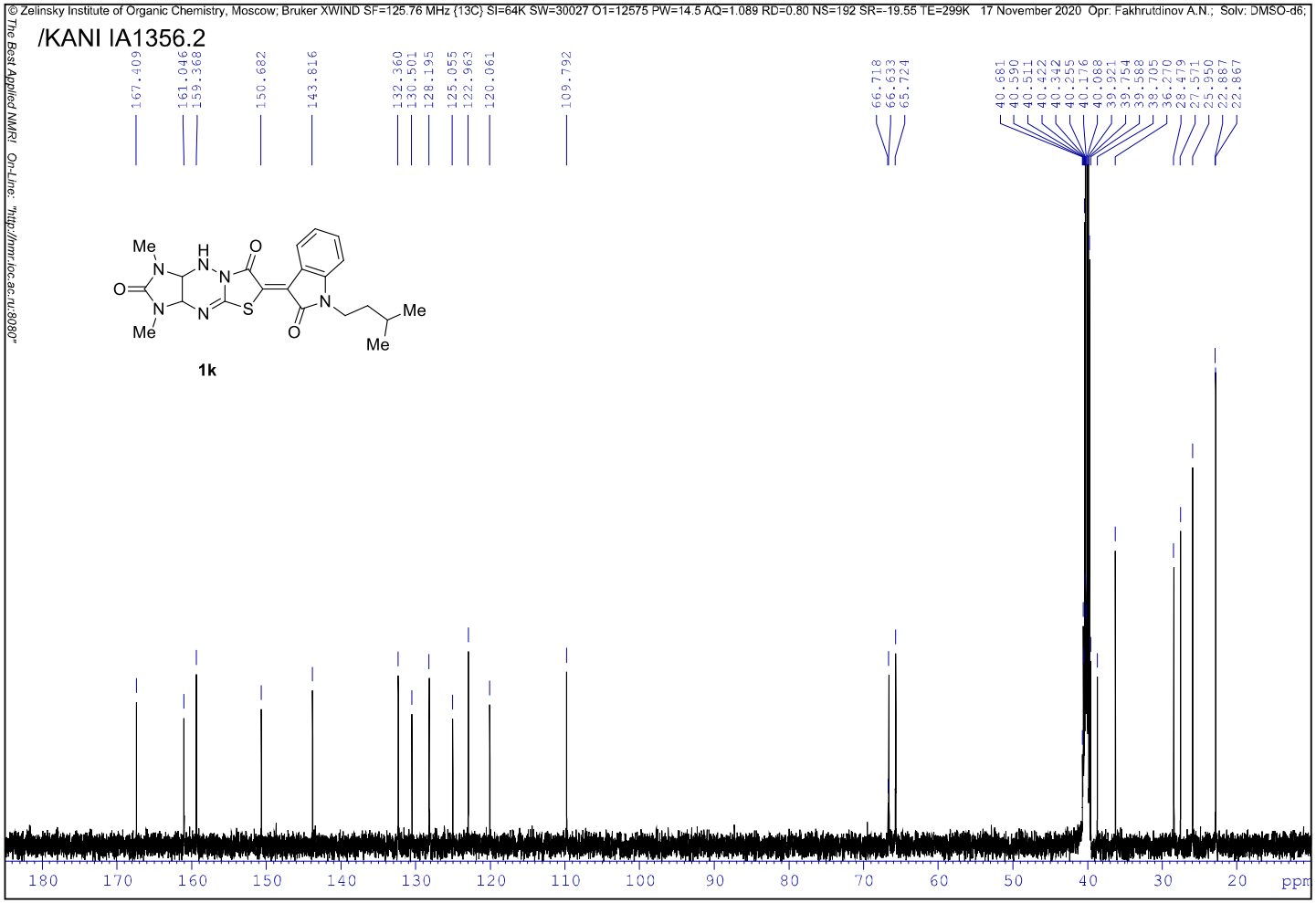
3.128
6.083


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker XWIND SF=125.76 MHz {13C} SI=64K SW=30027 O1=12575 PW=14.5 AQ=1.089 RD=0.80 NS=192 SR=-19.55 TE=299K 17 November 2020 Opr: Fakhrutdinov A.N.; Solv: DMSO-d6;
The Best Applied NMR!. On-Line. "http://nmr.ioc.ac.ru:8080/"
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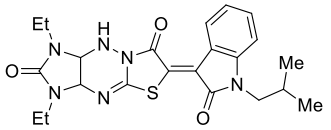
167.409
161.046
159.368
150.682
143.816
132.360
130.501
128.195
125.055
122.963
120.061
109.792
66.718
66.633
65.724
40.681
40.590
40.511
40.422
40.342
40.255
40.176
40.088
39.921
39.754
39.588
38.705
36.270
28.479
27.571
25.950
22.887
22.867
Me
H
O
N
N
N
N
S
O
N
Me
Me
O
Me
1k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

/KANI IA657.1



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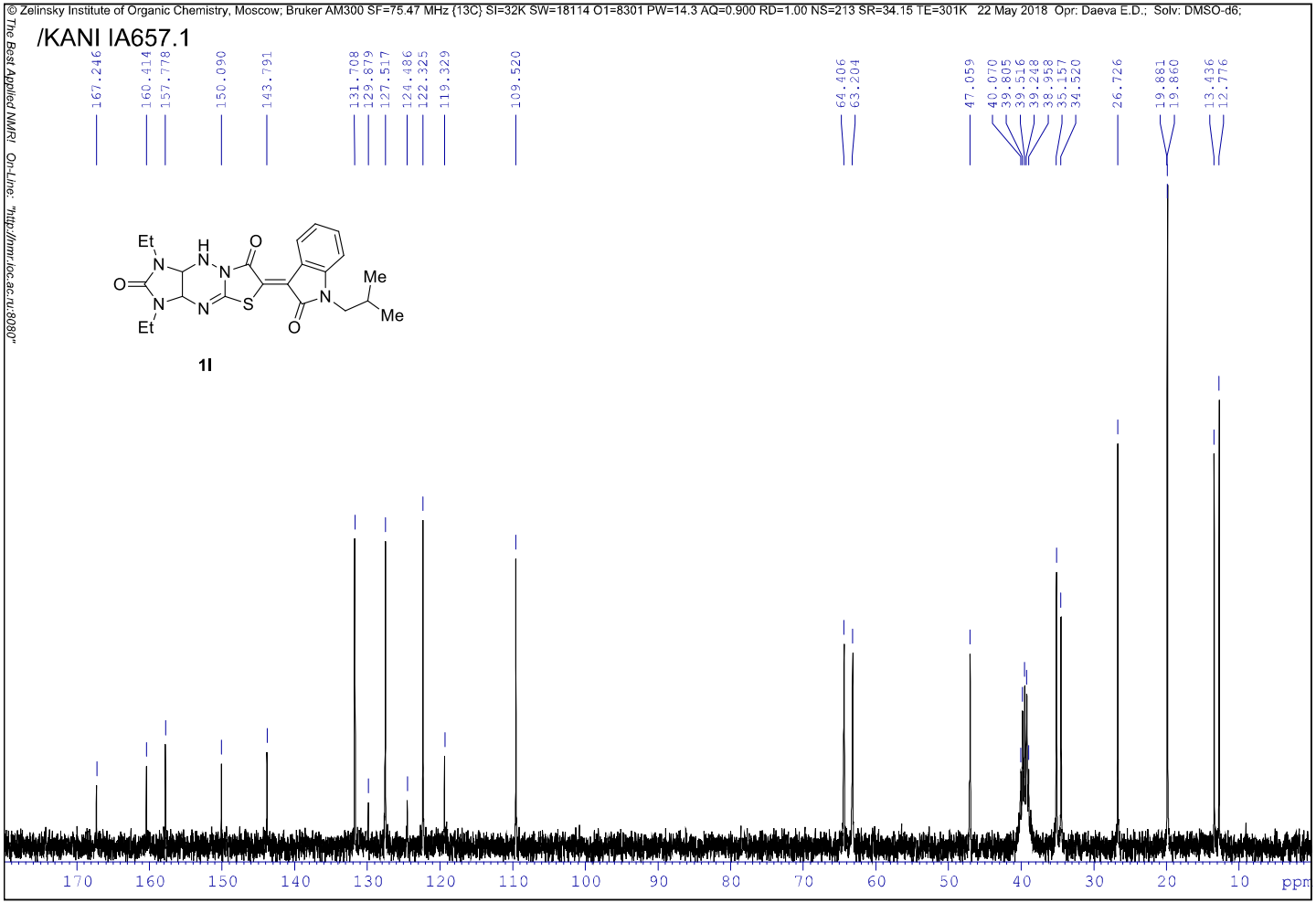
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=213 SR=34.15 TE=301K 22 May 2018 Opr: Daeva E.D.; Solv: DMSO-d6;
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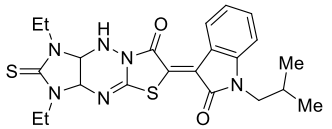
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
167.246
160.414
157.778
150.090
143.791
131.708
129.879
127.517
124.486
122.325
119.329
109.520
64.406
63.204
47.059
40.070
39.805
39.516
39.248
38.958
35.157
34.520
26.726
19.881
19.860
13.436
12.776
Et
N
H
N
N
O
O
N
N
S
Me
N
Me
Et
O
1l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

/KANI IA1382.1



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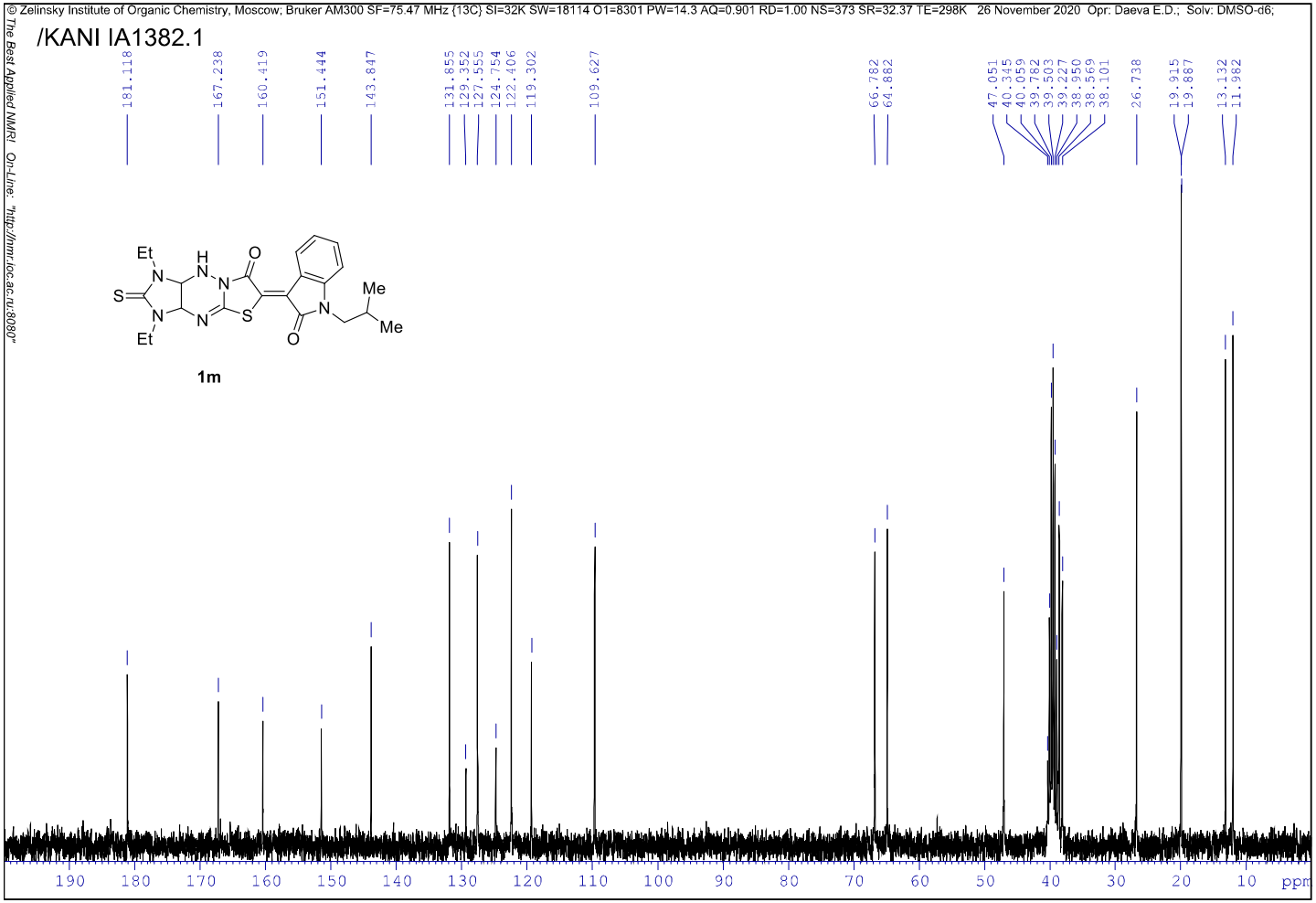
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=373 SR=32.37 TE=298K 26 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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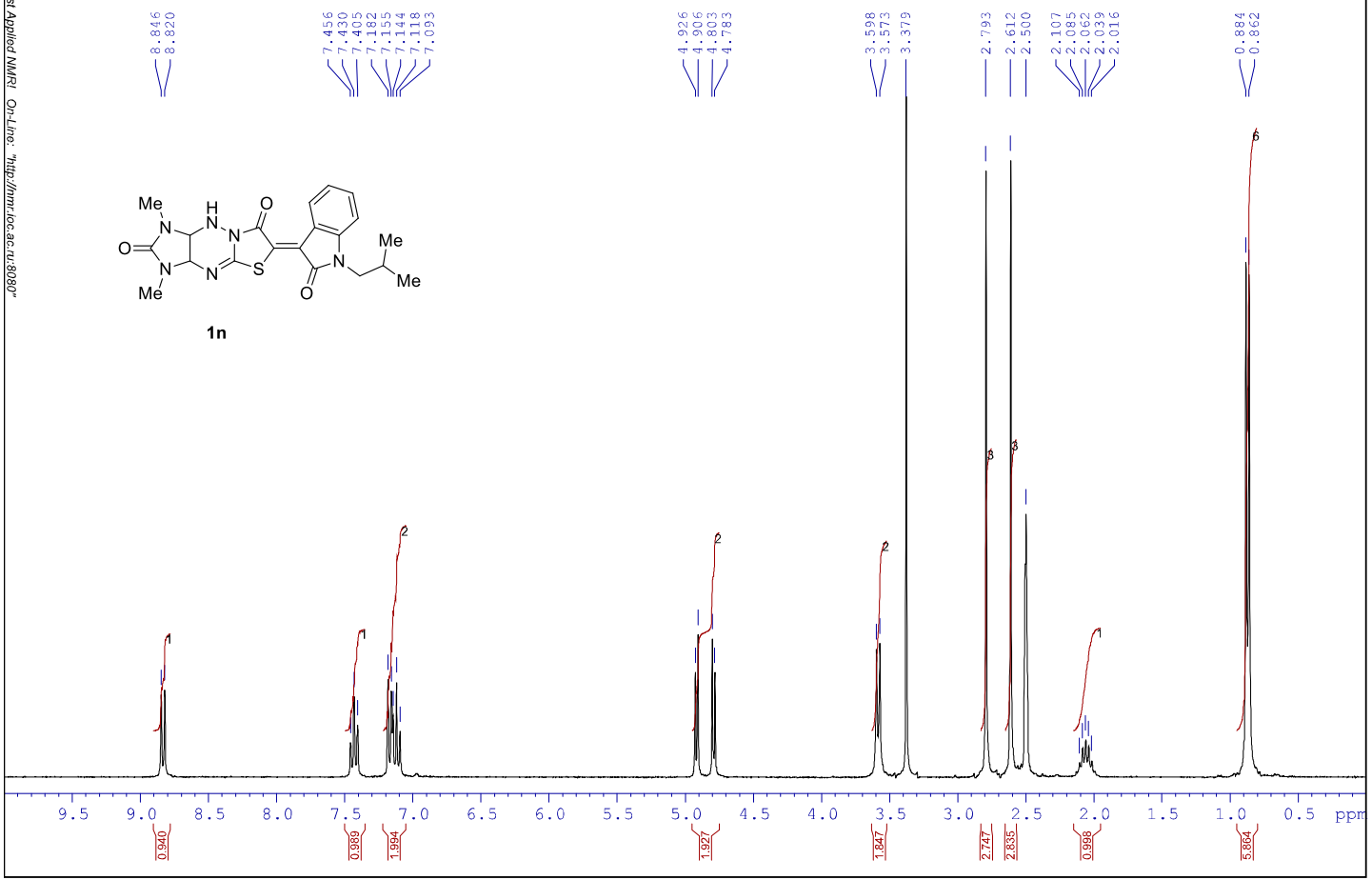
160.419
151.444
143.847
131.855
129.352
127.555
124.754
122.406
119.302
109.627
66.782
64.882
47.051
40.345
40.059
39.782
39.503
39.227
38.950
38.569
38.101
26.738
19.915
19.887
13.132
11.982
Et
N
H
N
O
S
N
N
S
Me
N
Me
Et
O
1m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

/KANI IA1378.1



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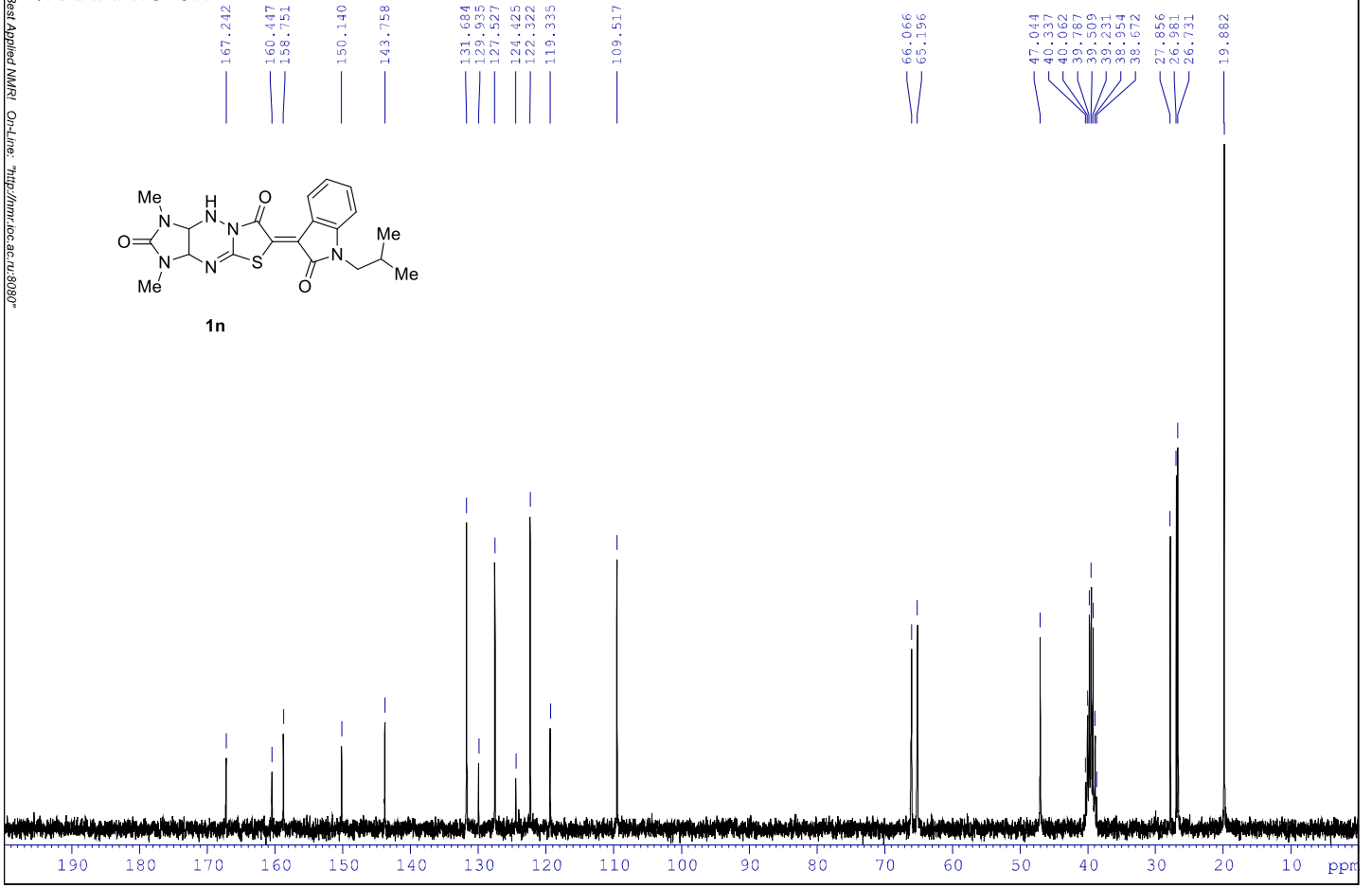
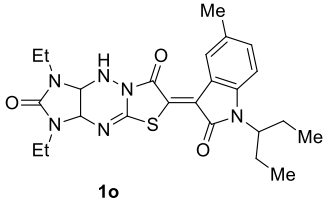


/KANI IA1332.1



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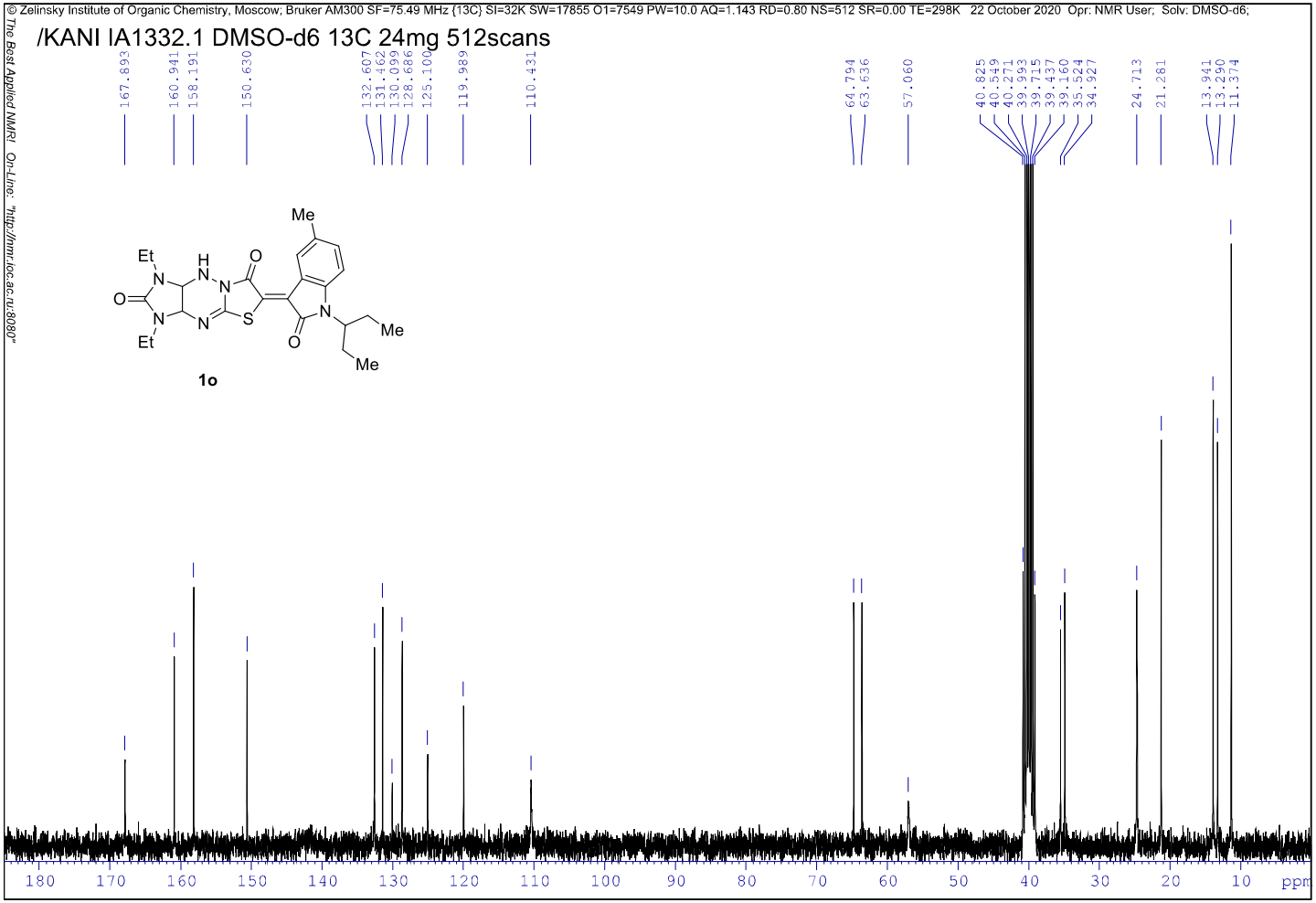
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=512 SR=0.00 TE=298K 22 October 2020 Opr: NMR User; Solv: DMSO-d6;
The Best Applied NMR! On-Line, "http://nmr.ioc.ac.ru:8080/"
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167.893
160.941
158.191
150.630
132.607
131.462
130.099
128.686
125.109
119.989
110.431
64.794
63.636
57.060
40.825
40.549
40.271
39.993
39.715
39.437
39.160
35.524
34.927
24.713
21.281
13.941
13.290
11.374
Me
Et
H
N
O
N
N
N
O
S
N
Me
Et
O
Me
1o
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

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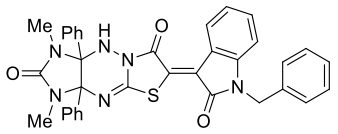

1p

/KANI osv178.01C

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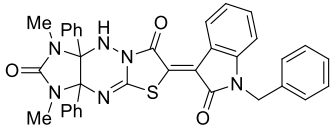
159.470
159.090
148.850
143.108
135.894
134.730
133.952
131.737
128.672
128.225
127.950
127.624
127.541
127.314
127.210
126.262
122.661
119.581
109.751
81.879
79.809
43.059
40.343
40.062
39.784
39.505
39.228
38.950
38.675
25.388
25.284



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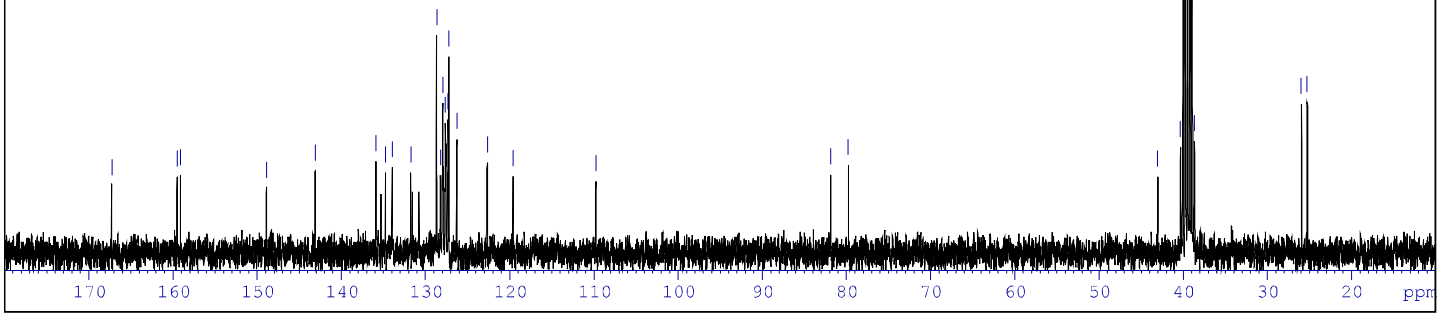

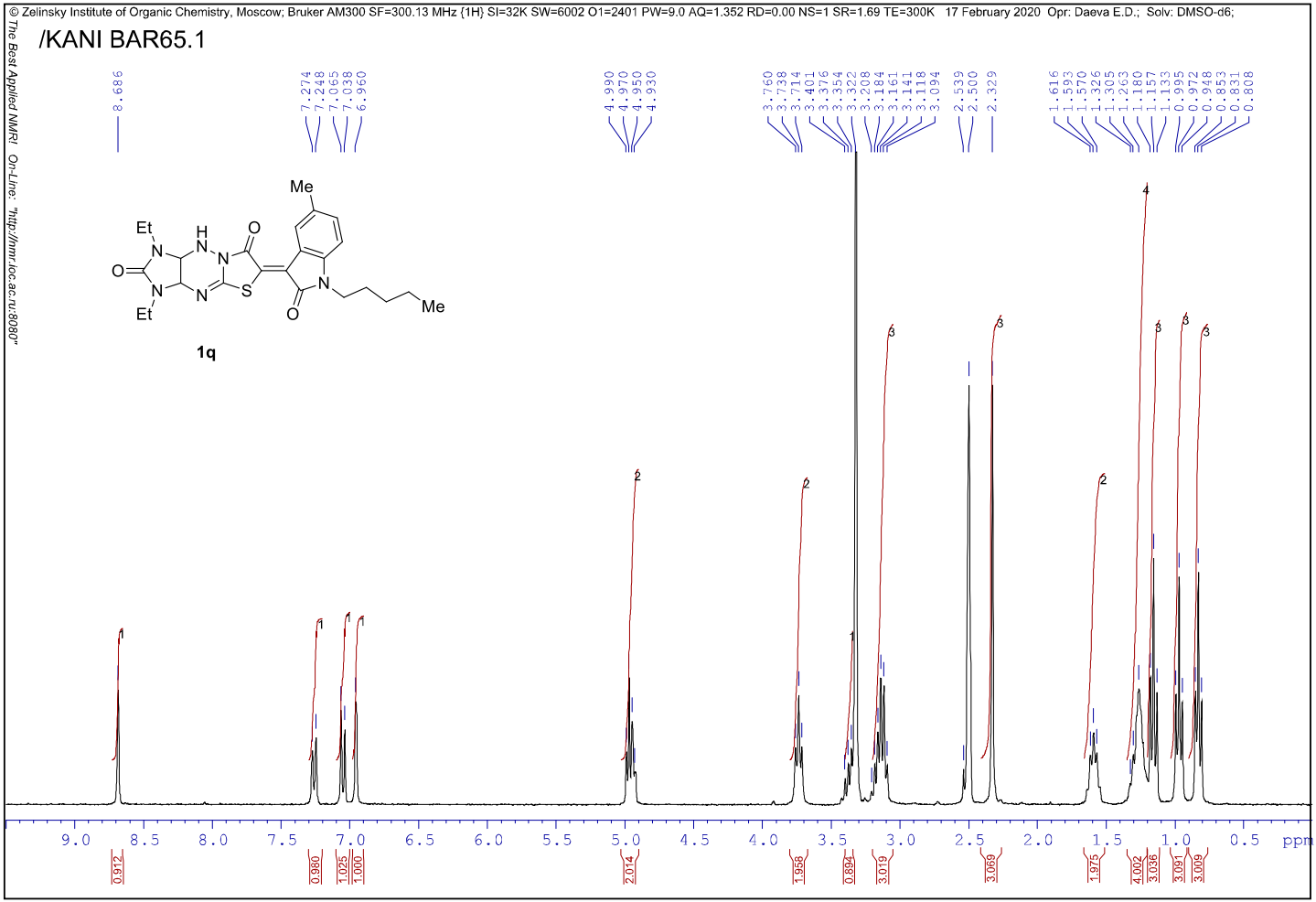
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=300K 17 February 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line: "http://nmr.ioc.ac.ru:8080"
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8.686
7.274
7.248
7.065
7.038
6.960
4.990
4.970
4.950
4.930
3.760
3.738
3.714
3.401
3.376
3.354
3.322
3.208
3.184
3.161
3.141
3.118
3.094
2.539
2.500
2.329
1.616
1.593
1.570
1.326
1.305
1.263
1.180
1.157
1.133
0.995
0.972
0.948
0.853
0.831
0.808
Et
N
H
N
O
O
N
N
S
N
Et
O
Me
N
Me
1q
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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0.980
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1.000
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0.894
3.019
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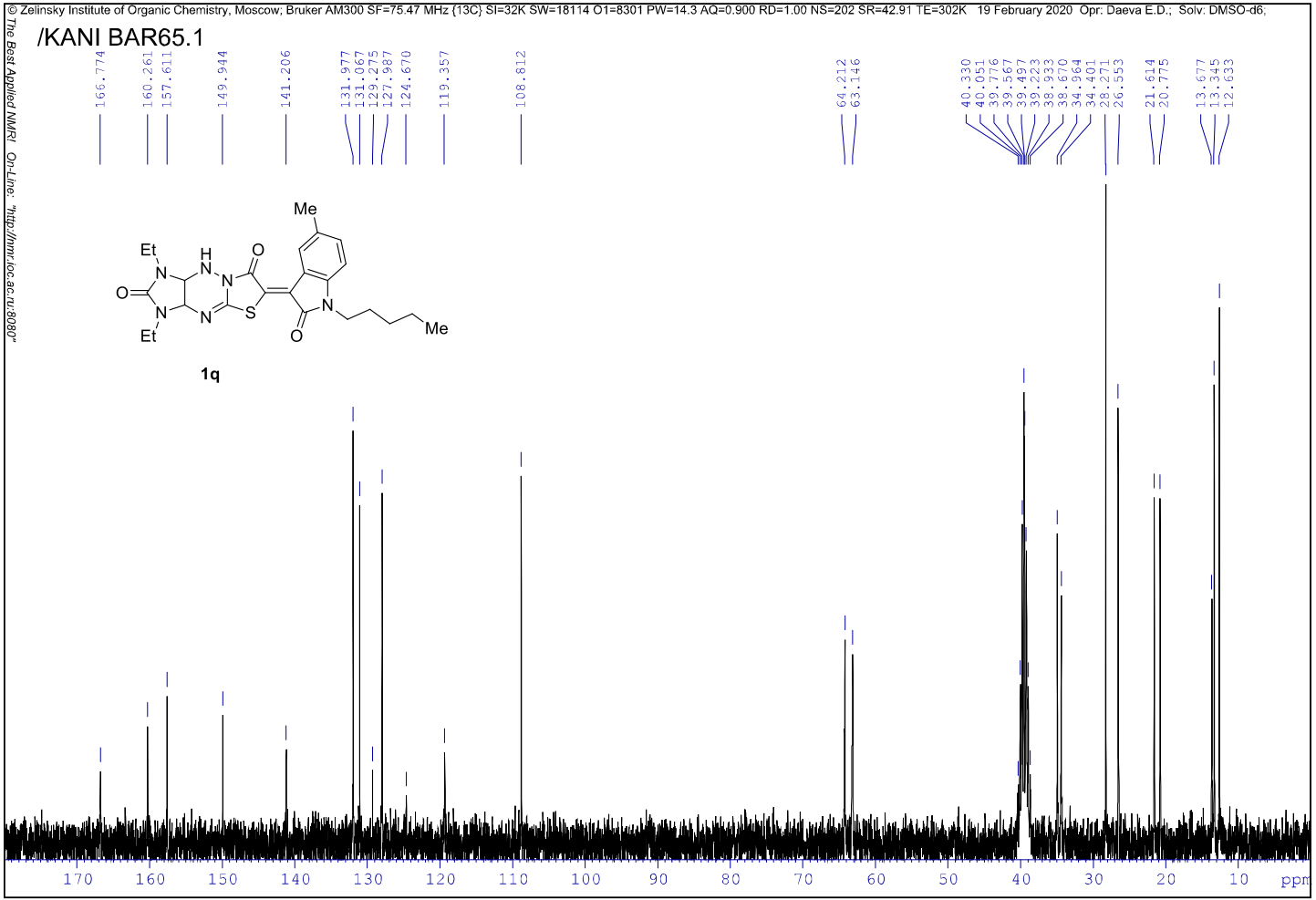
1.975
4.002
3.036
3.091
3.009


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=202 SR=42.91 TE=302K 19 February 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080"
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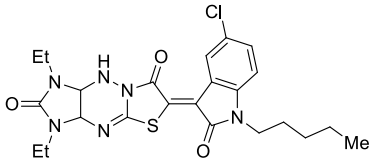
160.261
157.611
149.944
141.206
131.977
131.067
129.275
127.987
124.670
119.357
108.812
64.212
63.146
40.330
40.051
39.776
39.567
39.497
39.223
38.933
38.670
34.364
34.401
28.271
26.553
21.614
20.775
13.677
13.345
12.633
Me
Et
H
N
O
N
N
N
S
N
O
Et
Me
1q
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

/KANI BAR71.1 DMSO-d6 1H unknown mg



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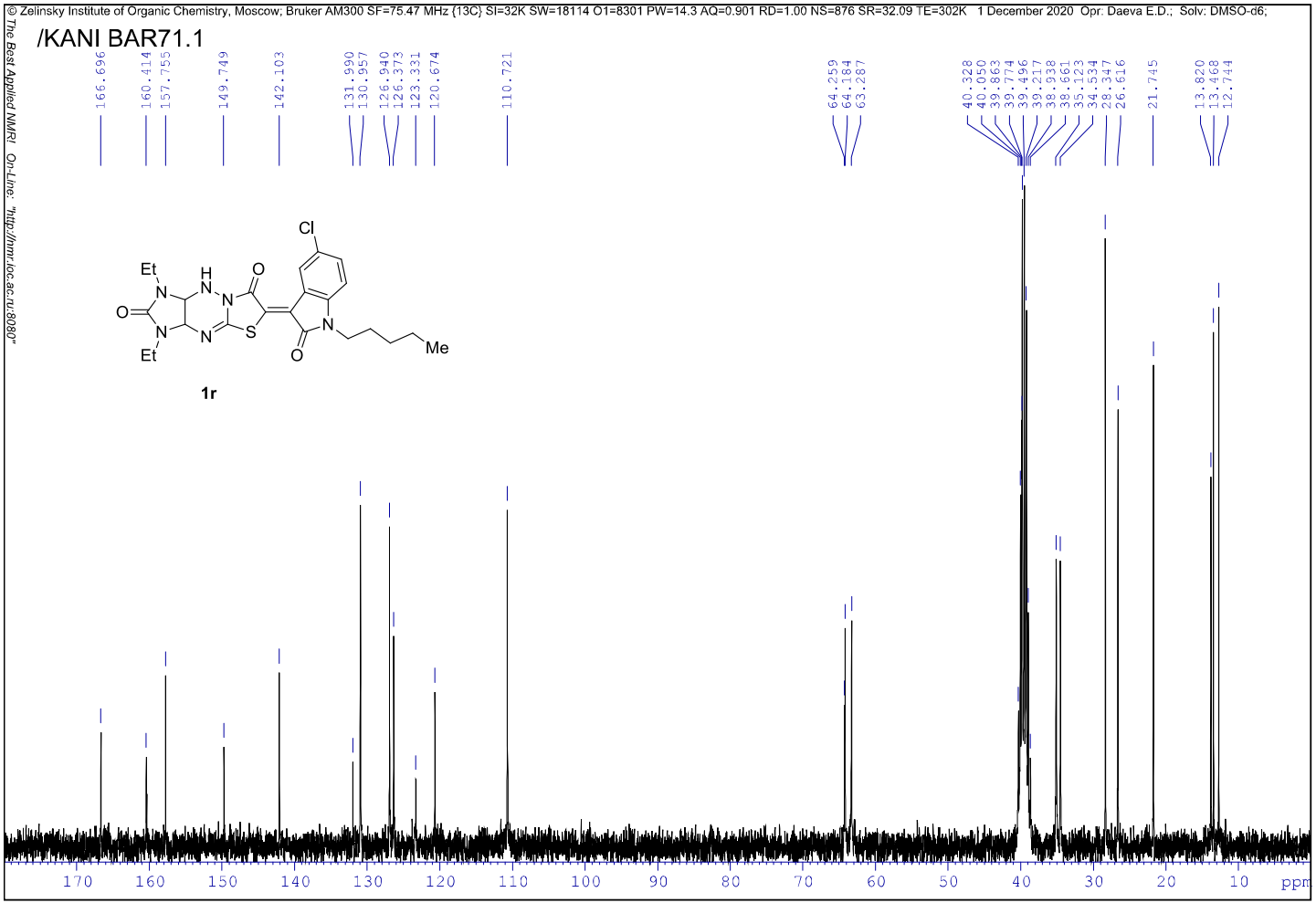
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=876 SR=32.09 TE=302K 1 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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157.755
149.749
142.103
131.990
130.957
126.940
126.373
123.331
120.674
110.721
64.259
64.184
63.287
40.328
40.050
39.863
39.774
39.496
39.217
38.938
38.661
35.123
34.534
29.347
26.616
21.745
13.820
13.468
12.744
Cl
Et
H
O
N
N
N
O
N
S
N
Et
O
Me
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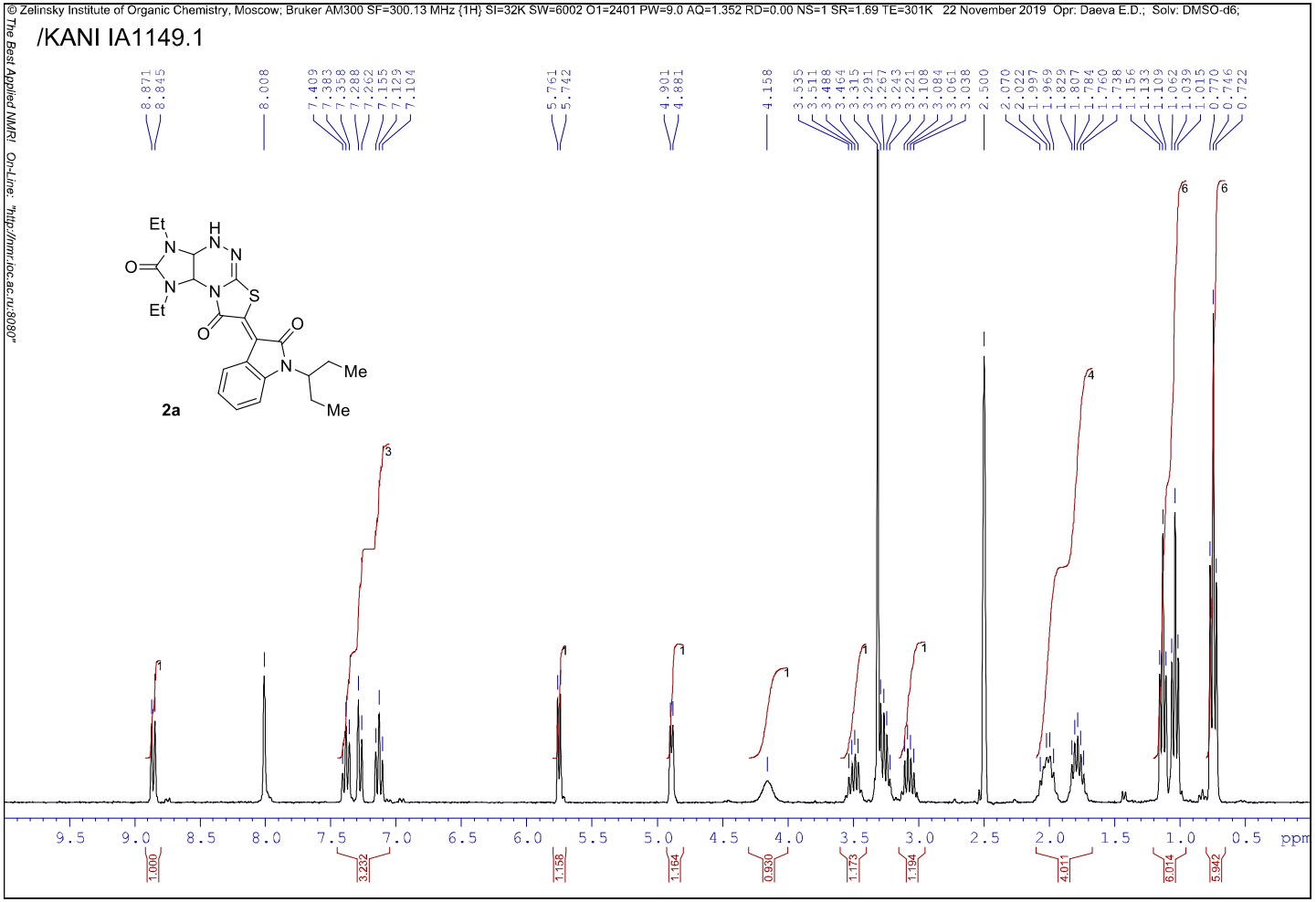
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=301K 22 November 2019 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line, "http://nmr.ioc.ac.ru:8080/"
/KANI IA1149.1
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8.845
8.008
7.409
7.383
7.358
7.288
7.262
7.155
7.129
7.104
5.761
5.742
4.901
4.881
4.158
3.535
3.511
3.488
3.464
3.315
3.291
3.267
3.243
3.221
3.108
3.084
3.061
3.038
2.500
2.070
2.022
1.997
1.969
1.829
1.807
1.784
1.760
1.738
1.156
1.133
1.109
1.062
1.039
1.015
0.770
0.746
0.722
Et
H
N
N
O
N
N
S
Et
O
O
N
Me
Me
2a
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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1.164
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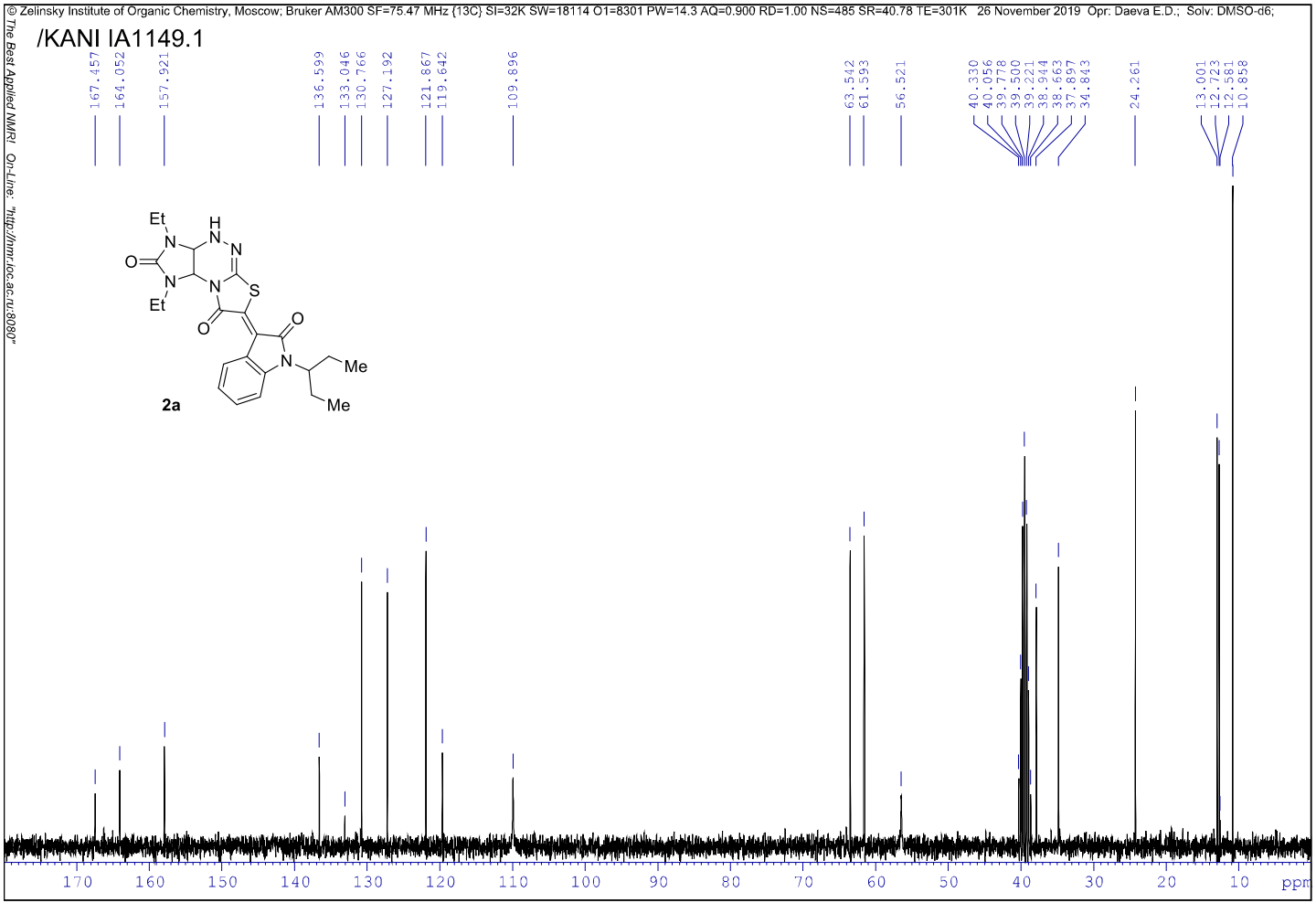
6.014
5.942


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=485 SR=40.78 TE=301K 26 November 2019 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
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164.052
157.921
136.599
133.046
130.766
127.192
121.867
119.642
109.896
63.542
61.593
56.521
40.330
40.056
39.778
39.500
39.221
38.944
38.663
37.897
34.843
24.261
13.001
12.723
12.581
10.858
Et
N
H
N
N
O
N
S
Et
O
O
N
Me
Me
2a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

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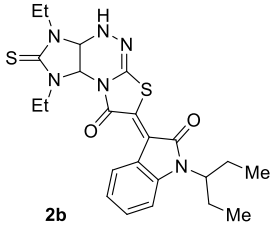
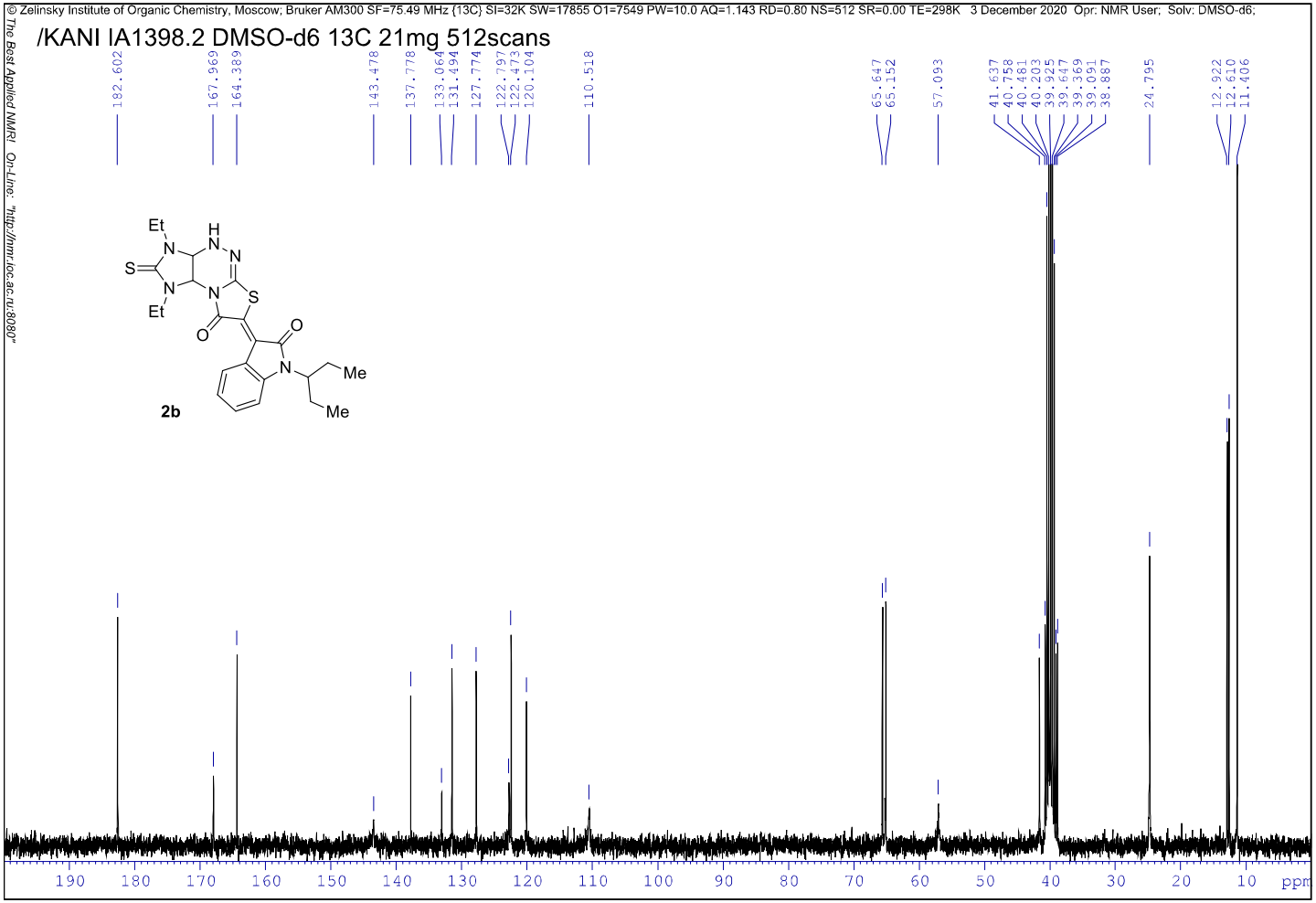


2b


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=512 SR=0.00 TE=298K 3 December 2020 Opr: NMR User; Solv: DMSO-d6;
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131.494
127.774
122.797
122.473
120.104
110.518
65.647
65.152
57.093
41.637
40.758
40.481
40.203
39.925
39.647
39.369
39.091
38.887
24.795
12.922
12.610
11.406
Et
N
H
N
S
N
N
S
N
Et
O
O
N
Me
Me
2b
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20
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ppm

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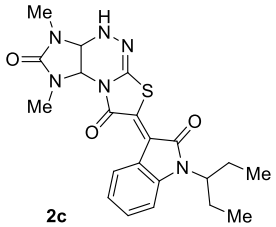

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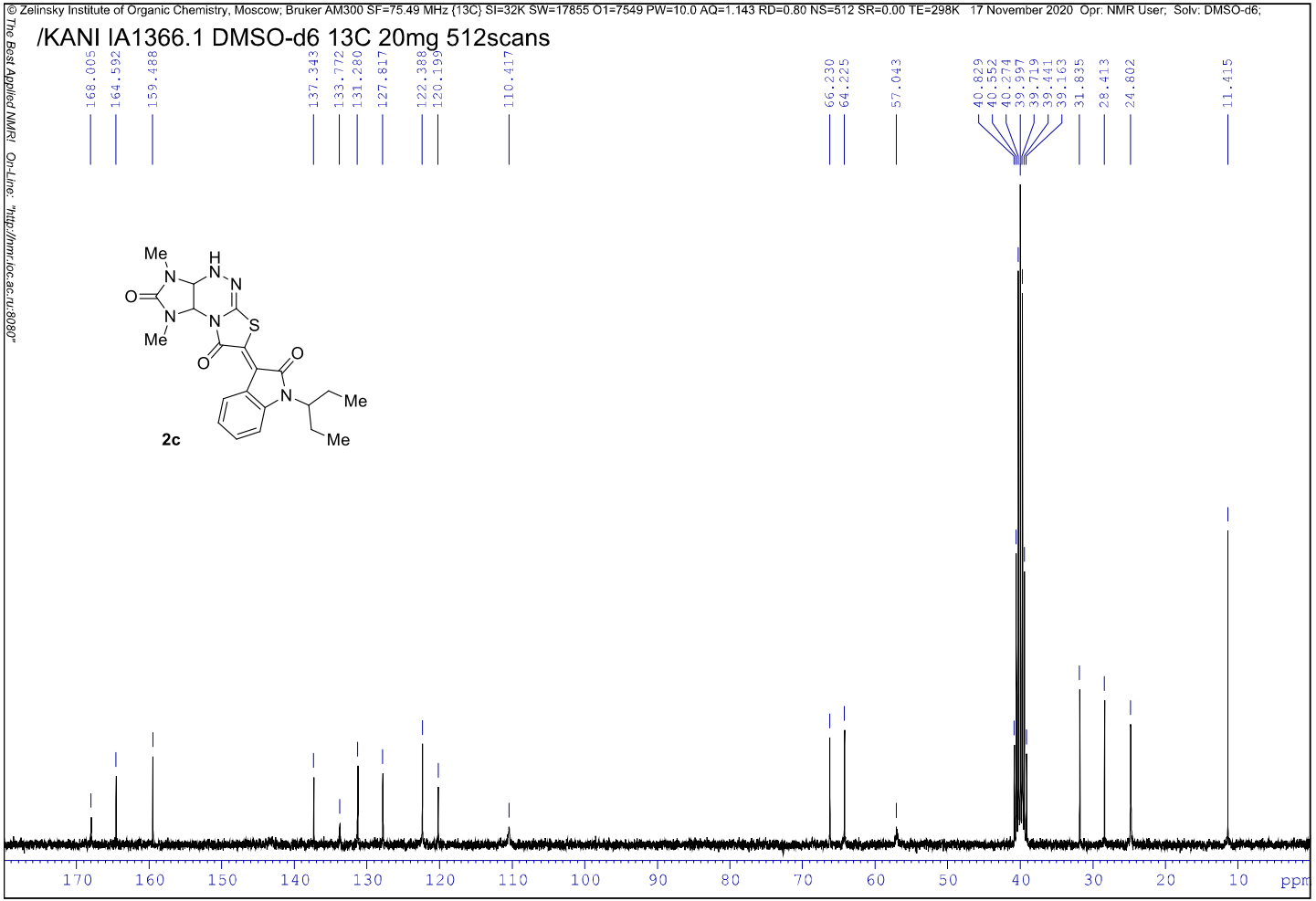
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=512 SR=0.00 TE=298K 17 November 2020 Opr: NMR User; Solv: DMSO-d6;
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122.388
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110.417
66.230
64.225
57.043
40.829
40.552
40.274
39.997
39.719
39.441
39.163
31.835
28.413
24.802
11.415
Me
H
N
N
O
N
N
S
Me
O
O
N
Me
Me
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30
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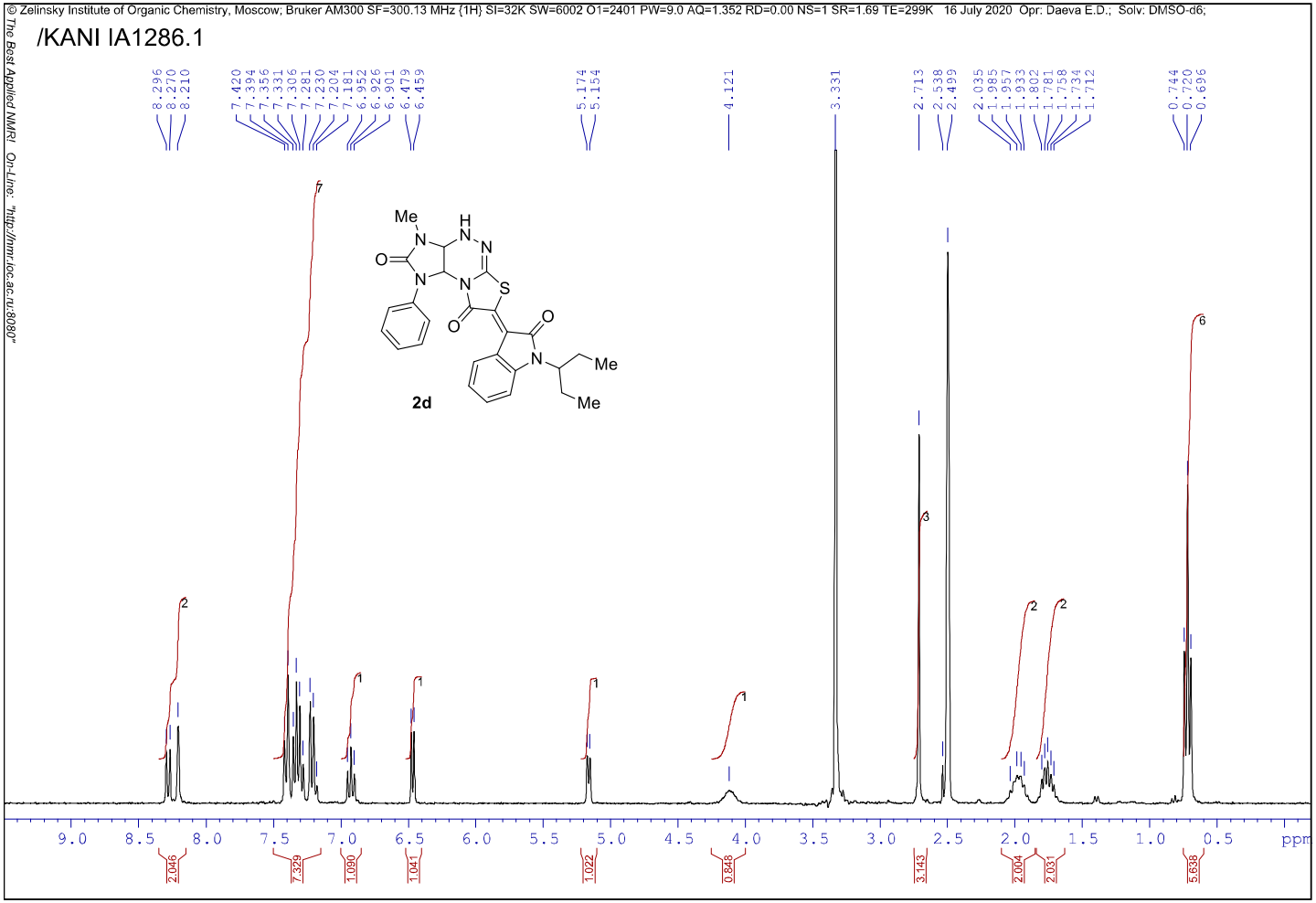
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=299K 16 July 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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8.210
7.420
7.394
7.356
7.331
7.306
7.281
7.230
7.204
7.181
6.952
6.926
6.901
6.479
6.459
5.174
5.154
4.121
3.331
2.713
2.538
2.499
2.035
1.985
1.957
1.933
1.802
1.781
1.758
1.734
1.712
0.744
0.720
0.696
Me
N
H
N
O
N
N
S
O
O
N
Me
Me
2d
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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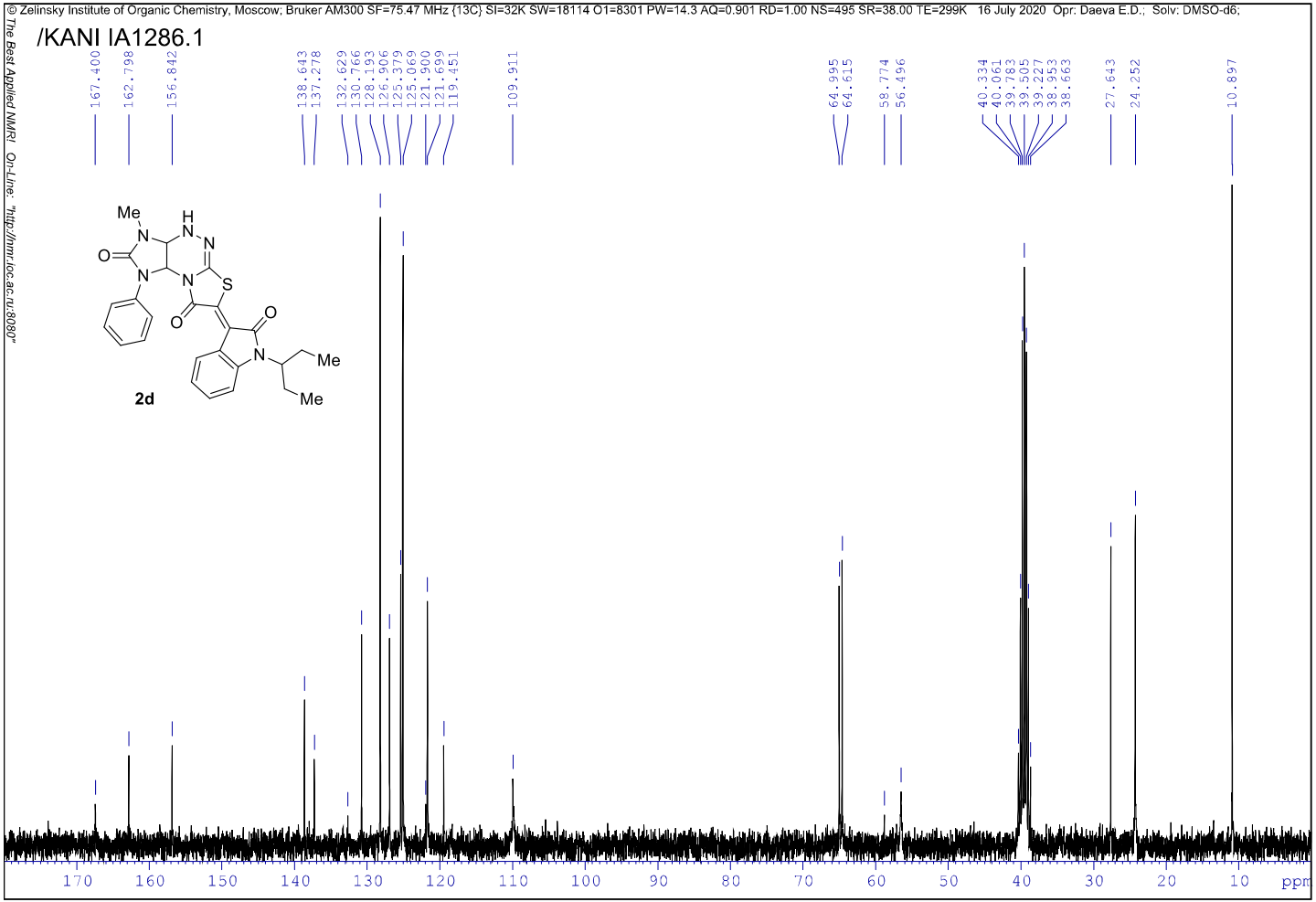
2.031
5.638


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=495 SR=38.00 TE=299K 16 July 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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138.643
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130.766
128.193
126.906
125.379
125.069
121.900
121.699
119.451
109.911
64.995
64.615
58.774
56.496
40.334
40.061
39.783
39.505
39.227
38.953
38.663
27.643
24.252
10.897
Me
H
N
N
O
N
N
S
O
O
N
Me
Me
2d
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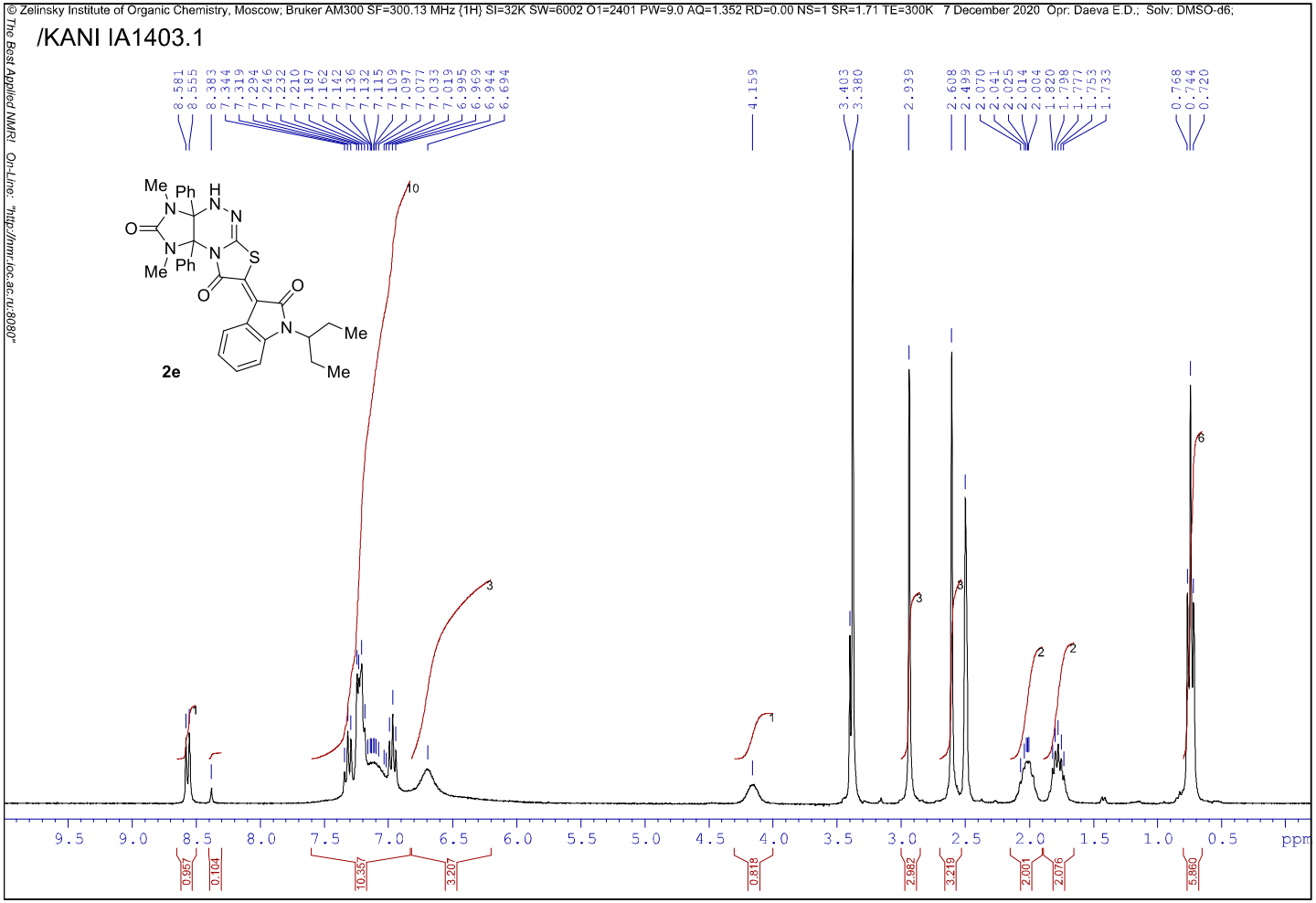
20
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.71 TE=300K 7 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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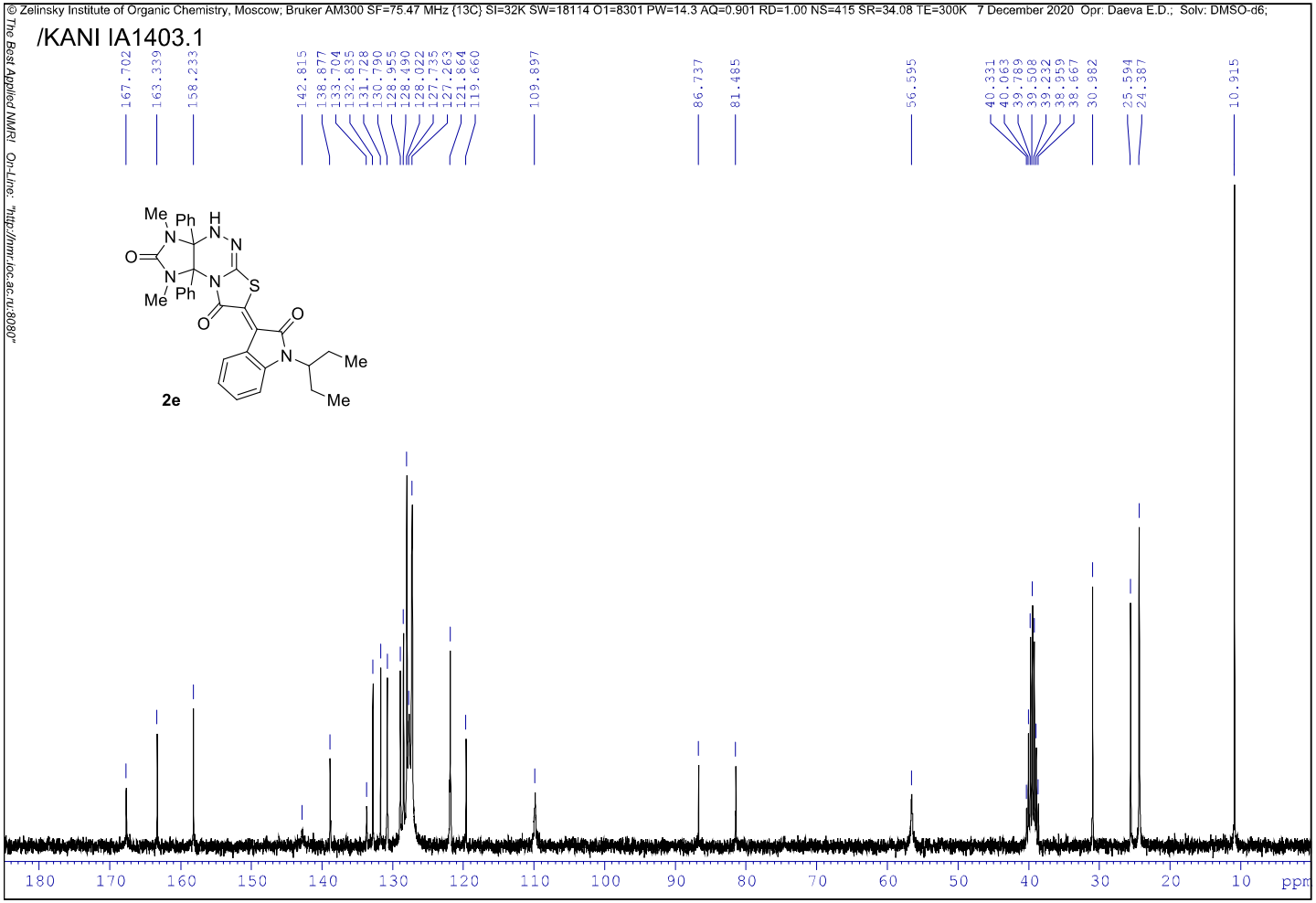
4.159
3.403 3.380
2.939
2.608 2.499 2.070 2.041 2.025 2.014 2.004 1.820 1.798 1.777 1.753 1.733
0.768 0.744 0.720
Me Ph H N N O N Ph Me S O O N Me Me
2e
10 3 1 3 3 2 2 6
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.957 0.104 10.357 3.207 0.818 2.982 3.219 2.001 2.076 5.860


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=415 SR=34.08 TE=300K 7 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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131.728
130.790
128.955
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128.022
127.735
127.263
121.864
119.660
109.897
86.737
81.485
56.595
40.331
40.063
39.789
39.508
39.232
38.959
38.667
30.982
25.594
24.387
10.915
Me
Ph
H
N
N
O
N
S
Me
Ph
O
O
N
Me
Me
2e
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170
160
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120
110
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90
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40
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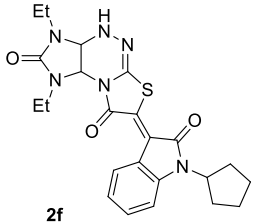
20
10
ppm

/KANI IA853.1



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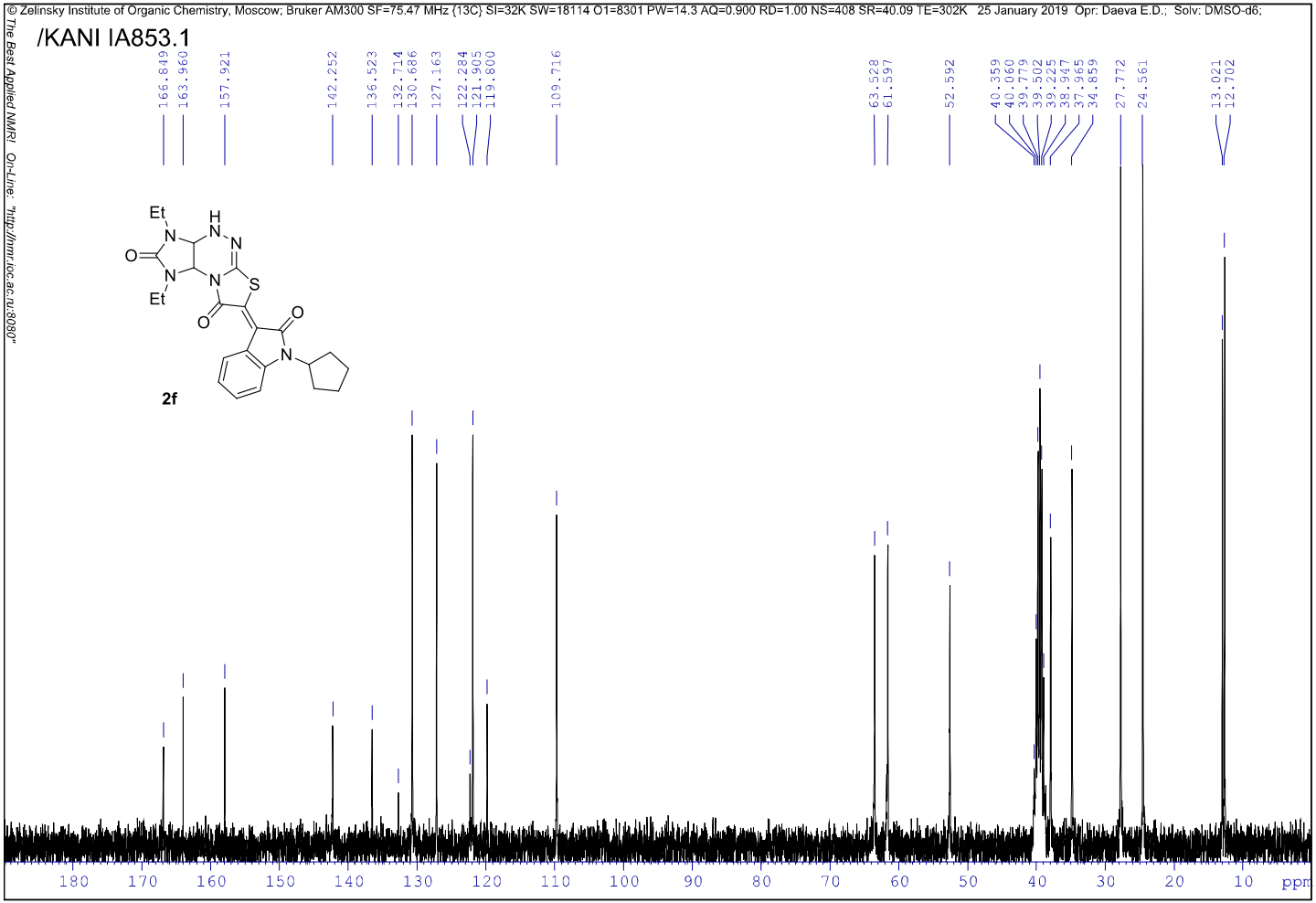
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=408 SR=40.09 TE=302K 25 January 2019 Opr: Daeva E.D.; Solv: DMSO-d6;
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109.716
63.528
61.597
52.592
40.359
40.060
39.779
39.502
39.225
38.947
37.965
34.859
27.772
24.561
13.021
12.702
Et
N
H
N
O
N
S
N
Et
O
O
N
2f
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40
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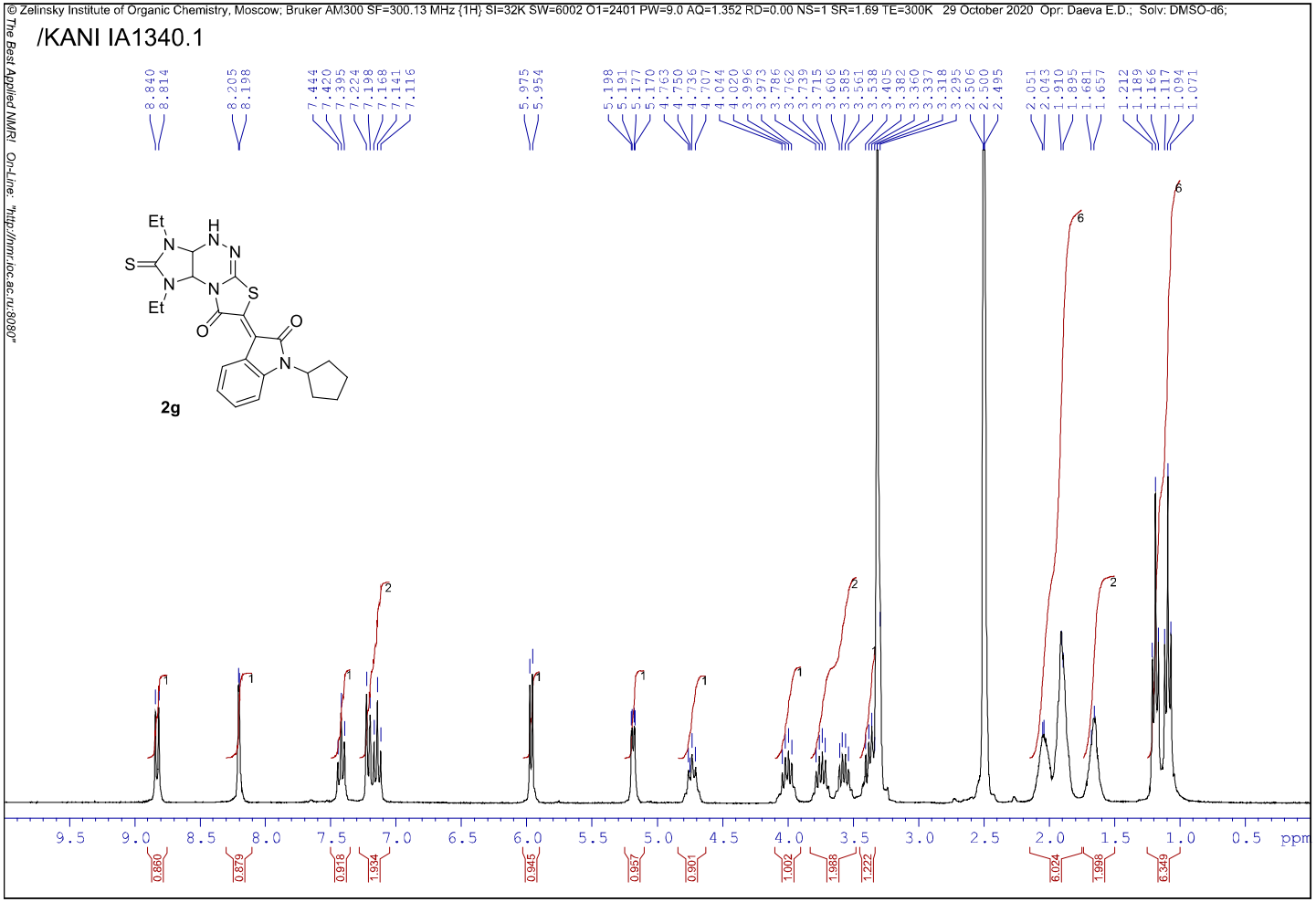
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=300K 29 October 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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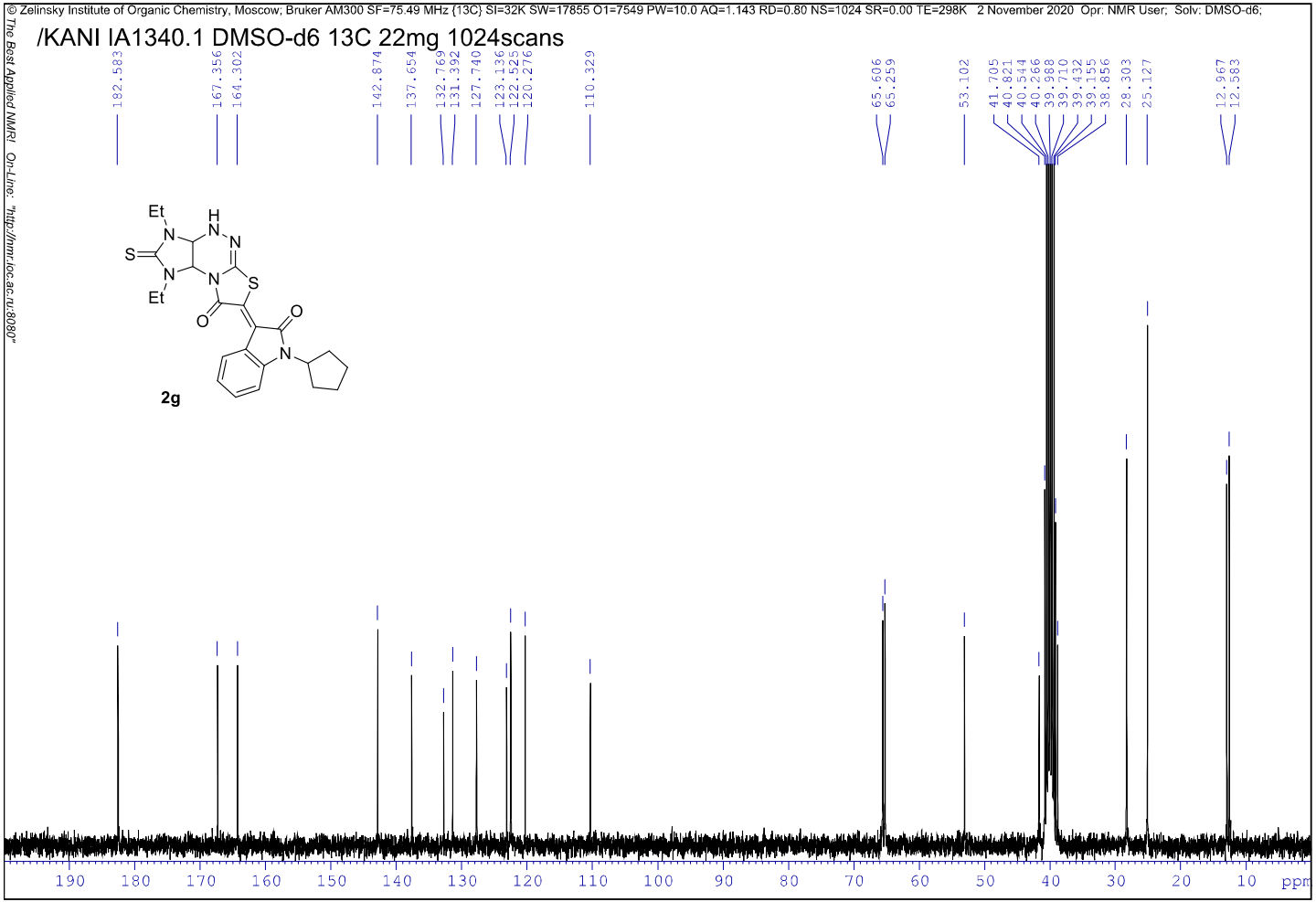
2g
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=1024 SR=0.00 TE=298K 2 November 2020 Opr: NMR User; Solv: DMSO-d6;
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122.525
120.276
110.329
65.606
65.259
53.102
41.705
40.821
40.544
40.266
39.988
39.710
39.432
39.155
38.856
28.303
25.127
12.967
12.583
2g
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70
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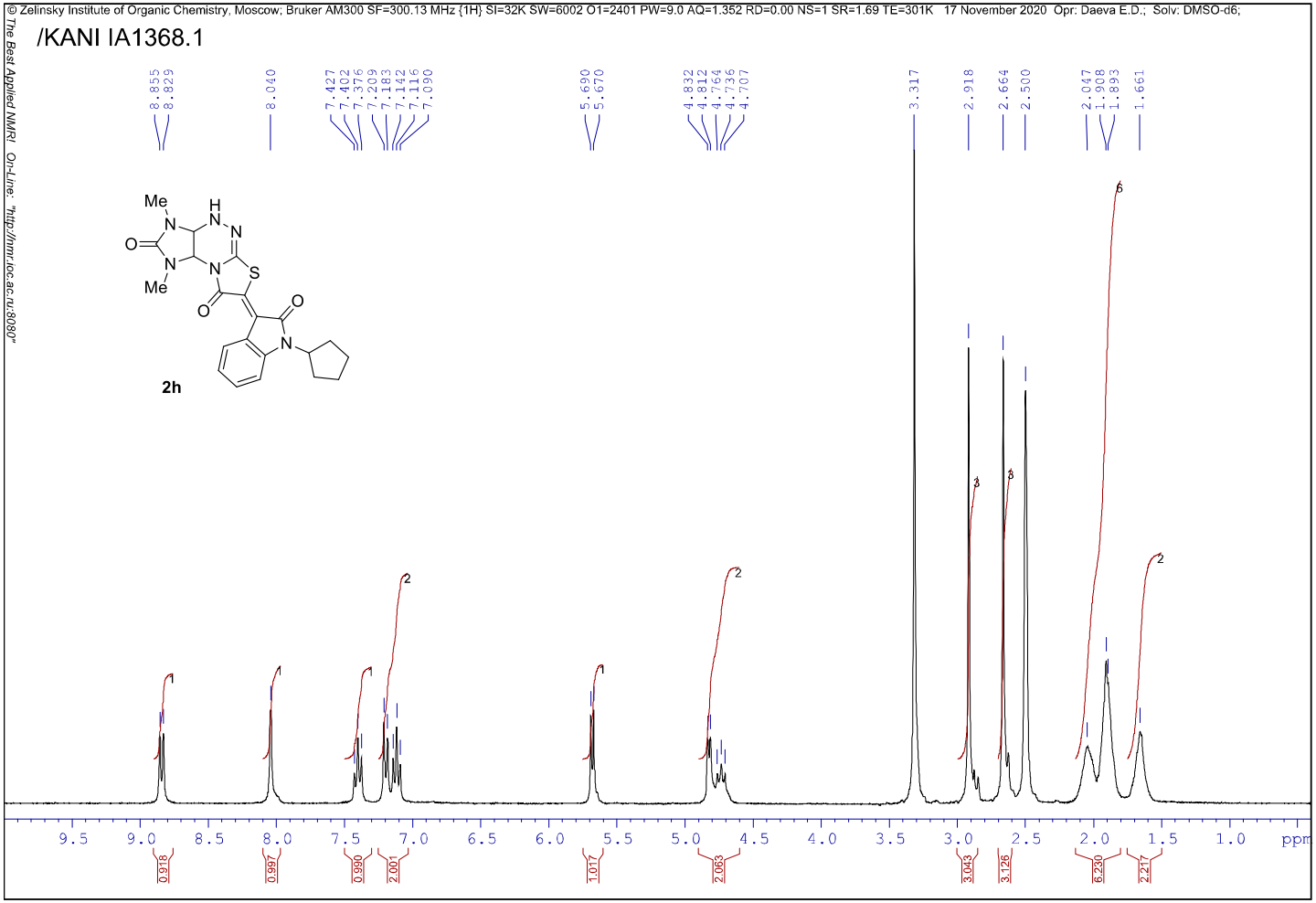
20
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=301K 17 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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5.670
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4.812
4.764
4.736
4.707
3.317
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2.664
2.500
2.047
1.908
1.893
1.661
Me
N
H
N
O
N
N
S
Me
O
O
N
2h
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
4.5
4.0
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1.5
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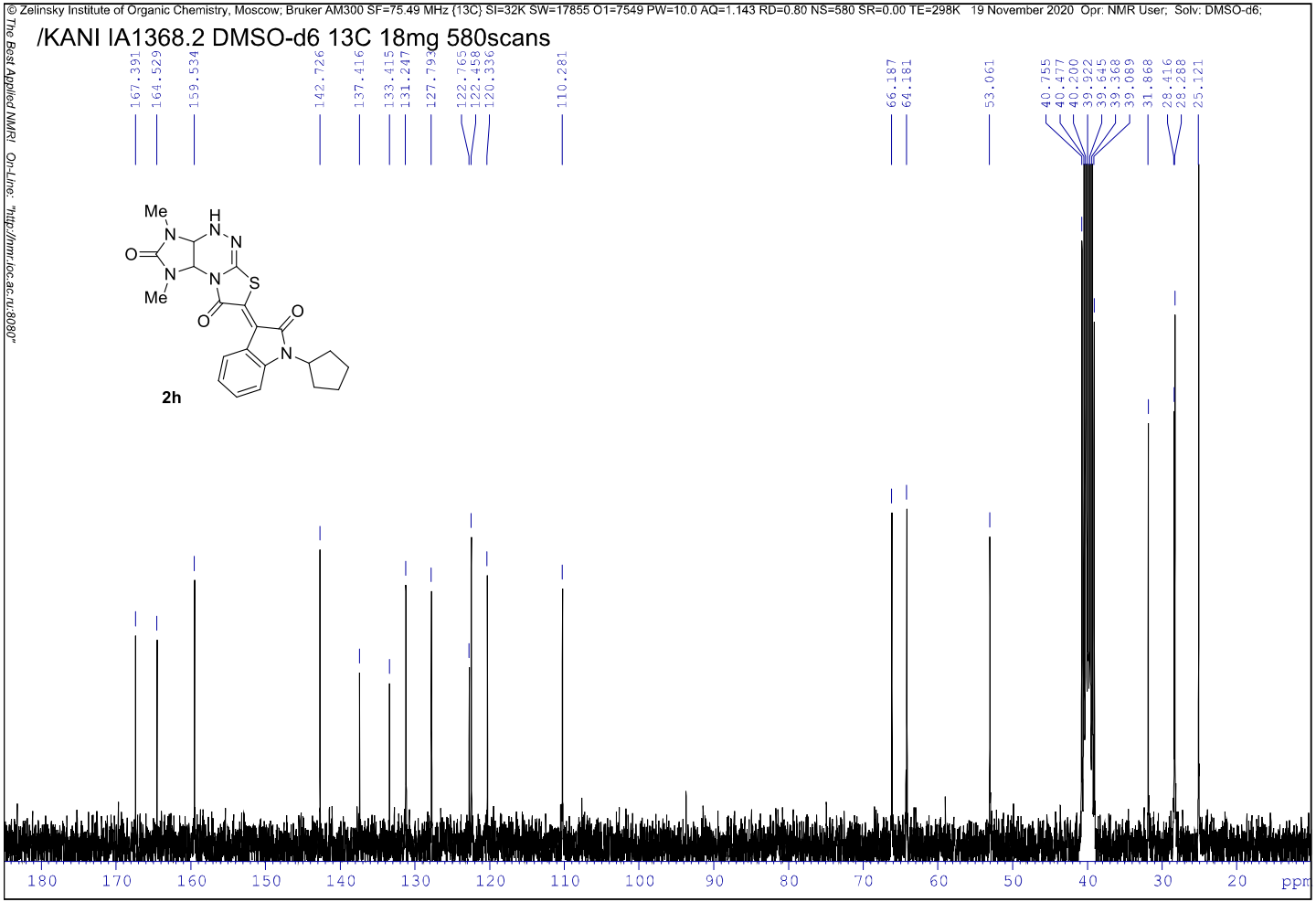
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=580 SR=0.00 TE=298K 19 November 2020 Opr: NMR User; Solv: DMSO-d6;
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133.415
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127.793
122.765
122.458
120.336
110.281
66.187
64.181
53.061
40.755
40.477
40.200
39.922
39.645
39.368
39.089
31.868
28.416
28.288
25.121
Me
H
N
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O
N
N
S
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O
O
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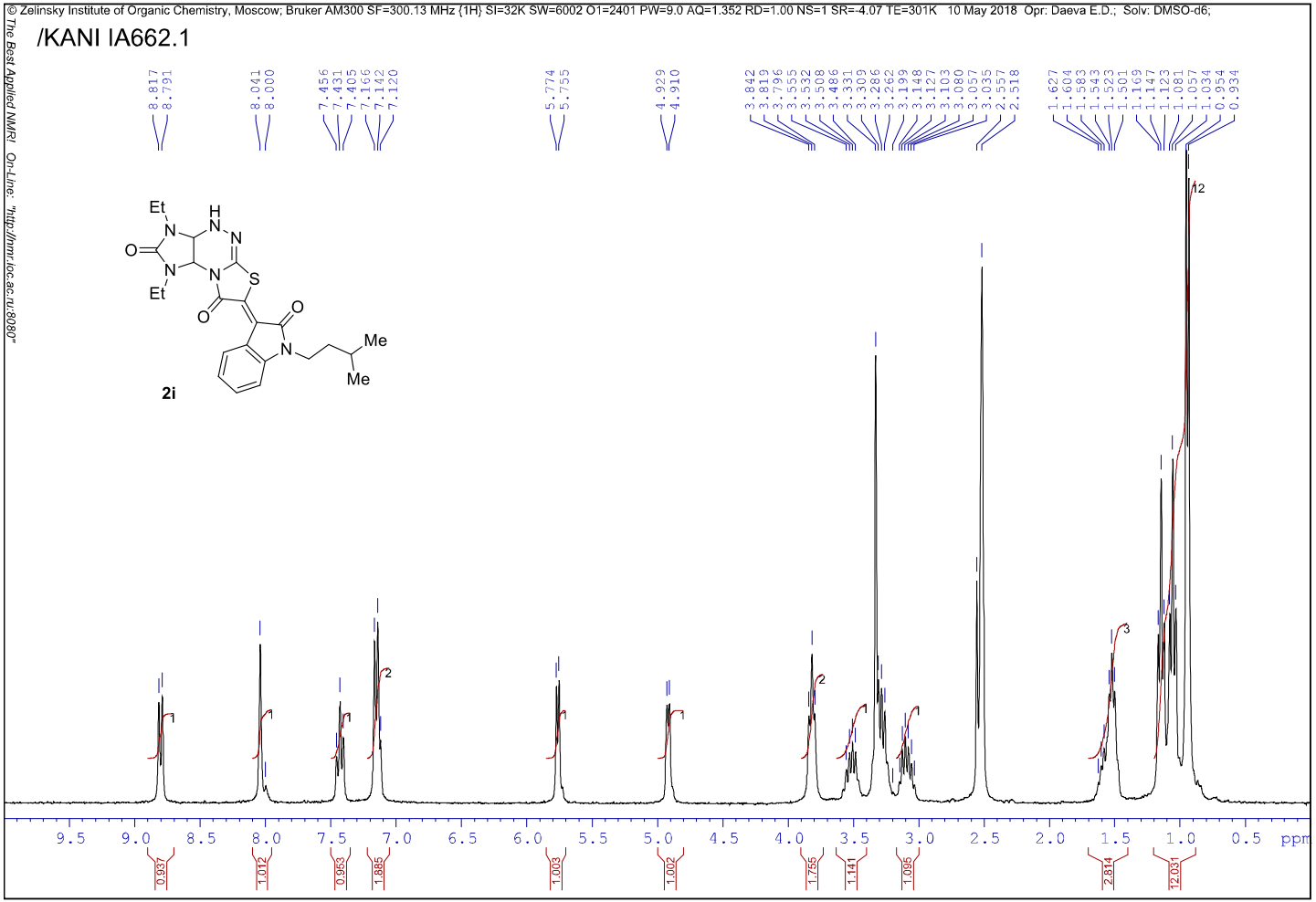
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=1.00 NS=1 SR=-4.07 TE=301K 10 May 2018 Opr: Daeva E.D.; Solv: DMSO-d6;
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3.796
3.555
3.532
3.508
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3.331
3.309
3.286
3.262
3.199
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3.127
3.103
3.080
3.057
3.035
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1.627
1.604
1.583
1.543
1.523
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1.169
1.147
1.123
1.081
1.057
1.034
0.954
0.934
Et
N
H
N
O
N
N
S
Et
O
O
N
Me
Me
2i
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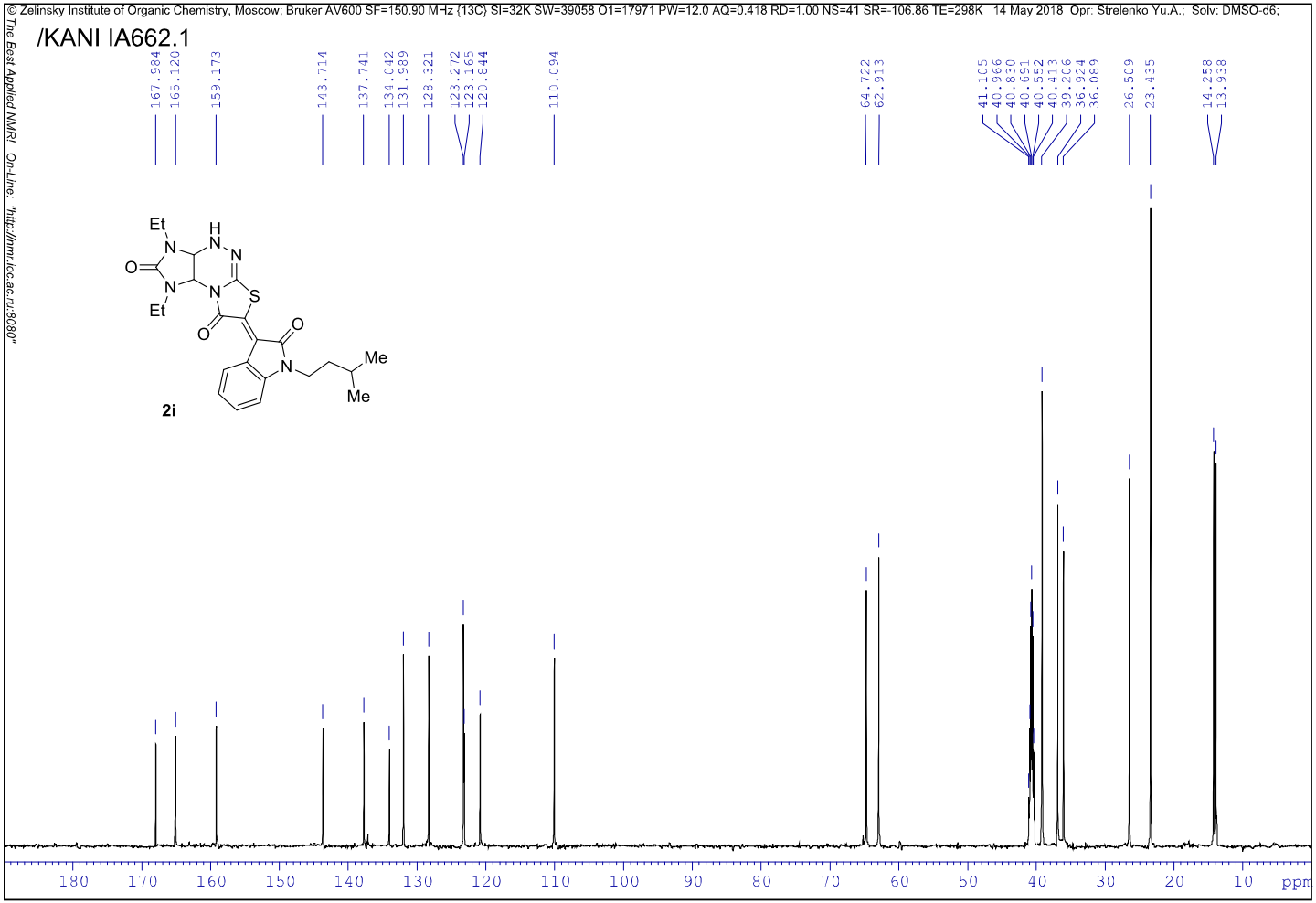
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AV600 SF=150.90 MHz {13C} SI=32K SW=39058 O1=17971 PW=12.0 AQ=0.418 RD=1.00 NS=41 SR=-106.86 TE=298K 14 May 2018 Opr: Strelenko Yu.A.; Solv: DMSO-d6;
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143.714
137.741
134.042
131.989
128.321
123.272
123.165
120.844
110.094
64.722
62.913
41.105
40.966
40.830
40.691
40.552
40.413
39.206
36.924
36.089
26.509
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N
Me
Me
2i
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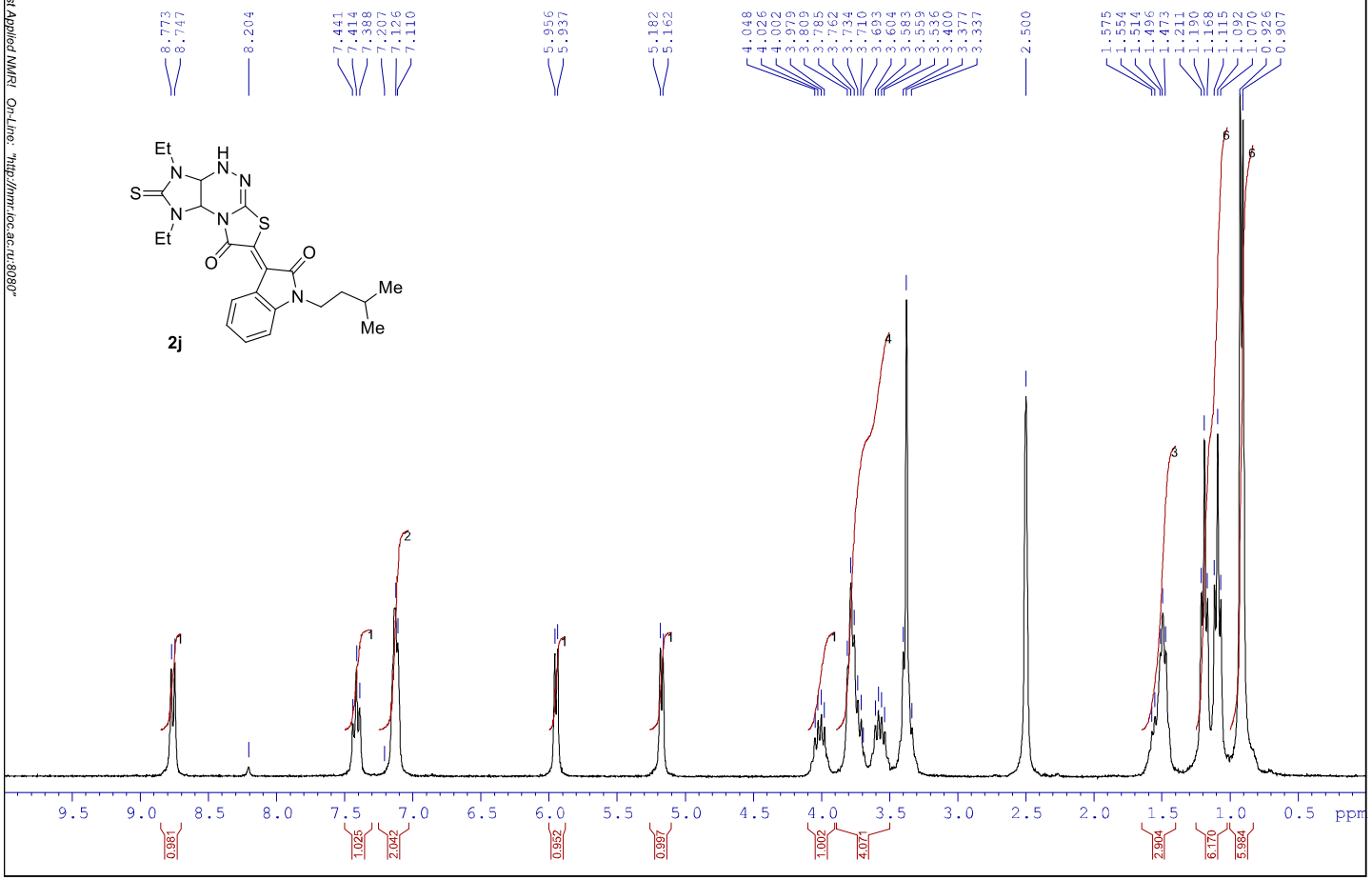

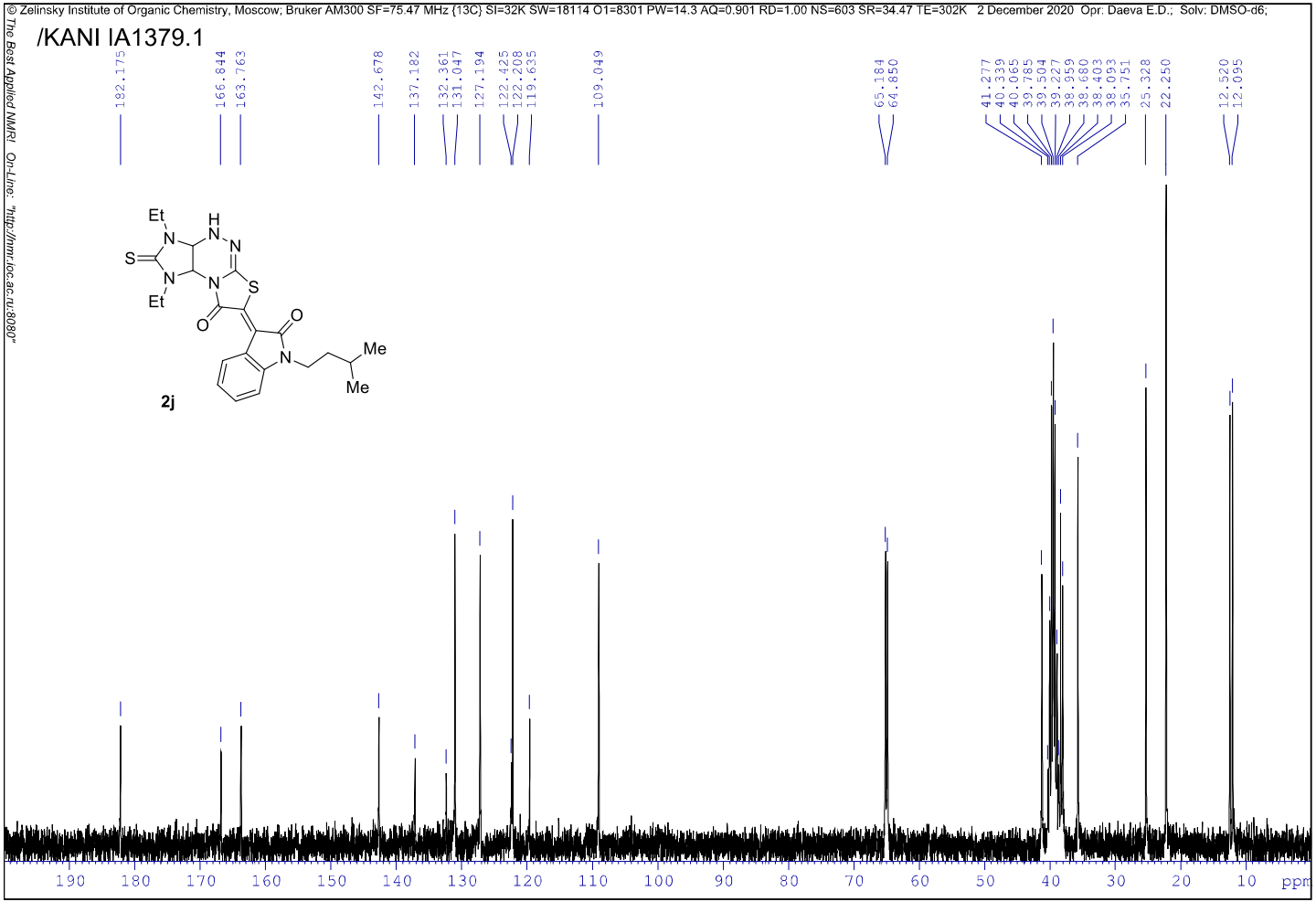
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=603 SR=34.47 TE=302K 2 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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127.194
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109.049
65.184
64.850
41.277
40.339
40.065
39.785
39.504
39.227
38.959
38.680
38.403
38.093
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22.250
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Et
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H
N
N
S
N
S
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Et
O
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N
Me
Me
2j
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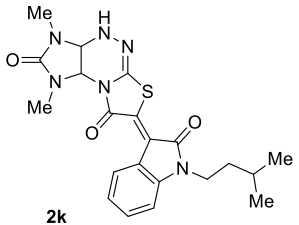

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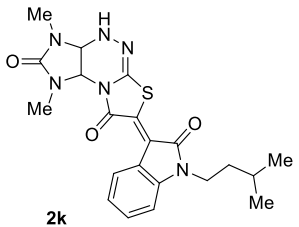

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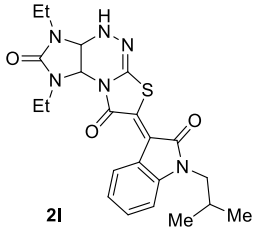

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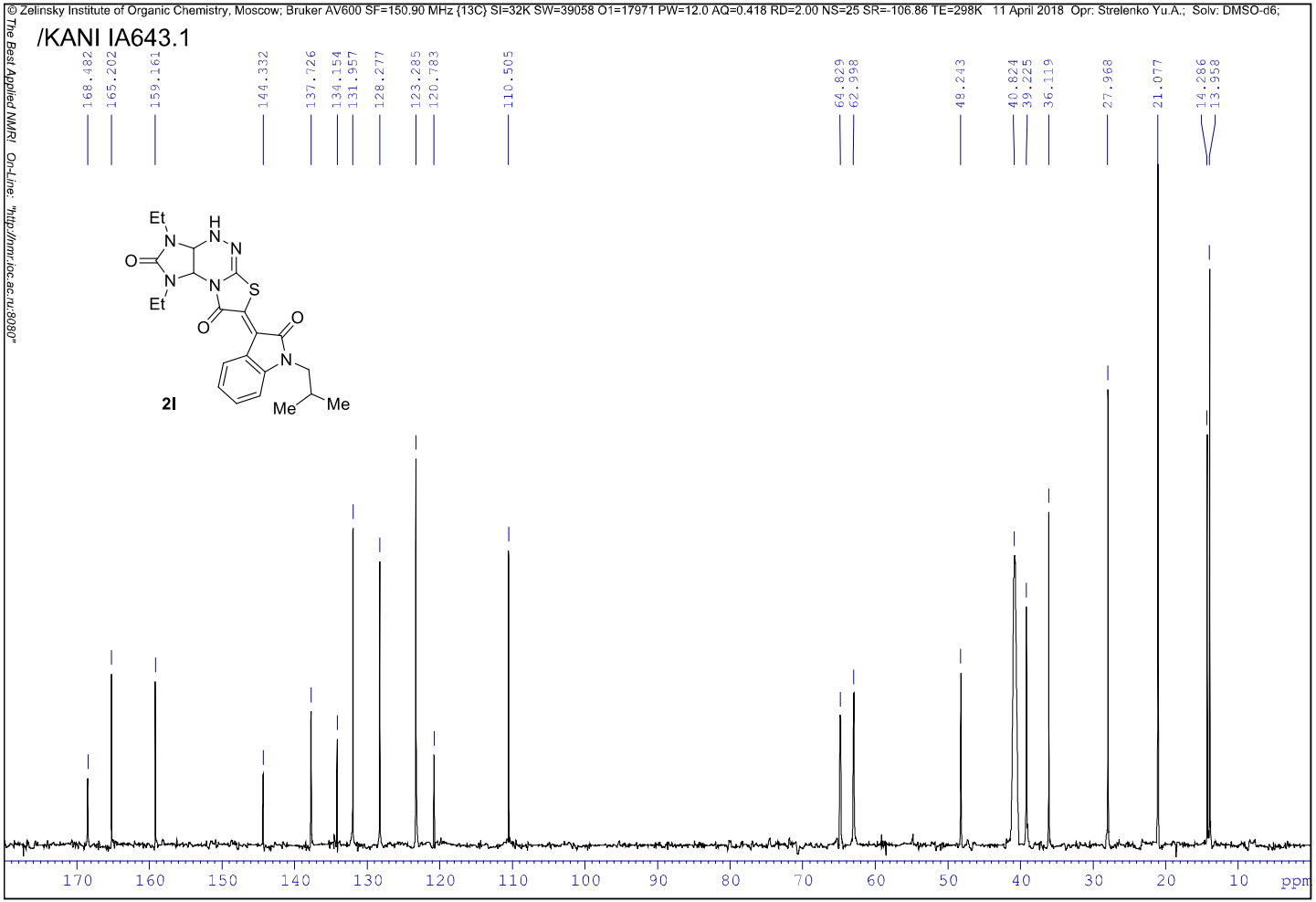
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AV600 SF=150.90 MHz {13C} SI=32K SW=39058 O1=17971 PW=12.0 AQ=0.418 RD=2.00 NS=25 SR=-106.86 TE=298K 11 April 2018 Opr: Strelenko Yu.A.; Solv: DMSO-d6;
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128.277
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120.783
110.505
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62.998
48.243
40.824
39.225
36.119
27.968
21.077
14.286
13.958
Et
N
H
N
N
O
N
S
Et
O
O
N
Me
Me
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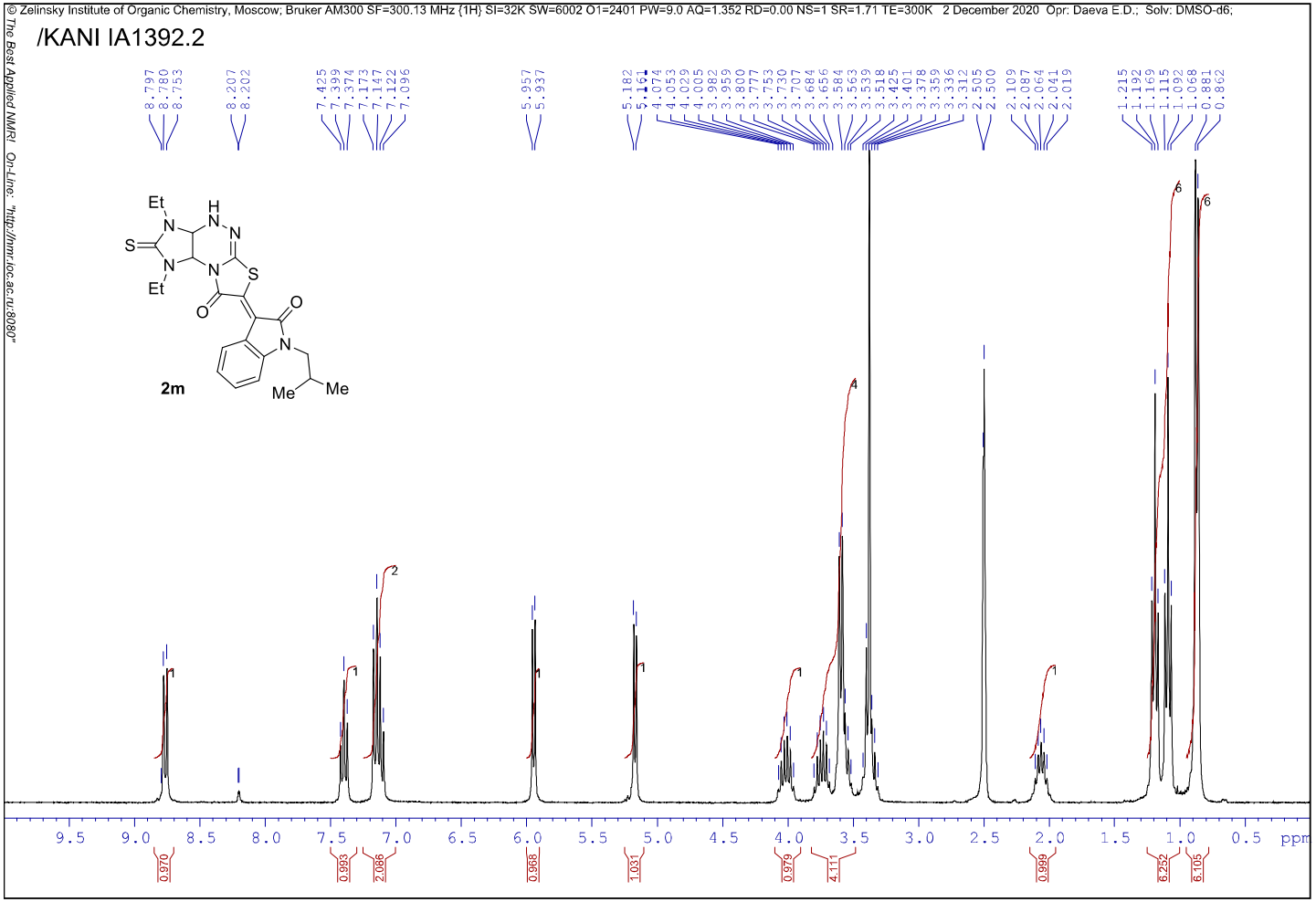
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.71 TE=300K 2 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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2m
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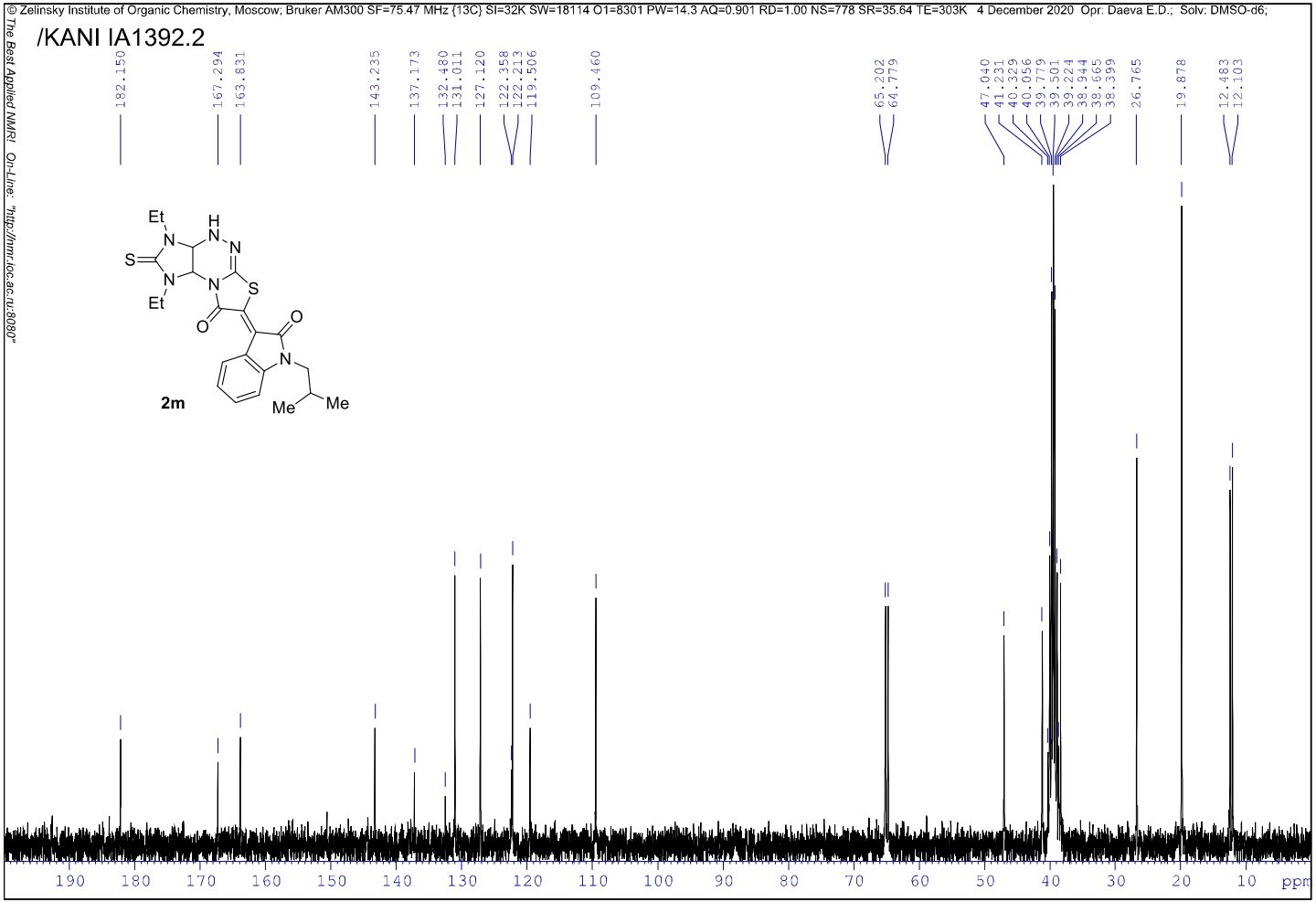
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=778 SR=35.64 TE=303K 4 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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122.213
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109.460
65.202
64.779
47.040
41.231
40.229
40.056
39.779
39.501
39.224
38.944
38.665
38.399
26.765
19.878
12.483
12.103
2m
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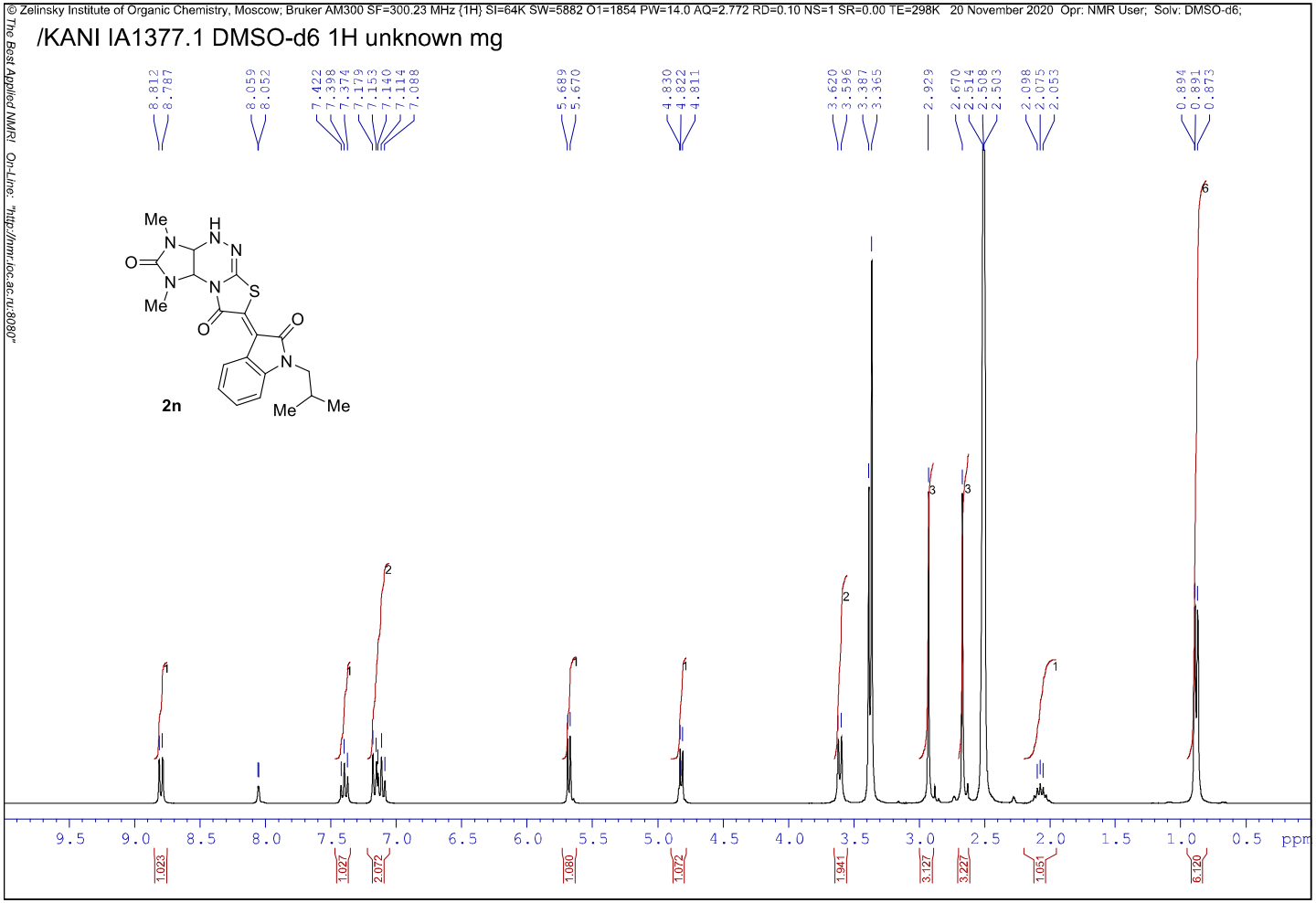
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.23 MHz {1H} SI=64K SW=5882 O1=1854 PW=14.0 AQ=2.772 RD=0.10 NS=1 SR=0.00 TE=298K 20 November 2020 Opr: NMR User; Solv: DMSO-d6;
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8.052
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7.398
7.374
7.179
7.153
7.140
7.114
7.088
5.689
5.670
4.830
4.822
4.811
3.620
3.596
3.387
3.365
2.929
2.670
2.514
2.508
2.503
2.098
2.075
2.053
0.894
0.891
0.873
Me
N
H
N
N
O
N
S
Me
O
O
N
Me
Me
2n
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9.0
8.5
8.0
7.5
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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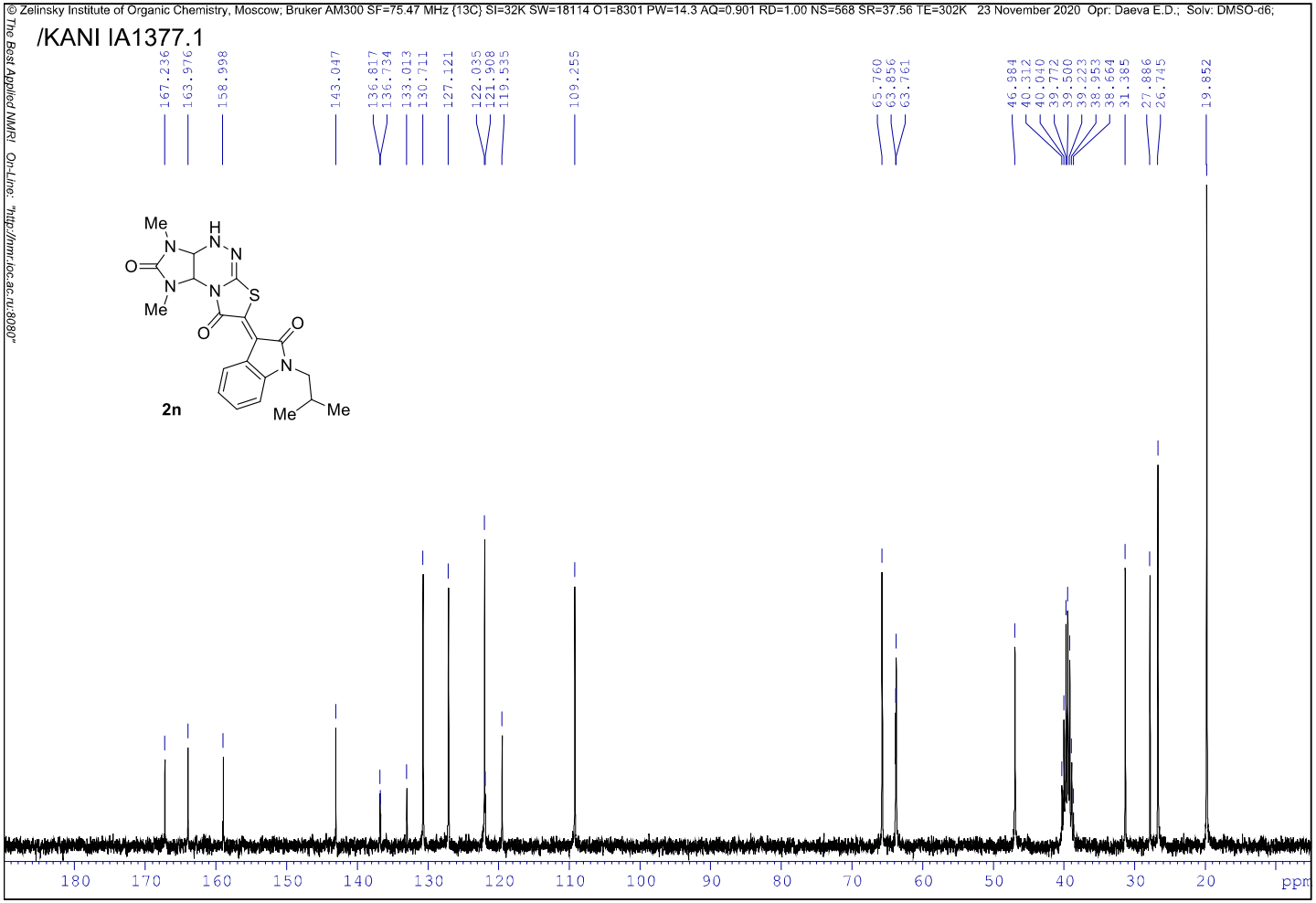
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=568 SR=37.56 TE=302K 23 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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130.711
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122.035
121.908
119.535
109.255
65.760
63.856
63.761
46.984
40.312
40.040
39.772
39.500
39.223
38.953
38.664
31.385
27.886
26.745
19.852
Me
N
H
N
O
N
N
S
Me
O
O
N
2n
Me
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50
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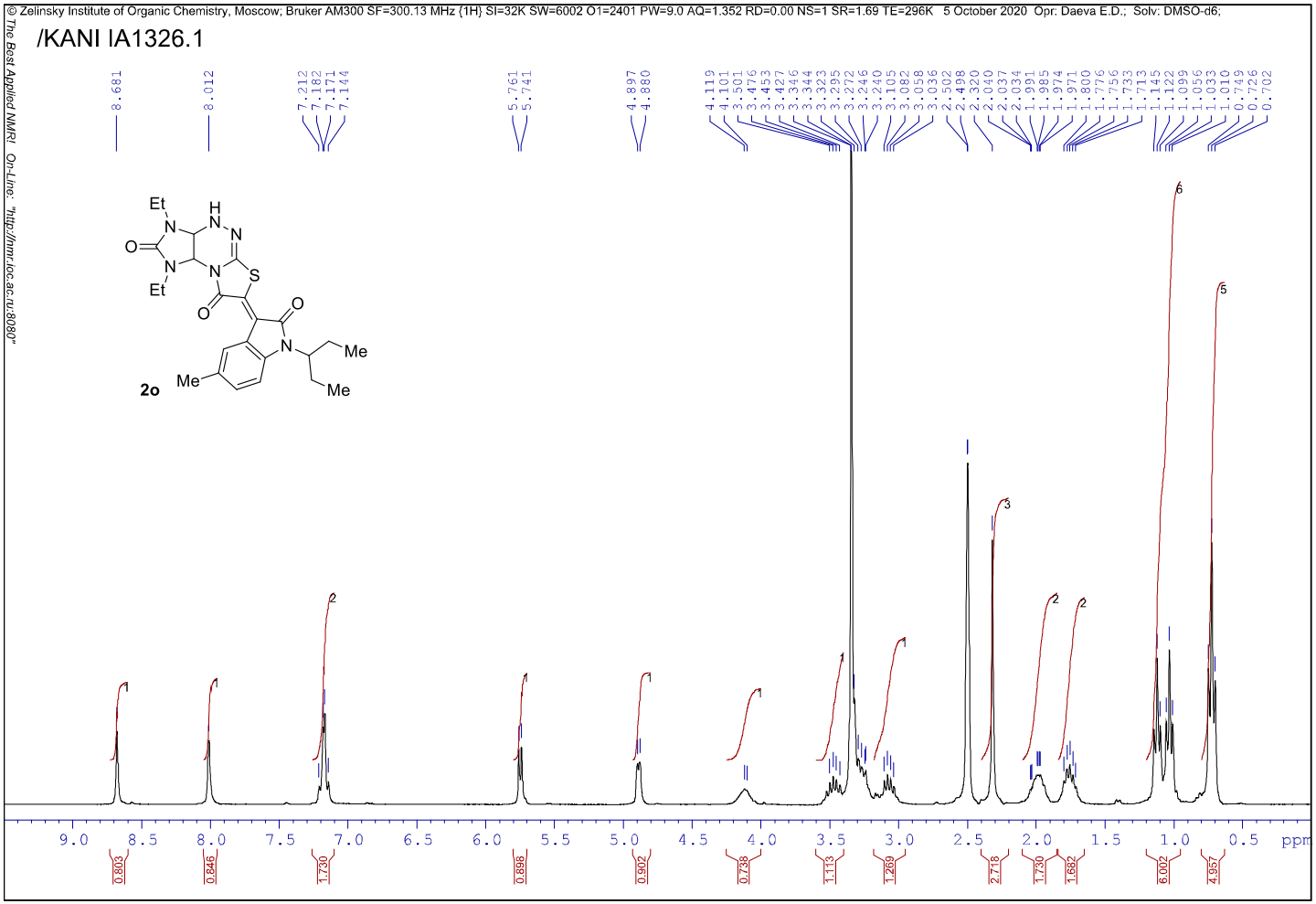
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=296K 5 October 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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7.182
7.171
7.144
5.761
5.741
4.897
4.880
4.119
4.101
3.501
3.476
3.453
3.427
3.344
3.323
3.295
3.272
3.246
3.240
3.105
3.082
3.058
3.036
2.502
2.498
2.320
2.040
2.037
2.034
1.991
1.985
1.974
1.971
1.800
1.776
1.756
1.733
1.713
1.145
1.122
1.099
1.056
1.033
1.010
0.749
0.726
0.702
Et
N
H
N
O
N
N
S
Et
O
O
O
N
Me
Me
Me
2o
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6.5
6.0
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5.0
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4.0
3.5
3.0
2.5
2.0
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1.0
0.5
ppm
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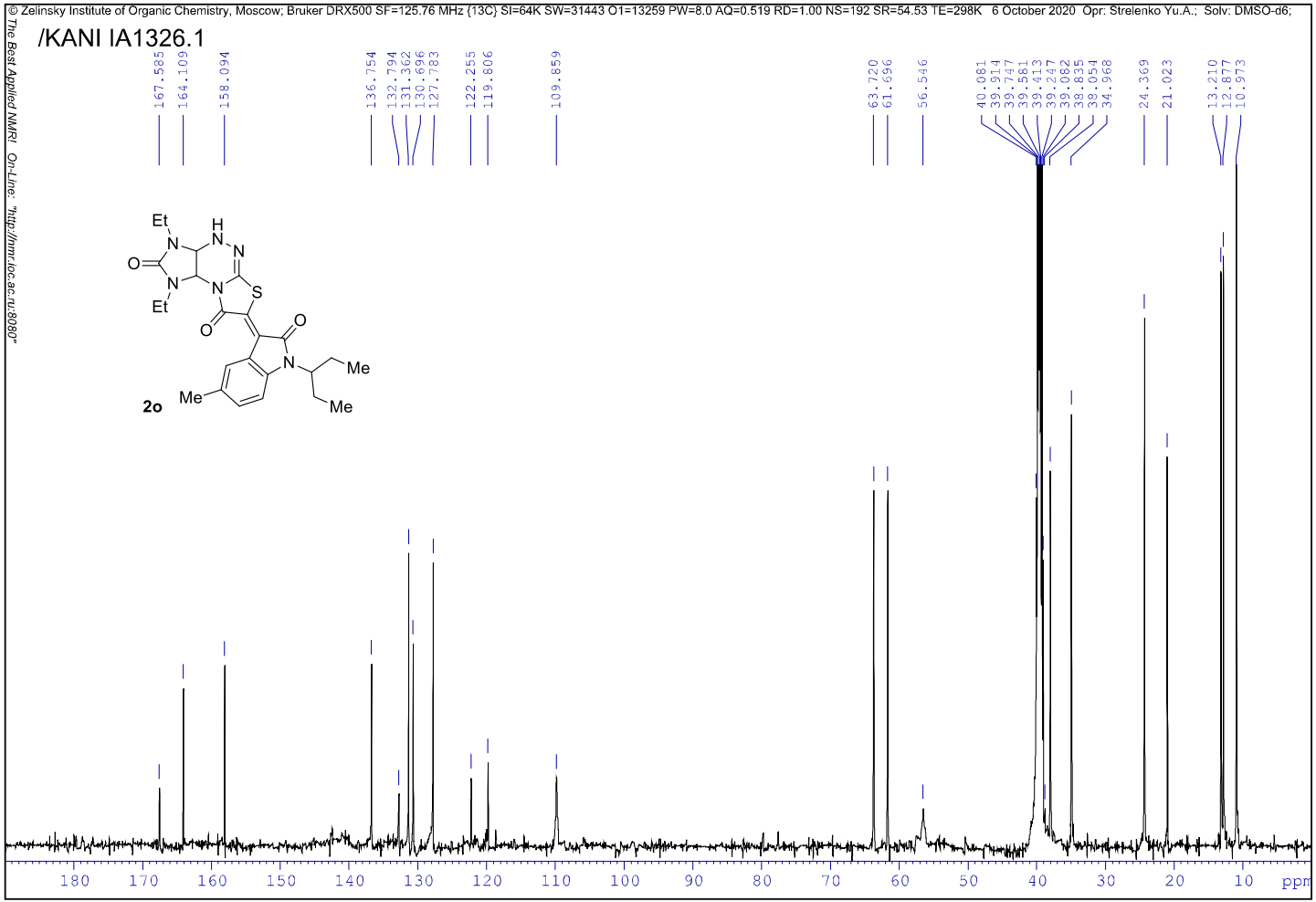
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz {13C} SI=64K SW=31443 O1=13259 PW=8.0 AQ=0.519 RD=1.00 NS=192 SR=54.53 TE=298K 6 October 2020 Opr: Strelenko Yu.A.; Solv: DMSO-d6;
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109.859
63.720
61.696
56.546
40.081
39.914
39.747
39.581
39.413
39.247
39.082
38.835
38.054
34.968
24.369
21.023
13.210
12.877
10.973
Et
N
H
N
N
O
N
S
Et
O
O
N
Me
Me
Me
2o
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170
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ppm

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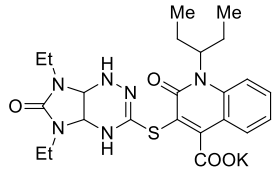

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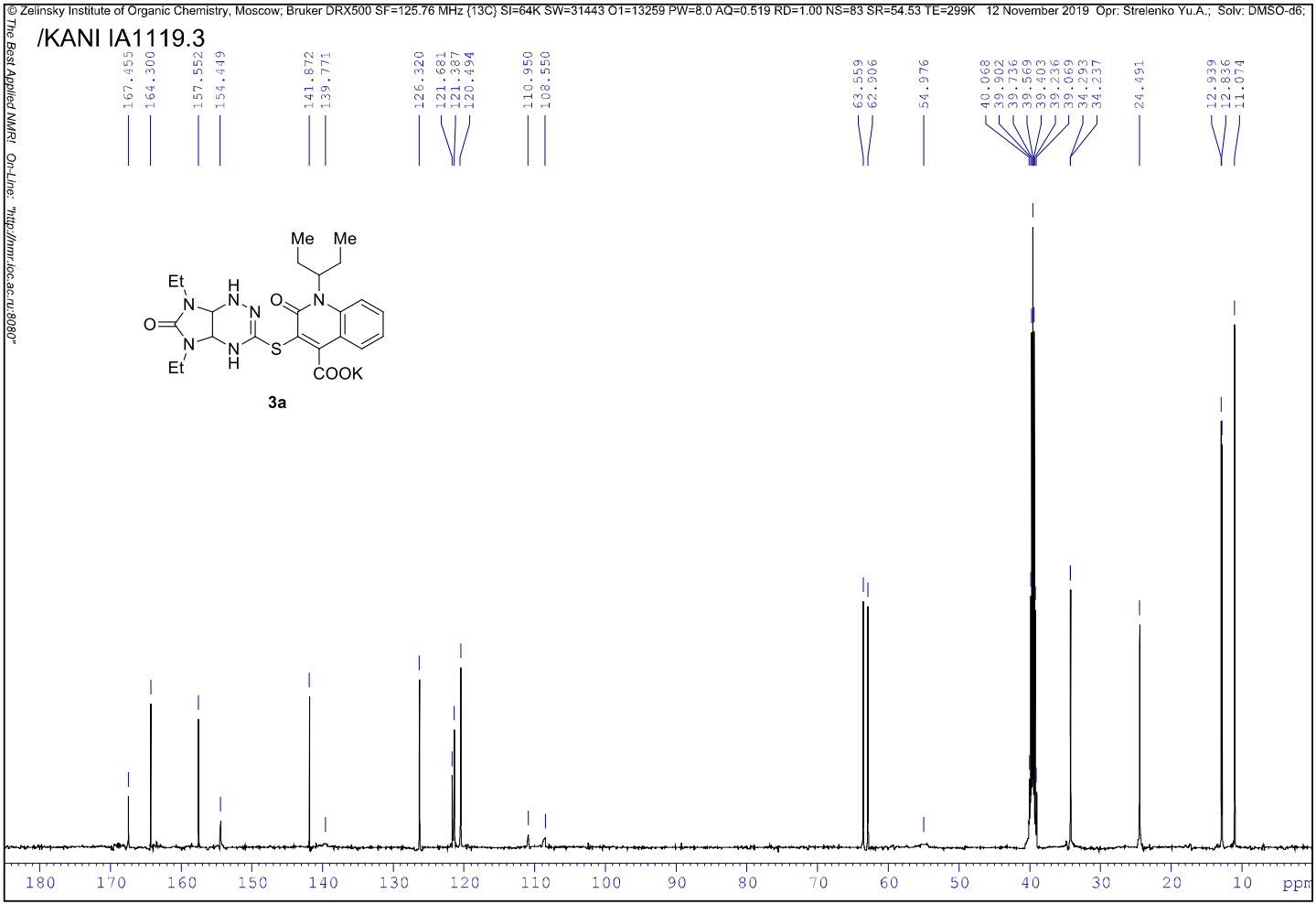
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz {13C} SI=64K SW=31443 O1=13259 PW=8.0 AQ=0.519 RD=1.00 NS=83 SR=54.53 TE=299K 12 November 2019 Opr: Strelenko Yu.A.; Solv: DMSO-d6;
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63.559
62.906
54.976
40.068
39.902
39.736
39.569
39.403
39.236
39.069
34.293
34.237
24.491
12.939
12.836
11.074
Me
Me
Et
Et
COOK
3a
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110
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70
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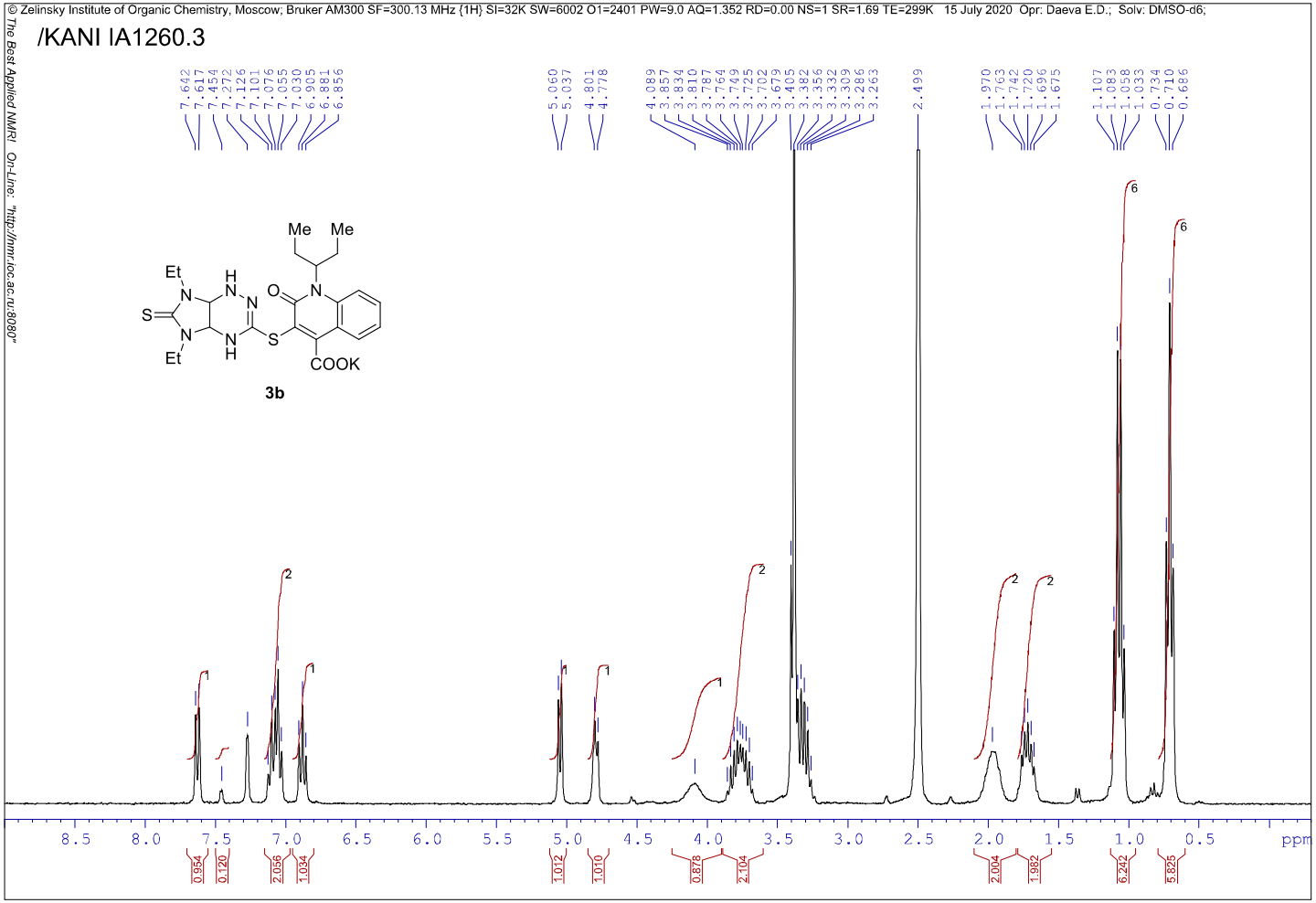
50
40
30
20
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=299K 15 July 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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5.060
5.037
4.801
4.778
4.089
3.857
3.834
3.810
3.787
3.764
3.749
3.725
3.702
3.679
3.405
3.382
3.356
3.332
3.309
3.286
3.263
2.499
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1.763
1.742
1.720
1.696
1.675
1.107
1.083
1.058
1.033
0.734
0.710
0.686
Me
Me
Et
Et
S
O
COOK
3b
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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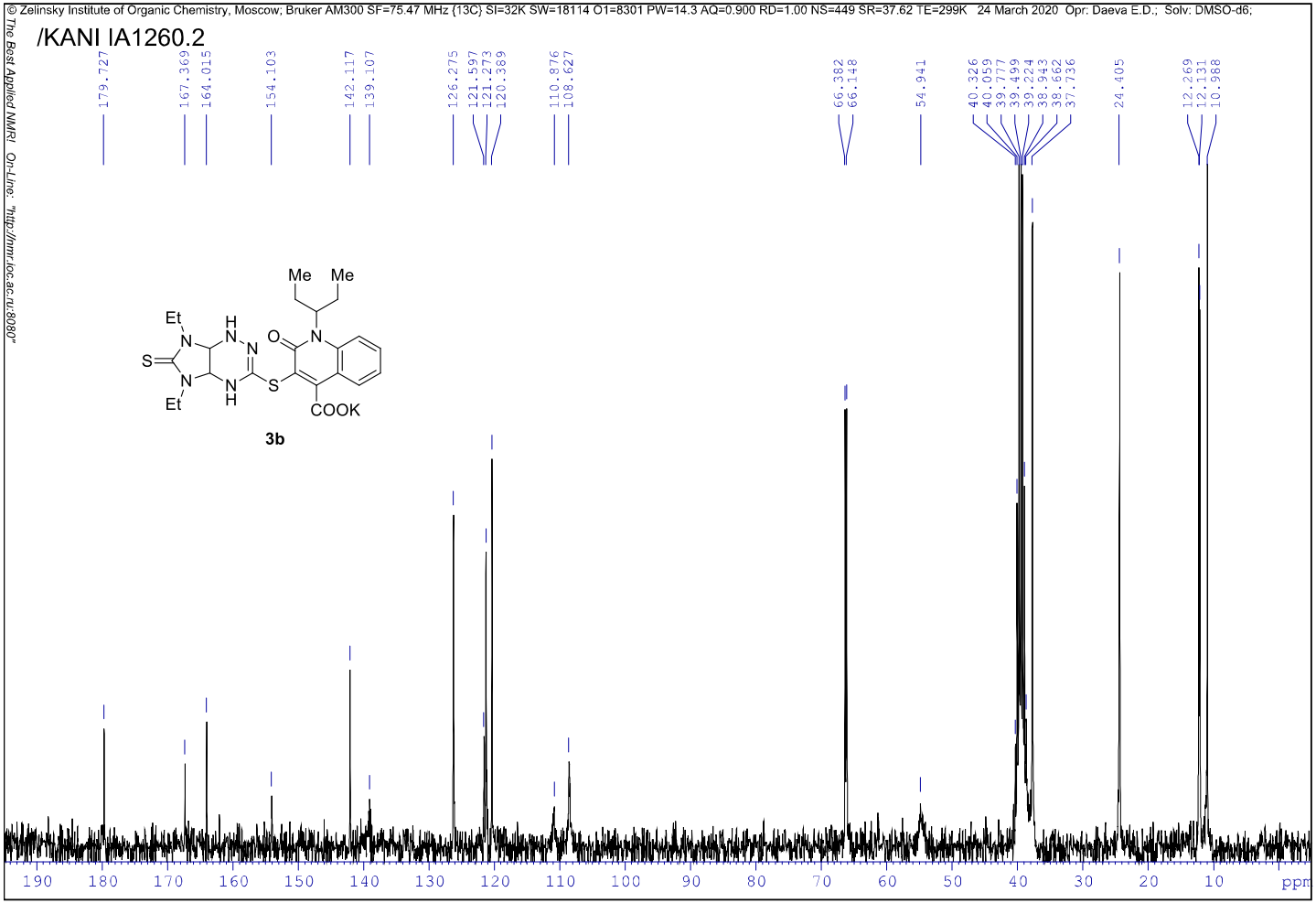
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=449 SR=37.62 TE=299K 24 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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66.382
66.148
54.941
40.326
40.059
39.777
39.499
39.224
38.943
38.662
37.736
24.405
12.269
12.131
10.988
Me
Me
Et
Et
H
N
N
N
N
N
O
S
S
H
COOK
3b
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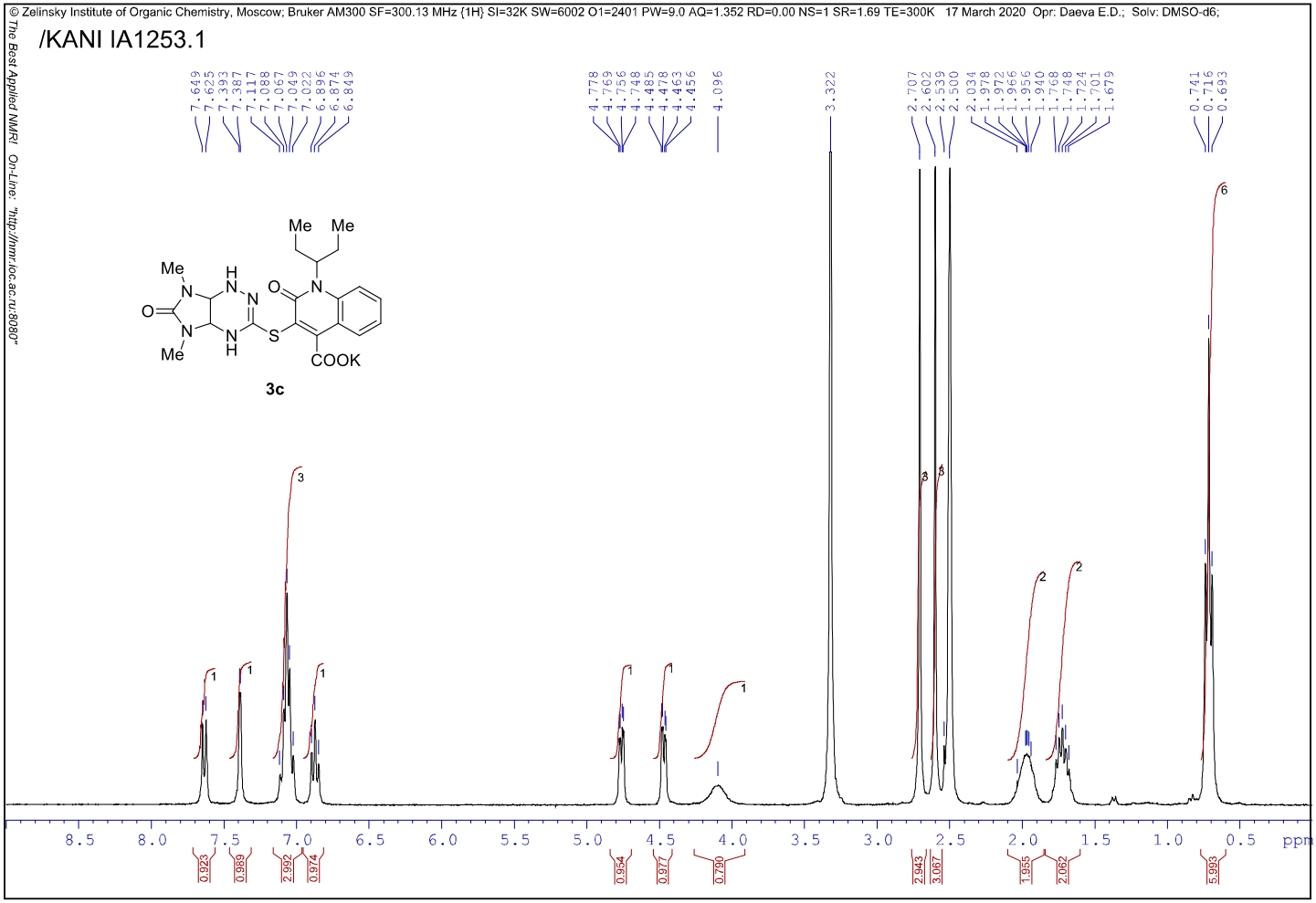
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=300K 17 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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Me
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N
H
S
COOK
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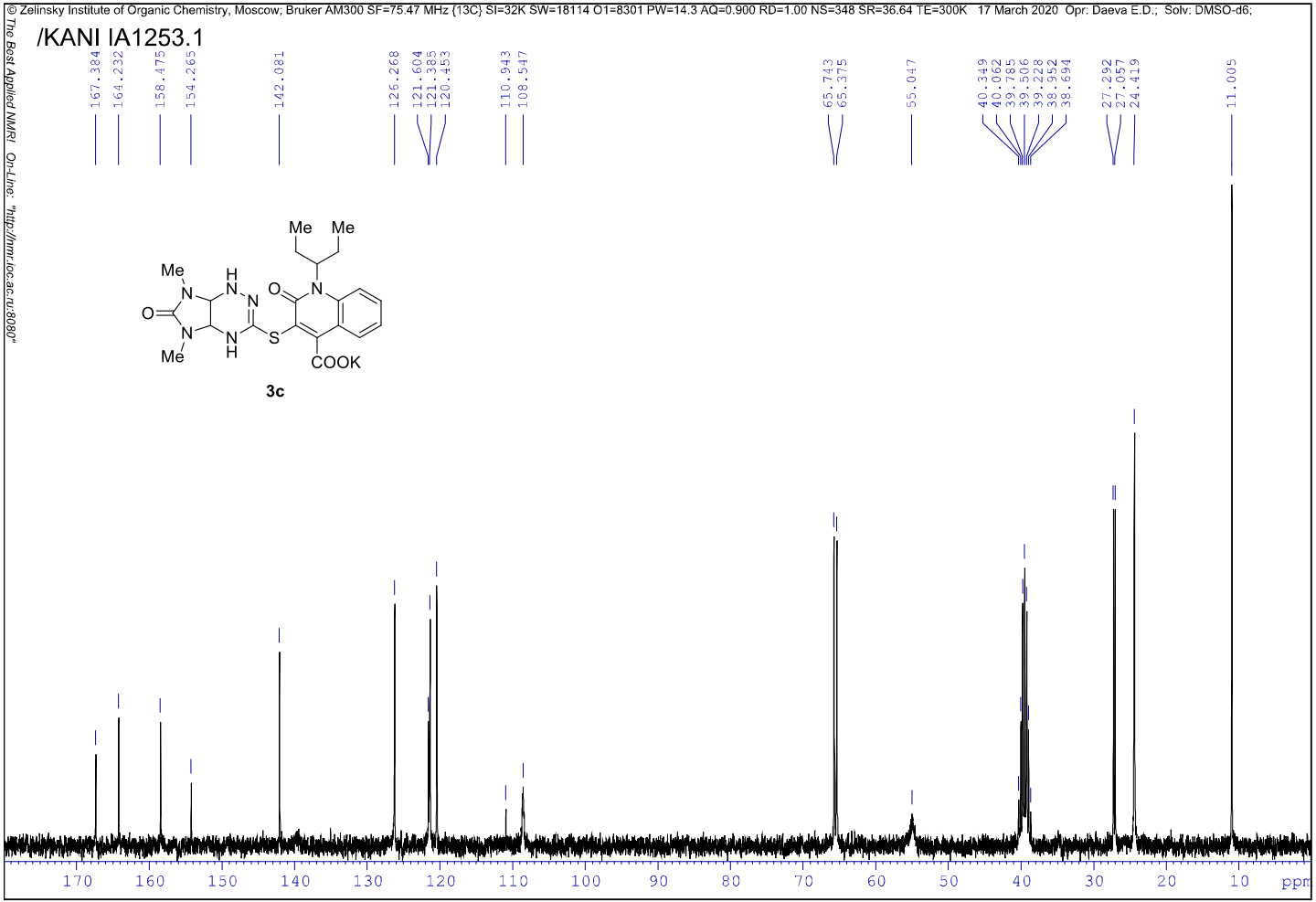
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=348 SR=36.64 TE=300K 17 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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65.743
65.375
55.047
40.349
40.062
39.785
39.506
39.228
38.952
38.694
27.292
27.057
24.419
11.005
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Me
Me
Me
N
H
N
N
H
N
O
O
N
S
COOK
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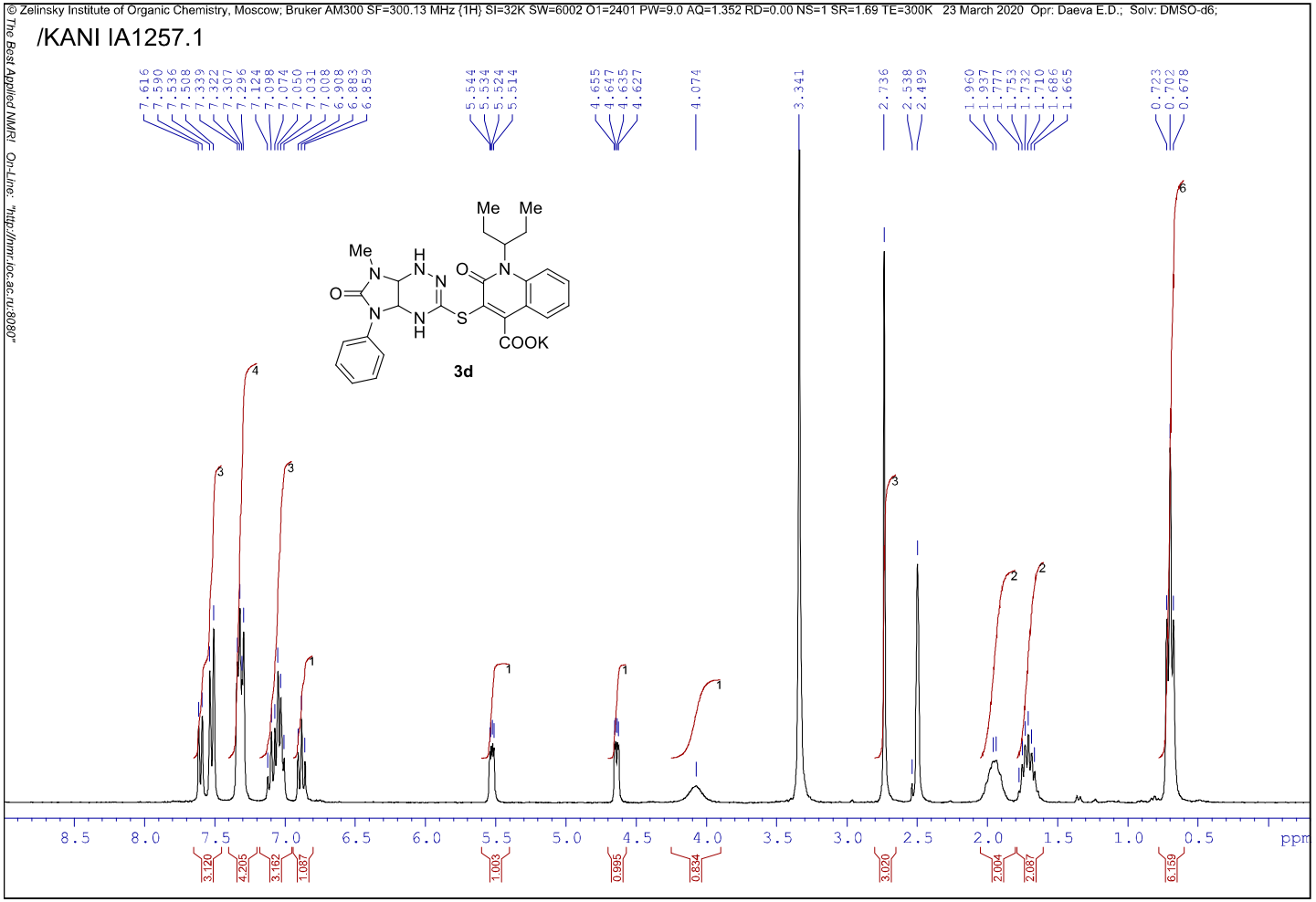
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=300K 23 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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1.665
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0.702
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O
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N
H
S
COOK
3d
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0.5
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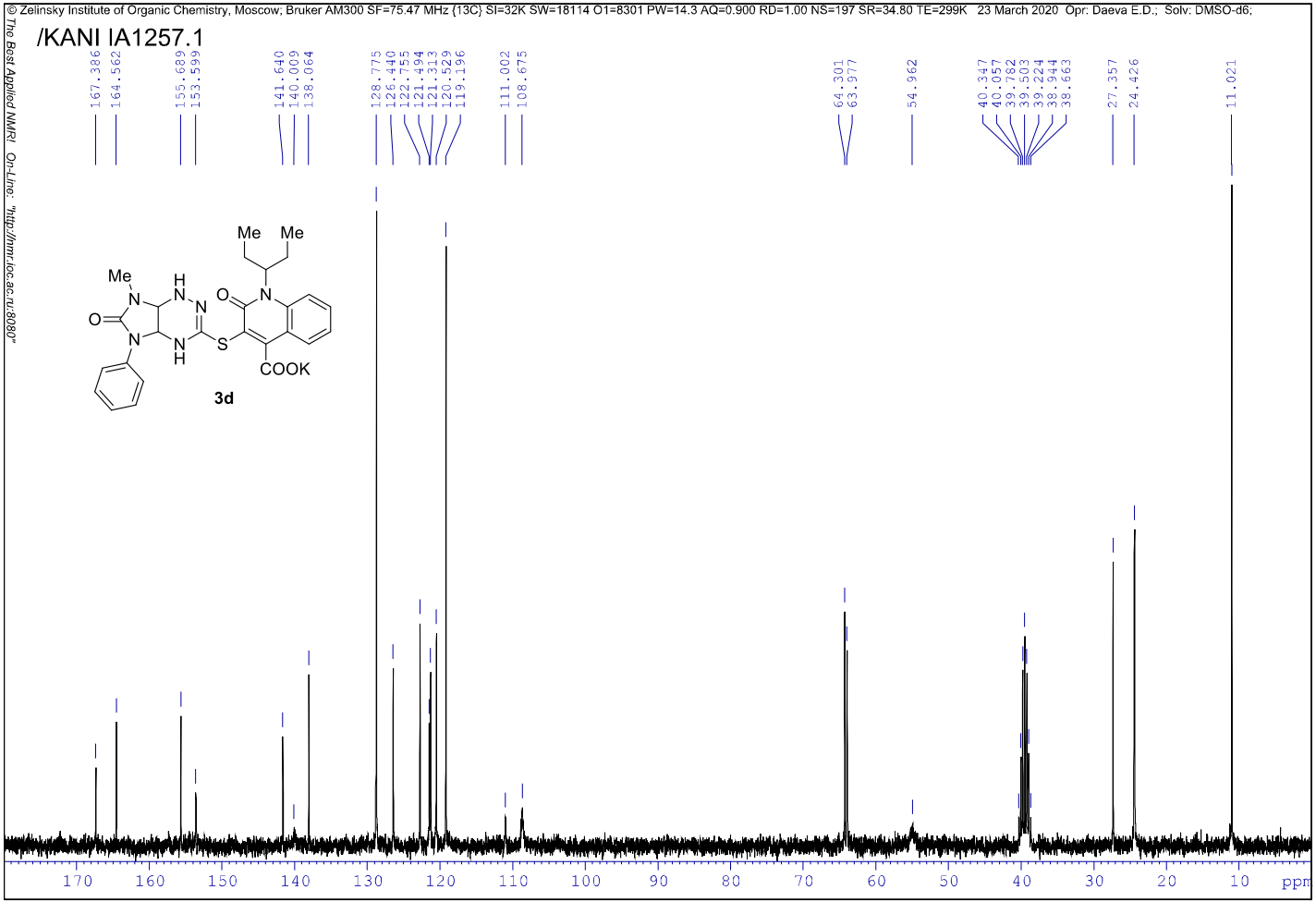
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.900 RD=1.00 NS=197 SR=34.80 TE=299K 23 March 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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120.529
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111.002
108.675
64.301
63.977
54.962
40.347
40.057
39.782
39.503
39.224
38.944
38.663
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Me
N
H
N
N
O
N
O
N
N
H
S
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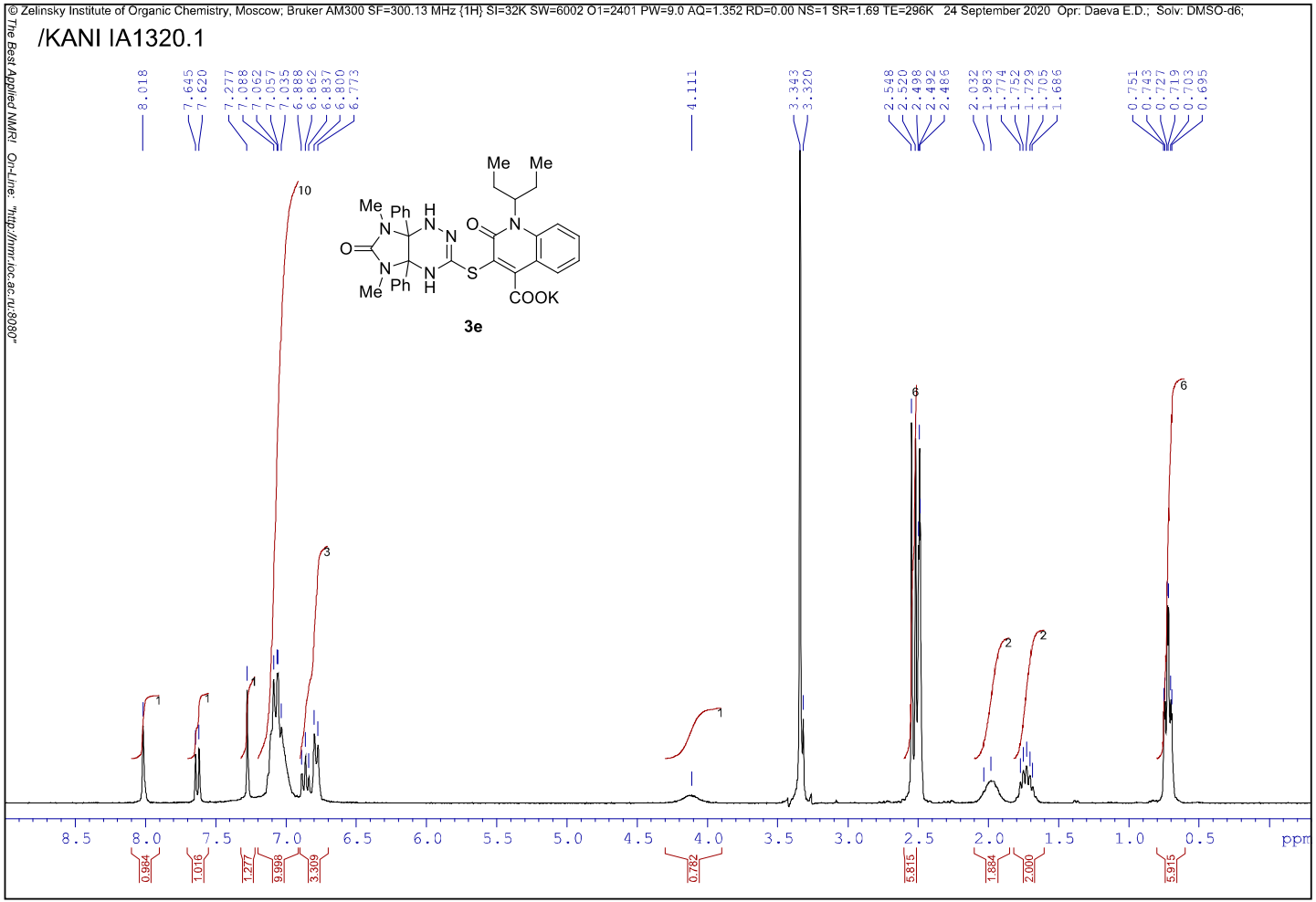
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=296K 24 September 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR!. On-Line: "http://nmr.ioc.ac.ru:8080/"
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1.705
1.686
0.751
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0.727
0.719
0.703
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Ph
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N
O
N
N
S
Me
Ph
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N
O
COOK
3e
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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9.996
3.309
0.782
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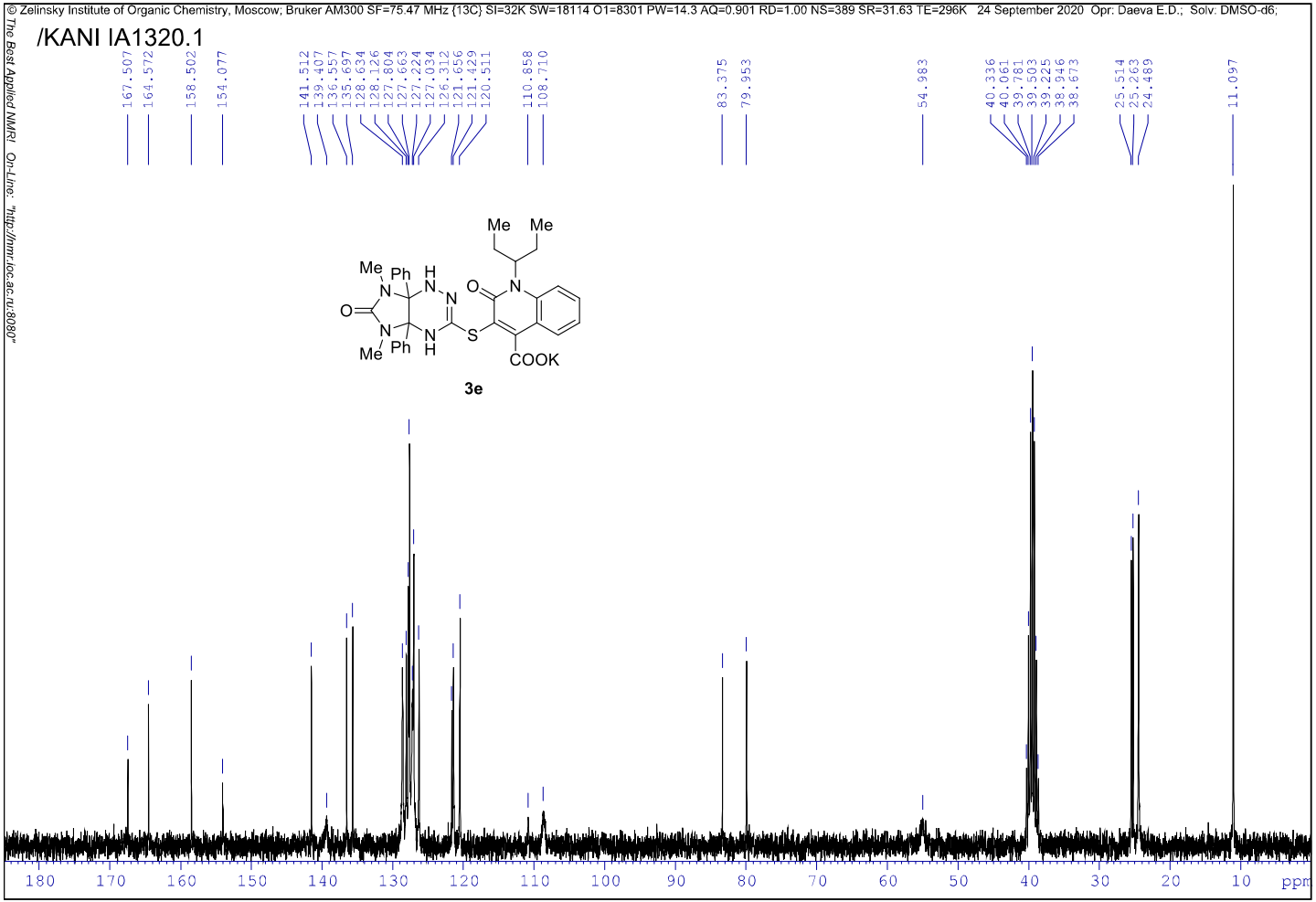
2.000
5.915


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=389 SR=31.63 TE=296K 24 September 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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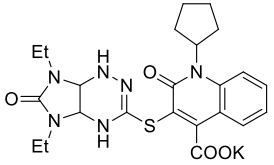
158.502
154.077
141.512
139.407
136.557
135.697
128.634
128.126
127.804
127.663
127.224
127.034
126.312
121.656
121.429
120.511
110.858
108.710
83.375
79.953
54.983
40.336
40.061
39.781
39.503
39.225
38.946
38.673
25.514
25.263
24.489
11.097
Me
Me
Ph
Ph
H
H
N
N
N
N
N
N
O
O
S
COOK
Me
Me
3e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

/KANI IA1301_1



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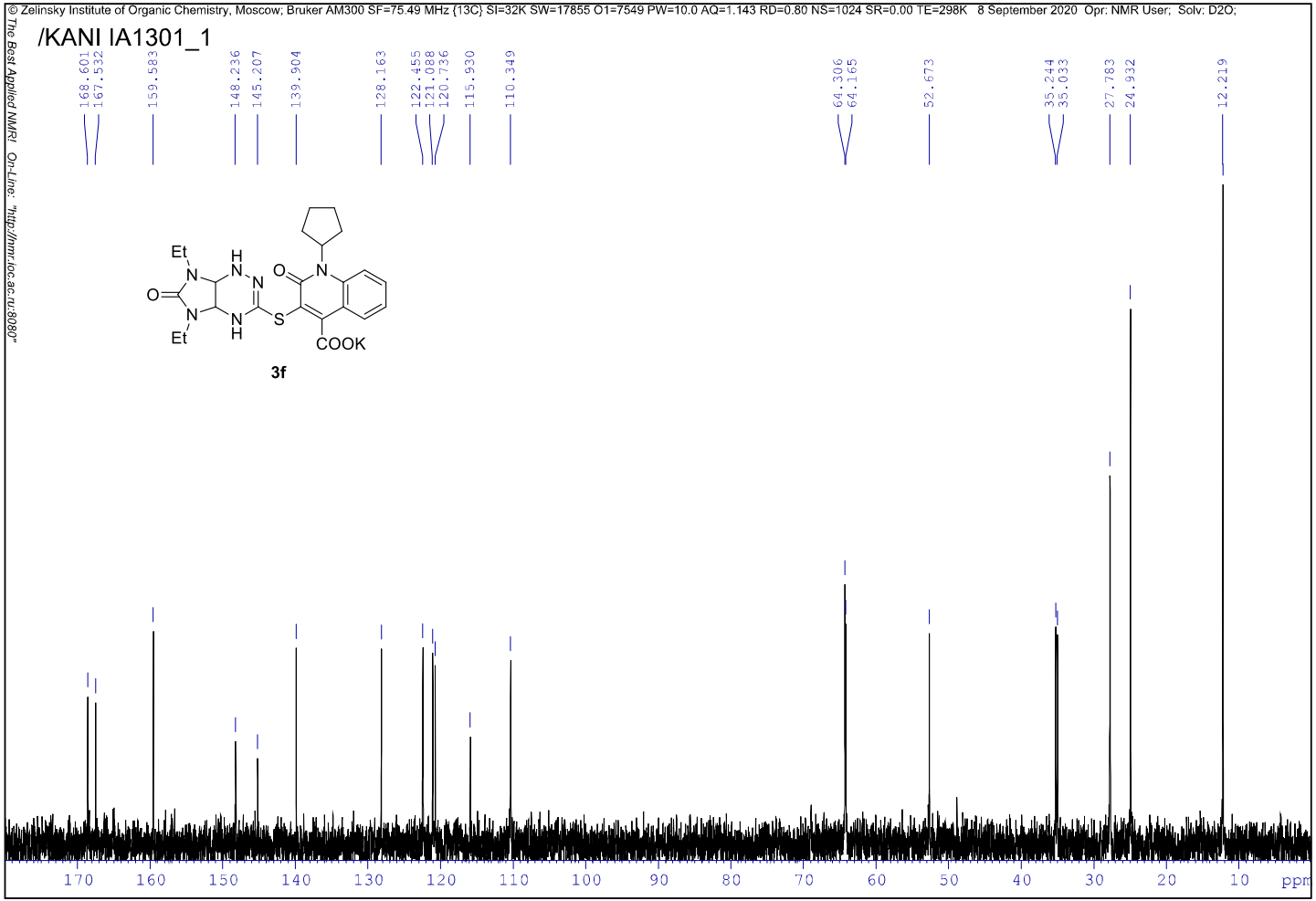
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=1024 SR=0.00 TE=298K 8 September 2020 Opr: NMR User; Solv: D2O;
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159.583
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145.207
139.904
128.163
122.455
121.088
120.736
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110.349
64.306
64.165
52.673
35.244
35.033
27.783
24.932
12.219
Et
N
H
N
N
O
N
S
O
N
N
H
Et
COOK
3f
170
160
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120
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100
90
80
70
60
50
40
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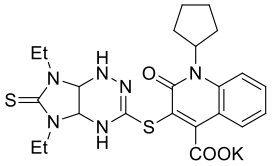
20
10
ppm

/KANI IA1313.2



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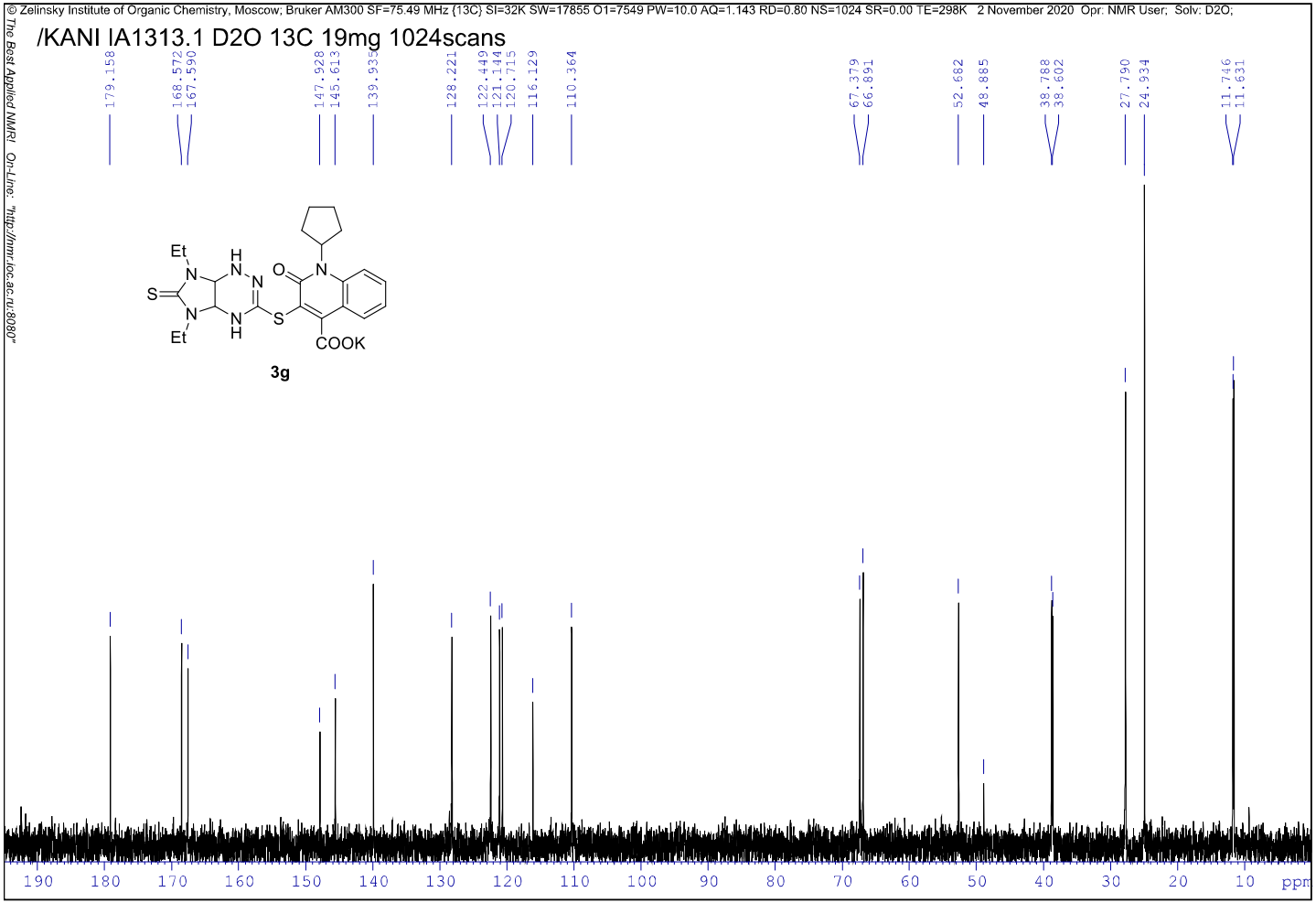
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=1024 SR=0.00 TE=298K 2 November 2020 Opr: NMR User; Solv: D2O;
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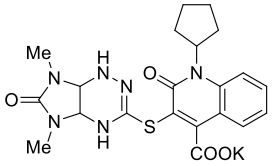
167.590
147.928
145.613
139.935
128.221
122.449
121.144
120.715
116.129
110.364
67.379
66.891
52.682
48.885
38.788
38.602
27.790
24.934
11.746
11.631
Et
N
H
N
N
O
N
S
N
N
H
S
Et
COOK
3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

/KANI IA1296_1



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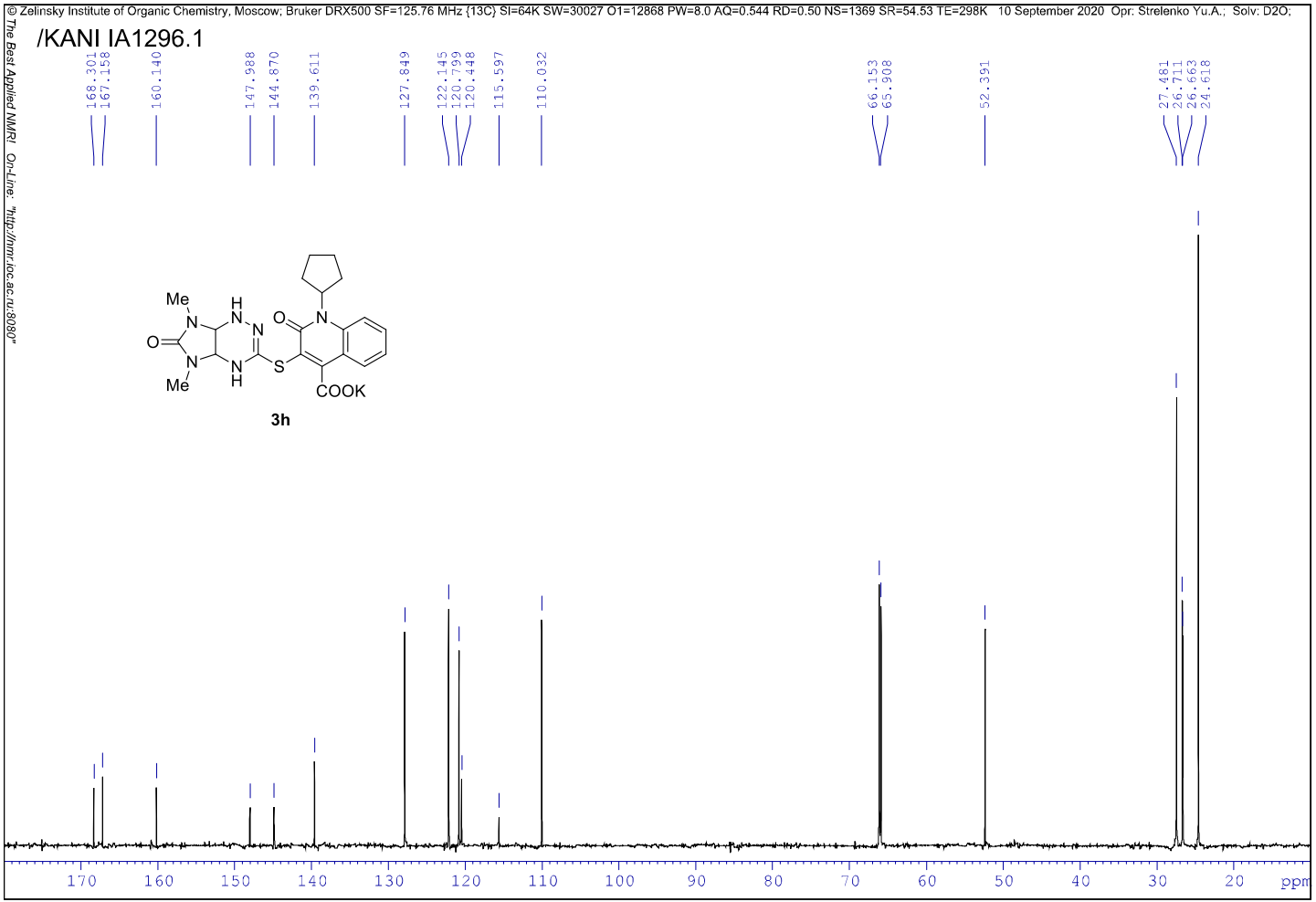
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz {13C} SI=64K SW=30027 O1=12868 PW=8.0 AQ=0.544 RD=0.50 NS=1369 SR=54.53 TE=298K 10 September 2020 Opr: Strelenko Yu.A.; Solv: D2O;
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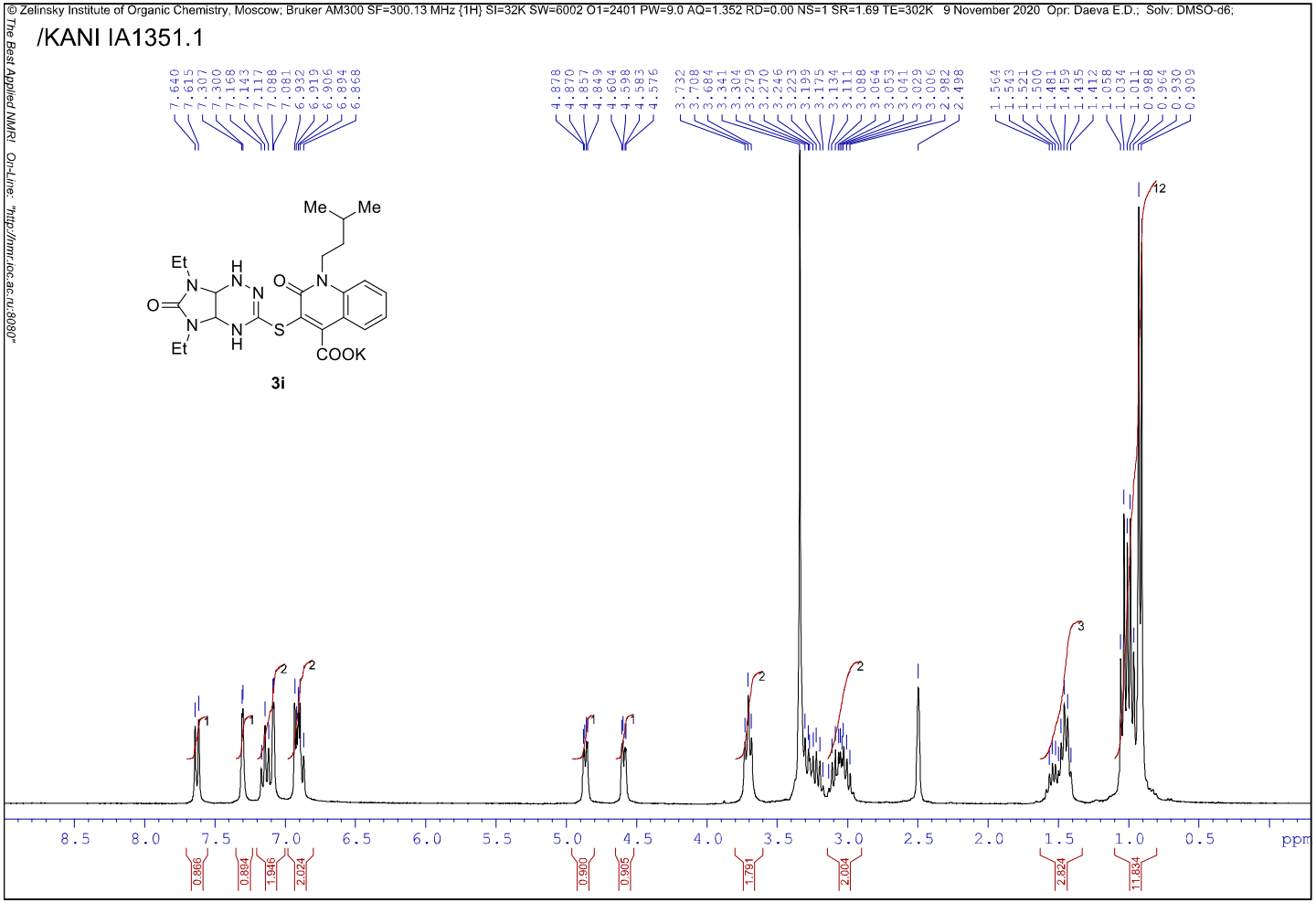
144.870
139.611
127.849
122.145
120.799
120.448
115.597
110.032
66.153
65.908
52.391
27.481
26.711
26.463
24.618
Me
N
H
N
N
O
N
O
N
S
N
H
Me
COOK
3h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=302K 9 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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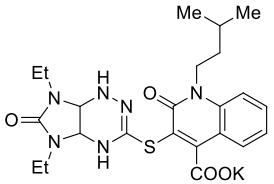
4.878 4.870 4.857 4.849 4.604 4.598 4.583 4.576
3.732 3.708 3.684 3.341 3.304 3.279 3.270 3.246 3.223 3.199 3.175 3.134 3.111 3.088 3.064 3.053 3.041 3.029 3.006 2.982 2.498
1.564 1.543 1.521 1.500 1.481 1.459 1.435 1.412 1.058 1.034 1.011 0.988 0.964 0.930 0.909
Me Me
Et
N
H
N
N
O
O
N
N
H
S
Et
COOK
3i
12
3
2
2
2
1
1
1
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.866 0.894 1.946 2.024 0.900 0.905 1.791 2.004 2.824 11.834

/KANI IA1358.2 DMSO-d6 13C 24mg 512scans

167.113 164.542 157.981 154.842 141.977 140.270 126.933 122.095 121.749 121.282 111.495 108.016 64.118 62.963 40.753 40.475 40.198 39.920 39.642 39.365 39.087 37.563 36.585 34.749 25.779 22.849 13.284



3i

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

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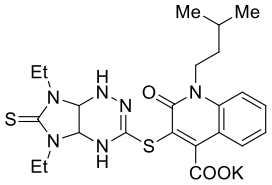
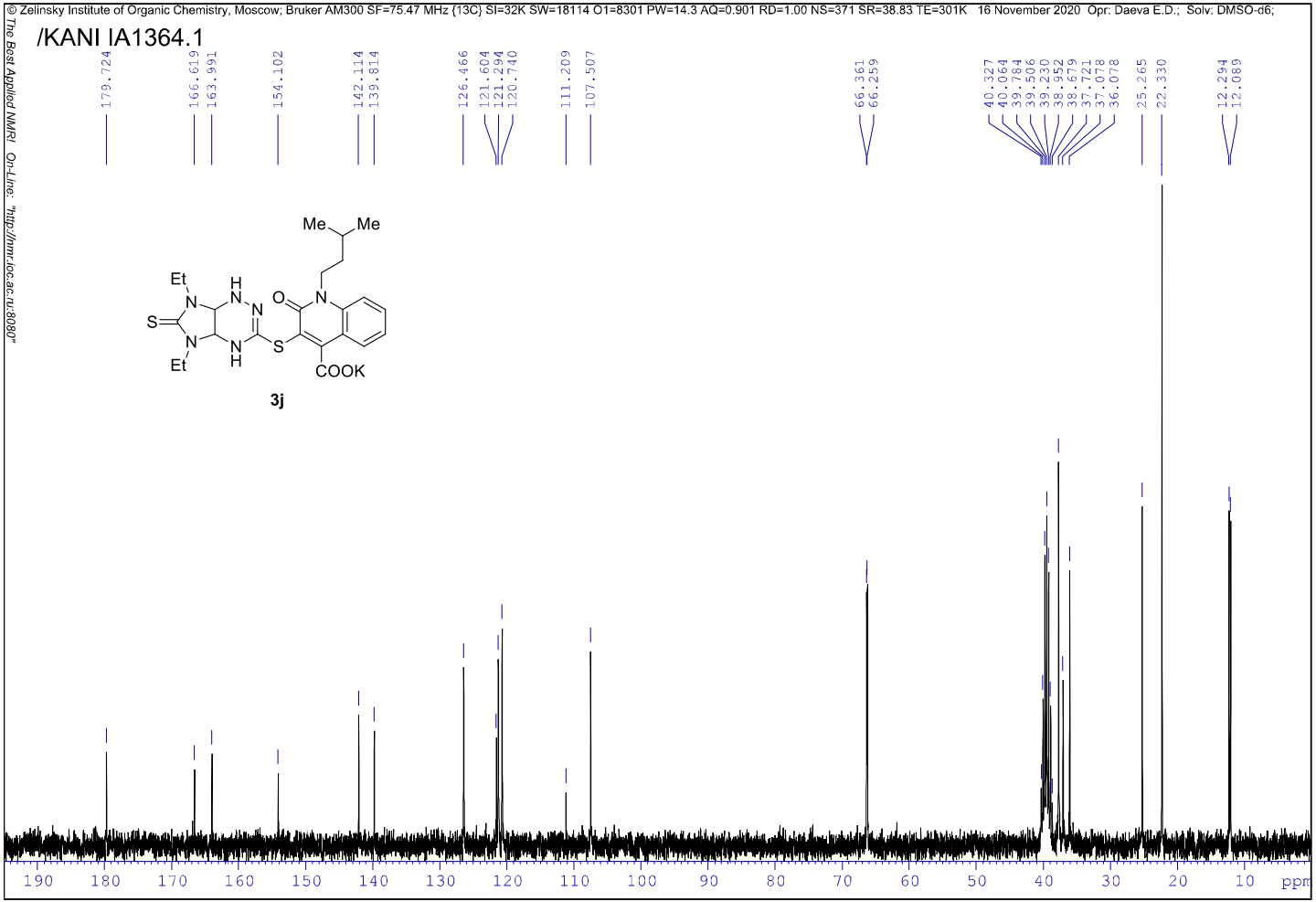


3j


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=371 SR=38.83 TE=301K 16 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
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163.991
154.102
142.114
139.814
126.466
121.604
121.294
120.740
111.209
107.507
66.361
66.259
40.327
40.064
39.784
39.506
39.230
38.952
38.679
37.721
37.078
36.078
25.265
22.330
12.294
12.089
Me
Me
Et
Et
COOK
3j
190
180
170
160
150
140
130
120
110
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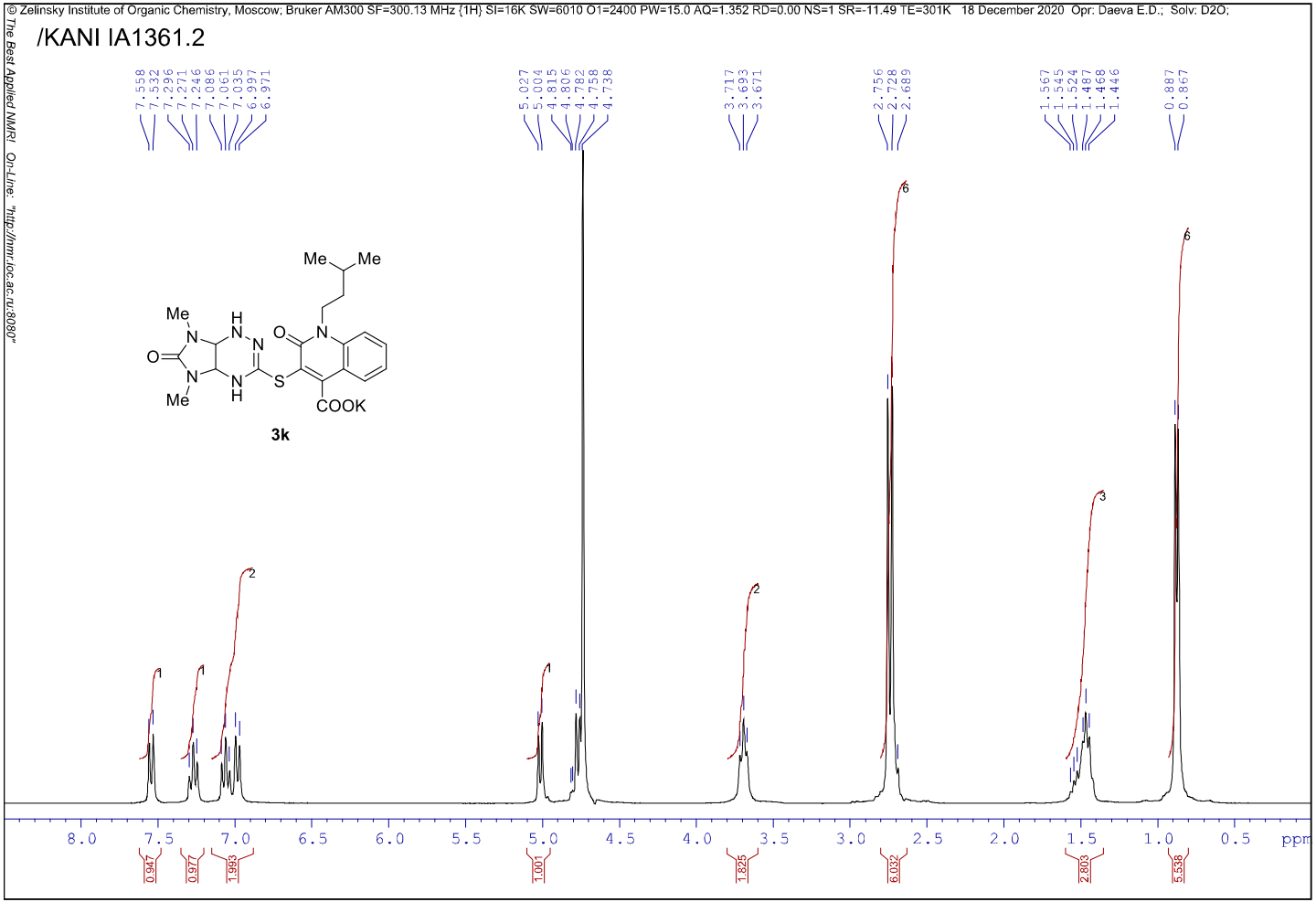
90
80
70
60
50
40
30
20
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=16K SW=6010 O1=2400 PW=15.0 AQ=1.352 RD=0.00 NS=1 SR=-11.49 TE=301K 18 December 2020 Opr: Daeva E.D.; Solv: D2O;
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
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7.271
7.246
7.086
7.061
7.035
6.997
6.971
5.027
5.004
4.815
4.806
4.782
4.758
4.738
3.717
3.693
3.671
2.756
2.728
2.689
1.567
1.545
1.524
1.487
1.468
1.446
0.887
0.867
Me
Me
Me
Me
H
N
N
N
N
N
O
O
S
COOK
3k
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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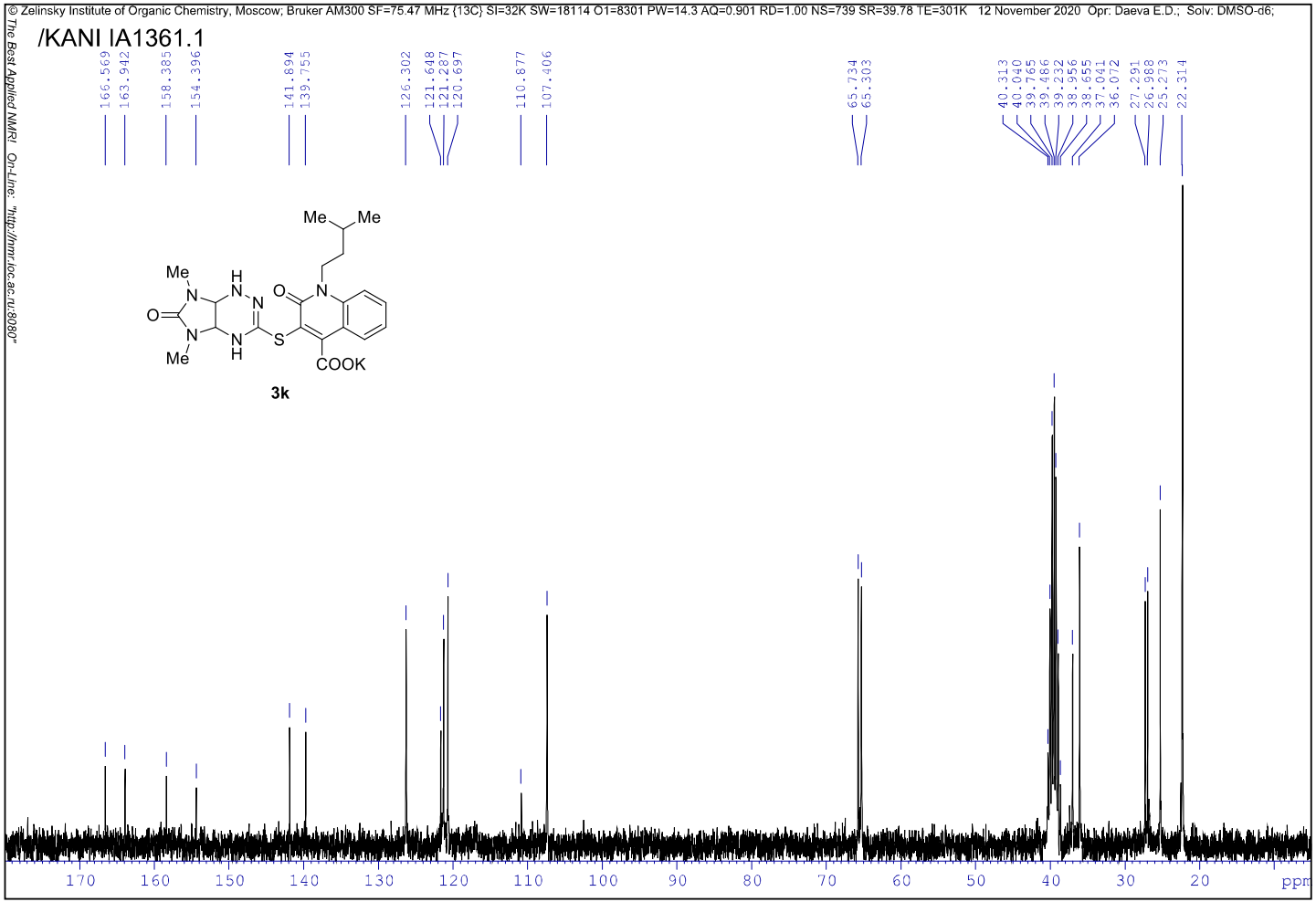
5.536


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=739 SR=39.78 TE=301K 12 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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121.287
120.697
110.877
107.406
65.734
65.303
40.313
40.040
39.765
39.486
39.232
38.956
38.655
37.041
36.072
27.291
26.988
25.273
22.314
Me
Me
Me
Me
O
O
N
N
N
N
H
H
S
COOK
3k
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120
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80
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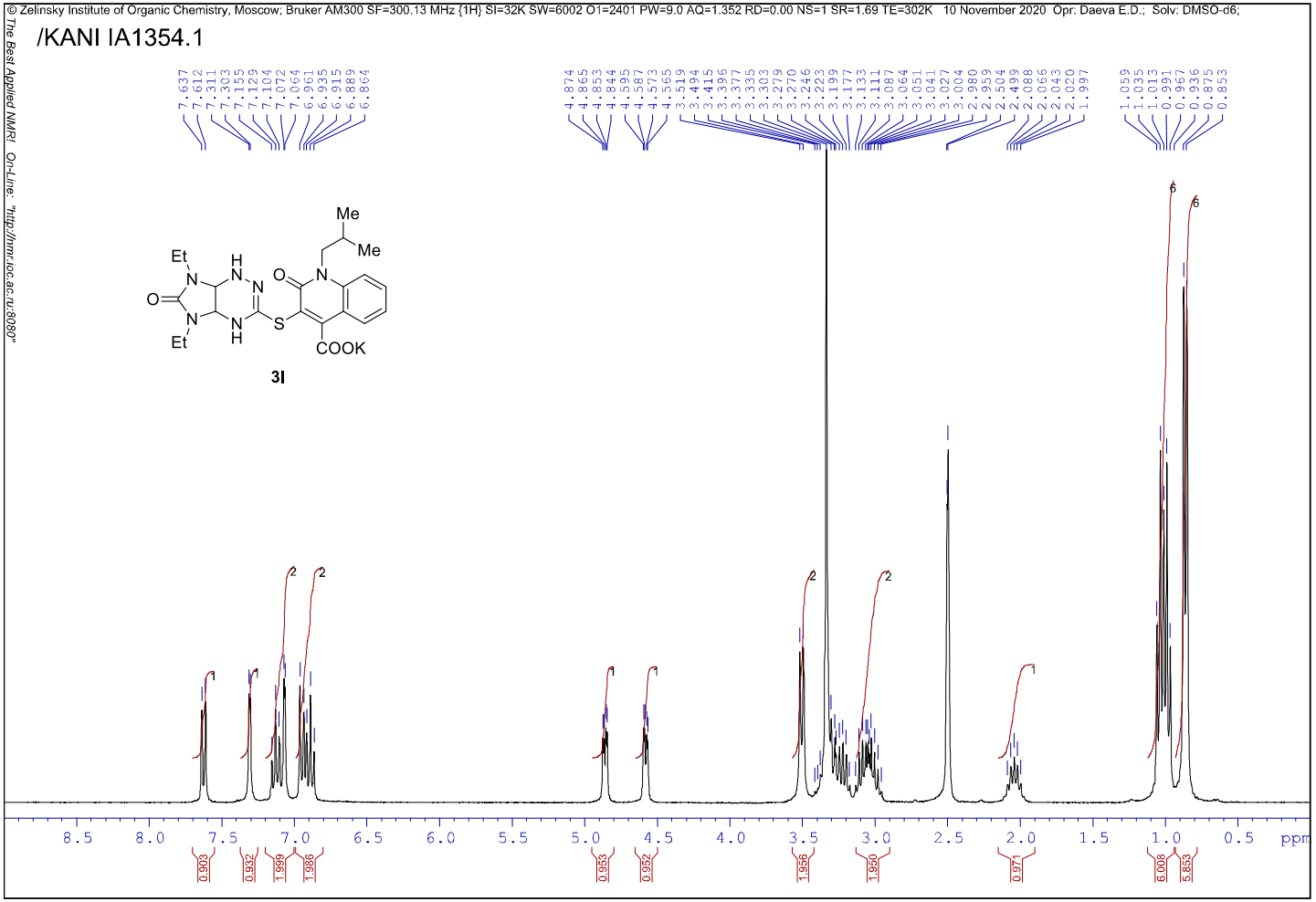
20
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.69 TE=302K 10 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
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4.874 4.865 4.853 4.844 4.595 4.587 4.573 4.565 3.519 3.494 3.415 3.396 3.377 3.335 3.303 3.279 3.270 3.246 3.223 3.199 3.177 3.133 3.111 3.087 3.064 3.051 3.041 3.027 3.004 2.980 2.959 2.504 2.499 2.088 2.066 2.043 2.020 1.997
1.059 1.035 1.013 0.991 0.967 0.936 0.875 0.853
Me
Me
Et
H
N
N
O
N
O
N
S
N
H
Et
COOK
3I
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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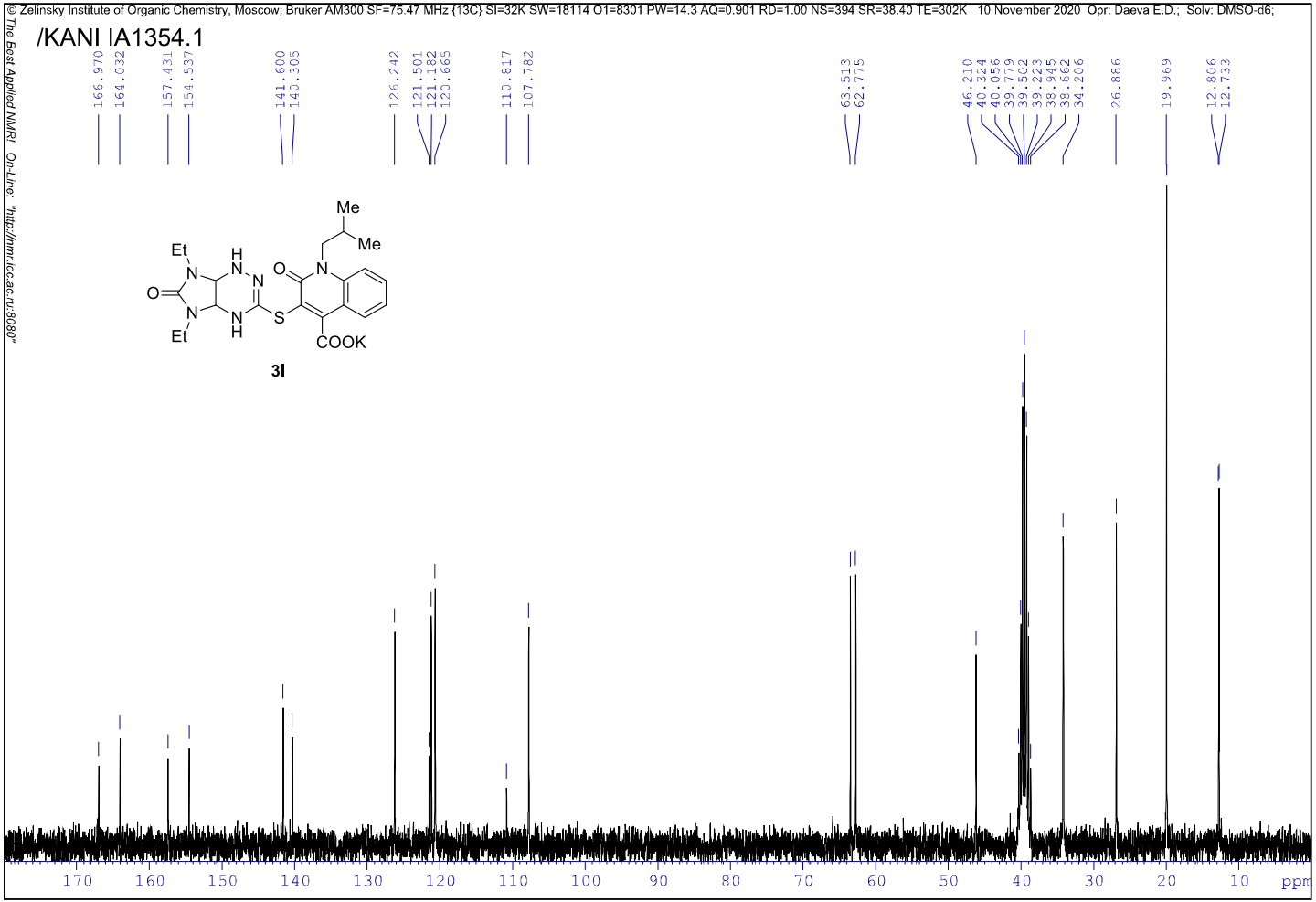
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=394 SR=38.40 TE=302K 10 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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141.600
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126.242
121.501
121.182
120.665
110.817
107.782
63.513
62.775
46.210
40.324
40.056
39.779
39.502
39.223
38.945
38.662
34.206
26.886
19.969
12.806
12.733
Me
Me
Et
Et
COOK
3l
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70
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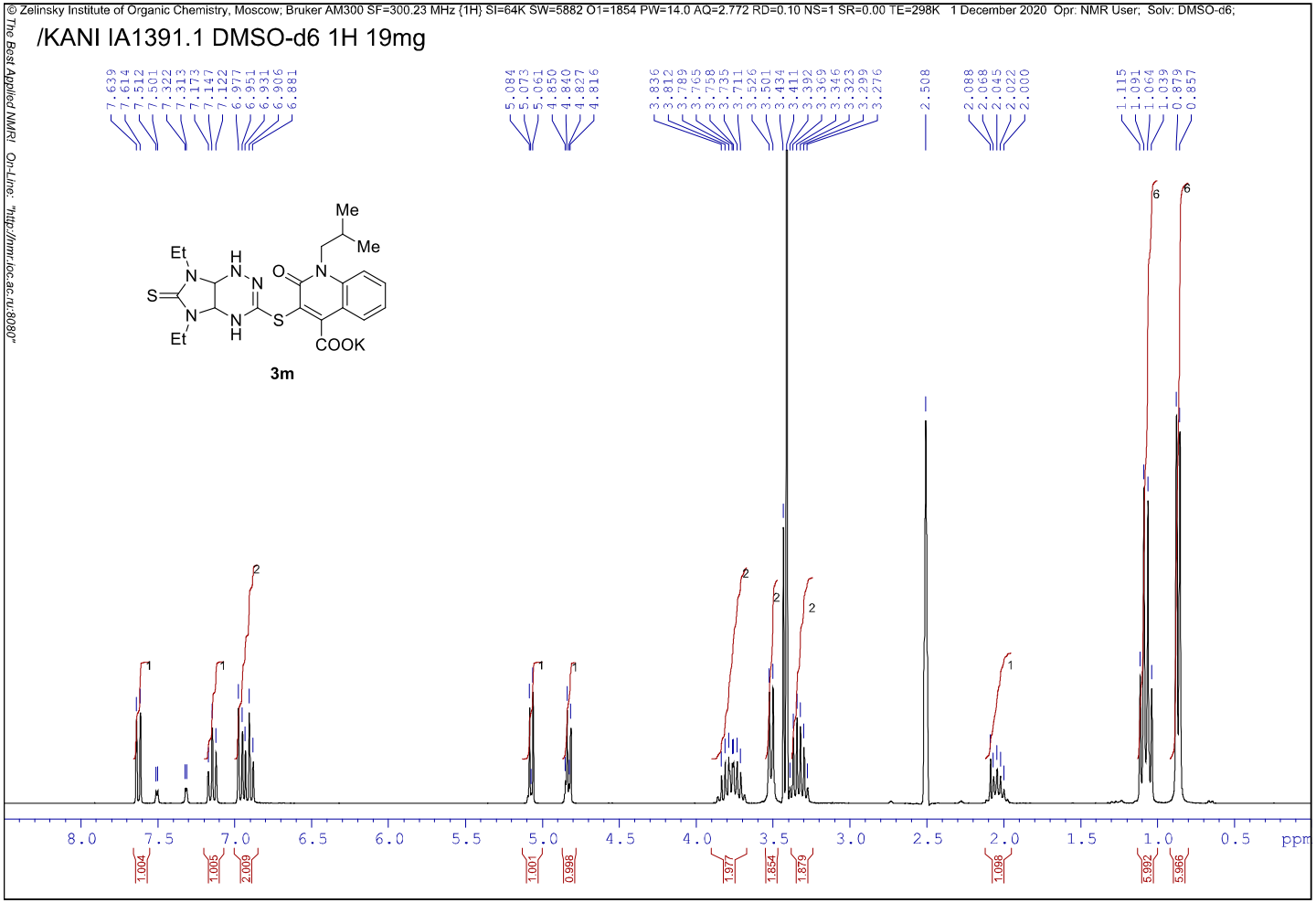
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.23 MHz {1H} SI=64K SW=5882 O1=1854 PW=14.0 AQ=2.772 RD=0.10 NS=1 SR=0.00 TE=298K 1 December 2020 Opr: NMR User; Solv: DMSO-d6;
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5.084 5.073 5.061 4.850 4.840 4.827 4.816
3.836 3.812 3.789 3.765 3.758 3.735 3.711 3.526 3.501 3.434 3.411 3.392 3.369 3.346 3.323 3.299 3.276
2.508
2.088 2.068 2.045 2.022 2.000
1.115 1.091 1.064 1.039 0.879 0.857
Me
Me
Et
N
H
N
N
O
N
S
N
H
S
Et
COOK
3m
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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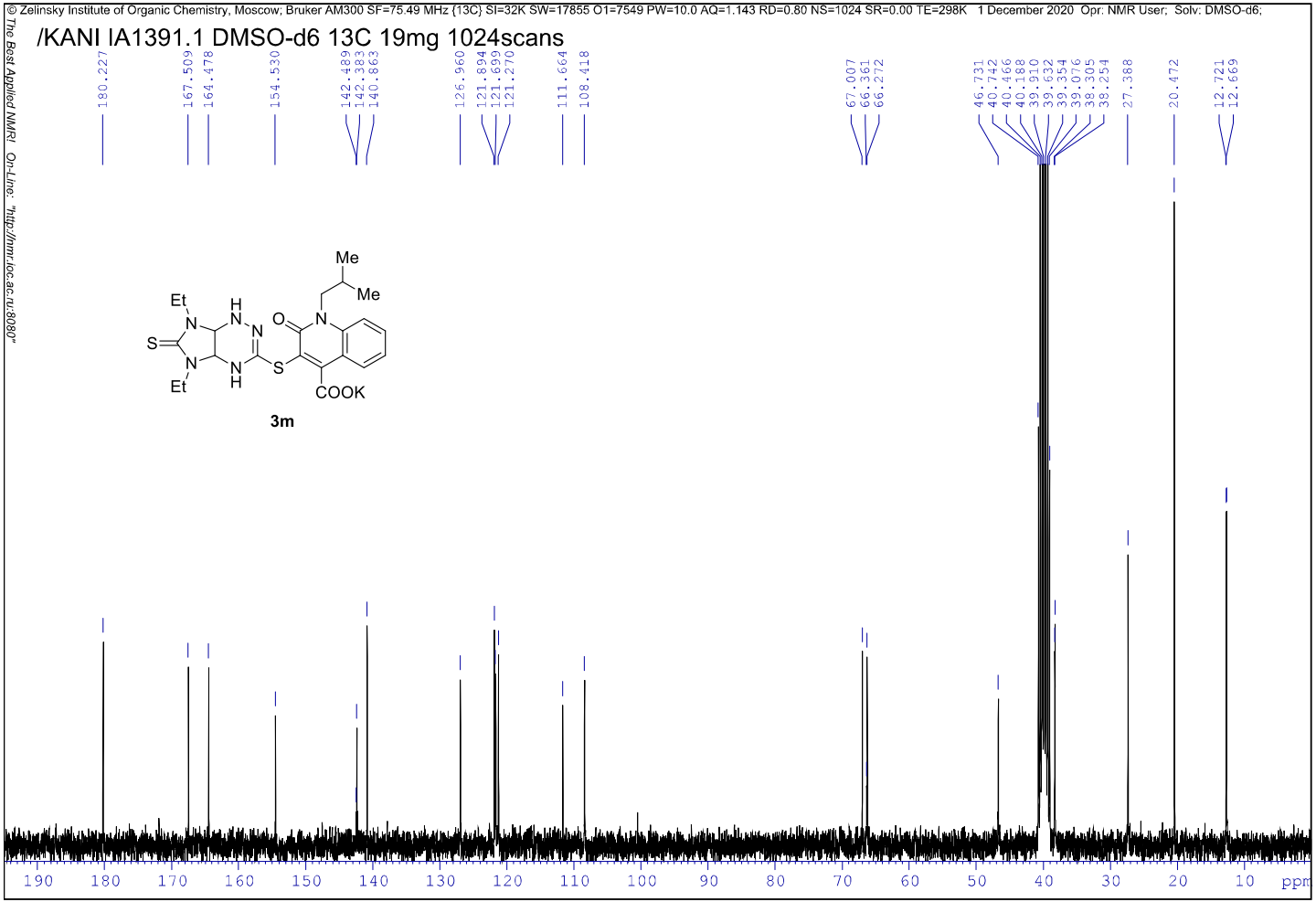
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=1024 SR=0.00 TE=298K 1 December 2020 Opr: NMR User; Solv: DMSO-d6;
The Best Applied NMR! On-Line, "http://nmr.ioc.ac.ru:8080/"
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167.509
164.478
154.530
142.489
142.383
140.863
126.960
121.894
121.699
121.270
111.664
108.418
67.007
66.361
66.272
46.731
40.742
40.466
40.188
39.910
39.632
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39.076
38.305
38.254
27.388
20.472
12.721
12.669
Et
N
H
N
N
S
O
N
Me
Me
S
N
H
N
Et
COOK
3m
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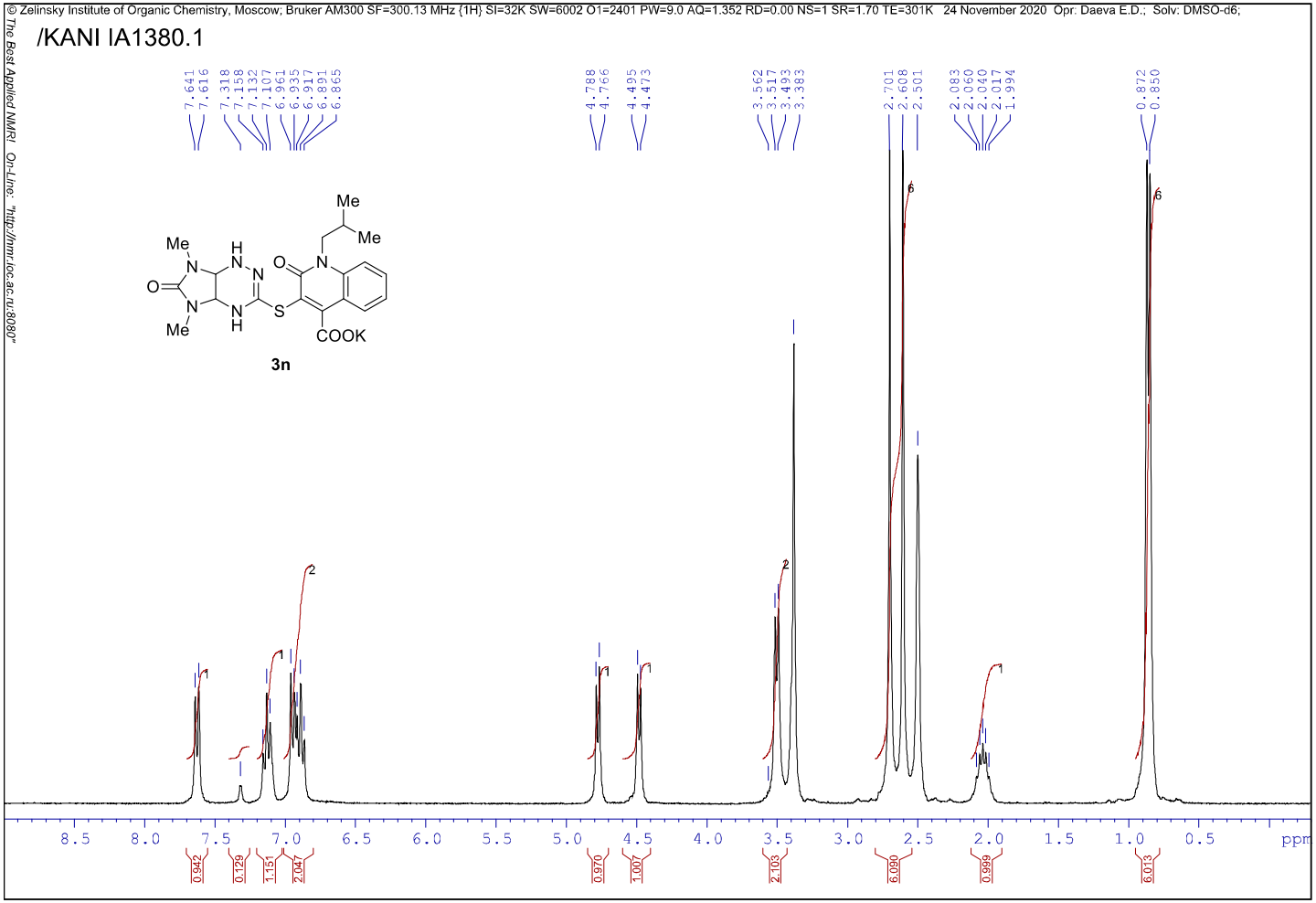
20
10
ppm


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=300.13 MHz {1H} SI=32K SW=6002 O1=2401 PW=9.0 AQ=1.352 RD=0.00 NS=1 SR=1.70 TE=301K 24 November 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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7.132
7.107
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6.935
6.917
6.891
6.865
4.788
4.766
4.495
4.473
3.562
3.517
3.493
3.383
2.701
2.608
2.501
2.083
2.060
2.040
2.017
1.994
0.872
0.850
Me
Me
Me
Me
N
H
N
N
O
O
N
N
H
S
COOK
3n
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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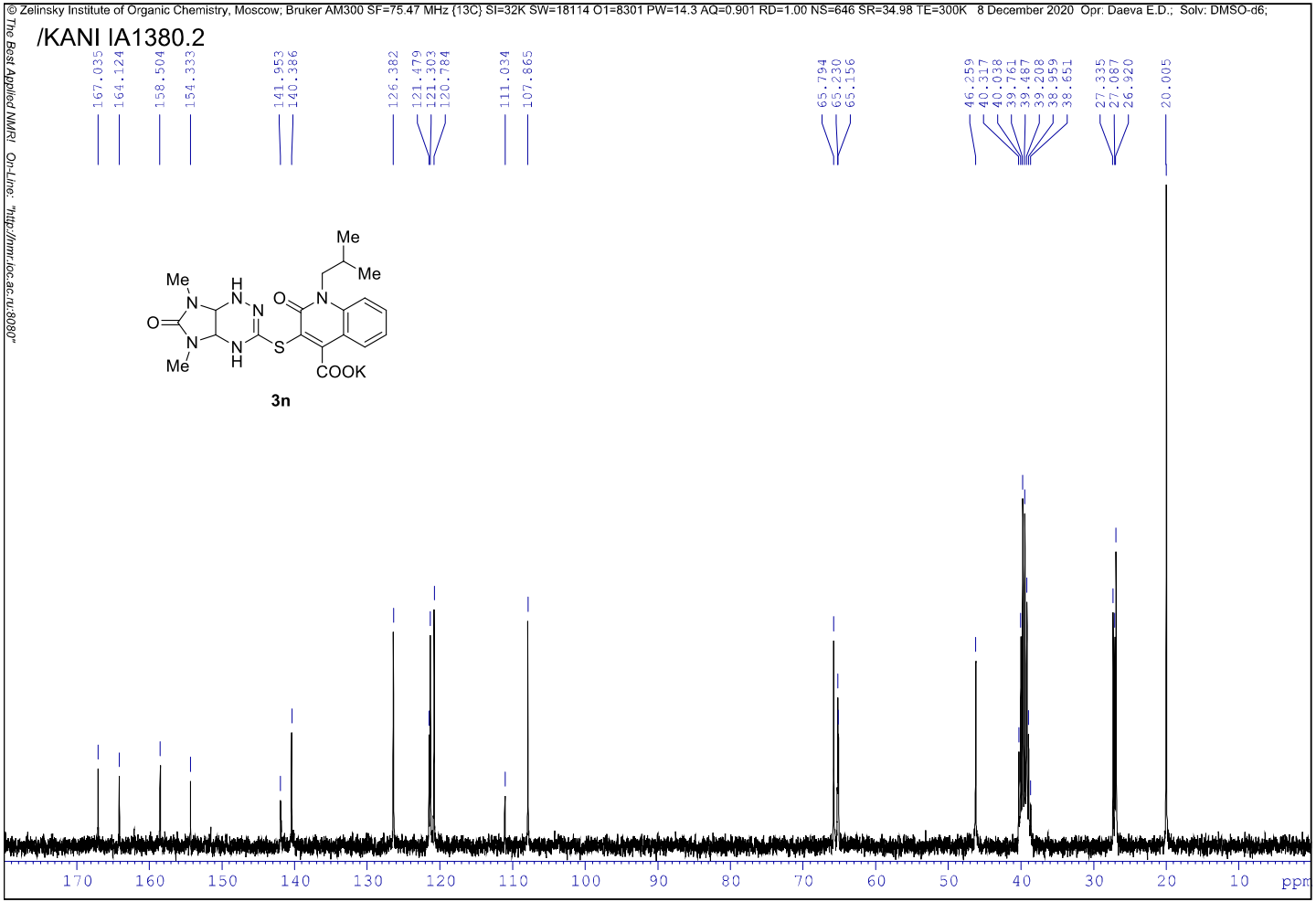
1.007
2.103
6.090
0.999
6.013


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=646 SR=34.98 TE=300K 8 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
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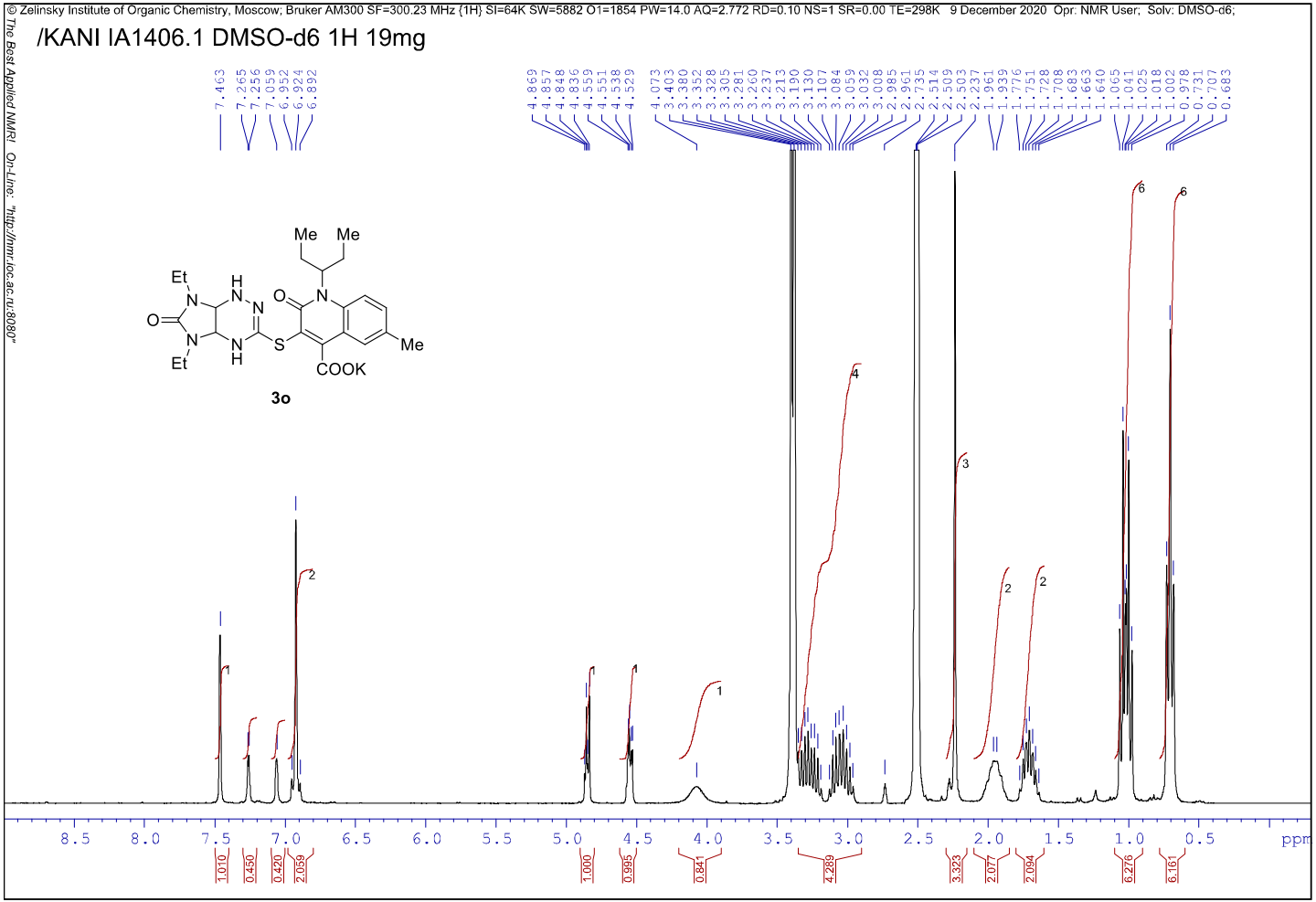
141.953
140.386
126.382
121.479
121.303
120.784
111.034
107.865
65.794
65.230
65.156
46.259
40.317
40.038
39.761
39.487
39.208
38.959
38.651
27.335
27.087
26.920
20.005
Me
Me
Me
Me
H
N
N
N
N
O
O
N
S
COOK
3n
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.265
7.256
7.059
6.932
6.924
6.892
4.869
4.857
4.848
4.836
4.559
4.551
4.538
4.529
4.073
3.403
3.380
3.352
3.328
3.305
3.281
3.260
3.237
3.213
3.190
3.130
3.107
3.084
3.059
3.032
3.008
2.985
2.961
2.735
2.514
2.509
2.503
2.237
1.961
1.939
1.776
1.751
1.728
1.708
1.683
1.663
1.640
1.055
1.041
1.025
1.018
1.002
0.978
0.731
0.707
0.683
Me
Me
Et
H
N
N
N
O
N
O
N
N
S
Me
Et
H
COOK
3o
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.010
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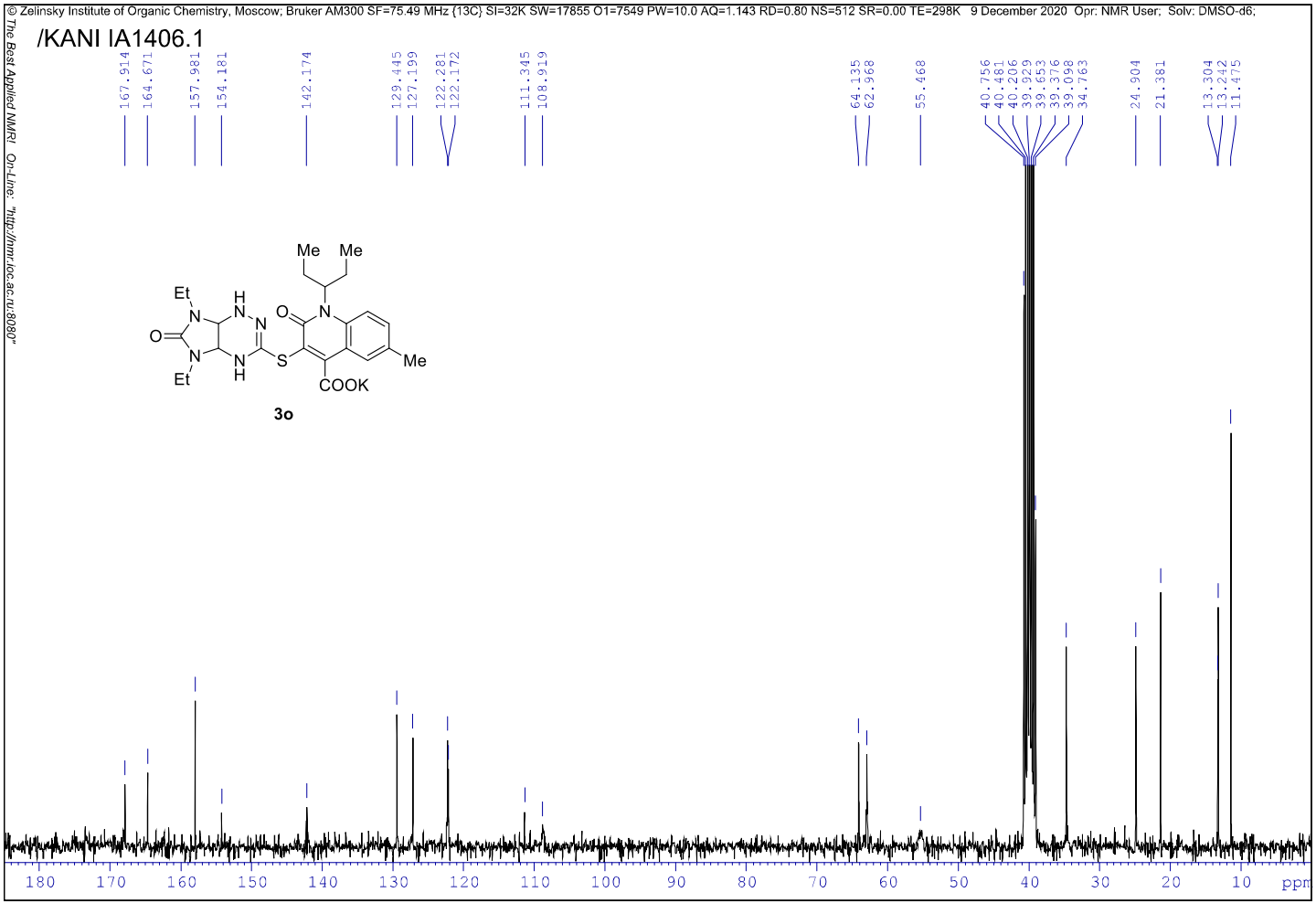
2.094
6.276
6.161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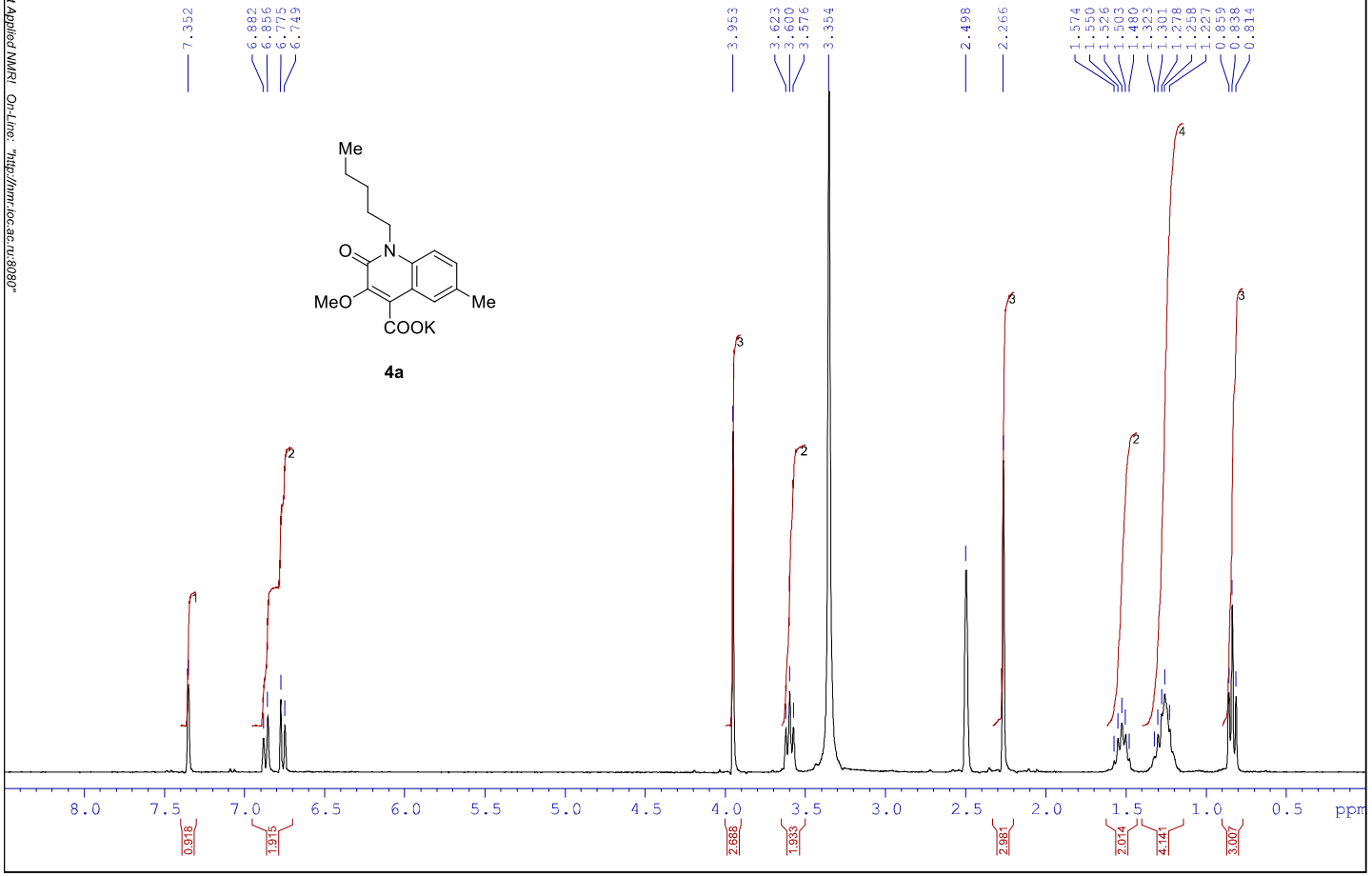
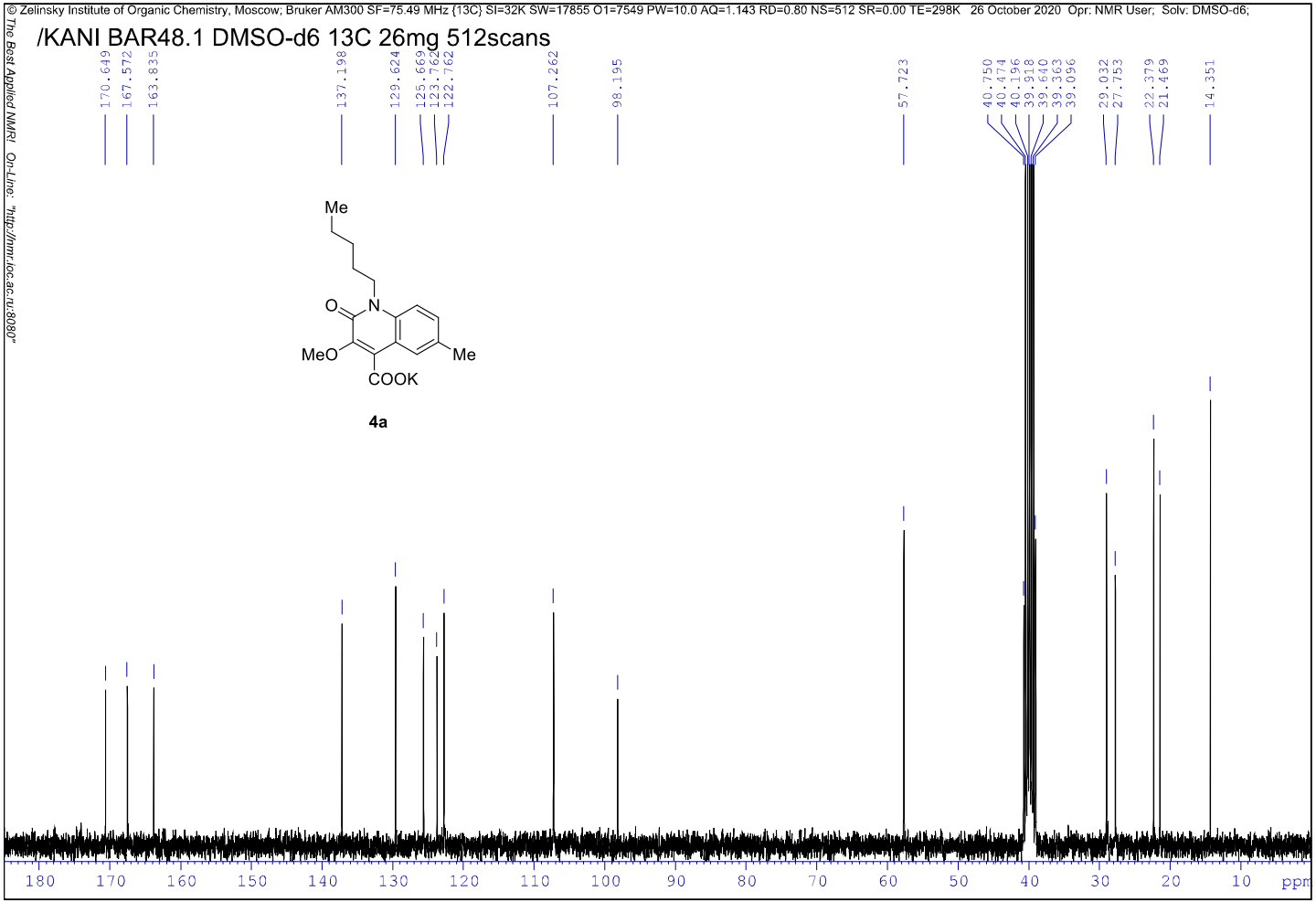
164.671
157.981
154.181
142.174
129.445
127.199
122.281
122.172
111.345
108.919
64.135
62.968
55.468
40.756
40.481
40.206
39.929
39.653
39.376
39.098
34.763
24.904
21.381
13.304
13.242
11.475
Me
Me
Et
H
N
N
O
N
O
N
S
Me
N
H
Et
COOK
3o
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

/KANI BAR48.1




© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.49 MHz {13C} SI=32K SW=17855 O1=7549 PW=10.0 AQ=1.143 RD=0.80 NS=512 SR=0.00 TE=298K 26 October 2020 Opr: NMR User; Solv: DMSO-d6;
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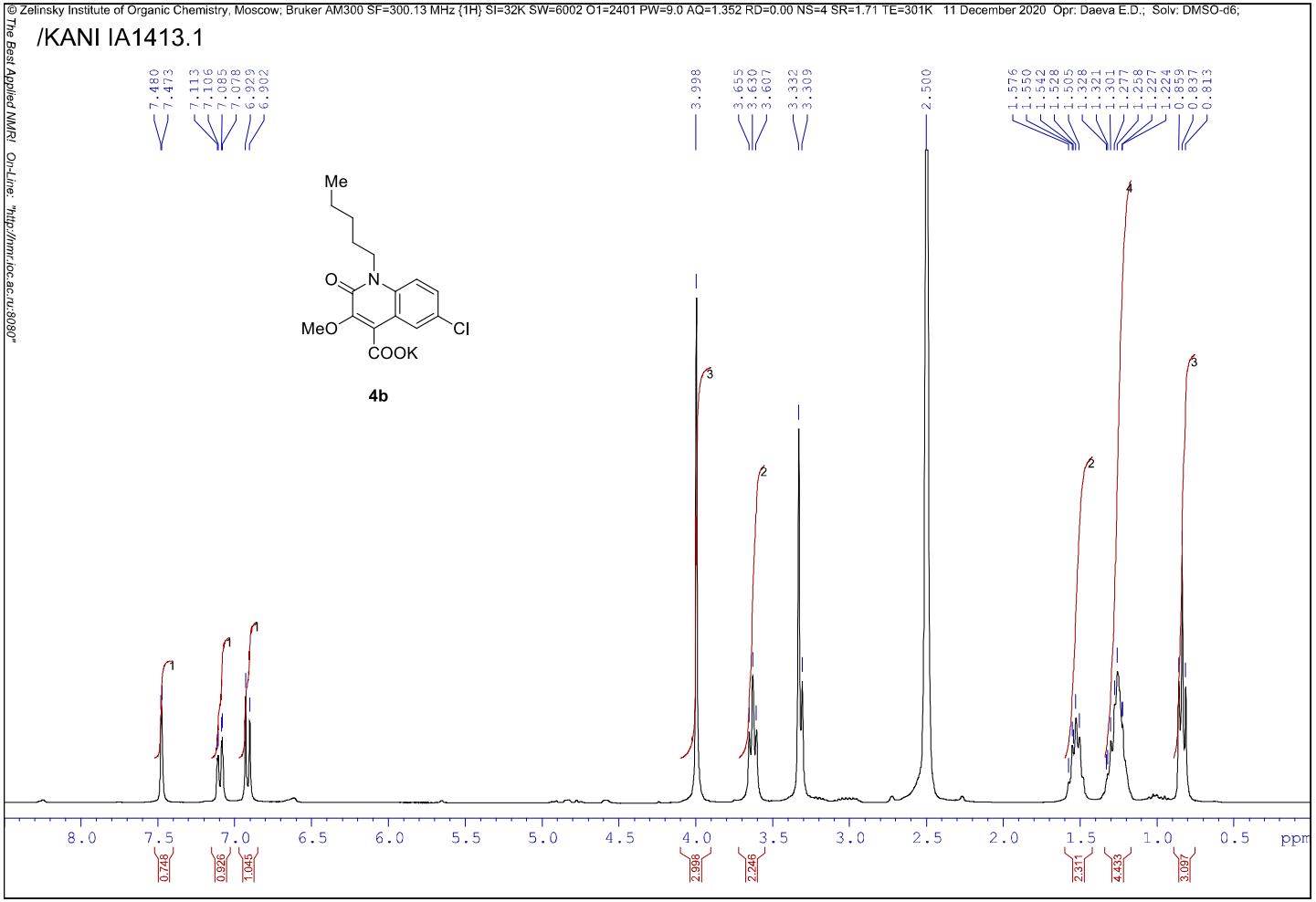
167.572
163.835
137.198
129.624
125.669
123.762
122.762
107.262
98.195
57.723
40.750
40.474
40.196
39.918
39.640
39.363
39.096
29.032
27.753
22.379
21.469
14.351
Me
O
N
MeO
Me
COOK
4a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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The Best Applied NMR! On-Line. "http://nmr.ioc.ac.ru:8080/"
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7.473
7.113
7.106
7.085
7.078
6.929
6.902
3.998
3.655
3.630
3.607
3.332
3.309
2.500
1.576
1.550
1.542
1.528
1.505
1.328
1.321
1.301
1.277
1.258
1.227
1.224
0.859
0.837
0.813
Me
O
N
MeO
Cl
COOK
4b
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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ppm
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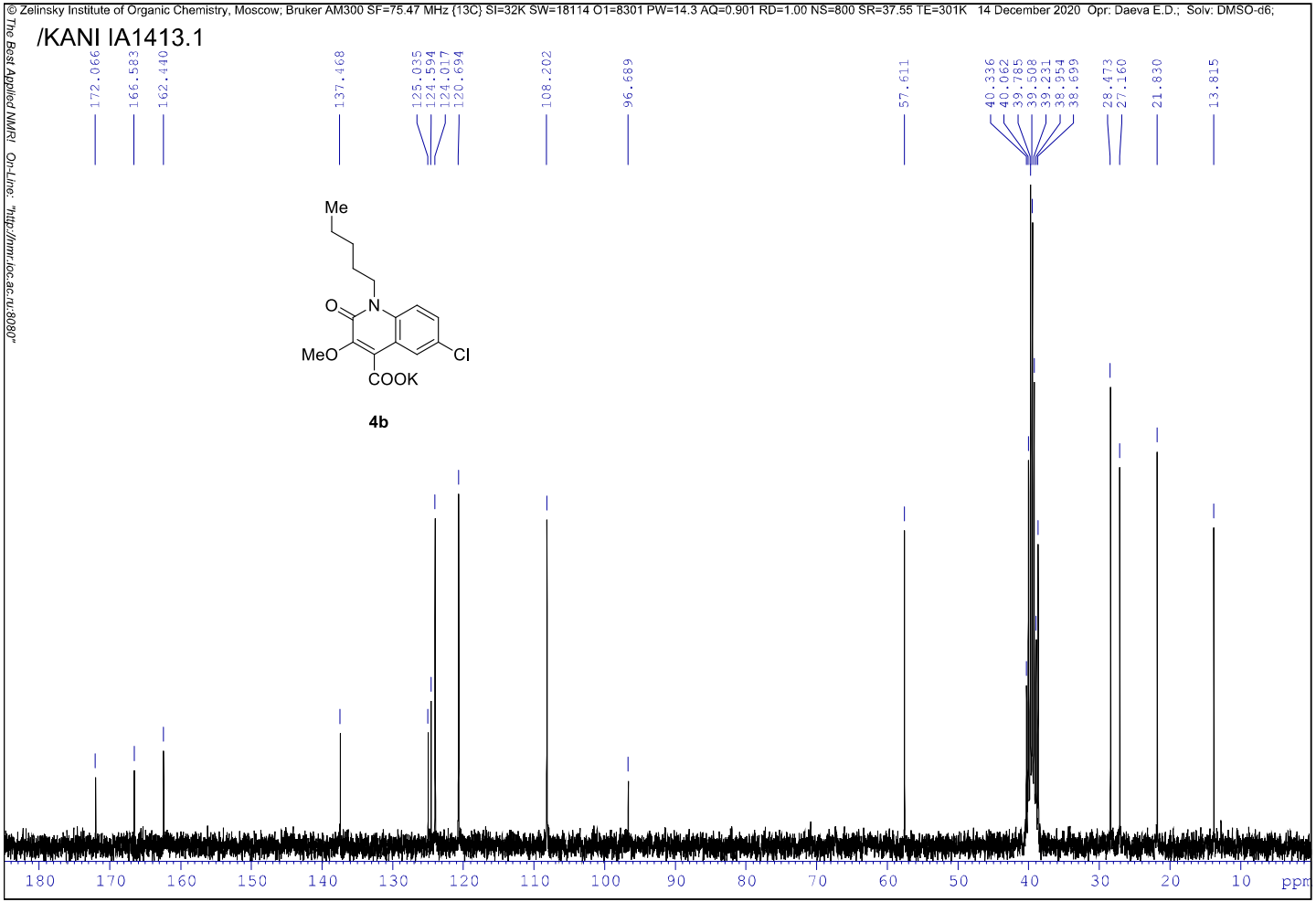
2.311
4.433
3.097


© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=800 SR=37.55 TE=301K 14 December 2020 Opr: Daeva E.D.; Solv: DMSO-d6;
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166.583
162.440
137.468
125.035
124.594
124.017
120.694
108.202
96.689
57.611
40.336
40.062
39.785
39.508
39.231
38.954
38.699
28.473
27.160
21.830
13.815
Me
O
N
MeO
Cl
COOK
4b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

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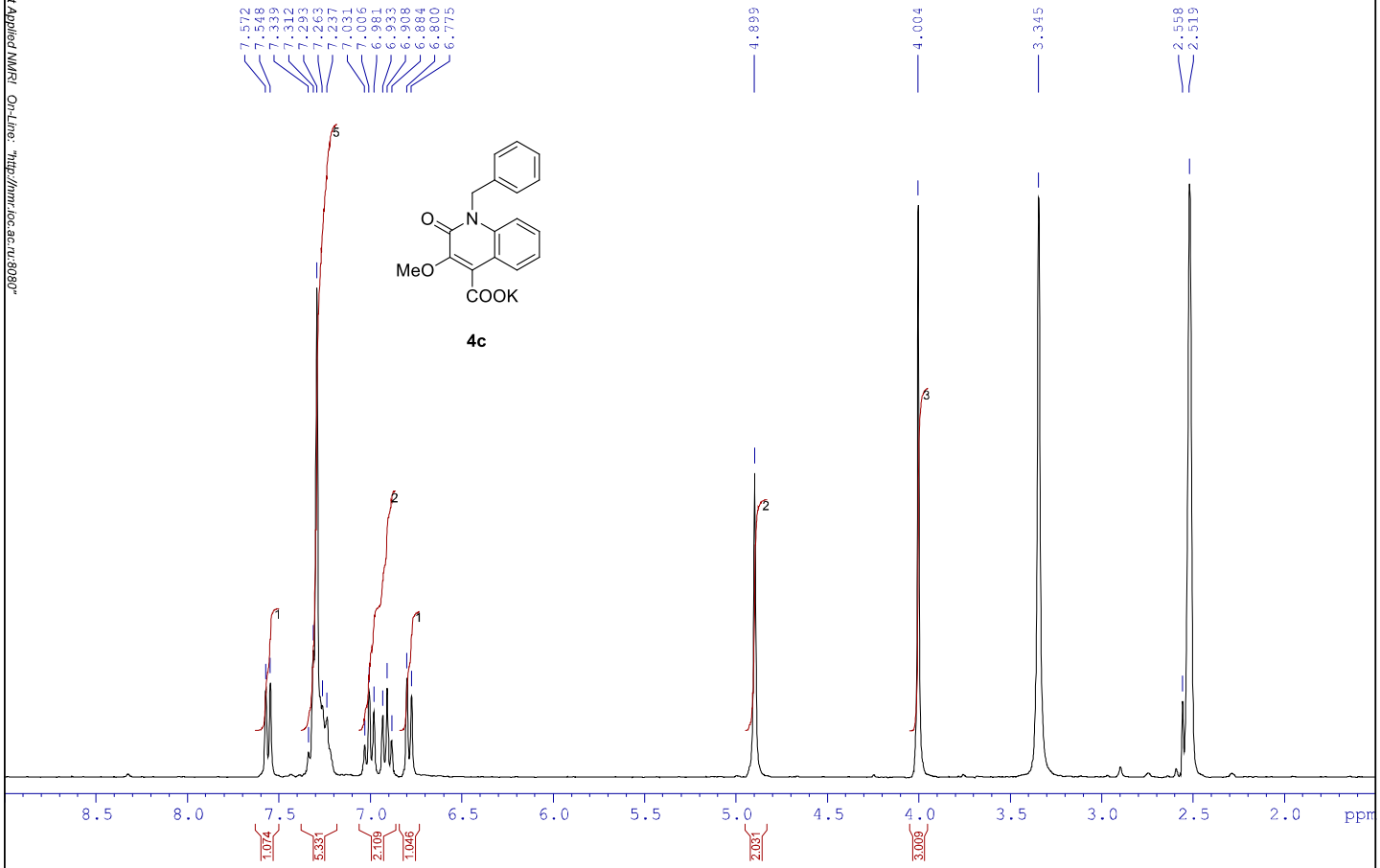

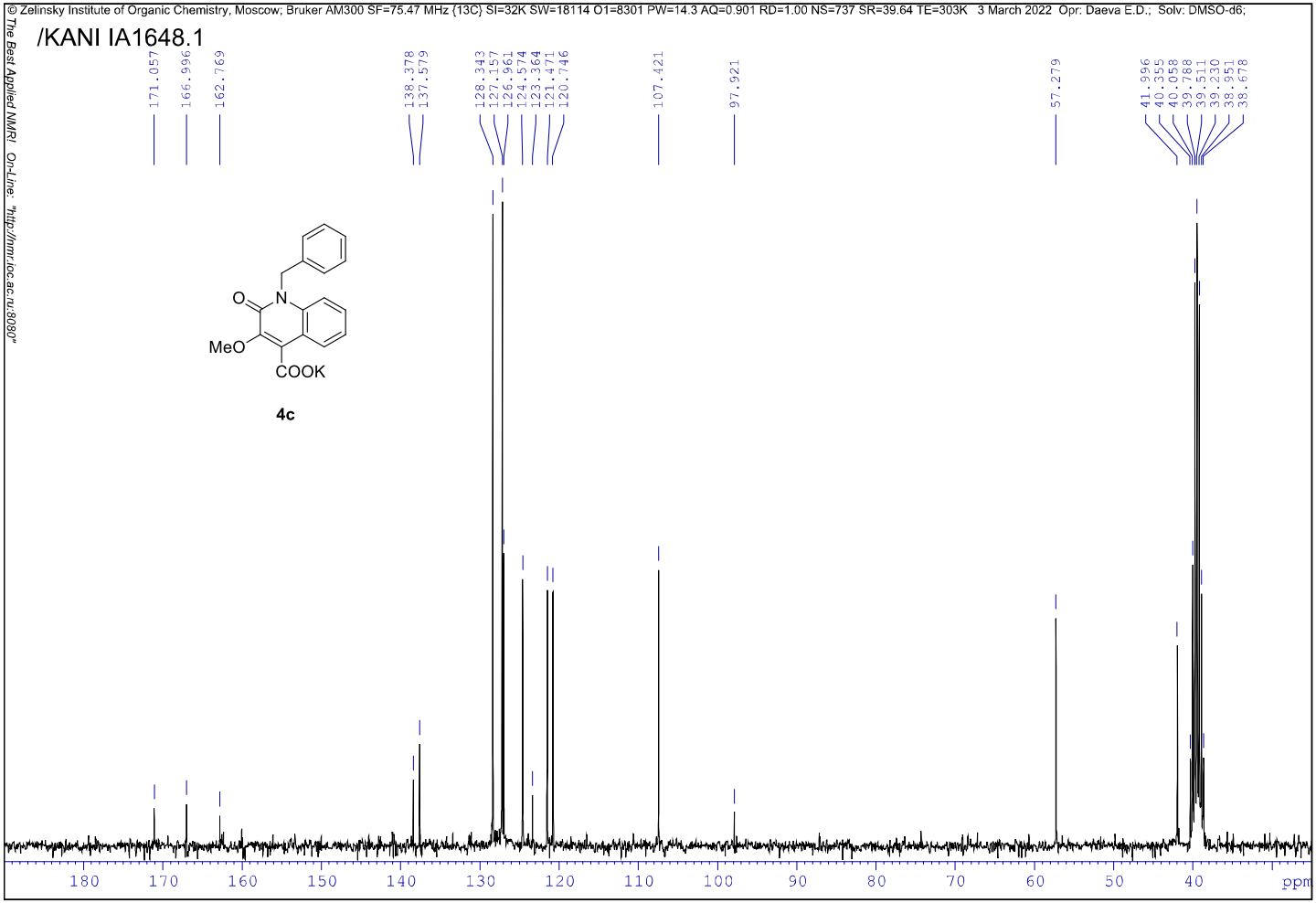
© Zelinsky Institute of Organic Chemistry, Moscow; Bruker AM300 SF=75.47 MHz {13C} SI=32K SW=18114 O1=8301 PW=14.3 AQ=0.901 RD=1.00 NS=737 SR=39.64 TE=303K 3 March 2022 Opr: Daeva E.D.; Solv: DMSO-d6;
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166.996
162.769
138.378
137.579
128.343
127.157
126.961
124.574
123.364
121.471
120.746
107.421
97.921
57.279
41.996
40.355
40.058
39.788
39.511
39.230
38.951
38.678
O
N
MeO
COOK
4c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

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