Electronic supplementary materials *Mendeleev Commun.*, 2025, **35**, 648–650

C–H functionalization of highly electrophilic azolopyridines as a way to donor–acceptor conjugated indoles

Victoria V. Ivanova, Alexey M. Starosotnikov, Mikhail E. Minyaev, Andrey A. Kruchinin, Artem N. Fakhrutdinov and Maxim A. Bastrakov

All chemicals were of commercial grade and used directly without purification. Melting points were measured on a Stuart SMP20 apparatus (Stuart (Bibby Scientific), UK). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AM-300 (at 300.13 and 75.13 MHz, respectively, Bruker Biospin, Germany) or Bruker Avance DRX 500 (at 500 and 125 MHz, respectively, Bruker Biospin, Germany) in DMSO-d_6 or $CDCl_3$. *J* values are given in Hz. HRMS spectra were recorded on a Bruker micrOTOF II mass spectrometer using ESI. UV–Vis absorption spectra were recorded in EtOH (1×10^{-4} M) in standard 10 × 10 × 45 mm quartz cuvettes on a Cary 60 UV–Vis spectrophotometer (Agilent Technologies, Santa Clara, CA, USA). All reactions were monitored by TLC analysis using ALUGRAM SIL G/UV254 plates, which were visualized with UV light. Dihydro compounds **4** and **5** were synthesized using previously described methods.[S1]

General method for the synthesis of compounds **6a-h, 7a-h**

To a solution of dihydro compound **4** or **5** (0.3 mmol) in MeOH (4 ml), DDQ (0.48 mmol) was added. The mixture was stirred for 1-24 h at 20 °C (TLC monitoring). The precipitate that formed was filtered off and dried in air, or the solvent was evaporated under reduced pressure, the residue was purified by column chromatography on silica gel (eluent: $CHCl_3$/MeOH 5:1).

Methyl 7-(1H-indol-3-yl)-[1,2,5]selenadiazolo[3,4-b]pyridine-6-carboxylate (**6a**), brown powder; yield 92%; mp 218–219 °C; ^{1}H NMR (300 MHz, DMSO-d_6): δ 3.58 (s, 3H), 7.08 (t, *J* = 7.0 Hz, 1H), 7.19 (t, *J* = 7.0 Hz, 1H), 7.30 (d, *J* = 7.9 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 8.03 (d, *J* = 2.8 Hz, 1H), 9.22 (s, 1H), 11.92 (s, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 53.0, 109.4, 112.8, 119.3, 120.7, 122.2, 122.4, 126.7, 131.3, 131.4, 136.6, 138.9, 152.7, 156.4, 165.2, 167.9. HRMS (ESI, m/z): calcd for $C_{15}H_{11}N_4O_2Se$ $[M+H]^+$: 359.0047; found: 359.0042.

7-(1H-Indol-3-yl)-6-nitro-[1,2,5]selenadiazolo[3,4-b]pyridine (**6b**), burgundy color powder; yield 99%; mp 242–243 °C; ^{1}H NMR (300 MHz DMSO-d_6): δ 7.11 – 7.26 (m, 3H), 7.56 (d, *J* = 8.1 Hz, 1H), 8.22 (d, *J* = 3.0 Hz, 1H), 9.46 (s, 1H), 12.22 (s, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 106.6, 113.3, 119.3, 121.4, 123.1, 125.6, 133.2, 133.8, 136.8, 140.0, 151.5, 151.9, 164.6.HRMS (ESI, m/z): calcd for $C_{13}H_8N_5O_2Se$ $[M+H]^+$: 345.9843; found: 345.9838.

*Methyl 7-(5-methoxy-1H-indol-3-yl)-[1,2,5]selenadiazolo[3,4-b]pyridine-6-carboxylate (**6c**);* burgundy color powder; yield 99%; mp 264–265 °C; ^{1}H NMR (300 MHz, DMSO-d_6): δ 3.61 (s, 3H), 3.70 (s, 3H), 6.76 – 6.88 (m, 2H), 7.41 (d, *J* = 8.7 Hz, 1H), 8.00 (d, *J* = 3.0 Hz, 1H), 9.21 (s, 1H), 11.82 (s, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 53.0, 55.6, 101.1, 109.3, 112.5, 113.5, 121.8, 127.2, 131.6, 132.0, 139.0, 152.7, 154.8, 156.5, 165.2, 168.0. HRMS (ESI, m/z): calcd for $C_{16}H_{13}N_4O_3Se$ $[M+H]^+$: 389.0153; found: 389.0148.

*7-(5-Methoxy-1H-indol-3-yl)-6-nitro-[1,2,5]selenadiazolo[3,4-b]pyridine (**6d**);* dark powder; yield 79%; mp >300 °C; ^{1}H NMR (300 MHz, DMSO-d_6) : δ 3.68 (s, 3H), 6.59 (d, *J* = 2.4 Hz, 1H), 6.87 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.45 (d, *J* = 8.8 Hz, 1H), 8.20 (d, *J* = 2.9 Hz, 1H), 9.44 (s, 1H), 12.12 (s, 1H). ^{13}C

NMR (126 MHz, DMSO-d_6) δ 55.0, 100.9, 105.9, 112.2, 113.4, 125.8, 131.0, 132.6, 133.6, 139.2, 151.0, 151.3, 154.5, 164.0. HRMS (ESI, m/z): calcd for $C_{14}H_{10}N_5O_3Se$ $[M+H]^+$: 375.9949; found: 375.9944.

*7-(1H-Indol-3-yl)-6-(trifluoromethyl)-[1,2,5]selenadiazolo[3,4-b]pyridine (**6e**);* brown powder; yield 99%; mp 257-258 °C; ^{1}H NMR (300 MHz, DMSO-d_6): δ 6.99 (t, J = 7.5 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 7.24 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 8.1 Hz, 1H), 7.66 (d, J = 2.7 Hz, 1H), 9.35 (s, 1H), 11.76 (s, 1H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 78.1, 106.5, 110.7, 118.6, 119.1, 119.3 (q, $^2J_{CF}$= 28.6 Hz), 120.7, 122.8 (q, $^1J_{CF}$ = 274.9 Hz), 126.3, 134.9, 139.4, 150.90 (q, $^3J_{CF}$ = 5.1 Hz), 151.2, 163.7. HRMS (ESI, m/z): calcd for $C_{14}H_8F_3N_4Se$ $[M+H]^+$: 368.9866; found: 368.9861.

*7-(5-Methoxy-1H-indol-3-yl)-6-(trifluoromethyl)-[1,2,5]selenadiazolo[3,4-b]pyridine (**6f**);* red powder; yield 90%; mp 266-267 °C; ^{1}H NMR (300 MHz, DMSO-d_6): δ 3.59 (s, 3H), 6.75 (d, J = 2.4 Hz, 1H), 6.81 (dd, J = 8.8, 2.4 Hz, 1H), 7.39 (d, J = 8.8 Hz, 1H), 7.61 (s, 1H), 9.34 (s, 1H), 11.63 (s, 1H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 53.1, 78.1, 106.5, 110.7, 118.7, 119.1, 119.3 (q, $^2J_{CF}$ = 28.6 Hz), 120.7, 122.8 (q, $^1J_{CF}$ = 274.9 Hz), 126.3, 134.9, 139.4, 150.9 (q, $^3J_{CF}$ = 5.1 Hz), 151.2, 163.7. HRMS (ESI, m/z): calcd for $C_{15}H_{10}F_3N_4OSe$ $[M+H]^+$: 398.9972; found: 398.9967.

*Methyl 7-(1H-indol-3-yl)-[1,2,5]thiadiazolo[3,4-b]pyridine-6-carboxylate (**6g**);* orange powder; yield 71%; mp 228-229 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.62 (s, 3H), 7.11 (t, J = 7.5 Hz, 1H), 7.21 (t, J = 7.5 Hz, 1H), 7.35 (d, J = 7.9 Hz, 1H), 7.54 (d, J = 8.0 Hz, 1H), 8.10 (d, J = 2.8 Hz, 1H), 9.26 (s, 1H), 12.01 (s, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) 52.84, 108.90, 112.72, 119.38, 120.73, 122.47, 123.45, 126.43, 130.69, 130.87, 136.81, 138.07, 147.37, 155.98, 156.00, 162.87, 167.56.HRMS (ESI, m/z): calcd for $C_{15}H_{11}N_4O_2S$ $[M+H]^+$: 311.0603; found: 311.0597.

*Methyl 7-(5-methoxy-1H-indol-3-yl)-[1,2,5]thiadiazolo[3,4-b]pyridine-6-carboxylate (**6h**)*; red powder; yield 99%; mp 267-268 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.64 (s, 3H), 3.70 (s, 3H), 6.81 – 6.87 (m, 2H), 7.43 (d, J = 8.6 Hz, 1H), 8.06 (d, J = 2.9 Hz, 1H), 9.25 (s, 1H), 11.90 (s, 1H). ^{13}C NMR (151 MHz, DMSO) 52.65, 55.15, 100.62, 108.23, 112.22, 113.13, 122.34, 126.39, 131.20, 131.27, 137.62, 146.79, 154.45, 155.70, 162.41, 167.44. HRMS (ESI, m/z): calcd for $C_{16}H_{13}N_4O_3S$ $[M+H]^+$: 341.0708; found: 341.0703.

*2-(3,5-Dinitrophenyl)-5-(1H-indol-3-yl)-6,8-dinitro-[1,2,4]triazolo[1,5-a]pyridine (**7a**);* orange powder; yield 76%; mp >300 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.18 – 7.35 (m, 3H), 7.65 (d, J = 8.1 Hz, 1H), 8.74 (d, J = 2.7 Hz, 1H), 8.99 (t, J = 2.2 Hz, 1H), 9.22 (d, J = 2.1 Hz, 2H), 9.35 (s, 1H), 12.65 (s, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) 102.12, 113.56, 119.76, 120.84, 121.92, 123.54, 125.66, 126.96, 127.26, 131.54, 132.63, 135.10, 135.31, 136.67, 140.72, 147.46, 149.33, 162.90. HRMS (ESI, m/z): calcd for $C_{20}H_{11}N_8O_8$ $[M+H]^+$: 491.0700; found: 491.0694.

*2-(4-Methoxyphenyl)-5-(1-methyl-1H-indol-3-yl)-6,8-dinitro-[1,2,4]triazolo[1,5-a]pyridine (**7b**)*; orange powder; yield 70%; mp >300 °C; ^{1}H NMR (300 MHz, DMSO-d_6): δ 3.85 (s, 3H), 4.08 (s, 3H), 7.14 (d, J = 8.8 Hz, 2H), 7.21 – 7.40 (m, 3H), 7.71 (d, J = 8.2 Hz, 1H), 8.22 (d, J = 8.5 Hz, 2H), 8.69 (s, 1H), 9.21 (s, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): δ 33.55, 55.44, 101.04, 111.50, 114.24, 114.61, 119.47, 121.58, 121.71, 123.04, 125.68, 125.74, 129.34, 130.48, 134.01, 136.81, 137.65, 139.21, 146.74, 161.94, 166.22. HRMS (ESI, m/z): calcd for $C_{22}H_{17}N_6O_5$ $[M+H]^+$: 445.1255; found: 445.1247.

*5-(1H-Indol-3-yl)-2-(4-methoxy-3,5-dinitrophenyl)-6,8-dinitro-[1,2,4]triazolo[1,5-a]pyridine (**7c**);* orange powder; yield 78%; mp 265-266 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 4.03 (s, 3H), 7.19 – 7.34 (m, 3H), 7.64 (d, J = 8.1 Hz, 1H), 8.74 (d, J = 3.0 Hz, 1H), 8.99 (s, 2H), 9.30 (s, 1H), 12.61 (d, J = 3.3 Hz, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 65.1, 102.1, 113.7, 119.3, 122.2, 123.7, 125.5, 125.6, 127.3, 128.2, 130.9, 134.8, 136.0, 136.6, 140.6, 145.3, 147.5, 148.8, 162.8. HRMS (ESI, m/z): calcd for $C_{21}H_{13}N_8O_9$ $[M+H]^+$: 521.0806; found: 521.0800.

*2-(4-Fluorophenyl)-5-(1H-indol-3-yl)-6,8-dinitro-[1,2,4]triazolo[1,5-a]pyridine (**7d**);* red-orange powder; yield 90%; mp .>300 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.16 – 7.33 (m, 3H), 7.37 – 7.46 (t, J = 8.8 Hz, 2H), 7.64 (d, *J* = 8.1 Hz, 1H), 8.20 – 8.33 (m, 2H), 8.63 (d, *J* = 3.0 Hz, 1H), 9.23 (s, 1H), 12.52 (d, *J* = 3.2 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 101.74, 113.09, 116.25 (d, J = 22.1 Hz), 118.99, 121.46, 123.00, 125.03, 125.61 (d, J = 2.9 Hz), 126.14, 129.84 (d, J = 8.9 Hz), 130.41, 134.04, 134.76, 135.97, 139.86, 146.76, 163.91 (d, J = 248.9 Hz), 165.04. HRMS (ESI, m/z): calcd for $C_{20}H_{12}FN_6O_4$ $[M+H]^+$: 419.0904; found: 419.0899.

*5-(5-Methoxy-1H-indol-3-yl)-2-(4-methoxy-3,5-dinitrophenyl)-6,8-dinitro-[1,2,4]triazolo[1,5-a]-pyridine (**7e**)*; orange powder; yield 80%; mp .229-230°C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.69 (s, 3H), 4.04 (s, 3H), 6.67 (s, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 7.52 (d, *J* = 8.8 Hz, 1H), 8.70 (s, 1H), 9.00 (s, 2H), 9.29 (s, 1H), 12.51 (s, 1H). HRMS (ESI, m/z): calcd for $C_{22}H_{15}N_8O_{10}$ $[M+H]^+$: 551.0911; found: 551.0906.

*2-(4-Fluorophenyl)-5-(5-methoxy-1H-indol-3-yl)-6,8-dinitro-[1,2,4]triazolo[1,5-a]pyridine (**7f**);* red-orange powder; yield 99%; mp .>300 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 3.68 (s, 3H), 6.71 (d, *J* = 2.4 Hz, 1H), 6.93 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.44 (t, *J* = 8.7 Hz, 2H), 7.53 (d, *J* = 8.8 Hz, 1H), 8.30 (dd, *J* = 8.6, 5.6 Hz, 2H), 8.58 (s, 1H), 9.24 (s, 1H), 12.41 (s, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 55.69, 101.90, 102.18, 113.33, 114.38, 116.77 (d, J = 22.1 Hz), 126.21 (d, *J* = 2.4 Hz), 126.51, 126.70, 130.35 (d, *J* = 8.9 Hz), 130.65, 131.35, 134.44, 135.47, 140.38, 147.24, 155.47, 164.49 (d, *J* = 248.9 Hz), 165.59. HRMS (ESI, m/z): calcd for $C_{21}H_{14}FN_6O_5$ $[M+H]^+$: 449.1010; found: 449.1004.

*2-(4-Chlorophenyl)-5-(1H-indol-3-yl)-6,8-dinitro-[1,2,4]triazolo[1,5-a]pyridine (**7g**);* red-orange powder; yield 63%; mp >300 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.16 – 7.33 (m, 3H), 7.63 – 7.67 (m, 3H), 8.23 (d, *J* = 8.3 Hz, 2H), 8.63 (d, *J* = 2.6 Hz, 1H), 9.25 (s, 1H), 12.51 (s, 1H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 102.3, 113.7, 119.6, 122.1, 123.6, 125.6, 126.7, 128.4, 129.6, 129.7, 130.9, 134.6, 135.4, 136.6, 136.6, 140.4, 147.2, 165.5. HRMS (ESI, m/z): calcd for $C_{20}H_{12}ClN_6O_4$ $[M+H]^+$: 435.0609; found: 435.0603

*One-pot procedure for the preparation of 5-(1H-indol-3-yl)-6,8-dinitro-[1,2,4]triazolo-[1,5-a]pyridines **7** from 6,8-dinitro-[1,2,4]triazolo-[1,5-a]pyridines **2** and indoles **3***. A mixture of compound **2c** or **2d** (1 mmol) in MeCN (5 ml) and indole **3a** (0.12g, 1.0 mmol) was stirred at 20 °C for 24 h. After full conversion of starting compound (TLC monitoring), DDQ (0.3 g, 1.3 mmol) was added, and the solution was stirred at 20 °C for more 24 h. The solvent was evaporated under reduced pressure, the residue was purified by column chromatography on silica gel (eluent: $CHCl_3$/MeOH 5:1) to afford compounds **7c** (40%) or **7d** (73%) identical to those obtained from dihydro analogs **5c** and **5d**, respectively.

X-ray crystallographic data and refinement details.

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program.[S2] The structure was solved by dual methods using SHELXT[S3] and refined on F^2 using SHELXL-2018[S4] in the OLEX2 program.[S5] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. The location of amino hydrogen atom (H6) was found from the electron density-difference map (e-map), all other hydrogen atoms (with the exception of the disordered acetone molecule) were also found from the e-map but placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters.

Acknowledgment

Crystal structure determination was performed in the Department of Structural Studies of Zelinsky Institute of Organic Chemistry, Moscow.

Table S1. Crystal data and structure refinement for **7a**.

Identification code	**7a**	
Empirical formula	C23 H16 N8 O9	
Formula weight	548.44	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 12.7454(3) Å	α = 90°.
	b = 6.87168(18) Å	β = 93.1454(19)°.
	c = 27.0983(5) Å	γ = 90°.
Volume	2369.76(9) $Å^3$	
Z	4	
Density (calculated)	1.537 g/cm^3	
Absorption coefficient	1.046 mm^{-1}	
F(000)	1128	
Crystal size	0.162 x 0.080 x 0.026 mm	
Theta range for data collection	3.267 to 81.693°.	
Index ranges	-16<=h<=16, -8<=k<=7, -34<=l<=34	
Reflections collected	27515	
Independent reflections	5129 [R(int) = 0.0342]	
Observed reflections	4346	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.818	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5129 / 52 / 391	
Goodness-of-fit on F^2	1.065	
Final R indices [I>2σ(I)]	R1 = 0.0447, wR2 = 0.1204	
R indices (all data)	R1 = 0.0527, wR2 = 0.1266	
Largest diff. peak and hole	0.220 and -0.298 $ē \cdot Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **7a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2780(1)	5761(2)	4745(1)	40(1)
O(2)	3657(1)	7386(2)	5318(1)	39(1)
O(3)	7266(1)	8974(2)	5131(1)	41(1)
O(4)	7987(1)	8399(3)	4441(1)	47(1)
O(5)	3111(1)	1628(2)	1430(1)	29(1)
O(6)	4267(1)	2831(2)	954(1)	39(1)
N(1)	6042(1)	5407(2)	3038(1)	29(1)
N(2)	4254(1)	5150(2)	3053(1)	25(1)
N(3)	4579(1)	4624(2)	2600(1)	24(1)
N(4)	3555(1)	6659(2)	4902(1)	30(1)
N(5)	7236(1)	8393(2)	4703(1)	34(1)
N(6)	1249(1)	4198(2)	2615(1)	27(1)
N(7)	3889(1)	2620(2)	1359(1)	27(1)
C(1)	5159(1)	5580(2)	3294(1)	25(1)
C(2)	3904(1)	4062(2)	2205(1)	24(1)
C(3)	4438(1)	3564(2)	1784(1)	26(1)
C(4)	5520(1)	3784(3)	1748(1)	29(1)
C(5)	6130(1)	4396(3)	2148(1)	30(1)
N(8)	7258(4)	4499(9)	2116(2)	31(1)
O(7)	7594(8)	4557(13)	1698(3)	35(1)
O(8)	7826(4)	4586(12)	2501(2)	50(1)
N(8A)	7219(8)	4989(16)	2079(4)	31(1)
O(7A)	7533(16)	4980(20)	1662(5)	35(1)
O(8A)	7763(7)	5366(17)	2447(3)	50(1)
C(6)	5664(1)	4800(3)	2599(1)	27(1)
C(7)	5214(1)	6229(2)	3813(1)	26(1)
C(8)	6170(1)	6949(2)	4010(1)	28(1)
C(9)	6227(1)	7629(2)	4493(1)	28(1)
C(10)	5373(1)	7600(2)	4786(1)	28(1)
C(11)	4450(1)	6821(2)	4582(1)	27(1)
C(12)	4340(1)	6142(2)	4097(1)	26(1)
C(13)	2792(1)	4175(2)	2256(1)	24(1)
C(14)	2283(1)	3918(2)	2693(1)	25(1)
C(15)	1030(1)	4760(2)	2128(1)	26(1)
C(16)	77(1)	5350(3)	1904(1)	30(1)
C(17)	88(1)	5992(3)	1419(1)	32(1)
C(18)	1026(1)	6041(3)	1175(1)	31(1)
C(19)	1970(1)	5409(2)	1397(1)	27(1)
C(20)	1981(1)	4739(2)	1886(1)	25(1)
C(21)	435(5)	3059(9)	4232(2)	65(1)
C(22)	-368(11)	3490(50)	3823(4)	42(1)
C(23)	-1494(7)	3582(19)	3941(5)	69(2)
O(9)	-134(4)	3783(7)	3399(2)	51(1)
C(21A)	176(14)	2660(20)	4343(6)	65(1)
C(22A)	-300(30)	3370(130)	3859(10)	42(1)
C(23A)	-1428(18)	3930(50)	3863(13)	69(2)
O(9A)	211(9)	3366(17)	3488(4)	51(1)

Table S3. Bond lengths [Å] and angles [°] for **7a**.

O(1)-N(4)	1.221(2)
O(2)-N(4)	1.2329(18)
O(3)-N(5)	1.2241(18)
O(4)-N(5)	1.223(2)
O(5)-N(7)	1.2275(18)
O(6)-N(7)	1.2304(17)
N(1)-C(1)	1.359(2)
N(1)-C(6)	1.3254(19)
N(2)-N(3)	1.3644(17)
N(2)-C(1)	1.327(2)
N(3)-C(2)	1.3912(18)
N(3)-C(6)	1.388(2)
N(4)-C(11)	1.474(2)
N(5)-C(9)	1.475(2)
N(6)-H(6)	0.90(2)
N(6)-C(14)	1.337(2)
N(6)-C(15)	1.386(2)
N(7)-C(3)	1.4651(19)
C(1)-C(7)	1.472(2)
C(2)-C(3)	1.402(2)
C(2)-C(13)	1.433(2)
C(3)-C(4)	1.396(2)
C(4)-H(4)	0.9500
C(4)-C(5)	1.365(2)
C(5)-N(8)	1.447(6)
C(5)-N(8A)	1.467(10)
C(5)-C(6)	1.417(2)
N(8)-O(7)	1.234(6)
N(8)-O(8)	1.237(6)
N(8A)-O(7A)	1.222(11)
N(8A)-O(8A)	1.210(10)
C(7)-C(8)	1.394(2)
C(7)-C(12)	1.391(2)
C(8)-H(8)	0.9500
C(8)-C(9)	1.388(2)
C(9)-C(10)	1.381(2)
C(10)-H(10)	0.9500
C(10)-C(11)	1.380(2)
C(11)-C(12)	1.393(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.394(2)
C(13)-C(20)	1.452(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.389(2)
C(15)-C(20)	1.410(2)
C(16)-H(16)	0.9500
C(16)-C(17)	1.387(2)
C(17)-H(17)	0.9500
C(17)-C(18)	1.397(3)
C(18)-H(18)	0.9500

C(18)-C(19)	1.385(2)
C(19)-H(19)	0.9500
C(19)-C(20)	1.403(2)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(21)-C(22)	1.495(9)
C(22)-C(23)	1.488(8)
C(22)-O(9)	1.221(6)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(21A)-H(21D)	0.9800
C(21A)-H(21E)	0.9800
C(21A)-H(21F)	0.9800
C(21A)-C(22A)	1.496(13)
C(22A)-C(23A)	1.493(14)
C(22A)-O(9A)	1.226(15)
C(23A)-H(23D)	0.9800
C(23A)-H(23E)	0.9800
C(23A)-H(23F)	0.9800

C(6)-N(1)-C(1)	102.45(13)
C(1)-N(2)-N(3)	101.80(12)
N(2)-N(3)-C(2)	124.10(13)
N(2)-N(3)-C(6)	109.23(12)
C(6)-N(3)-C(2)	126.65(13)
O(1)-N(4)-O(2)	124.40(15)
O(1)-N(4)-C(11)	118.12(13)
O(2)-N(4)-C(11)	117.43(14)
O(3)-N(5)-C(9)	117.60(15)
O(4)-N(5)-O(3)	124.32(15)
O(4)-N(5)-C(9)	118.07(13)
C(14)-N(6)-H(6)	124.9(13)
C(14)-N(6)-C(15)	109.68(13)
C(15)-N(6)-H(6)	125.3(13)
O(5)-N(7)-O(6)	124.36(13)
O(5)-N(7)-C(3)	118.58(12)
O(6)-N(7)-C(3)	117.01(13)
N(1)-C(1)-C(7)	121.09(14)
N(2)-C(1)-N(1)	116.69(13)
N(2)-C(1)-C(7)	122.21(14)
N(3)-C(2)-C(3)	112.76(13)
N(3)-C(2)-C(13)	118.88(13)
C(3)-C(2)-C(13)	128.21(13)
C(2)-C(3)-N(7)	120.97(14)
C(4)-C(3)-N(7)	115.13(13)
C(4)-C(3)-C(2)	123.74(14)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-C(3)	120.02(15)
C(5)-C(4)-H(4)	120.0
C(4)-C(5)-N(8)	119.5(3)

C(4)-C(5)-N(8A)	119.1(4)
C(4)-C(5)-C(6)	119.87(15)
C(6)-C(5)-N(8)	120.4(3)
C(6)-C(5)-N(8A)	119.9(4)
O(7)-N(8)-C(5)	116.8(6)
O(7)-N(8)-O(8)	123.8(7)
O(8)-N(8)-C(5)	119.4(5)
O(7A)-N(8A)-C(5)	118.5(12)
O(8A)-N(8A)-C(5)	117.3(9)
O(8A)-N(8A)-O(7A)	124.1(13)
N(1)-C(6)-N(3)	109.82(13)
N(1)-C(6)-C(5)	133.43(15)
N(3)-C(6)-C(5)	116.69(13)
C(8)-C(7)-C(1)	117.93(15)
C(12)-C(7)-C(1)	121.23(14)
C(12)-C(7)-C(8)	120.85(14)
C(7)-C(8)-H(8)	120.7
C(9)-C(8)-C(7)	118.69(15)
C(9)-C(8)-H(8)	120.7
C(8)-C(9)-N(5)	118.93(15)
C(10)-C(9)-N(5)	118.73(14)
C(10)-C(9)-C(8)	122.34(15)
C(9)-C(10)-H(10)	121.4
C(11)-C(10)-C(9)	117.19(14)
C(11)-C(10)-H(10)	121.4
C(10)-C(11)-N(4)	117.66(13)
C(10)-C(11)-C(12)	123.13(15)
C(12)-C(11)-N(4)	119.18(14)
C(7)-C(12)-C(11)	117.76(15)
C(7)-C(12)-H(12)	121.1
C(11)-C(12)-H(12)	121.1
C(2)-C(13)-C(20)	128.17(14)
C(14)-C(13)-C(2)	125.77(13)
C(14)-C(13)-C(20)	105.85(13)
N(6)-C(14)-C(13)	110.30(13)
N(6)-C(14)-H(14)	124.8
C(13)-C(14)-H(14)	124.8
N(6)-C(15)-C(16)	128.54(15)
N(6)-C(15)-C(20)	107.81(13)
C(16)-C(15)-C(20)	123.58(15)
C(15)-C(16)-H(16)	121.5
C(17)-C(16)-C(15)	116.97(16)
C(17)-C(16)-H(16)	121.5
C(16)-C(17)-H(17)	119.7
C(16)-C(17)-C(18)	120.63(15)
C(18)-C(17)-H(17)	119.7
C(17)-C(18)-H(18)	118.9
C(19)-C(18)-C(17)	122.17(15)
C(19)-C(18)-H(18)	118.9
C(18)-C(19)-H(19)	120.8
C(18)-C(19)-C(20)	118.47(15)
C(20)-C(19)-H(19)	120.8

C(15)-C(20)-C(13)	106.25(13)
C(19)-C(20)-C(13)	135.20(15)
C(19)-C(20)-C(15)	118.15(14)
H(21A)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(22)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21C)	109.5
C(23)-C(22)-C(21)	118.5(6)
O(9)-C(22)-C(21)	122.5(8)
O(9)-C(22)-C(23)	119.0(8)
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
H(21D)-C(21A)-H(21E)	109.5
H(21D)-C(21A)-H(21F)	109.5
H(21E)-C(21A)-H(21F)	109.5
C(22A)-C(21A)-H(21D)	109.5
C(22A)-C(21A)-H(21E)	109.5
C(22A)-C(21A)-H(21F)	109.5
C(23A)-C(22A)-C(21A)	114.9(15)
O(9A)-C(22A)-C(21A)	120.9(18)
O(9A)-C(22A)-C(23A)	124.1(19)
C(22A)-C(23A)-H(23D)	109.5
C(22A)-C(23A)-H(23E)	109.5
C(22A)-C(23A)-H(23F)	109.5
H(23D)-C(23A)-H(23E)	109.5
H(23D)-C(23A)-H(23F)	109.5
H(23E)-C(23A)-H(23F)	109.5

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7a**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	33(1)	60(1)	27(1)	-1(1)	0(1)	-7(1)
O(2)	44(1)	51(1)	21(1)	-7(1)	2(1)	2(1)
O(3)	45(1)	55(1)	23(1)	-7(1)	-8(1)	-9(1)
O(4)	37(1)	73(1)	31(1)	-5(1)	0(1)	-14(1)
O(5)	29(1)	34(1)	24(1)	-4(1)	-1(1)	-4(1)
O(6)	40(1)	60(1)	18(1)	-5(1)	4(1)	-8(1)
N(1)	28(1)	38(1)	20(1)	-3(1)	-2(1)	0(1)
N(2)	30(1)	29(1)	14(1)	-1(1)	-2(1)	2(1)
N(3)	25(1)	29(1)	16(1)	-1(1)	-1(1)	1(1)
N(4)	34(1)	36(1)	21(1)	1(1)	-2(1)	3(1)
N(5)	36(1)	41(1)	24(1)	-1(1)	-5(1)	-6(1)

N(6)	27(1)	32(1)	22(1)	-1(1)	3(1)	-2(1)
N(7)	29(1)	35(1)	18(1)	-2(1)	0(1)	1(1)
C(1)	28(1)	28(1)	18(1)	0(1)	-2(1)	0(1)
C(2)	27(1)	27(1)	17(1)	1(1)	-2(1)	-1(1)
C(3)	29(1)	31(1)	17(1)	-1(1)	-3(1)	0(1)
C(4)	30(1)	36(1)	20(1)	-2(1)	3(1)	2(1)
C(5)	24(1)	43(1)	24(1)	-4(1)	1(1)	-1(1)
N(8)	26(1)	43(3)	25(1)	-4(2)	2(1)	1(1)
O(7)	29(1)	52(4)	25(1)	-3(2)	5(1)	1(2)
O(8)	26(1)	97(4)	26(1)	-7(2)	-4(1)	1(2)
N(8A)	26(1)	43(3)	25(1)	-4(2)	2(1)	1(1)
O(7A)	29(1)	52(4)	25(1)	-3(2)	5(1)	1(2)
O(8A)	26(1)	97(4)	26(1)	-7(2)	-4(1)	1(2)
C(6)	26(1)	36(1)	21(1)	-1(1)	-2(1)	0(1)
C(7)	32(1)	26(1)	18(1)	1(1)	-4(1)	2(1)
C(8)	32(1)	32(1)	20(1)	2(1)	-2(1)	-1(1)
C(9)	33(1)	30(1)	21(1)	2(1)	-6(1)	-3(1)
C(10)	38(1)	29(1)	17(1)	1(1)	-5(1)	1(1)
C(11)	33(1)	28(1)	19(1)	2(1)	-2(1)	4(1)
C(12)	31(1)	26(1)	19(1)	2(1)	-5(1)	2(1)
C(13)	29(1)	26(1)	17(1)	-1(1)	-2(1)	-1(1)
C(14)	28(1)	27(1)	20(1)	0(1)	0(1)	0(1)
C(15)	29(1)	28(1)	21(1)	-3(1)	-1(1)	-2(1)
C(16)	27(1)	31(1)	31(1)	-7(1)	-3(1)	-1(1)
C(17)	33(1)	32(1)	31(1)	-6(1)	-11(1)	2(1)
C(18)	40(1)	31(1)	22(1)	-2(1)	-9(1)	2(1)
C(19)	32(1)	30(1)	19(1)	-2(1)	-2(1)	0(1)
C(20)	28(1)	27(1)	20(1)	-2(1)	-3(1)	-1(1)
C(21)	78(4)	48(3)	68(3)	15(2)	-4(2)	5(2)
C(22)	52(2)	36(5)	39(2)	-3(2)	15(2)	-4(2)
C(23)	54(2)	82(5)	72(4)	-11(3)	22(2)	-6(2)
O(9)	53(2)	61(2)	41(2)	-7(1)	20(2)	-14(2)
C(21A)	78(4)	48(3)	68(3)	15(2)	-4(2)	5(2)
C(22A)	52(2)	36(5)	39(2)	-3(2)	15(2)	-4(2)
C(23A)	54(2)	82(5)	72(4)	-11(3)	22(2)	-6(2)
O(9A)	53(2)	61(2)	41(2)	-7(1)	20(2)	-14(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7a**.

	x	y	z	U(eq)
H(6)	778(17)	4130(30)	2848(8)	32
H(4)	5832	3509	1445	35
H(8)	6771	6973	3818	34
H(10)	5419	8095	5113	34
H(12)	3689	5637	3966	31
H(14)	2622	3591	3003	30
H(16)	-554	5315	2075	36
H(17)	-547	6403	1251	39
H(18)	1015	6523	846	37
H(19)	2595	5428	1222	33
H(21A)	1140	3225	4111	97
H(21B)	350	1716	4344	97
H(21C)	341	3954	4507	97
H(23A)	-1922	3938	3644	103
H(23B)	-1582	4562	4199	103
H(23C)	-1718	2309	4060	103
H(21D)	937	2512	4321	97
H(21E)	-134	1405	4424	97
H(21F)	36	3607	4603	97
H(23D)	-1704	4175	3524	103
H(23E)	-1496	5117	4060	103
H(23F)	-1828	2877	4007	103

Table S6. Torsion angles [°] for **7a**.

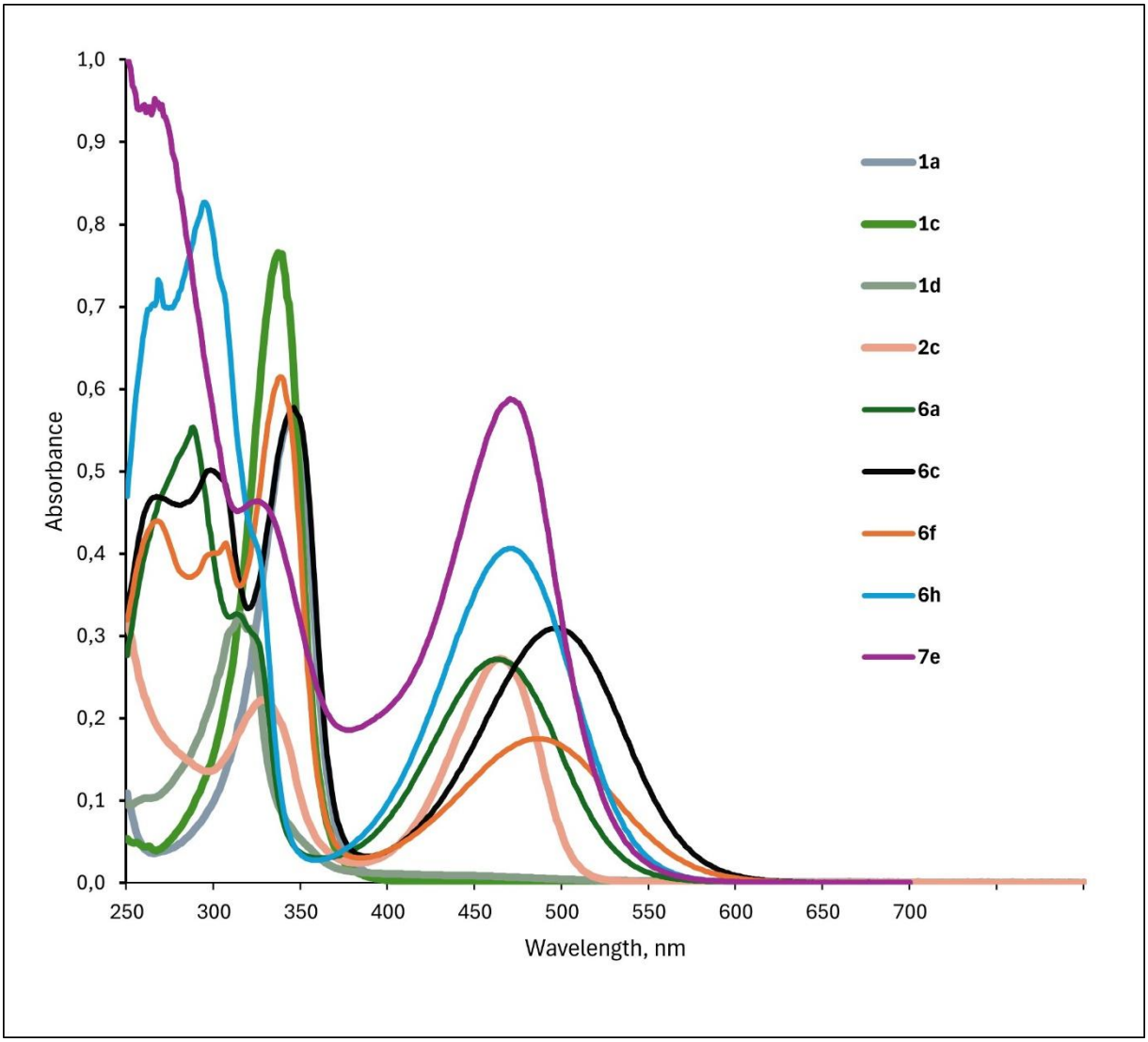
O(1)-N(4)-C(11)-C(10)	-171.27(16)
O(1)-N(4)-C(11)-C(12)	7.0(2)
O(2)-N(4)-C(11)-C(10)	6.3(2)
O(2)-N(4)-C(11)-C(12)	-175.46(15)
O(3)-N(5)-C(9)-C(8)	-179.62(16)
O(3)-N(5)-C(9)-C(10)	-0.3(2)
O(4)-N(5)-C(9)-C(8)	0.2(2)
O(4)-N(5)-C(9)-C(10)	179.52(16)
O(5)-N(7)-C(3)-C(2)	-27.0(2)
O(5)-N(7)-C(3)-C(4)	148.53(15)
O(6)-N(7)-C(3)-C(2)	155.27(16)
O(6)-N(7)-C(3)-C(4)	-29.2(2)
N(1)-C(1)-C(7)-C(8)	9.8(2)
N(1)-C(1)-C(7)-C(12)	-170.64(15)
N(2)-N(3)-C(2)-C(3)	-179.01(14)
N(2)-N(3)-C(2)-C(13)	5.1(2)
N(2)-N(3)-C(6)-N(1)	0.43(19)
N(2)-N(3)-C(6)-C(5)	-177.15(14)
N(2)-C(1)-C(7)-C(8)	-169.72(15)
N(2)-C(1)-C(7)-C(12)	9.8(2)
N(3)-N(2)-C(1)-N(1)	0.83(18)
N(3)-N(2)-C(1)-C(7)	-179.62(14)
N(3)-C(2)-C(3)-N(7)	169.40(14)
N(3)-C(2)-C(3)-C(4)	-5.8(2)
N(3)-C(2)-C(13)-C(14)	-31.6(2)
N(3)-C(2)-C(13)-C(20)	142.33(16)
N(4)-C(11)-C(12)-C(7)	-176.90(14)
N(5)-C(9)-C(10)-C(11)	-178.05(15)
N(6)-C(15)-C(16)-C(17)	174.88(16)
N(6)-C(15)-C(20)-C(13)	-1.27(18)
N(6)-C(15)-C(20)-C(19)	-175.06(14)
N(7)-C(3)-C(4)-C(5)	-170.96(16)
C(1)-N(1)-C(6)-N(3)	0.06(18)
C(1)-N(1)-C(6)-C(5)	177.08(19)
C(1)-N(2)-N(3)-C(2)	-179.04(14)
C(1)-N(2)-N(3)-C(6)	-0.72(16)
C(1)-C(7)-C(8)-C(9)	177.80(14)
C(1)-C(7)-C(12)-C(11)	-178.71(14)
C(2)-N(3)-C(6)-N(1)	178.70(15)
C(2)-N(3)-C(6)-C(5)	1.1(2)
C(2)-C(3)-C(4)-C(5)	4.5(3)
C(2)-C(13)-C(14)-N(6)	177.53(15)
C(2)-C(13)-C(20)-C(15)	-175.57(15)
C(2)-C(13)-C(20)-C(19)	-3.3(3)
C(3)-C(2)-C(13)-C(14)	153.18(17)
C(3)-C(2)-C(13)-C(20)	-32.9(3)
C(3)-C(4)-C(5)-N(8)	176.0(3)
C(3)-C(4)-C(5)-N(8A)	-168.0(5)
C(3)-C(4)-C(5)-C(6)	0.2(3)
C(4)-C(5)-N(8)-O(7)	19.7(6)

C(4)-C(5)-N(8)-O(8)	-162.6(4)
C(4)-C(5)-N(8A)-O(7A)	2.6(13)
C(4)-C(5)-N(8A)-O(8A)	-173.9(7)
C(4)-C(5)-C(6)-N(1)	-179.66(19)
C(4)-C(5)-C(6)-N(3)	-2.8(3)
N(8)-C(5)-C(6)-N(1)	4.5(4)
N(8)-C(5)-C(6)-N(3)	-178.6(3)
N(8A)-C(5)-C(6)-N(1)	-11.6(6)
N(8A)-C(5)-C(6)-N(3)	165.3(5)
C(6)-N(1)-C(1)-N(2)	-0.58(19)
C(6)-N(1)-C(1)-C(7)	179.86(15)
C(6)-N(3)-C(2)-C(3)	3.0(2)
C(6)-N(3)-C(2)-C(13)	-172.95(15)
C(6)-C(5)-N(8)-O(7)	-164.5(5)
C(6)-C(5)-N(8)-O(8)	13.3(5)
C(6)-C(5)-N(8A)-O(7A)	-165.6(9)
C(6)-C(5)-N(8A)-O(8A)	17.9(11)
C(7)-C(8)-C(9)-N(5)	-179.99(15)
C(7)-C(8)-C(9)-C(10)	0.7(3)
C(8)-C(7)-C(12)-C(11)	0.8(2)
C(8)-C(9)-C(10)-C(11)	1.3(2)
C(9)-C(10)-C(11)-N(4)	175.90(14)
C(9)-C(10)-C(11)-C(12)	-2.3(2)
C(10)-C(11)-C(12)-C(7)	1.3(2)
C(12)-C(7)-C(8)-C(9)	-1.7(2)
C(13)-C(2)-C(3)-N(7)	-15.2(3)
C(13)-C(2)-C(3)-C(4)	169.68(16)
C(14)-N(6)-C(15)-C(16)	-174.13(17)
C(14)-N(6)-C(15)-C(20)	2.86(18)
C(14)-C(13)-C(20)-C(15)	-0.67(17)
C(14)-C(13)-C(20)-C(19)	171.56(18)
C(15)-N(6)-C(14)-C(13)	-3.37(19)
C(15)-C(16)-C(17)-C(18)	-0.3(2)
C(16)-C(15)-C(20)-C(13)	175.91(15)
C(16)-C(15)-C(20)-C(19)	2.1(2)
C(16)-C(17)-C(18)-C(19)	1.8(3)
C(17)-C(18)-C(19)-C(20)	-1.4(3)
C(18)-C(19)-C(20)-C(13)	-172.05(17)
C(18)-C(19)-C(20)-C(15)	-0.5(2)
C(20)-C(13)-C(14)-N(6)	2.47(18)
C(20)-C(15)-C(16)-C(17)	-1.7(2)

Table S7. Hydrogen bonds for **7a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6)...O(9)	0.90(2)	1.96(2)	2.848(4)	173(2)
N(6)-H(6)...O(9A)	0.90(2)	1.99(2)	2.831(10)	156.9(19)

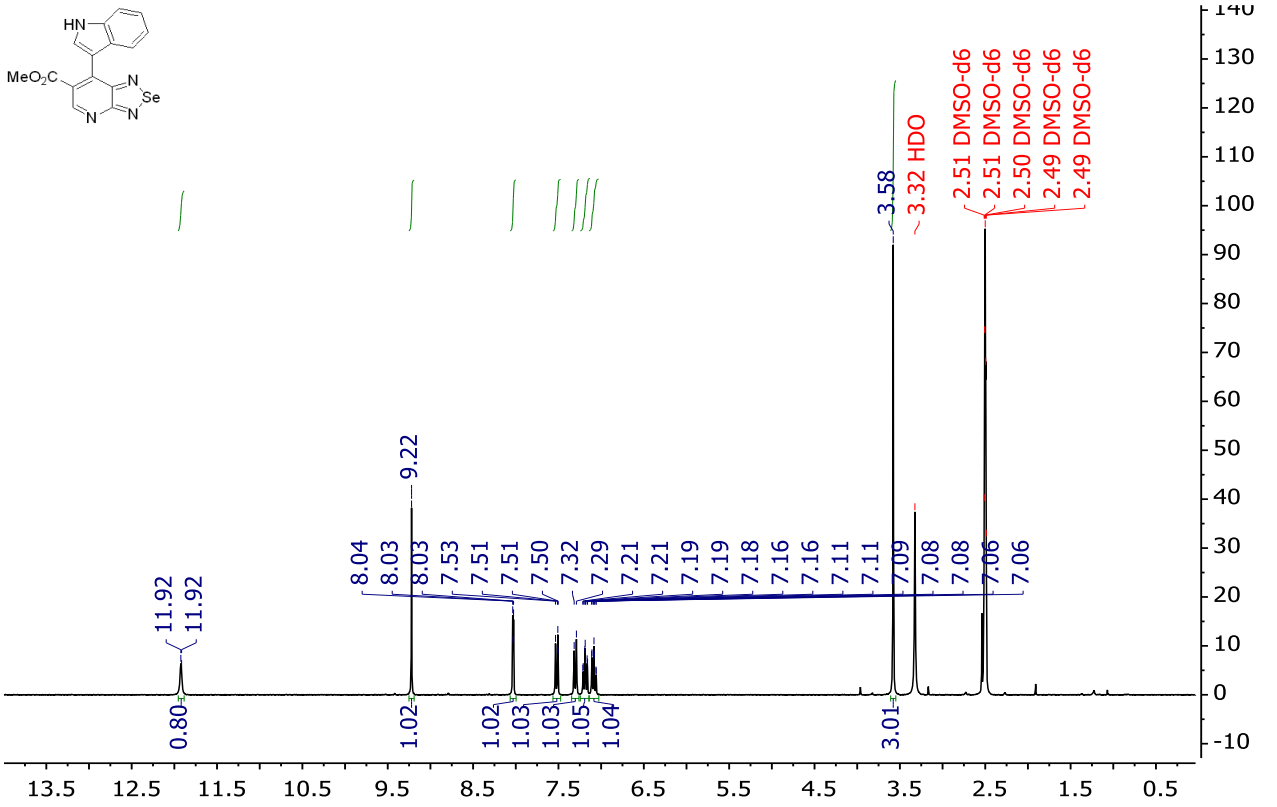
UV-Vis spectra of compounds **1a**, **1c**, **1d, 2c**, **6a, 6c, 6f, 6h, 7e**

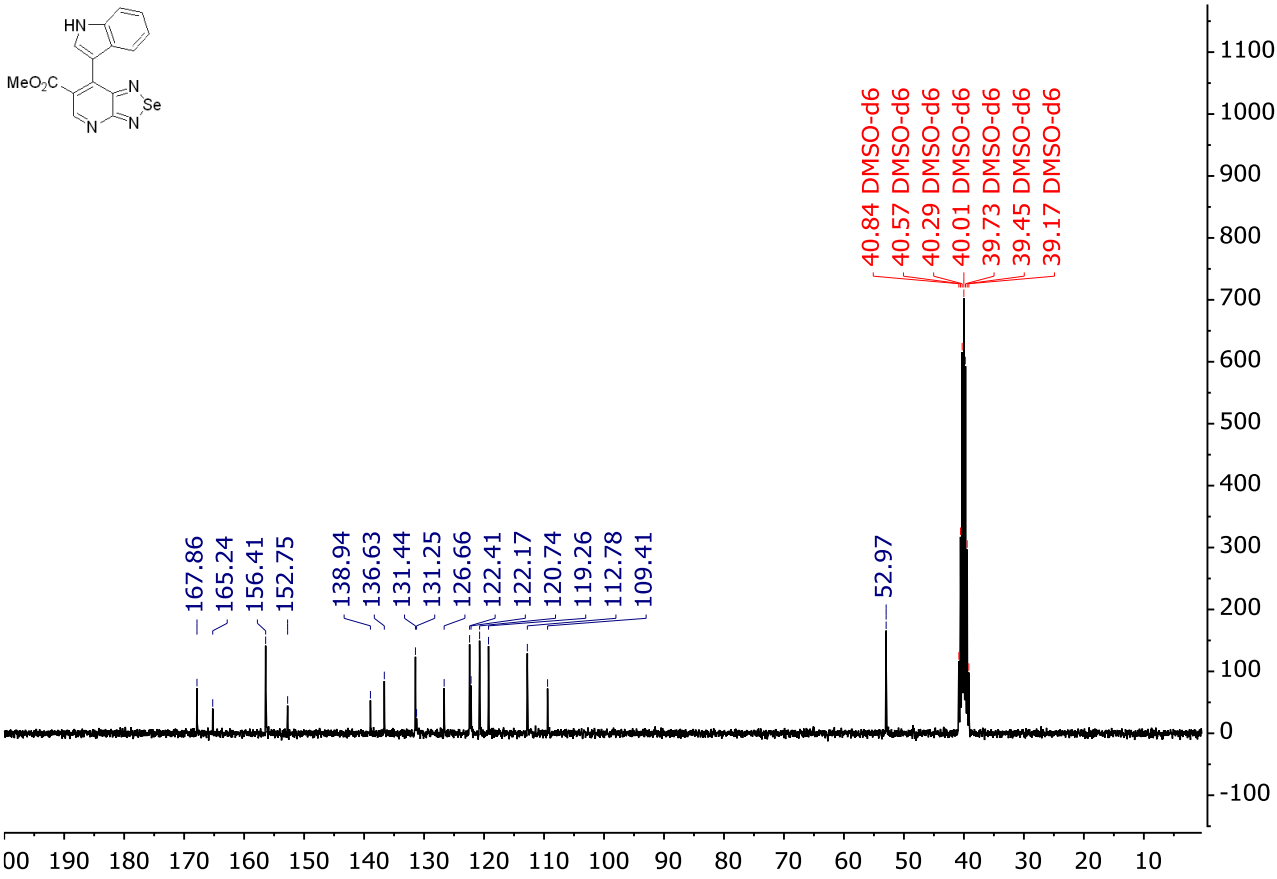


Sample	λ_{max1}/nm	ε_1 /dm^{3}mol^{-1}cm^{-1}	λ_{max2}/nm	ε_2/dm^{3}mol^{-1}cm^{-1}
6a	288	16129	463	7921
6c	346	16825	495	9015
6f	338	17922	487	5110
6h	295	24095	470	11846
7e	325	13521	470	17146

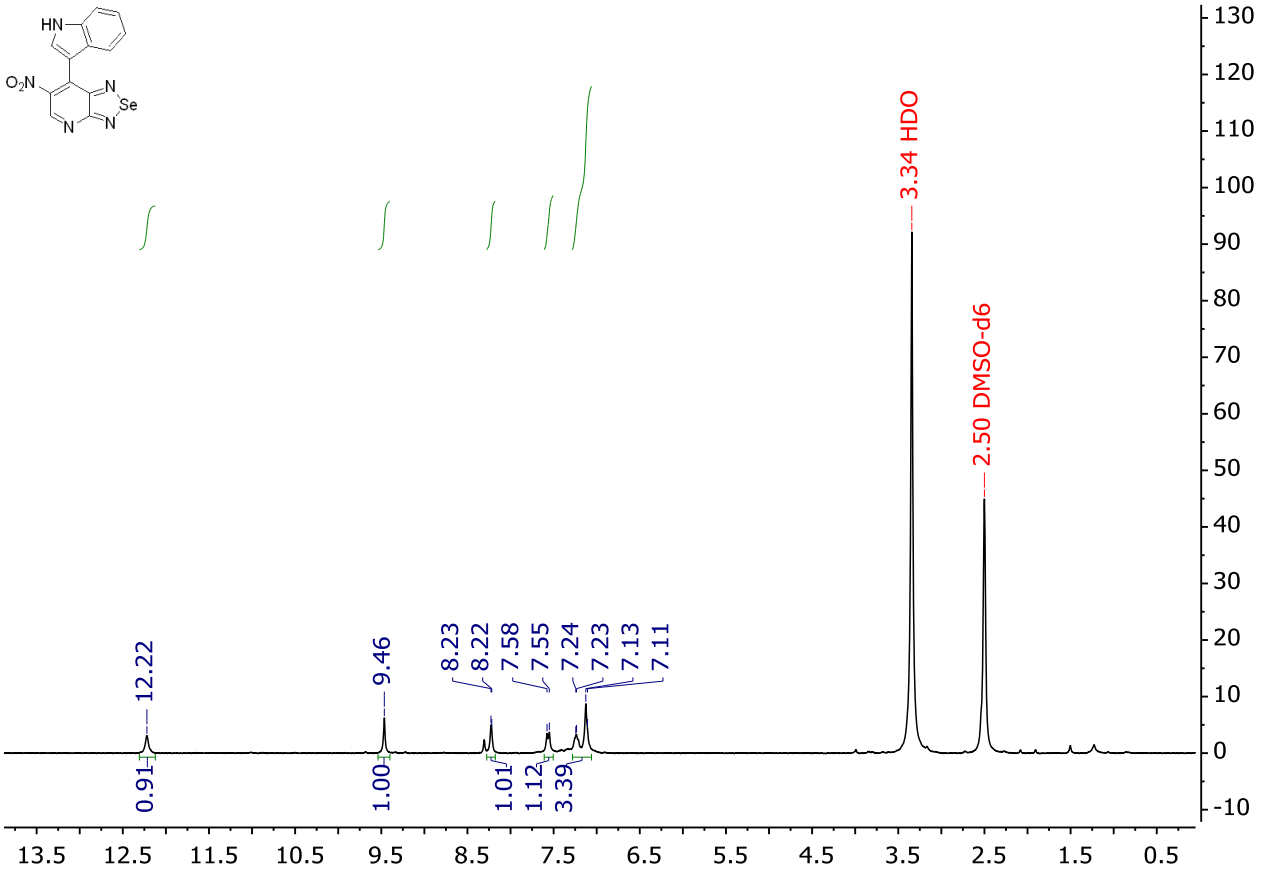
NMR spectra for compounds 6 and 7

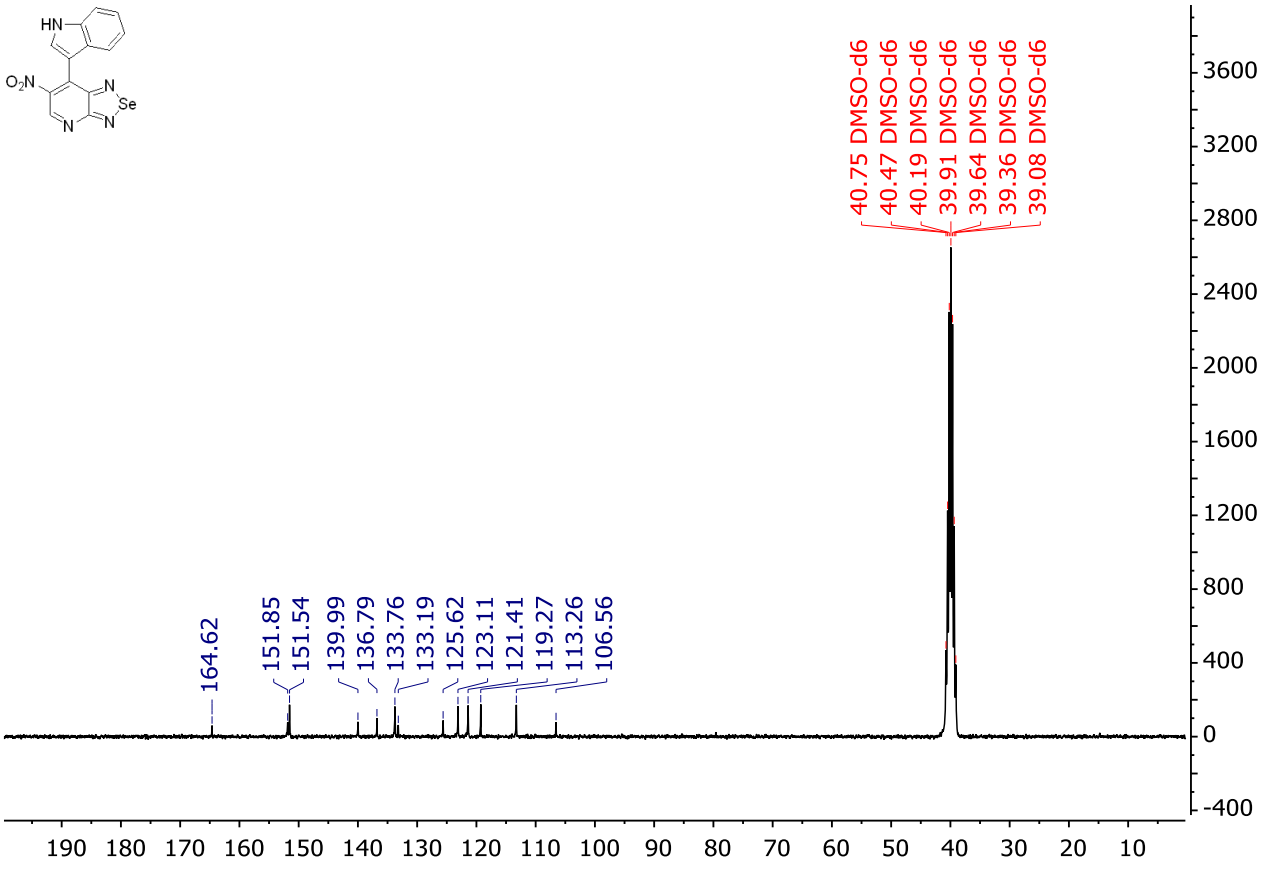
6a



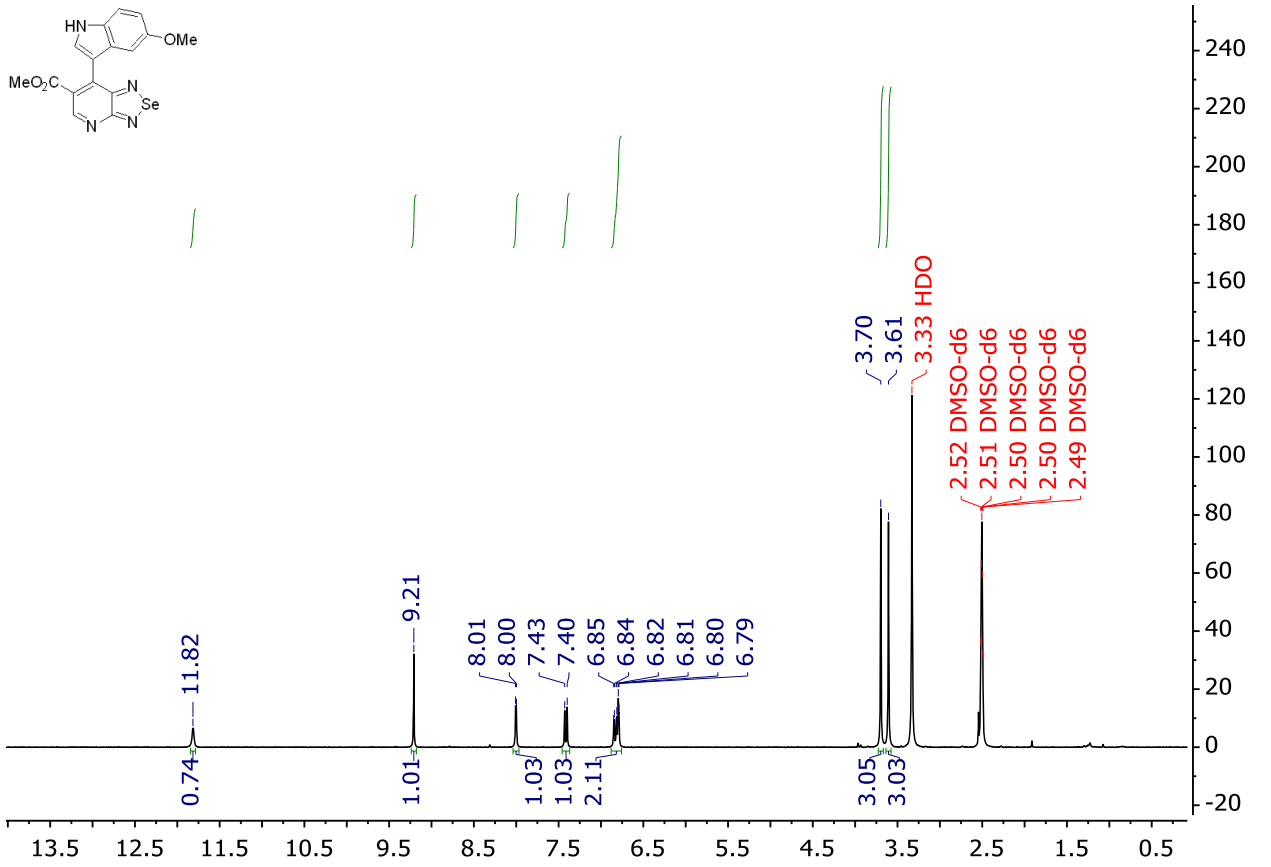


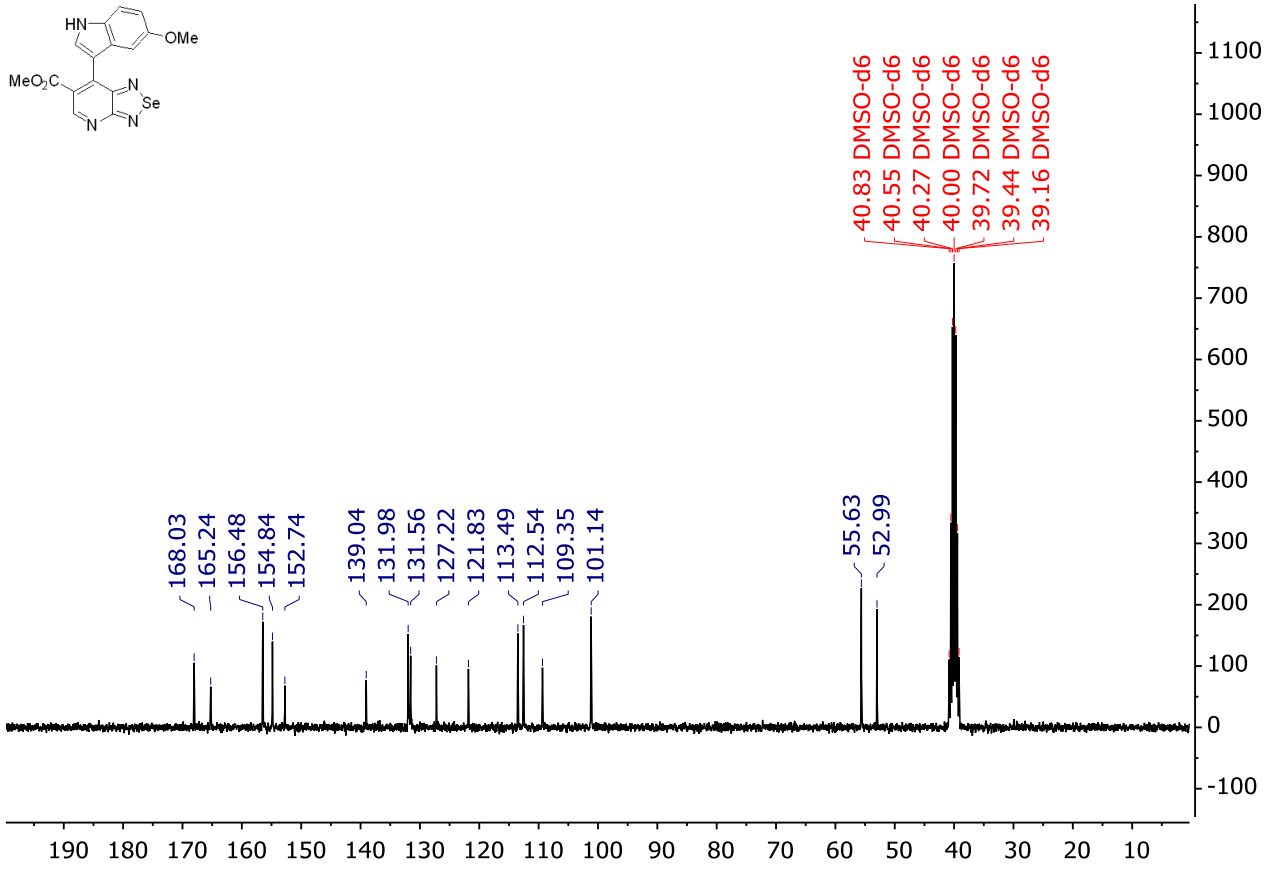
6b


HN
O2N
N
Se
N
N
12.22
9.46
8.23
8.22
7.58
7.55
7.24
7.23
7.13
7.11
3.34 HDO
2.50 DMSO-d6
0.91
1.00
1.01
1.12
3.39
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

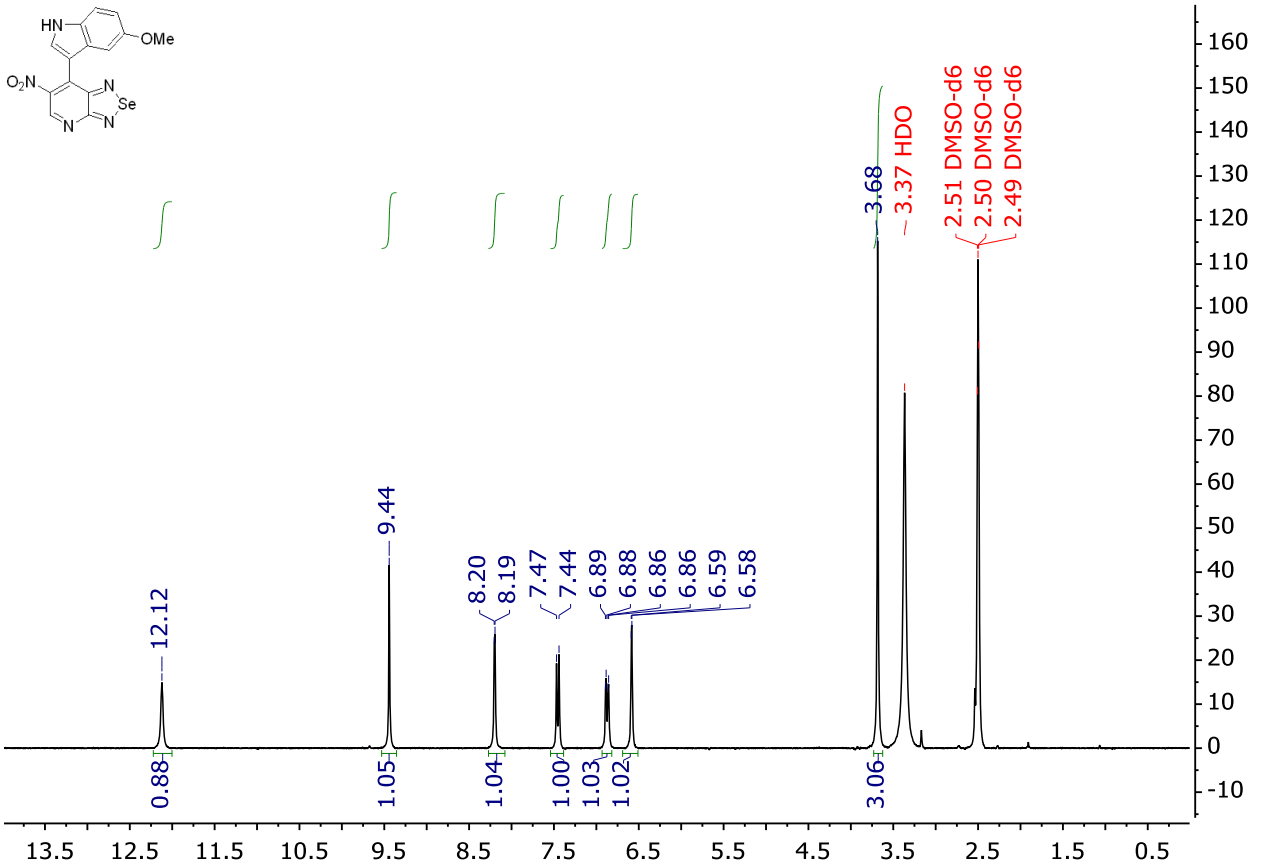

HN
O2N
N
Se
N
N
164.62
151.85
151.54
139.99
136.79
133.76
133.19
125.62
123.11
121.41
119.27
113.26
106.56
40.75 DMSO-d6
40.47 DMSO-d6
40.19 DMSO-d6
39.91 DMSO-d6
39.64 DMSO-d6
39.36 DMSO-d6
39.08 DMSO-d6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

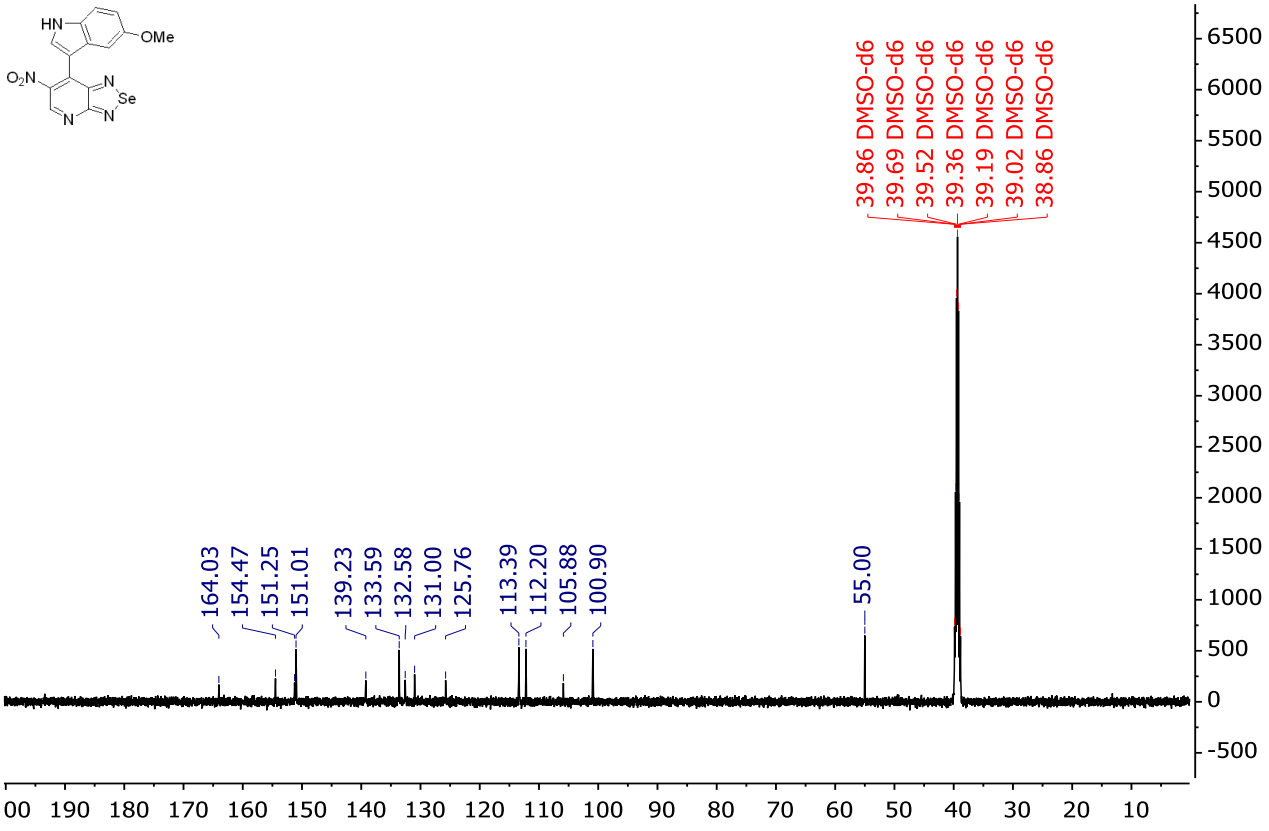
6c


HN
OMe
MeO2C
N
Se
N
N
11.82
9.21
8.01
8.00
7.43
7.40
6.85
6.84
6.82
6.81
6.80
6.79
3.70
3.61
3.33 HDO
2.52 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
0.74
1.01
1.03
1.03
2.11
3.05
3.03

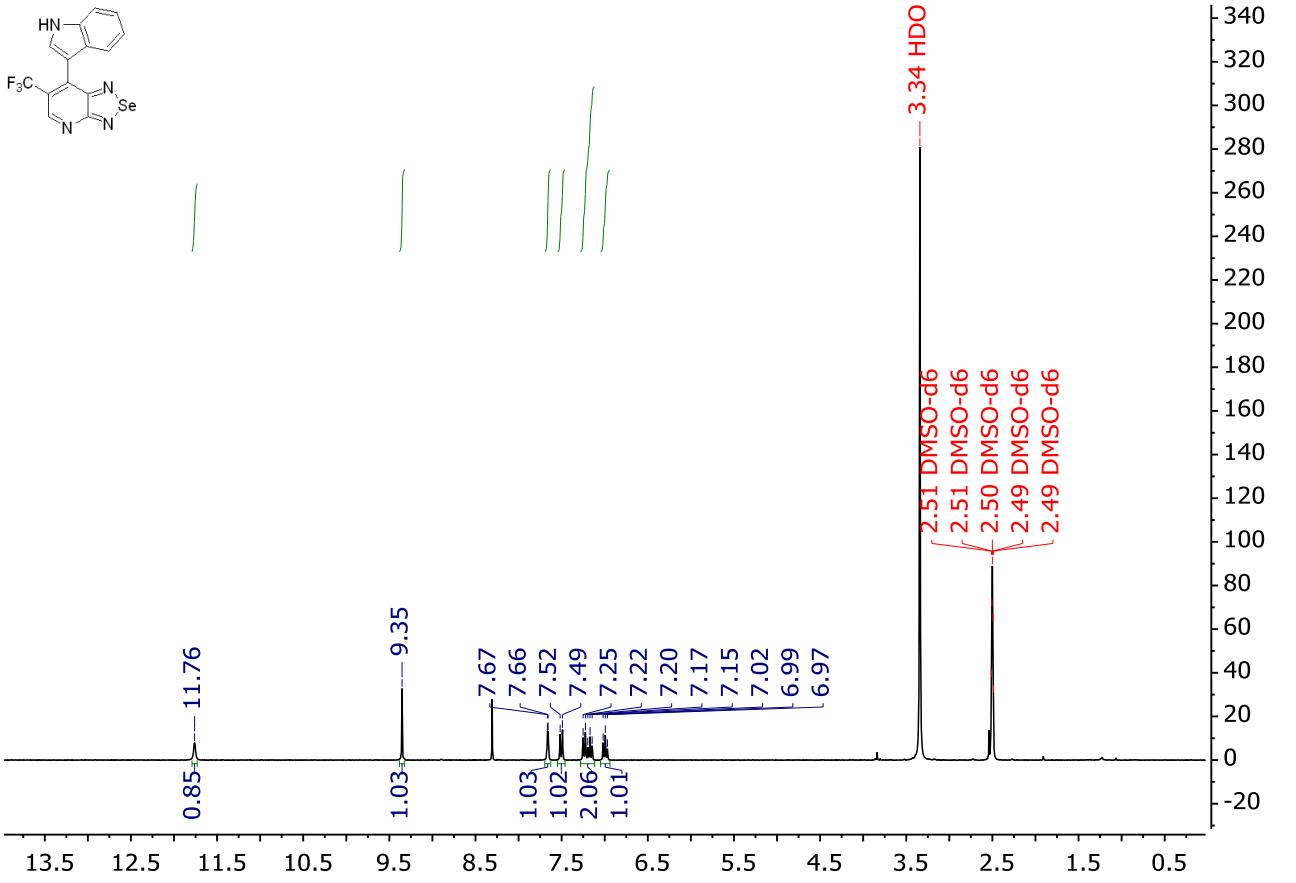

HN
OMe
MeO2C
N
Se
N
N
168.03
165.24
156.48
154.84
152.74
139.04
131.98
131.56
127.22
121.83
113.49
112.54
109.35
101.14
55.63
52.99
40.83 DMSO-d6
40.55 DMSO-d6
40.27 DMSO-d6
40.00 DMSO-d6
39.72 DMSO-d6
39.44 DMSO-d6
39.16 DMSO-d6

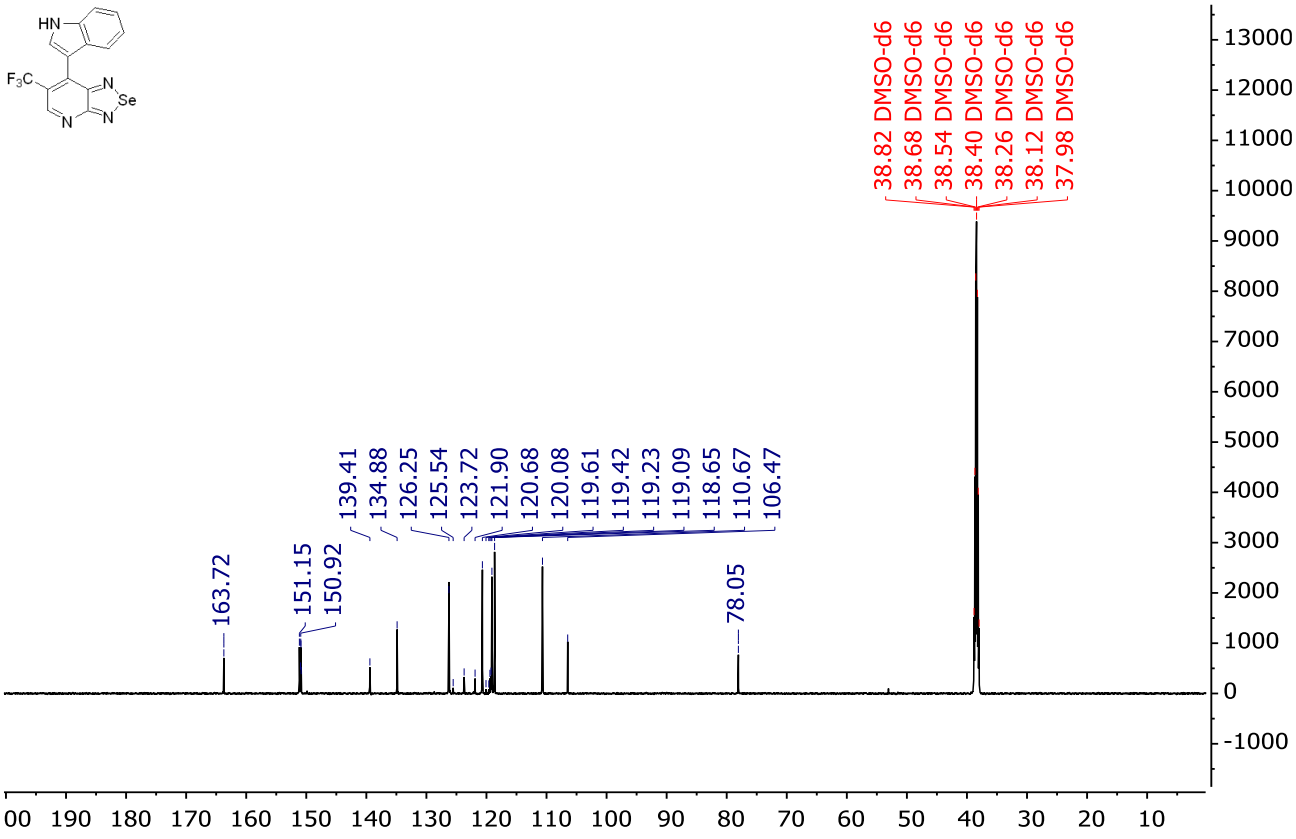
6d


HN
OMe
O2N
N
Se
N
12.12
9.44
8.20
8.19
7.47
7.44
6.89
6.88
6.86
6.86
6.59
6.58
3.68
3.37 HDO
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
0.88
1.05
1.04
1.00
1.03
1.02
3.06

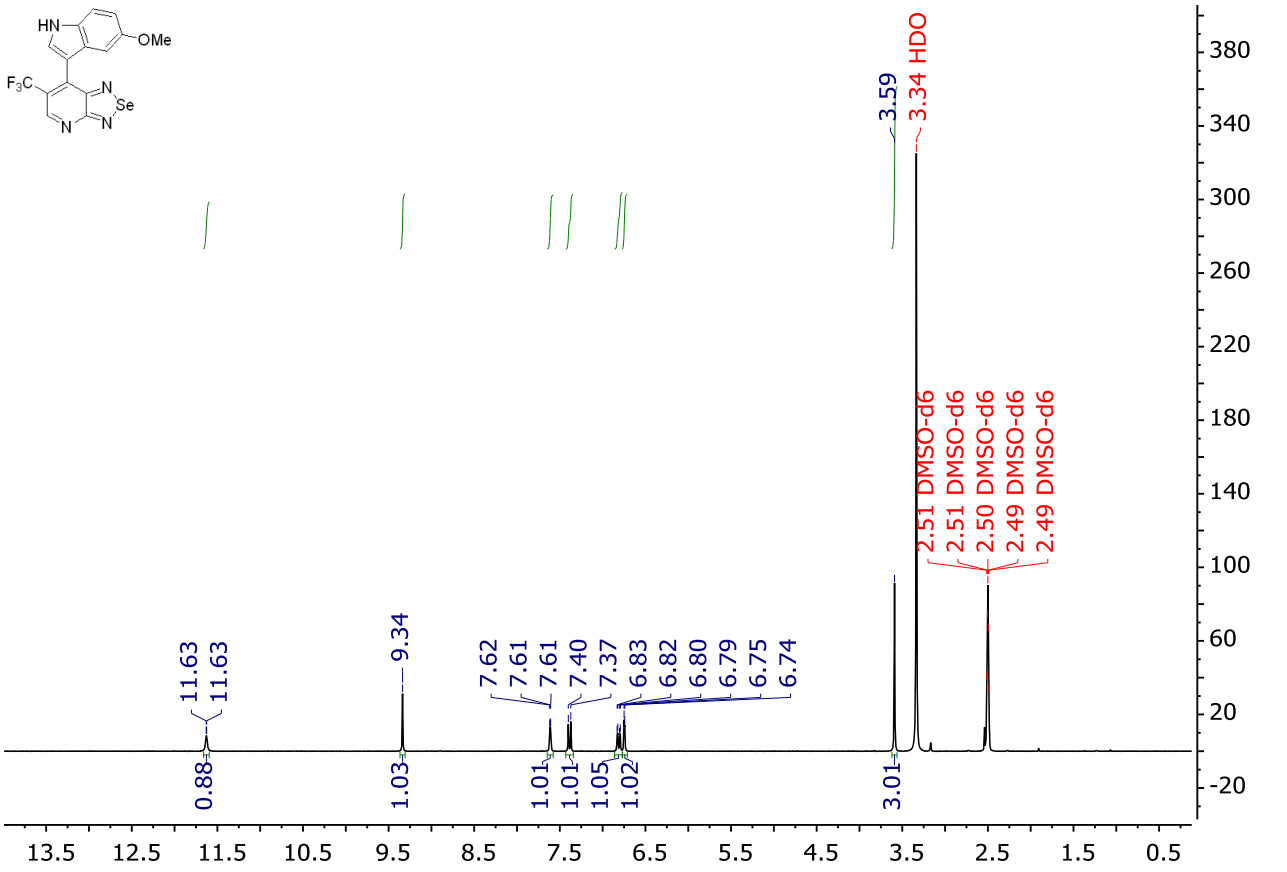

HN
OMe
O2N
N
Se
N
164.03
154.47
151.25
151.01
139.23
133.59
132.58
131.00
125.76
113.39
112.20
105.88
100.90
55.00
39.86 DMSO-d6
39.69 DMSO-d6
39.52 DMSO-d6
39.36 DMSO-d6
39.19 DMSO-d6
39.02 DMSO-d6
38.86 DMSO-d6

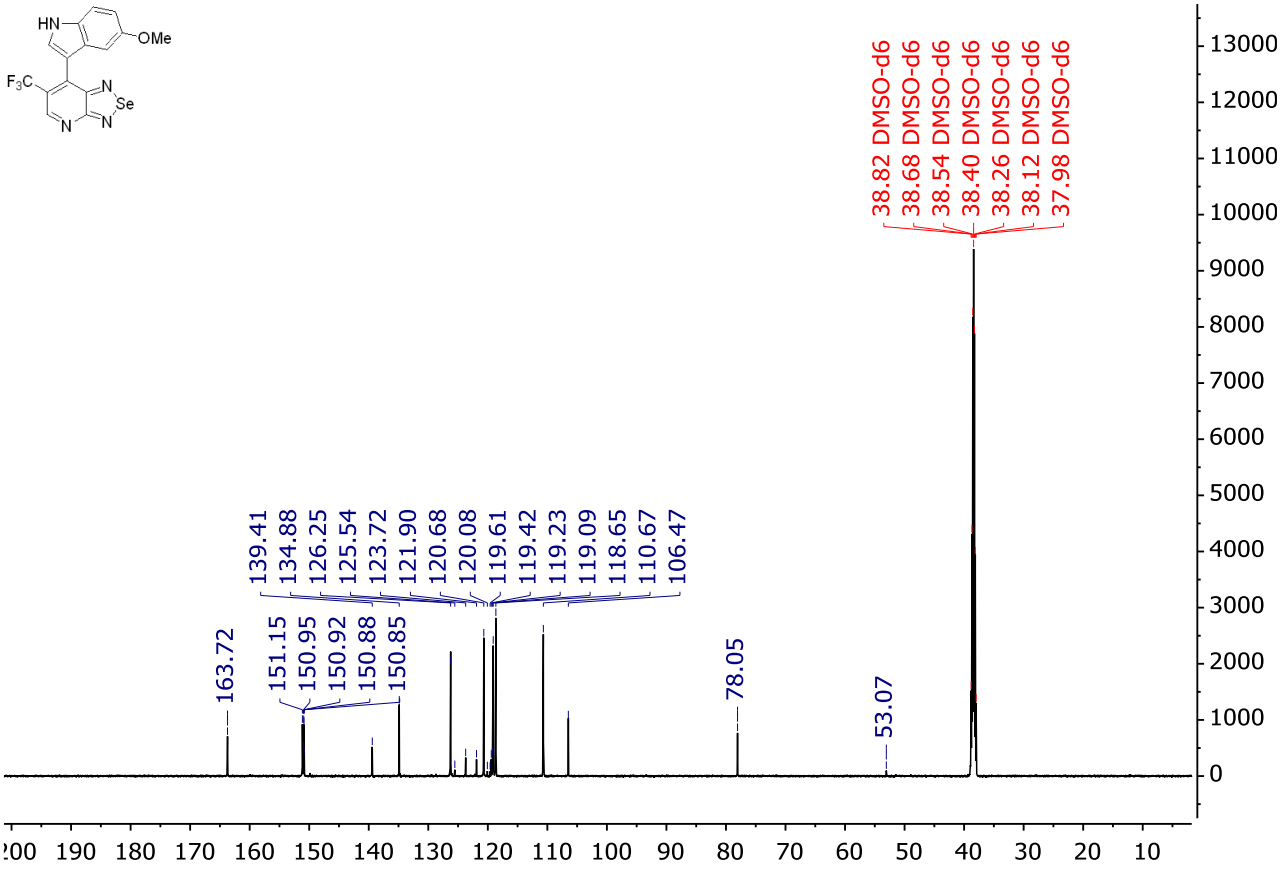
6e


HN
F3C
N
Se
N
N
3.34 HDO
2.51 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
11.76
9.35
7.67
7.66
7.52
7.49
7.25
7.22
7.20
7.17
7.15
7.02
6.99
6.97
0.85
1.03
1.03
1.02
2.06
1.01

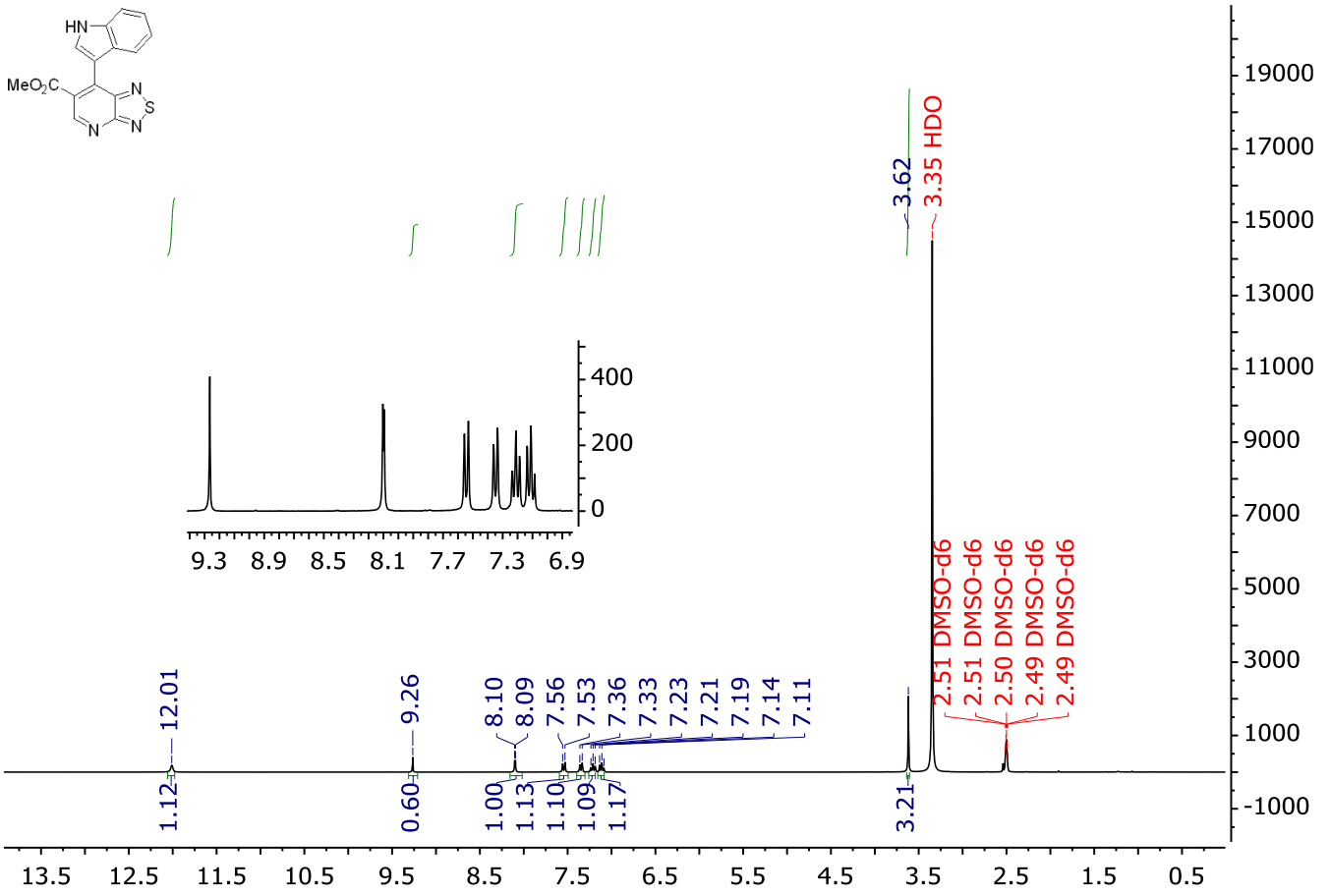

HN
F3C
N
Se
N
N
38.82 DMSO-d6
38.68 DMSO-d6
38.54 DMSO-d6
38.40 DMSO-d6
38.26 DMSO-d6
38.12 DMSO-d6
37.98 DMSO-d6
163.72
151.15
150.92
139.41
134.88
126.25
125.54
123.72
121.90
120.68
120.08
119.61
119.42
119.23
119.09
118.65
110.67
106.47
78.05

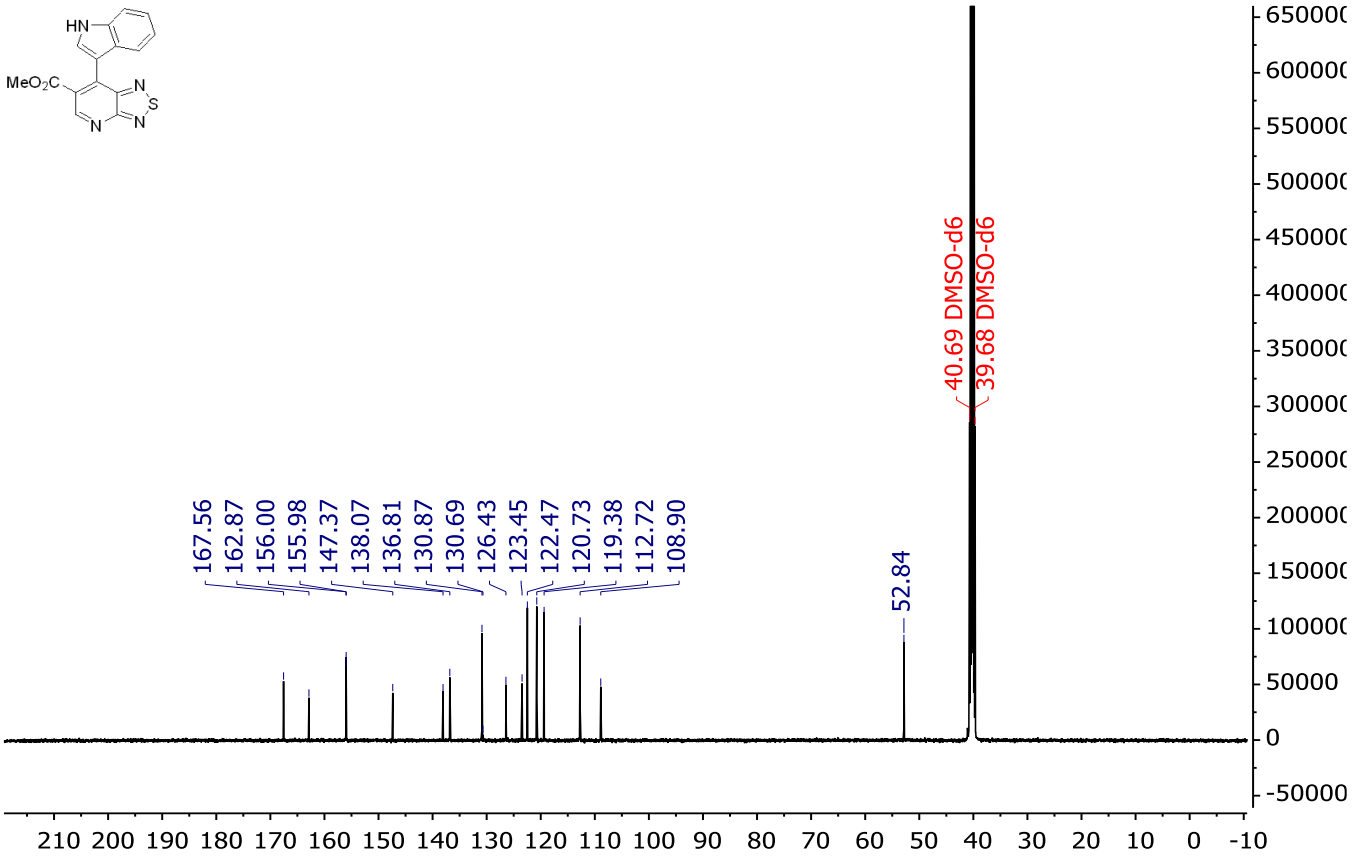
6f


HN
OMe
F3C
N
Se
N
N
11.63
11.63
9.34
7.62
7.61
7.61
7.40
7.37
6.83
6.82
6.80
6.79
6.75
6.74
3.59
3.34 HDO
2.51 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
0.88
1.03
1.01
1.01
1.05
1.02
3.01

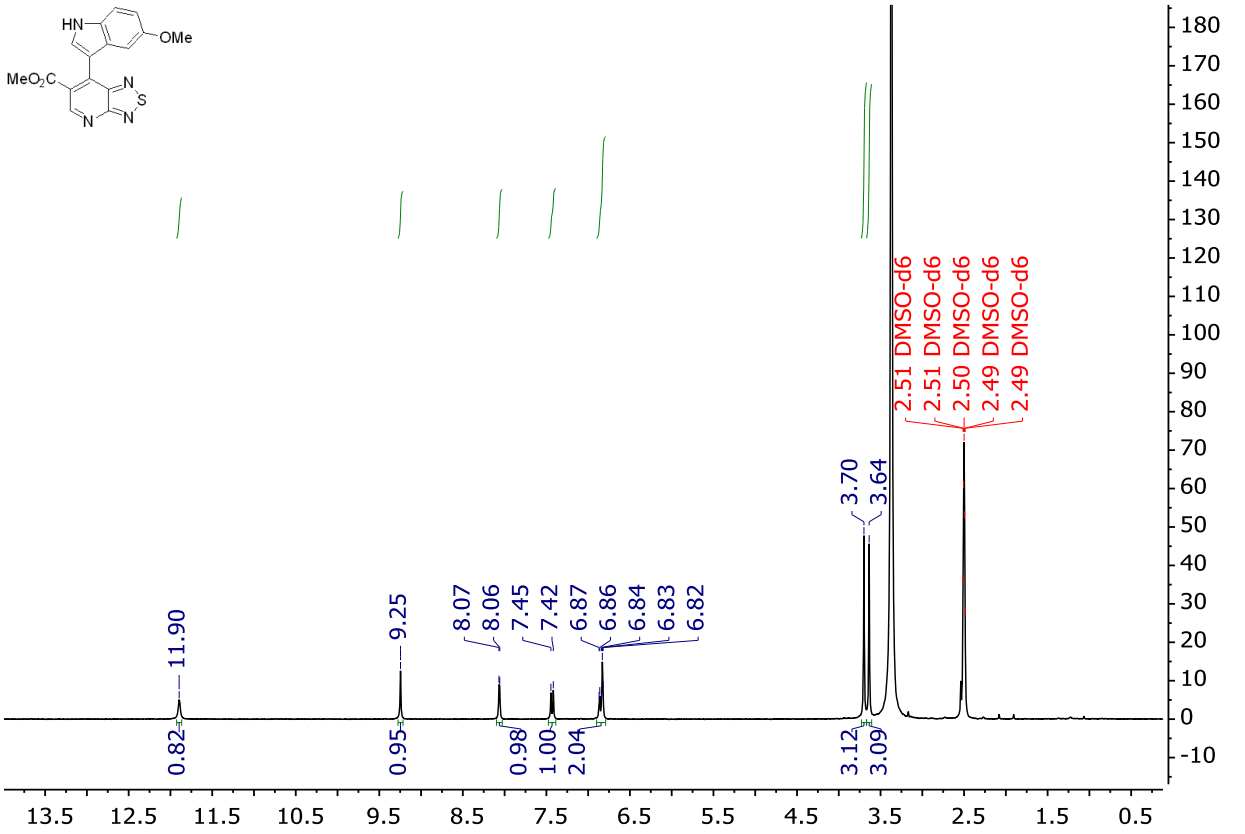

HN
OMe
F3C
N
Se
N
N
38.82 DMSO-d6
38.68 DMSO-d6
38.54 DMSO-d6
38.40 DMSO-d6
38.26 DMSO-d6
38.12 DMSO-d6
37.98 DMSO-d6
139.41
134.88
126.25
125.54
123.72
121.90
120.68
120.08
119.61
119.42
119.23
119.09
118.65
110.67
106.47
163.72
151.15
150.95
150.92
150.88
150.85
78.05
53.07

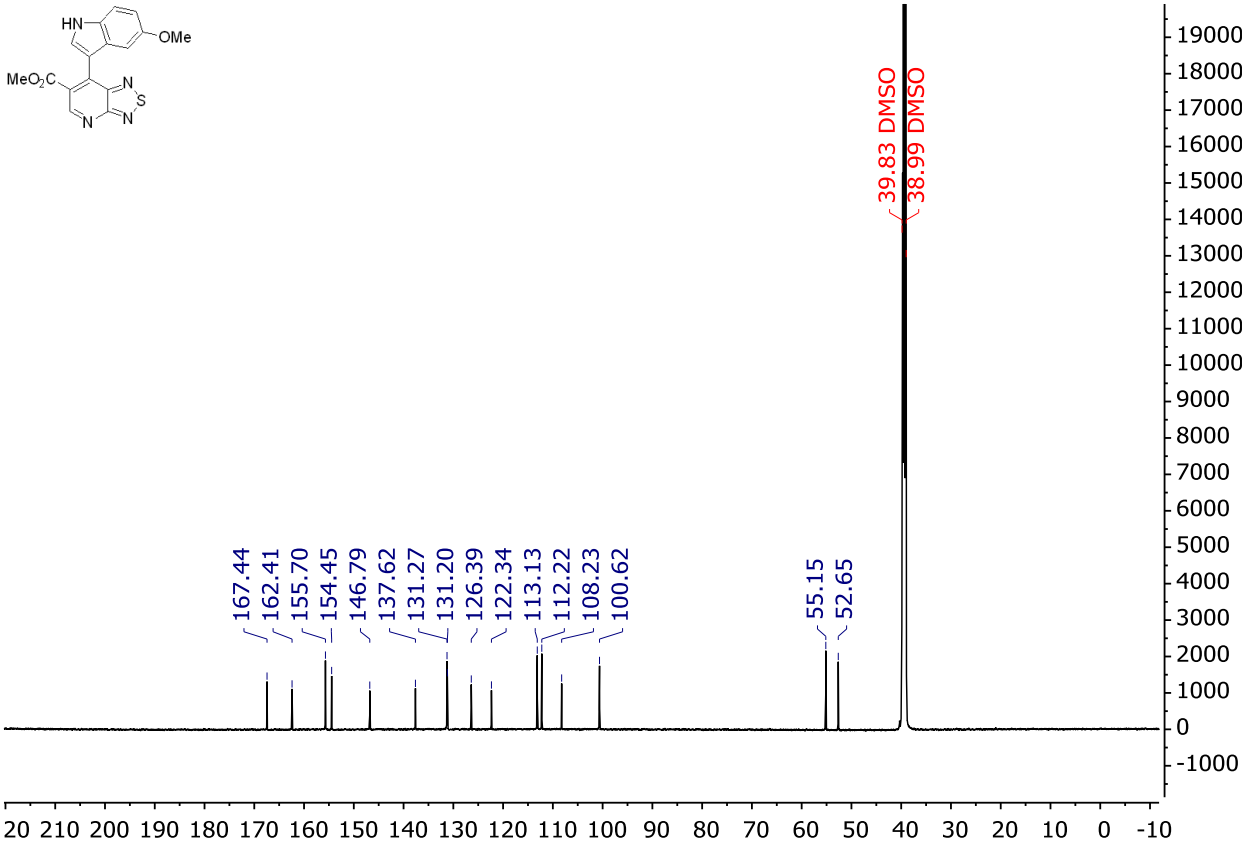
6g


HN
MeO2C
N
S
N
N
3.62
3.35 HDO
2.51 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
12.01
9.26
8.10
8.09
7.56
7.53
7.36
7.33
7.23
7.21
7.19
7.14
7.11
1.12
0.60
1.00
1.13
1.10
1.09
1.17
3.21

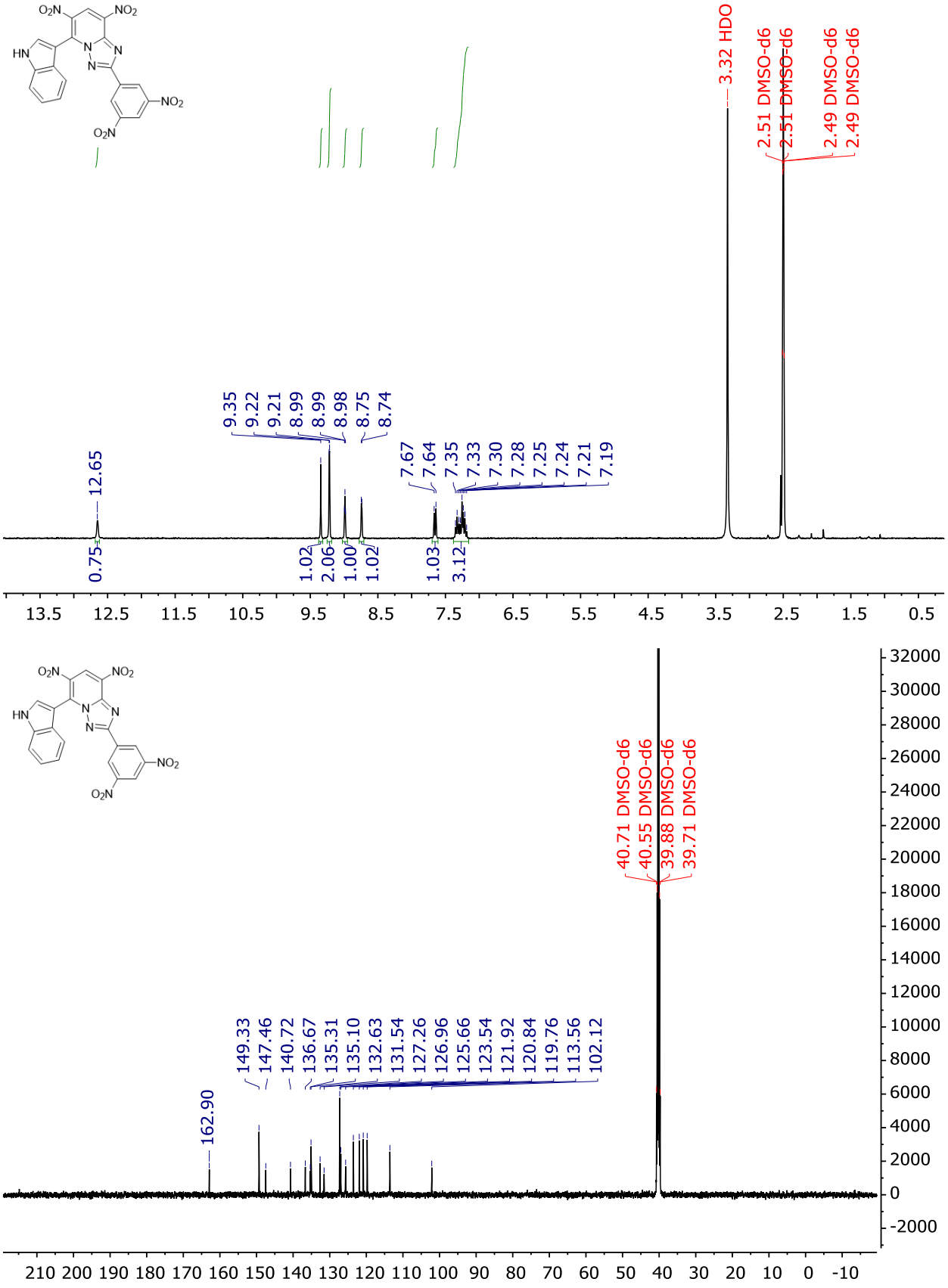

HN
MeO2C
N
S
N
N
40.69 DMSO-d6
39.68 DMSO-d6
167.56
162.87
156.00
155.98
147.37
138.07
136.81
130.87
130.69
126.43
123.45
122.47
120.73
119.38
112.72
108.90
52.84

6h

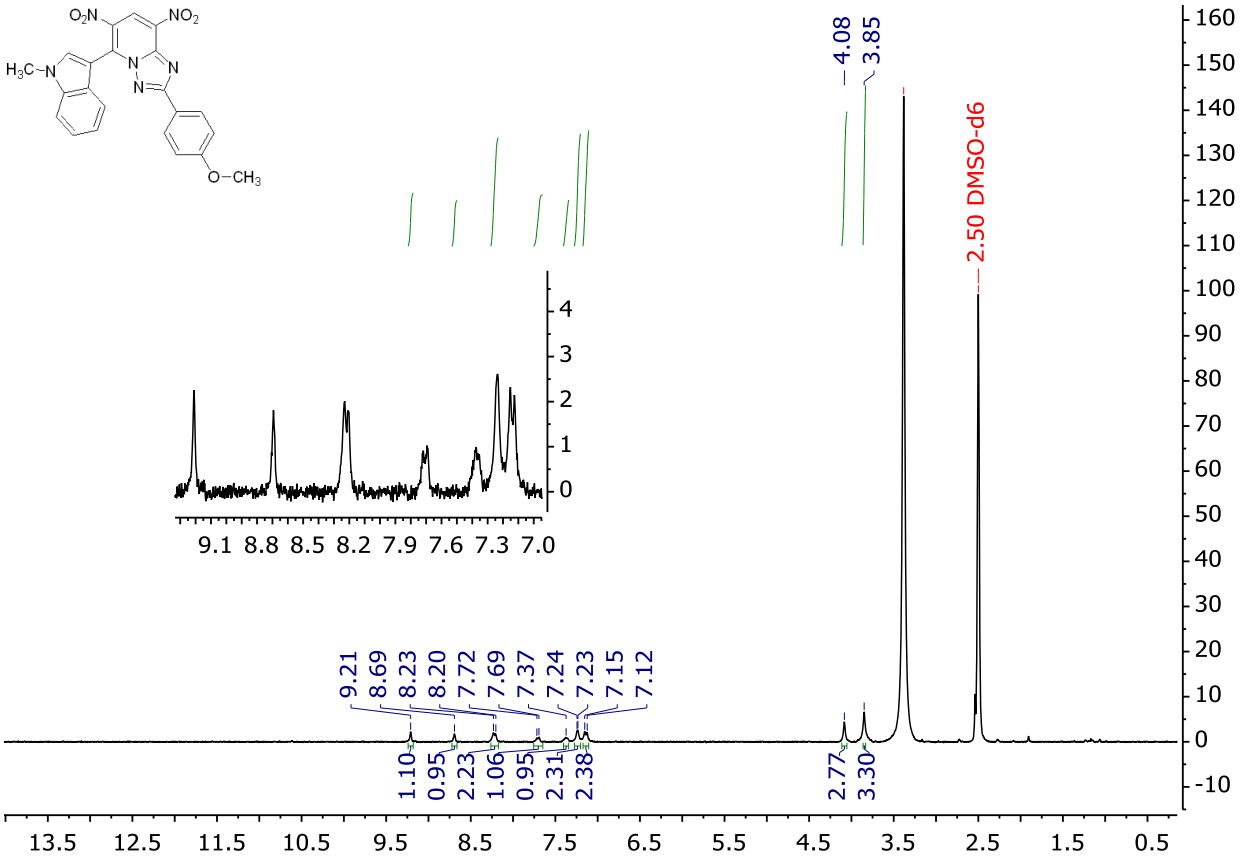

HN
OMe
MeO2C
N
S
N
N
11.90
9.25
8.07
8.06
7.45
7.42
6.87
6.86
6.84
6.83
6.82
3.70
3.64
2.51 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
0.82
0.95
0.98
1.00
2.04
3.12
3.09

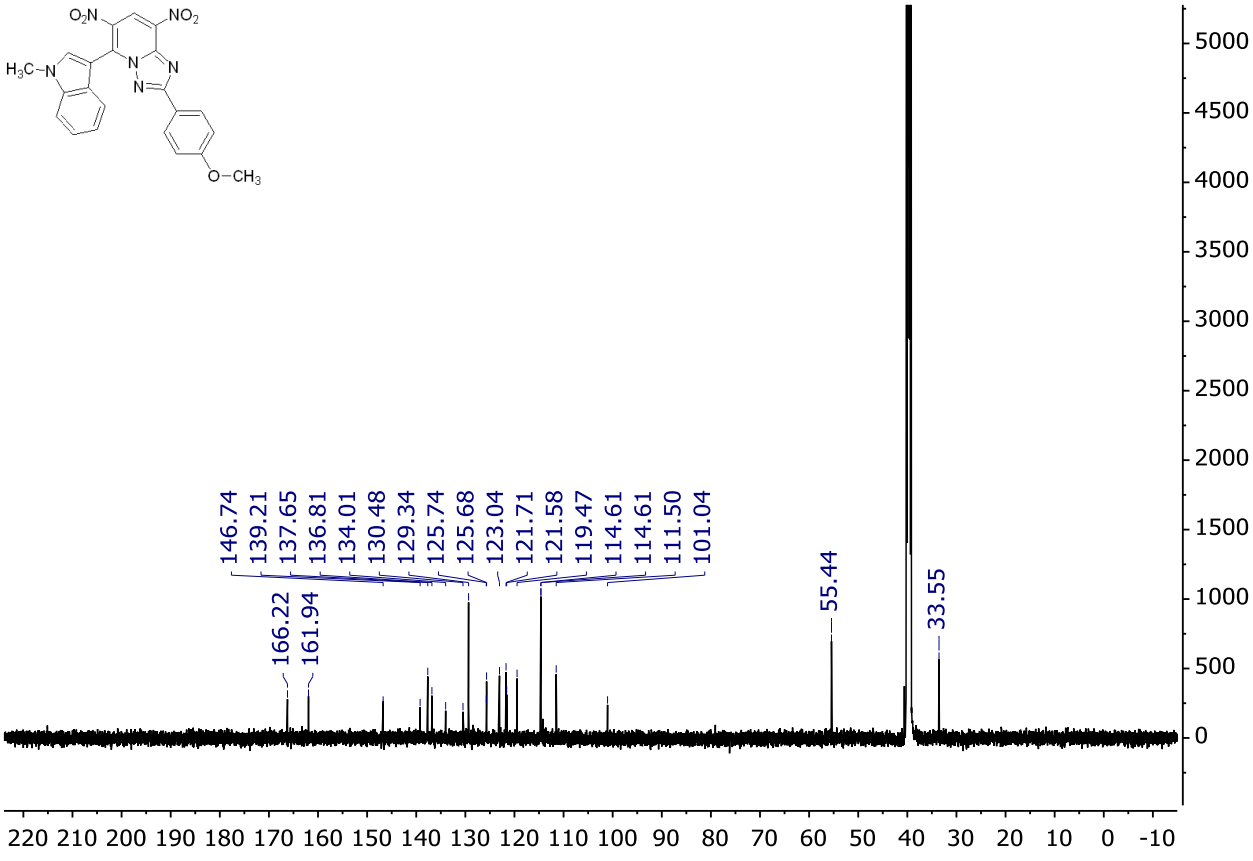

HN
OMe
MeO2C
N
S
N
N
39.83 DMSO
38.99 DMSO
167.44
162.41
155.70
154.45
146.79
137.62
131.27
131.20
126.39
122.34
113.13
112.22
108.23
100.62
55.15
52.65

7a

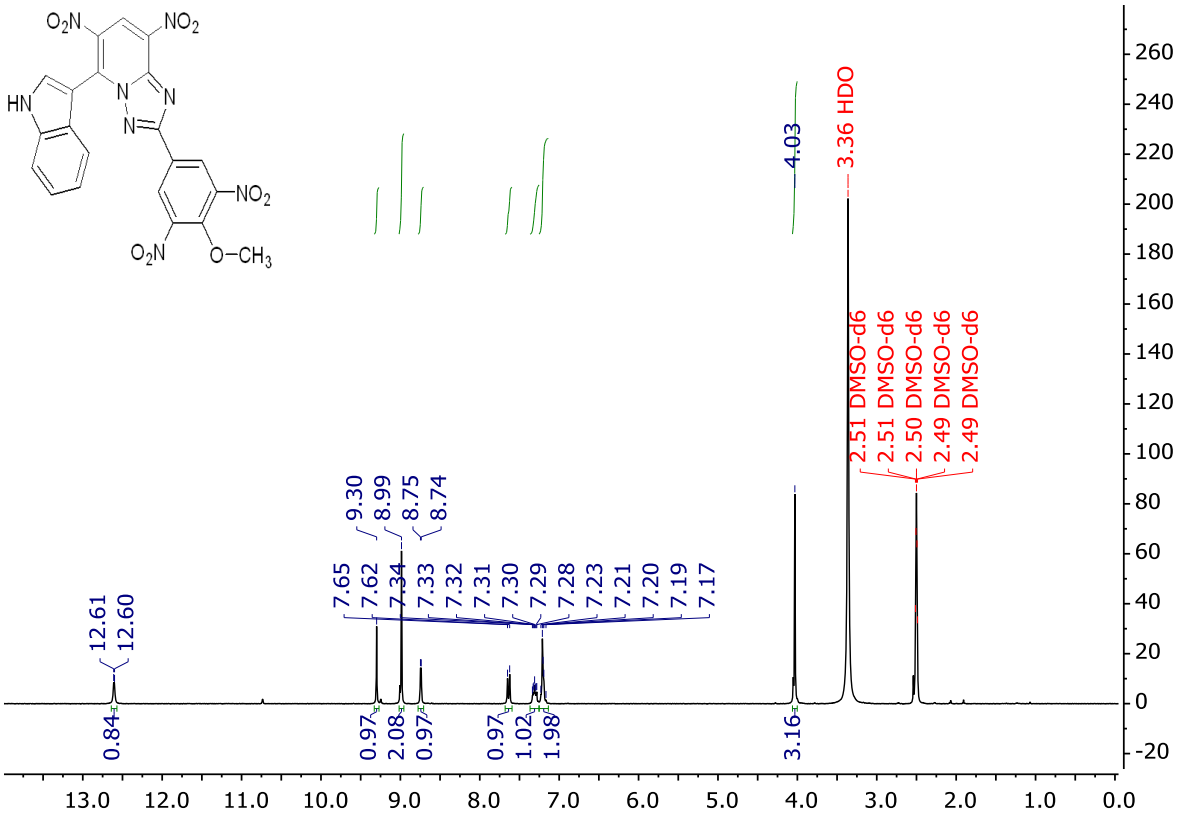

3.32 HDO
2.51 DMSO-d6
2.51 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
9.35
9.22
9.21
8.99
8.99
8.98
8.75
8.74
7.67
7.64
7.35
7.33
7.30
7.28
7.25
7.24
7.21
7.19
12.65
0.75
1.02
2.06
1.00
1.02
1.03
3.12
40.71 DMSO-d6
40.55 DMSO-d6
39.88 DMSO-d6
39.71 DMSO-d6
162.90
149.33
147.46
140.72
136.67
135.31
135.10
132.63
131.54
127.26
126.96
125.66
123.54
121.92
120.84
119.76
113.56
102.12

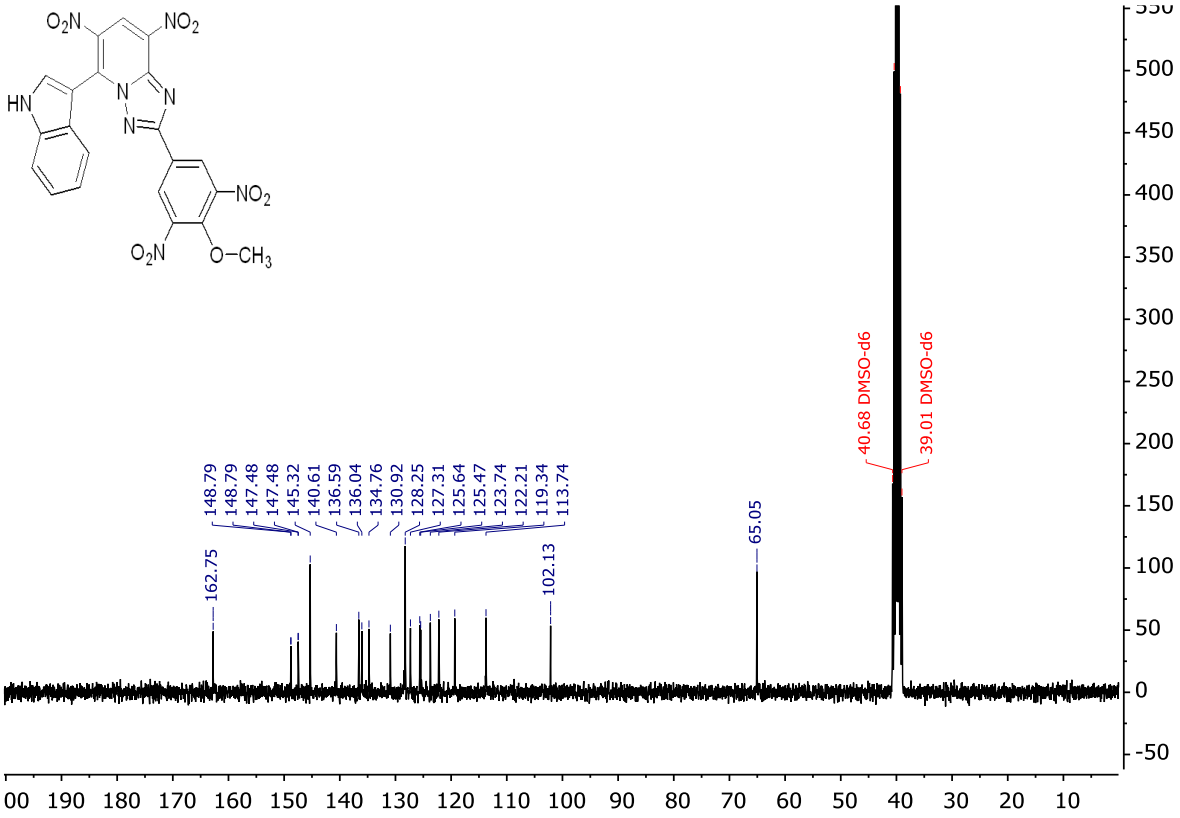
7b


4.08
3.85
2.50 DMSO-d6
9.21
8.69
8.23
8.20
7.72
7.69
7.37
7.24
7.23
7.15
7.12
1.10
0.95
2.23
1.06
0.95
2.31
2.38
2.77
3.30

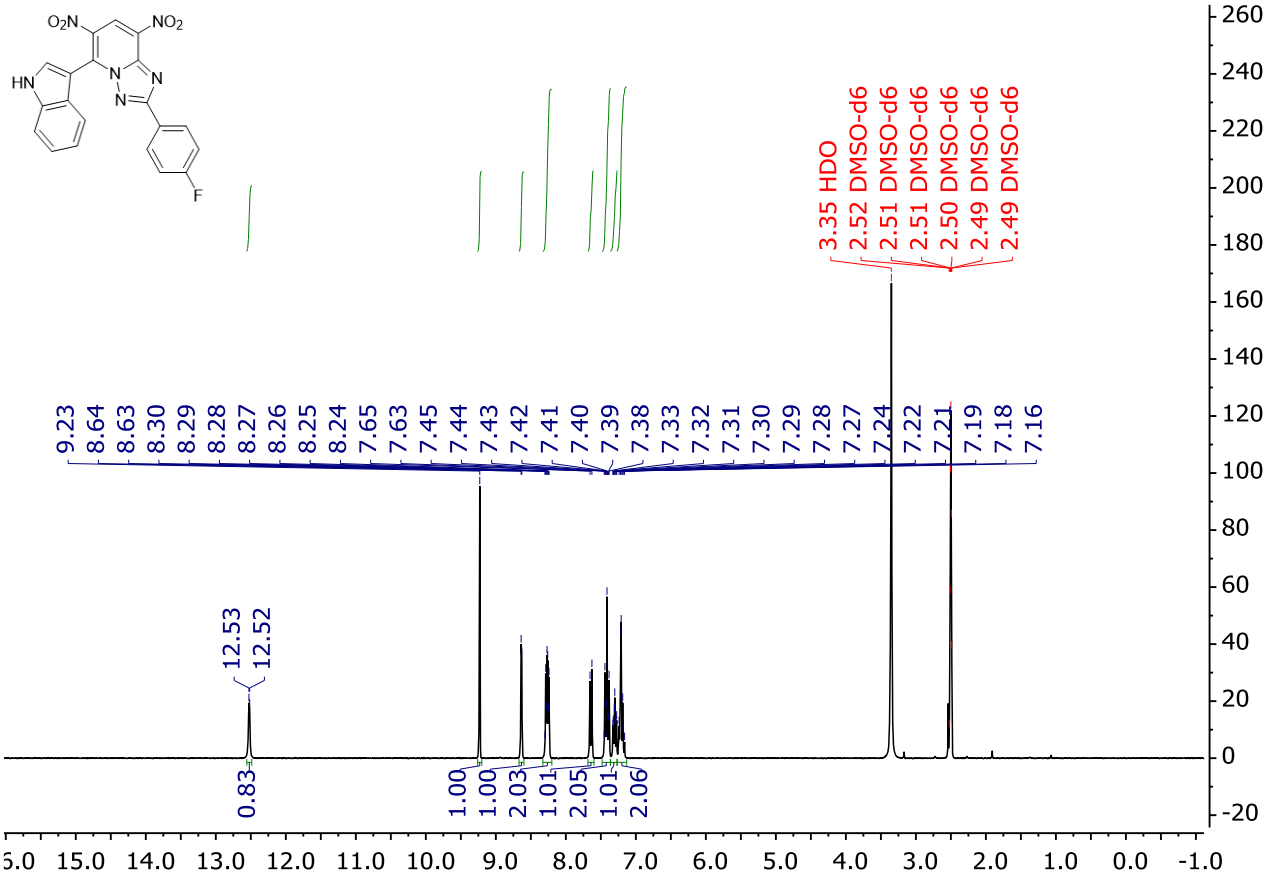

146.74
139.21
137.65
136.81
134.01
130.48
129.34
125.74
125.68
123.04
121.71
121.58
119.47
114.61
114.61
111.50
101.04
166.22
161.94
55.44
33.55

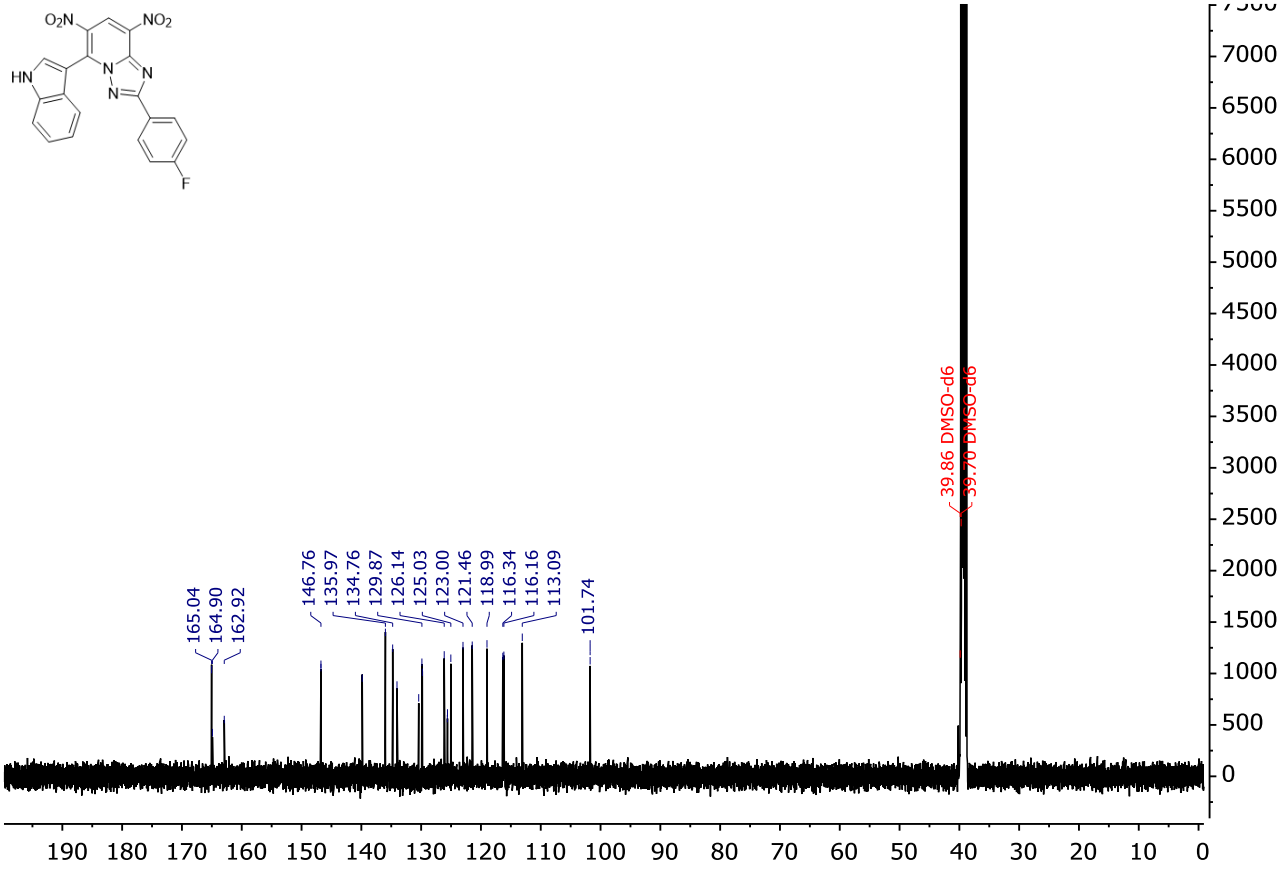
7c


O2N
NO2
HN
N
N
NO2
O2N
O-CH3
12.61
12.60
9.30
8.99
8.75
8.74
7.65
7.62
7.34
7.33
7.32
7.31
7.30
7.29
7.28
7.23
7.21
7.20
7.19
7.17
4.03
3.36 HDO
2.51 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
0.84
0.97
2.08
0.97
0.97
1.02
1.98
3.16

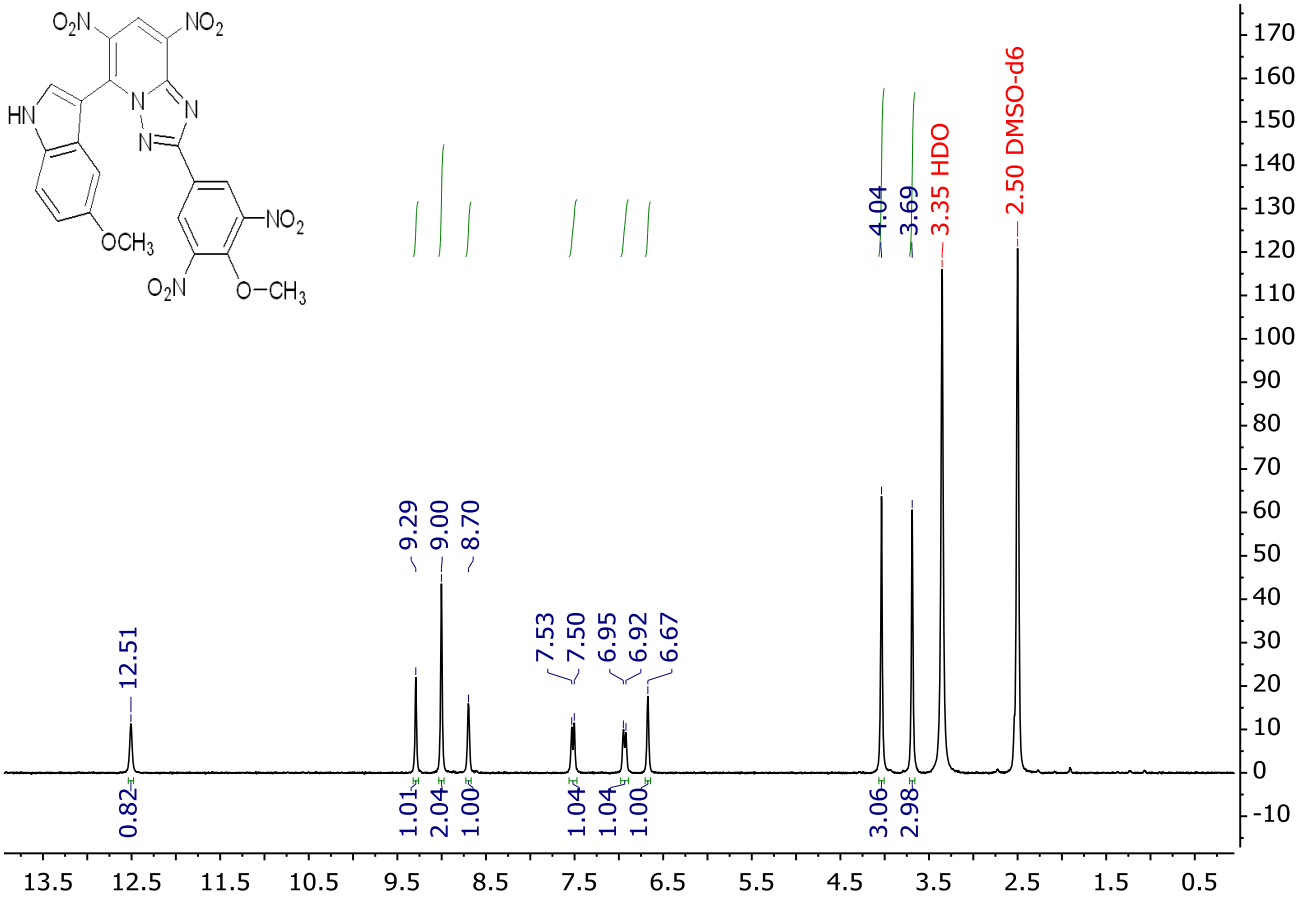

O2N
NO2
HN
N
N
NO2
O2N
O-CH3
148.79
148.79
147.48
147.48
145.32
140.61
136.59
136.04
134.76
130.92
128.25
127.31
125.64
125.47
123.74
122.21
119.34
113.74
162.75
102.13
65.05
40.68 DMSO-d6
39.01 DMSO-d6

7d

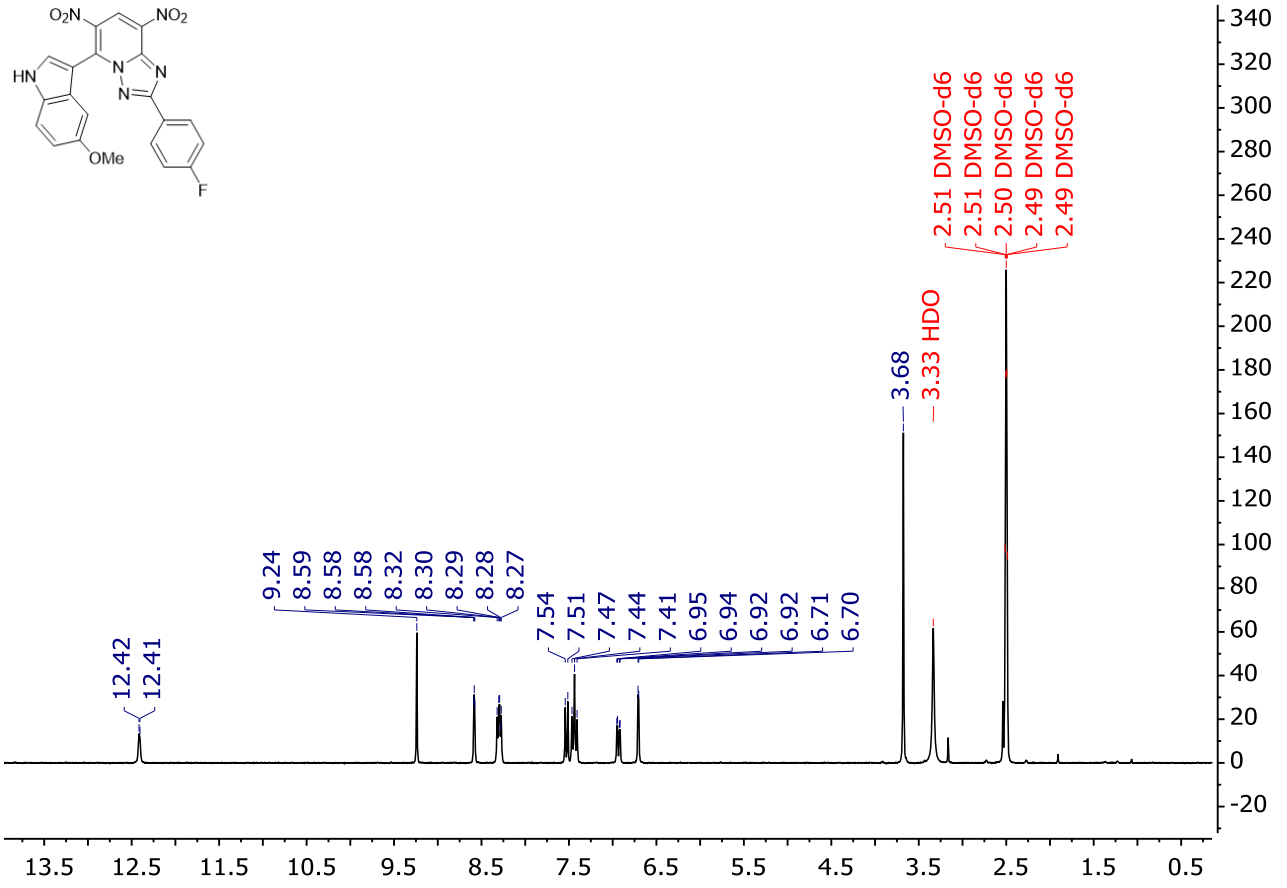

3.35 HDO
2.52 DMSO-d6
2.51 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
9.23
8.64
8.63
8.30
8.29
8.28
8.27
8.26
8.25
8.24
7.65
7.63
7.45
7.44
7.43
7.42
7.41
7.40
7.39
7.38
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.24
7.22
7.21
7.19
7.18
7.16
12.53
12.52
0.83
1.00
1.00
2.03
1.01
2.05
1.01
2.06

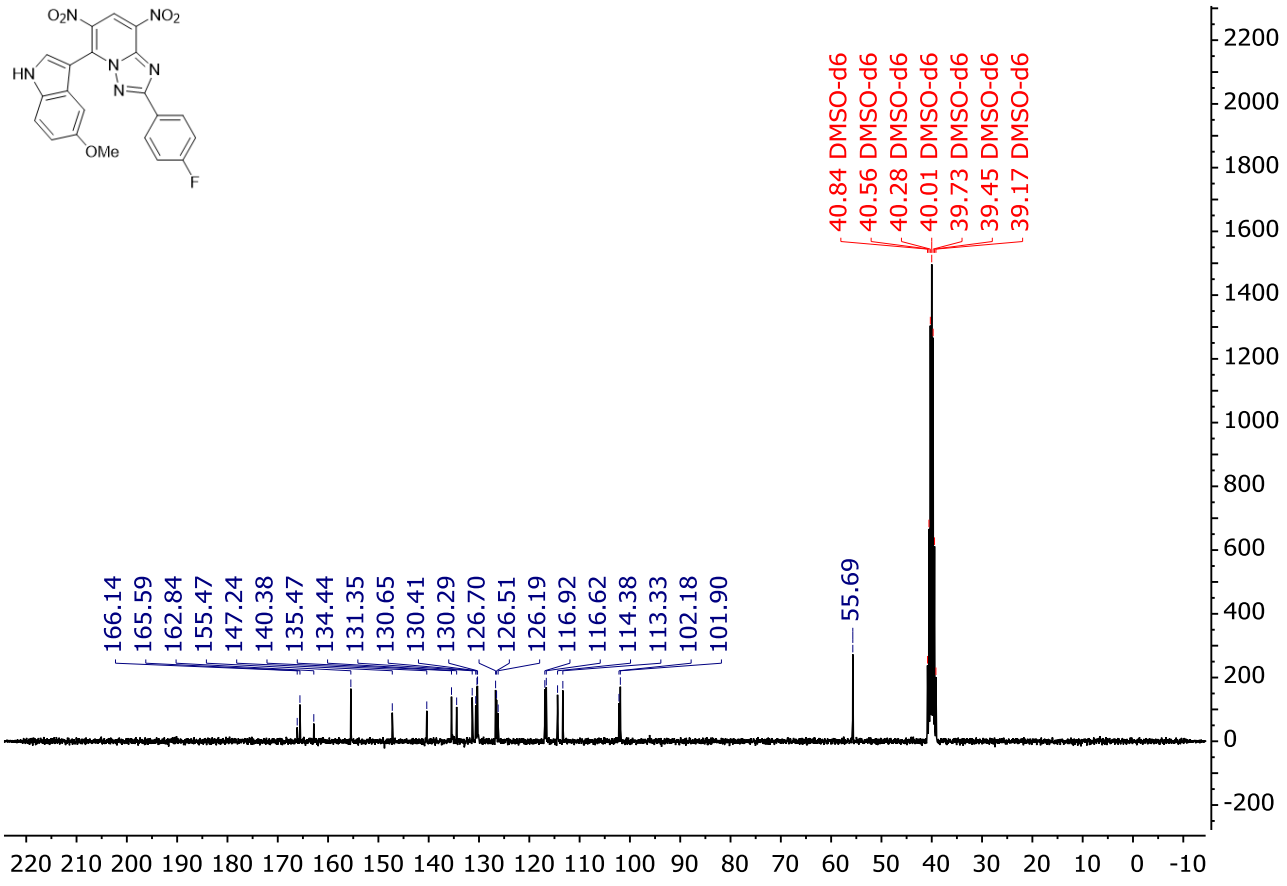

39.86 DMSO-d6
39.70 DMSO-d6
165.04
164.90
162.92
146.76
135.97
134.76
129.87
126.14
125.03
123.00
121.46
118.99
116.34
116.16
113.09
101.74

7e

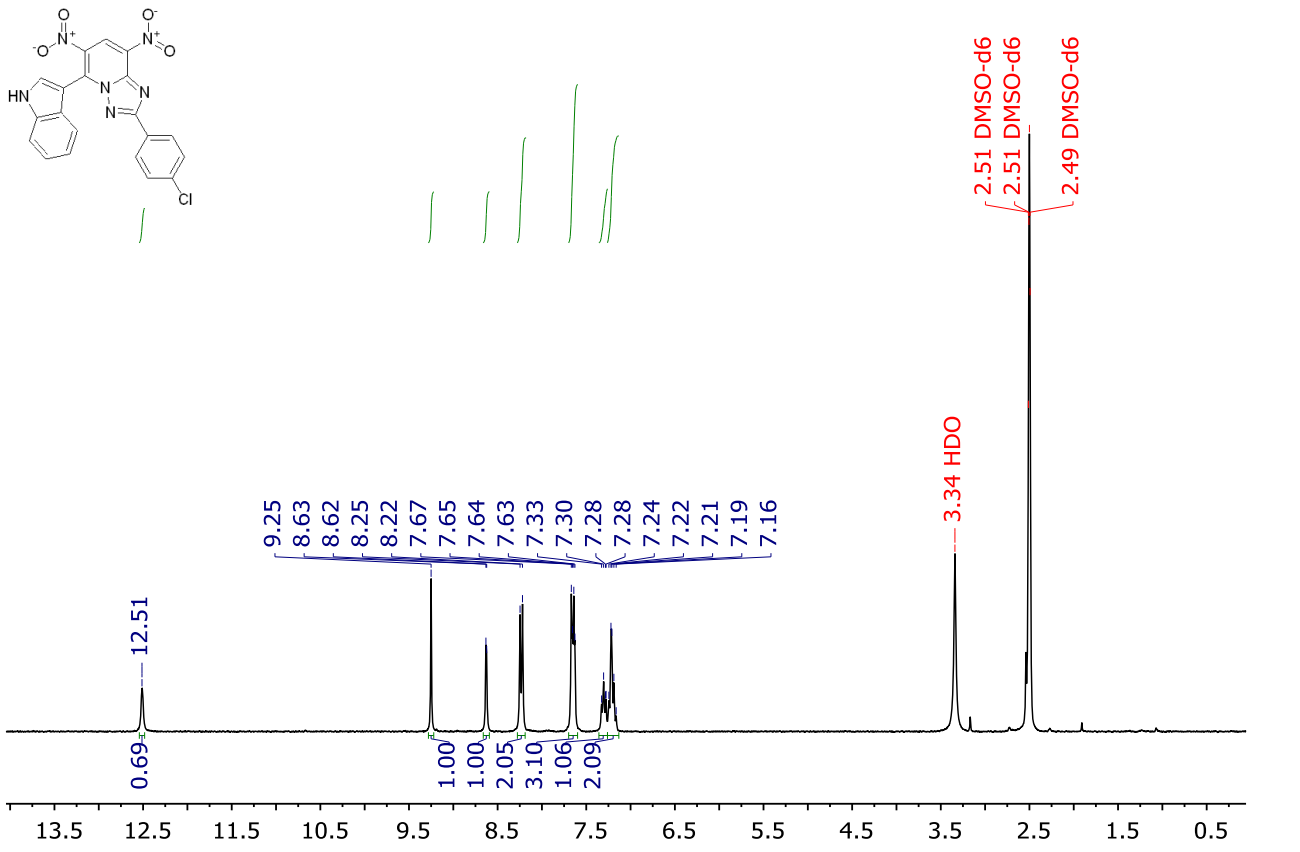

O2N
NO2
HN
N
N
N
OCH3
NO2
O2N
O−CH3
12.51
9.29
9.00
8.70
7.53
7.50
6.95
6.92
6.67
4.04
3.69
3.35 HDO
2.50 DMSO-d6
0.82
1.01
2.04
1.00
1.04
1.04
1.00
3.06
2.98
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

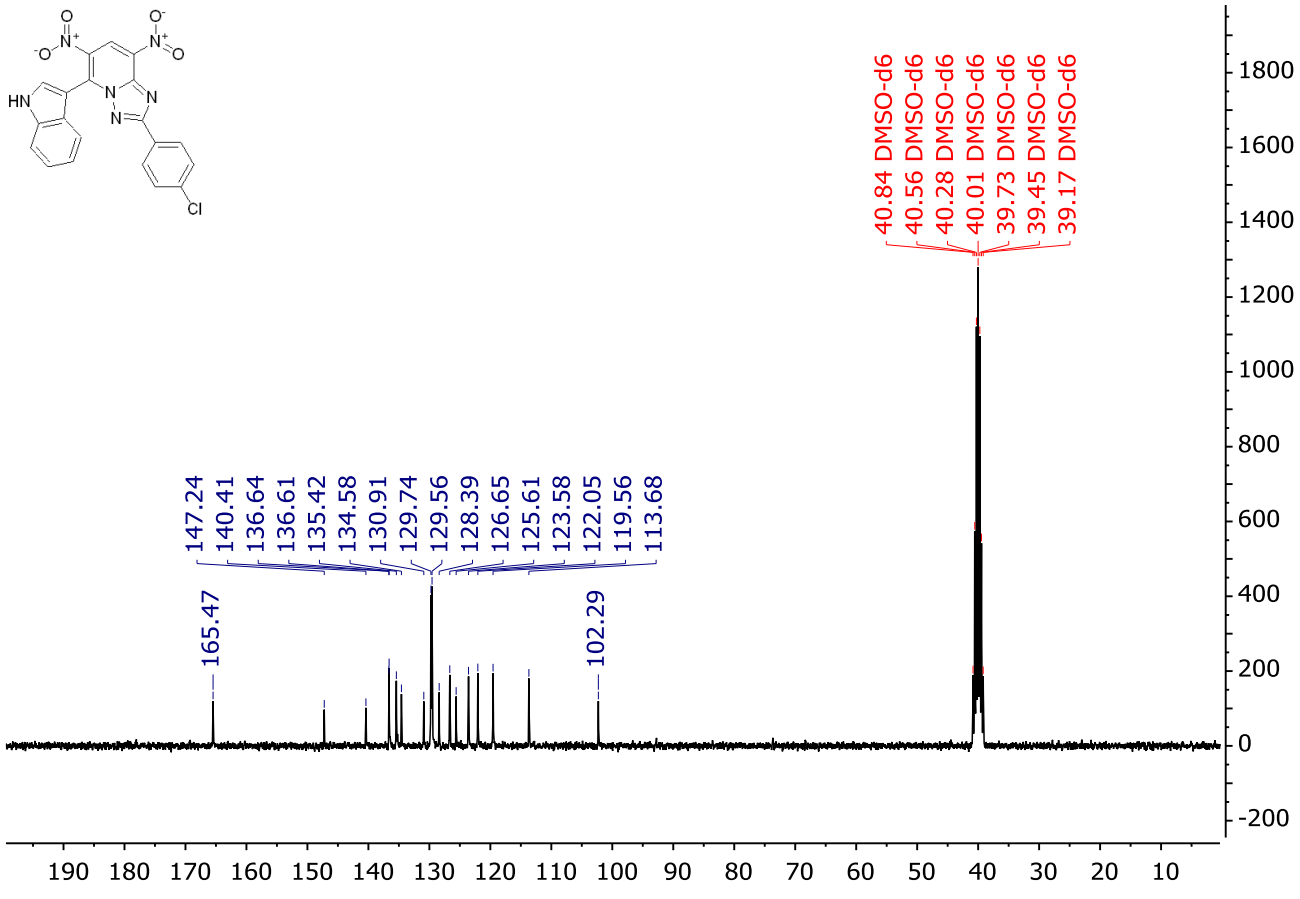
7f


O2N
NO2
HN
N
N
N
OMe
F
2.51 DMSO-d6
2.51 DMSO-d6
2.50 DMSO-d6
2.49 DMSO-d6
2.49 DMSO-d6
3.68
3.33 HDO
9.24
8.59
8.58
8.58
8.32
8.30
8.29
8.28
8.27
7.54
7.51
7.47
7.44
7.41
6.95
6.94
6.92
6.92
6.71
6.70
12.42
12.41


O2N
NO2
HN
N
N
N
OMe
F
40.84 DMSO-d6
40.56 DMSO-d6
40.28 DMSO-d6
40.01 DMSO-d6
39.73 DMSO-d6
39.45 DMSO-d6
39.17 DMSO-d6
166.14
165.59
162.84
155.47
147.24
140.38
135.47
134.44
131.35
130.65
130.41
130.29
126.70
126.51
126.19
116.92
116.62
114.38
113.33
102.18
101.90
55.69

7g


HN
N
N
N
Cl
2.51 DMSO-d6
2.51 DMSO-d6
2.49 DMSO-d6
3.34 HDO
9.25
8.63
8.62
8.25
8.22
7.67
7.65
7.64
7.63
7.33
7.30
7.28
7.28
7.24
7.22
7.21
7.19
7.16
12.51
0.69
1.00
1.00
2.05
3.10
1.06
2.09
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5


HN
N
N
N
Cl
40.84 DMSO-d6
40.56 DMSO-d6
40.28 DMSO-d6
40.01 DMSO-d6
39.73 DMSO-d6
39.45 DMSO-d6
39.17 DMSO-d6
147.24
140.41
136.64
136.61
135.42
134.58
130.91
129.74
129.56
128.39
126.65
125.61
123.58
122.05
119.56
113.68
165.47
102.29
1800
1600
1400
1200
1000
800
600
400
200
0
-200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

References

S1 (*a*) A. M. Starosotnikov, D. V. Shkaev, M. A. Bastrakov, I. V. Fedyanin, S. A. Shevelev and I. L. Dalinger, *Beilstein J. Org. Chem.*, 2017, **13,** 2854; (*b*) A. M. Starosotnikov, D. V. Shkaev, M. A. Bastrakov, I. V. Fedyanin, S. A. Shevelev and I. L. Dalinger, *Mendeleev Commun.*, 2018, **28**, 638; (*c*) V. V. Ivanova, A. K. Fedorenko, A. M. Starosotnikov and M. A. Bastrakov, *Russ. Chem. Bull*., 2022, **71**, 1826; (*d*) M. A Bastrakov, V. G. Nadykta, A. K Fedorenko and A. M. Starosotnikov, *Russ. Chem. Bull.,* 2023, **72**, 960; (*f*) A. K. Fedorenko, V. V. Ivanova, M. E. Minyaev, M. A. Bastrakov and A. M. Starosotnikov, *ChemistrySelect*, 2023, **43,** 202303122.

S2 *CrysAlisPro, Version 1.171.43*, Rigaku Oxford Diffraction, 2023.

S3 G. M. Sheldrick, *Acta Crystallogr.,* **2**015, **A71**, 3; https://doi.org/10.1107/S2053273314026370.

S3 G. M. Sheldrick, *Acta Crystallogr.,* 2015, **C71**, 3; https://doi.org/10.1107/S2053229614024218.

S4 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339; https://doi.org/10.1107/S0021889808042726