Electronic supplementary materials *Mendeleev Commun.*, 2024, **34**, 706–708

An alternative synthesis of 7-amino-6-nitro-substituted azolo[1,5-*a*]pyrimidines

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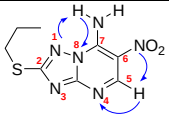
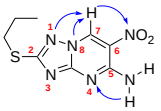
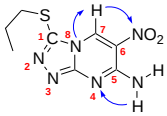
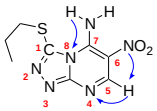
Table S1. Calculated isotropic shieldings for nitrogen nuclei and their association with real chemical shifts in ^{15}N NMR spectrum. Possible N-H HMBC interactions (2-3 bonds) are indicated by blue arrows

Nucleus	Calculated absolute shieldings (σ^{calc}) and associated real chemical shifts (δ^{real}), ppm							
	 **4c**		 **4'c**		 **4"c**		 **4"'c**	
	σ^{calc}	δ^{real}	σ^{calc}	δ^{real}	σ^{calc}	δ^{real}	σ^{calc}	δ^{real}
N8	22	208	6.7	234	52	208	58	208
N1 or C1	-16	257	-21	257	-	-	-	-
C2 or N2	-	-	-	-	-87	257	-129	257
N3	3	232	21	232	-42	234	-74	234
N4	0	234	34	208	40	232	-5	232
NH_2	156	96	148	96	151	96	146	96
NO_2	-143	366	-143	366	-144	366	-143	366
Bravais-Pearson correlation (exclude NO_2, NH_2 signals)	-1		-0.96		-0.87		-0.95	

*Chemical shifts at 96, 234, 366 ppm associated with cross peaks according to ^{1}H-^{15}N HMBC NMR

Table S2. Reaction conditions optimization for the preparation of some 7-amino-6-nitroazolo[1,5-*a*]pyrimidines

Target compound	Solvent, ml	Base (eq.)	Time, h	Temperature, °C	Yield, %
4b	CCl_4	NEt_3 (1)	2.5	77	<1
4b	H_2O	Na_2CO_3 (1)	1	100	n.d.
4d	*i*-PrOH	NEt_3 (1)	30	82	47.2
4d	-	Pyridine (8)	1	100	n.d.
4d	-	Piperidine (4)	1	100	n.d.
4f	*i*-PrOH	NEt_3 (1)	2	82	25.6
4f	*n*-BuOH	NEt_3 (1)	5	100	27.4
4f	*i*-PrOH	DIPEA (1)	9.75	82	8.2
4f	-	NEt_3 (10)	20.5	90	31.6
4f	Et_2O	-	5.5	35	n.d.
4f	THF	-	13	55	Trace (TLC)
4f	-	Morpholine (20)	1.5	120	n.d.

n.d. – not detected

Table S3. Varying the conditions for the preparation of 3,5-dinitro-*N*-(*p*-tolyl)pyridine-2,6-diamine **5**

Amino azole	Mole ratio			Yield of the compound **5**, %
	Amino azole **1**	Nitro synthon **2**	NEt_3	
1j	1	2	1	9
1j	1	1	1	33
1k	1	2	1	20
	0	1	1	-

Table S4. Crystallographic parameters and structure refinement results for compound **5**

Molecular formula	$C_{14.5}H_{13.5}N_{5.5}O_4$
M/g mol^{-1}	328.81
T/K	295(2)
System	triclinic
Space group	P-1
a/Å	6.6352(6)
b/Å	12.7380(17)
c/Å	18.3280(16)
α/°	86.951(9)
β/°	89.244(7)
γ/°	89.381(9)
V/Å^3	1546.7(3)
Z	4
ρ_{calc} г/cm^3	1.412
μ/mm^{-1}	0.107
F(000)	684.0
Crystal size/mm	0.39 × 0.31 × 0.18
Type of radiation	MoKα (λ = 0.71073)
Scattering angles 2Θ /°	7.172 to 56.552
Reflection indicies	-8 ≤ h ≤ 8, -16 ≤ k ≤ 15, -24 ≤ l ≤ 24
Reflections collected	15409
Independent reflections	7548 [R_{int} = 0.0687, R_{sigma} = 0.1428]
Reflections with [I≥2σ (I)]	2213
Number of parameters	7548/0/447
GooF по F^2	1.000
R factors [I≥2σ (I)]	R_1 = 0.0856, wR_2 = 0.1873
R factors [all reflections]	R_1 = 0.2471, wR_2 = 0.2692
$\Delta\rho_{\bar{e}}$/ ēÅ^{-3}	0.47/-0.22

Computational studies

DFT calculations were performed using the Orca 5.0.3 program.[S1,S2] Initial geometries (one conformer per structure) were generated using OpenBabel 2.4.1.[S3] The ground-state geometry optimizations were performed at the B3LYP/def2-TZVP level of theory with D3 correction in the gas phase. Frequency analyses were carried out at the same theoretical level to ensure that the optimized geometries correspond to a local minimum on the potential energy surface. Isotropic shieldings were calculated using the same level of theory with the Conductor-like Polarizable Continuum Model of DMSO.

Chemistry

All solvents and commercially available reagents were used as received unless otherwise stated. Non-commercial starting materials were prepared as described below or according to literature procedures. One-dimensional ^{1}H and ^{13}C NMR spectra were obtained on a Bruker AVANCE II - 400 (400 and 101 MHz, respectively) equipped with a Prodigy broadband gradient cryoprobe using DMSO-d_6 as solvent and TMS as internal standard. Two dimensional NMR spectra ^{1}H-^{13}C and ^{1}H-^{15}N (internal standard for ^{15}N: NH_3) were obtained on a «Bruker Avance NEO 600» (^{1}H: 600 MHz, ^{13}C: 151 MHz, ^{15}N: 61 MHz) equipped with a Prodigy broadband gradient cryoprobe using DMSO-d6 as solvent.

IR spectra were recorded on a Bruker Alpha FTIR spectrometer equipped with an ATR attachment. Mass spectra were recorded on a Shimadzu GCMS-QP2010 mass spectrometer using the EI ionization method (70 eV). The progress of the reaction was monitored by TLC on 0.25 mm plates with silica gel (Merck 60F 254), eluent - chloroform. Melting points were determined on a Stuart ST.PL.3 instrument at a heating rate of 1°C/min.

Starting potassium salt of nitroacetonitrile was synthesized as described in literature.[S4,S5]

2-Nitro-3-(*p*-tolylamino)acrylonitrile (**2**). To a suspension of potassium salt of nitroacetonitrile[S4] (13 mmol, 1.566 g) in 20 ml of *i*-PrOH were added 1.7 ml (16 mmol) of trifluoroacetic acid and kept with stirring at 20 ºC until a clear yellow solution is formed. Then, 1.351 g (13 mmol) of dry *p*-toluidine and 2.1 ml (13 mmol) of triethyl orthoformate were sequentially added to the mixture with vigorous stirring in small portions. A thick yellow suspension was formed immediately. The suspension was kept with stirring for 30 minutes, then filtered, the solid was washed with *i*-PrOH and dried on air. Yield 71%. Yellow powder. R_f = 0.1 ($CHCl_3$). m.p. (*i-PrOH*) = 215-217ºC (220 ºC, lit.[5]). ^{1}H NMR (400 MHz, DMSO-d6) δ, p.m.: 9.47 (s, 2H, NH_2), 9.14 (s, 1H, CH), 2.70 (s, 3H, CH_3) 12.14 (s, 1H, NH), 8.99 (s, 1H, CH), 7.40

(d, 2H, 2xCH (Ar)), 7.26 (d, 2H, 2xCH (Ar)), 2.39 (s, 3H, CH_3). Found, %: C, 59.07; H, 4.46; N, 20.65. Calc. for $C_{10}H_9N_3O_2$ (%): C, 59.11; H, 4.46; N, 20.68.

7-Amino-6-nitroazolo[1,5-*a*]pyrimidines (4a-i).

General procedure. The corresponding aminoazole 1 (1 mmol) was suspended in 3 ml of *i*-PrOH, then triethylamine (1 mmol) and dry 2-nitro-3-(*p*-tolylamino)acrylonitrile **2** (1 mmol) were added sequentially. The mixture was refluxed for the number of hours indicated in each case. The resulting suspension was filtered and the solid was washed with a minimum amount of *i*-PrOH. The precipitate was transferred to a new flask, suspended in 5 ml of water and refluxed for another 1 hour. Then the suspension was cooled to 20°C, precipitate was filtered, washed with water and dried in air.

2-Methylthio-6-nitro[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (4a). Yellow solid. Yield 20%. R_f = 0.09 ($CHCl_3$). m.p. 258-260°C (*i*-PrOH). IR 507, 524, 577, 612, 678, 689, 707, 751, 770, 837, 905, 944, 960, 989, 1063, 1160, 1213, 1253, 1288, 1311, 1340, 1394, 1435, 1481, 1574, 1643, 1709, 3079, 3386, 3540, 3646, 3741, 3829, 3900. ^{1}H NMR (400 MHz, DMSO-d_6) δ, p.m.: 9.47 (s, 2H, NH_2), 9.14 (s, 1H, CH), 2.70 (s, 3H, CH_3) ^{13}C NMR (101 MHz, DMSO) δ, p.m. : 168.36, 156.61, 152.56, 145.10, 119.00, 13.91. Found, %: C 31.98; H 2.67; N 36.86. Calculated, %: C 31.86; H 2.65; N 37.17. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 226.

2-Ethylthio-6-nitro[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (4b) Refluxing time: 9 hours. Beige powder. Yield 28%. R_f = 0.13 ($CHCl_3$). m.p. 219-222°C (*i*-PrOH). IR 523, 569, 610, 660, 675, 690, 705, 748, 770, 796, 837, 902, 956, 979, 1066, 1211, 1250, 1303, 1338, 1383, 1436, 1481, 1567, 1584, 1643, 1704, 1906, 2872, 2931, 2972, 2989, 3112, 3234, 3390, 3419. ^{1}H NMR (400 MHz, DMSO-d_6) δ, p.m.: 9.54 (s, 2H, NH_2), 9.15 (s, 1H, CH), 3.27 (q, J = 7.4 Hz, 2H, CH_2), 1.46 (t, J = 7.3 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, DMSO) δ, p.m.: 167.92, 156.53, 152.46, 145.13, 119.03, 25.67, 15.52. Found, %: C 35.14; H 3.39; N 35.01, S 13.39. Calc. for $C_7H_8N_6O_2S$ (%): C 35.00; H 3.36; N 34.98, S 13.35. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 240.

6-Nitro-2-propylthio[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (4c) Refluxing time: 5 hours. Brown powder. Yield 11%. R_f = 0.14 ($CHCl_3$). m.p. 224°C (*i*-PrOH). IR 512, 524, 574, 596, 689, 708, 752, 768, 836, 898, 951, 983, 1067, 1159, 1233, 1259, 1295, 1341, 1392, 1435, 1482, 1573, 1642, 2873, 2963, 3207, 3616, 3667, 3750, 3816, 3852, 3884, 3902, 3912

^{1}H NMR (600 MHz, DMSO-d_6) δ, p.m.: 9.55 (s, 2H, NH_2), 9.14 (s, 1H, CH), 3.23 (t, J = 7.2 Hz, 2H, CH_2), 1.76 (h, J = 7.3 Hz, 2H, CH_2), 1.01 (t, 3H, J = 7.3 Hz, CH_3) ^{13}C NMR (101 MHz, DMSO) δ, p.m.: 167.81, 156.50, 152.53, 145.09, 119.01, 33.02, 23.15, 13.53. ^{15}N NMR (61 MHz, DMSO) δ 365.87, 257.21, 231.55, 208.81, 95.94. Found, %: C 37.75; H 3.97; N

32.92, S 12.65. Calc. for $C_8H_9N_6O_2S$ (%): C 37.79; H 3.96; N 33.05, S 12.61. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 254.

6-Nitro-2-(thiophen-2-yl)[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (4d) Refluxing time: 5 hours. Light yellow powder. Yield 26%. R_f = 0.12 ($CHCl_3$). m.p. 368-369°C (*i*-PrOH). IR 522, 587, 596, 669, 687, 714, 769, 836, 854, 904, 1069, 1103, 1213, 1276, 1360, 1435, 1468, 1577, 1646, 3085, 3382. ^{1}H NMR (400 MHz, DMSO-d_6) δ, p.m.: 9.74 (s, 1H, NH_2), .: 9.51 (s, 1H, NH_2), 9.21 (s, 1H, CH), 7.89 (dd, J = 3.6, 1.3 Hz, 1H, CH (thien-2-yl)), 7.83 (dd, J = 5.0, 1.3 Hz, 1H, CH (thien-2-yl)), 7.27 (dd, J = 5.0, 3.6 Hz, 1H, CH (thien-2-yl)) ^{13}C NMR (101 MHz, DMSO) δ, p.m.: 161.80, 156.72, 152.82, 145.97, 132.90, 130.51, 129.39, 128.84, 119.23. Found, %: C 41.28; H 2.33; N 32.15, S 12.29. Calc. for $C_9H_6N_6O_2S$ (%): C 41.22; H 2.31; N 32.05, S 12.23. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 262.

2-(Furan-2-yl)-6-nitro[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (4e) Refluxing time: 3 hours. Light yellow powder. Yield 55%. R_f = 0.08 ($CHCl_3$). m.p. 260°C (*i*-PrOH). IR 570, 587, 638, 703, 747, 767, 830, 882, 898, 970, 1010, 1067, 1084, 1122, 1158, 1180, 1215, 1286, 1344, 1423, 1478, 1504, 1562, 1621, 1648, 2865, 3411. ^{1}H NMR (400 MHz, DMSO-d_6) δ, p.m.: 9.62 (s, 2H, NH_2), 9.17 (s, 1H, CH), 7.87 (dd, J = 1.8, 0.8 Hz, 1H, CH(furan-2-yl)), 7.22 (dd, J = 3.4, 0.9 Hz, 1H, CH(furan-2-yl)), 6.68 (dd, J = 3.4, 1.8 Hz, 1H, CH(furan-2-yl)), ^{13}C NMR (101 MHz, DMSO) δ, p.m.: 158.27, 156.64, 153.01, 146.18, 146.13, 145.51, 119.17, 113.71, 112.80. Found, %: C 43.85; H 2.40; N 34.11. Calc. for $C_9H_6N_6O_3$ (%): C 43.91; H 2.46; N 34.14. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 246.

2-Benzylthio-6-nitro[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (4f) Refluxing time: 2 hours. Brown powder. Yield 31%. R_f = 0.17 ($CHCl_3$). m.p. 217-219°C (*i*-PrOH). IR 525, 565, 577, 648, 693, 709, 756, 836, 920, 967, 987, 1029, 1067, 1090, 1158, 1232, 1261, 1300, 1343, 1392, 1434, 1454, 1480, 1569, 1650, 2993, 3198, 3646, 3708, 3813, 3850, 3868. ^{1}H NMR (400 MHz, DMSO-d_6) δ, p.m.: 9.60 (s, 2H, NH_2), 9.17 (s, 1H, CH), 7.52 (d, J = 7.4 Hz, 2H, 2CH (Ar)), 7.24-7.34 (m, 3CH(Ar)), 4.56 (s, 2H, CH_2). ^{13}C NMR (101 MHz, DMSO) δ, p.m.: 167.32, 156.55, 152.64, 145.14, 138.08, 129.51, 128.93, 127.83, 119.11, 34.91. Found, %: C 47.64; H 3.41; N 27.75, S 10.69. Calc. for $C_{12}H_{10}N_6O_2S$ (%): C 47.68; H 3.33; N 27.80, S 10.61. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 302

6-Nitro-2-(prop-2-yn-1-ylthio)[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (4g) Refluxing time: 24 hours. The final product was additionally recrystallized from AcOH. Dark yellow powder. Yield 26%. R_f = 0.12 ($CHCl_3$). m.p. 214-216 °C (AcOH). IR 525, 556, 632, 680, 690, 704, 716, 752, 770, 836, 858, 908, 967, 982, 1073, 1183, 1229, 1259, 1291, 1308, 1342, 1381, 1426, 1470, 1520, 1574, 1644, 1930, 2116, 2359, 2929, 3061, 3194, 3194, 3235, 3305, 3400. ^{1}H NMR (600 MHz, DMSO-d_6) δ, p.m.: 9.73 (s, 1H, NH_2), 9.53 (s, 1H, NH_2), 9.19 (s, 1H, CH),

4.17 (d, *J* = 2.6 Hz, 2H, CH_2), 3.25 (t, *J* = 2.6 Hz, 1H). ^{13}C NMR (151 MHz, DMSO) δ 166.15, 156.61, 152.77, 145.24, 119.22, 80.34, 74.68, 19.63. Found, %: C, 38.44; H, 2.43; N, 33.59; S, 12.75. Calc. for $C_8H_6N_6O_2S$ (%): C, 38.40; H, 2.42; N, 33.58; S, 12.81. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 250

7-Amino-6-nitropyrazolo[1,5-*a*]pyrimidine-3-carbonitrile (4h) Refluxing time: 4 hours. Brown powder. Yield 13%. R_f = 0.06 ($CHCl_3$). m.p. 246-249°C (*i*-PrOH). IR 534, 585, 625, 657, 704, 759, 836, 864, 909, 923, 942, 1026, 1075, 1144, 1176, 1247, 1283, 1338, 1367, 1436, 1478, 1565, 1578, 1652, 2840, 2313, 2225, 2313, 2839, 3114, 3186, 3264, 3373, 3595 ^1H NMR (400 MHz, DMSO-d_6) δ, p.m.: 9.74 (br s, 2H, NH_2), 9.13 (s, 1H, CH), 8.71 (s, 1H, CH) ^{13}C NMR (101 MHz, DMSO) δ, p.m.: 151.70, 150.63, 148.83, 146.21, 119.04, 113.25, 83.75. Found, %: C 41.17; H 2.01; N 41.12. Calc. for $C_7H_4N_6O_2$ (%): C 41.18; H 1.97; N 41.17. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 204.

Ethyl 7-amino-6-nitropyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4i) Refluxing time: 10 hours. Beige powder. Yield 28%. R_f = 0.10 ($CHCl_3$). m.p. 362-364°C (*i*-PrOH). IR 525, 567, 630, 642, 675, 688, 718, 749, 781, 824, 848, 862, 909, 972, 1026, 1092, 1129, 1169, 1183, 1214, 1255, 1294, 1327, 1349, 1367, 1394, 1430, 1477, 1569, 1648, 1709, 1812, 1937, 2937, 2981, 3066, 3372 ^1H NMR (400 MHz, DMSO-d_6) δ, p.m.: 9.64 (br s, 1H, NH_2), 9.14 (s, 1H, CH), 8.64 (s, 1H, CH), 4.30 (q, J = 7.1 Hz, 2H, CH_2), 1.31 (t, J = 7.1 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, DMSO) δ 161.89, 150.03, 148.62, 148.46, 146.10, 118.43, 104.54, 60.34, 14.85. Found, %: C 43.01; H 3.62; N 27.86. Calc. for $C_9H_9N_5O_4$ (%): C 43.04; H 3.61; N 27.88. Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 251.

3,5-Dinitro-*N*-(*p*-tolyl)pyridine-2,6-diamine (5).

m.p. 234-235°C ($CHCl_3$), 235-236°C (*i*-PrOH). R_f = 0.56 ($CHCl_3$). IR 547, 608, 631, 658, 698, 718, 757, 771, 818, 865, 893, 1028, 1097, 1123, 1195, 1221, 1260, 1291, 1307, 1338, 1374, 1417, 1443, 1484, 1510, 1572, 1615, 1908, 2855, 3119, 3324, 3445, 3462, 3504 ^1H NMR (400 MHz, DMSO-d_6) δ, p.m.: 10.46 (s, 1H, 1NH), 9.15 (s, 1H, CH), 8.81 (s, 1H, NH_2), 8.40 (s, 1H, NH_2), 7.69 (d, J = 8.0 Hz, 2H, 2CH), 7.18 (d, J = 8.2 Hz, 2H, 2CH), 2.37 (s, 3H, CH_3) ^{13}C NMR (101 MHz, DMSO) δ, p.m.: 154.85, 150.79, 136.02, 135.39, 134.67, 129.63, 123.07, 121.33, 120.81, 21.00. Found, %: C 49.84; H 3.82; N 24.24. Calculated, %: C 49.83; H 3.81; N 24.22 Mass spectrum (EI, 70 eV, m/z): $[M]^+$ = 289.

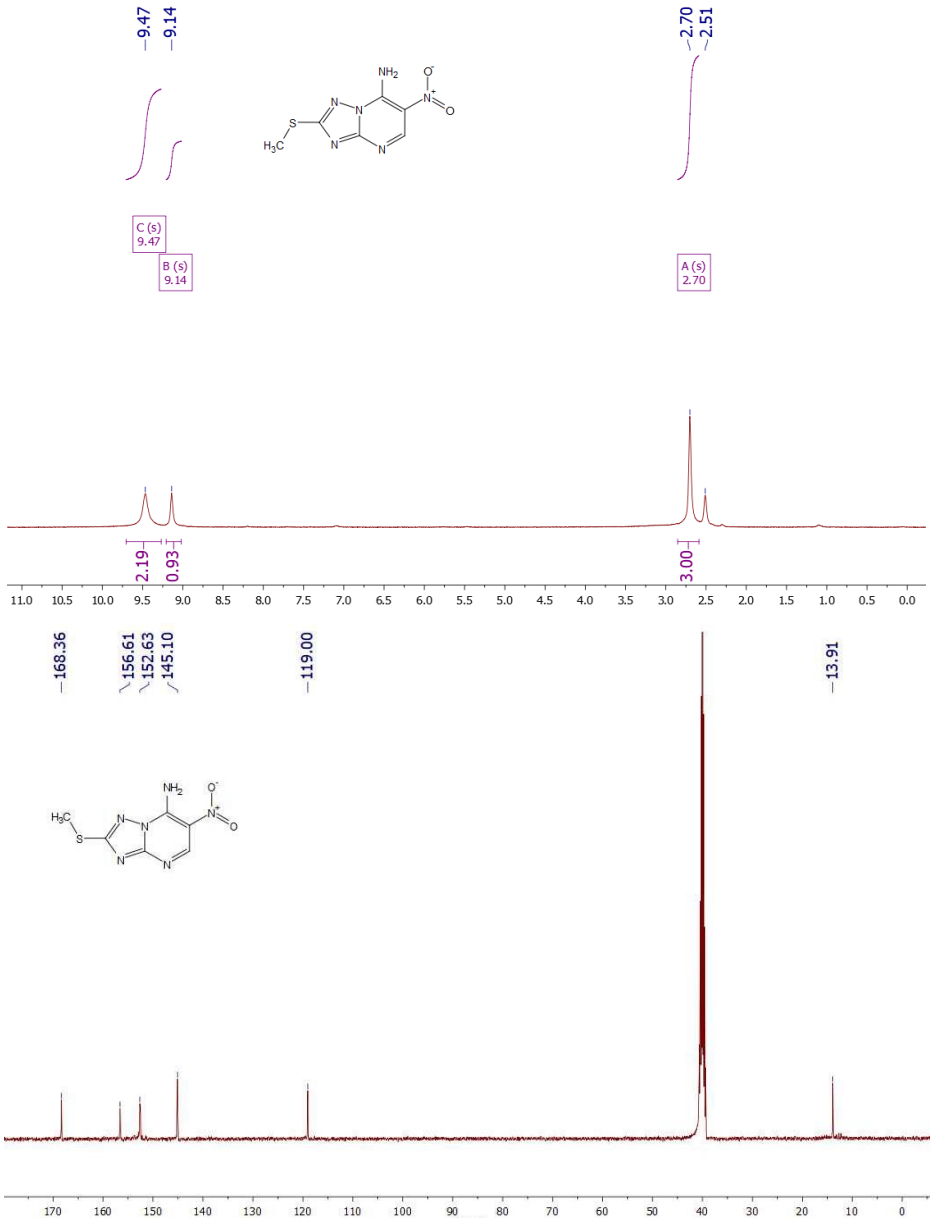


Figure S1. ^{1}H and ^{13}C NMR spectra of compound **4a**

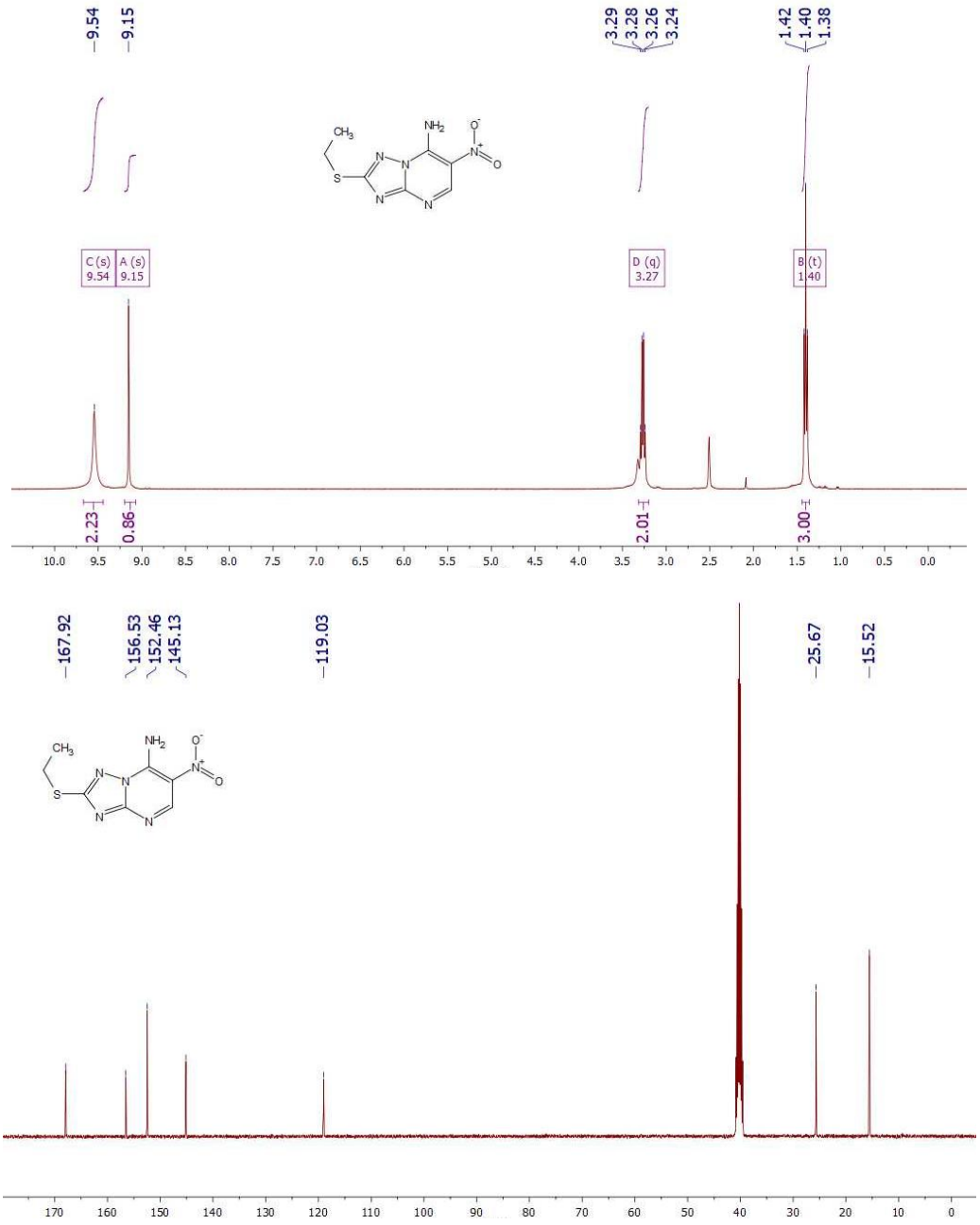


Figure S2. ^{1}H and ^{13}C NMR spectra of compound **4b**

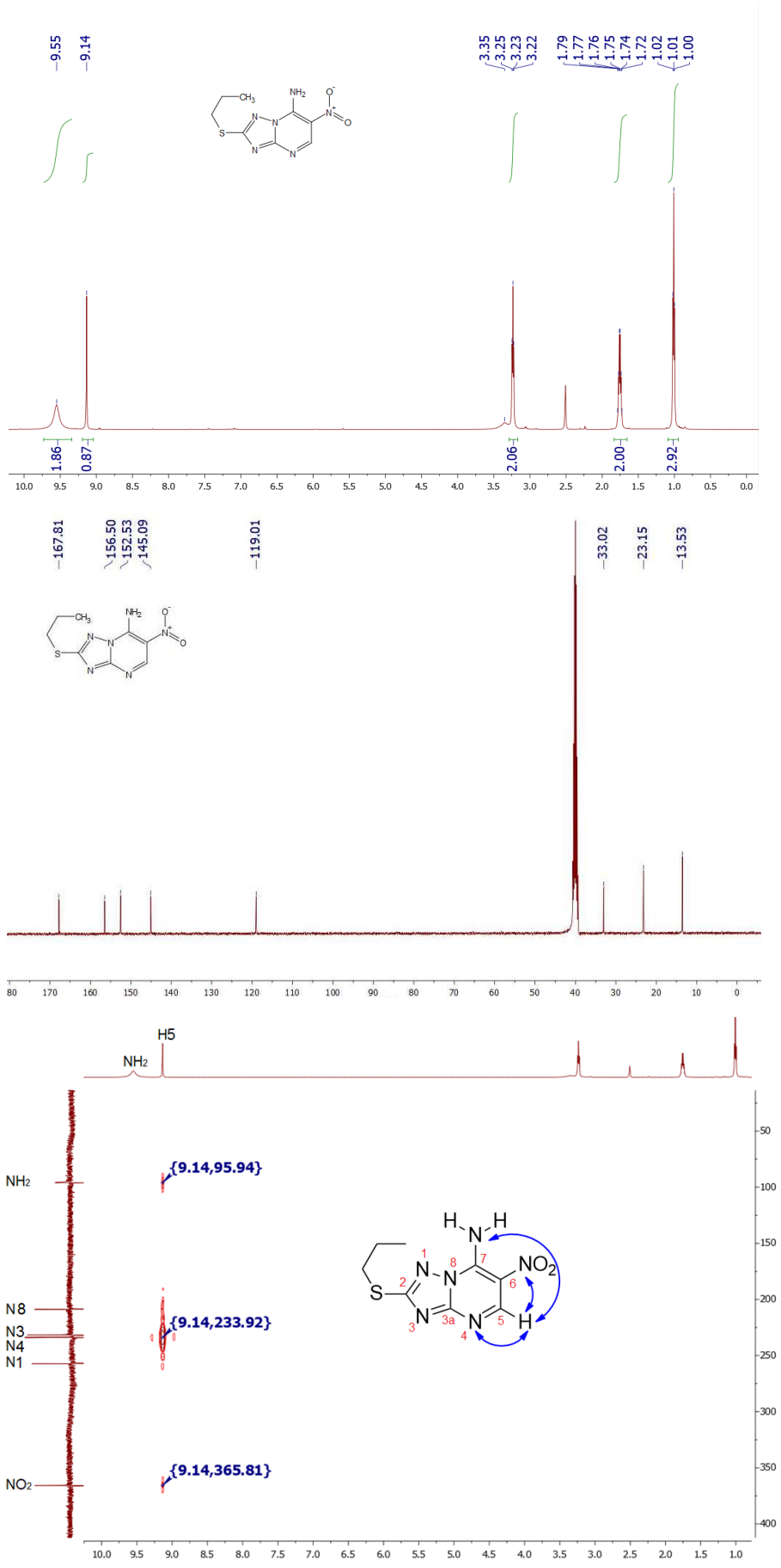


Figure S3. ^{1}H, ^{13}C and ^{1}H-^{15}N HMBC NMR spectra of compound **4c.** Cross interactions are indicated by blue arrows

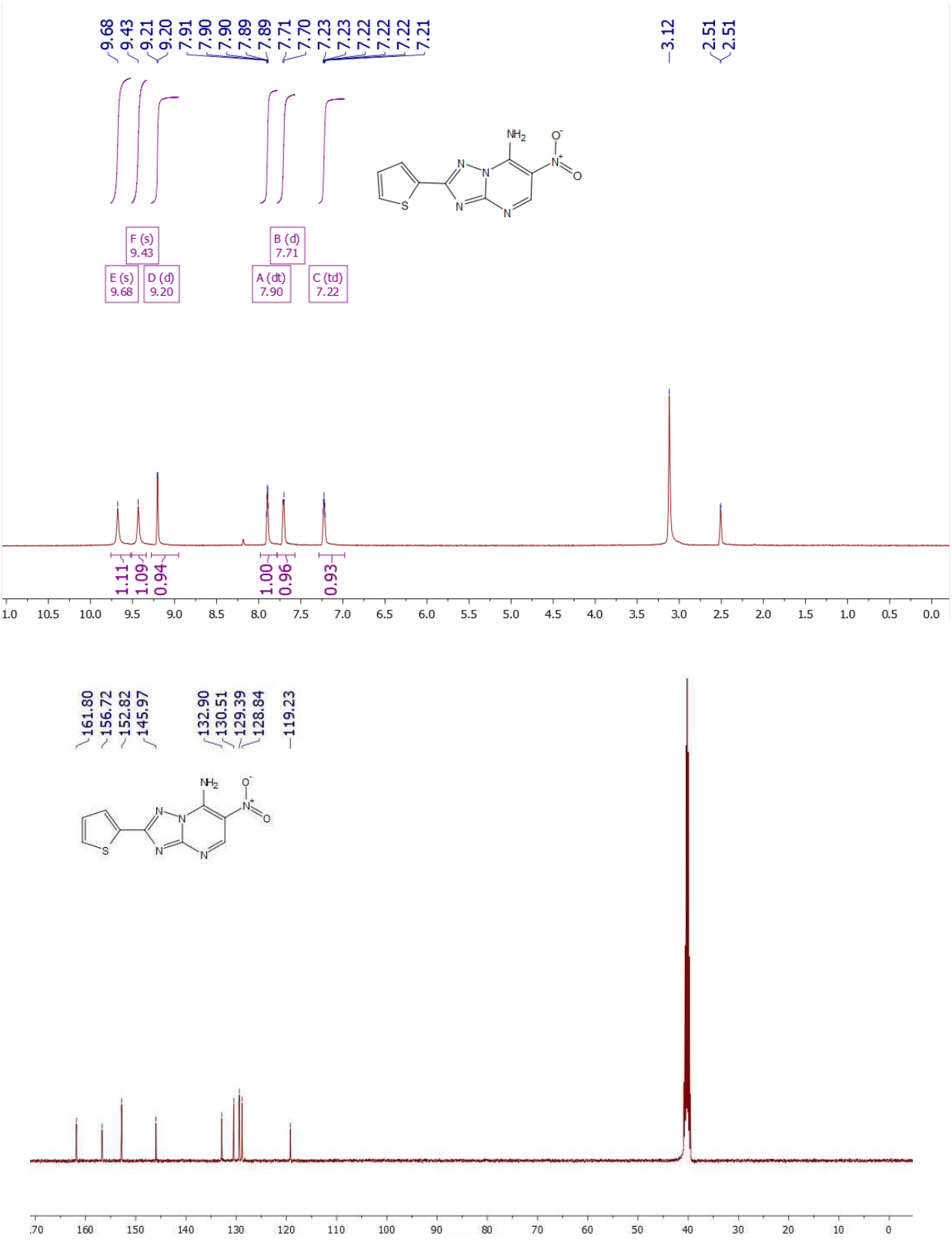


Figure S4. ^{1}H and ^{13}C NMR spectra of compound **4d**

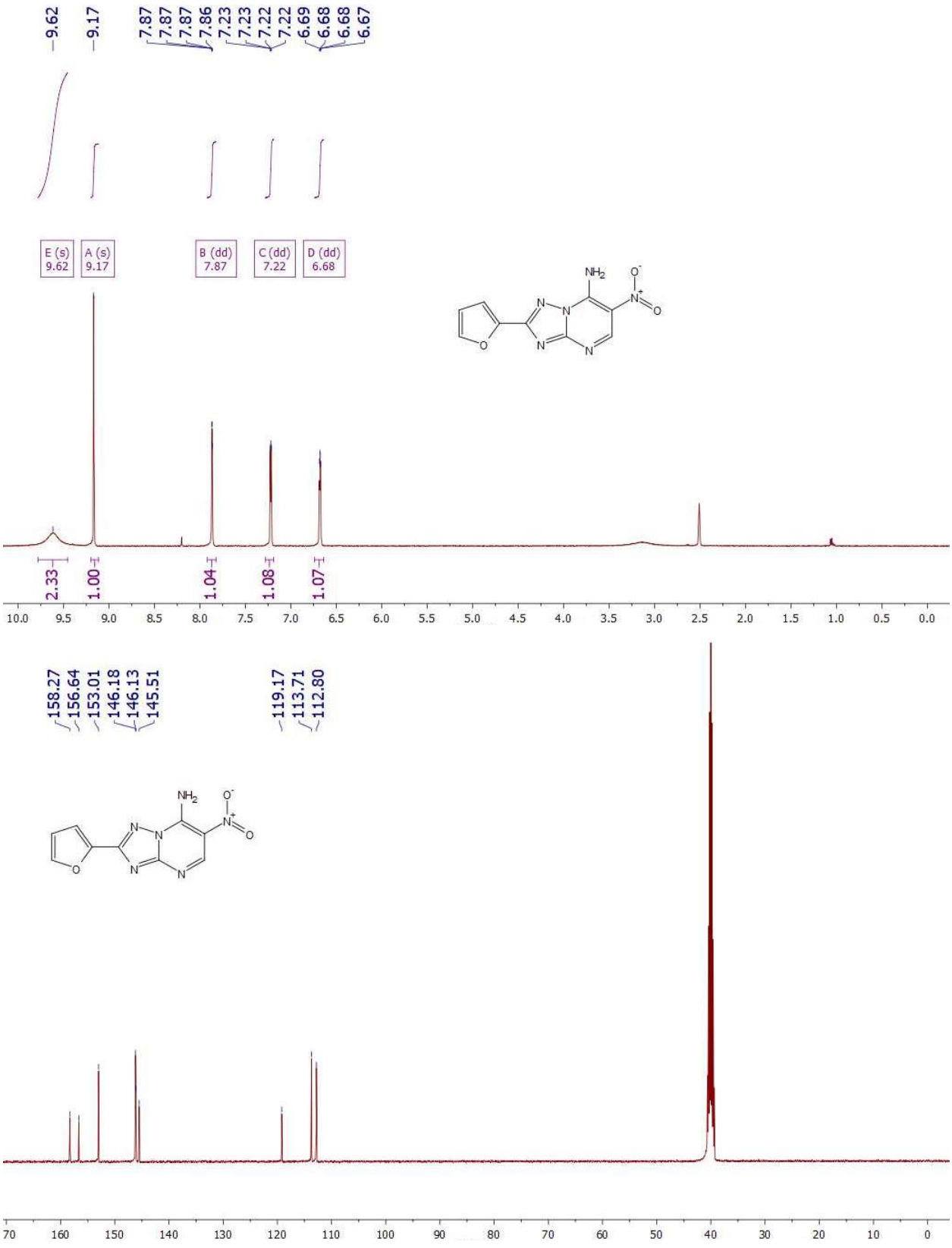


Figure S5. ^{1}H and ^{13}C NMR spectra of compound **4e**

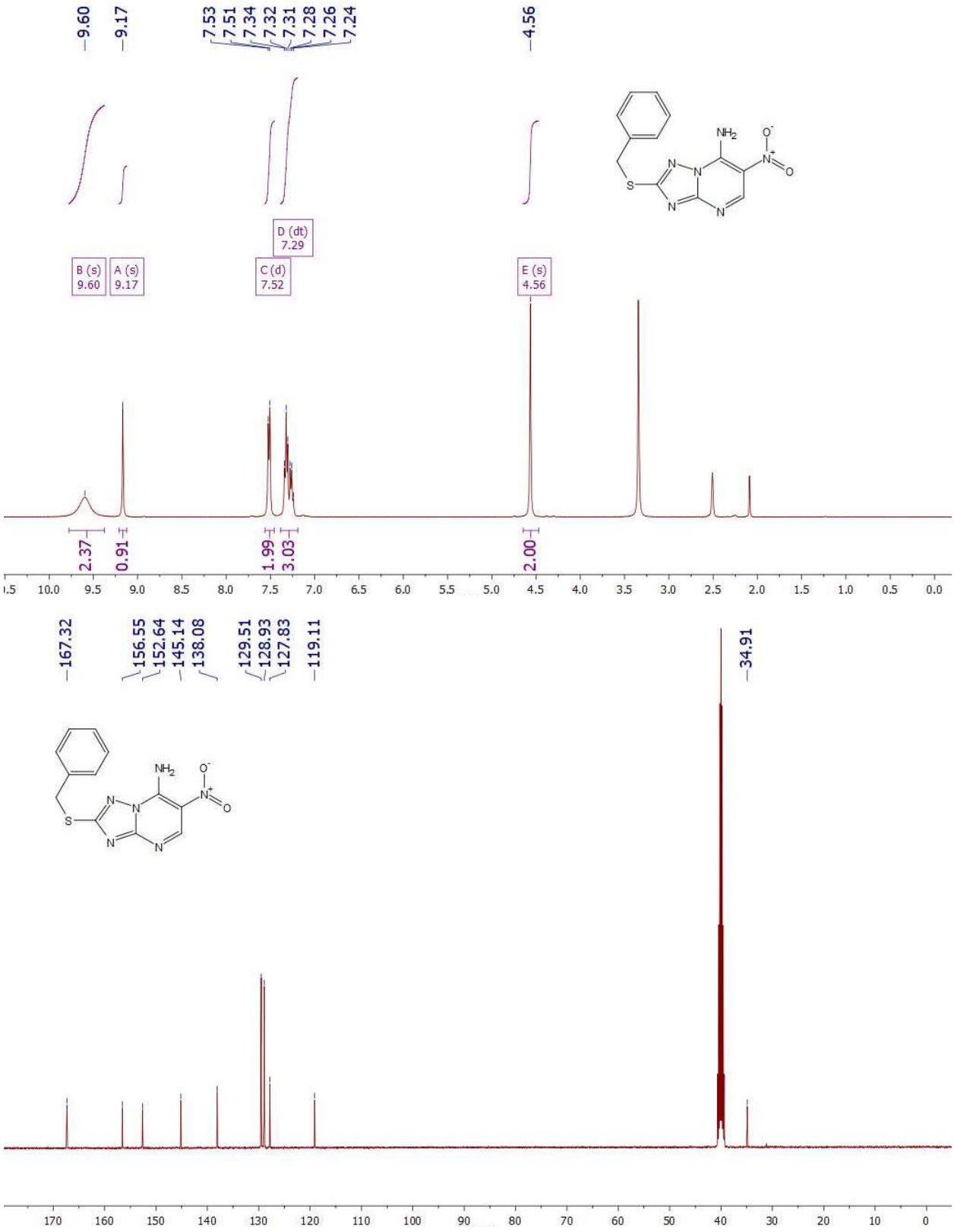


Figure S6. ^{1}H and ^{13}C NMR spectra of compound **4f**

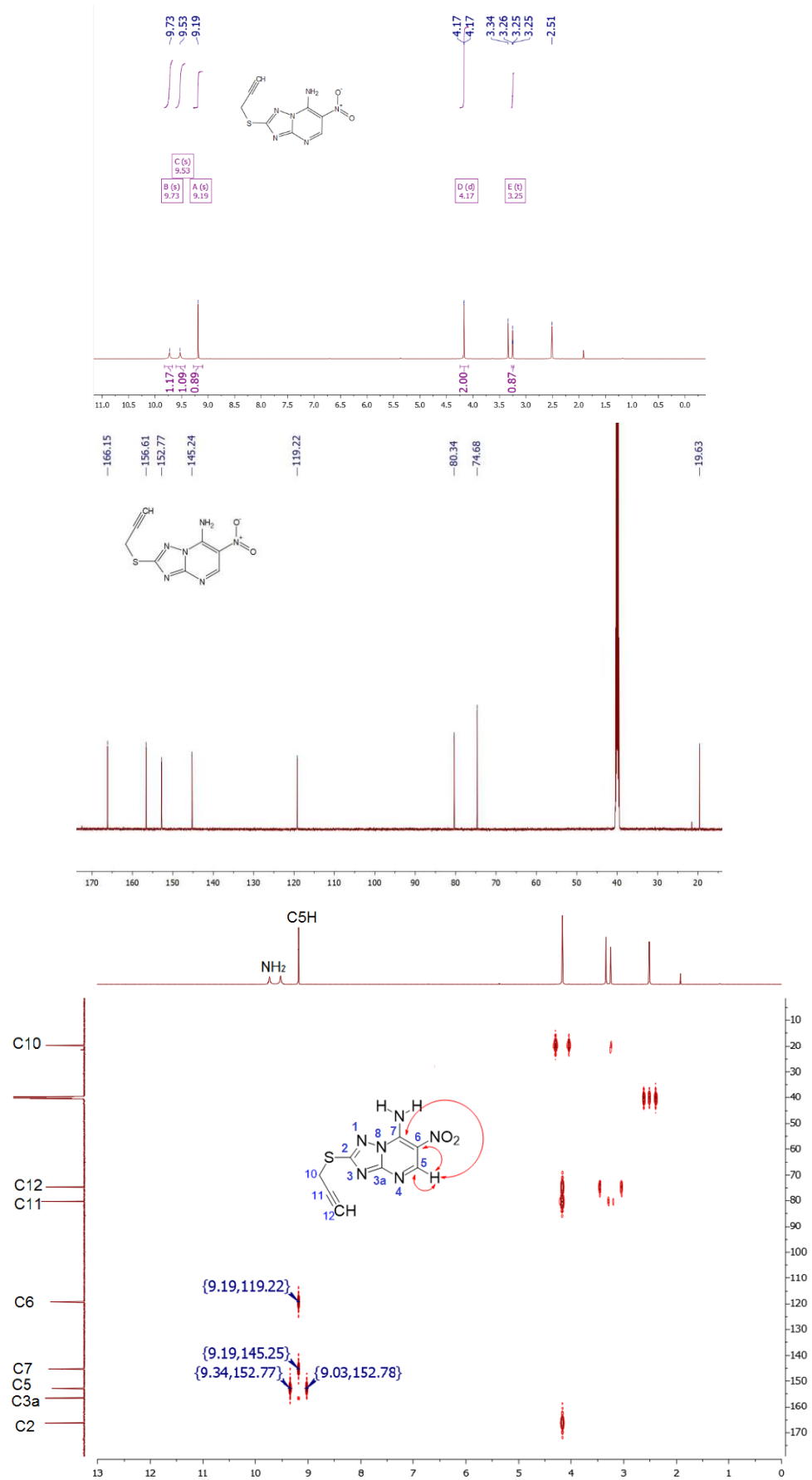


Figure S7. ^{1}H, ^{13}C and ^{1}H-^{13}C HMBC spectra of compound **4g**. ^{1}H-^{13}C cross interactions (excluding interactions in prop-2-yn-1-yl moiety) are indicated by red arrows.

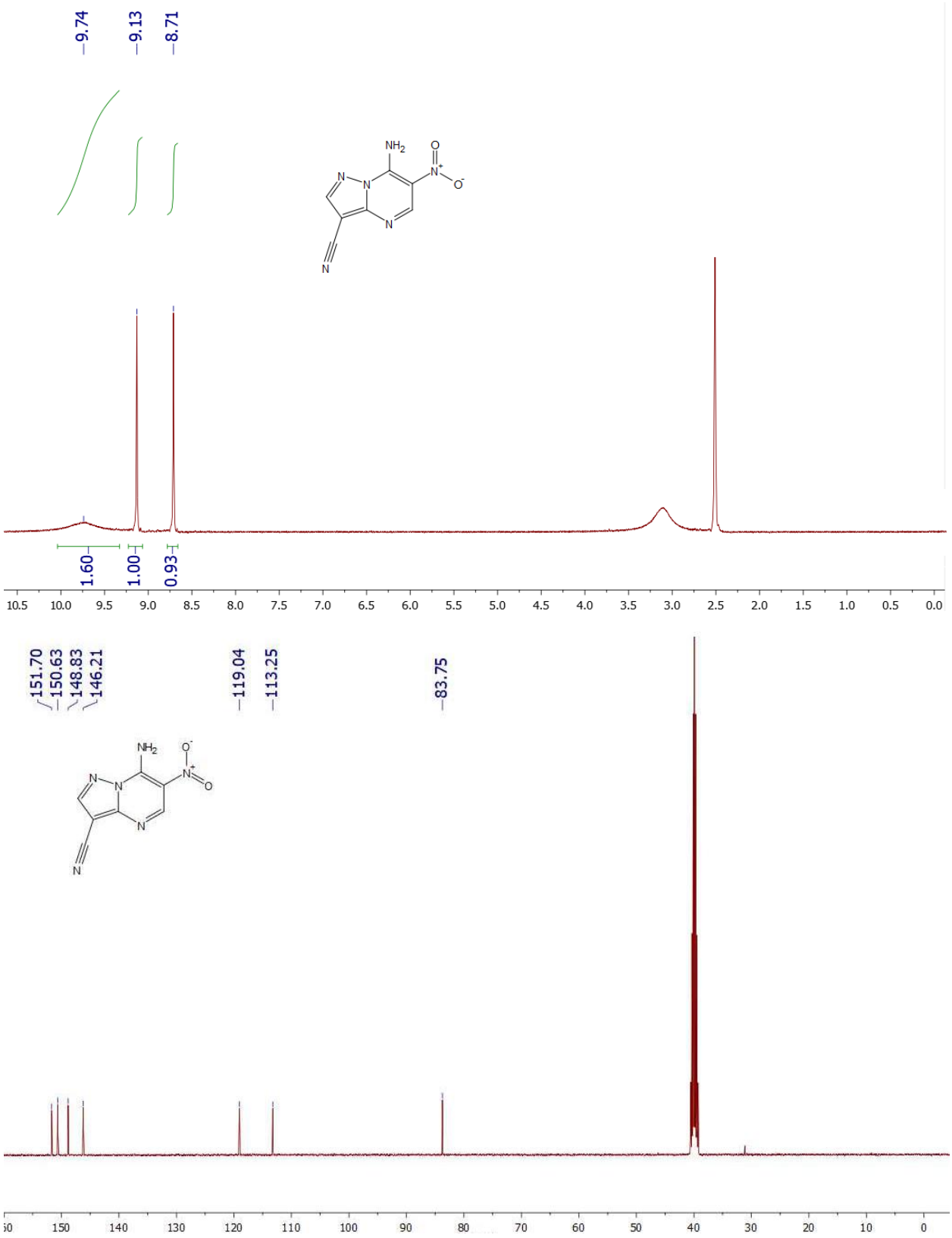


Figure S8. ^{1}H and ^{13}C NMR spectra of compound **4h**

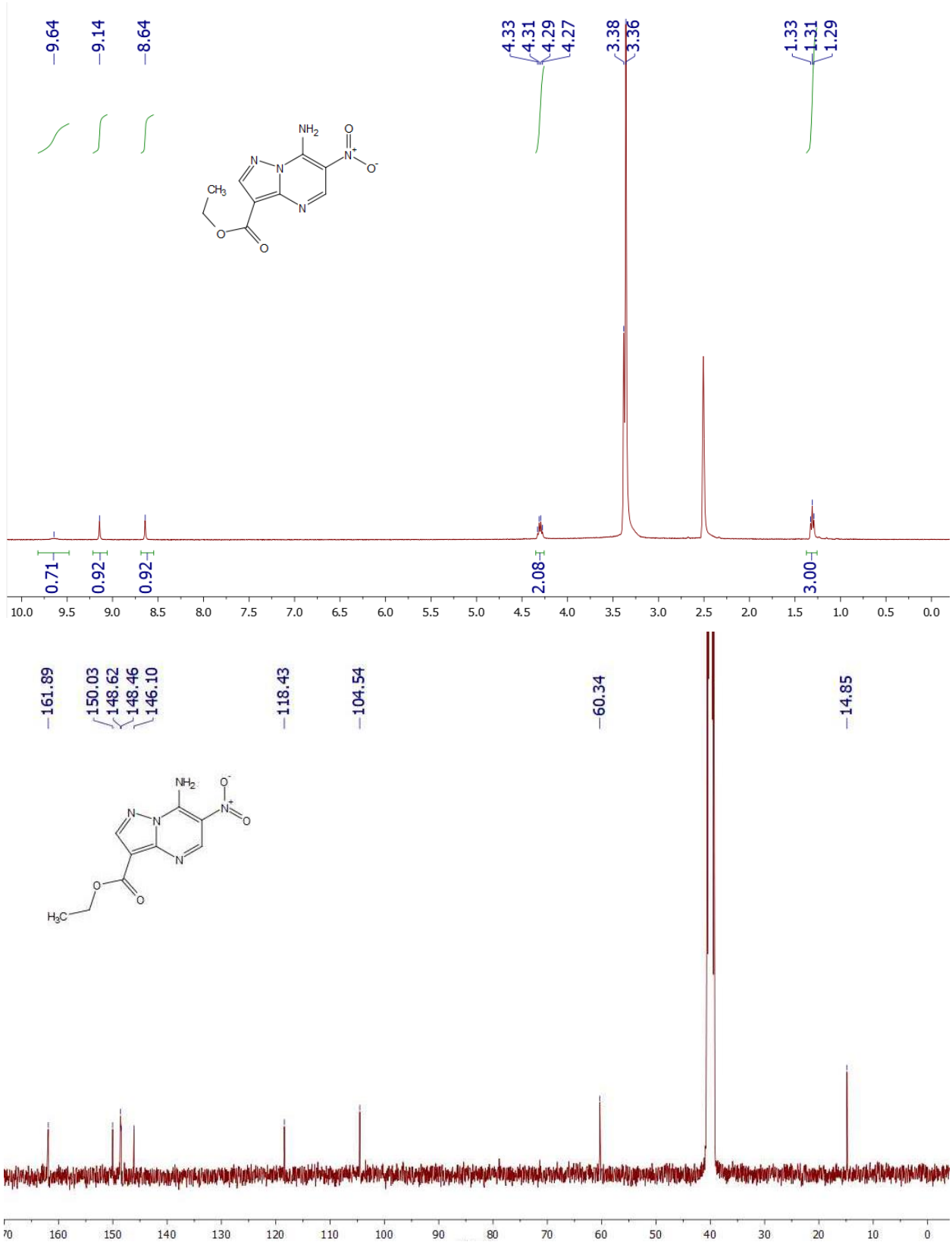


Figure S9. ^{1}H and ^{13}C NMR spectra of compound **4i**

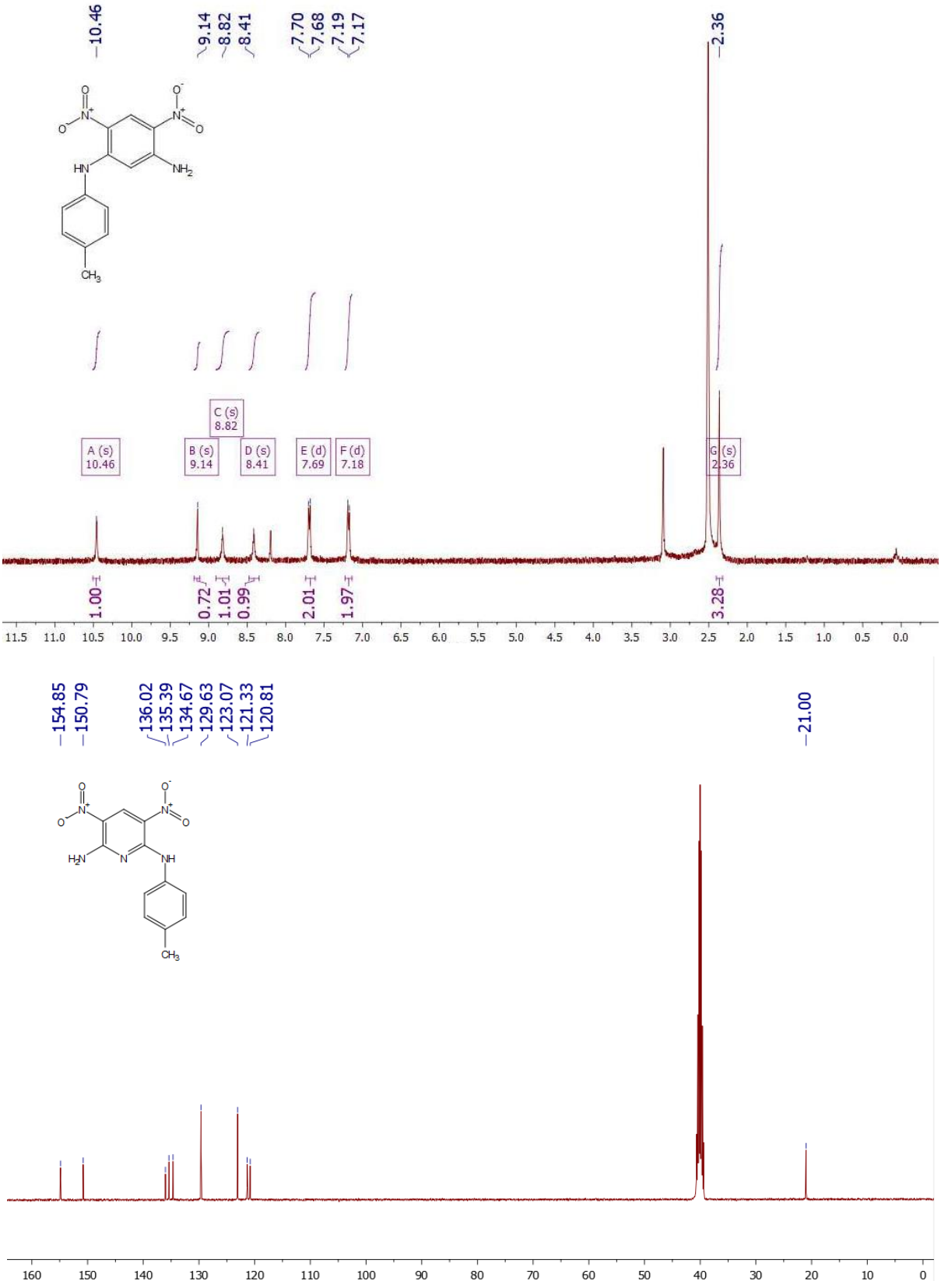


Figure S10. ^{1}H and ^{13}C NMR spectra of compound **5**

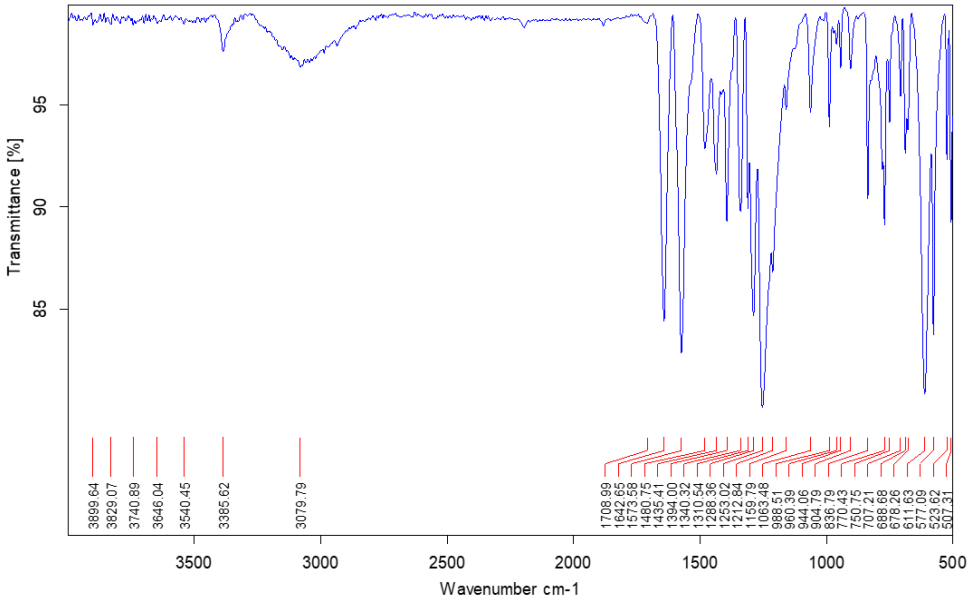


Figure S11. IR spectrum of compound **4a**

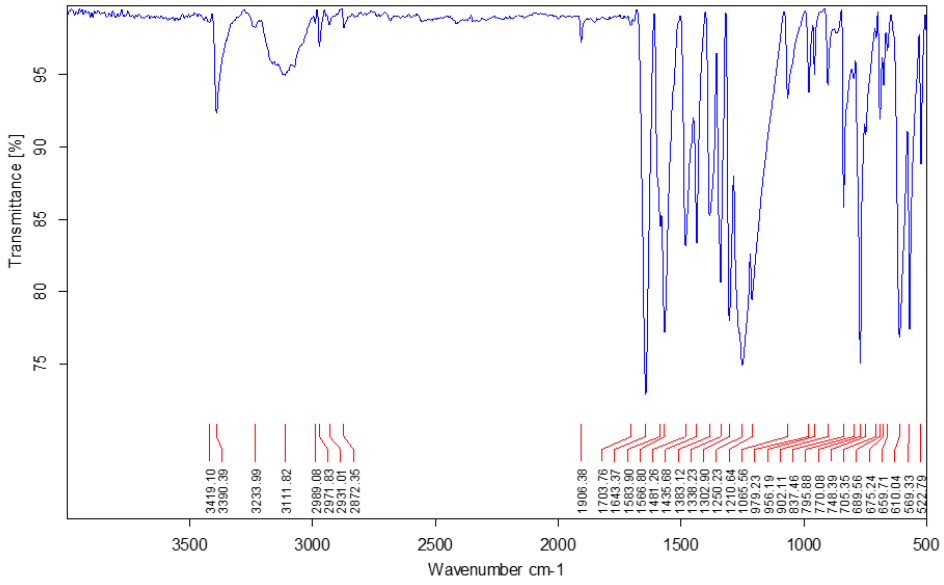


Figure S12. IR spectrum of compound **4b**

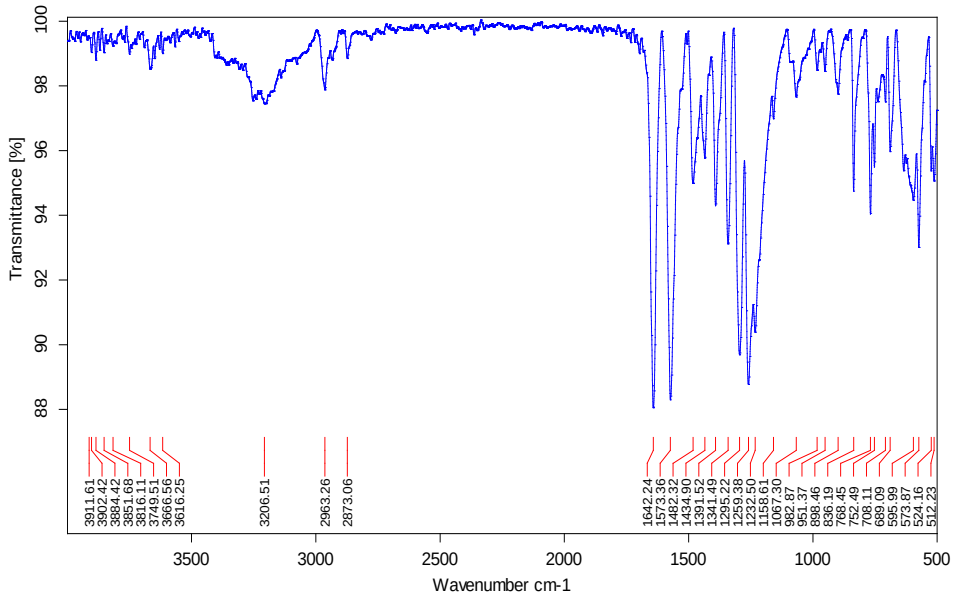


Figure S13. IR spectrum of compound **4c**

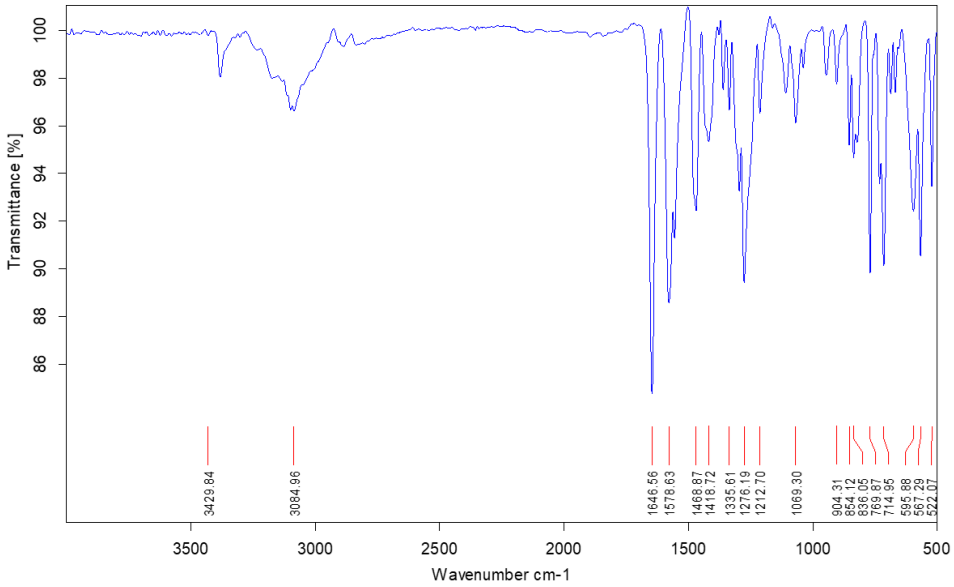


Figure S14. IR spectrum of compound **4d**

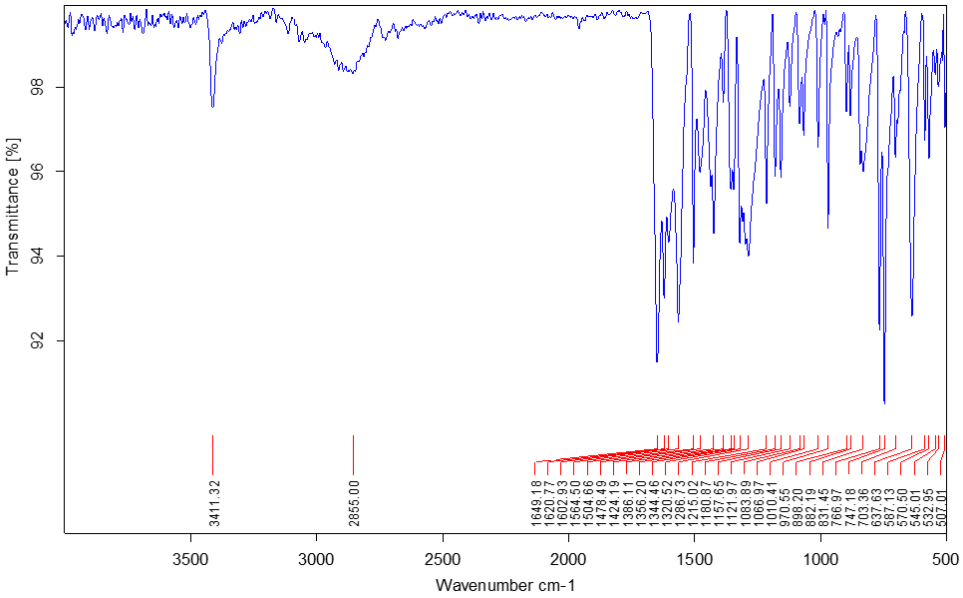


Figure S15. IR spectrum of compound **4e**

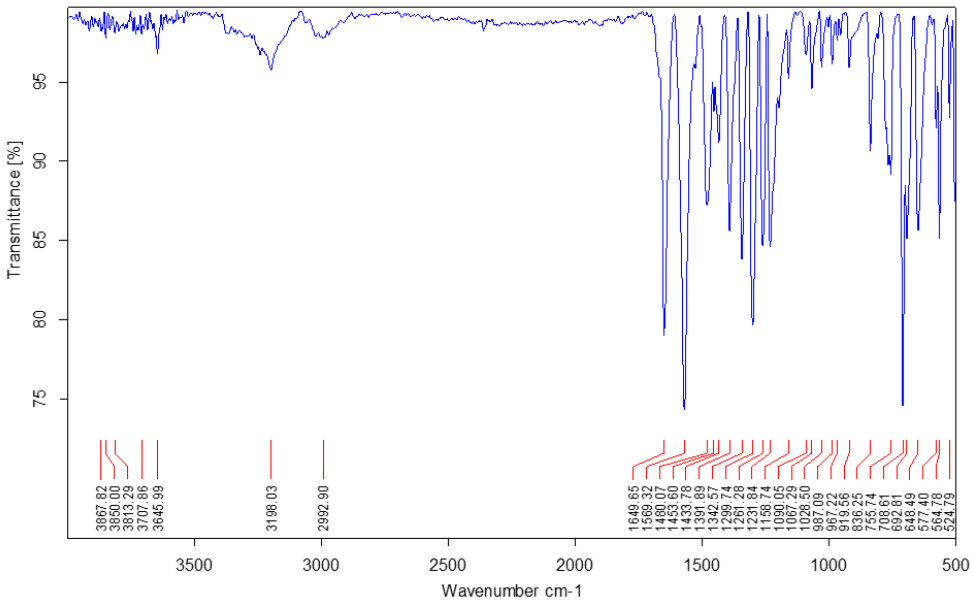


Figure S16. IR spectrum of compound **4f**

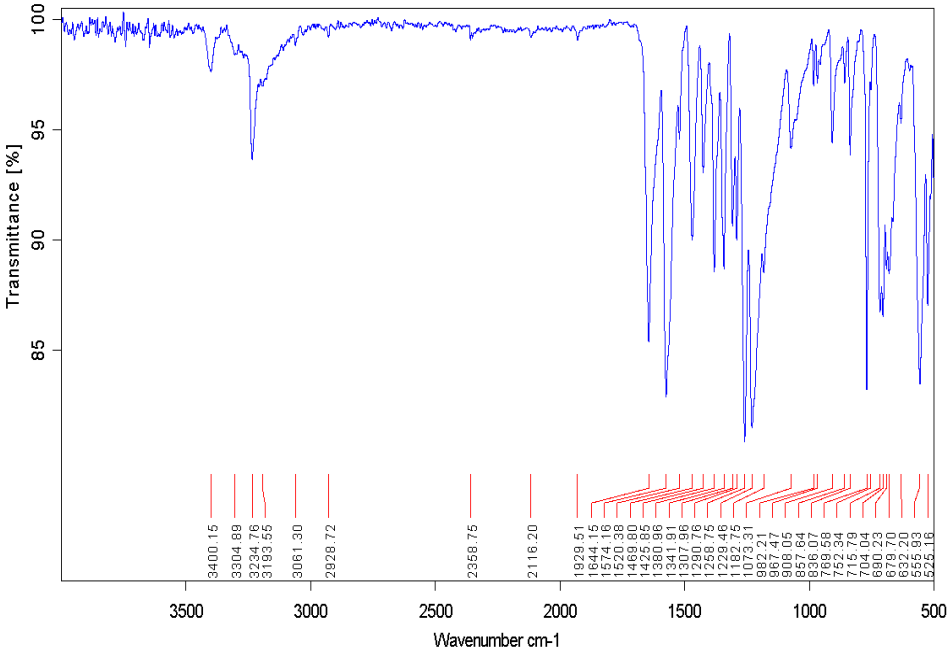


Figure S17. IR spectrum of compound **4g**

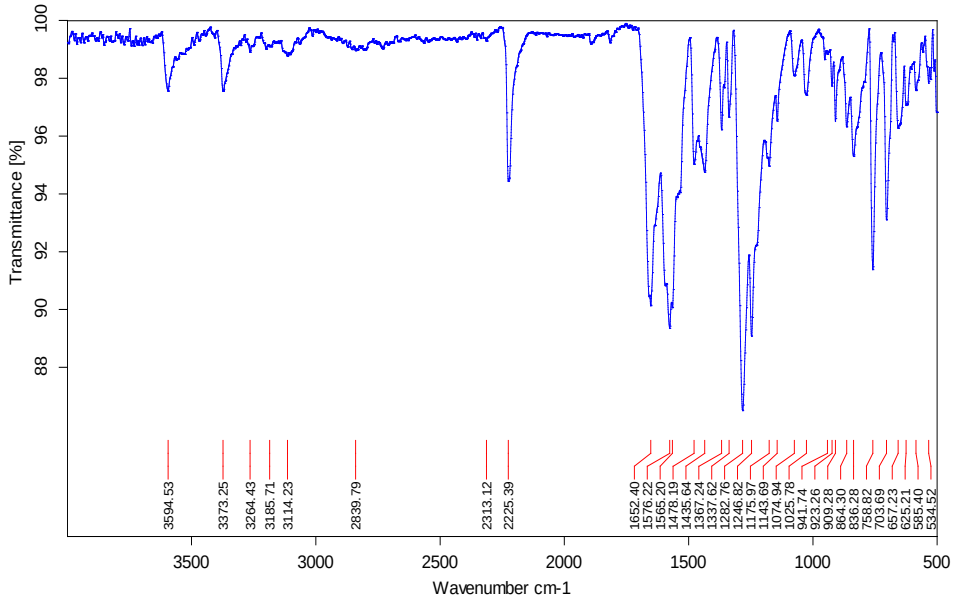


Figure S18. IR spectrum of compound **4h**

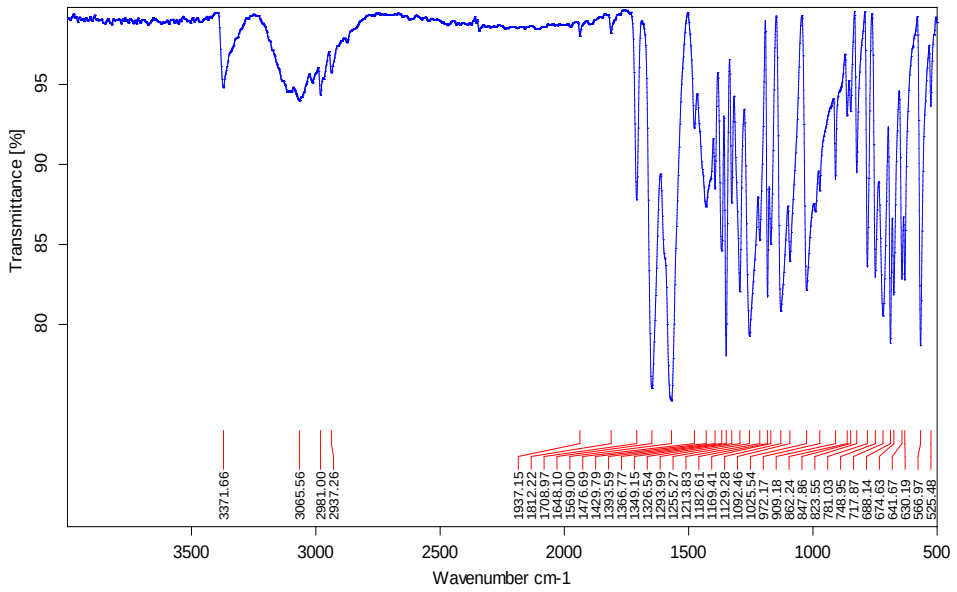


Figure S19. IR spectrum of compound **4i**

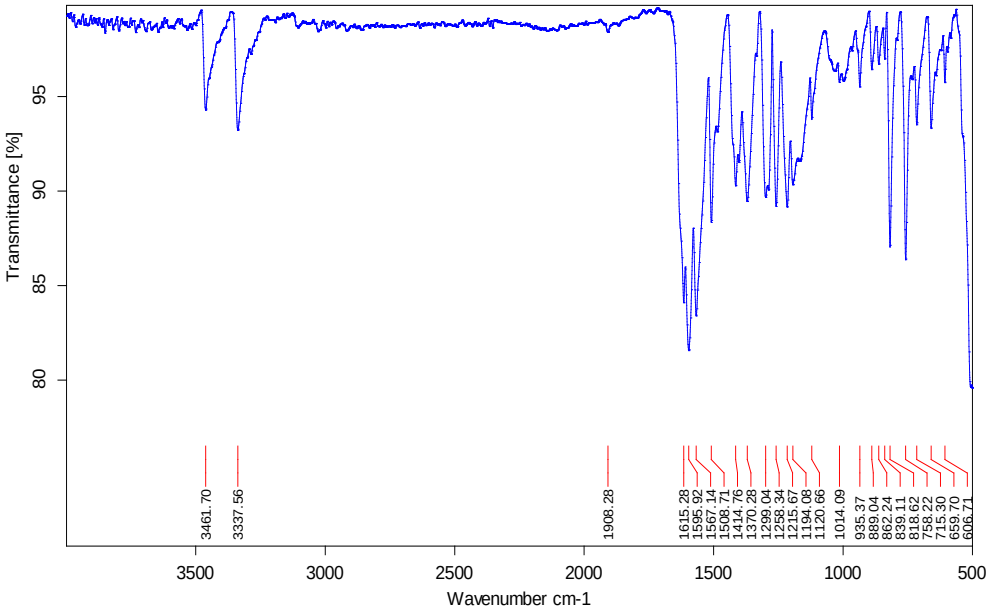
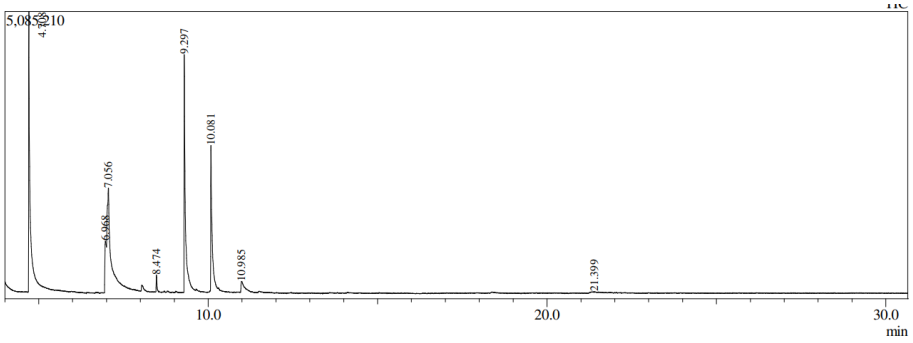


Figure S20. IR spectrum of compound **5**

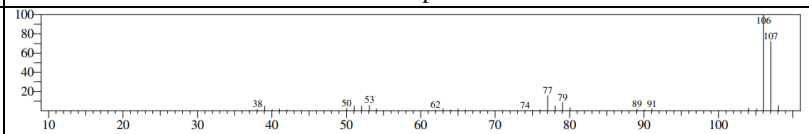
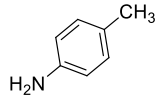
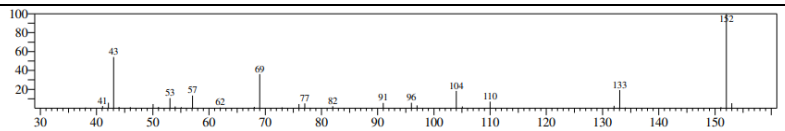
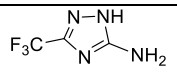
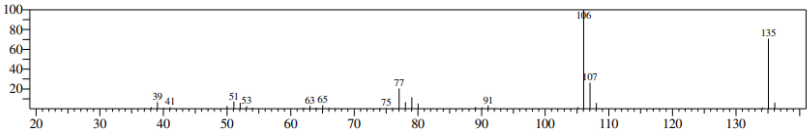
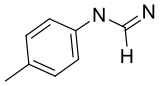
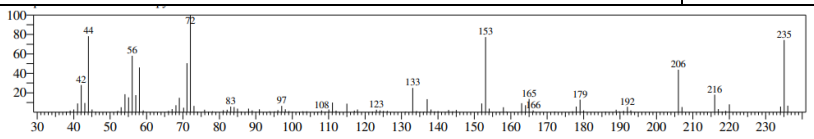
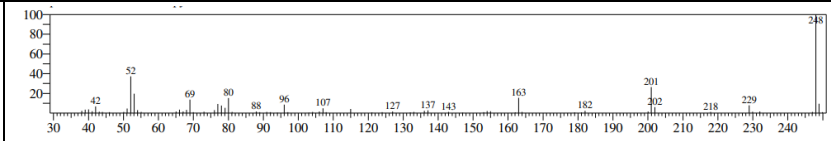
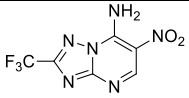
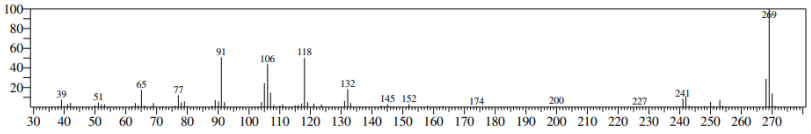
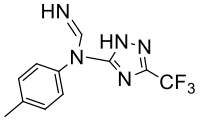
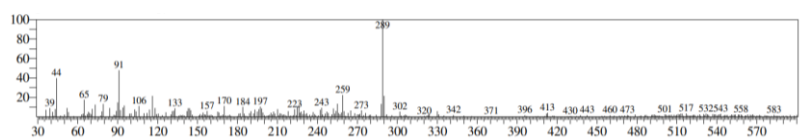
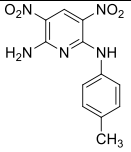


Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	Name
1	4.708	4.679	5.050	13495390	27.71	4951621	33.06	p-Aminotoluene
2	6.968	6.933	7.004	2895726	5.95	907937	6.06	1,2,4-Triazole, 3-trifluoromethyl-5-amino-
3	7.056	7.004	7.575	13462516	27.64	1835255	12.25	
4	8.474	8.433	8.583	491293	1.01	304927	2.04	
5	9.297	9.250	9.592	10265106	21.07	4204137	28.07	
6	10.081	10.050	10.271	6947347	14.26	2567572	17.14	
7	10.985	10.929	11.158	949151	1.95	184150	1.23	
8	21.399	21.221	21.596	201223	0.41	21472	0.14	
				48707752	100.00	14977071	100.00	

Figure S21. GCMS chromatogram for the filtrate from the preparation of compound **5** (method A)

Table S5. MS spectra for the peaks according to chromatogram (Fig. S22)

Line	Mass spectrum	Structure
1		 Exact Mass: 107,0735 $[M]^+$ = 107
2		 Exact Mass: 152,0310 $[M]^+$ = 152
3		 Exact Mass: 134,0844 $[M+1]^+$ = 135
4		
5		 Exact Mass: 248,0270 $[M]^+$ = 248
6		 Exact Mass: 269,0888 $[M]^+$ = 269
8		 Exact Mass: 289,0811 $[M]^+$ = 289

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