

Unusual cyclization of *N*-imidazolyl quinone imines with the formation of thiadiazole ring and its subsequent recyclization

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Experimental

General remarks

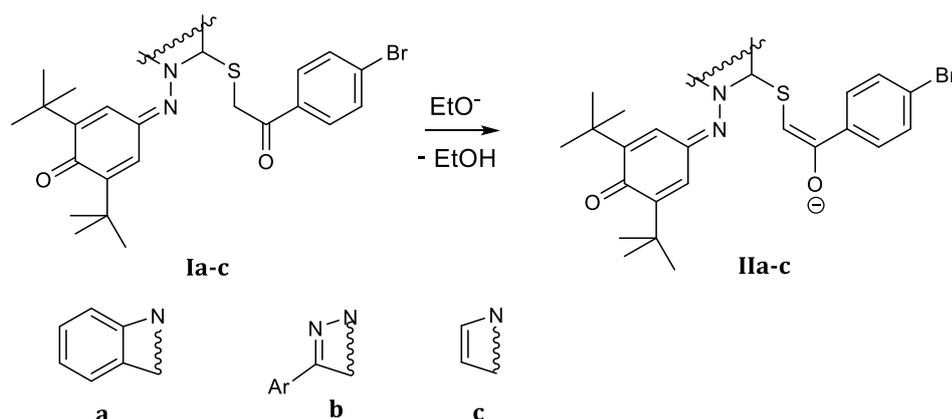
All commercial products and solvents were used without further purification. All reactions were performed in air unless noted otherwise.

TLC analyses were performed on Merck 60 F254 aluminum plates in combination with UV detection (254 nm). Melting points were determined using the Mel-Temp II Laboratory Devices apparatus; the values are uncorrected. ^1H and ^{13}C NMR spectra were acquired on a Bruker Avance HD 400 spectrometer (400 and 100 MHz, respectively) in $\text{DMSO-}d_6$ or in CDCl_3 , using the residual solvent signals ($\text{DMSO-}d_6$: 2.50 ppm for ^1H nuclei, 40.5 ppm for ^{13}C nuclei; CDCl_3 : 7.26 ppm for ^1H nuclei, 77.2 ppm for ^{13}C nuclei) as internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets), integration and coupling constants (J). The structure of the key products **3b**, **4b,d,f**, **5a-g**, **6e** was confirmed by 2D NMR experiments on the same instrument; mixing time for NOESY experiment was 0.3 s. HRMS-ESI spectra were recorded on Bruker UHR-TOF MaxisTM Impact mass spectrometer (electrospray ionization). Mass spectra were recorded using Kratos MS-30 instrument with EI ionization at 70 eV and 200 °C.

The quantum chemical calculations presented in this work were performed using the Gaussian 16 software package [S1]. To solve the Schrödinger equation, the density functional theory (DFT) approximation was used using the hybrid exchange-correlation functional wB97XD, which includes a correction for long-range order exchange interactions. The electron density was described by the standard three-exponential split valence basis set 6-311++G(d,p). The nature of the detected stationary points was checked by calculating the force constant matrix (Hessian). The effects of solvation were taken into account in the framework of the polarizable continuum model (PCM). Ethanol was chosen as a solvent.

Estimation of the probability of methylene proton elimination

We estimated the probability of proton cleavage from the methylene group at the phenacyl bromide substituent under basic catalysis conditions. The calculation results showed that the hydrogen atom in the methylene group with the phenacyl bromide substituent is capable of being easily split off under basic conditions, generating the anionic form of reagent **II** (Scheme S1).



Scheme S1

The calculated total energies and energy effects of this process, taking into account the effect of solvation, are shown in Table S1.

Table S1. Total (a.u) and relative (in kcal·mol⁻¹) energies of compounds calculated by the wB97XD/6-311++G** method in solution. The effects of solvation were taken into account within the polarizable continuum model (PCM); ethanol was chosen as the solvent.

Compound	a	b	c
I (<i>E</i> , a.u)	-4410.11230	-4519.57120	-4256.47677
EtO ⁻ (<i>E</i> , a.u)	-154.52835	-154.52835	-154.52835
II (<i>E</i> , a.u)	-4409.62235	-4519.08423	-4255.98067
EtOH (<i>E</i> , a.u)	-155.04634	-155.04634	-155.04634
ΔE , kcal·mol ⁻¹	-17.6	-19.5	-13.7

From the data presented in Table S1, it can be seen that for all derivatives of compound **I**, the proton elimination reaction is energetically favorable, since such a process is always accompanied by a decrease in the total energy of the system by 13.7 – 19.5 kcal mol⁻¹.

The results of the reaction mechanism (Scheme S2) calculations are presented in Tables S2 and S3.

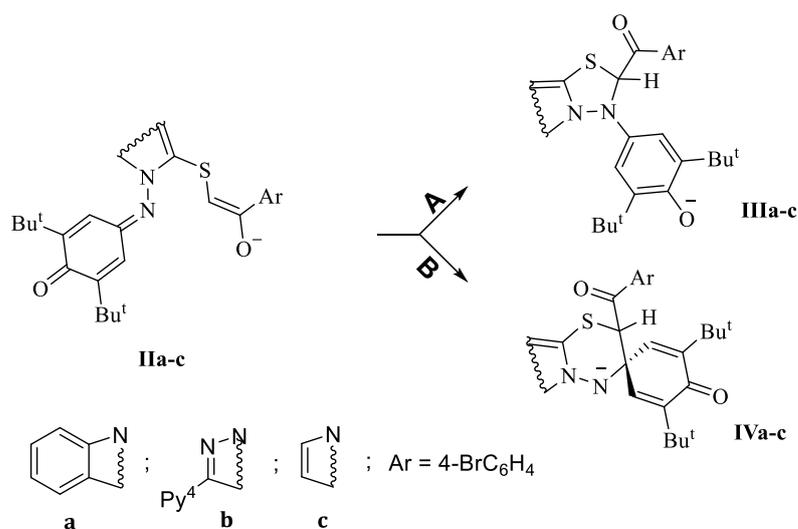


Table S2. Total (in a.u.) and relative (in kcal·mol⁻¹) energies of compounds calculated by the wB97XD/6-311++G** method in solution for the reaction proceeding along route **A**. The solvation effects were taken into account using the polarizable continuum model (PCM), ethanol was chosen as the solvent.

System	a		b		c	
	<i>E</i> , a.u	ΔE , kcal·mol ⁻¹	<i>E</i> , a.u	ΔE , kcal·mol ⁻¹	<i>E</i> , a.u	ΔE , kcal·mol ⁻¹
II	-4409.62235	0.0	-4519.08423	0.0	-4255.98067	0.0
TS	-4409.59812	15.2	-4519.06363	12.9	-4255.96271	11.3
III	-4409.63854	-10.2	-4519.10237	-11.4	-4256.00166	-13.2

Table S3. Total (in a.u.) and relative (in kcal·mol⁻¹) energies of compounds calculated by the wB97XD/6-311++G** method in solution for the reaction proceeding via pathway **B**. The solvation effects were taken into account using the polarizable continuum model (PCM), ethanol was chosen as the solvent.

System	a		b		c	
	<i>E</i> , a.u	ΔE , kcal·mol ⁻¹	<i>E</i> , a.u	ΔE , kcal·mol ⁻¹	<i>E</i> , a.u	ΔE , kcal·mol ⁻¹
II	-4409.62235	0.0	-4519.08423	0.0	-4255.98067	0.0
TS	-4409.60470	11.1	-4519.07452	6.1	-4255.97161	5.7
IV	-4409.61113	7.0	-4519.08476	-0.3	-4255.97819	1.6

In order to explain the obtained picture of the regioselectivity of the cyclization processes, we performed an NBO analysis, the results of which are shown in Table S4.

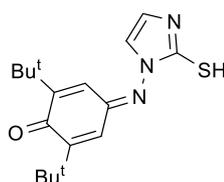
Table S4. Occupancy values of the natural orbital corresponding to the lone electron pair at the oxygen and nitrogen atom in the corresponding products **III** and **IV** (Scheme S2). NBO analysis was carried out by wB97XD/6-311++G**. The solvation effects were taken into account using the polarizable continuum model (PCM), and ethanol was chosen as the solvent.

Compound	Occupancy of lone electron pair in \bar{e}		
	a	b	c
III (O ⁻)	1.65431	1.66193	1.65875
IV (N ⁻)	1.72550	1.70546	1.72194

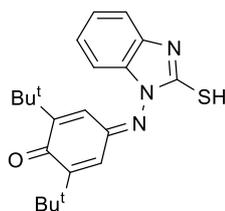
General procedure for the synthesis of compounds 3

The starting 1-amino-1*H*-imidazole-2-thiol hydrochloride and 1-amino-1*H*-benzo[*d*]imidazole-2-thiol were obtained according to the procedure described earlier [S2,S3].

A solution of 1-amino-1*H*-imidazole-2-thiol hydrochloride or 1-amino-1*H*-benzo[*d*]imidazole-2-thiol (15 mmol) and 2,6-di-*tert*-butyl-*p*-quinone (15 mmol) in EtOH was refluxed for 2 h. After cooling, the reaction mixture was diluted with water (30 ml). The precipitate that formed was filtered off. The product was isolated by column chromatography (Al₂O₃, eluent: CHCl₃) and was recrystallized from methanol.



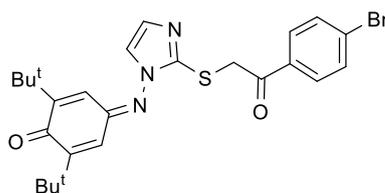
2,6-Di-*tert*-butyl-4-((2-thioxo-2,3-dihydro-1*H*-imidazol-1-yl)imino)cyclohexa-2,5-dien-1-one (3a), dark red solid, yield 44%, mp 193-195°C. ¹H NMR (CDCl₃, δ , ppm): 1.28 (s, 9H), 1.34 (s, 9H), 6.85-6.93 (m, 3H), 7.22 (d, 1H, $J = 2.6$ Hz). ¹³C NMR (CDCl₃, δ , ppm): 29.4 (3C), 29.43 (3C), 35.8, 36.1, 117.9, 120.2, 131.4, 154.3, 154.8, 162.3, 186.8. MS, m/z , (%): 317 (15.0) [M]⁺, 302 (10), 260 (20), 218 (10), 202 (5), 188 (5), 100 (15), 77 (8), 57 (48), 41 (100). HRMS (ESI): m/z [M + Na]⁺ calcd C₁₇H₂₃N₃NaOS: 340.1454; found: 340.1455.



2,6-Di-*tert*-butyl-4-((2-thioxo-2,3-dihydro-1*H*-benzo[*d*]imidazol-1-yl)imino)cyclohexa-2,5-dien-1-one (3b), dark red solid, yield 55%, mp 205-207°C. ¹H NMR (CDCl₃, δ, ppm): 1.24 (s, 9H), 1.39 (s, 9H), 6.87 (d, 1H, *J* = 2.4 Hz), 7.16 (d, 1H, *J* = 7.7 Hz), 7.22-7.37 (m, 4H). ¹³C NMR (CDCl₃, δ, ppm): 29.4 (3C), 29.5 (3C), 35.8, 35.9, 110.2, 110.3, 121.7, 123.4, 124.6, 129.6, 130.2, 131.1, 132.4, 153.4, 154.5, 164.6, 187.0. MS, *m/z*, (%): 367 (5.0) [M]⁺, 350 (4), 310 (10), 218 (4), 150 (15), 134 (10), 122 (15), 108 (10), 91 (15), 77 (15), 57 (50), 41 (100). HRMS (ESI): *m/z* [M + Na]⁺ calcd C₂₁H₂₅N₃NaOS: 390.1611; found: 390.1609.

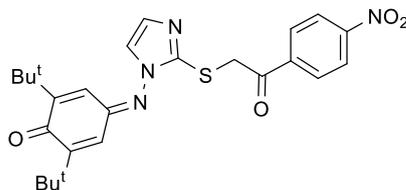
General procedure for the synthesis of compounds 4

A solution of sodium hydroxide (3 mmol) in methanol (10 ml) was added to solution of quinone imine **3** (3 mmol) in methanol (10 ml). Then phenacyl bromide (or phenacyl chloride for **4f**, 3 mmol) was added. The reaction mixture was stirred for 15 min at 40-50 °C, then poured into water (50 ml), the precipitate was filtered off. The product was isolated by column chromatography (Al₂O₃, eluent: CHCl₃).

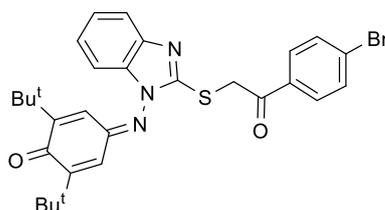


4-[(2-{[2-(4-Bromophenyl)-2-oxoethyl]thio}-1*H*-imidazol-1-yl)imino]-2,6-di-*tert*-butylcyclohexa-2,5-dien-1-one (4a), red solid, yield 57%, mp 135-137°C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.25 (s, 9H), 1.28 (s, 9H), 4.75 (s, 2H), 7.01 (d, 1H, *J* = 2.6 Hz), 7.08-7.13 (m, 2H), 7.70 (d, 1H, *J* = 1.7 Hz), 7.76 (d, 2H, *J* = 8.2 Hz), 7.95 (d, 2H, *J* = 8.2 Hz). ¹³C NMR (DMSO-*d*₆, δ, ppm): 29.3 (3C), 29.5 (3C), 35.6, 36.2, 40.1, 120.7, 121.3, 128.2, 129.6, 130.8 (2C), 132.3 (2C), 134.9, 140.9, 142.5, 153.0,

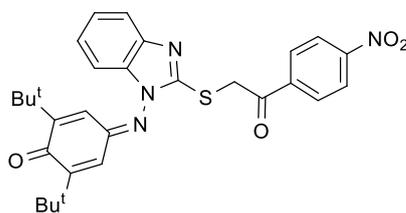
154.4, 155.9, 187.2, 193.3. HRMS (ESI): m/z $[M + Na]^+$ calcd $C_{25}H_{28}BrN_3NaO_2S$: 536.0978; found: 536.0979.



2,6-Di-tert-butyl-4-[(2-[[2-(4-nitrophenyl)-2-oxoethyl]thio]-1H-imidazol-1-yl)imino]cyclohexa-2,5-dien-1-one (4b), red solid, yield 67%, mp 146-148°C. 1H NMR (DMSO- d_6 , δ , ppm): 1.25 (s, 9H), 1.28 (s, 9H), 4.83 (s, 2H), 7.02 (d, 1H, $J = 2.6$ Hz), 7.09 (d, 1H, $J = 1.5$ Hz), 7.12 (d, 1H, $J = 2.6$ Hz), 8.71 (d, 1H, $J = 1.5$ Hz), 8.25 (d, 2H, $J = 8.9$ Hz), 8.36 (d, 2H, $J = 8.9$ Hz). ^{13}C NMR (DMSO- d_6 , δ , ppm): 29.3 (3C), 29.5 (3C), 35.6, 36.2, 40.1, 120.7, 121.4, 124.3 (2C), 129.7, 130.3 (2C), 132.2, 140.7, 142.5, 150.5, 153.0, 154.5, 155.8, 187.1, 193.4. HRMS (ESI): m/z $[M + Na]^+$ calcd $C_{25}H_{28}N_4NaO_4S$: 503.1723; found: 503.1722.

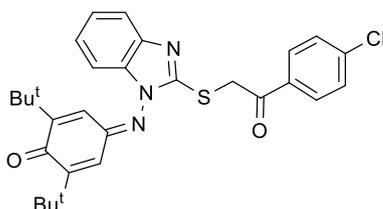


4-[(2-[[2-(4-Bromophenyl)-2-oxoethyl]thio]-1H-benzo[d]imidazol-1-yl)imino]-2,6-di-tert-butylcyclohexa-2,5-dien-1-one (4c), red solid, yield 61%, mp 153-155°C. 1H NMR (DMSO- d_6 , δ , ppm): 1.15 (s, 9H), 1.34 (s, 9H), 5.08 (s, 2H), 6.90 (d, 1H, $J = 2.6$ Hz), 7.22-7.27 (m, 4H), 7.53-7.56 (m, 1H), 7.81 (d, 2H, $J = 8.6$ Hz), 8.02 (d, 2H, $J = 8.6$ Hz). ^{13}C NMR (DMSO- d_6 , δ , ppm): 29.3 (3C), 29.5 (3C), 35.8, 36.1, 40.4, 110.3, 118.7, 121.5, 123.2, 123.7, 128.4, 130.9 (2C), 131.6, 132.4 (2C), 134.4, 134.9, 142.2, 152.1, 153.6, 153.9, 159.4, 187.1, 193.0. HRMS (ESI): m/z $[M + Na]^+$ calcd $C_{29}H_{30}BrN_3NaO_2S$: 586.1134; found: 586.1118.



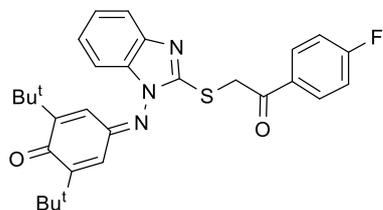
2,6-Di-*tert*-butyl-4-[(2-{[2-(4-nitrophenyl)-2-oxoethyl]thio}-1*H*-

benzo[*d*]imidazol-1-yl)imino]cyclohexa-2,5-dien-1-one (4d), red solid, yield 64%, mp 180-182 °C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.15 (s, 9H), 1.34 (s, 9H), 5.15 (s, 2H), 6.90 (d, 1H, *J* = 2.6 Hz), 7.22-7.29 (m, 4H), 7.51-7.55 (m, 1H), 8.32 (d, 2H, *J* = 8.9 Hz), 8.40 (d, 2H, *J* = 8.9 Hz). ¹³C NMR (DMSO-*d*₆, δ, ppm): 29.3 (3C), 29.6 (3C), 35.8, 36.1, 40.5, 110.4, 118.8, 121.5, 123.2, 123.7, 124.4 (2C), 130.3 (2C), 131.6, 134.5, 140.7, 142.3, 150.6, 152.0, 153.6, 154.0, 159.4, 187.1, 193.2. HRMS (ESI): *m/z* [M + Na]⁺ calcd C₂₉H₃₀N₄NaO₄S: 553.1880; found: 553.1878.



2,6-Di-*tert*-butyl-4-[(2-{[2-(4-chlorophenyl)-2-oxoethyl]thio}-1*H*-

benzo[*d*]imidazol-1-yl)imino]cyclohexa-2,5-dien-1-one (4e), red solid, yield 81%, mp 122-124 °C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.15 (s, 9H), 1.34 (s, 9H), 5.09 (s, 2H), 6.90 (d, 1H, *J* = 2.6 Hz), 7.22-7.29 (m, 4H), 7.53-7.56 (m, 1H), 7.67 (d, 2H, *J* = 8.6 Hz), 8.11 (d, 2H, *J* = 8.6 Hz). ¹³C NMR (DMSO-*d*₆, δ, ppm): 29.3 (3C), 29.6 (3C), 35.8, 36.1, 40.4, 110.3, 118.8, 121.5, 123.2, 123.7, 129.5 (2C), 130.8 (2C), 131.6, 134.4, 134.7, 139.2, 142.3, 152.1, 153.6, 153.9, 159.4, 187.1, 192.8. HRMS (ESI): *m/z* [M + Na]⁺ calcd C₂₉H₃₀ClN₃NaO₂S: 542.1639; found: 542.1635.



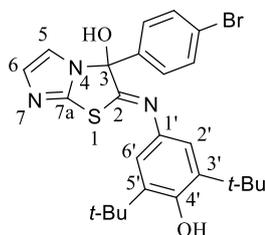
2,6-Di-*tert*-butyl-4-[(2-{[2-(4-fluorophenyl)-2-oxoethyl]thio}-1*H*-

benzo[*d*]imidazol-1-yl)imino]cyclohexa-2,5-dien-1-one (4f), red solid, yield 70%, mp 173-175 °C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.15 (s, 9H), 1.34 (s, 9H), 5.10 (s, 2H), 6.90 (d, 1H, *J* = 2.6 Hz), 7.22-7.29 (m, 4H), 7.40-7.45 (m, 2H), 7.53-7.57 (m, 1H), 8.15-8.21 (m, 2H). ¹³C NMR (DMSO-*d*₆, δ, ppm): 29.3 (3C), 29.6 (3C), 35.8,

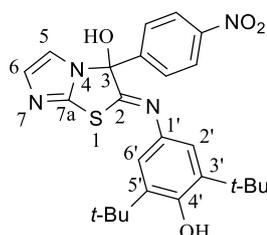
36.1, 40.1, 110.4, 116.4 (d, 2C, $J = 22.0$ Hz), 118.7, 121.5, 123.2, 123.7, 131.6, 132.0 (d, 2C, $J = 9.6$ Hz), 132.7 (d, 1C, $J = 2.9$ Hz), 134.4, 142.2, 152.2, 153.6, 153.9, 159.4, 165.8 (d, 1C, $J = 252.4$ Hz), 187.1, 192.2. HRMS (ESI): m/z $[M + Na]^+$ calcd $C_{29}H_{30}FN_3NaO_2S$: 526.1935; found: 526.1936.

General procedure for the synthesis of compounds 5

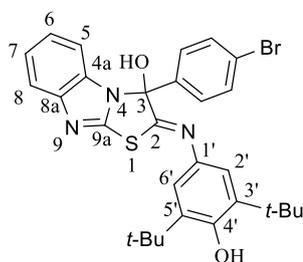
Compound 4 (1 mmol) was dissolved in DMF (5 ml), a solution of KOH (1 mmol) in EtOH (3 ml) was added dropwise. The reaction mixture was stirred at 50-60 °C for 30 min, then was diluted with water (30 ml) and neutralized with diluted AcOH. The precipitate formed was filtered off. The product was isolated by column chromatography (Al_2O_3 , eluent: CH_2Cl_2).



(Z)-2-((3,5-Di-*tert*-butyl-4'-hydroxyphenyl)imino)-3-(4-bromophenyl)-2,3-dihydroimidazo[2,1-*b*]thiazol-3-ol (5a), light pink solid, yield 45%, mp 190 °C. 1H NMR ($DMSO-d_6$, δ , ppm): 1.37 (s, 18H, $C(CH_3)_3$), 6.77 (s, 2H, H-2',6'), 7.11 (d, 1H, $J = 1.4$ Hz, H-6), 7.22 (br.s, 1H, HO-4'), 7.26 (d, 2H, $J = 8.5$ Hz, H-2,6 (C_6H_4Br-4)), 7.33 (d, 1H, $J = 1.4$ Hz, H-5), 7.64 (d, 2H, $J = 8.5$ Hz, H-3,5 (C_6H_4Br-4)), 8.64 (br.s, 1H, HO-3). ^{13}C NMR ($DMSO-d_6$, δ , ppm): 30.6 (6C, $C(CH_3)_3$), 35.2 (2C, $C(CH_3)_3$), 90.8 (C-3), 117.1 (C-5), 117.2 (2C, C-2',6'), 122.9 (C-4 (C_6H_4Br-4)), 128.3 (2C, C-2,6 (C_6H_4-Br-4)), 132.0 (2C, C3,5 (C_6H_4Br-4)), 133.6 (C-6), 140.2 (C-1 (C_6H_4Br-4)), 141.0 (C-1'), 141.1 (2C, C-3',5'), 141.2 (C-7a), 153.1 (C-4'), 164.2 (C-2). HRMS (ESI): m/z $[M + Na]^+$ calcd $C_{25}H_{28}BrN_3NaO_2S$: 536.0978; found: 536.0978.



(Z)-2-((3,5-Di-*tert*-butyl-4-hydroxyphenyl)imino)-3-(4-nitrophenyl)-2,3-dihydroimidazo[2,1-*b*]thiazol-3-ol (5b), colorless solid, yield 44%, mp 192 °C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.37 (s, 18H, C(CH₃)₃), 6.78 (s, 2H, H-2',6'), 7.14 (d, 1H, *J* = 1.4 Hz, H-6), 7.24 (br.s, 1H, HO-4'), 7.36 (d, 1H, *J* = 1.4 Hz, H-5), 7.60 (d, 2H, *J* = 8.9 Hz, H-2,6 (C₆H₄NO₂-4)), 8.30 (d, 2H, *J* = 8.9 Hz, H-3,5 (C₆H₄NO₂-4)), 8.89 (br.s, 1H, HO-3). ¹³C NMR (DMSO-*d*₆, δ, ppm): 30.6 (6C, C(CH₃)₃), 35.2 (2C, C(CH₃)₃), 90.6 (C-3), 117.1 (C-5), 117.2 (2C, C-2',6'), 124.3 (2C, C-3,5 (C₆H₄NO₂-4)), 127.7 (2C, C-2,6 (C₆H₄NO₂-4)), 133.9 (C-6), 140.8 (C-1'), 141.1 (2C, C-3',5'), 141.4 (C-7a), 147.3 (C-1 (C₆H₄NO₂-4)), 148.3 (C-NO₂) 153.2 (C-4'), 163.6 (C-2). HRMS (ESI): *m/z* [M + H]⁺ calcd C₂₅H₂₉N₄O₄S: 481.1904; found: 481.1904.



(Z)-3-(4-Bromophenyl)-2-((3,5-di-*tert*-butyl-4-hydroxyphenyl)imino)-2,3-dihydrobenzo[4,5]imidazo[2,1-*b*]thiazol-3-ol (5c), light pink solid, yield 43%, mp 207-208 °C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.39 (s, 18H, C(CH₃)₃), 6.82 (s, 2H, H-2',6'), 6.97 (d, 1H, *J* = 7.9 Hz, H-5), 7.11 (dd, 1H, *J* = 7.9 and 7.5 Hz, H-6), 7.22 (dd, 1H, *J* = 7.8 and 7.5 Hz, H-7), 7.26 (br.s, 1H, HO-4'), 7.40 (d, 2H, *J* = 8.5 Hz, H-2,6 (C₆H₄Br-4)), 7.64 (d, 2H, *J* = 8.5 Hz, H-3,5 (C₆H₄Br-4)), 7.66 (d, 1H, *J* = 7.8 Hz, H-8), 8.71 (br.s, 1H, HO-3). ¹³C NMR (DMSO-*d*₆, δ, ppm): 30.6 (6C, C(CH₃)₃), 35.3 (2C, C(CH₃)₃), 90.6 (C-3), 110.8 (C-5), 117.1 (2C, C-2',6'), 119.4 (C-8), 123.0 (C-6), 123.1 (C-7), 123.2 (C-Br), 128.6 (2C, C-2,6 (C₆H₄Br-4)), 131.8 (C-4a), 132.1 (2C, C-3,5 (C₆H₄Br-4)), 138.8 (C-1 (C₆H₄Br-4)), 141.0 (C-1'), 141.2 (2C, C-3',5'), 147.2 (C-8a), 150.6 (C-9a) 153.2 (C-4'), 163.0 (C-2). HRMS (ESI): *m/z* [M + H]⁺ calcd C₂₉H₃₁BrN₃O₂S: 564.1315; found: 564.1305.

To establish the structure of compound **5c**, a complete assignment of the signals from its ¹H and ¹³C NMR spectra was carried out based on the characteristic values

of chemical shifts and analysis of cross peaks in two-dimensional spectra of ^1H - ^1H COSY, NOESY correlations, as well as ^1H - ^{13}C HSQC, HMBC correlations (Figure S1). The coordinates of the cross peaks of the ^1H - ^{13}C HMQC and HMBC heteronuclear correlation spectra of compound **5c** are shown in Table S5. The most important HMBC and COSY correlations for the analysis of our structure are schematically shown in Figures S2 and S3, respectively.

Assignment of the signals of ^1H and ^{13}C NMR spectra for other compounds of this series was performed similarly based on the characteristic values of chemical shifts and analysis of cross peaks in two-dimensional spectra of ^1H - ^1H COSY, NOESY correlations, as well as ^1H - ^{13}C HSQC, HMBC correlations.

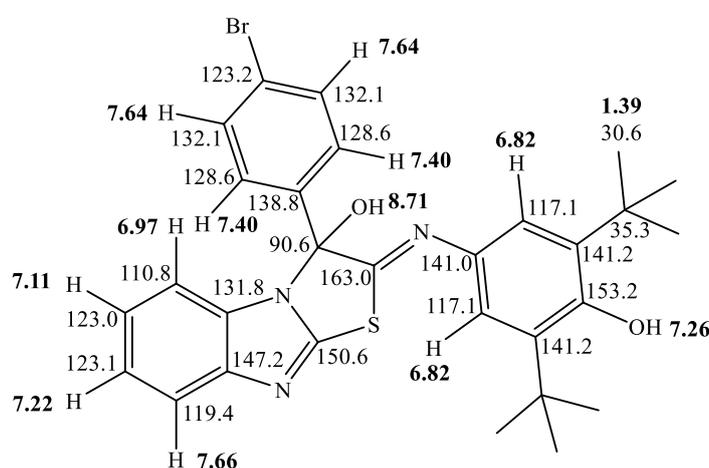


Figure S1 ^1H (bold) and ^{13}C signals of compound **5c**.

Table S5 Coordinates of cross-peaks in ^1H - ^{13}C HSQC and HMBC correlation spectra of compound **5c**

^1H , δ , ppm	^{13}C , δ , ppm	
	HSQC	HMBC
8.71 (HO-3)		163.0 (w), 138.8, 90.6
7.66 (H-8)	119.4	131.8, 123.0
7.64 (H-3,5 (C ₆ H ₄ Br-4))	132.1	138.8
7.40 (H-2,6 (C ₆ H ₄ Br-4))	128.6	123.2, 90.6
7.26 (HO-4')	-	-
7.22 (H-7)	123.1	147.2, 110.8
7.11 (H-6)	123.0	131.8, 119.4
6.97 (H-5)	110.8	147.2, 123.1
6.82 (H-2',6')	117.1	163.0 (w), 153.2, 141.2, 141.0, 117.1, 35.3
1.39 (Bu ^l)	30.6	141.2, 30.6

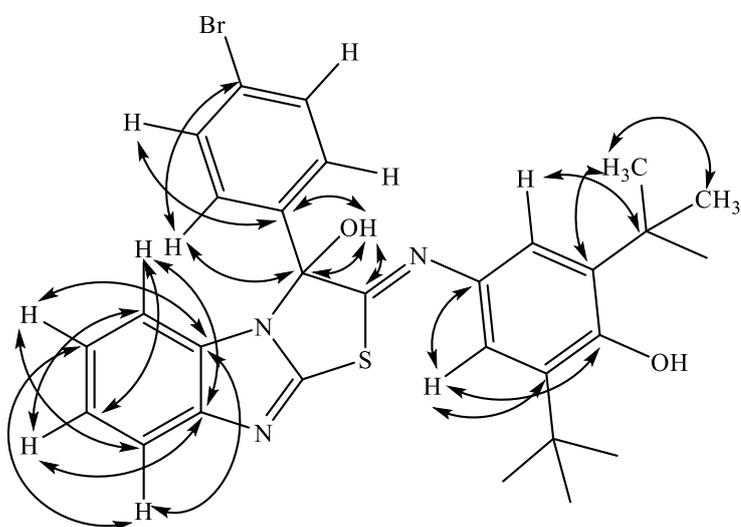


Figure S2 The scheme of the main ^1H - ^{13}C HMBC correlations of compound **5c**

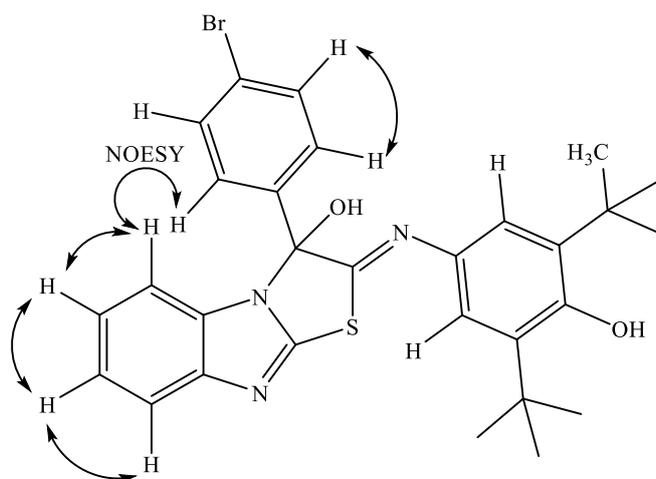
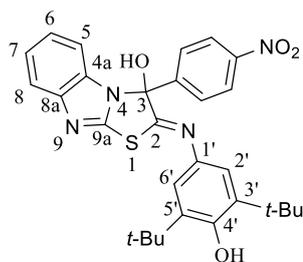
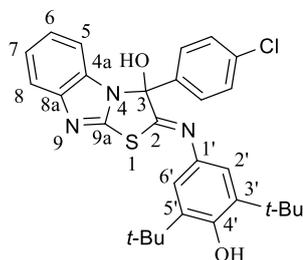


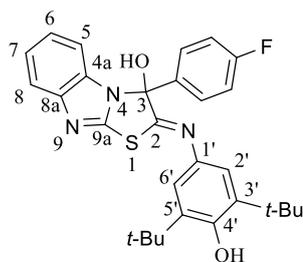
Figure S3 The scheme of the main COSY and NOESY correlations of compound **5c**



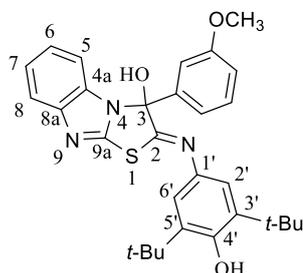
(Z)-2-((3,5-Di-*tert*-butyl-4-hydroxyphenyl)imino)-2,3-dihydro-3-(4-nitrophenyl)benzo[4,5]imidazo[2,1-*b*]thiazol-3-ol (5d), beige solid, yield 56%, mp 205-207°C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.39 (s, 18H, C(CH₃)₃), 6.82 (s, 2H, H-2',6'), 6.93 (d, 1H, *J* = 7.9 Hz, H-5), 7.11 (dd, 1H, *J* = 7.9 and 7.5 Hz, H-6), 7.23 (dd, 1H, *J* = 8.0 and 7.5 Hz, H-7), 7.29 (br.s, 1H, HO-4'), 7.67 (d, 1H, *J* = 8.0 Hz, H-8), 7.75 (d, 2H, *J* = 8.7 Hz, H-2,6 (C₆H₄NO₂-4)), 8.29 (d, 2H, *J* = 8.7 Hz, H-3,5 (C₆H₄NO₂-4)), 8.94 (br.s, 1H, HO-3). ¹³C NMR (DMSO-*d*₆, δ, ppm): 30.6 (6C, C(CH₃)₃), 35.3 (2C, C(CH₃)₃), 90.3 (C-3), 110.7 (C-5), 117.2 (2C, C-2',6'), 119.5 (C-8), 123.2 (C-6), 123.3 (C-7), 124.4 (2C, C-3,5 (C₆H₄NO₂-4)), 128.0 (2C, C-2,6 (C₆H₄NO₂-4)), 131.7 (C-4a), 140.8 (C-1'), 141.2 (2C, C-3',5'), 146.6 (C-1 (C₆H₄NO₂-4)), 147.2 (C-8a), 148.4 (C-NO₂), 150.8 (C-9a) 153.4 (C-4'), 162.5 (C-2). HRMS (ESI): *m/z* [M + Na]⁺ calcd C₂₉H₃₀N₄NaO₄S: 553.1875; found: 553.1871.



(Z)-2-((3,5-Di-*tert*-butyl-4-hydroxyphenyl)imino)-3-(4-chlorophenyl)-2,3-dihydrobenzo[4,5]imidazo[2,1-*b*]thiazol-3-ol (5e), white solid, yield 56%, mp 176-178 °C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.39 (s, 18H, C(CH₃)₃), 6.81 (s, 2H, H-2',6'), 6.97 (d, 1H, *J* = 7.9 Hz, H-5), 7.11 (dd, 1H, *J* = 7.9 and 7.2 Hz, H-6), 7.22 (dd, 1H, *J* = 8.0 and 7.2 Hz, H-7), 7.26 (br.s, 1H, HO-4'), 7.46 (d, 2H, *J* = 8.9 Hz, H-2,6 (C₆H₄Cl-4)), 7.50 (d, 2H, *J* = 8.9 Hz, H-3,5 (C₆H₄Cl-4)), 7.65 (d, 1H, *J* = 8.0 Hz, H-8), 8.71 (br.s, 1H, HO-3). ¹³C NMR (DMSO-*d*₆, δ, ppm): 30.6 (6C, C(CH₃)₃), 35.3 (2C, C(CH₃)₃), 90.5 (C-3), 110.8 (C-5), 117.1 (2C, C-2',6'), 119.4 (C-8), 123.1 (C-6), 123.2 (C-7), 128.3 (2C, C-2,6 (C₆H₄Cl-4)), 129.2 (2C, C-3,5 (C₆H₄Cl-4)), 131.8 (C-4a), 134.3 (C-Cl), 138.4 (C-1 (C₆H₄Cl-4)), 141.0 (C-1'), 141.2 (2C, C-3',5'), 147.2 (C-8a), 150.6 (C-9a) 153.2 (C-4'), 163.1 (C-2). HRMS (ESI): *m/z* [M + H]⁺ calcd C₂₉H₃₁ClN₃O₂S: 520.1829; found: 520.1819.

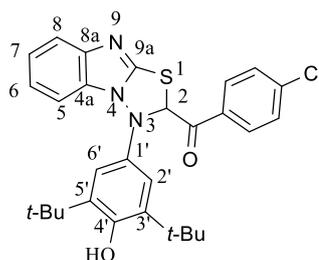


(Z)-2-((3,5-Di-*tert*-butyl-4-hydroxyphenyl)imino)-3-(4-fluorophenyl)-2,3-dihydrobenzo[4,5]imidazo[2,1-*b*]thiazol-3-ol (5f), light pink solid, yield 49%, mp 199-201 °C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.39 (s, 18H, C(CH₃)₃), 6.80 (s, 2H, H-2',6'), 6.97 (d, 1H, *J* = 7.8 Hz, H-5), 7.11 (m, 1H, H-6), 7.21 (m, 1H, H-7), 7.23-7.28 (m, 3H, HO-4', H-3,5 (C₆H₄F-4)), 7.45-7.52 (m, 2H, H-2,6 (C₆H₄F-4)), 7.63 (d, 1H, *J* = 7.2 Hz, H-8), 8.67 (br.s, 1H, HO-3). ¹³C NMR (DMSO-*d*₆, δ, ppm): 30.6 (6C, C(CH₃)₃), 35.3 (2C, C(CH₃)₃), 90.6 (C-3), 110.8 (C-5), 116.0 (d, 2C, *J* = 21.8 Hz, C-3,5 (C₆H₄Cl-4)), 117.1 (2C, C-2',6'), 119.4 (C-8), 123.0 (C-6), 123.1 (C-7), 128.66 (d, 2C, *J* = 8.7 Hz, C-2,6 (C₆H₄F-4)), 131.9 (C-4a), 135.7 (d, 1C, *J* = 2.5 Hz, C-1 (C₆H₄F-4)), 141.0 (C-1'), 141.2 (2C, C-3',5'), 147.2 (C-8a), 150.6 (C-9a) 153.2 (C-4'), 163.2 (C-2). HRMS (ESI): *m/z* [M + H]⁺ calcd C₂₉H₃₁FN₃O₂S: 504.2116; found: 504.2116.

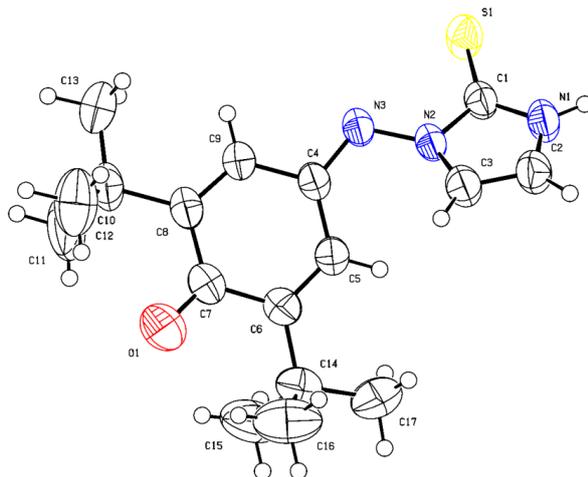


(Z)-2-((3,5-Di-*tert*-butyl-4-hydroxyphenyl)imino)-2,3-dihydro-3-(3-methoxyphenyl)benzo[4,5]imidazo[2,1-*b*]thiazol-3-ol (5g). Compound **3b** (1 mmol) was dissolved in DMF (5 ml), a solution of KOH (1 mmol) in EtOH (3 ml) was added. Then 3-methoxyphenacyl bromide (1 mmol) was added. This was kept for 15 min, then more KOH (1 mmol) solution in EtOH was added. The mixture was stirred at 50-60 °C for 30 min, then was diluted with water (30 ml) and neutralized with diluted AcOH. The precipitate formed was filtered off. The product was isolated by column chromatography (Al₂O₃, eluent: CH₂Cl₂), beige solid, yield 42%, mp 221-223°C. ¹H NMR (DMSO-*d*₆, δ, ppm): 1.39 (s, 18H, C(CH₃)₃), 3.76 (s, 3H, OCH₃), 6.81 (s, 2H, H-2',6'), 6.84 (d, 1H, *J* = 7.8 Hz, H-6 (C₆H₄OCH₃-3)), 6.98 (d, 1H, *J* = 8.1 Hz, H-4 (C₆H₄OCH₃-3)), 7.01 (d, 1H, *J* = 7.9 Hz, H-5), 7.09 (s, 1H, H-2 (C₆H₄OCH₃-3)), 7.10 (dd, 1H, *J* = 7.9 and 7.5 Hz, H-6), 7.20 (dd, 1H, *J* = 8.0 and 7.5 Hz, H-7), 7.26

(br.s, 1H, HO-4'), 7.32 (dd, 1H, $J = 7.8$ and 8.1 Hz, H-5 (C₆H₄OCH₃-3)), 7.63 (d, 1H, $J = 8.0$ Hz, H-8), 8.64 (br.s, 1H, HO-3). ¹³C NMR (DMSO-*d*₆, δ , ppm): 30.6 (6C, C(CH₃)₃), 35.3 (2C, C(CH₃)₃), 55.6 (OCH₃), 90.7 (C-3), 110.9 (C-5), 112.3 (C-2 (C₆H₄OCH₃-3)), 114.5 (C-4 (C₆H₄OCH₃-3)), 117.0 (2C, C-2',6'), 118.2 (C-6 (C₆H₄OCH₃-3)), 119.3 (C-8), 122.9 (C-6), 123.0 (C-7), 130.4 (C-5 (C₆H₄OCH₃-3)), 132.0 (C-4a), 141.1 (C-1'), 141.2 (C-1 (C₆H₄OCH₃-3)), 141.3 (2C, C-3',5'), 147.1 (C-8a), 150.6 (C-9a) 153.2 (C-4'), 159.7 (C-OCH₃), 163.4 (C-2). HRMS (ESI): m/z [M + H]⁺ calcd C₃₀H₃₄N₃O₃S: 516.2315; found: 516.2312.



3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-2-(4-chlorobenzoyl)-2,3-dihydrobenzo[4,5]imidazo[2,1-*b*][1,3,4]thiadiazole (6e). Compound **4e** (1 mmol) was poured into a solution of NaOEt (3 mmol) in EtOH (10 ml), while cooling in an ice bath. The mixture was quenched with water (30 ml), and the precipitate was filtered off. The product was isolated by column chromatography (Al₂O₃, eluent: CHCl₃). Orange solid, yield 45%, yield 51%, mp 187-189 °C. ¹H NMR (CDCl₃, δ , ppm): 1.40 (s, 18H, C(CH₃)₃), 5.29 (c, 1H, H-2), 6.03 (br.s, 1H, OH), 6.86 (s, 2H, H-2',6'), 6.91-7.09 (m, 3H, H-5,6,7), 7.31 (d, 2H, $J = 8.8$ Hz, H-2,6 (C₆H₄Cl-4)), 7.37 (d, 2H, $J = 8.8$ Hz, H-3,5 (C₆H₄Cl-4)), 7.47 (d, 1H, $J = 7.7$ Hz, H-8). ¹³C NMR (CDCl₃, δ , ppm): 30.6 (6C, C(CH₃)₃), 34.9 (2C, C(CH₃)₃), 91.1 (C-2), 111.2 (C-5), 118.6 (2C, C-2',6'), 119.4 (C-8), 123.4(C-6), 123.5 (C-7), 127.9 (2C, C-3,5 (4-ClC₆H₄)), 129.4 (2C, C-2,6 (4-ClC₆H₄)), 131.8 (C-4a), 135.7 (C-Cl), 137.4 (2C, C3',5'), 139.7 (2C, C-1', C-1 (4-ClC₆H₄)), 146.8 (C-8a), 151.8 (C-9a), 153.4 (C-4'), 161.1 (C=O). HRMS (ESI): m/z [M + H]⁺ calcd C₂₉H₃₁ClN₃O₂S: 520.1820; found: 520.1825.

Table S6 Crystal data and structure refinement for **3a**.

CCDC Number	2109334
Empirical formula	C ₁₇ H ₂₃ N ₃ OS
Formula weight	317.44
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	16.0957(4)
b/Å	10.7722(2)
c/Å	11.3986(2)
α/°	90
β/°	104.602(2)
γ/°	90
Volume/Å ³	1912.52(7)
Z	4
ρ _{calc} /cm ³	1.102
μ/mm ⁻¹	1.534
F(000)	680.0
Crystal size/mm ³	0.412 × 0.233 × 0.055
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	5.674 to 153.132
Index ranges	-20 ≤ h ≤ 20, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	7572
Independent reflections	7572 [R _{sigma} = 0.0141]
Data/restraints/parameters	7572/0/206
Goodness-of-fit on F ²	1.099
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0472, wR ₂ = 0.1460
Final R indexes [all data]	R ₁ = 0.0543, wR ₂ = 0.1513
Largest diff. peak/hole / e Å ⁻³	0.30/-0.23

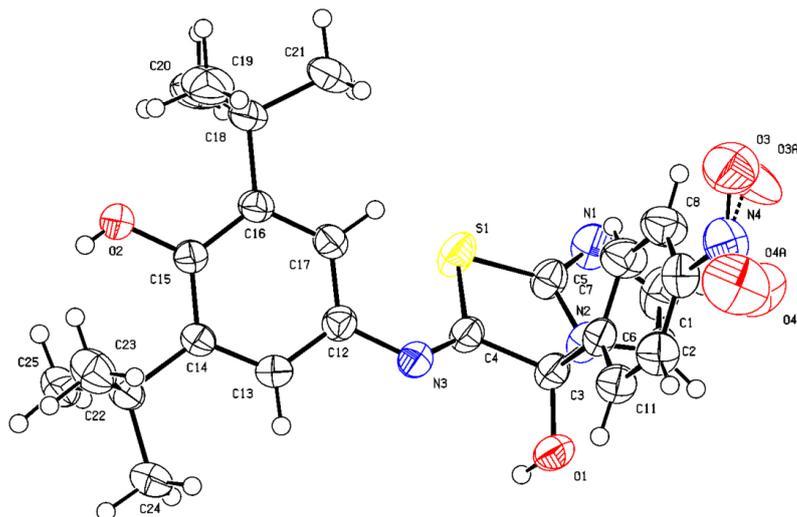
Table S7 Bond lengths for **3a**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C1	1.6718(19)	C6	C7	1.499(3)
N2	N3	1.391(2)	C8	C10	1.528(3)
N2	C1	1.368(2)	C8	C7	1.487(3)
N2	C3	1.396(3)	C3	C2	1.339(3)
N3	C4	1.306(2)	O1	C7	1.214(3)
N1	C1	1.342(3)	C14	C16	1.519(4)
N1	C2	1.370(3)	C14	C17	1.525(4)
C4	C9	1.450(3)	C14	C15	1.525(4)
C4	C5	1.442(3)	C10	C13	1.517(4)
C9	C8	1.336(3)	C10	C11	1.524(4)
C6	C5	1.338(3)	C10	C12	1.521(4)
C6	C14	1.523(3)			

Table S8 Bond angles for **3a**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	N2	C3	128.99(15)	C7	C8	C10	119.48(19)
C1	N2	N3	119.21(16)	C2	C3	N2	106.02(18)
C1	N2	C3	110.26(16)	C3	C2	N1	107.76(19)
C4	N3	N2	116.70(16)	C6	C14	C17	110.6(2)
C1	N1	C2	111.39(16)	C6	C14	C15	110.1(2)
N3	C4	C9	113.61(17)	C16	C14	C6	110.6(2)
N3	C4	C5	127.67(17)	C16	C14	C17	108.9(3)
C5	C4	C9	118.70(16)	C16	C14	C15	110.0(3)
N2	C1	S1	126.27(14)	C15	C14	C17	106.5(3)
N1	C1	S1	129.24(14)	C13	C10	C8	111.3(2)
N1	C1	N2	104.48(16)	C13	C10	C11	108.9(3)
C8	C9	C4	122.25(19)	C13	C10	C12	107.4(3)
C5	C6	C14	123.3(2)	C11	C10	C8	109.2(2)
C5	C6	C7	118.01(19)	C12	C10	C8	110.4(2)
C7	C6	C14	118.65(18)	C12	C10	C11	109.5(3)
C6	C5	C4	122.00(18)	C8	C7	C6	119.20(18)
C9	C8	C10	122.6(2)	O1	C7	C6	119.8(2)
C9	C8	C7	117.96(18)	O1	C7	C8	121.0(2)

Details: Twinned data refinement Scales: 0.6997(12) 0.3003(12)

Table S9 Crystal data and structure refinement for **5b**

CCDC Number	2109338
Empirical formula	C ₂₅ H ₂₈ N ₄ O ₄ S
Formula weight	480.57
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	11.71400(10)
b/Å	9.61590(10)
c/Å	21.90520(10)
α/°	90
β/°	90.3090(10)
γ/°	90
Volume/Å ³	2467.38(4)
Z	4
ρ _{calc} /cm ³	1.294
μ/mm ⁻¹	1.482
F(000)	1016.0
Crystal size/mm ³	0.26 × 0.197 × 0.092
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	7.548 to 152.766
Index ranges	-14 ≤ h ≤ 14, -12 ≤ k ≤ 12, -21 ≤ l ≤ 27
Reflections collected	50172
Independent reflections	5170 [R _{int} = 0.0261, R _{sigma} = 0.0139]
Data/restraints/parameters	5170/0/340
Goodness-of-fit on F ²	1.063
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0380, wR ₂ = 0.1047
Final R indexes [all data]	R ₁ = 0.0403, wR ₂ = 0.1070
Largest diff. peak/hole / e Å ⁻³	0.31/-0.31

Table S10 Bond lengths for **5b**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C5	1.7413(14)	C17	C16	1.3874(18)
S1	C4	1.8081(13)	C16	C18	1.5403(17)
O1	C3	1.3766(17)	N4	O3	1.270(9)
O2	C15	1.3725(16)	N4	O4	1.247(10)
N3	C12	1.4189(17)	N4	C9	1.474(2)
N3	C4	1.2528(18)	N4	O4A	1.172(13)
N2	C3	1.4667(17)	N4	O3A	1.160(12)
N2	C5	1.3507(18)	C3	C4	1.5617(17)
N2	C2	1.3768(19)	C22	C25	1.5406(19)
N1	C5	1.3074(19)	C22	C24	1.530(2)
N1	C1	1.388(2)	C22	C23	1.540(2)
C13	C14	1.3923(18)	C11	C10	1.386(2)
C13	C12	1.3856(18)	C18	C19	1.529(2)
C15	C14	1.4123(17)	C18	C21	1.530(2)
C15	C16	1.4044(18)	C18	C20	1.529(2)
C14	C22	1.5404(17)	C9	C10	1.372(2)
C12	C17	1.3881(19)	C9	C8	1.377(2)
C6	C3	1.5294(19)	C2	C1	1.348(2)
C6	C11	1.3866(19)	C7	C8	1.383(2)
C6	C7	1.389(2)			

Table S11 Bond angles for **5b**.

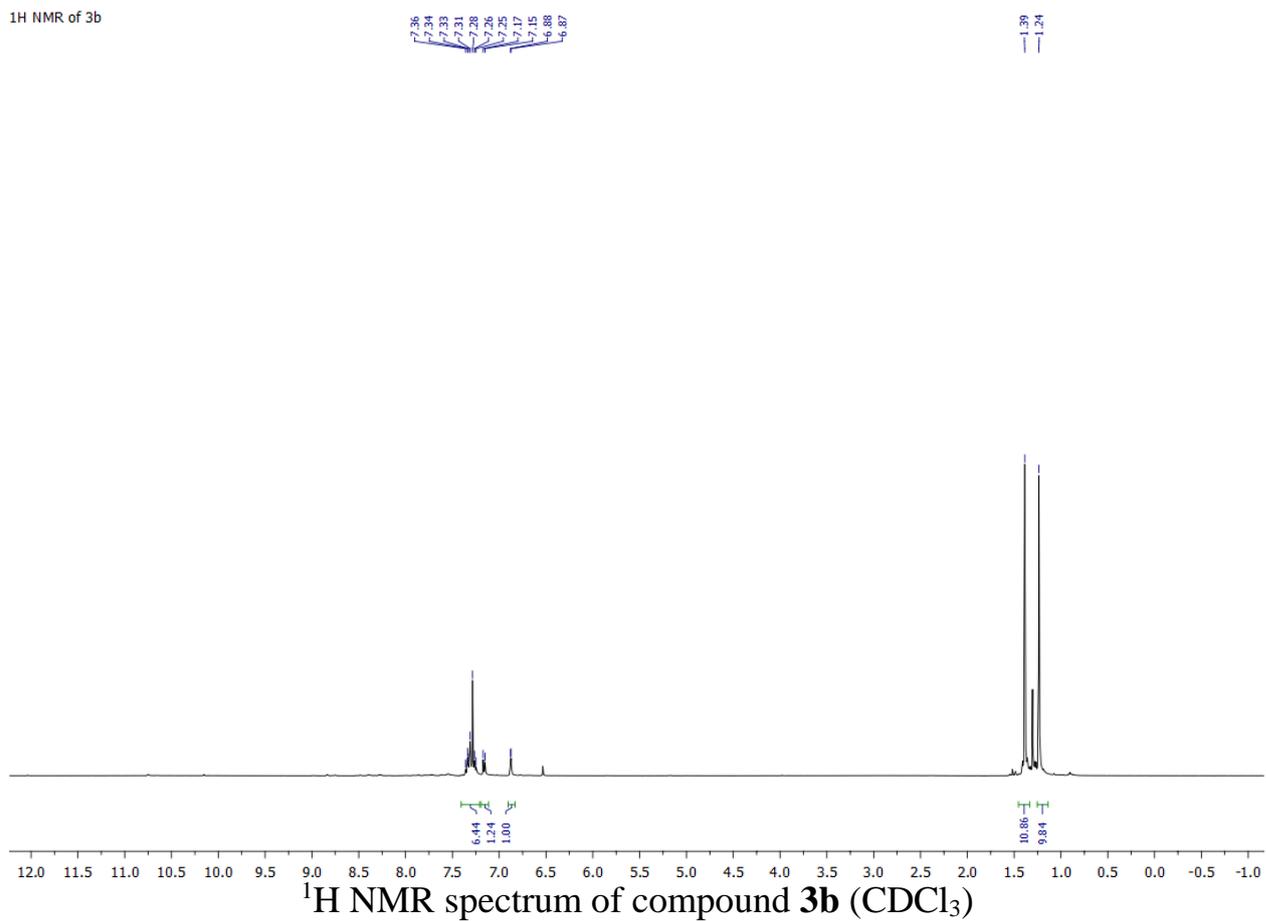
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	S1	C4	89.68(6)	O1	C3	C4	114.37(11)
C4	N3	C12	122.30(12)	N2	C3	C6	110.27(11)
C5	N2	C3	117.94(11)	N2	C3	C4	102.69(10)
C5	N2	C2	106.32(12)	C6	C3	C4	108.15(11)
C2	N2	C3	133.40(12)	C14	C22	C25	111.48(11)
C5	N1	C1	103.57(13)	C24	C22	C14	110.95(11)
C12	C13	C14	121.42(12)	C24	C22	C25	107.08(12)
O2	C15	C14	120.17(11)	C24	C22	C23	106.37(13)
O2	C15	C16	116.96(11)	C23	C22	C14	110.23(11)
C16	C15	C14	122.87(12)	C23	C22	C25	110.57(13)
C13	C14	C15	117.00(11)	N2	C5	S1	114.60(10)
C13	C14	C22	121.34(11)	N1	C5	S1	132.07(11)
C15	C14	C22	121.63(11)	N1	C5	N2	113.29(13)
C13	C12	N3	118.18(12)	N3	C4	S1	127.48(10)
C13	C12	C17	119.75(12)	N3	C4	C3	120.57(12)
C17	C12	N3	121.88(12)	C3	C4	S1	111.94(9)

C11	C6	C3	119.72(13)	C10	C11	C6	120.68(14)
C11	C6	C7	119.12(14)	C19	C18	C16	110.66(12)
C7	C6	C3	121.12(12)	C19	C18	C21	107.10(15)
C16	C17	C12	121.80(12)	C19	C18	C20	109.61(16)
C15	C16	C18	122.44(12)	C21	C18	C16	111.42(12)
C17	C16	C15	116.98(12)	C20	C18	C16	110.45(12)
C17	C16	C18	120.58(12)	C20	C18	C21	107.49(16)
O3	N4	C9	117.2(5)	C10	C9	N4	118.90(14)
O4	N4	O3	124.3(8)	C10	C9	C8	122.61(15)
O4	N4	C9	118.6(6)	C8	C9	N4	118.48(15)
O4A	N4	C9	117.2(9)	C9	C10	C11	118.45(13)
O3A	N4	C9	119.1(6)	C1	C2	N2	105.58(14)
O3A	N4	O4A	123.7(11)	C8	C7	C6	120.93(14)
O1	C3	N2	112.87(11)	C9	C8	C7	118.18(15)
O1	C3	C6	108.33(11)	C2	C1	N1	111.22(14)

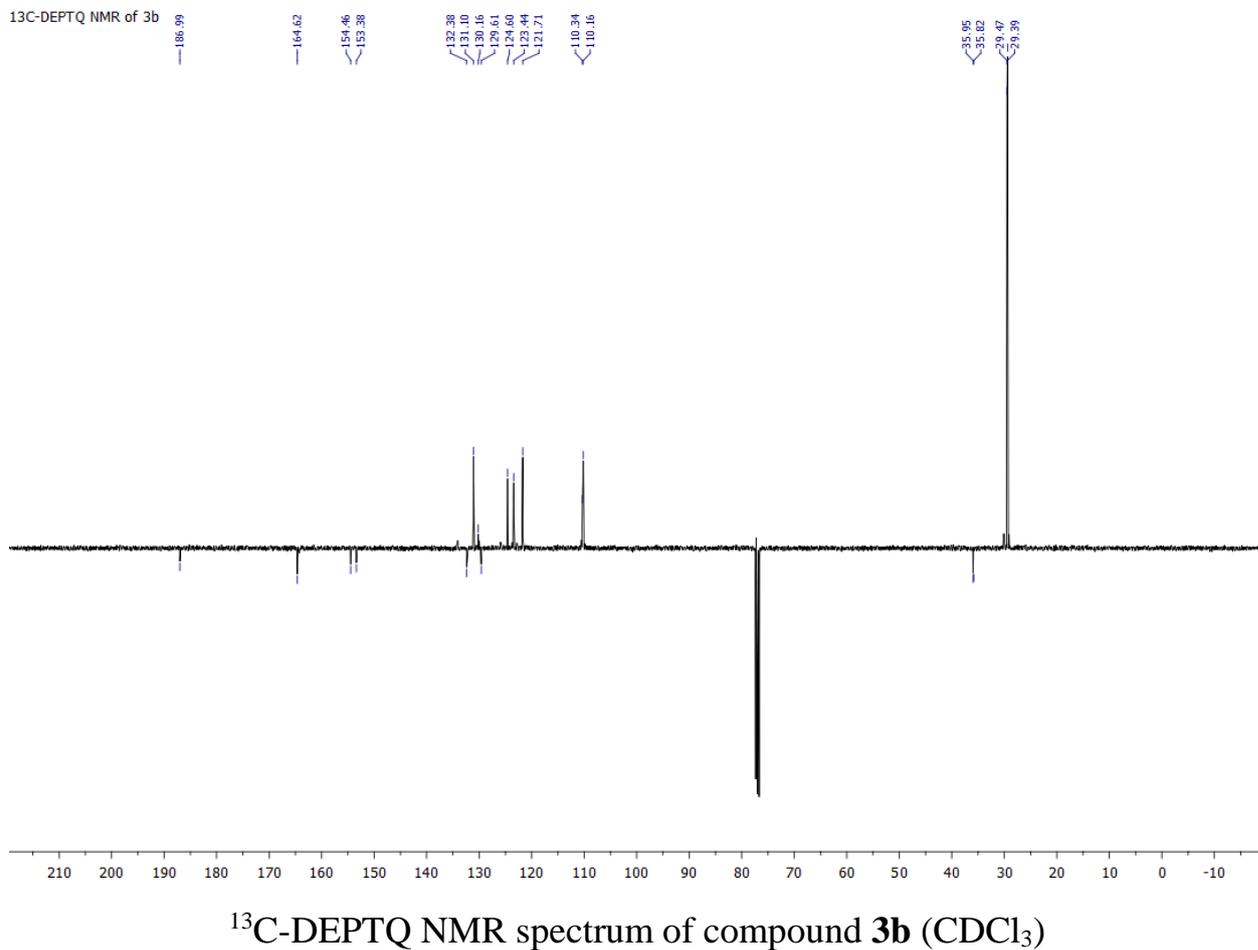
Supplementary references

- S1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, *Gaussian 16, Revision C.01*, Gaussian, Inc., Wallingford CT, 2016.
- S2. W. Thorwart, U. Gebert, R. Schleyerbach and R. Bartlett, *Ger. Patent. Appl. DE 3702757 A1*.
- S3. O. V. Kryshtalyuk, V.V. Kuz'menko and A. F. Pozharskii, *Zh. Org. Khim.*, 1992, **28**, 2328 (in Russian).

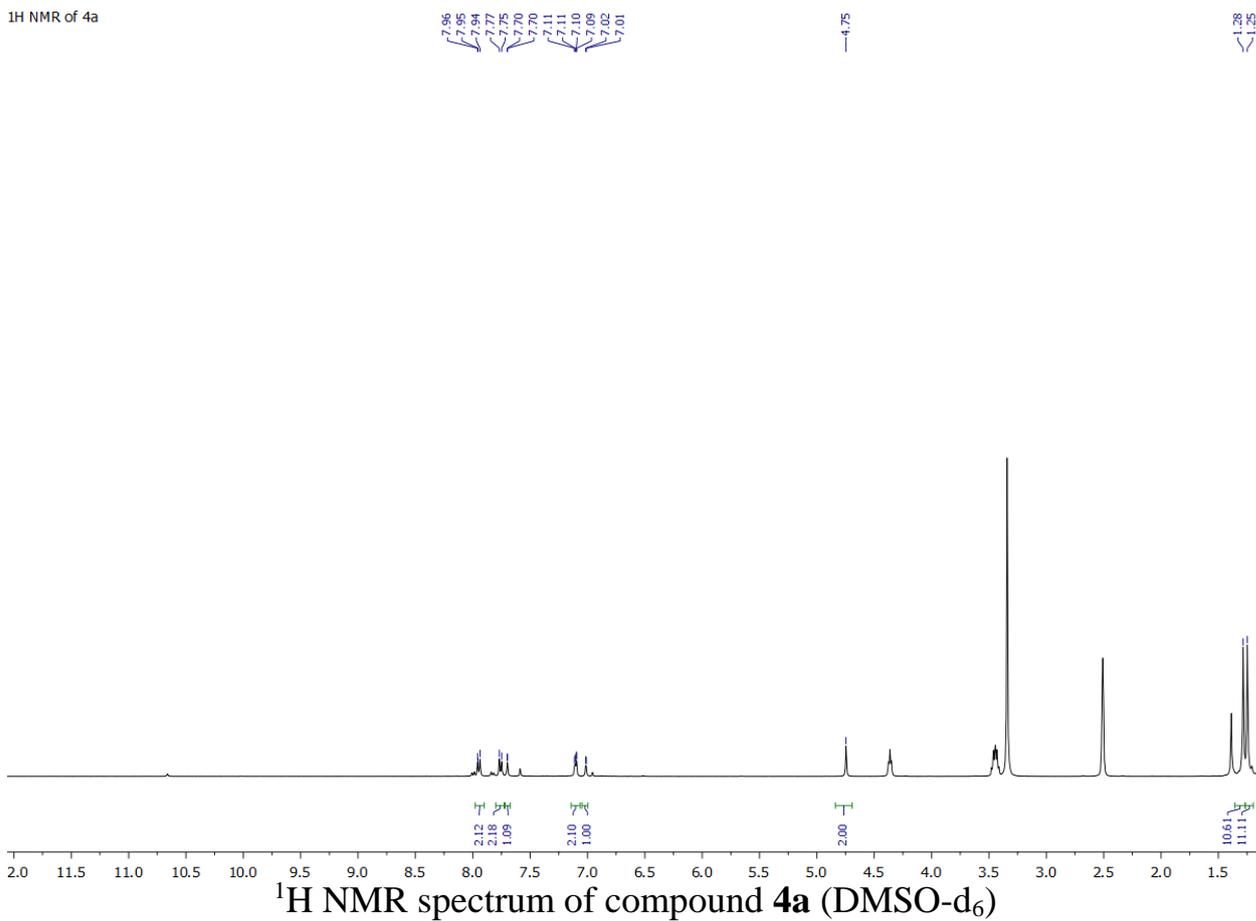
¹H NMR of 3b



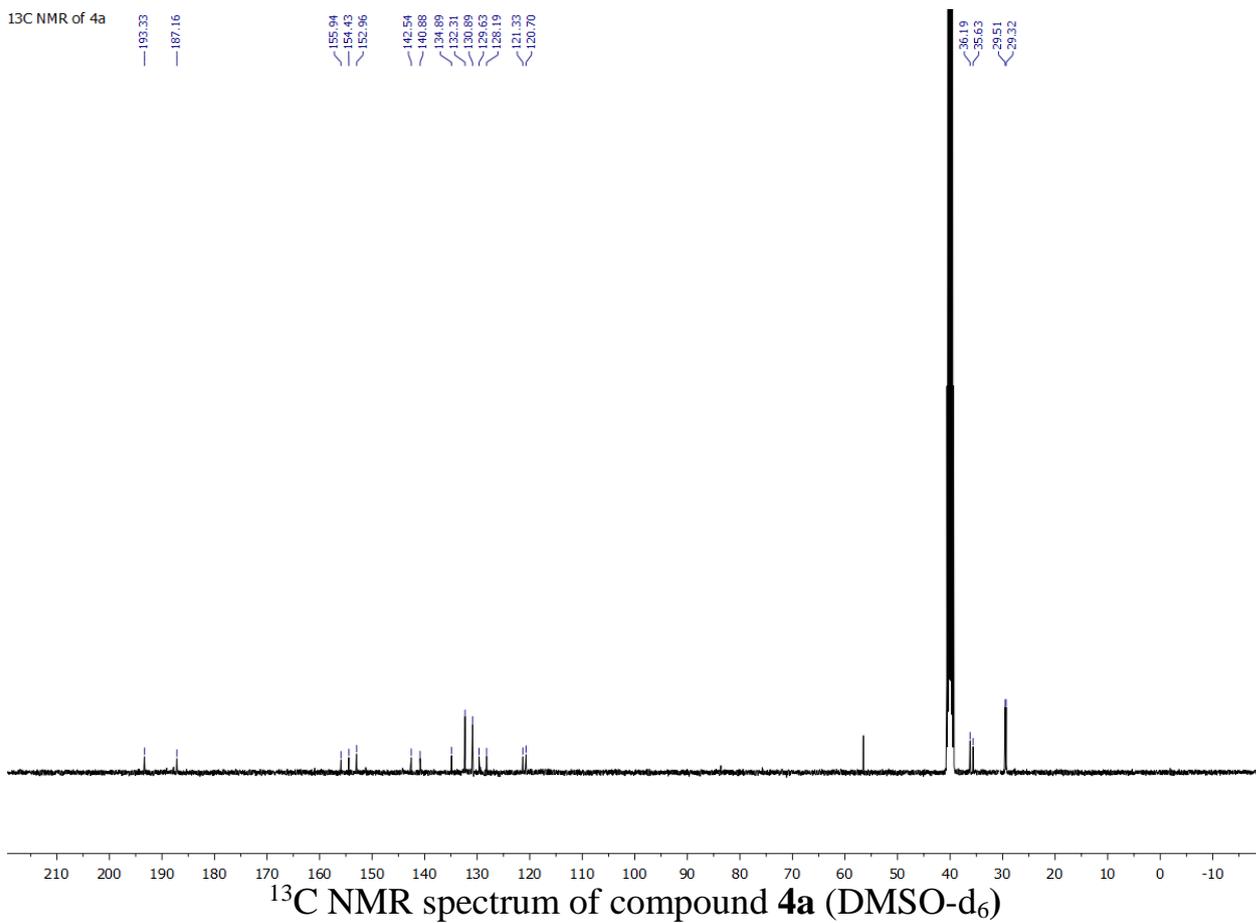
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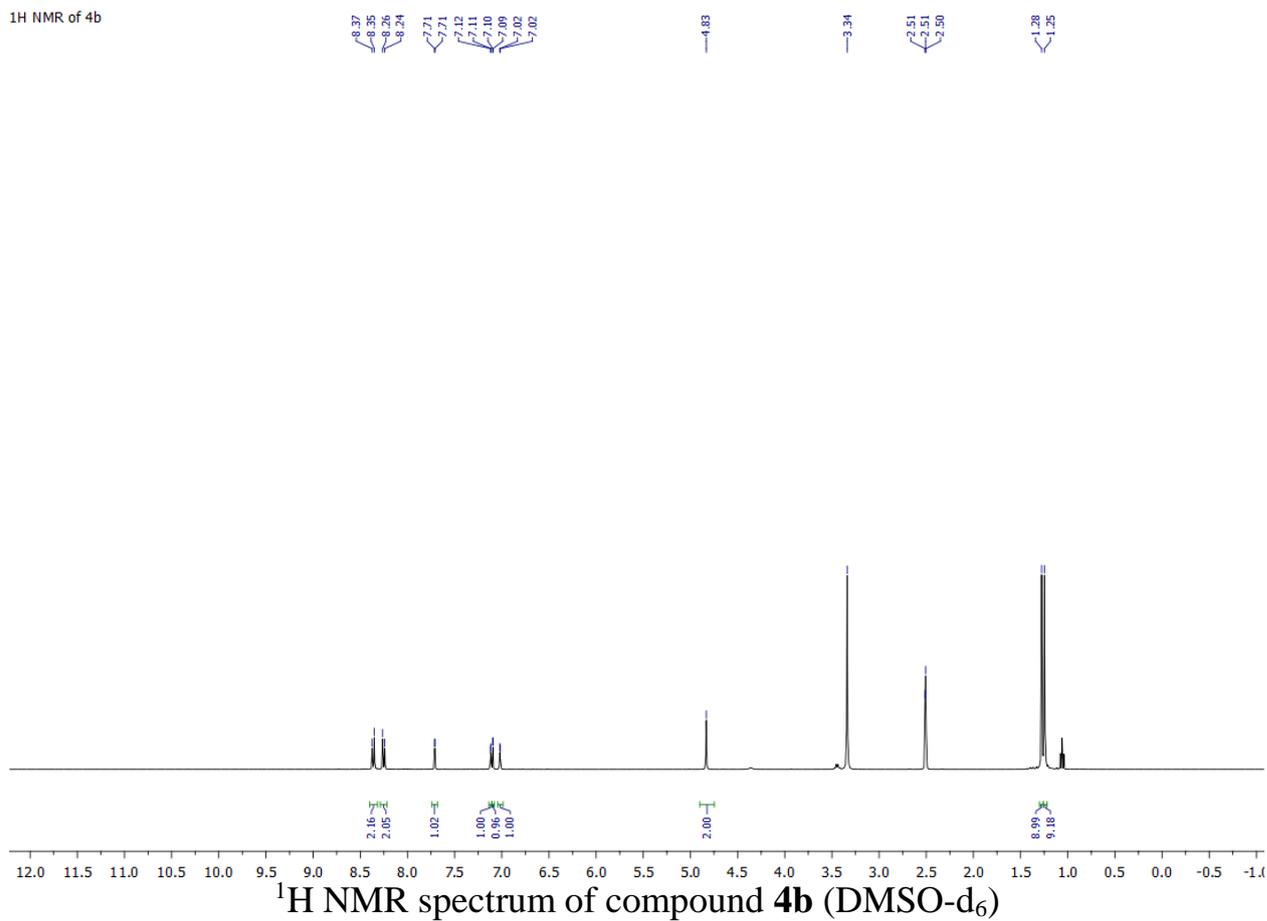
¹H NMR of 4a



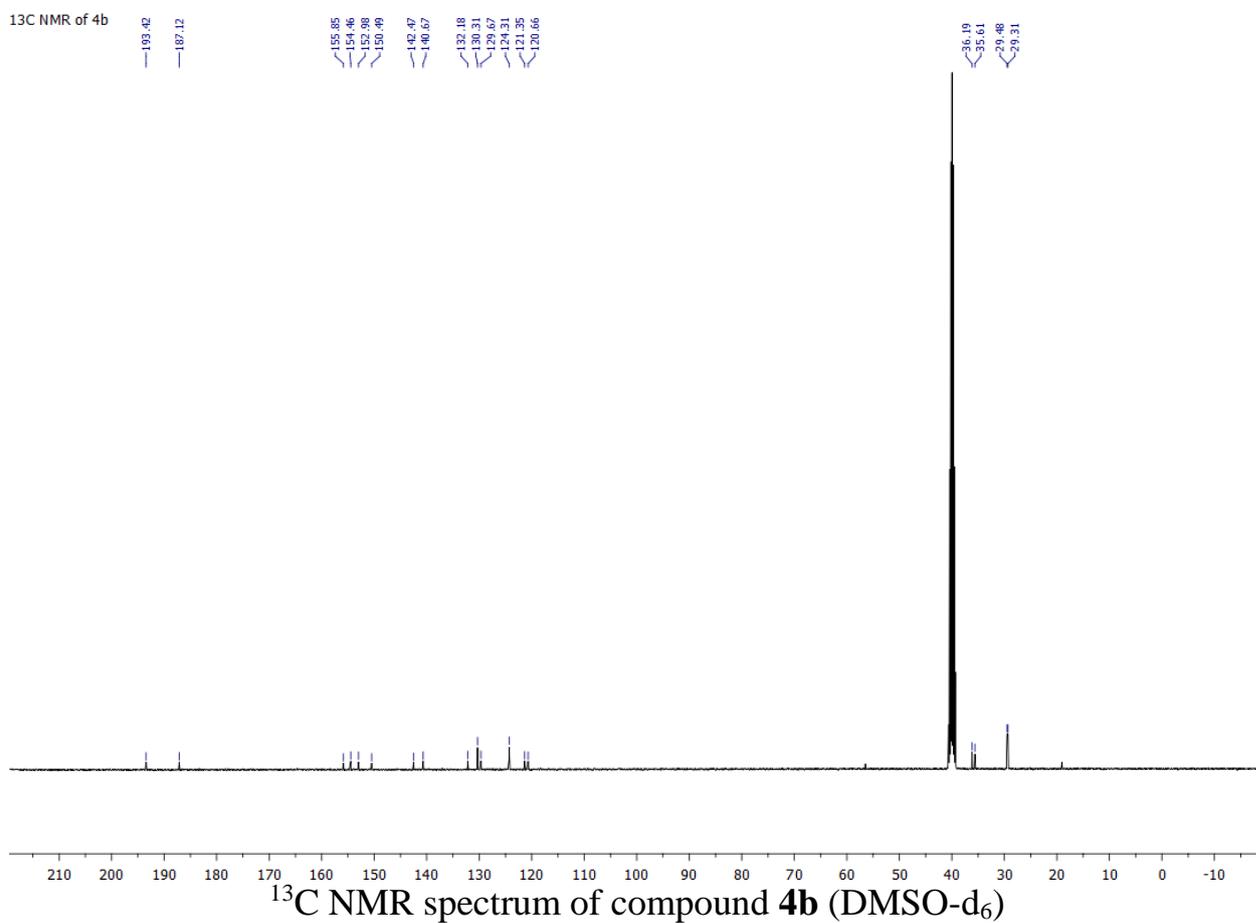
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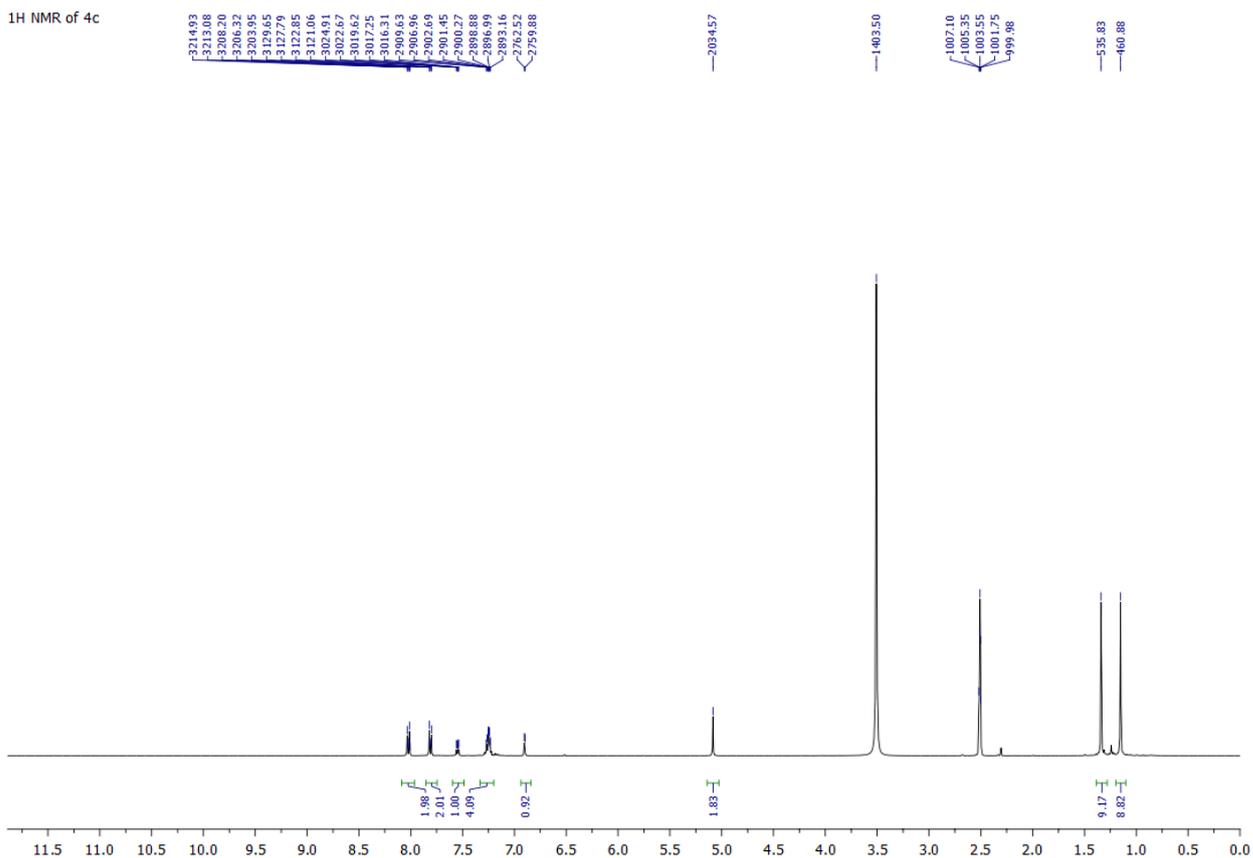
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¹³C NMR of 4b

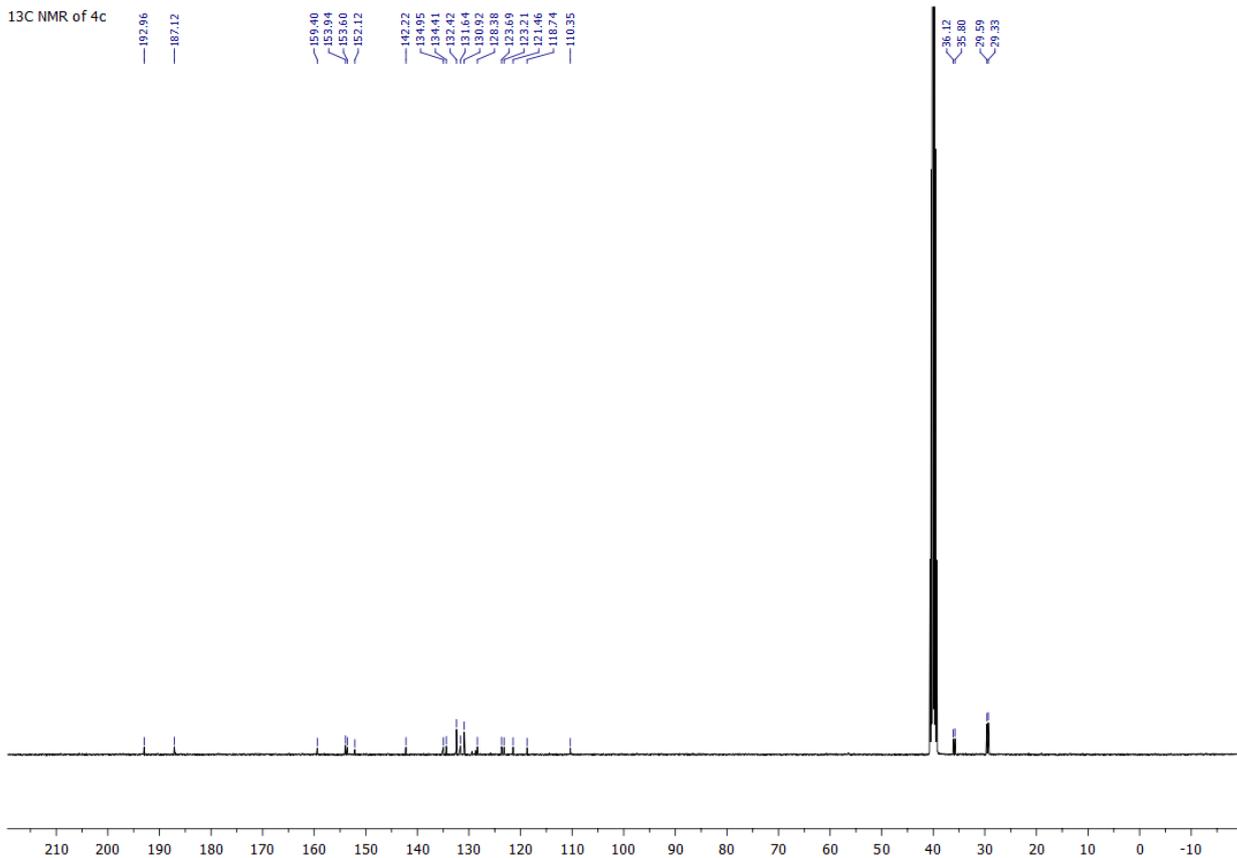


¹H NMR of 4c



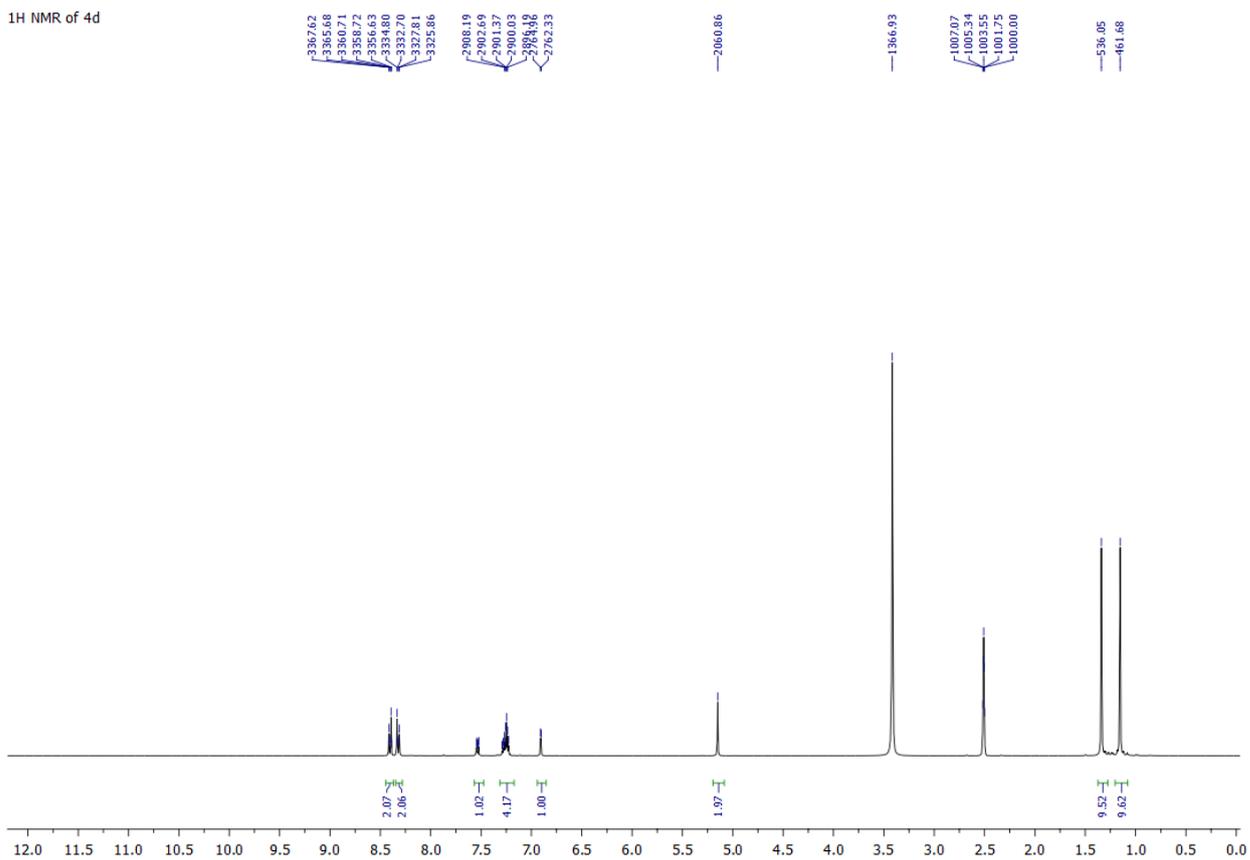
¹H NMR spectrum of compound 4c (DMSO-d₆)

¹³C NMR of 4c

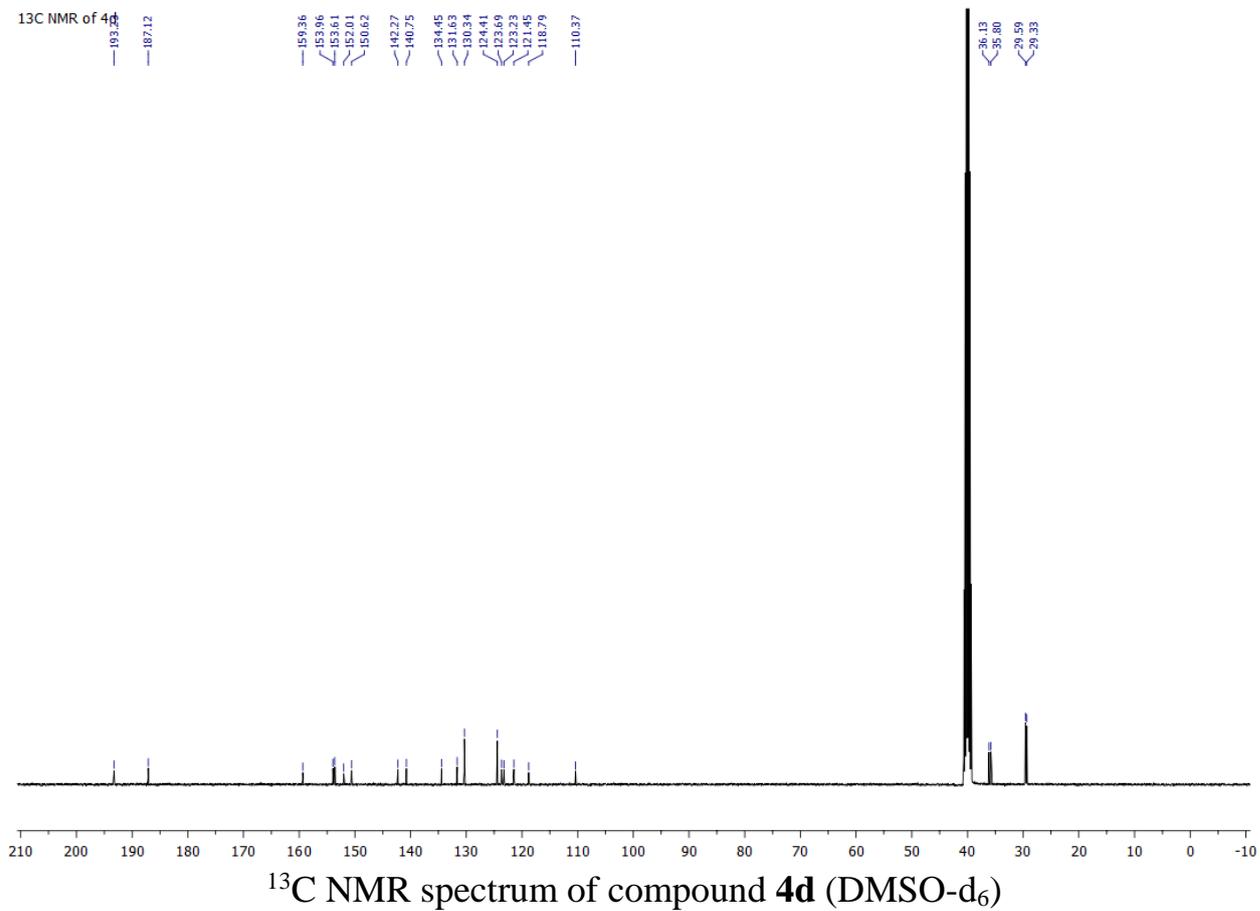


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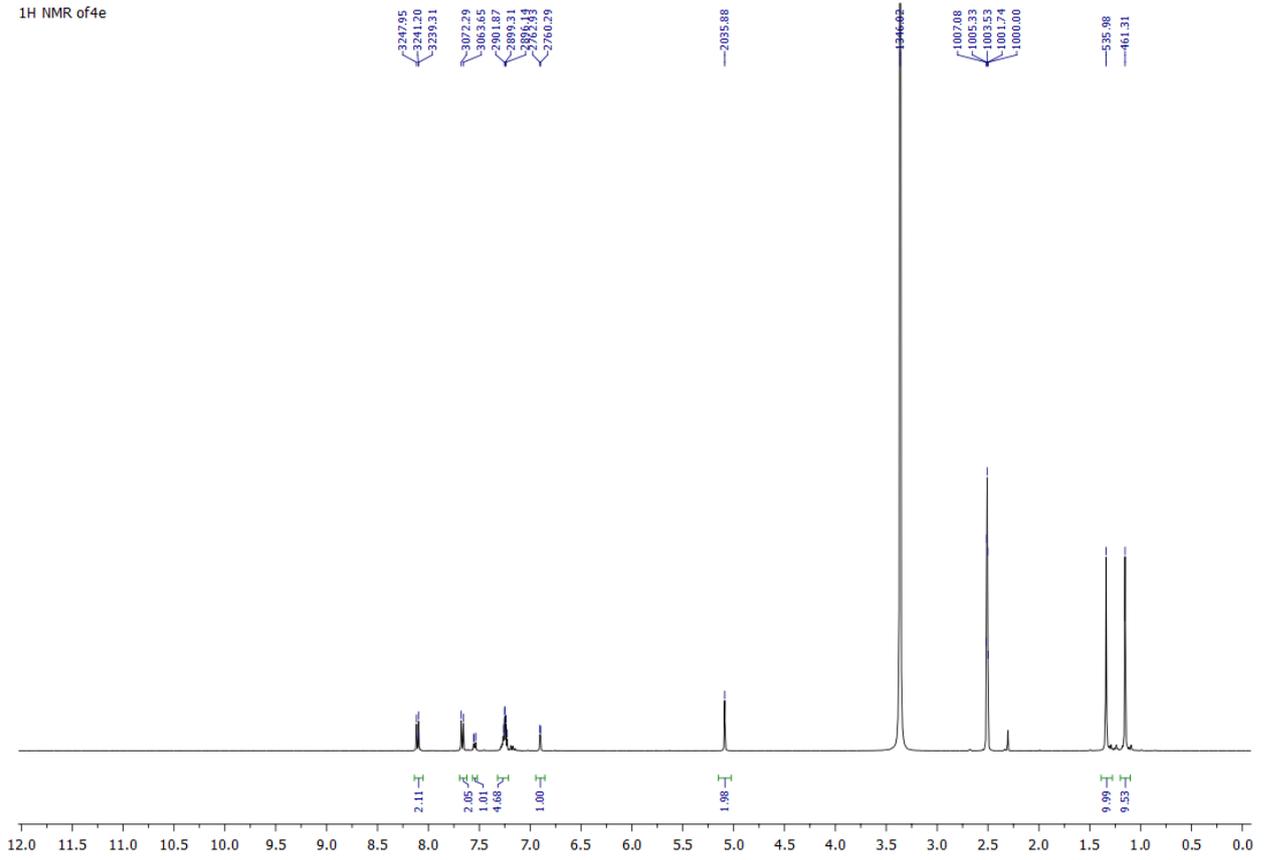
¹H NMR of 4d



¹³C NMR of 4d

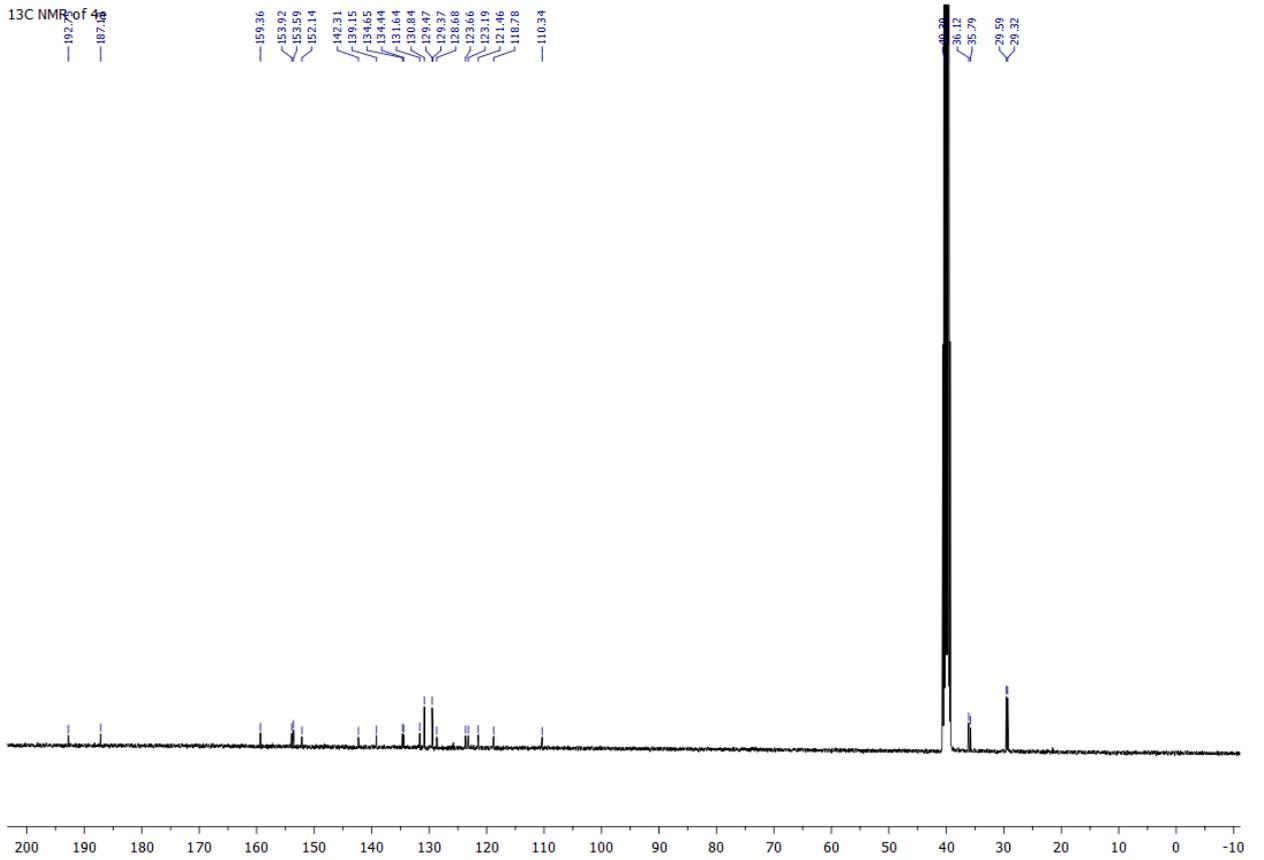


¹H NMR of 4e



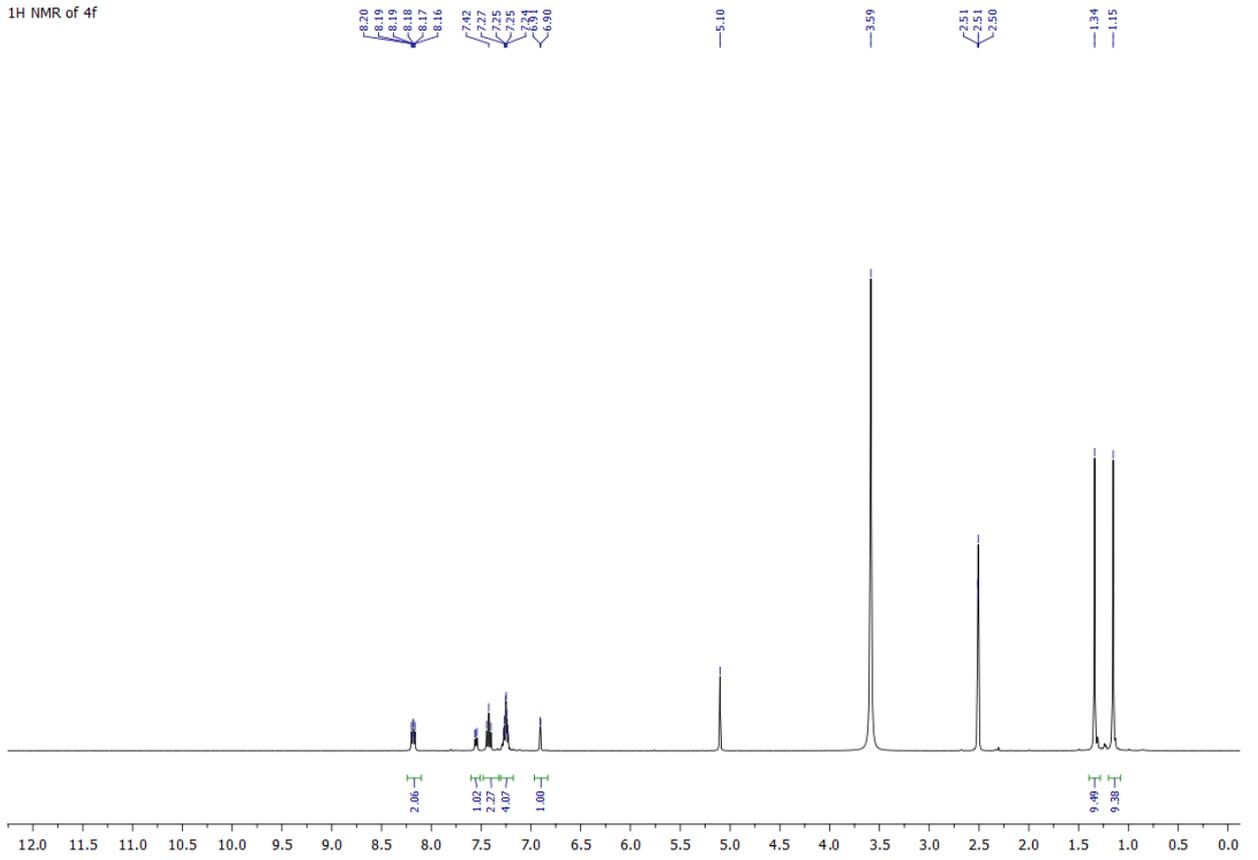
¹H NMR spectrum of compound **4e** (DMSO-d₆)

¹³C NMR of 4e



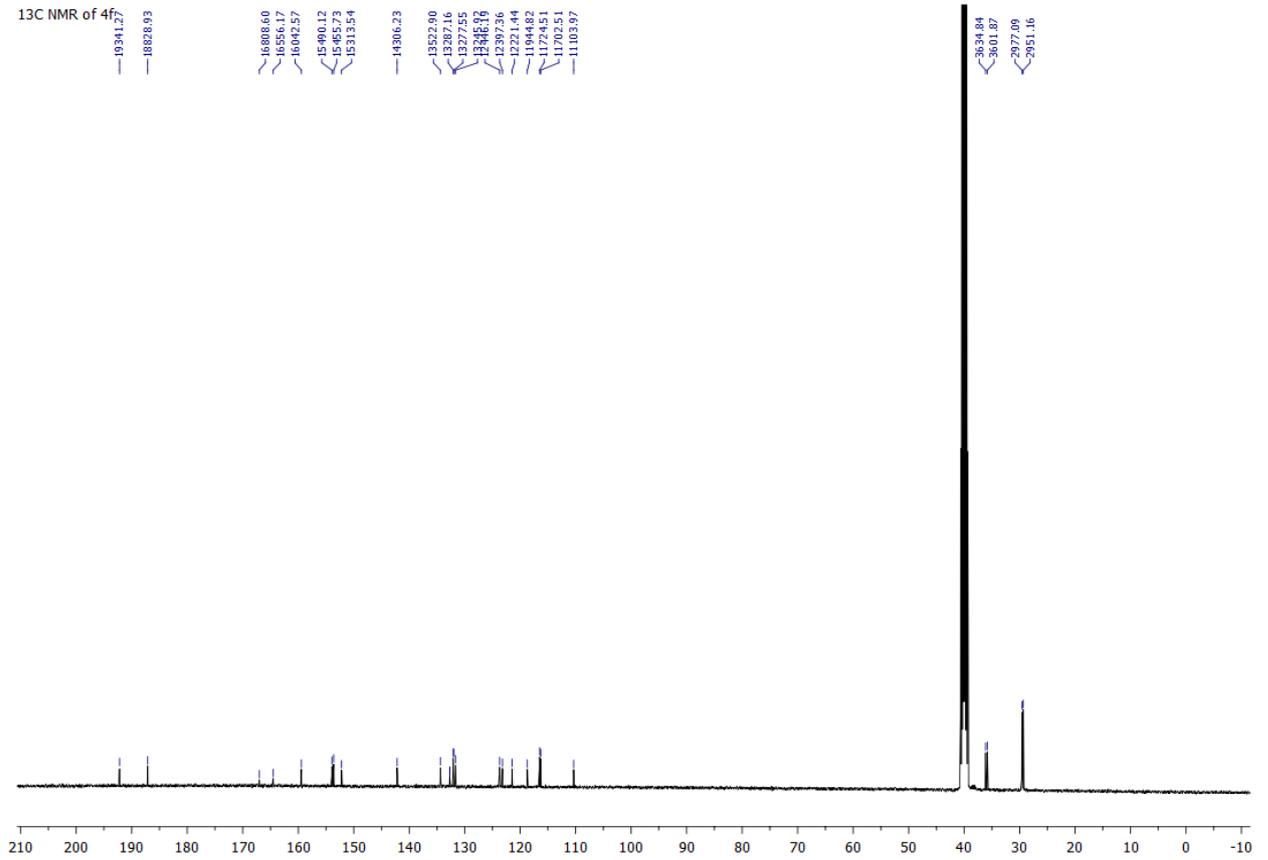
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¹H NMR of 4f



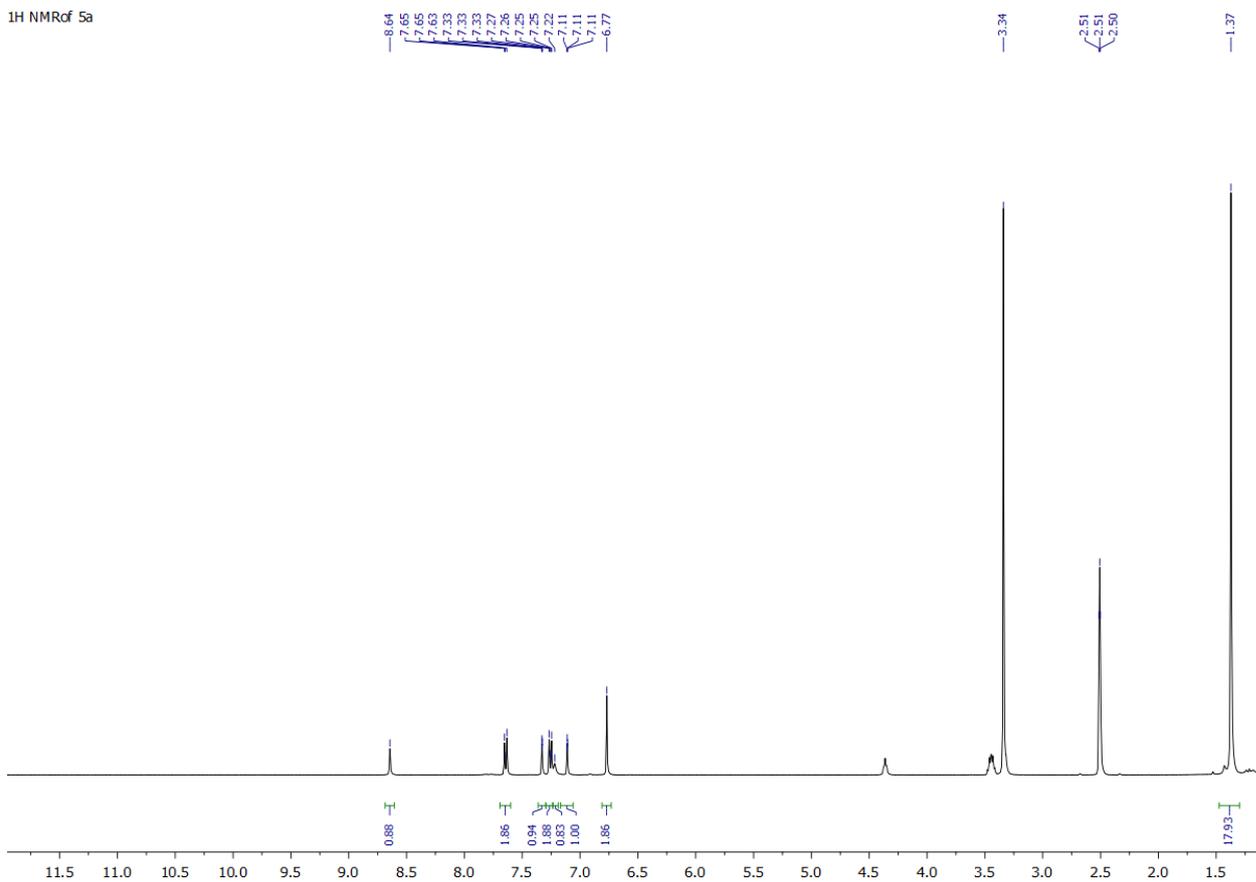
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¹³C NMR of 4f



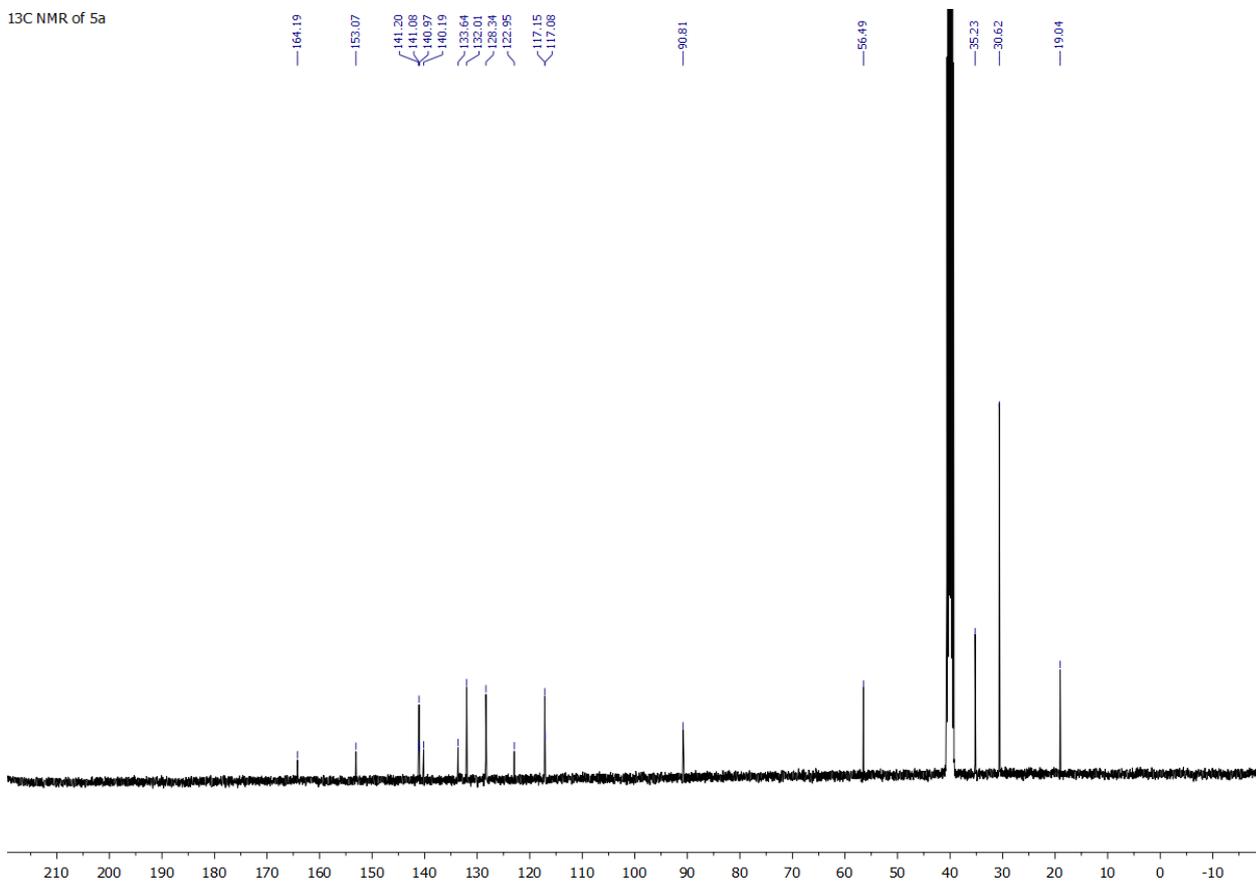
¹³C NMR spectrum of compound 4f (DMSO-d₆)

^1H NMR of 5a



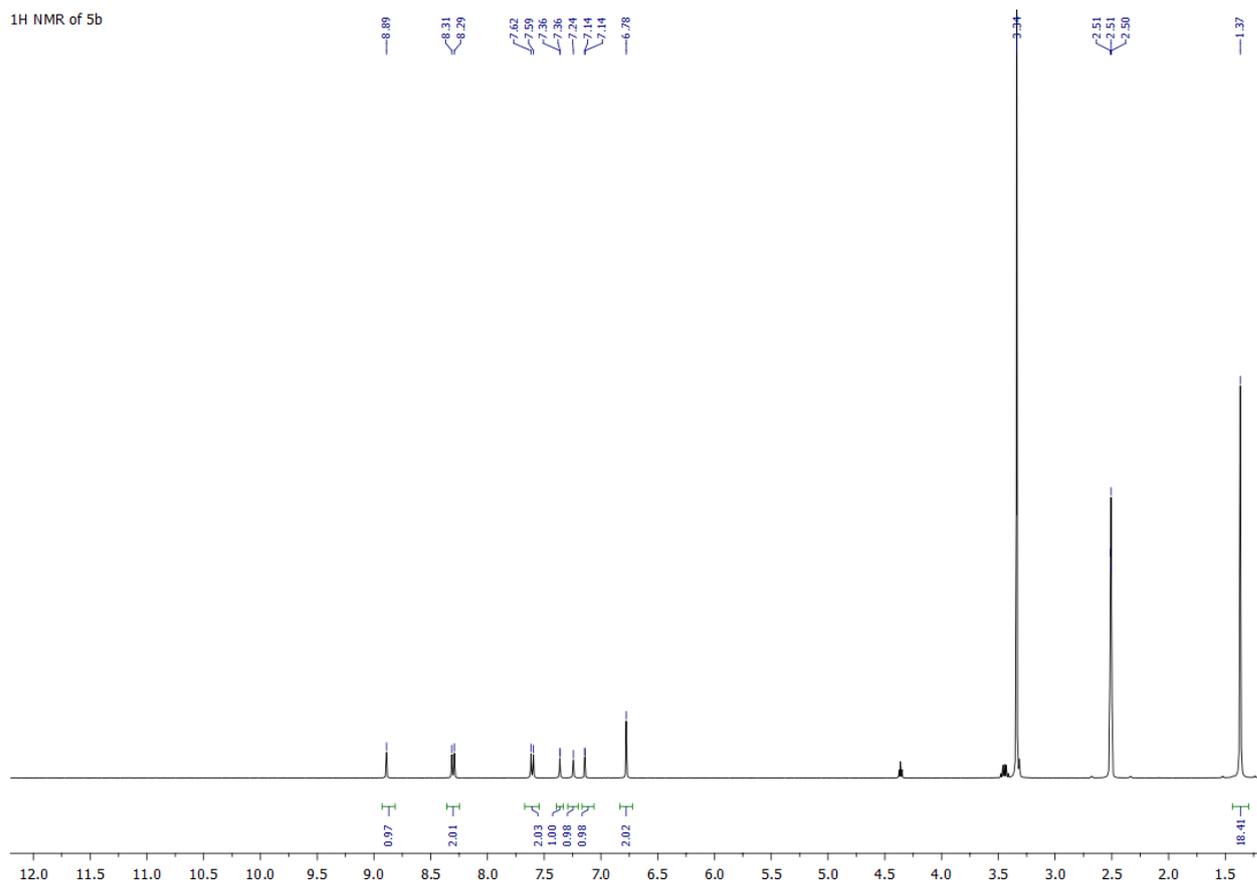
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^{13}C NMR of 5a



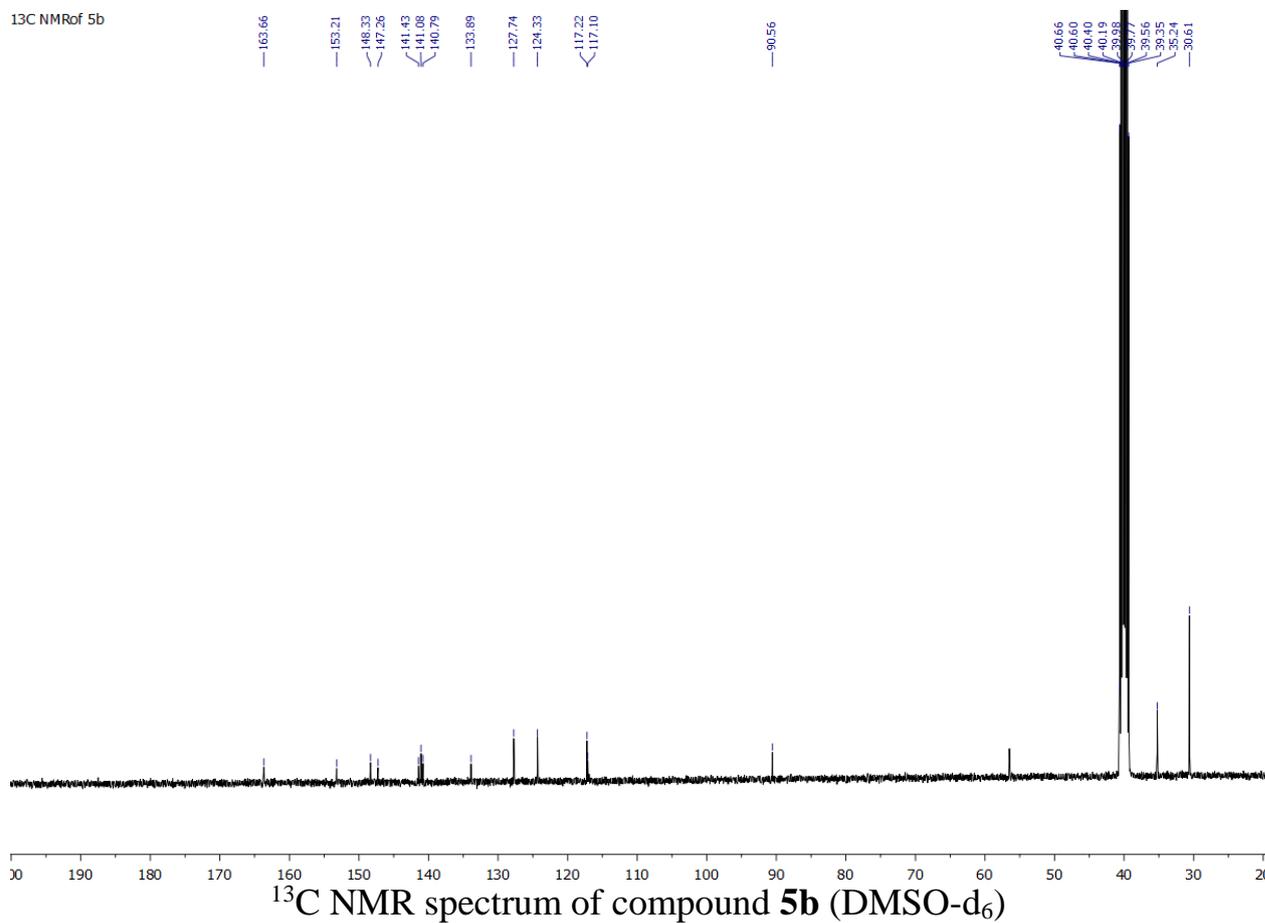
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¹H NMR of 5b



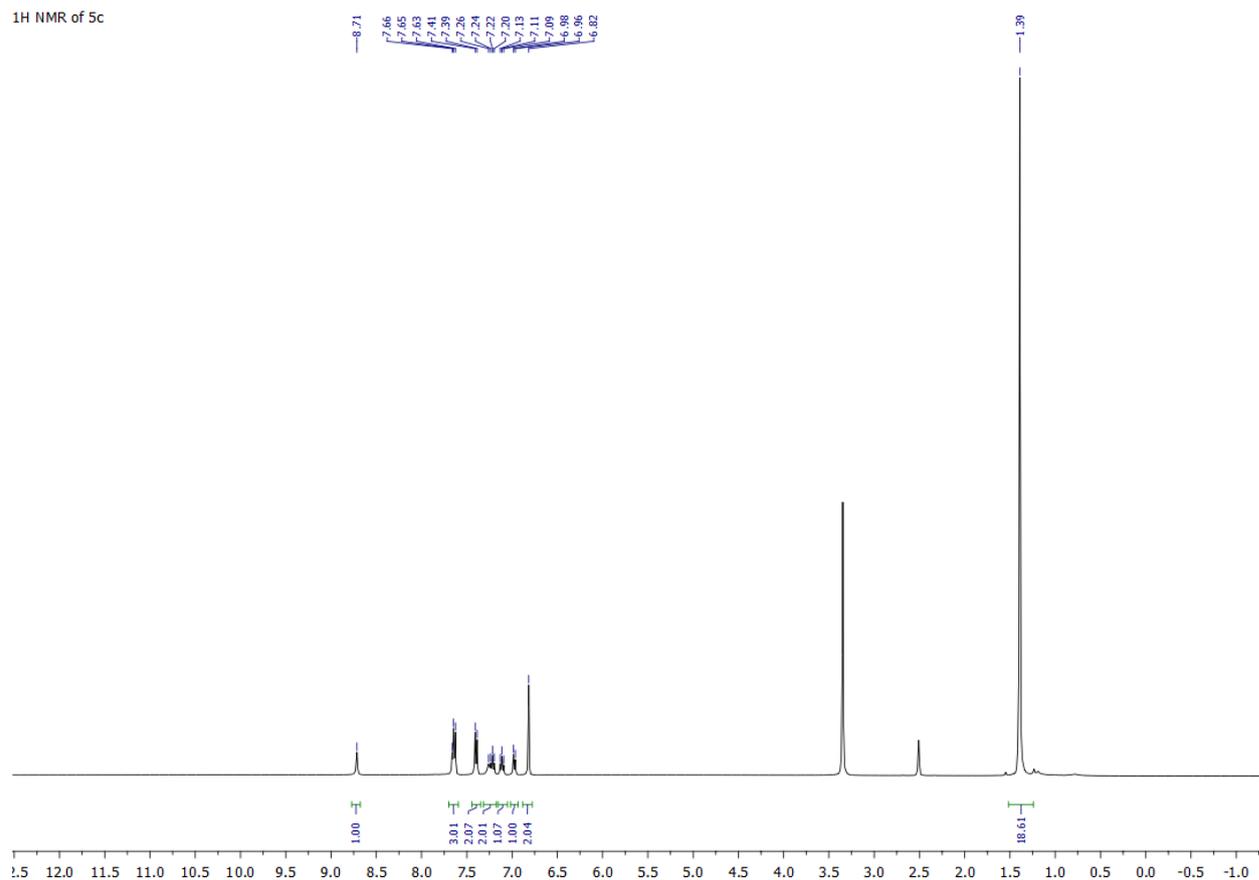
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¹³C NMR of 5b



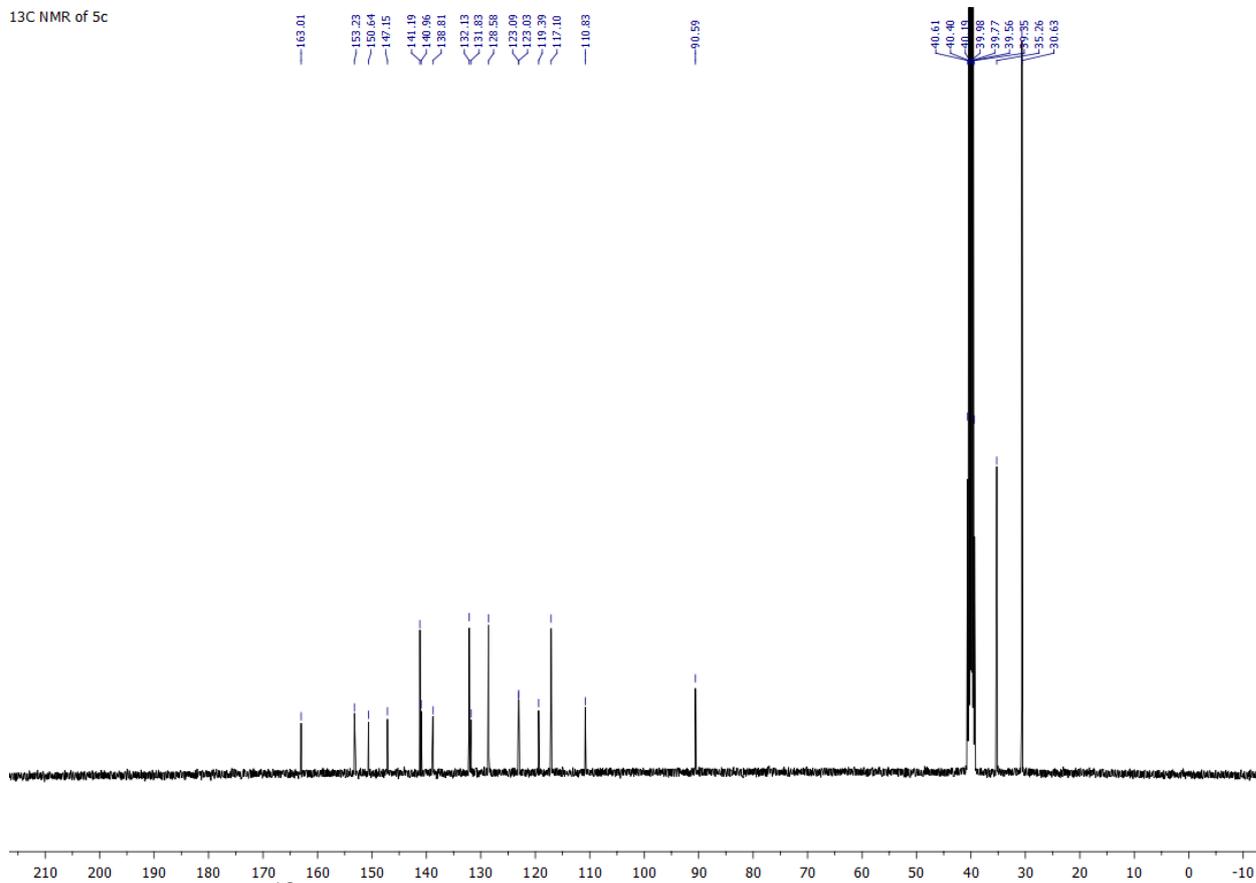
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¹H NMR of 5c



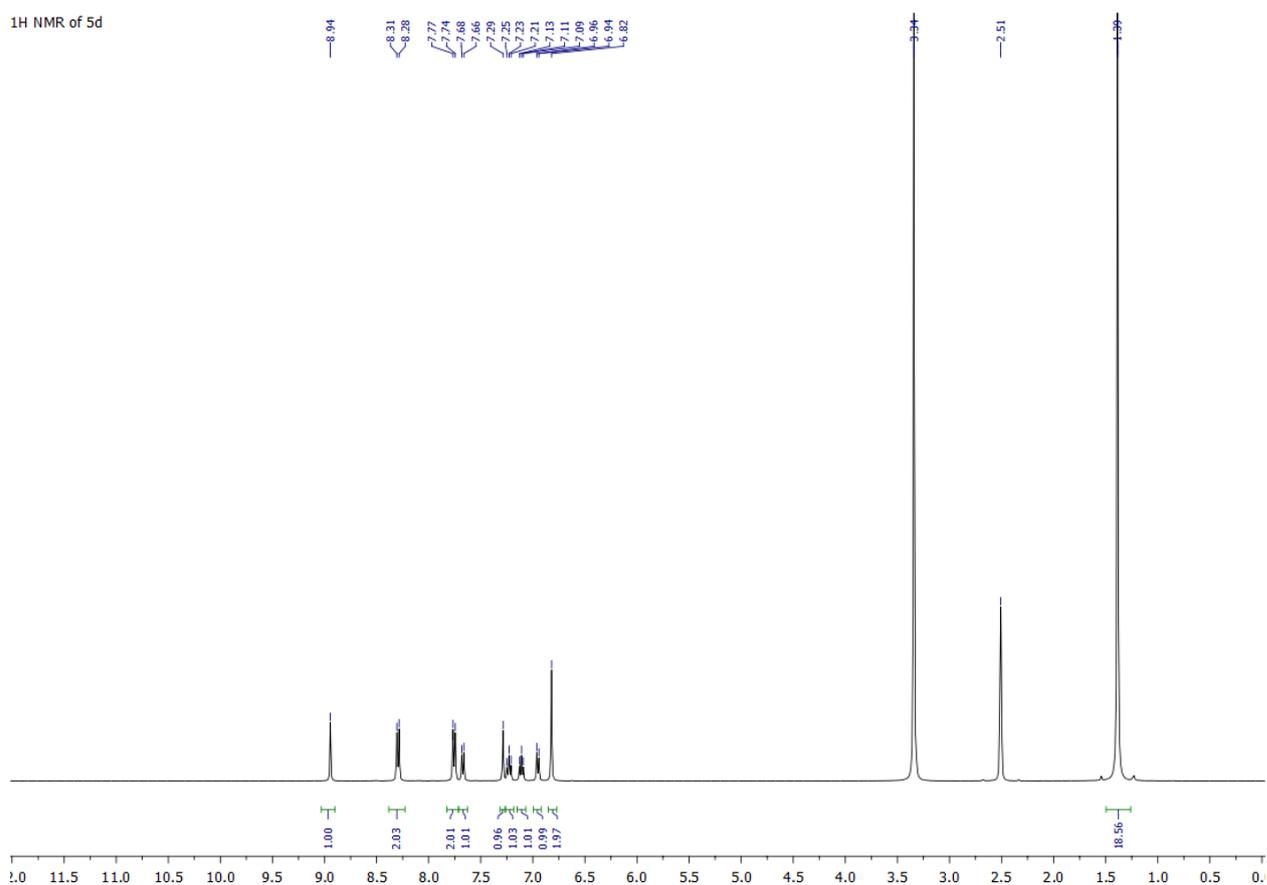
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¹³C NMR of 5c



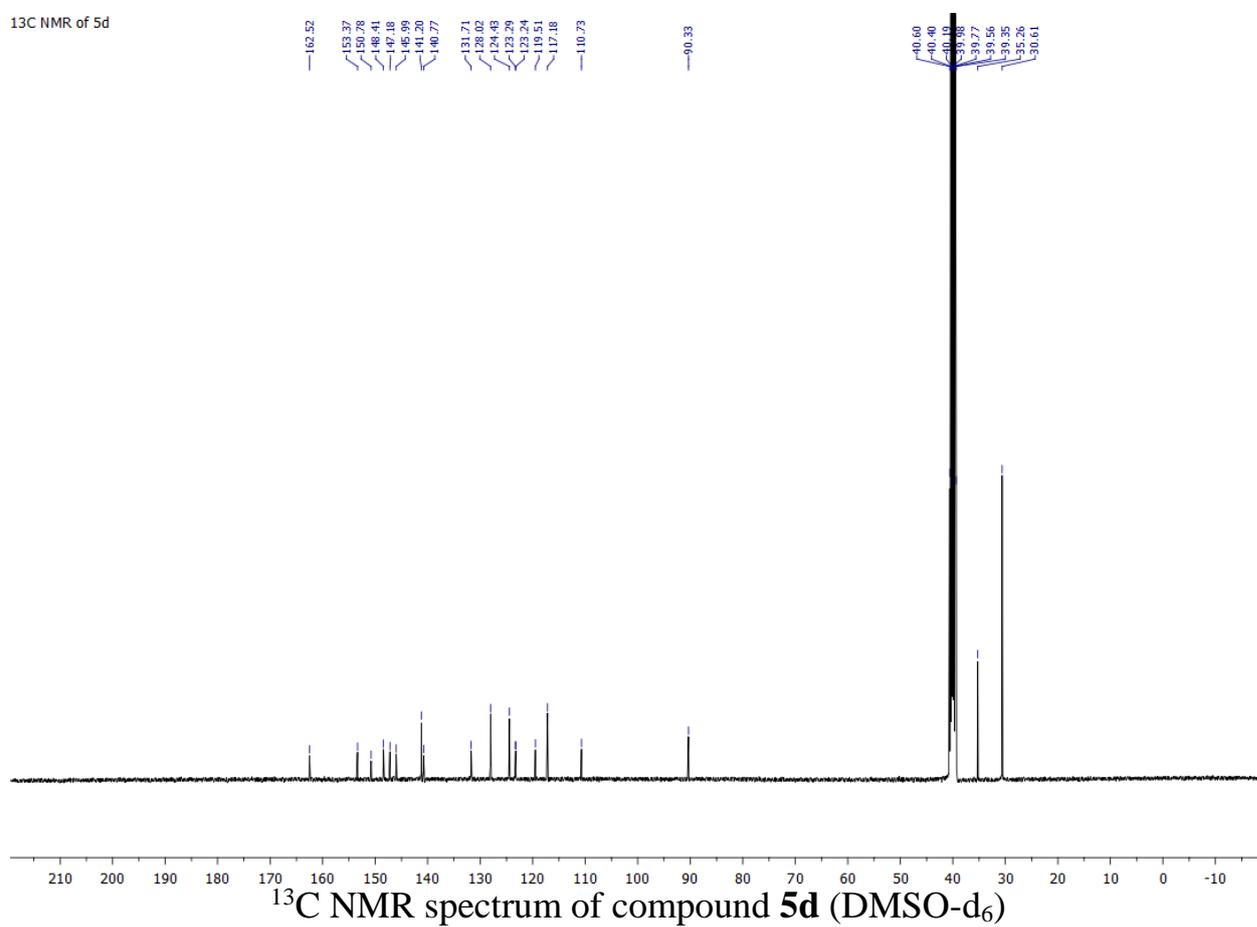
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¹H NMR of 5d



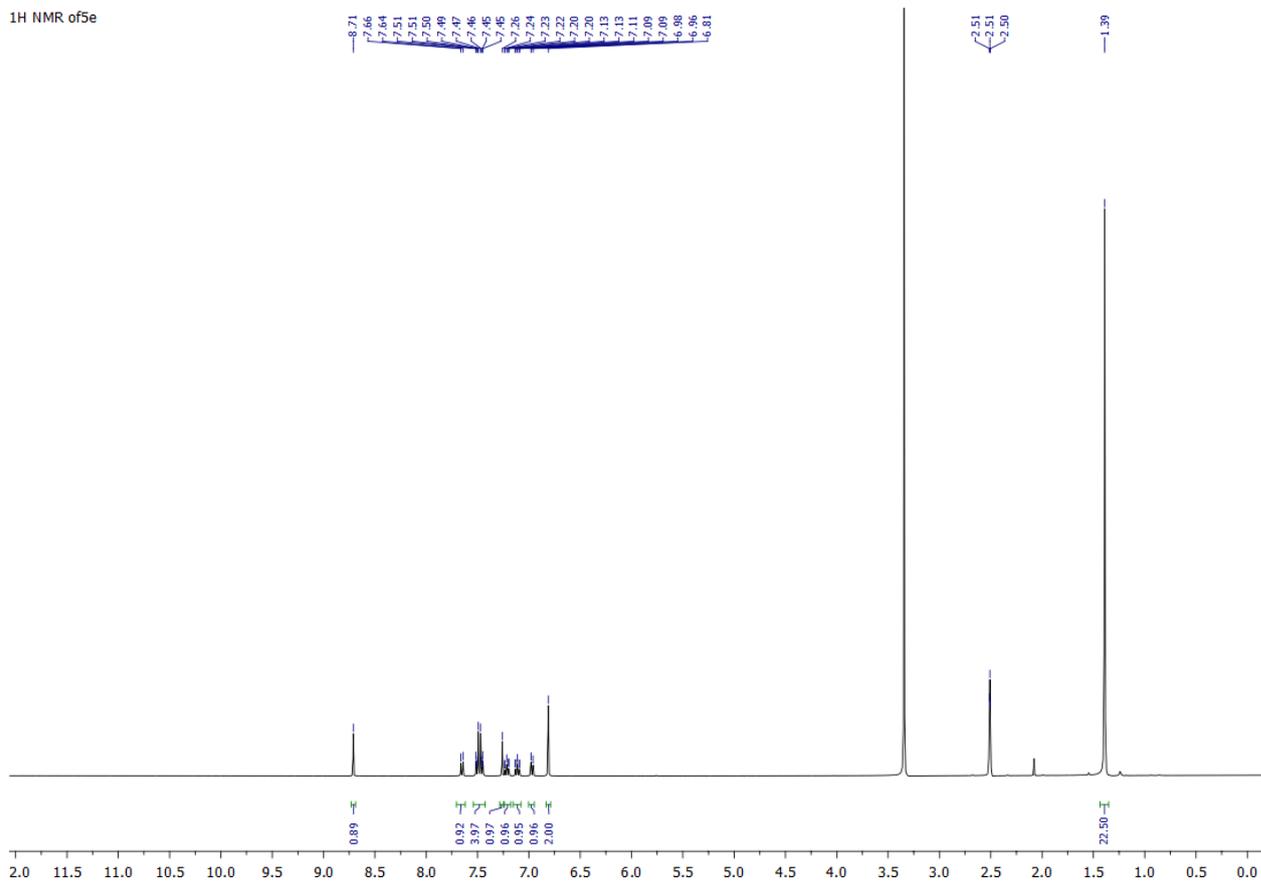
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¹³C NMR of 5d



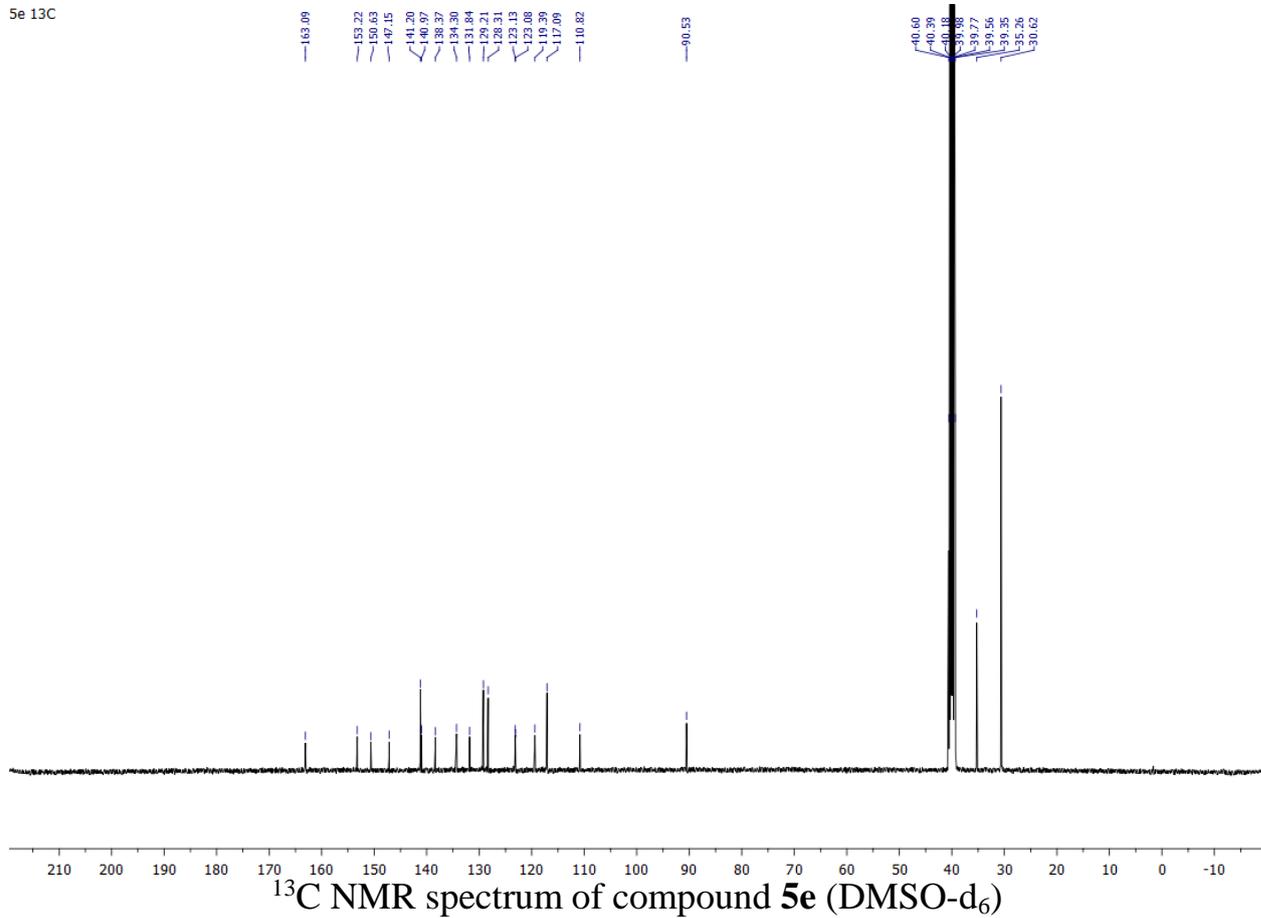
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^1H NMR of 5e



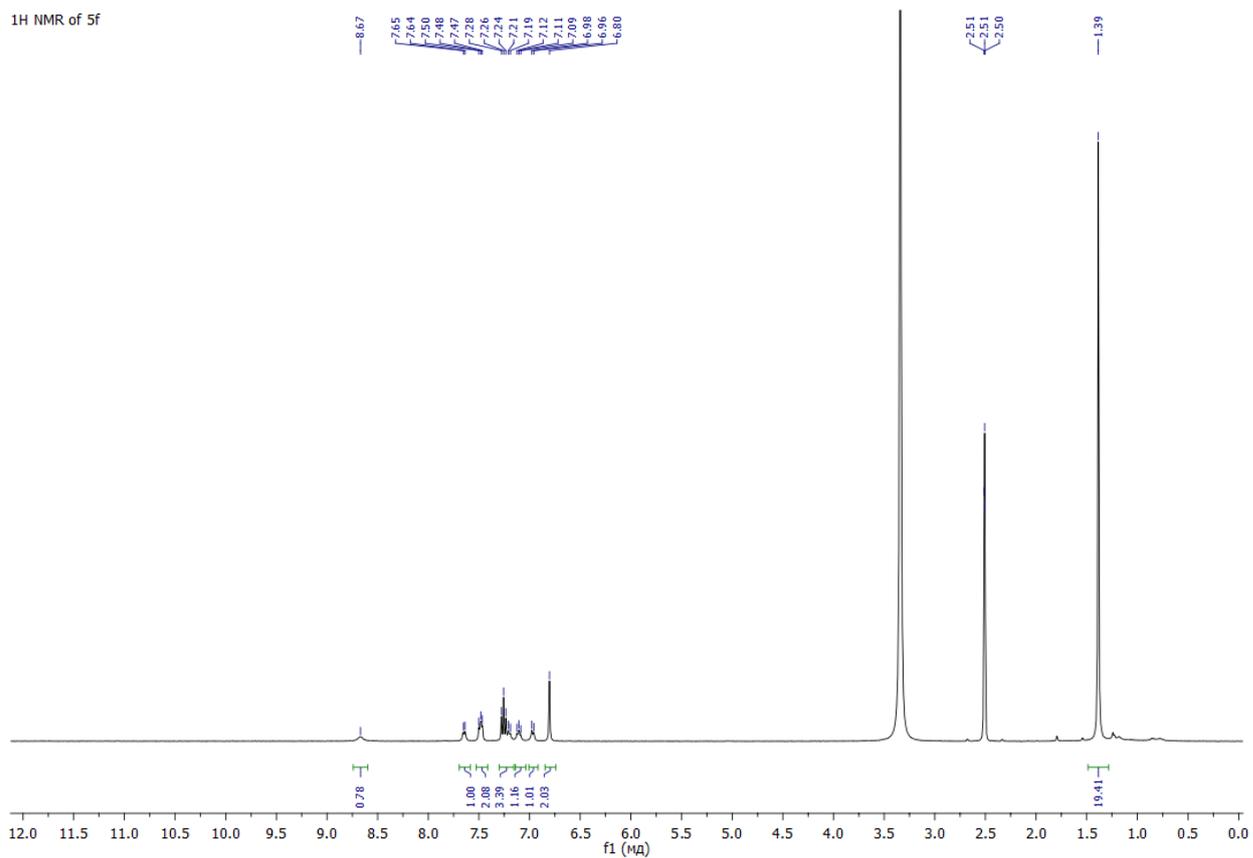
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5e ^{13}C



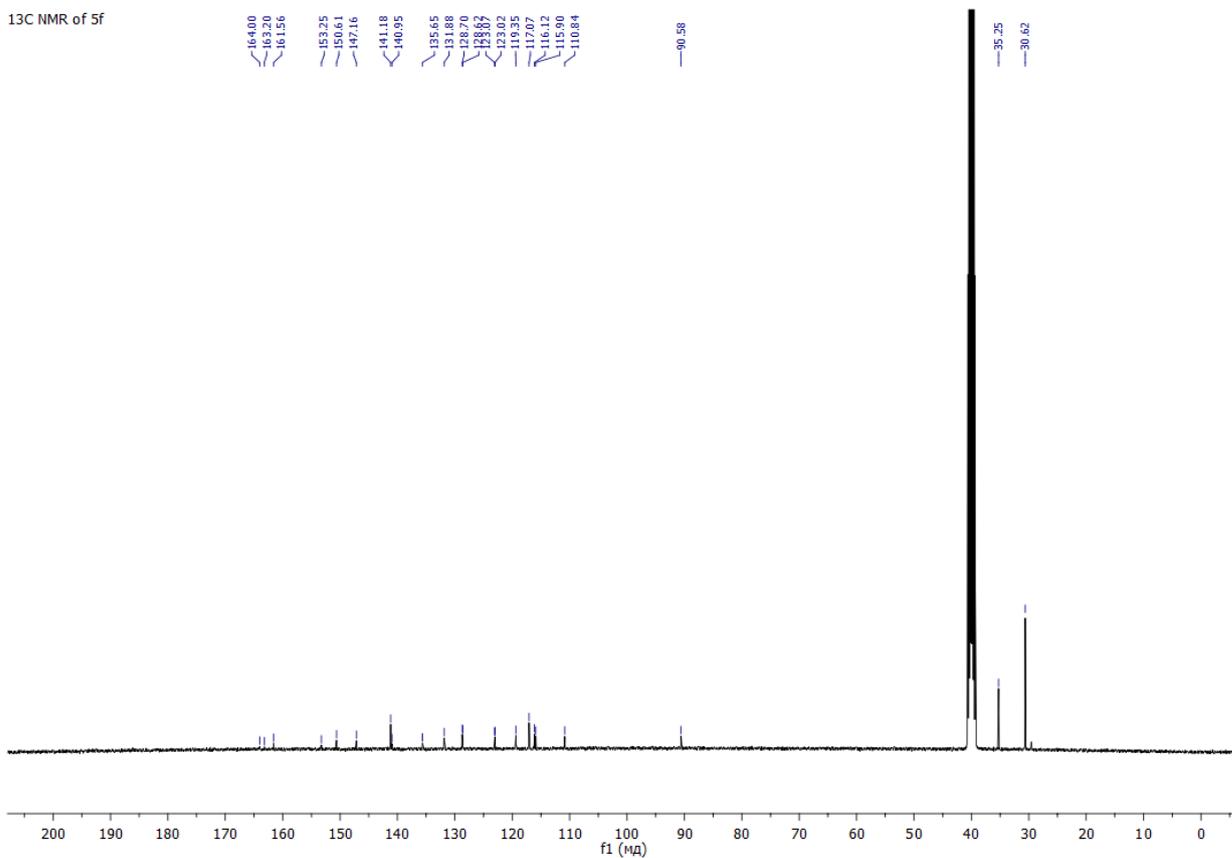
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¹H NMR of 5f



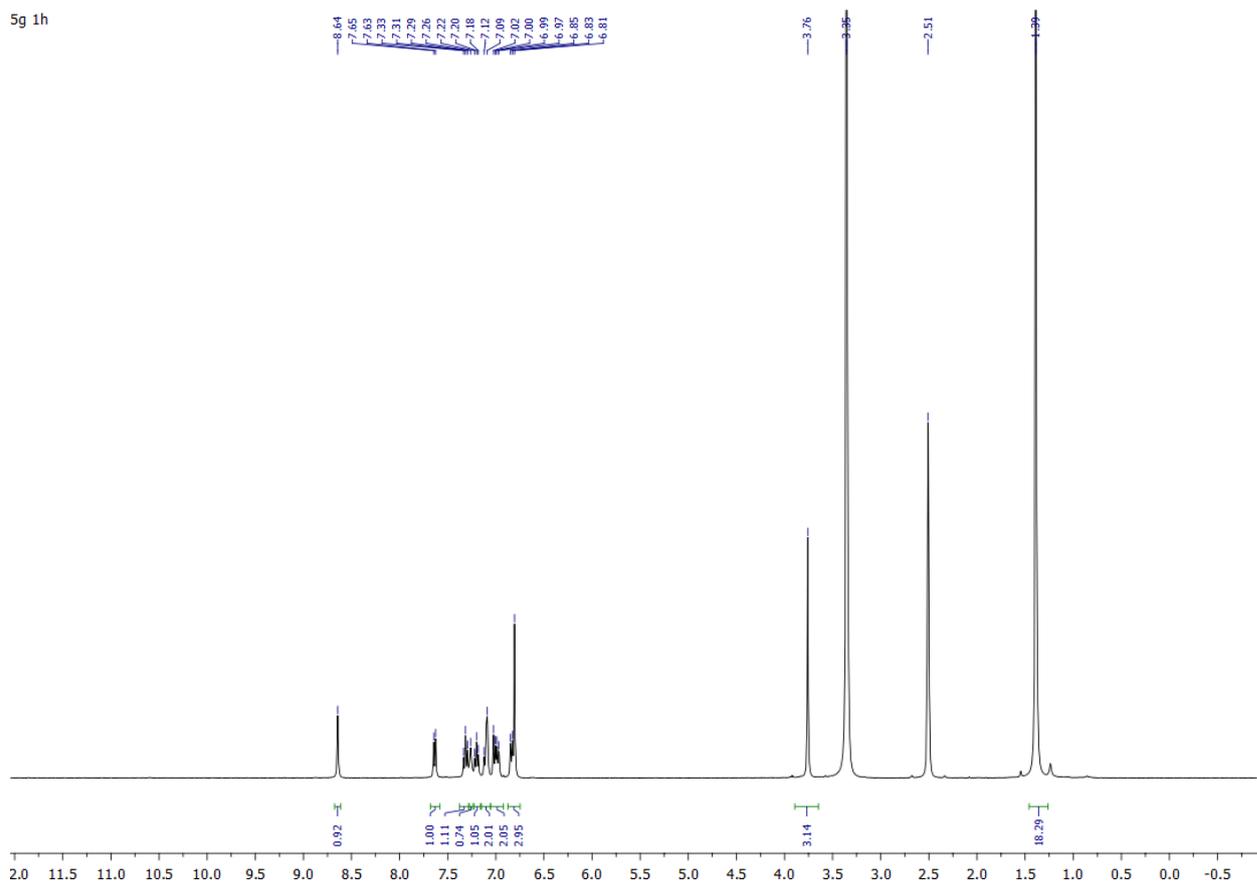
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¹³C NMR of 5f



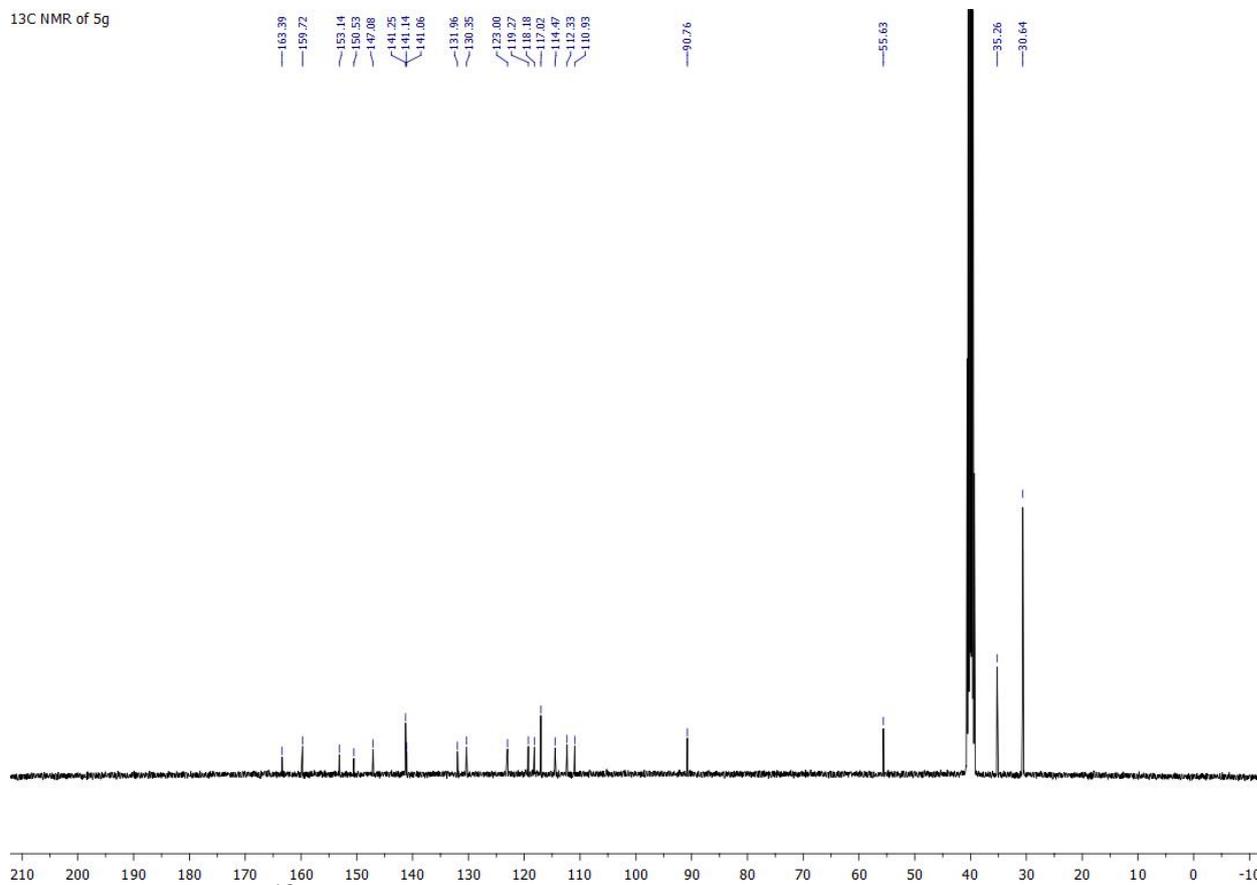
¹³C NMR spectrum of compound **5f** (DMSO-d₆)

5g 1h

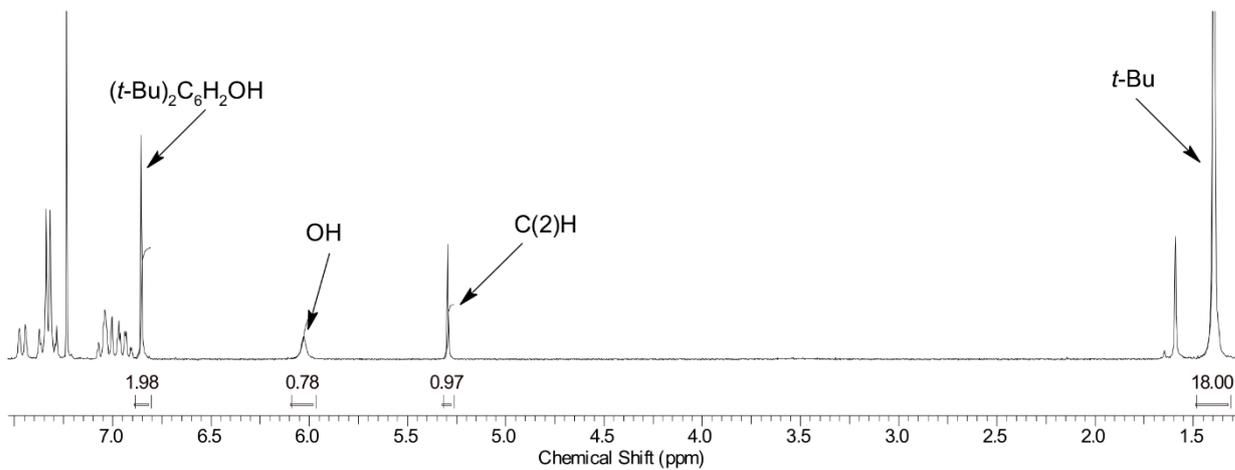


¹H NMR spectrum of compound **5g** (DMSO-d₆)

¹³C NMR of 5g

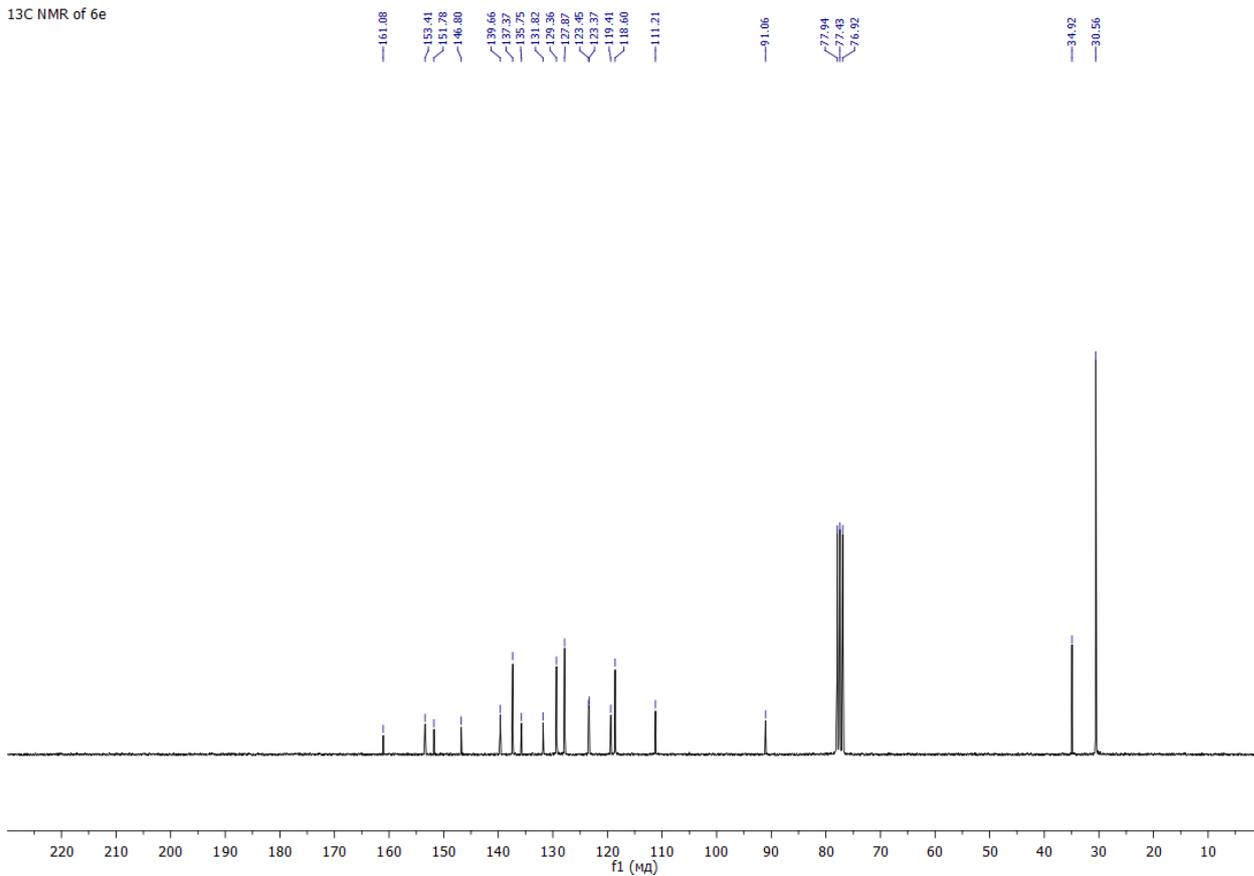


¹³C NMR spectrum of compound **5g** (DMSO-d₆)

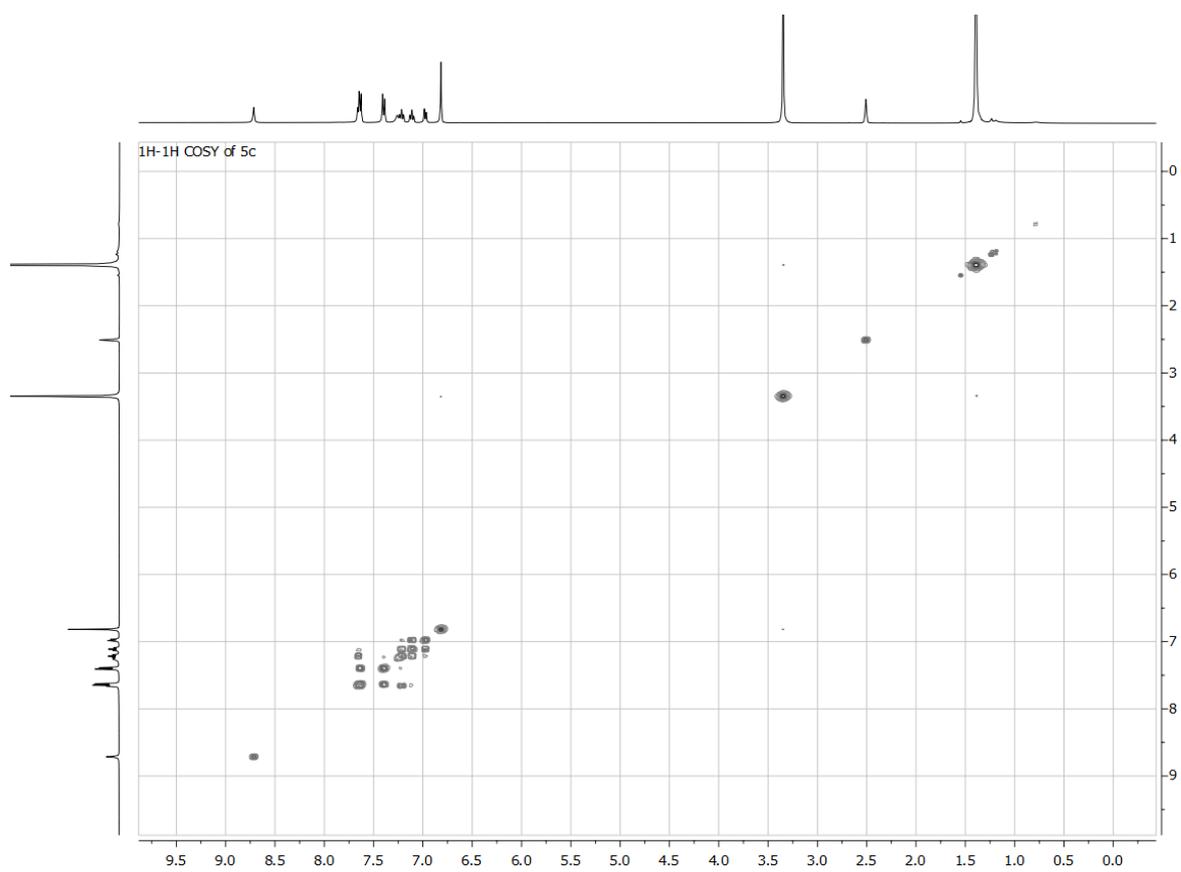


^1H NMR spectrum of compound **6e** (DMSO-d_6)

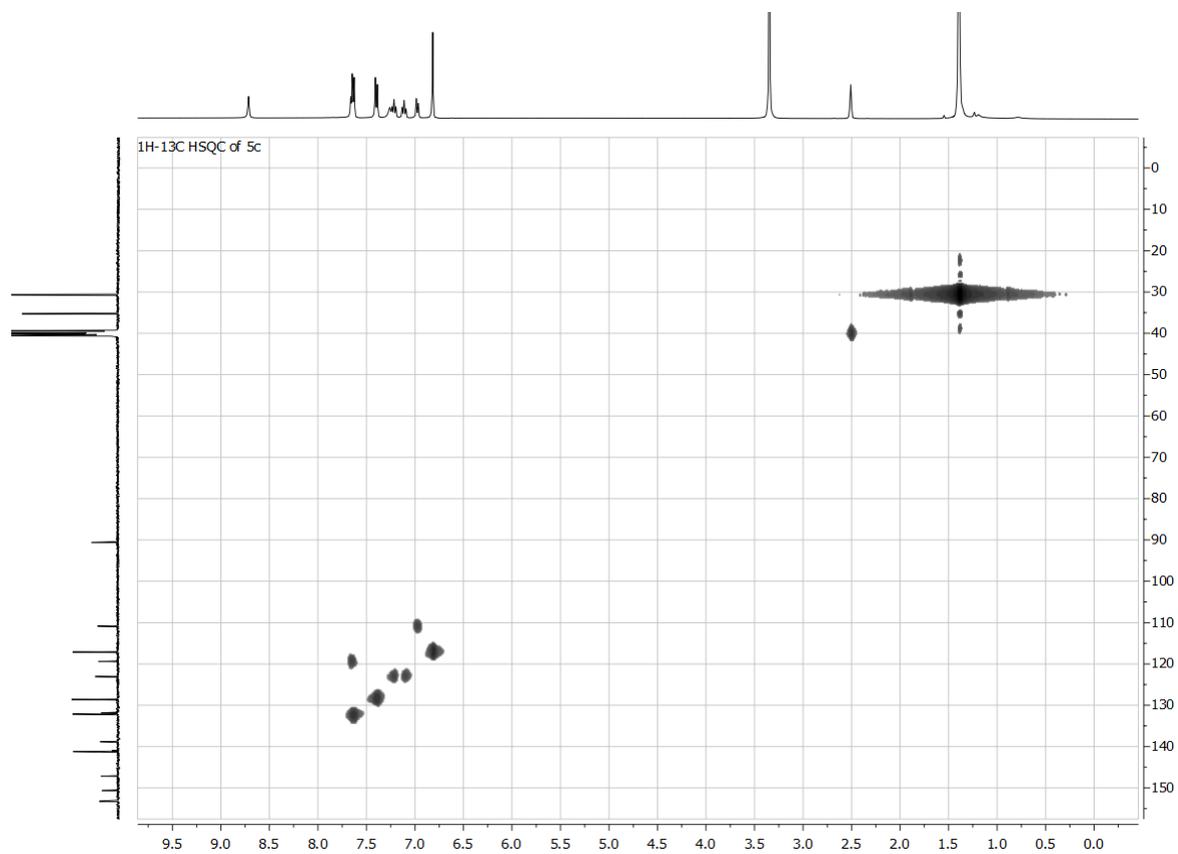
^{13}C NMR of **6e**



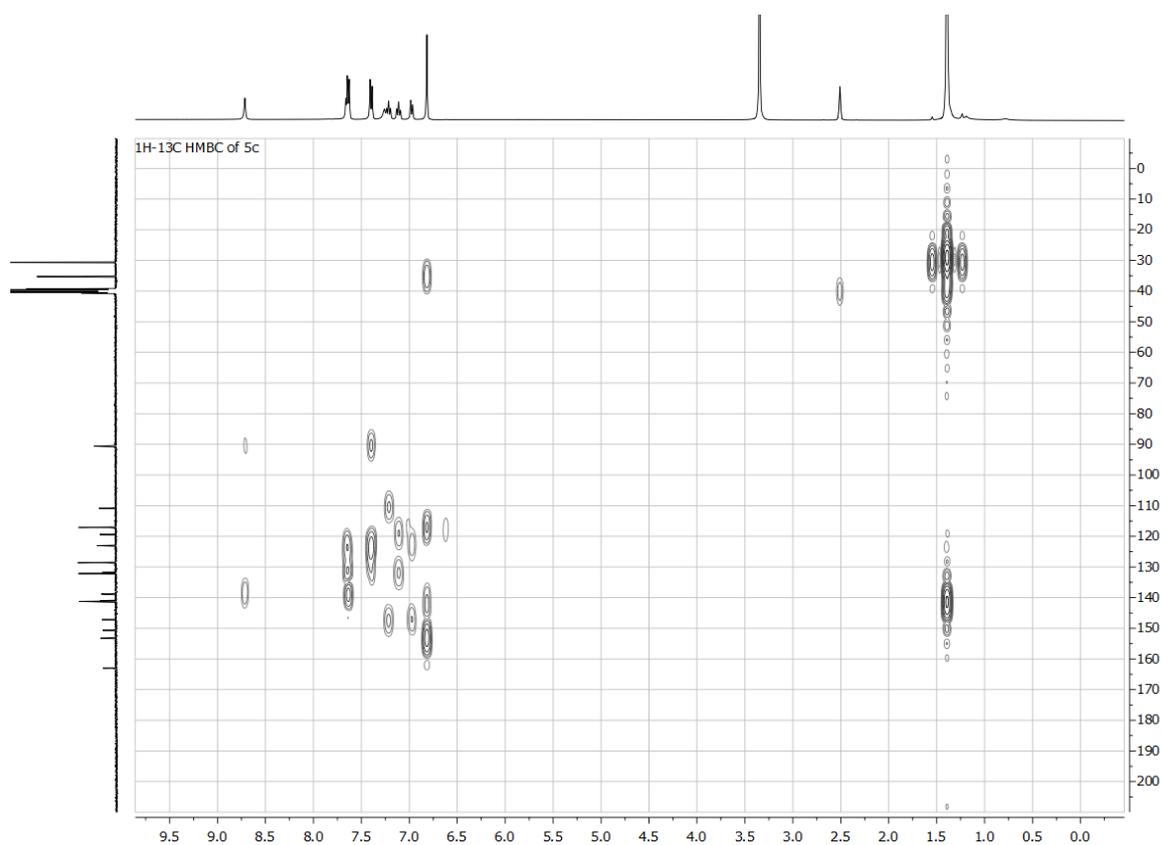
^{13}C NMR spectrum of compound **6e** (DMSO-d_6)



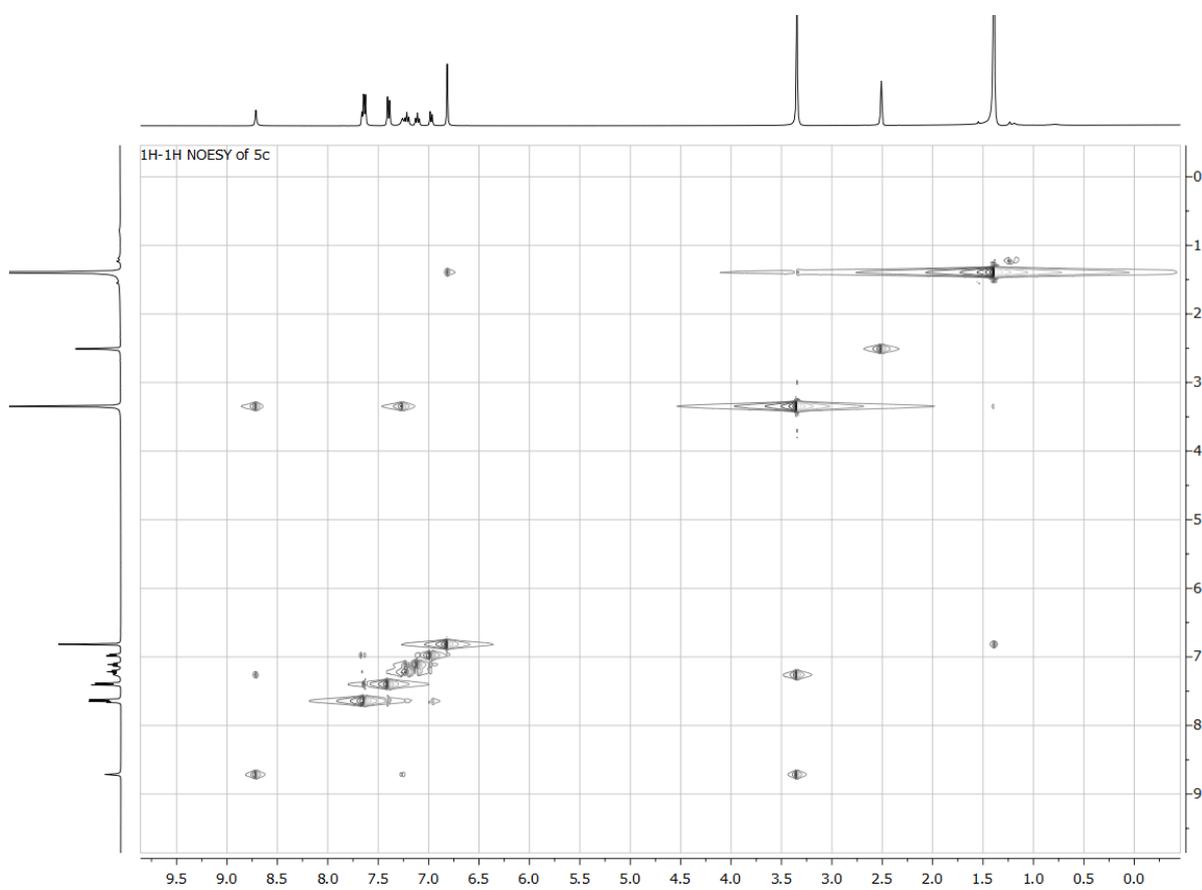
¹H-¹H COSY NMR spectrum of compound **5c**



¹H-¹³C HMQC NMR spectrum of compound **5c**



^1H - ^{13}C HMBC NMR spectrum of compound **5c**



^1H - ^1H NOESY NMR spectrum of compound **5c**