Organic & Biomolecular Chemistry

Supporting Information

Three-Component Cascade Reaction of 3-Ketonitriles, 2-Unsubstituted Imidazole *N*-oxides, and Aldehydes

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General information

All reagents were purchased from commercial suppliers and used without further purification unless otherwise specified. ^{1}H and ^{13}C NMR spectra were recorded using a Bruker Avance 300, 400, or 600 MHz spectrometer in DMSO-d_6; chemical shift values for ^{1}H and ^{13}C NMR spectra are reported in parts per million (ppm), with the solvent resonance as the internal standard (DMSO-d_6: δ_H = 2.50 ppm, δ_C = 39.52 ppm).

High-resolution mass spectra (HRMS) were recorded using a Bruker MicrOTOF ESI-TOF mass spectrometer.

TLC analysis was performed using Merck silica gel 60 F254 pre-coated plates, visualization was performed with UV and/or iodine vapor. Column chromatography purifications were performed using silica gel 60 (40-63 μm) from Merck. Chloroform and its mixtures with methanol were used as eluents.

IR spectra were recorded using a Shimadzu IRAffinity-1 FTIR spectrophotometer.

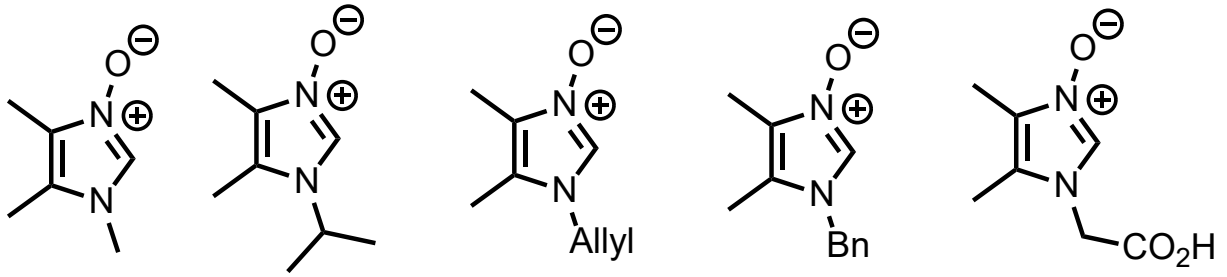
The melting points were determined using a Kofler hot stage.

X-ray diffraction data for **4x**, **4j**, **5b** and **5k** were collected at 100 K with a Bruker Quest D8 CMOS diffractometer, using graphite monochromated Mo-Kα radiation (lλ = 0.71073 Å).

General procedures

Starting materials.

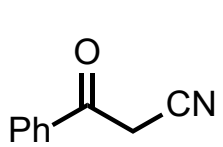
1,4,5-Trimethyl-1*H*-imidazole *N*-oxide (**1a**),[1] 1-isopropyl-4,5-dimethyl-1*H*-imidazole *N*-oxide (**1b**),[2] 1-allyl-4,5-dimethyl-1*H*-imidazole *N*-oxide (**1c**),[3] 1-benzyl-4,5-dimethyl-1*H*-imidazole *N*-oxide (**1d**),[1] and 1-(carboxymethyl)-4,5-dimethyl-1*H*-imidazole *N*-oxide (**1e**)[4] were obtained according to earlier works.



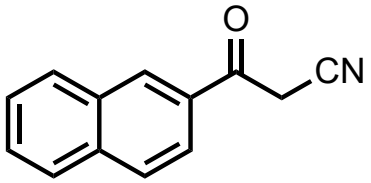
1a **1b** **1c** **1d** **1e**

General procedure for preparation (aroyl)acetonitriles. To a solution of methyl or ethyl ester of corresponding acid (40 mmol, 1 equiv.) in absolute THF (30 ml) and MeCN (2.00 g, 49 mmol, 1.2 equiv.) potassium *tert*-butoxide (5.8 g, 52 mmol, 1.3 equiv.) was added in one portion. The reaction mixture was stirred at reflux for 3 h, and then the solvent was removed under reduced pressure. The residue was dissolved in cold water (150 ml) and acetic acid (5 ml) was added. The product was filtered off and washed with cold water (100 ml) and dried at an ambient

temperature. The using of the described procedure allowed to obtain each of the (aroyl)acetonitriles in sufficiently pure form for further synthetic utility.



2a



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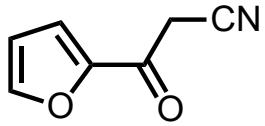

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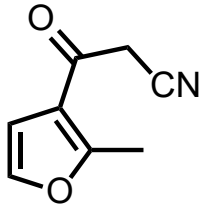


2d

Benzoylacetonitrile (2a). Yield 18.9 g (65% from 0.2 mole of ethyl benzoate).[5]

2-Naphthoylacetonitrile (2b)[6].

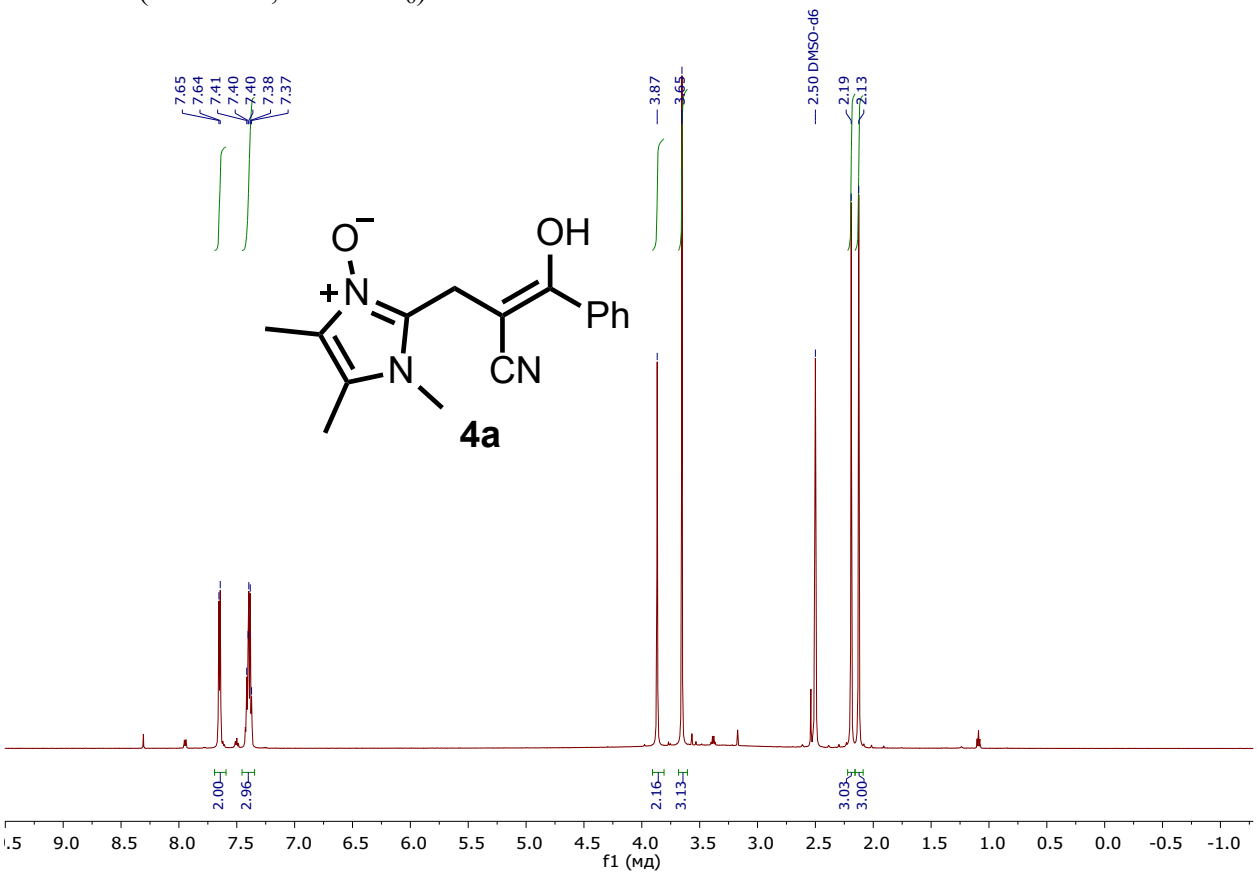
(2-Furoyl)acetonitrile (2c). Yield 7.0 g (51% from 0.1 mole of methyl 2-furoate). **^{1}H NMR**[7] (400 MHz, DMSO-d_6) δ: 8.09 (dd, J = 1.7, 0.7 Hz, 1H), 7.56 (dd, J = 3.7, 0.7 Hz, 1H), 6.78 (dd, J = 3.7, 1.7 Hz, 1H), 4.53 (s, 2H).

(2-Methylfur-3-oyl)acetonitrile (2d).[8] Yield 4.54 g (61% from 0.05 mole methyl 3-methyl-2-furoate). **^{1}H NMR** (600 MHz, DMSO-d_6) δ: 7.62 (d, J = 1.9 Hz, 1H), 6.84 (d, J = 1.9 Hz, 1H), 4.45 (s, 2H), 2.54 (s, 3H).

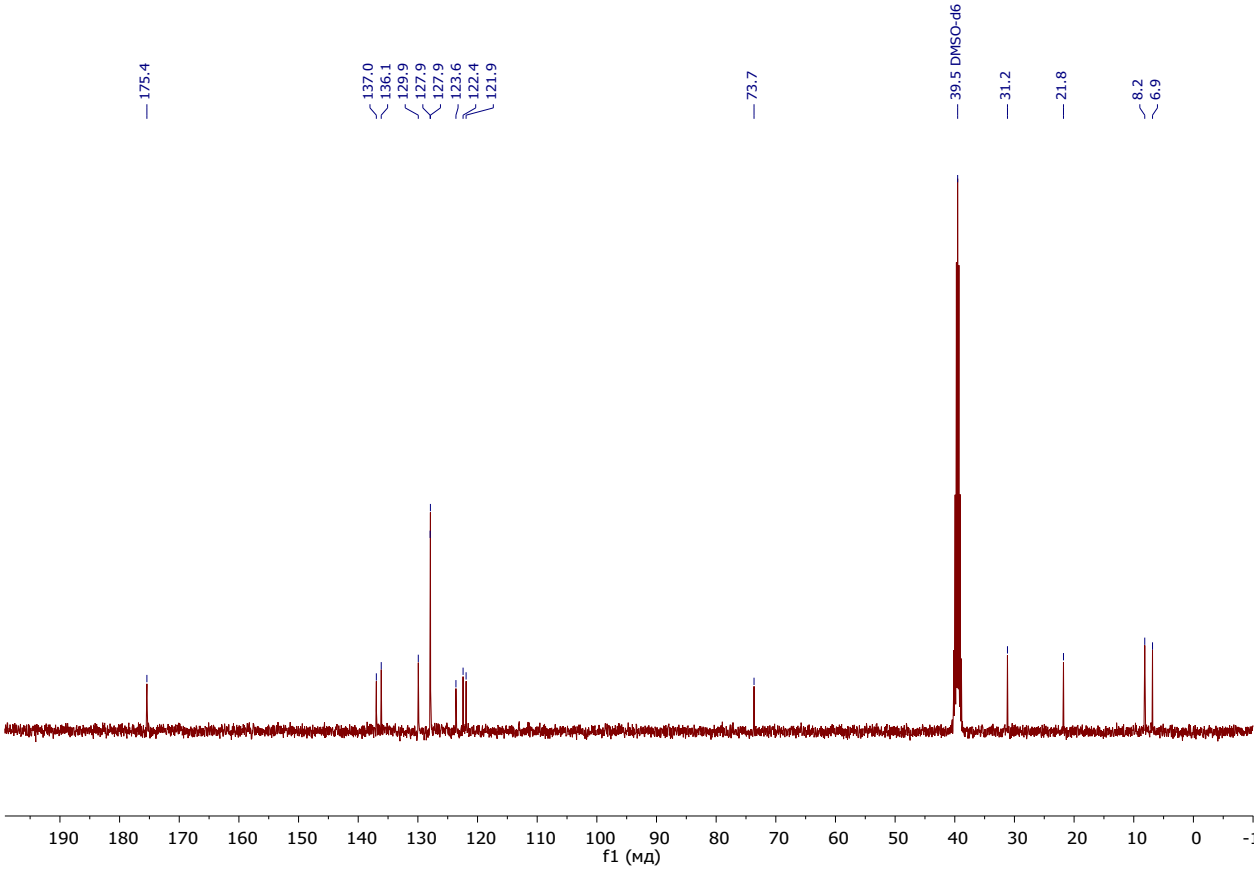
(*E*)-2-benzoyl-3-(4-methoxyphenyl)acrylonitrile (3). A mixture of benzoylacetonitrile (730 mg, 5 mmol), 4-anisaldehyde (700 mg, 5.1 mmol), piperidine (100 mg), and AcOH (100 mg) in EtOH (10 ml) was stirred under reflux for 5 h. After cooling, the product was filtered off and washed with EtOH (10 ml). Pale yellow powder; yield 720 mg (55%). **^{1}H NMR**[9] (400 MHz, DMSO-d_6) δ: 8.12-8.09 (m, 3H), 7.84-7.81 (m, 2H), 7.72-7.67 (m, 1H), 7.60-7.56 (m, 2H), 7.18-7.16 (m, 2H), 3.88 (s, 3H).

Copies of ^{1}H and ^{13}C NMR spectra

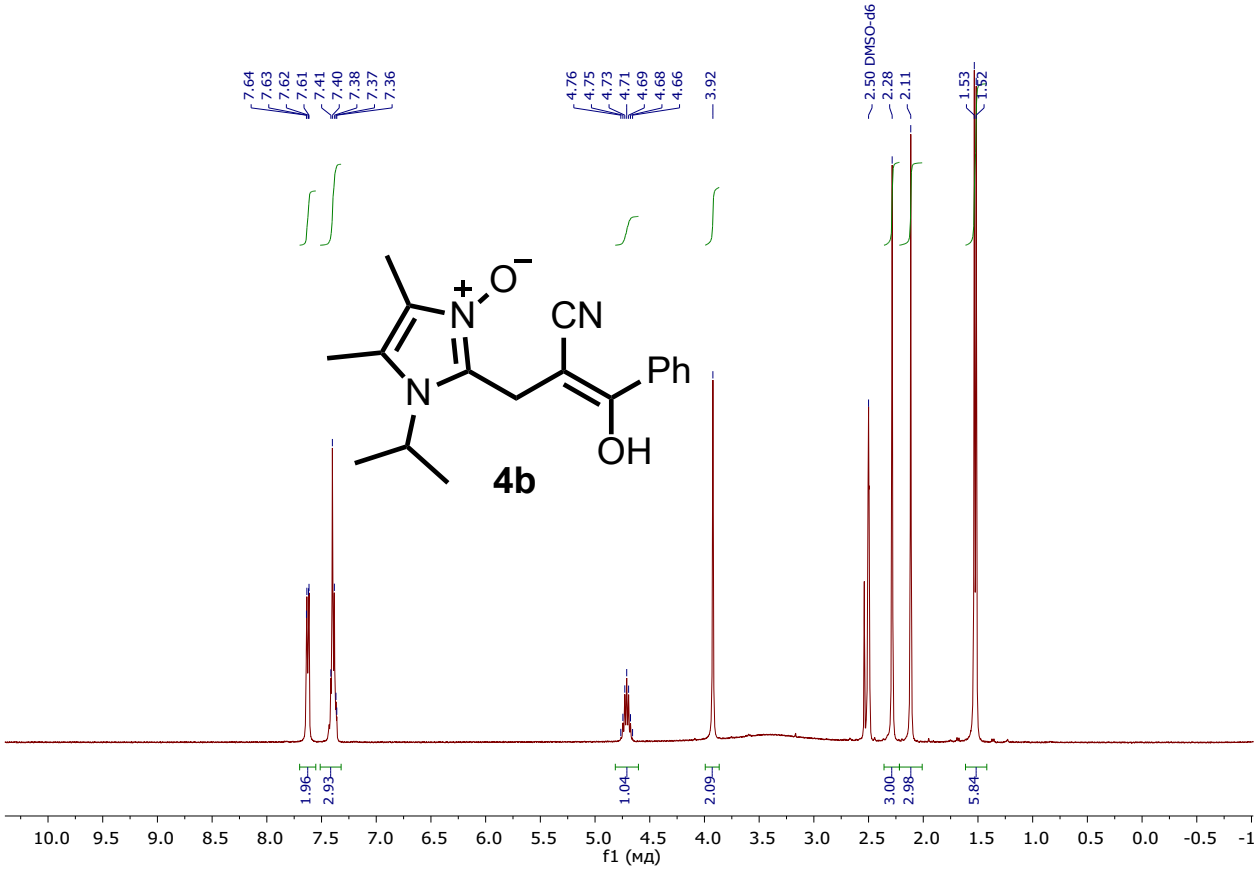
^{1}H NMR (600 MHz, DMSO-d_6) of **4a**



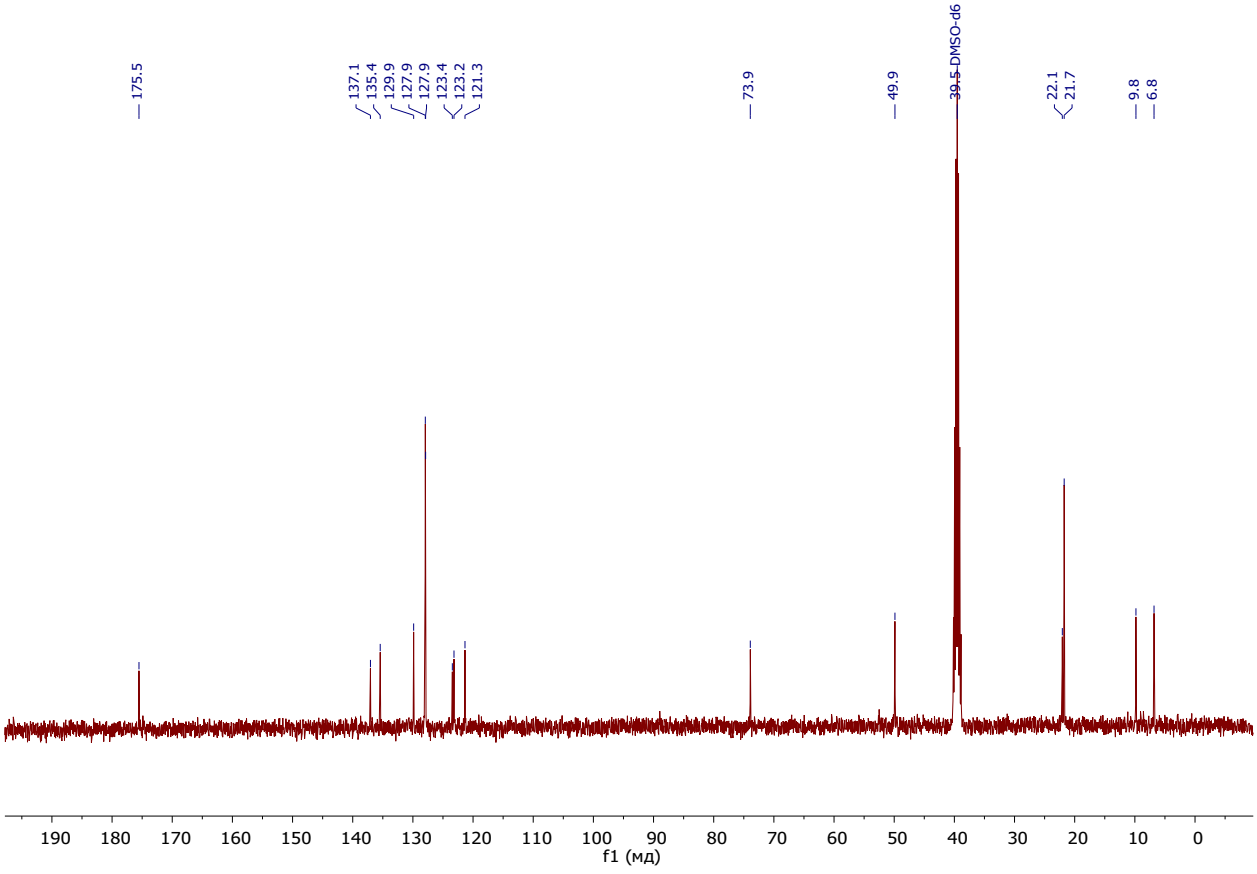
$^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) of **4a**



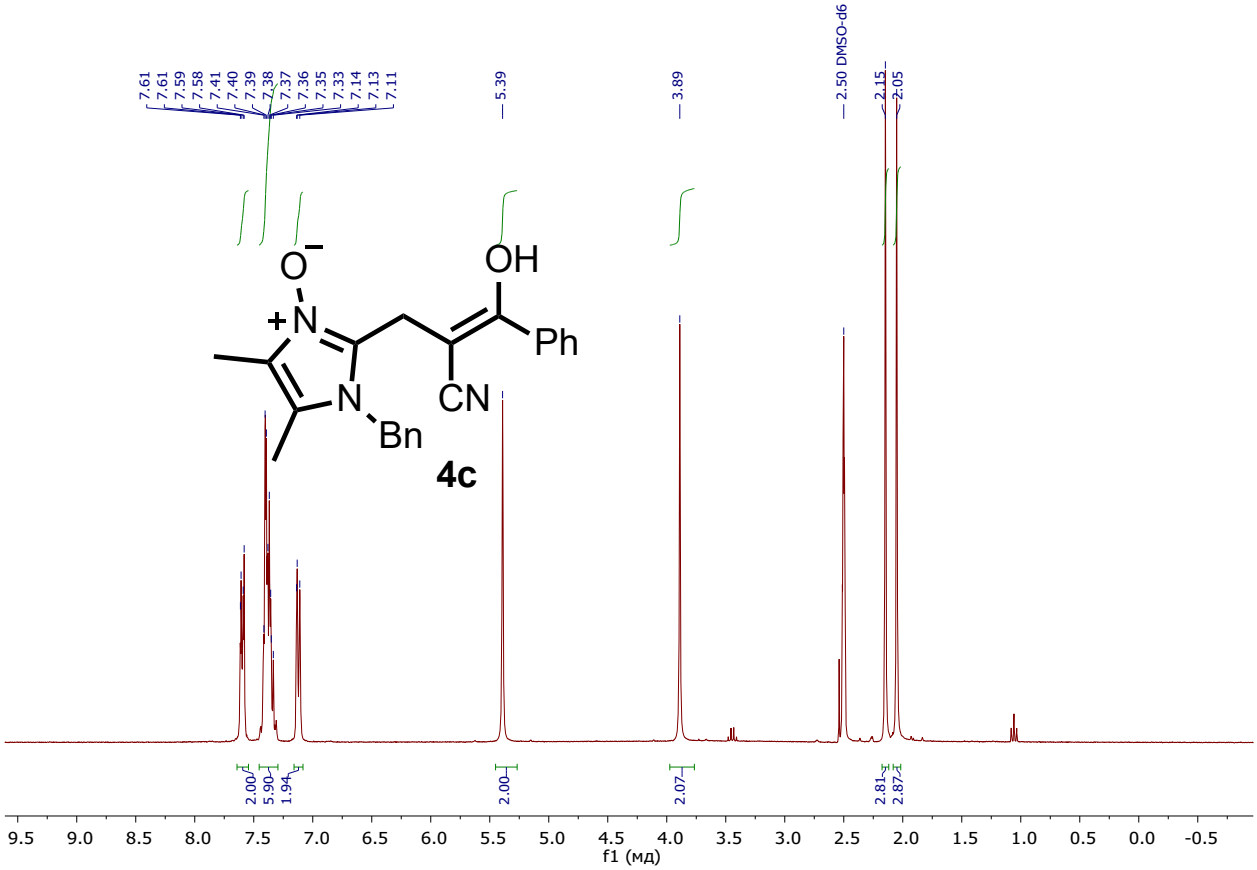
^{1}H NMR (400 MHz, DMSO-d_6) of **4b**



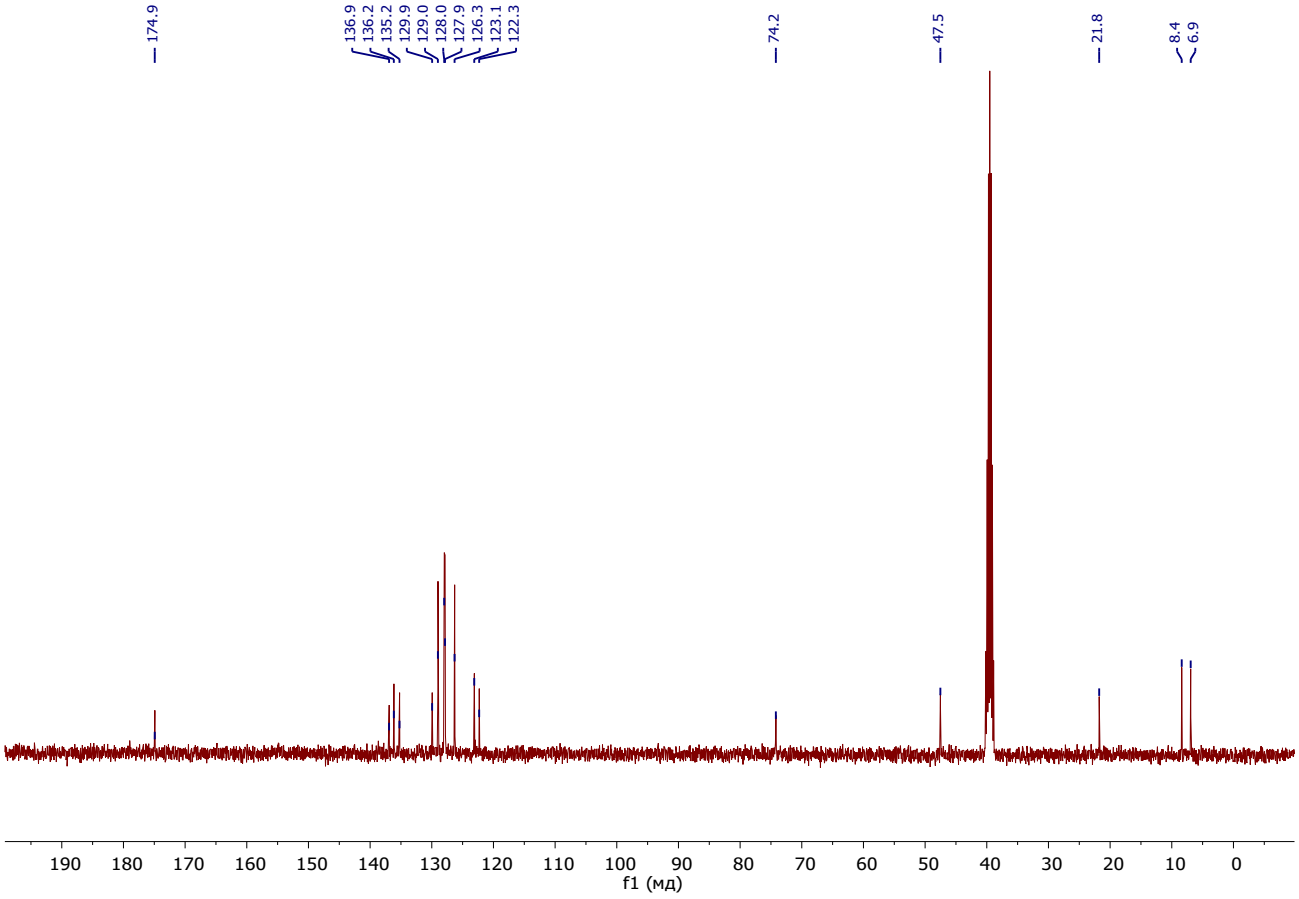
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4b**



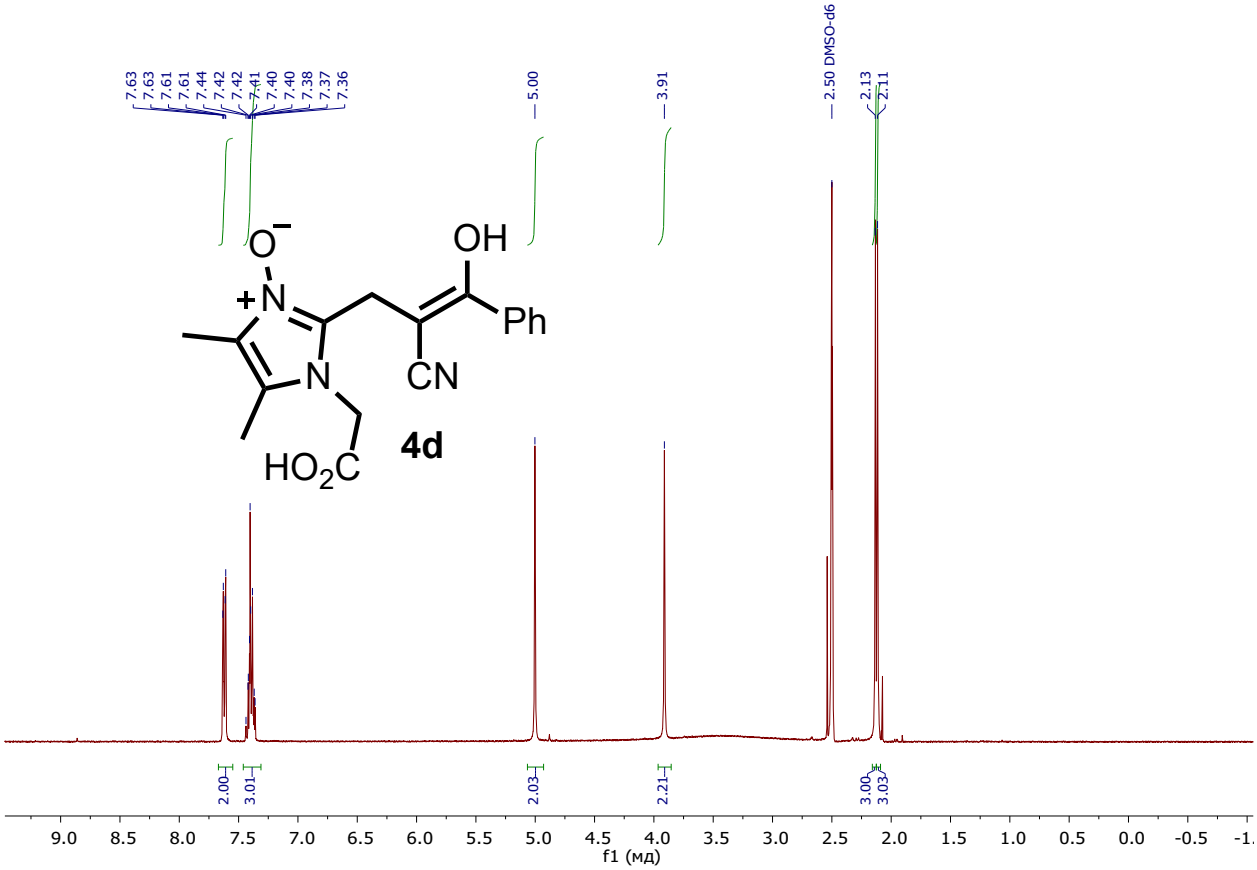
^{1}H NMR (300 MHz, DMSO-d_6) of **4c**



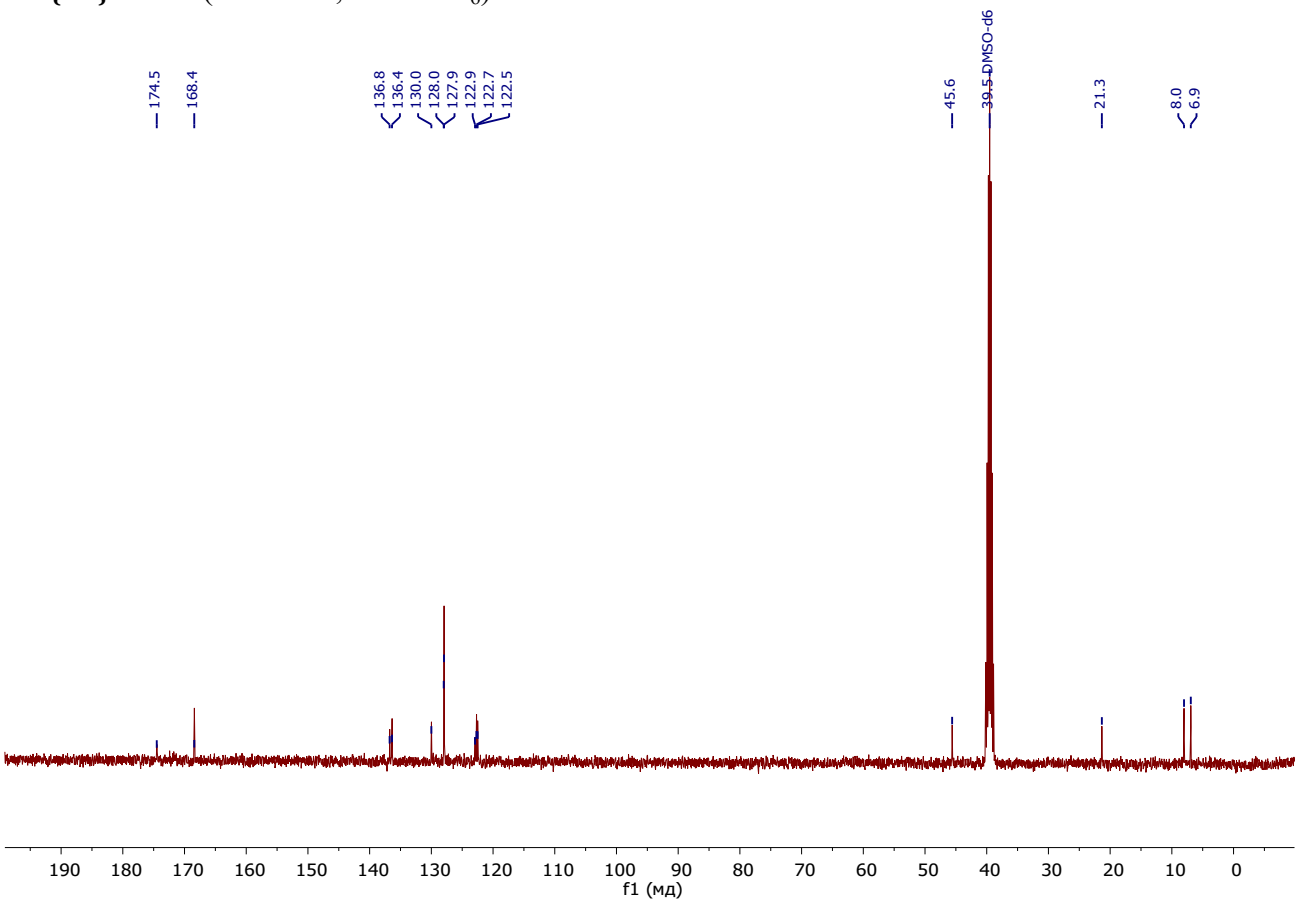
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4c**



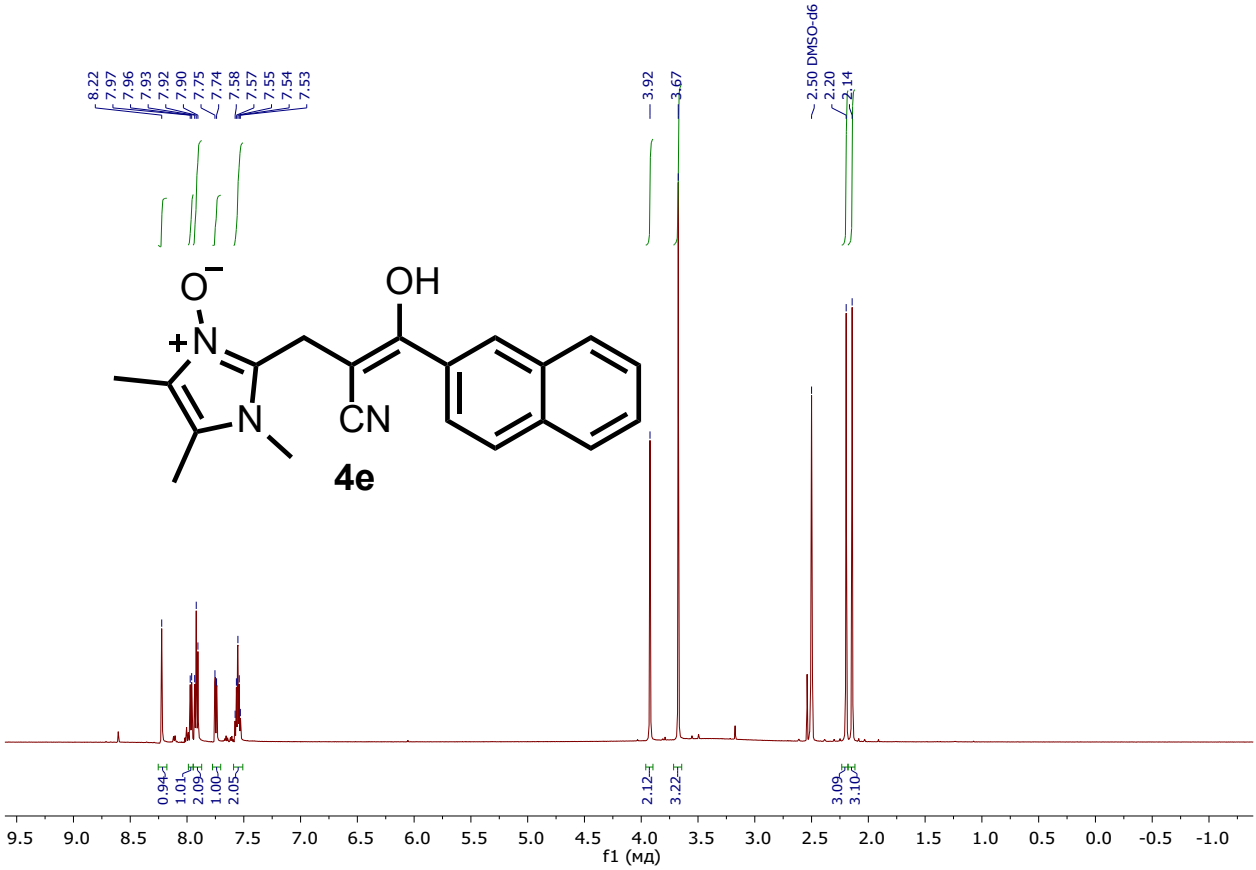
^{1}H NMR (400 MHz, DMSO-d_6) of **4d**



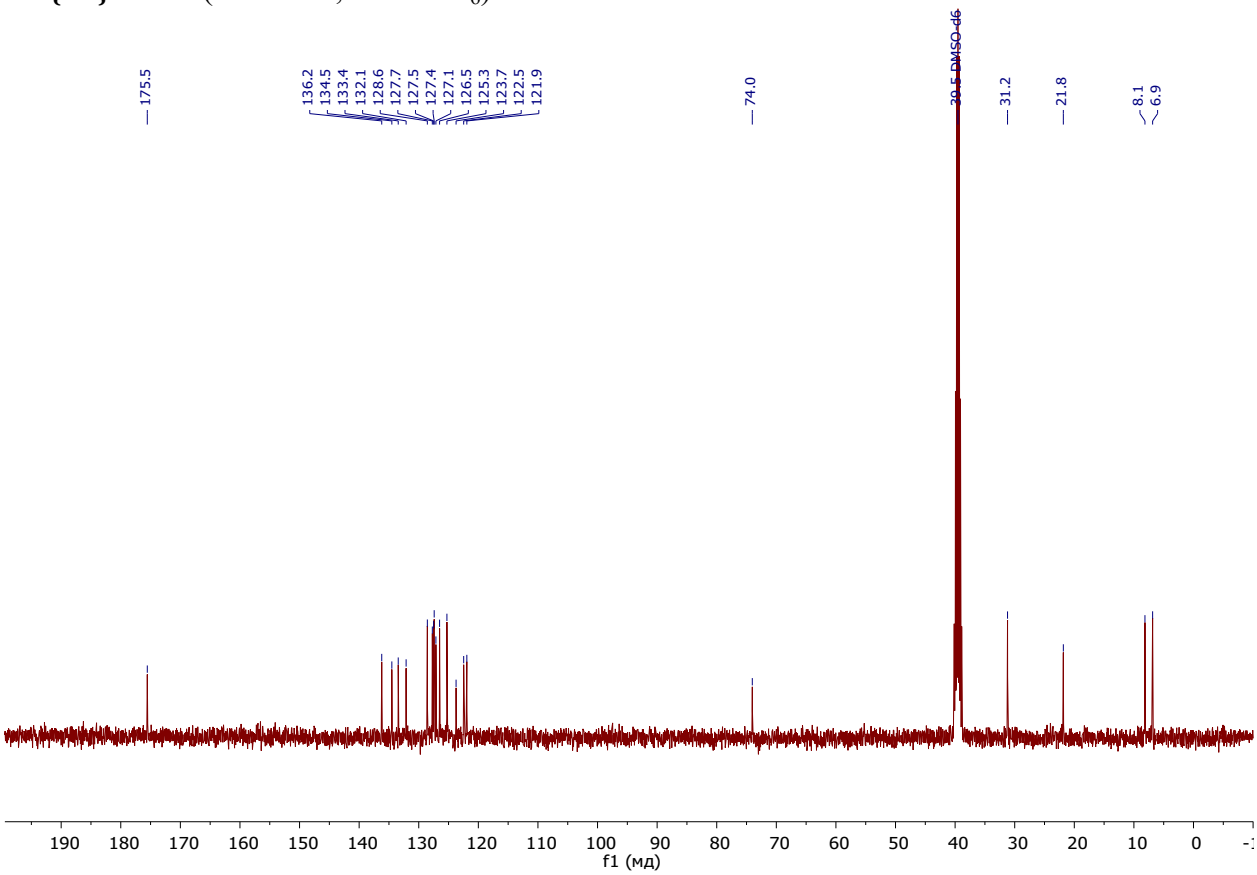
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4d**



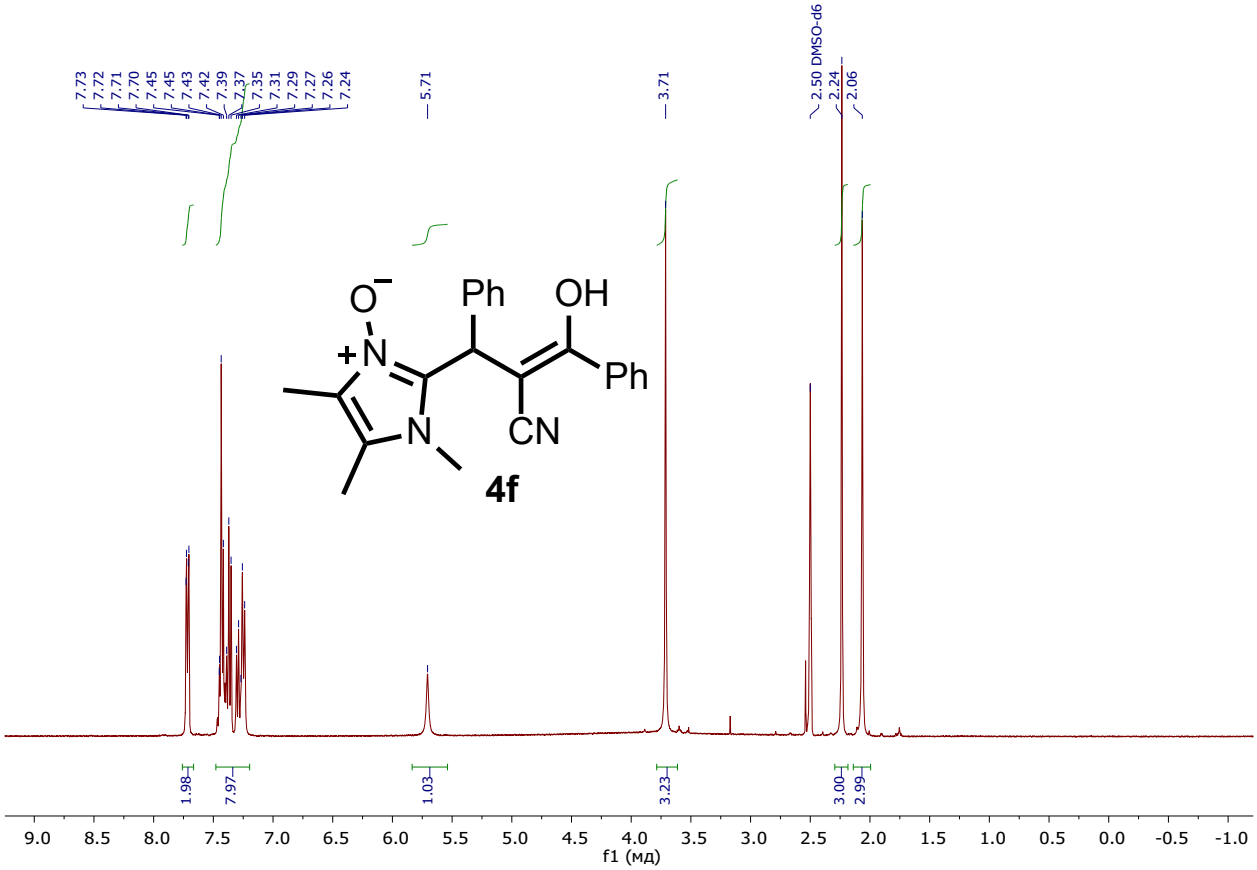
^{1}H NMR (600 MHz, DMSO-d_6) of **4e**



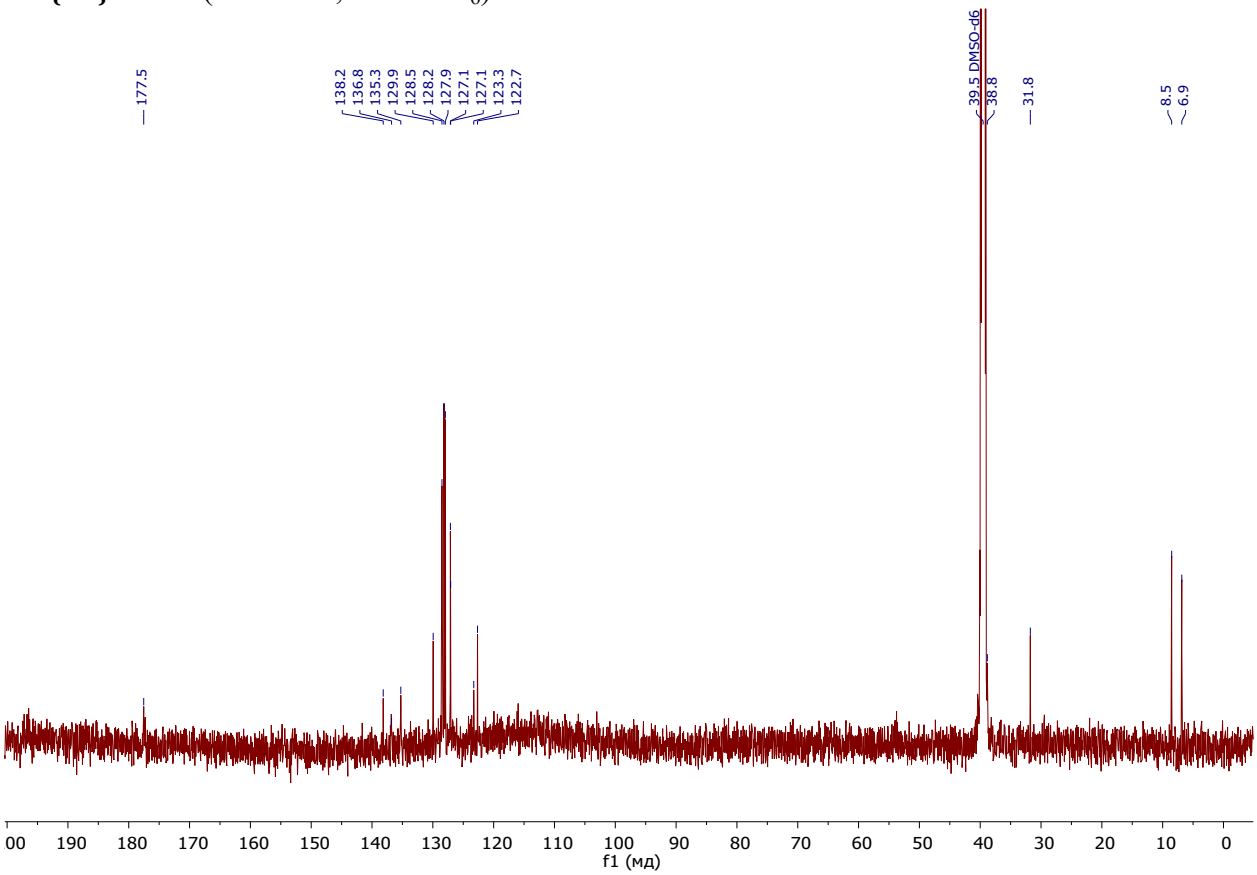
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4e**



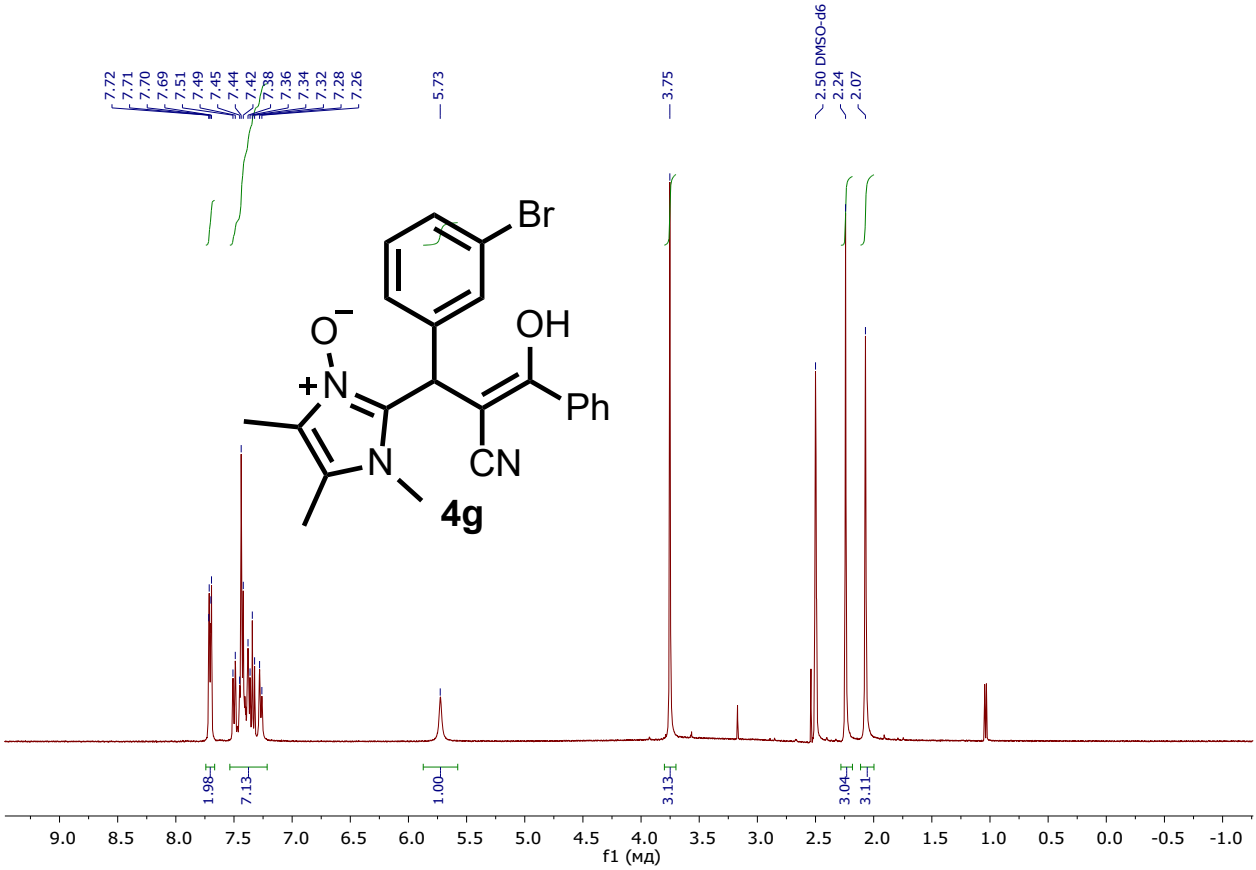
^{1}H NMR (400 MHz, DMSO-d_6) **4f**



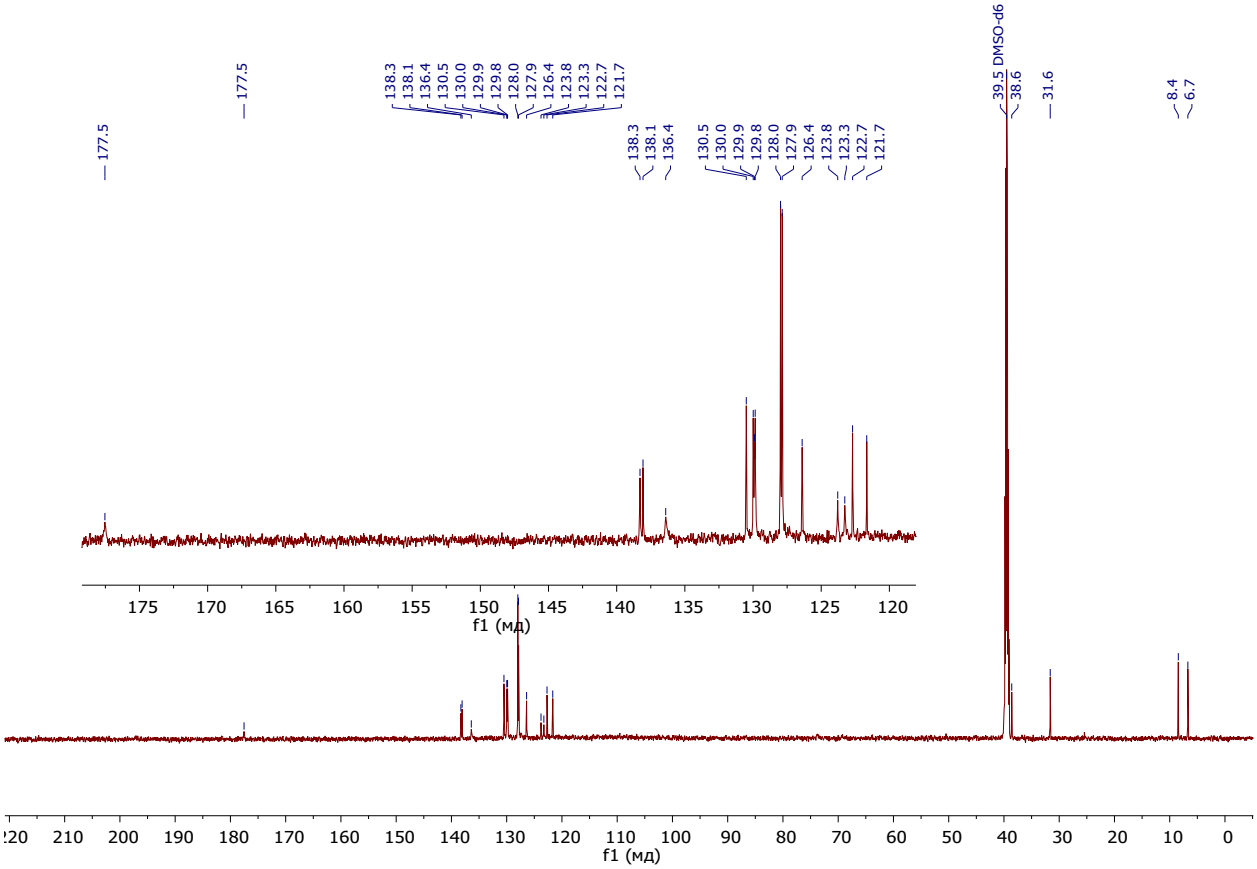
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4f**



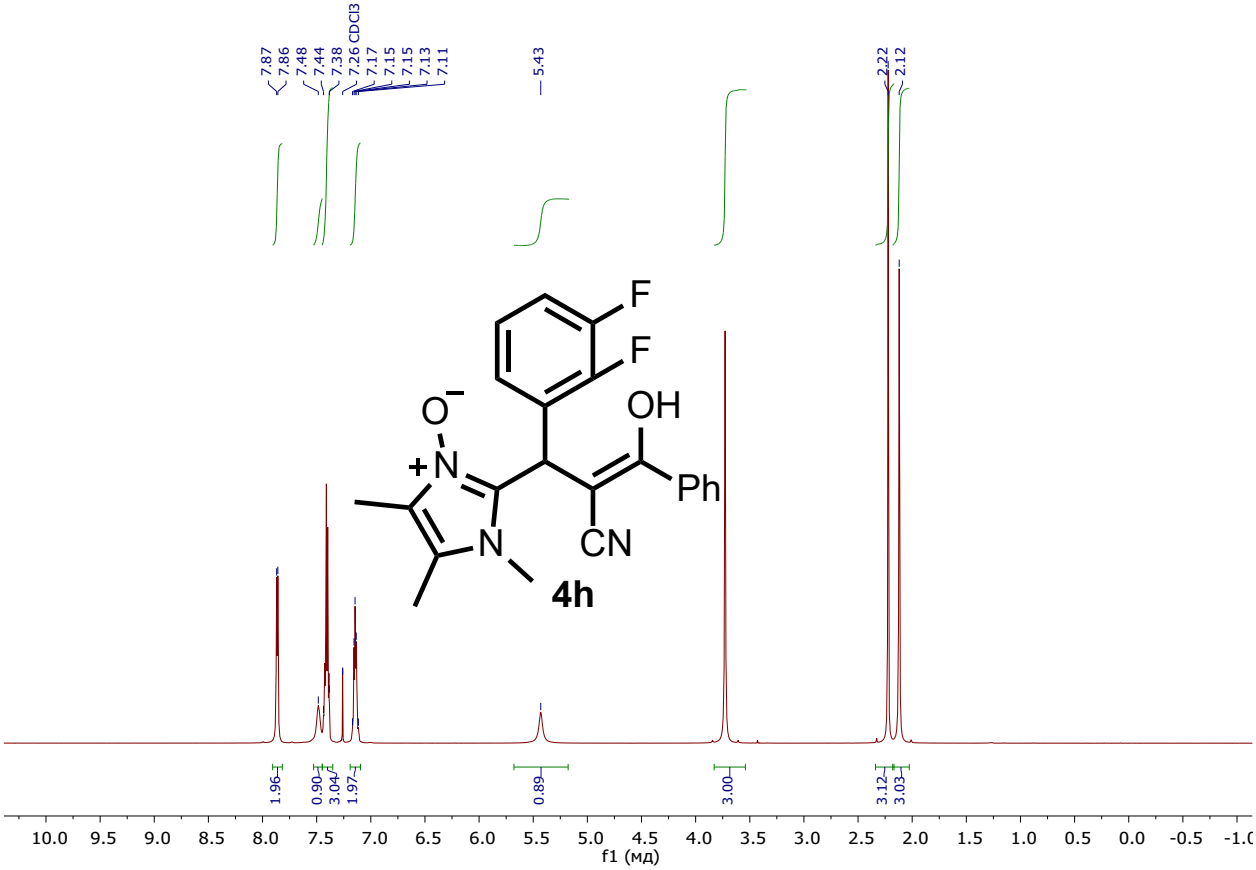
^{1}H NMR (400 MHz, DMSO-d_6) of **4g**



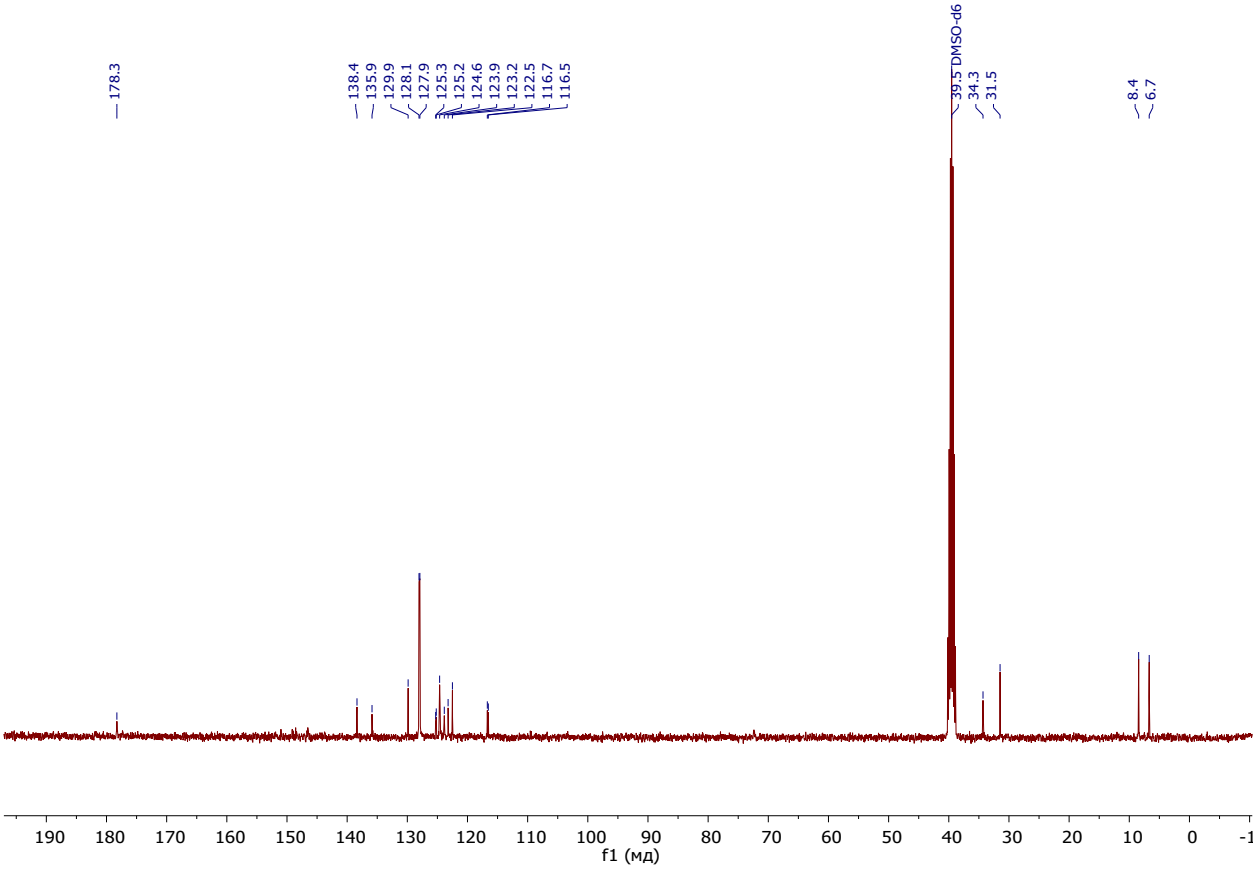
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4g**



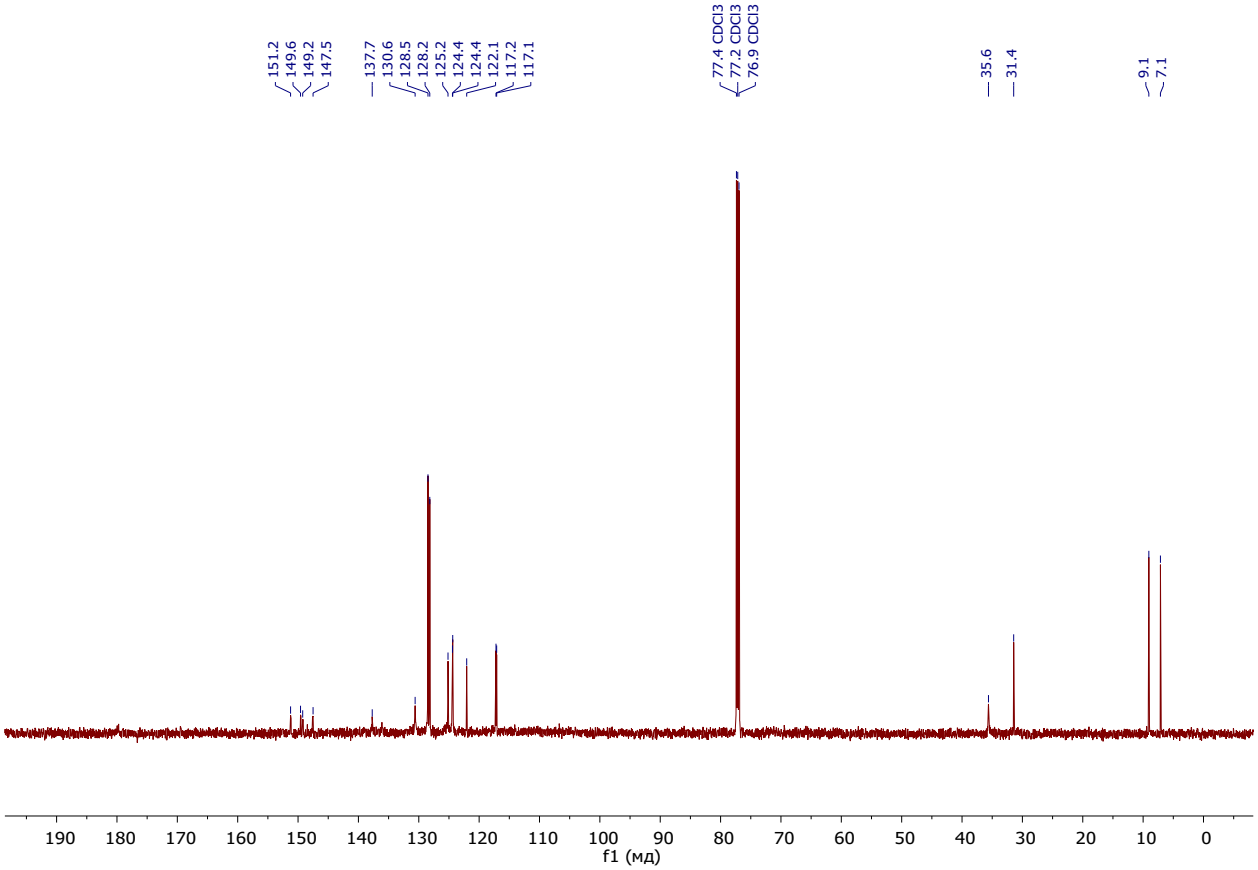
^{1}H NMR (600 MHz, $CDCl_3$) of **4h**



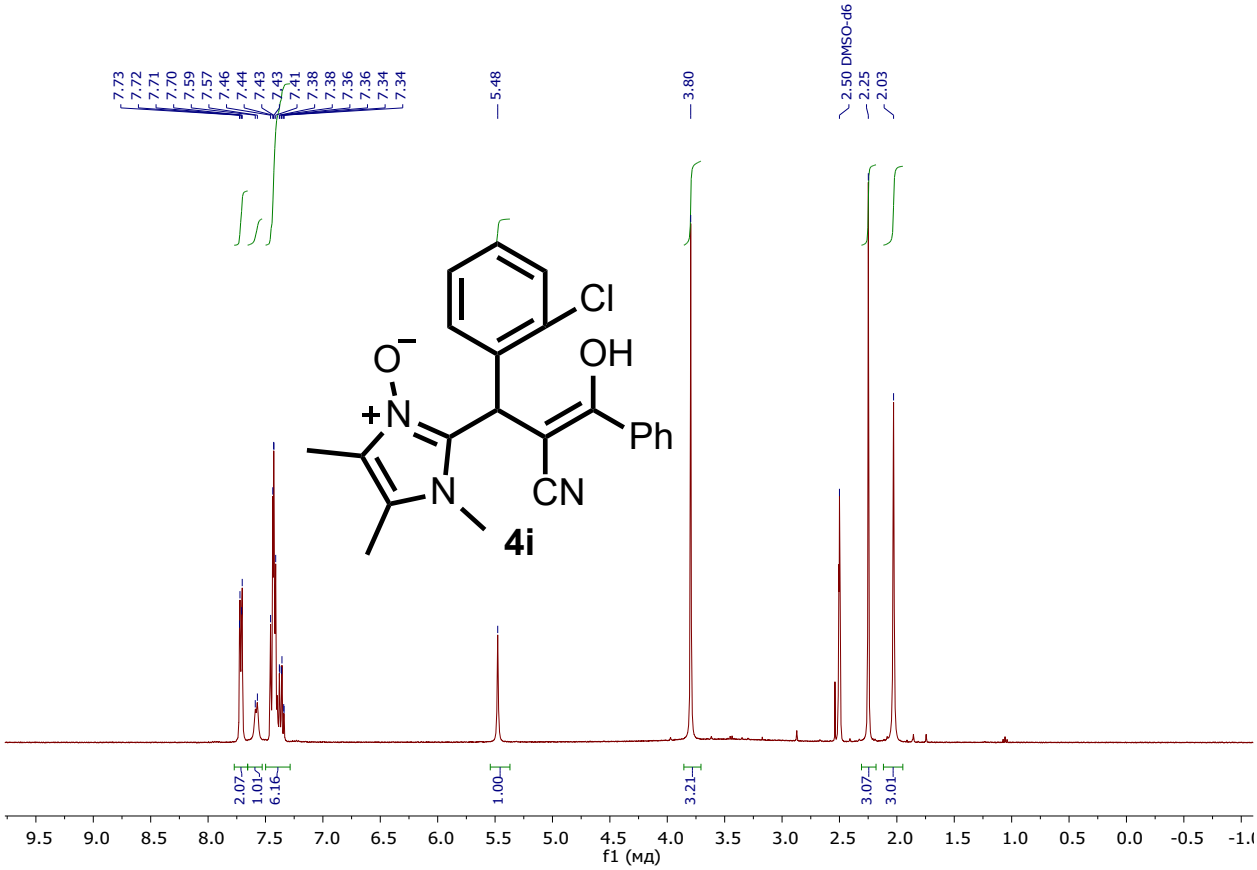
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4h**



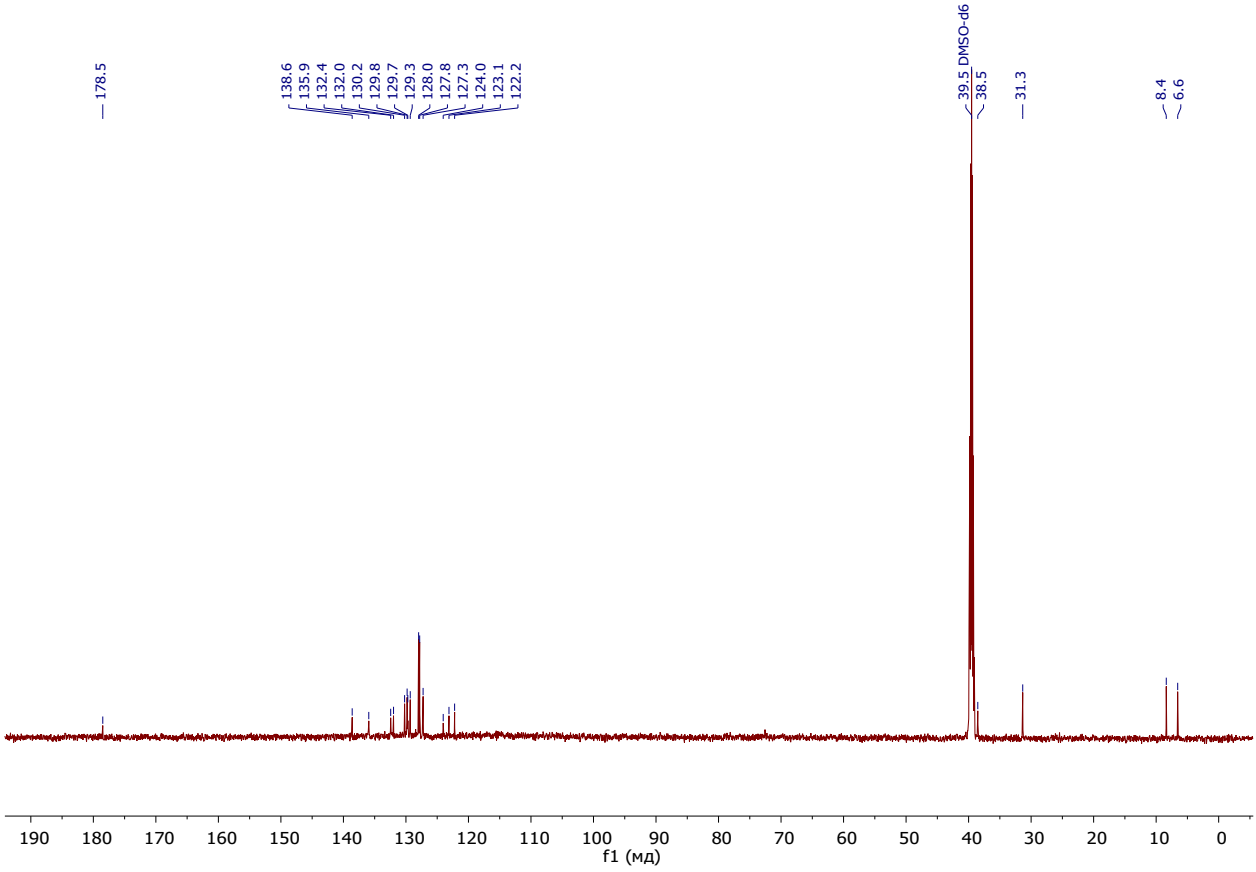
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) of **4h**



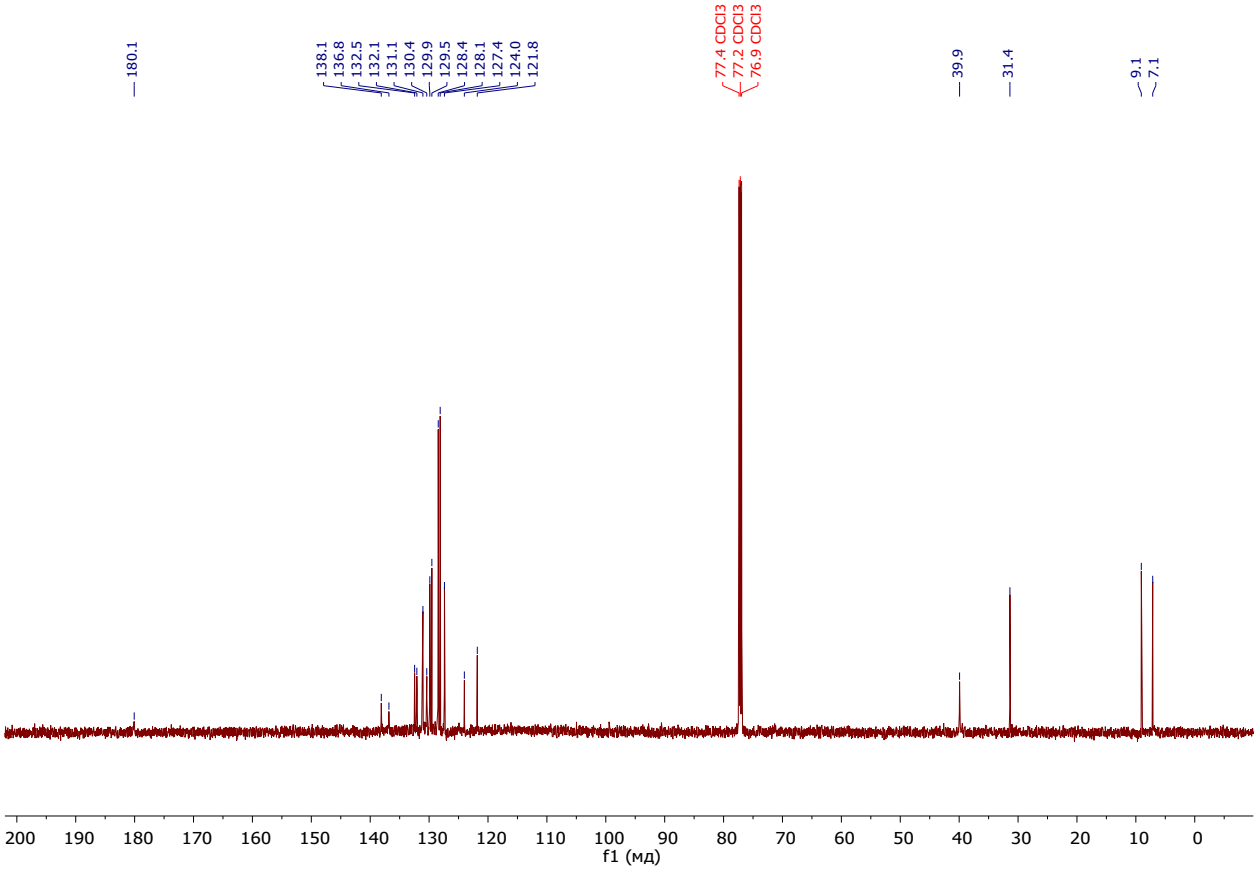
^{1}H NMR (400 MHz, DMSO-d_6) of **4i**



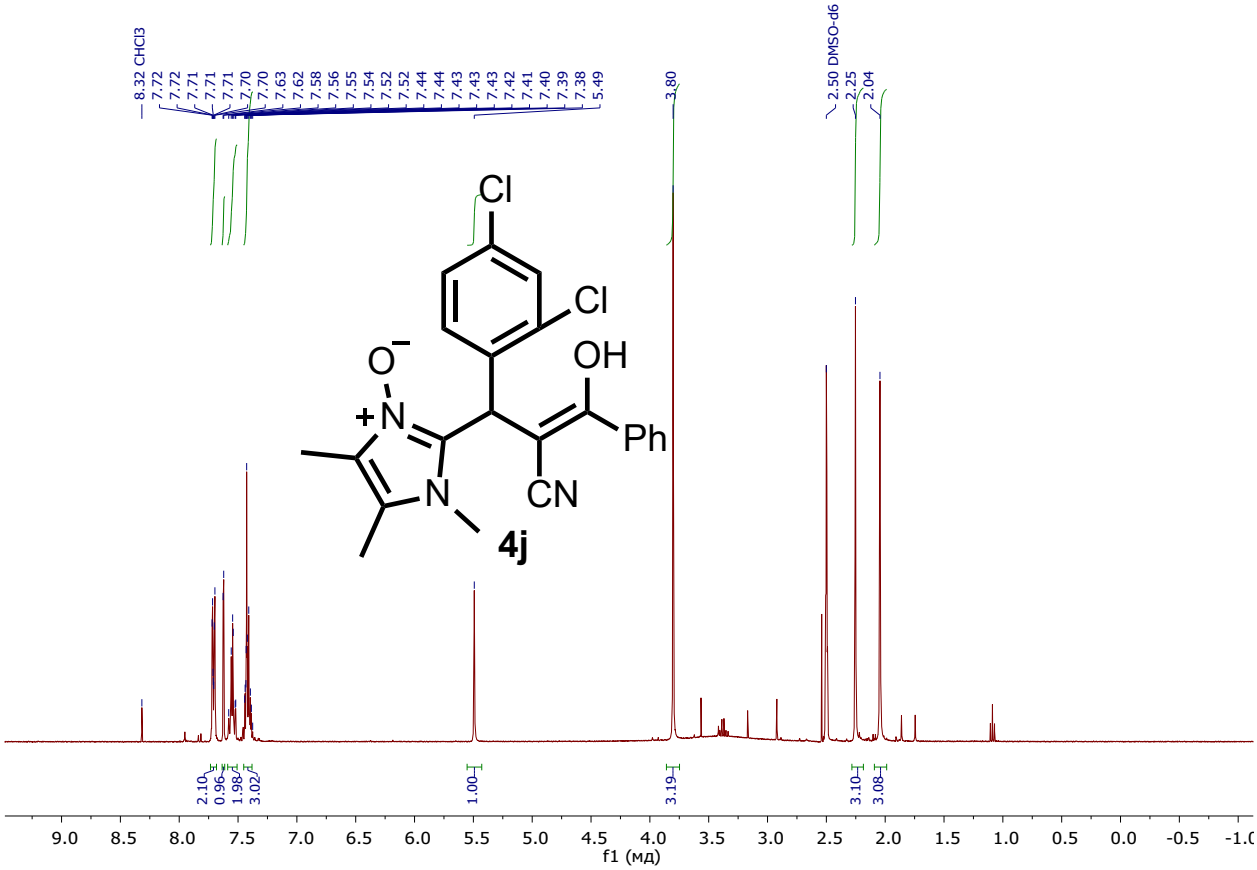
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4i**



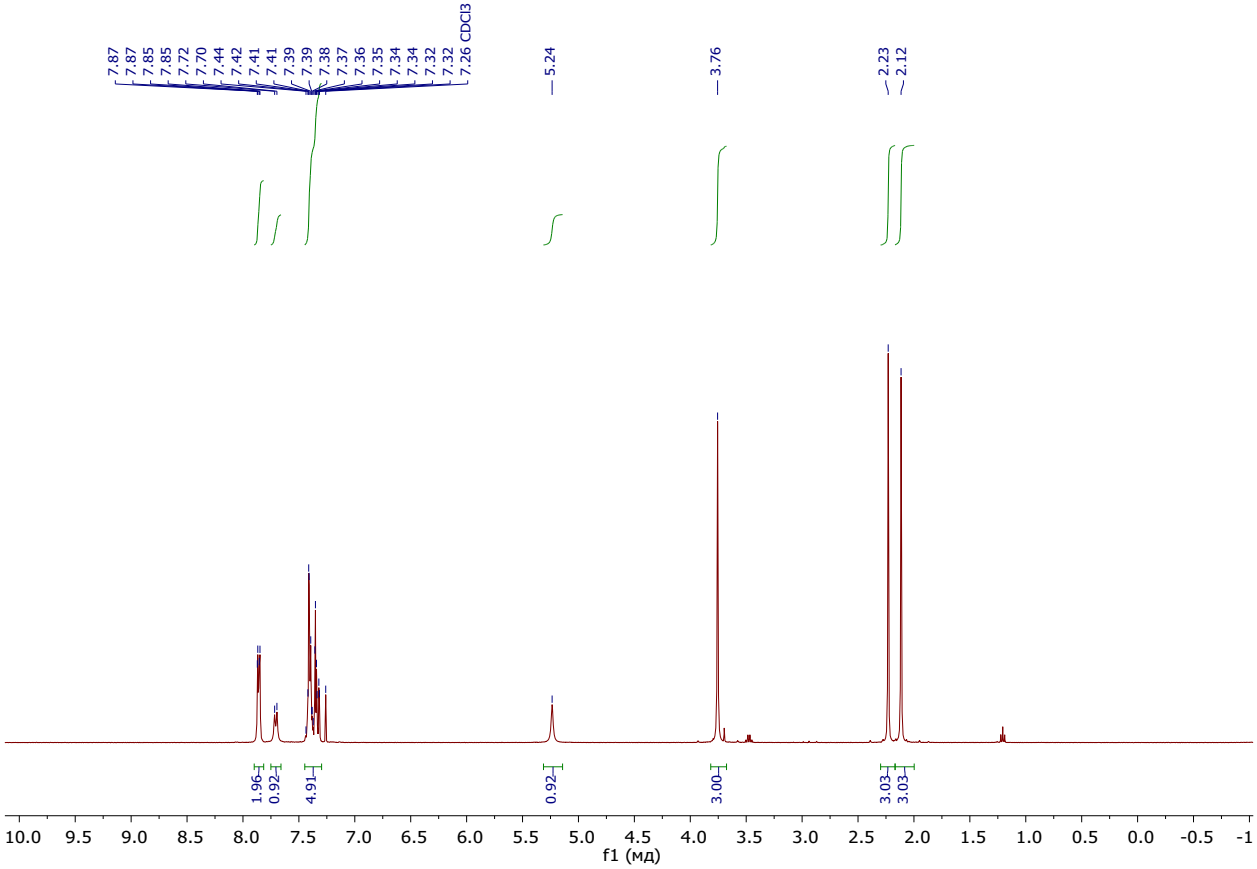
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) of **4i**



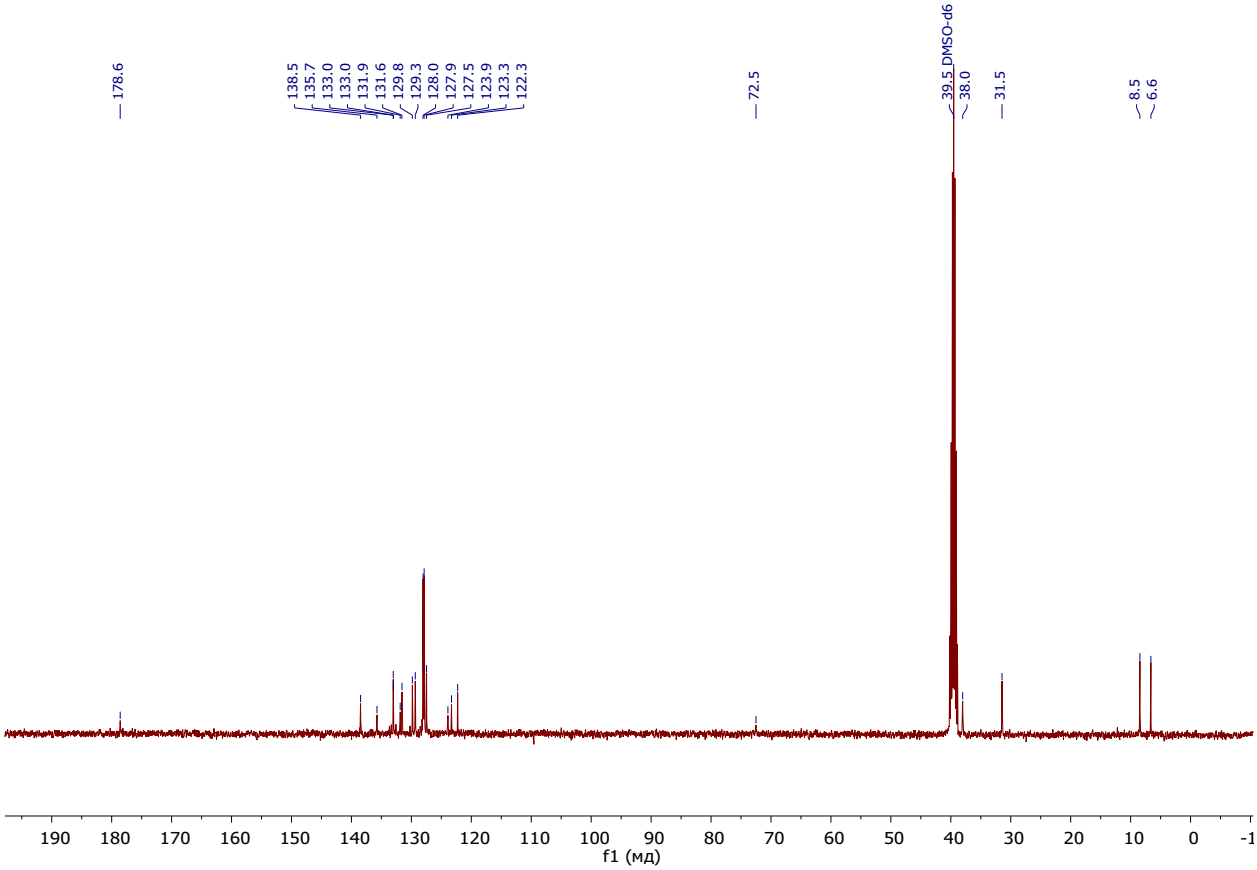
^{1}H NMR (400 MHz, DMSO-d_6) of **4j**



^{1}H NMR (400 MHz, $CDCl_3$) of **4j**



$^{13}C\{^1H\}$ NMR (101 MHz, DMSO-d_6) of **4j**



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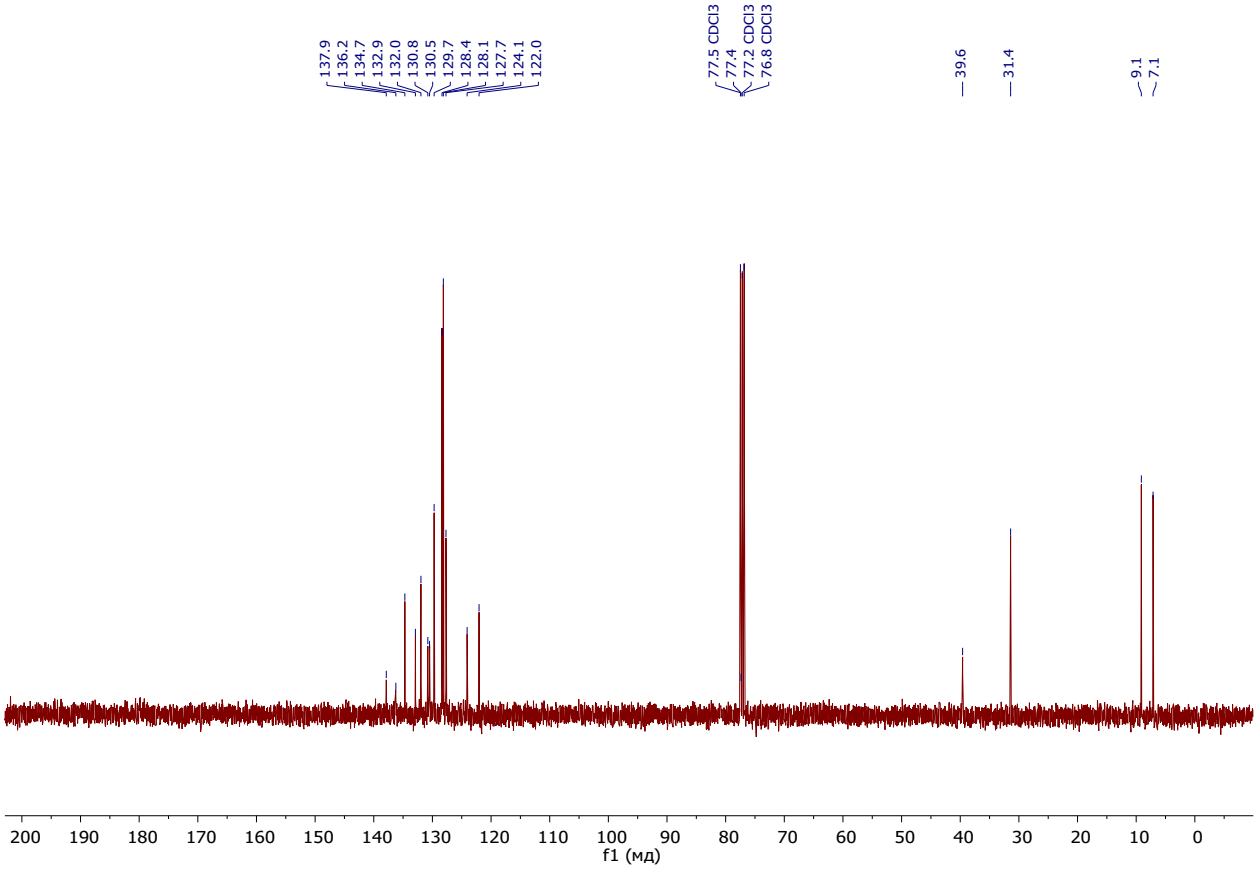

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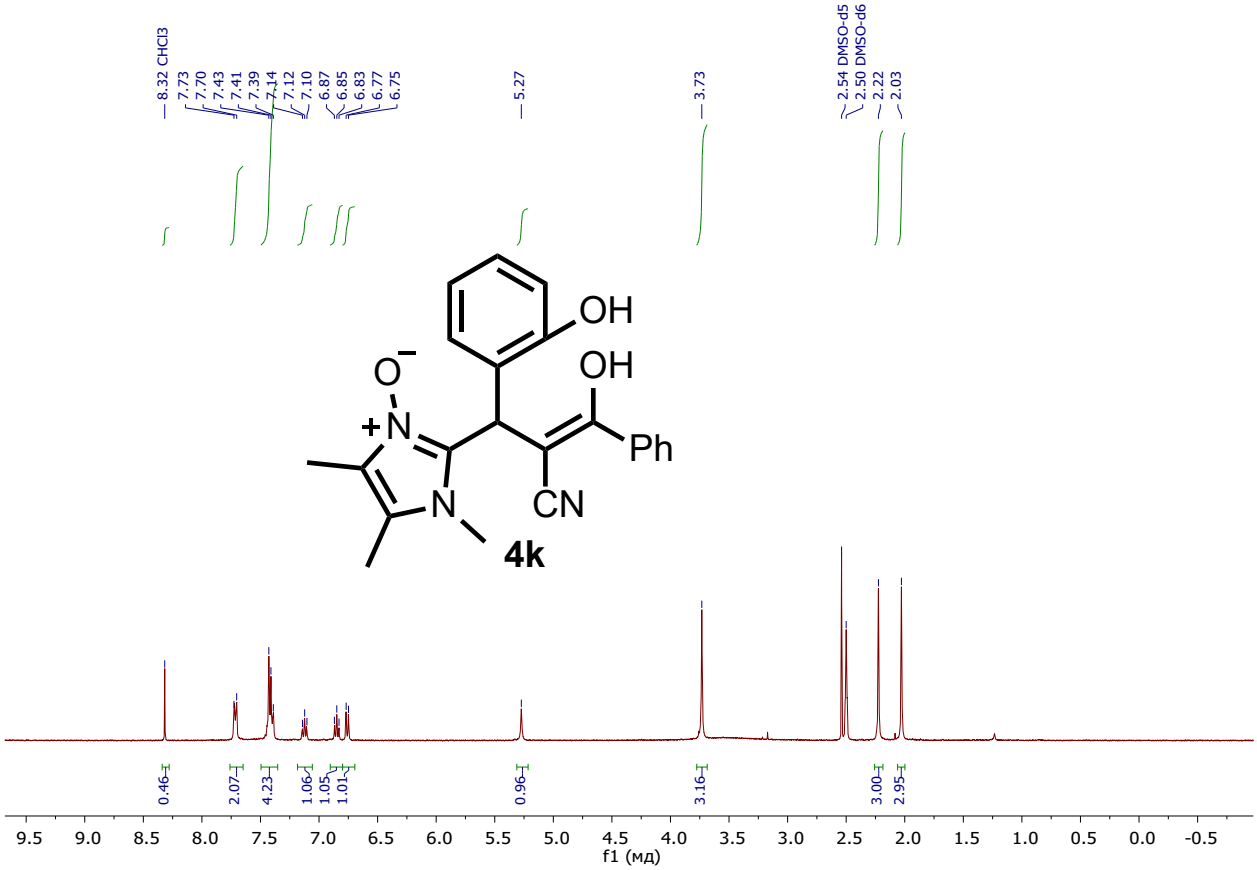
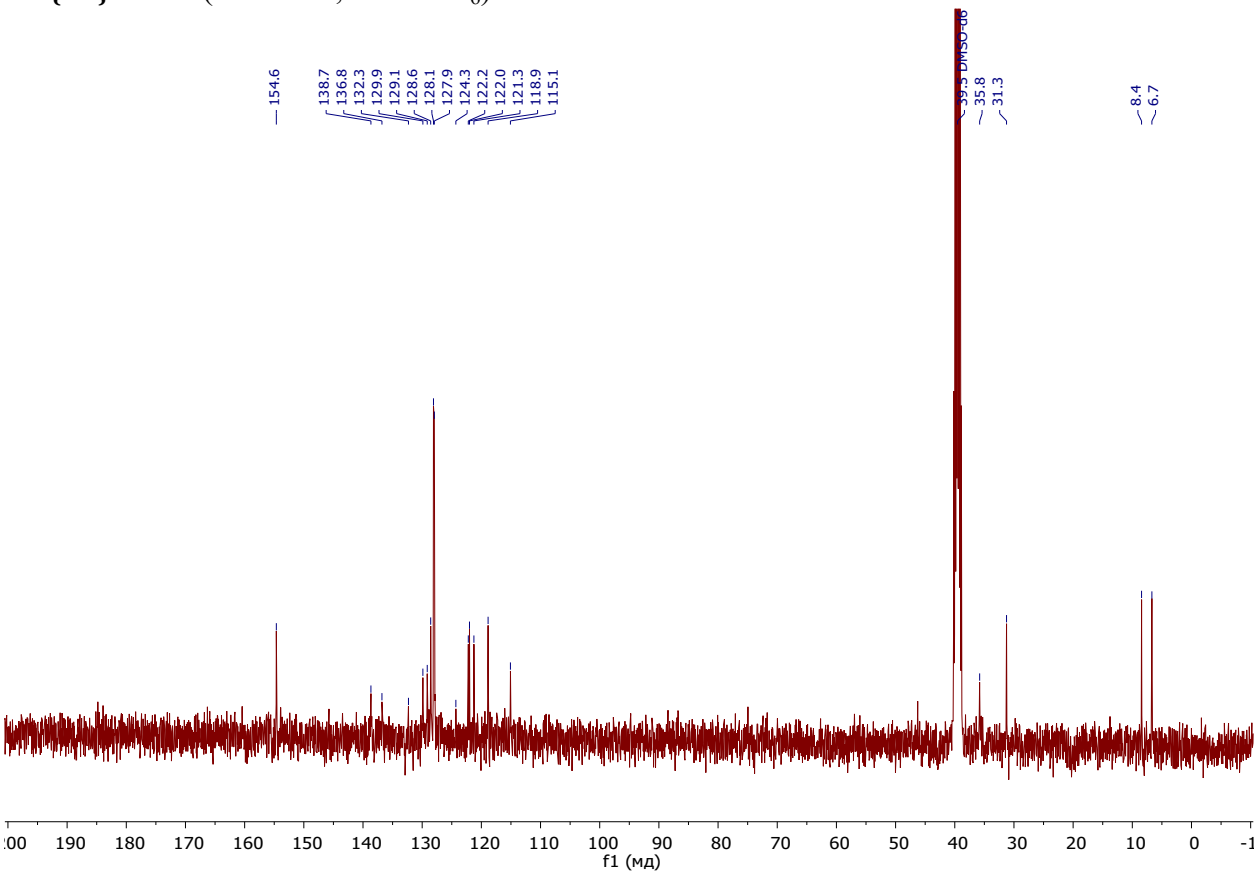
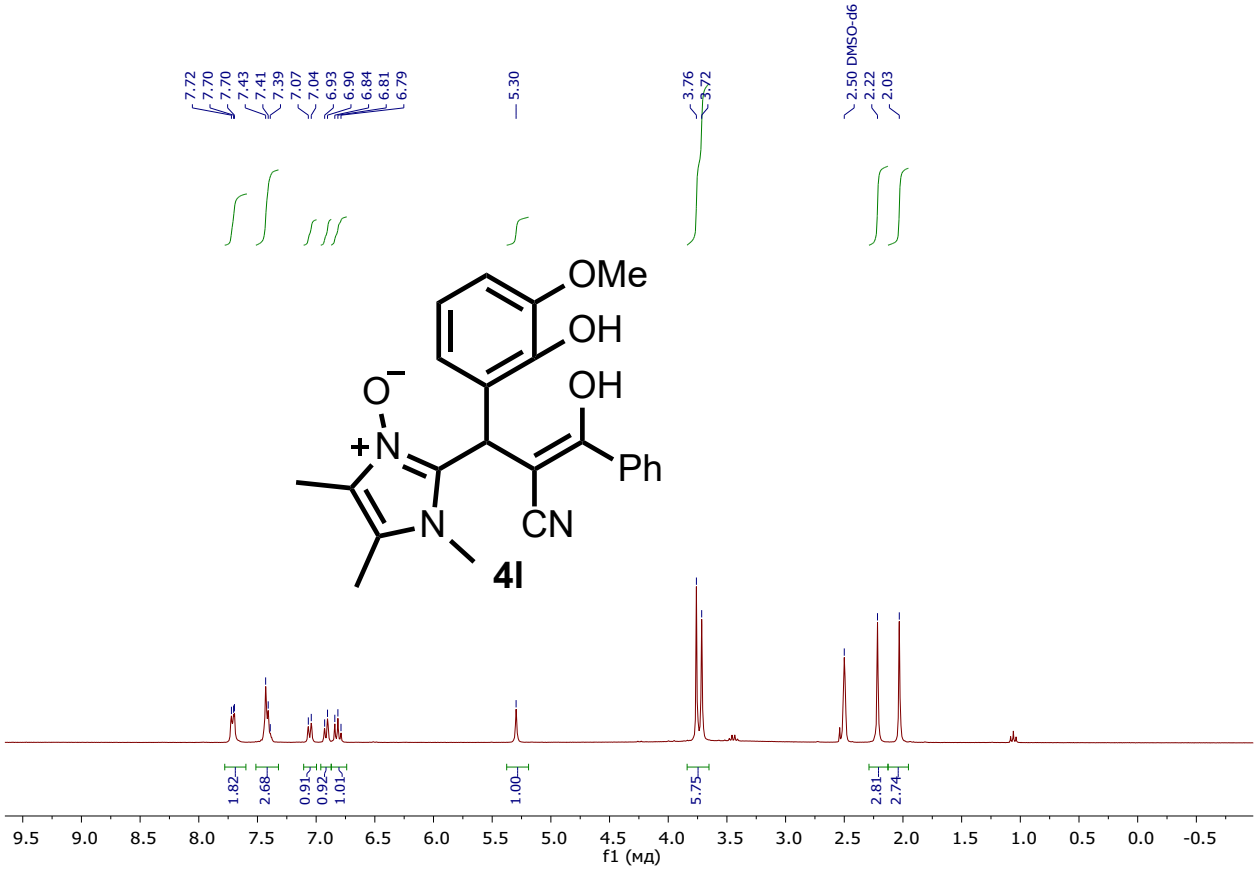


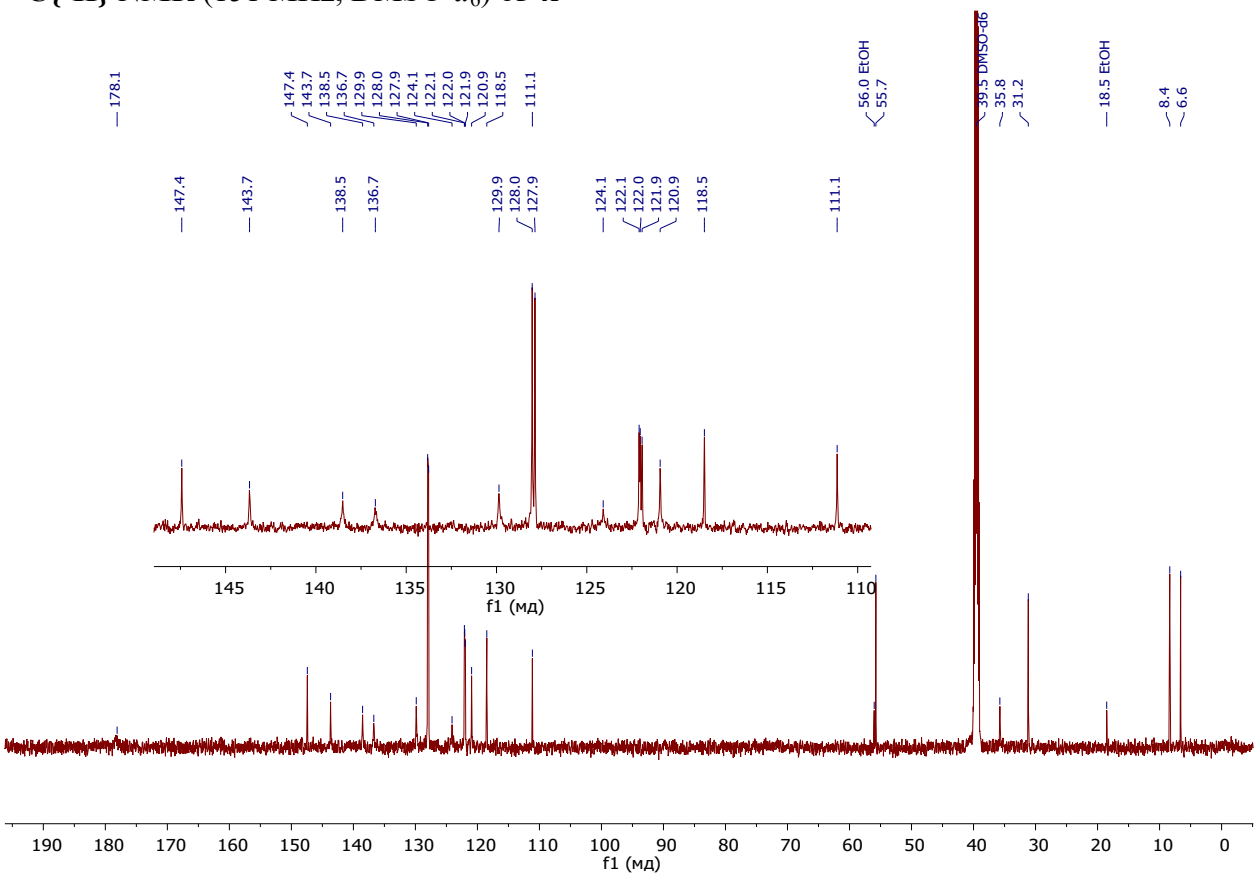
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4k**



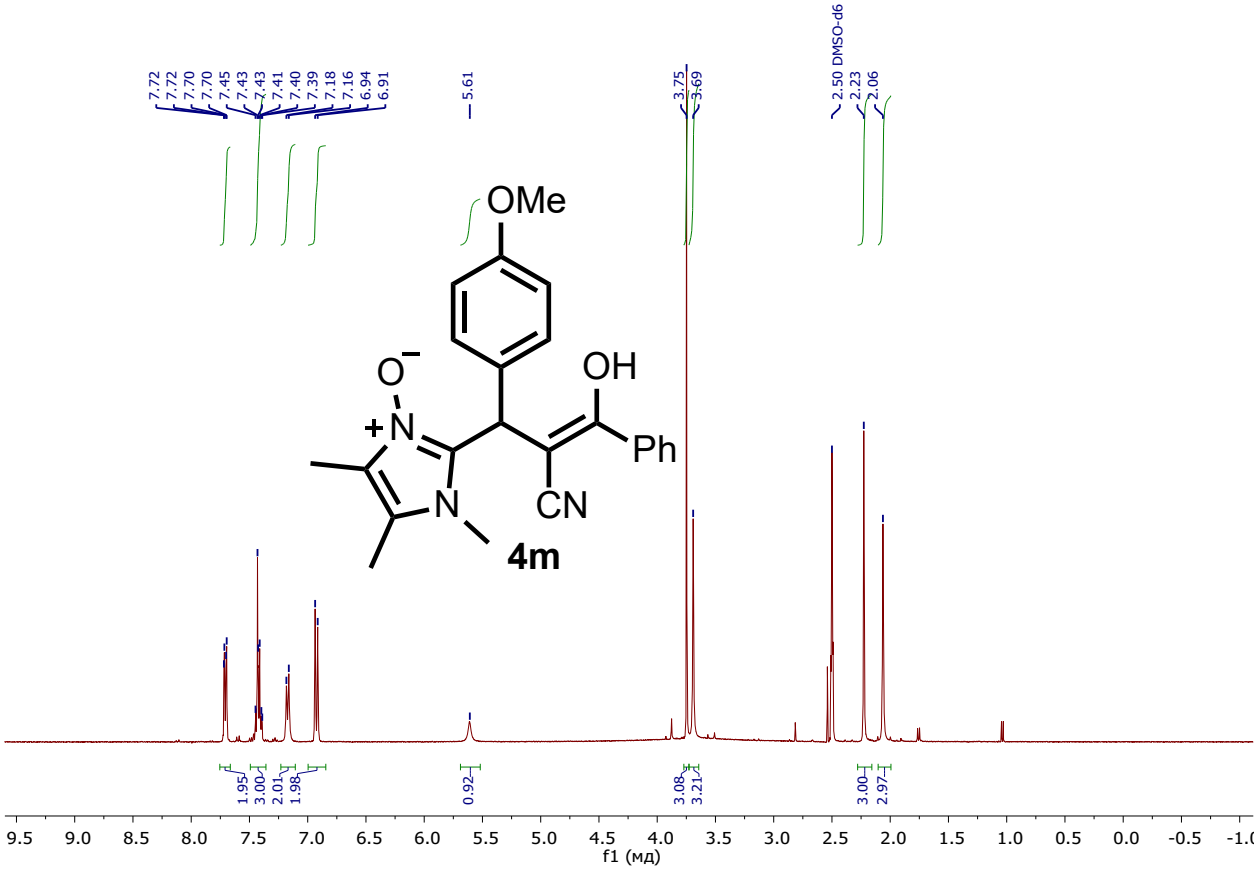
^{1}H NMR (300 MHz, DMSO-d_6) of **4l**



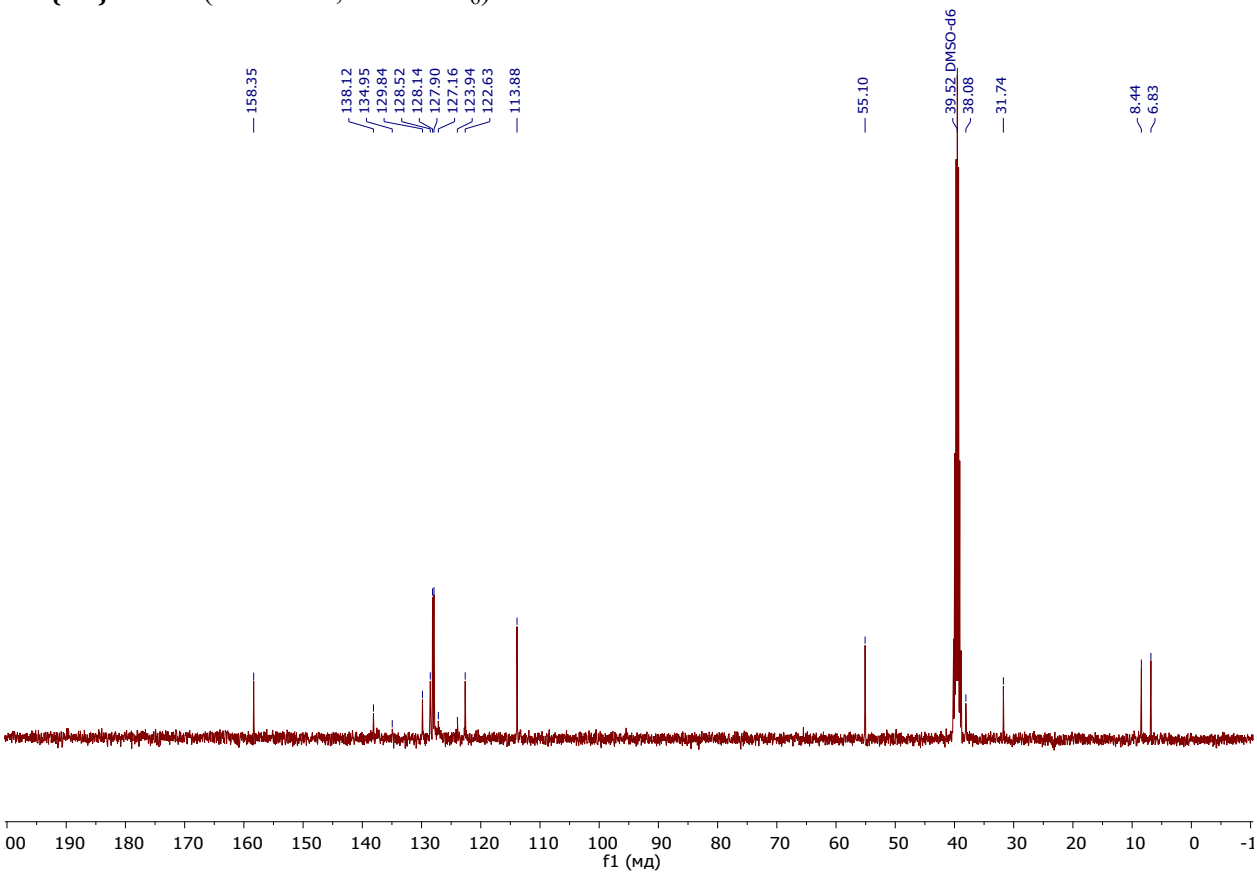
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4l**



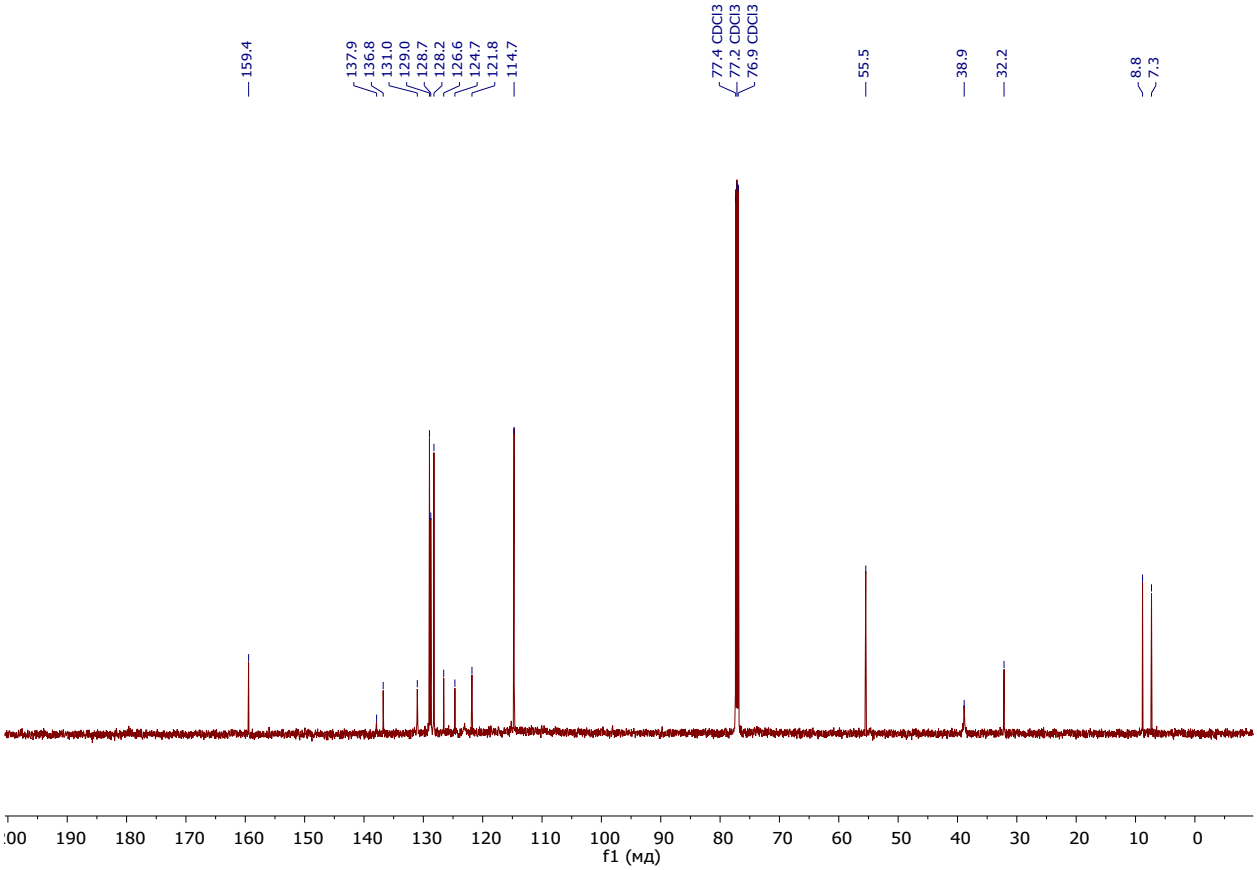
^{1}H NMR (400 MHz, DMSO-d_6) of **4m**



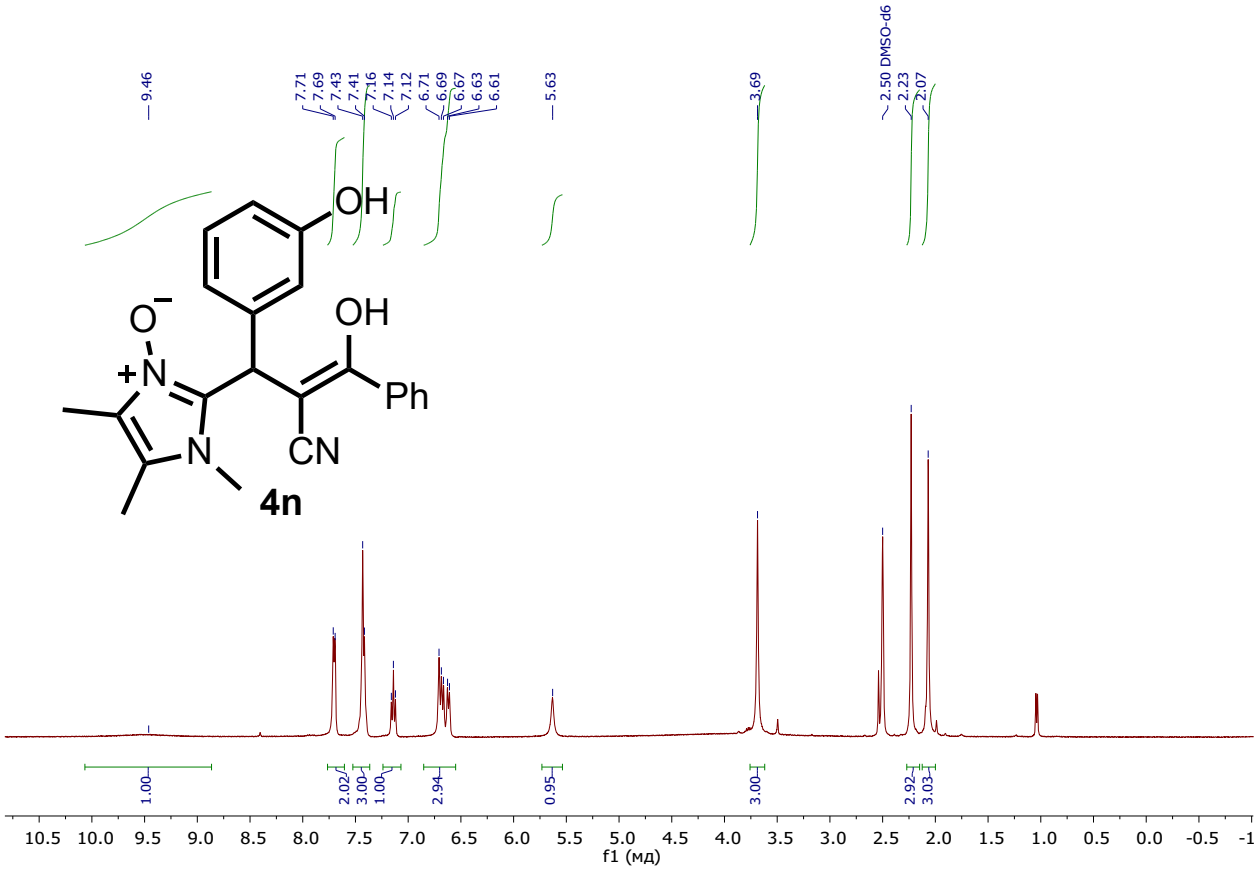
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4m**



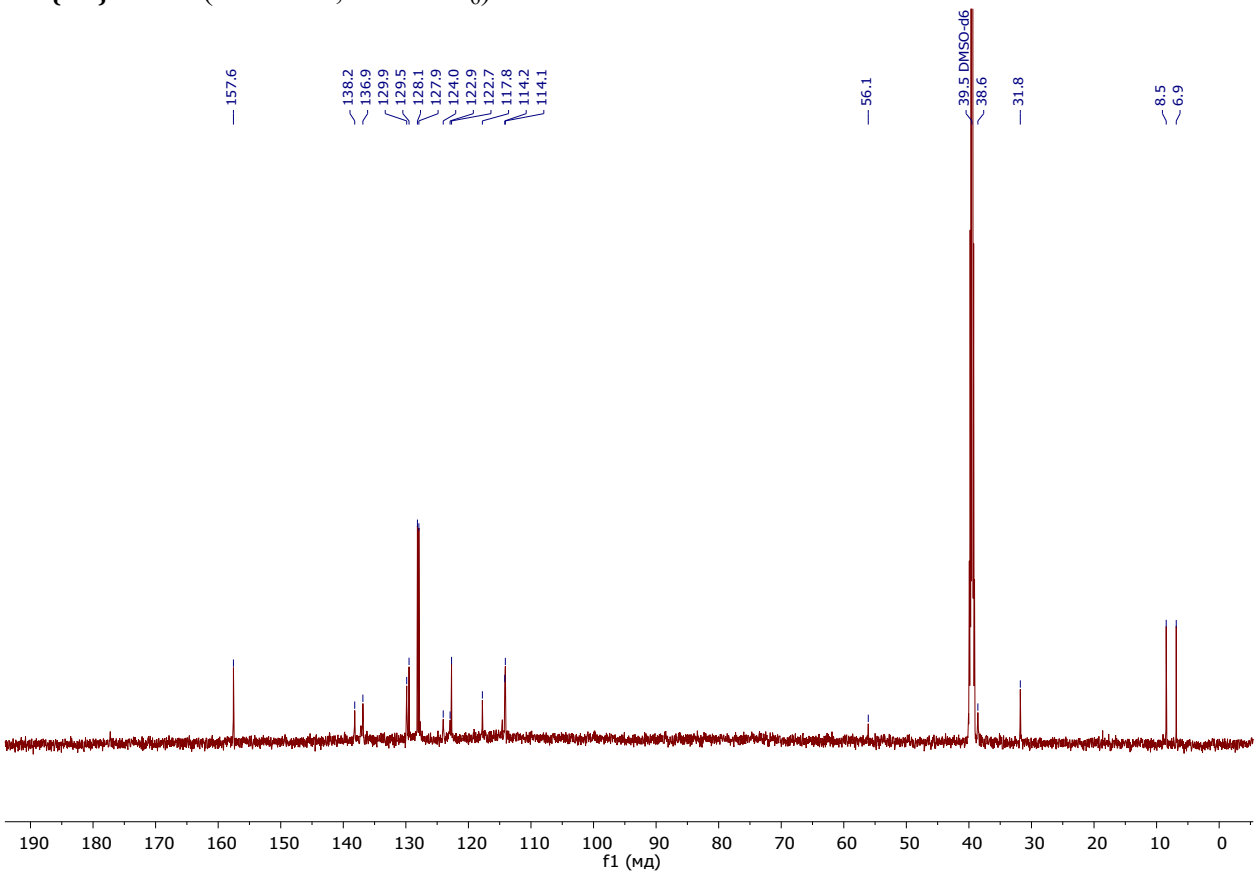
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$, 333K) of **4m**



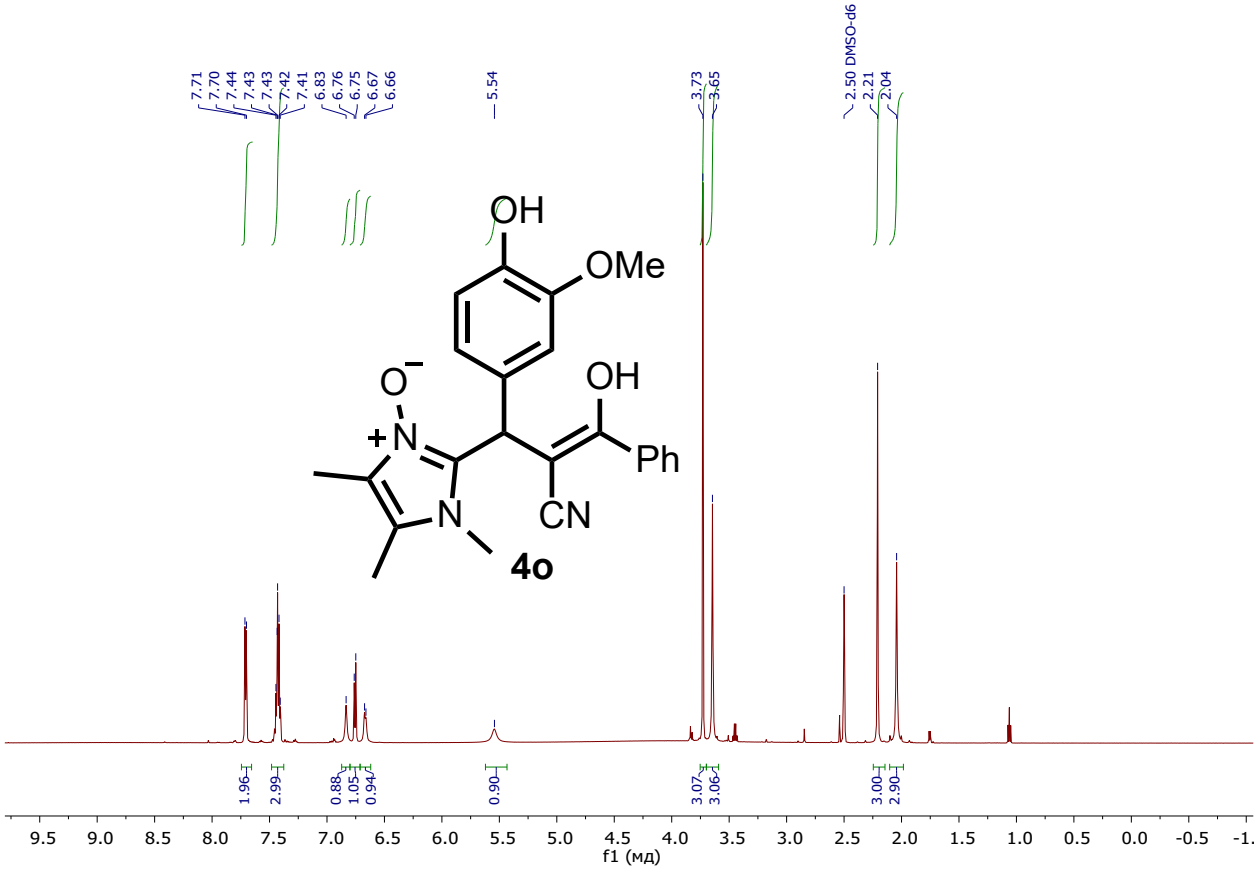
^{1}H NMR (400 MHz, DMSO-d_6) of **4n**



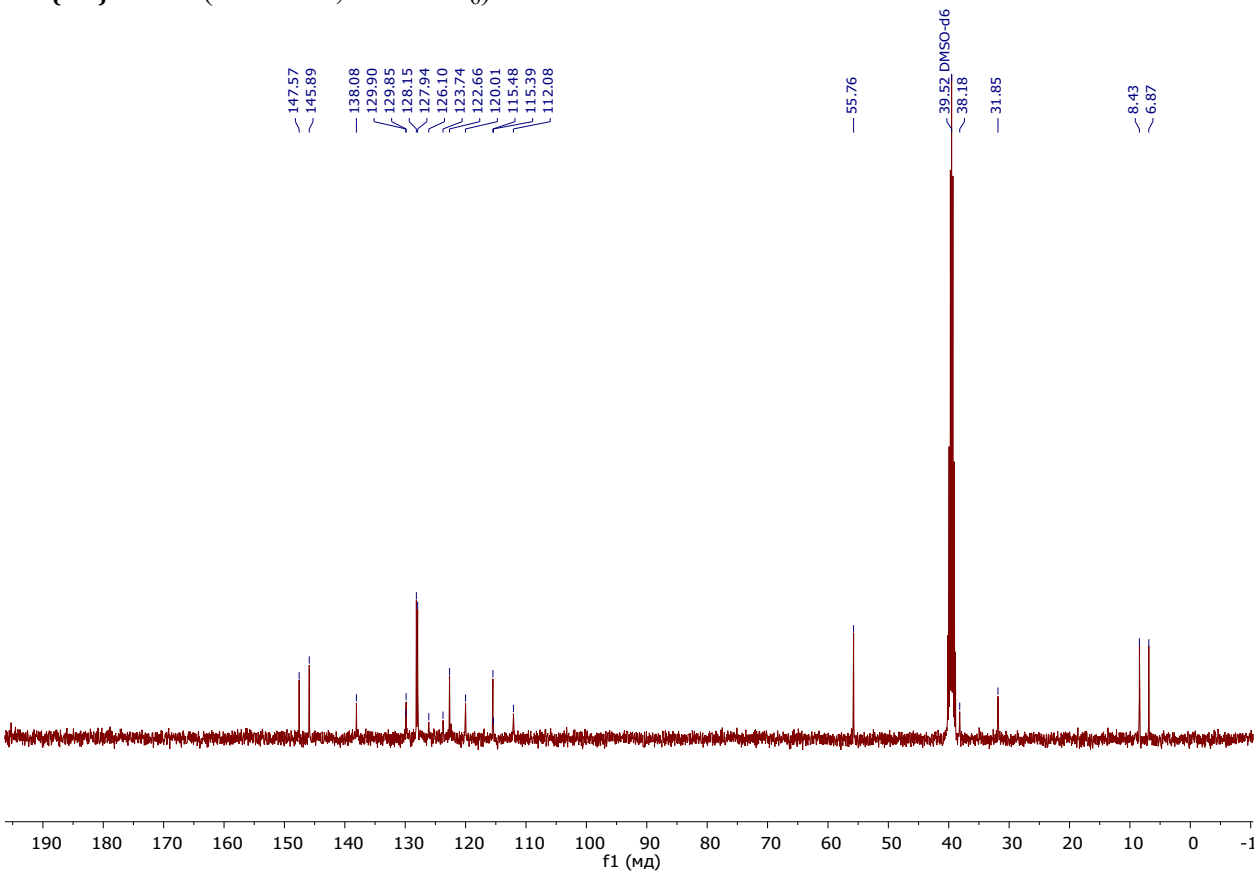
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4n**



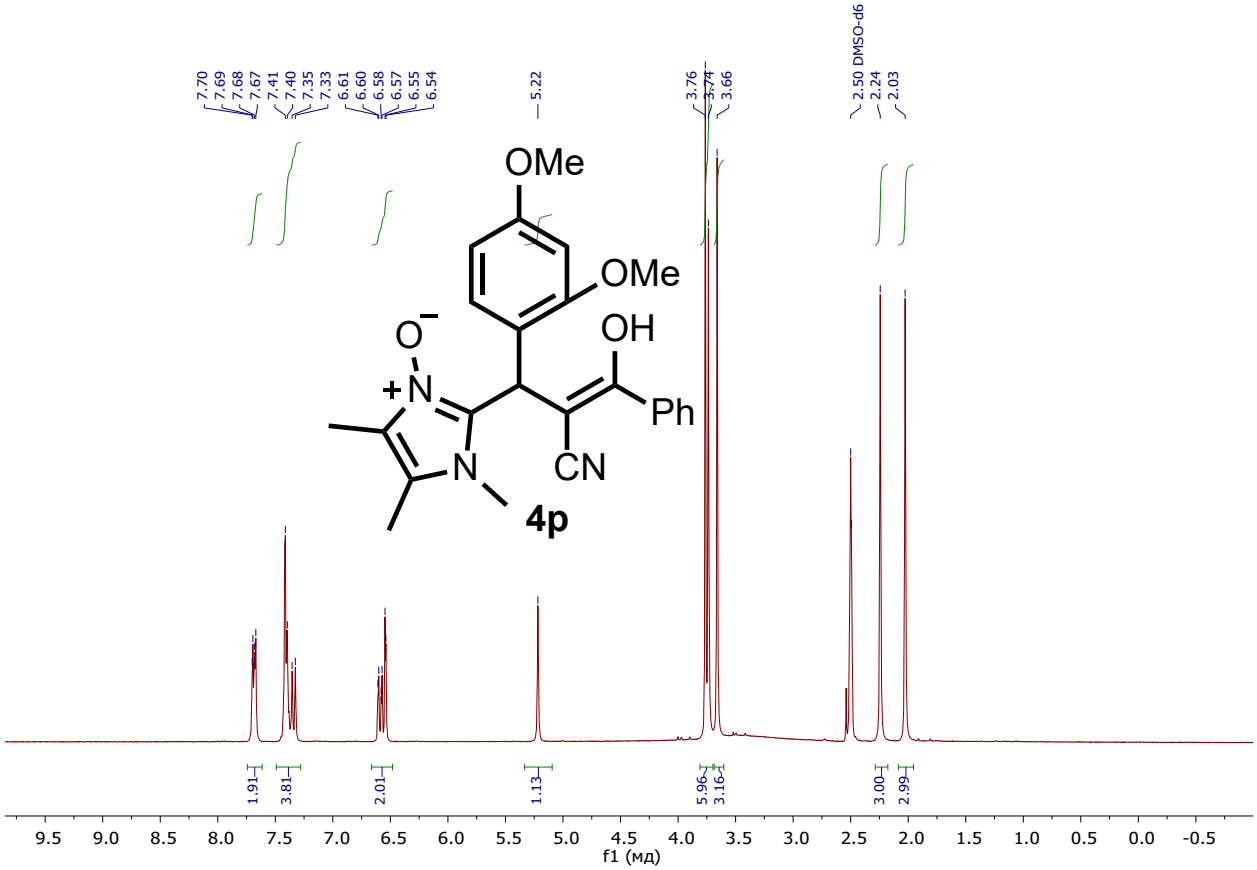
^{1}H NMR (600 MHz, DMSO-d_6) of **4o**



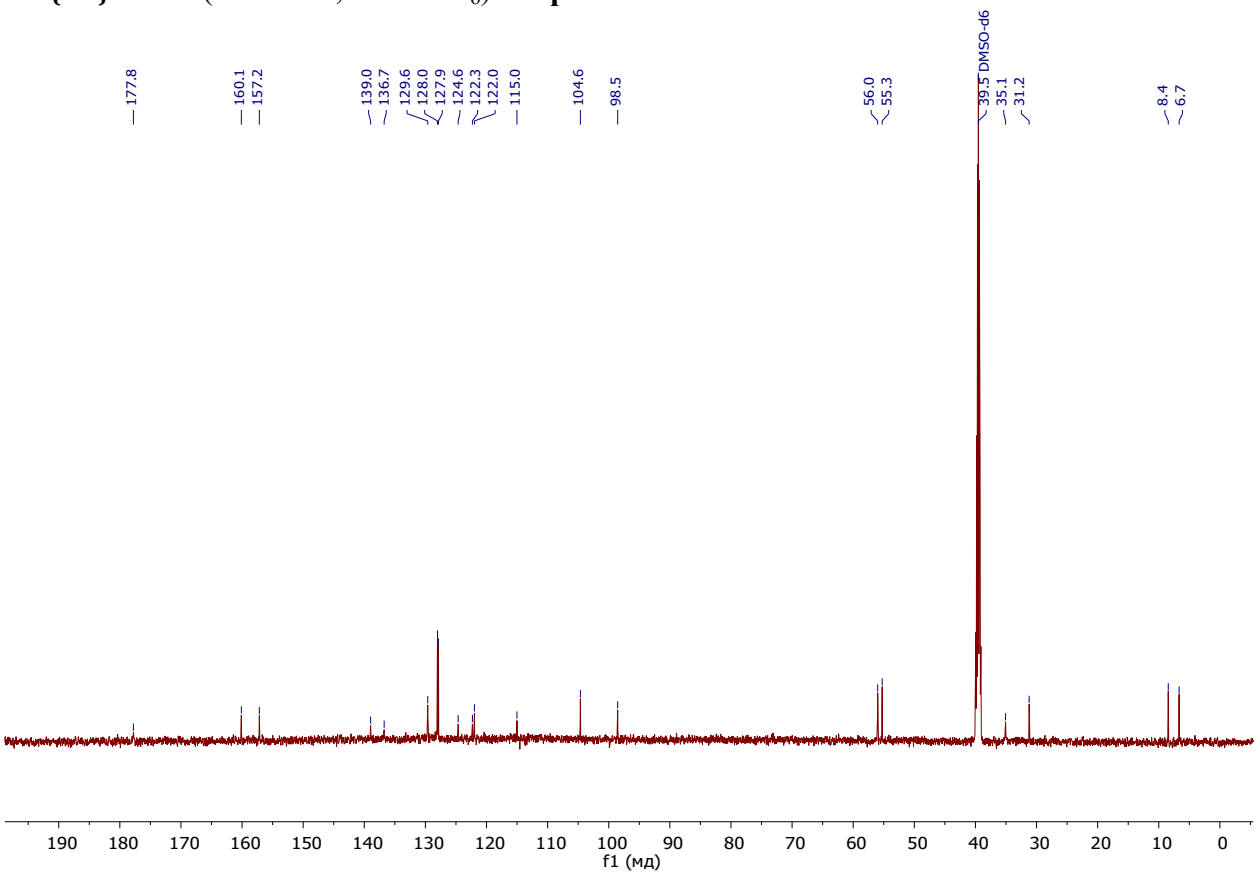
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4o**



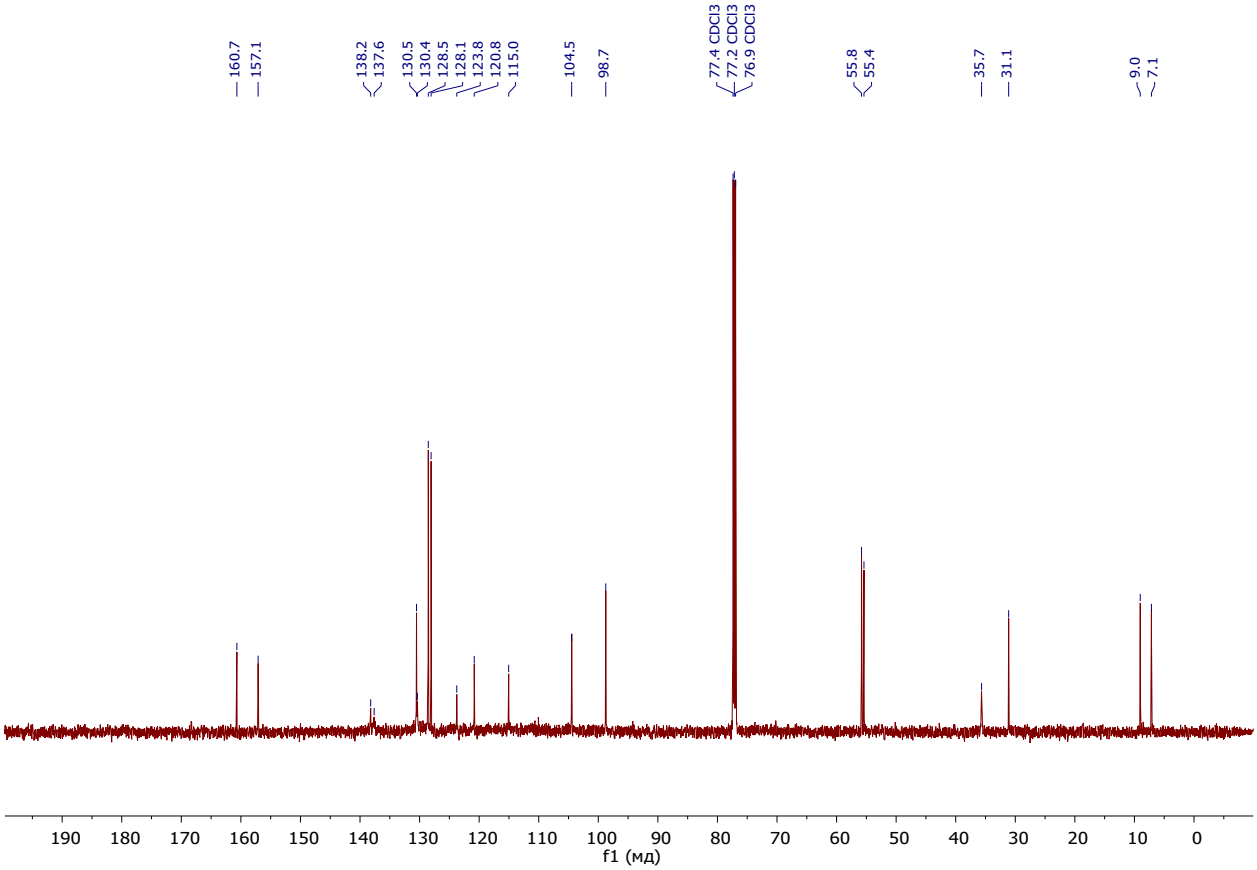
^{1}H NMR (300 MHz, DMSO-d_6) of **4p**



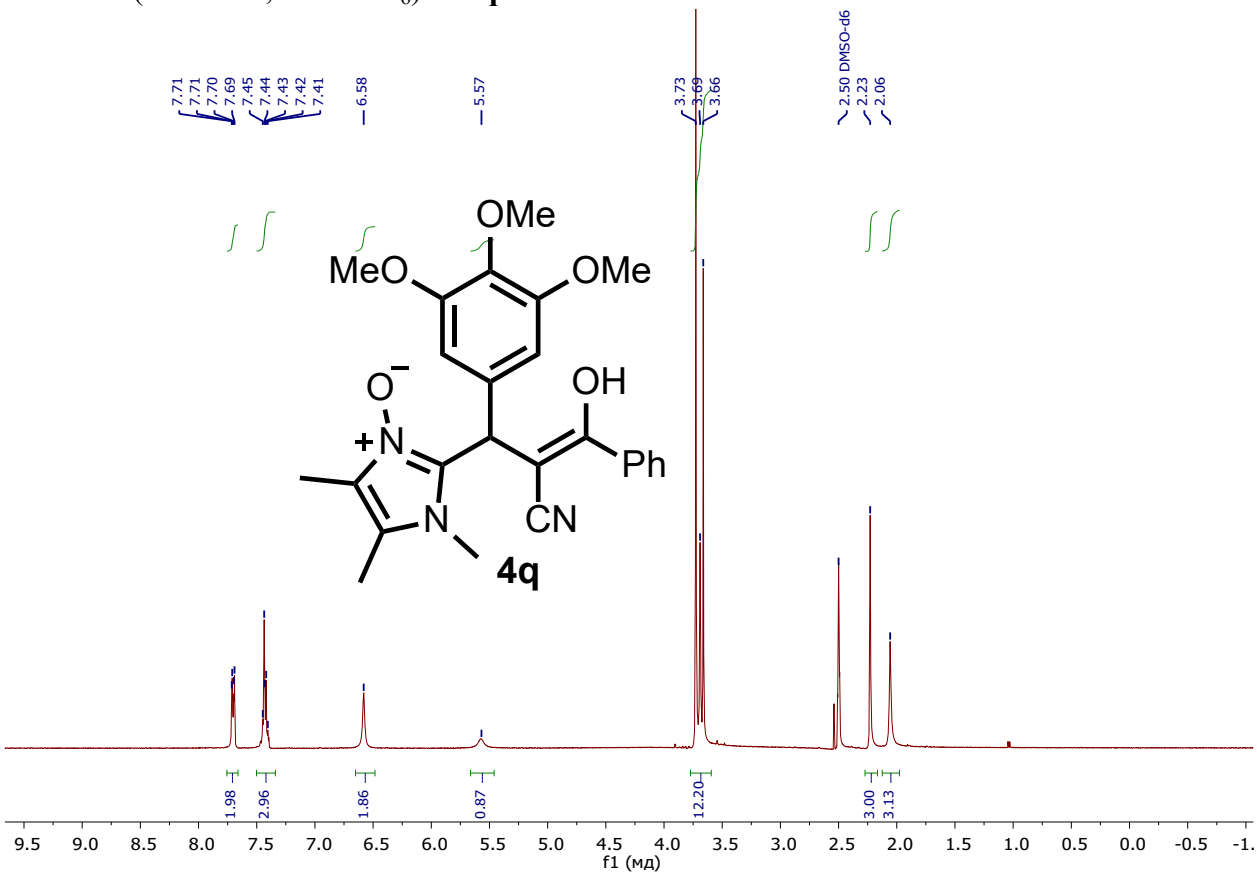
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4p**



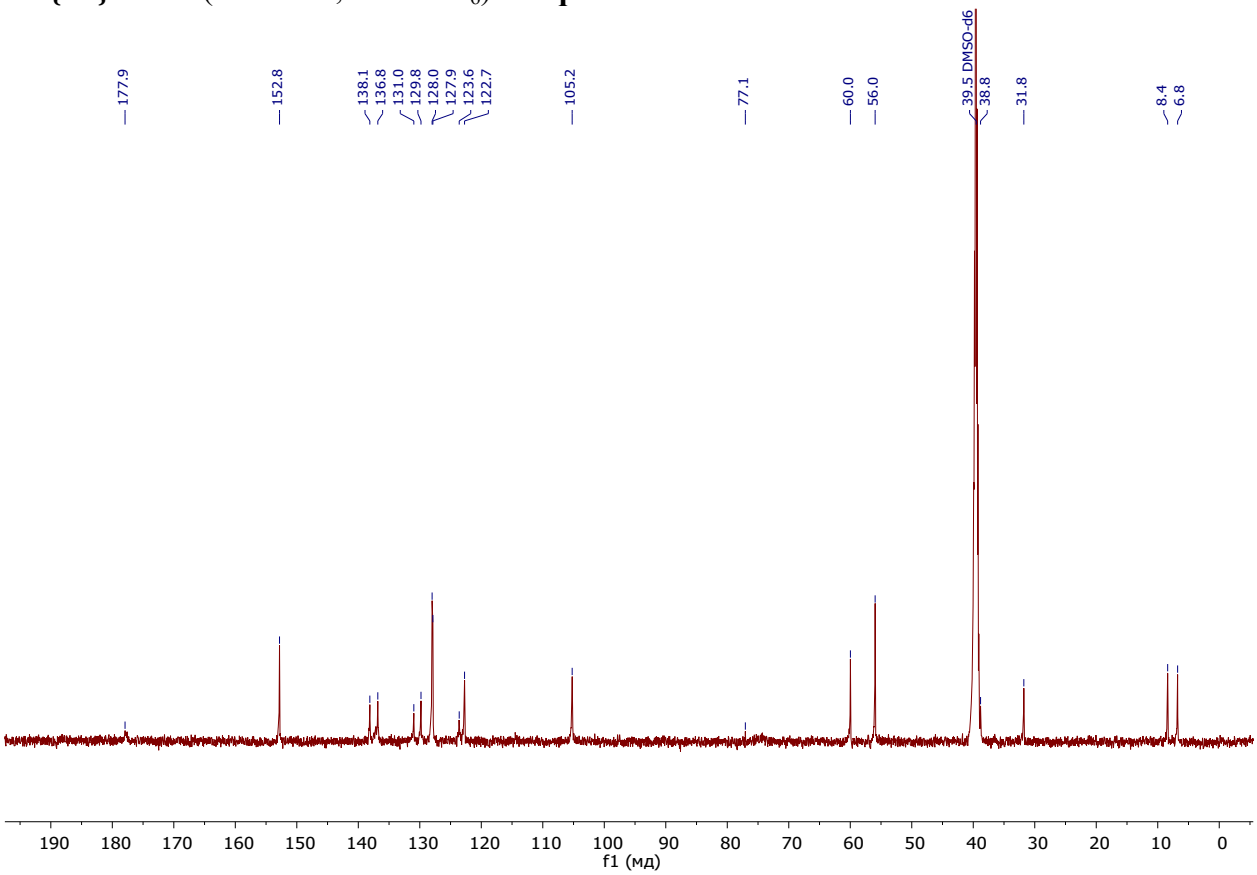
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) of **4p**



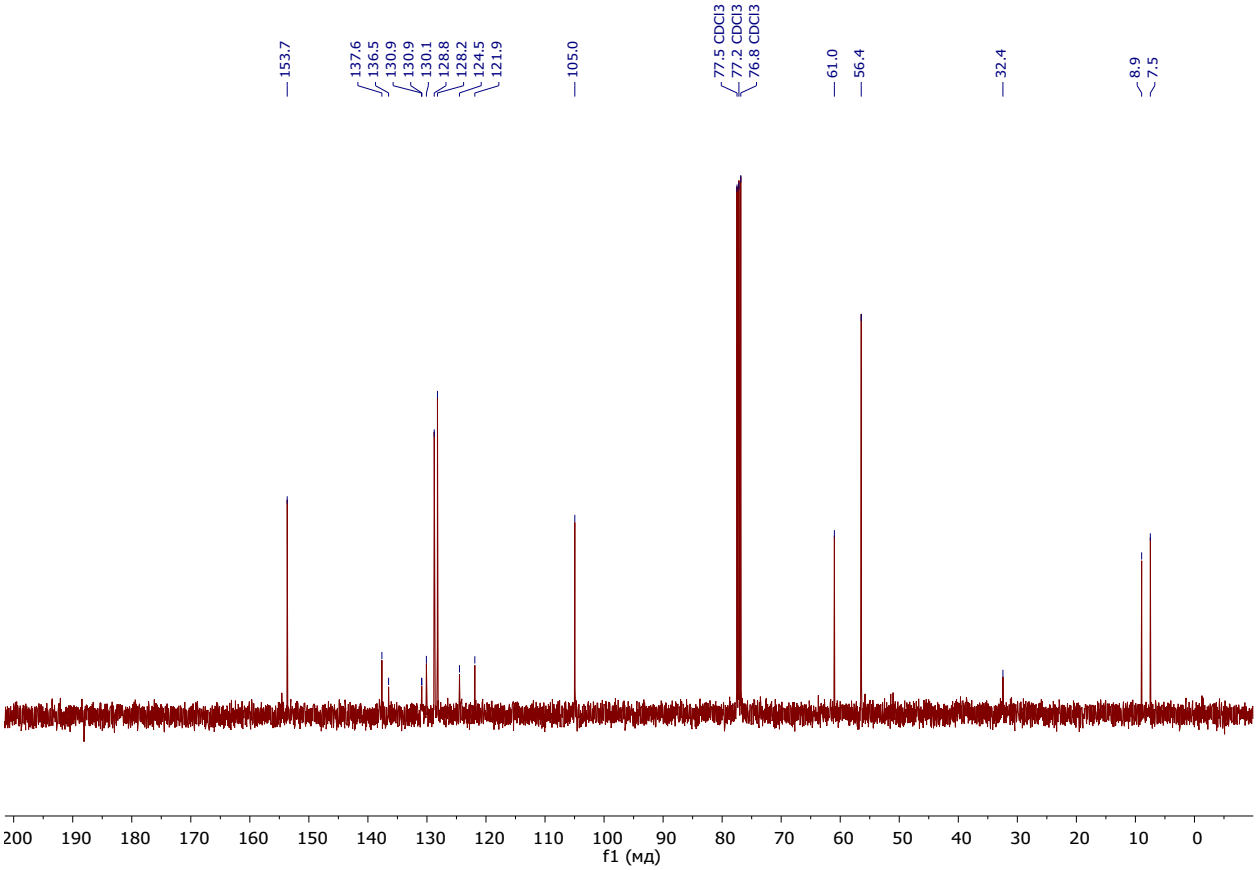
^{1}H NMR (400 MHz, DMSO-d_6) of **4q**



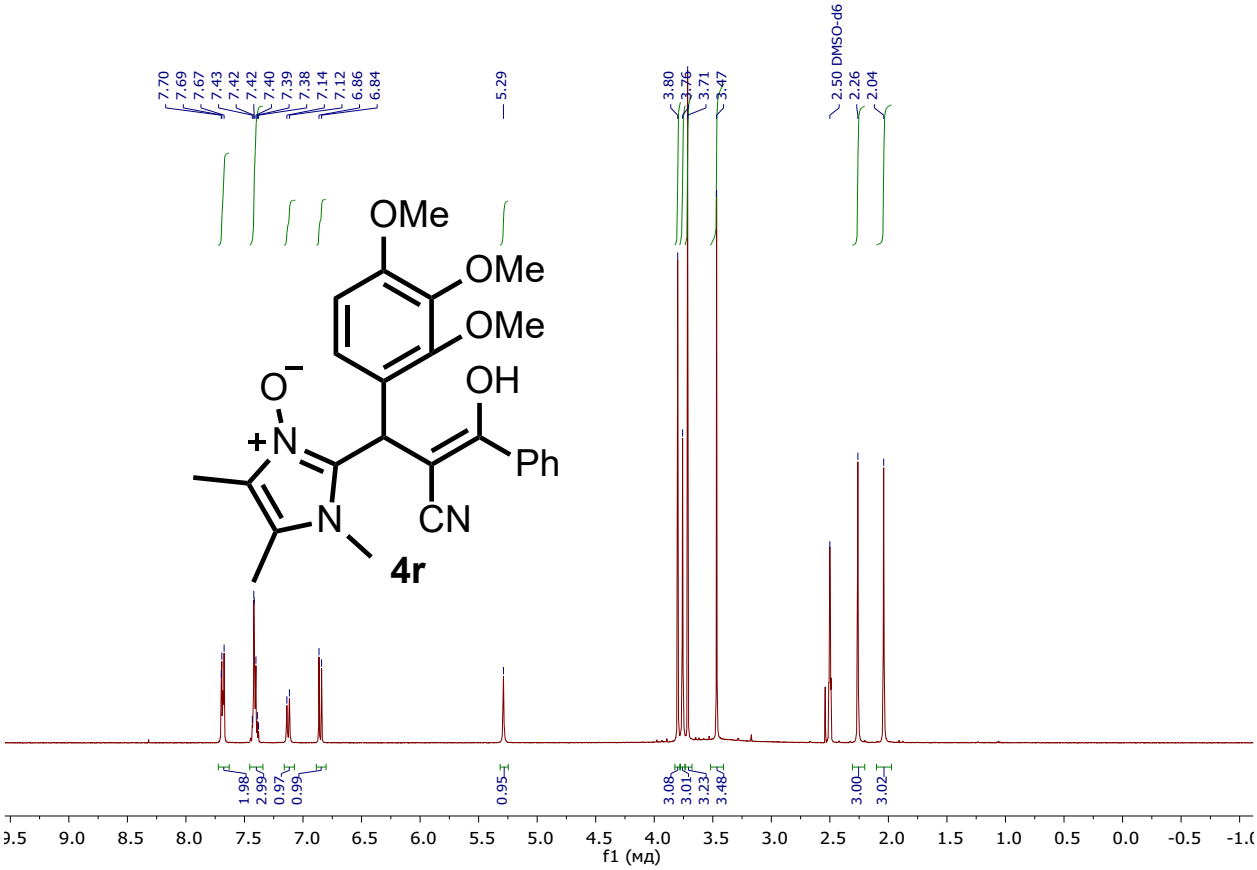
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4q**



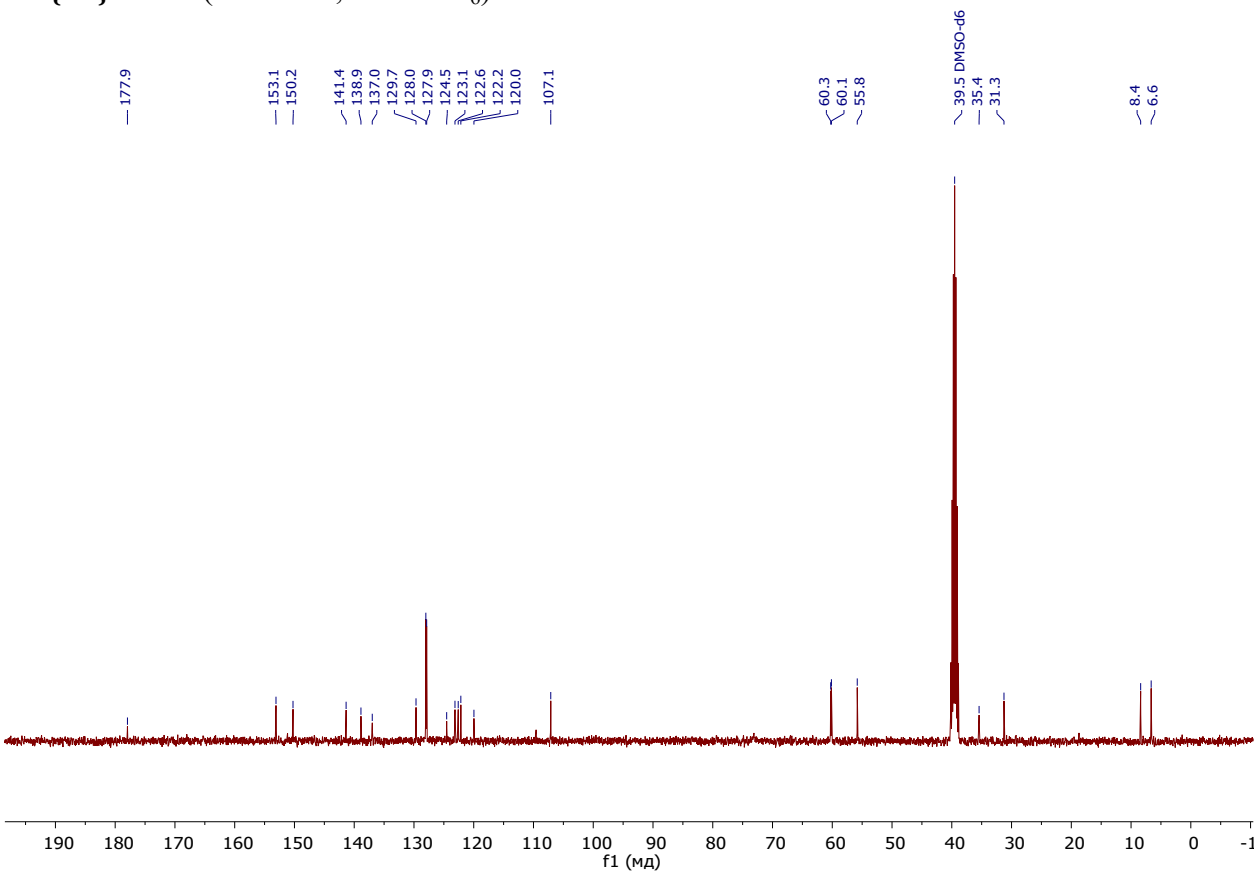
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of **4q**



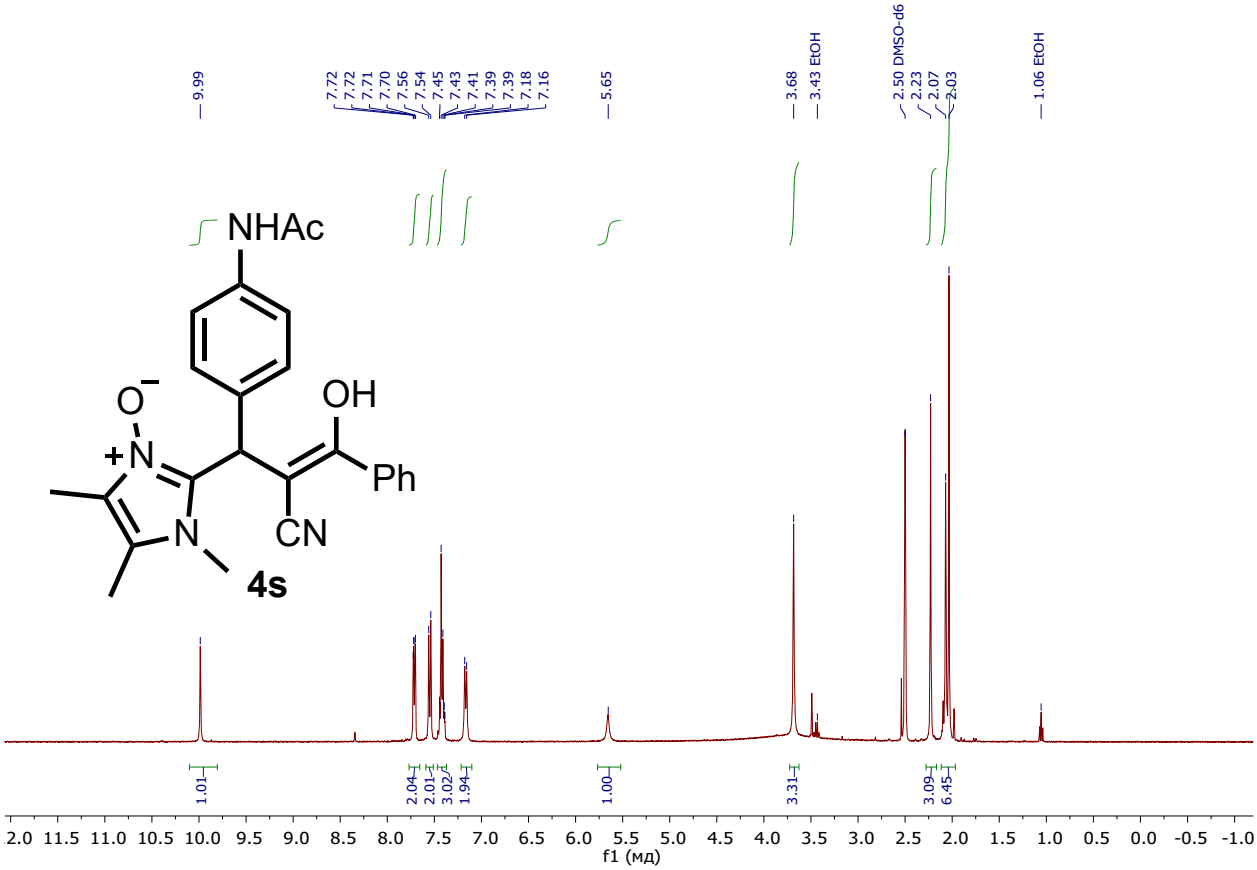
^{1}H NMR (400 MHz, DMSO-d_6) of **4r**



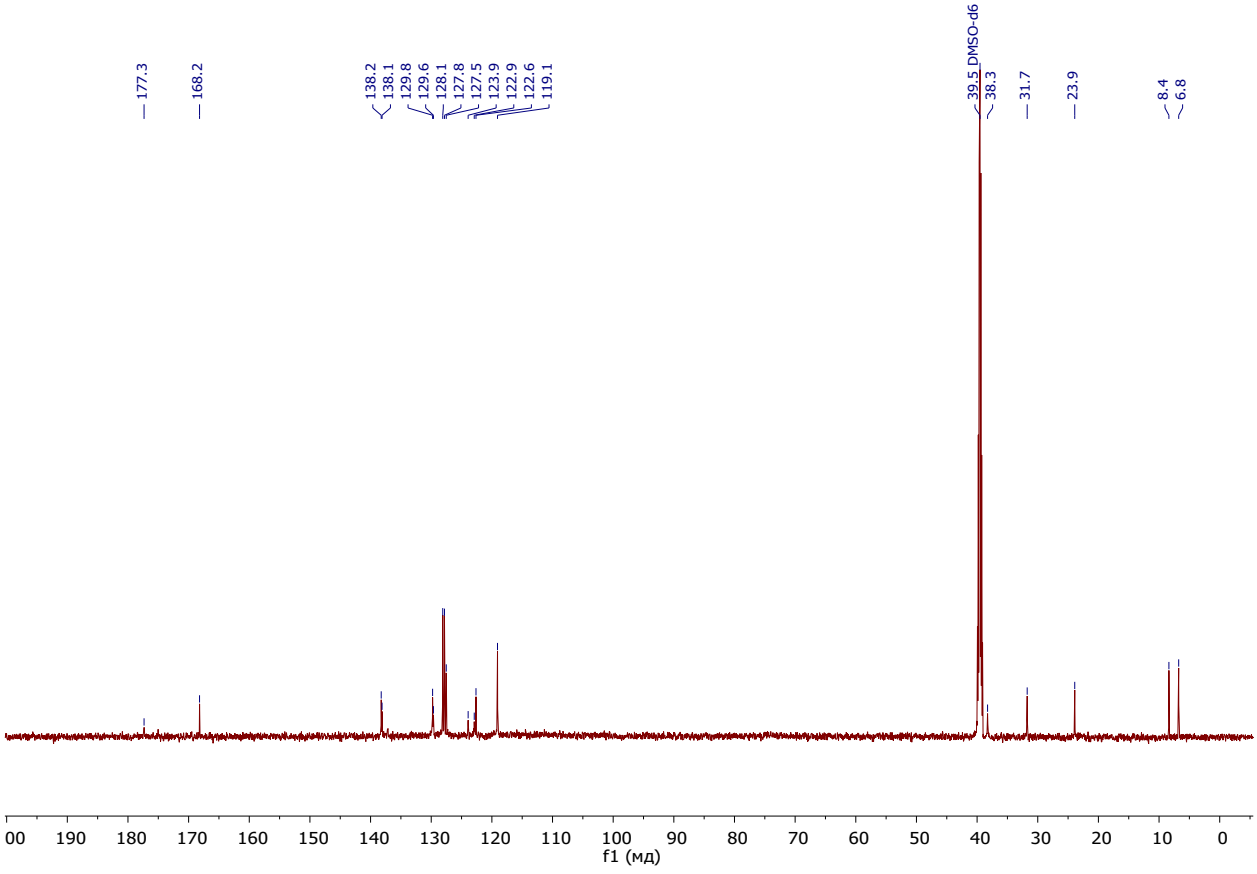
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4r**



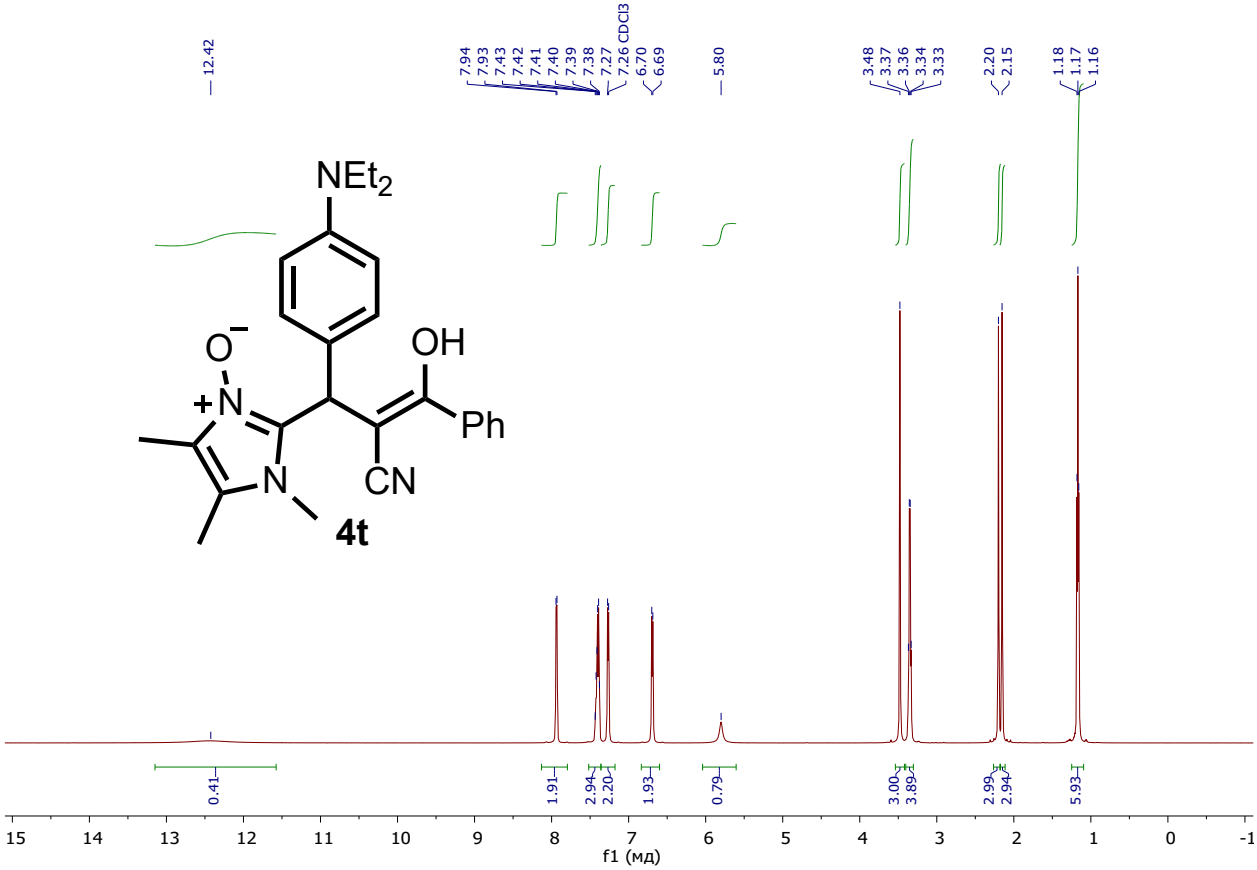
^{1}H NMR (400 MHz, DMSO-d_6) of **4s**



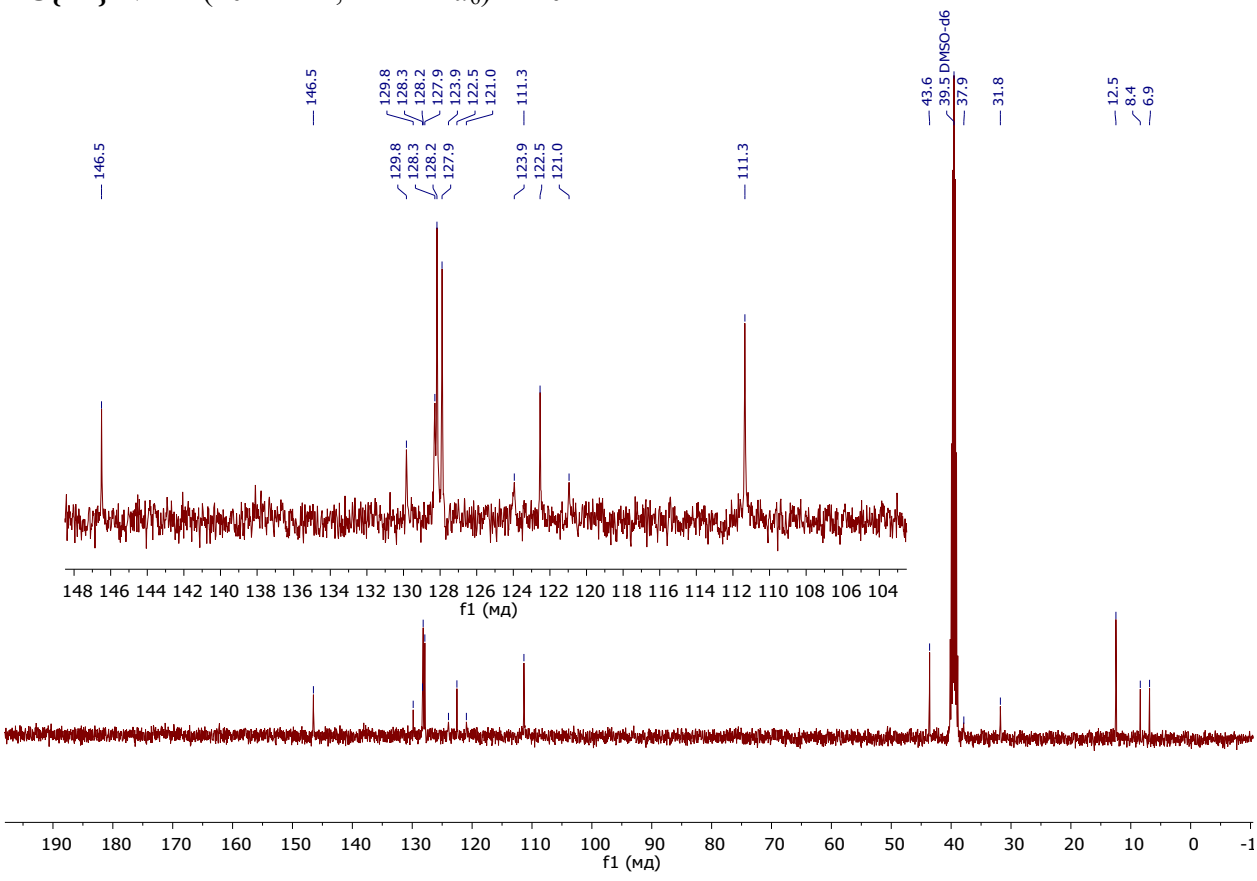
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4s**



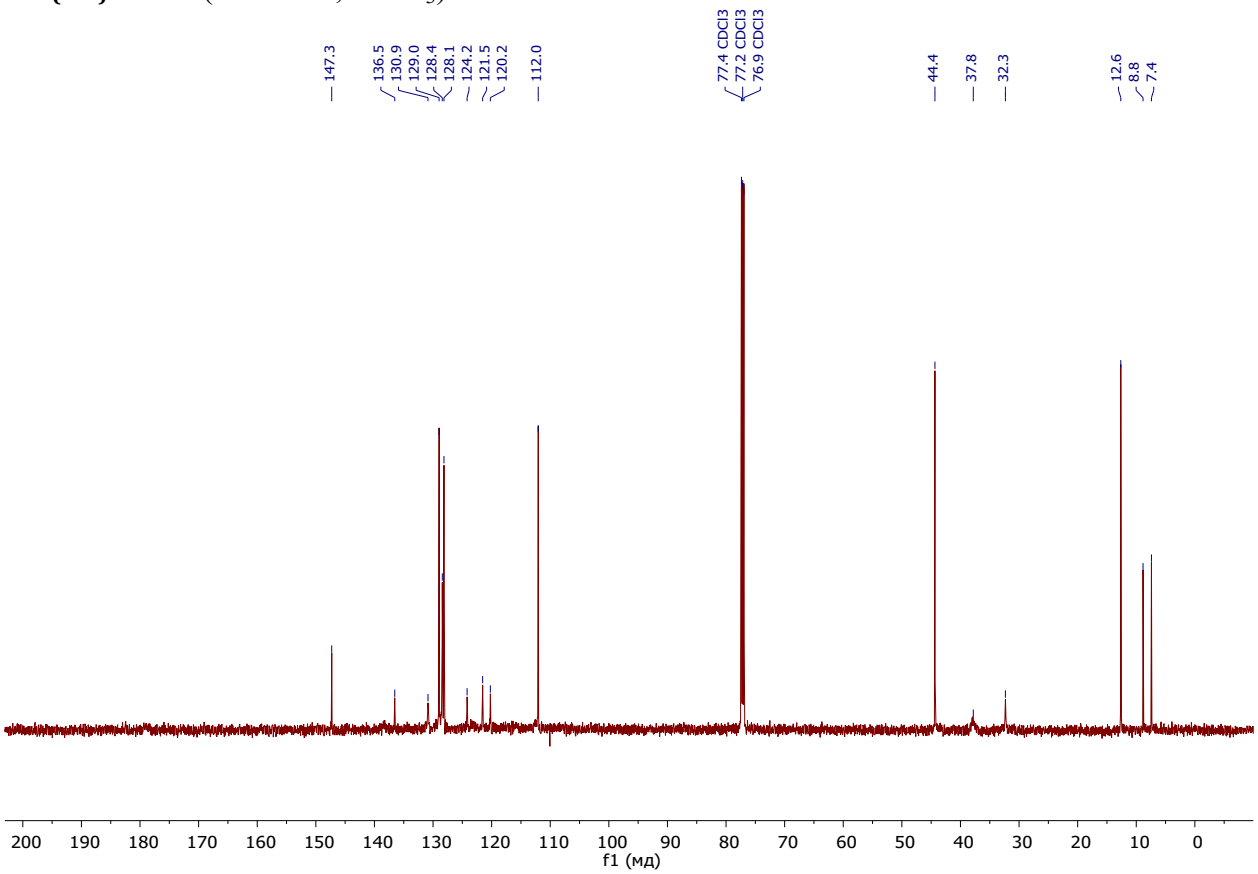
^{1}H NMR (600 MHz, $CDCl_3$, 333K) of **4t**



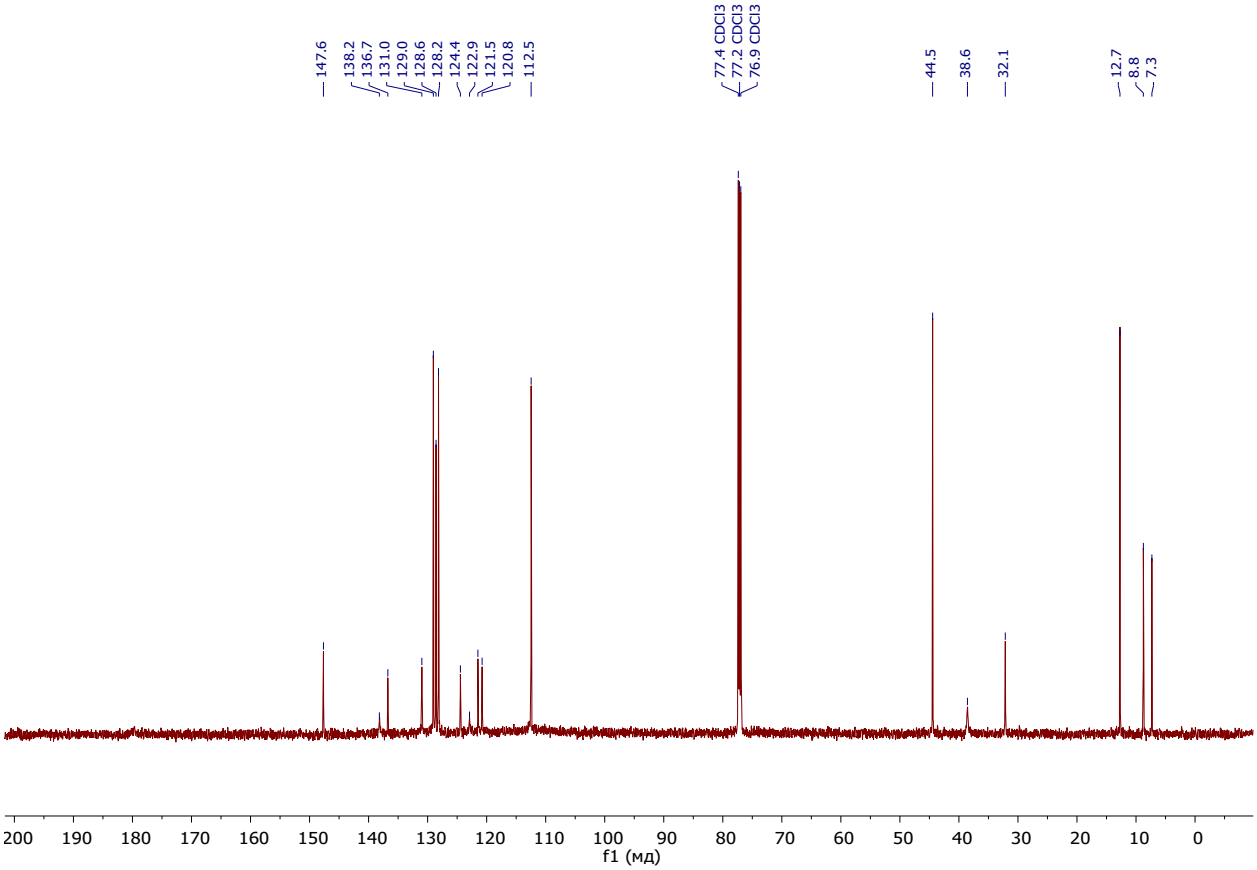
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4t**



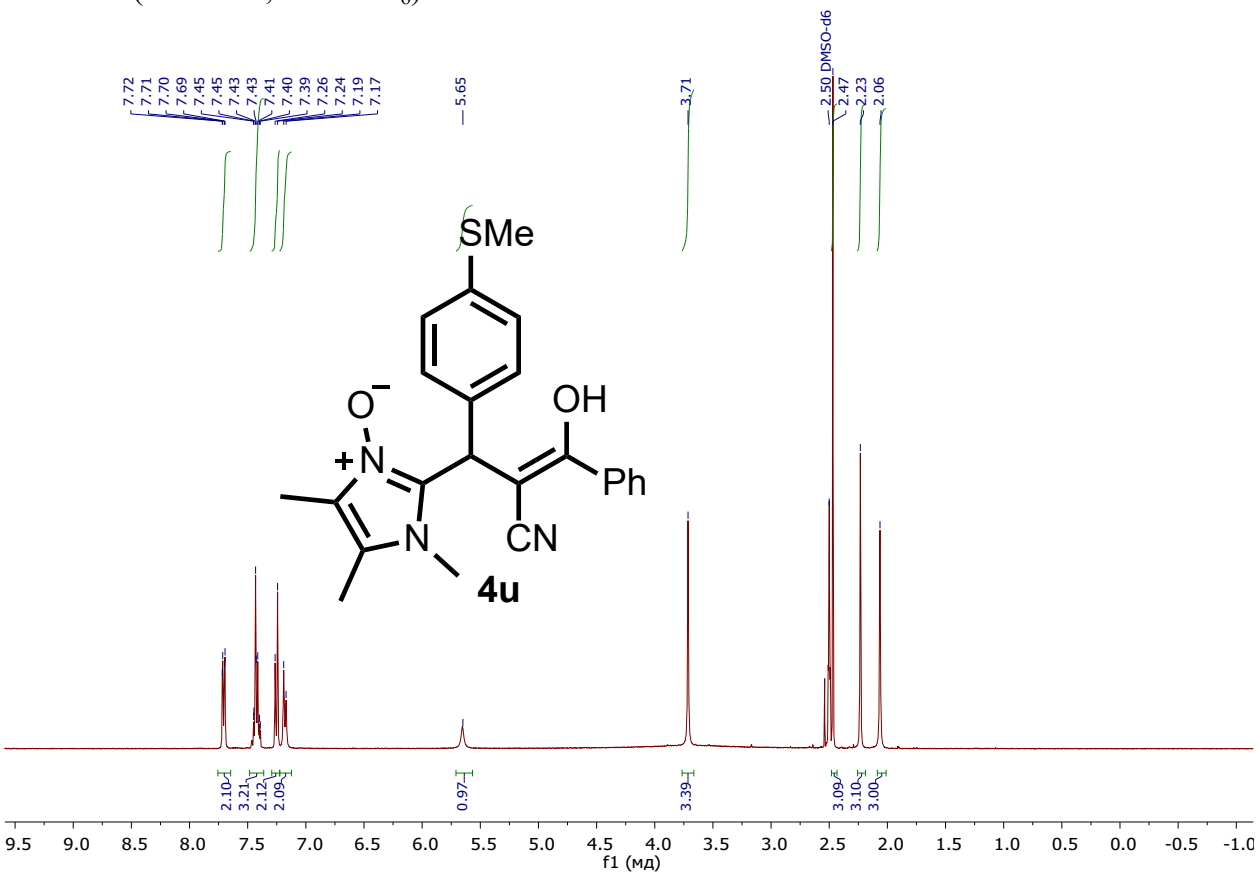
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) of **4t**



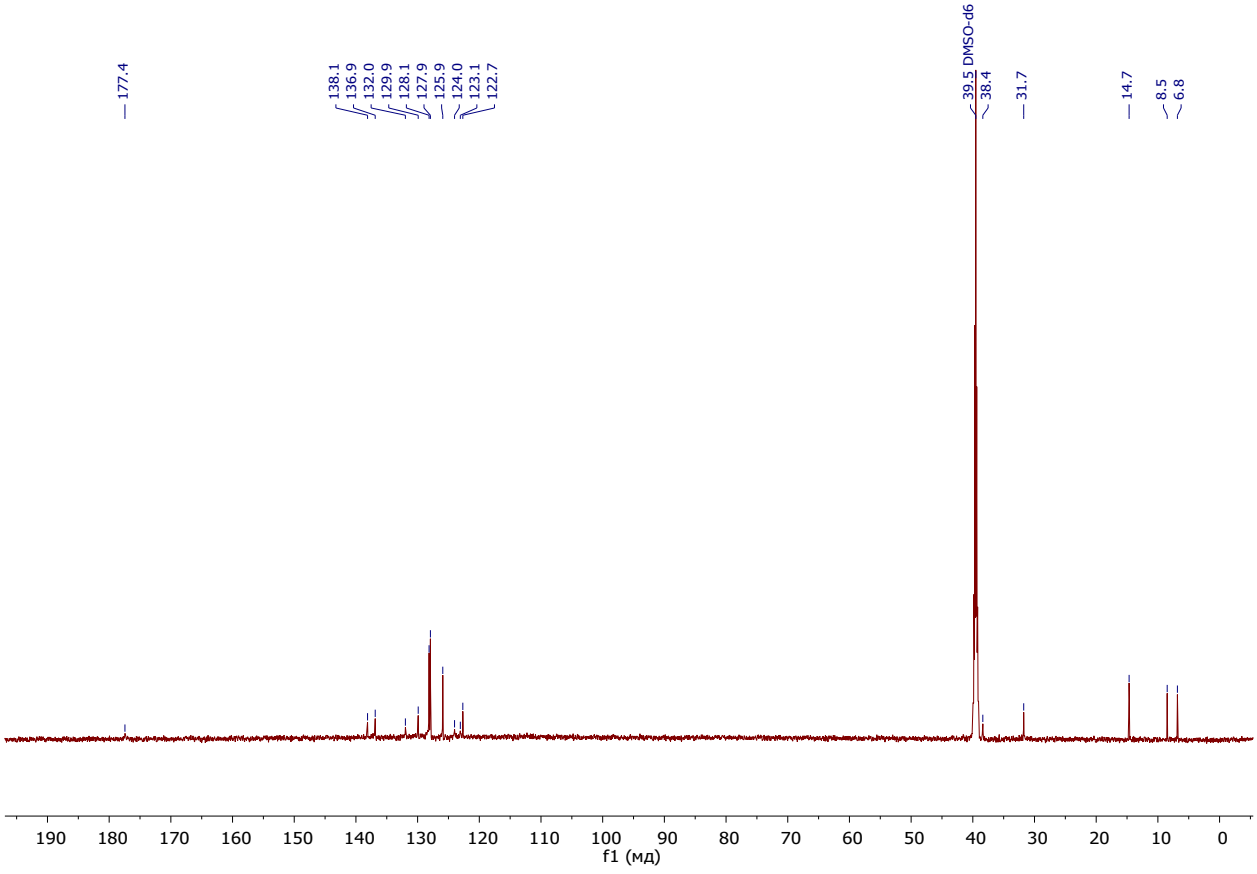
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$, 333K) of **4t**



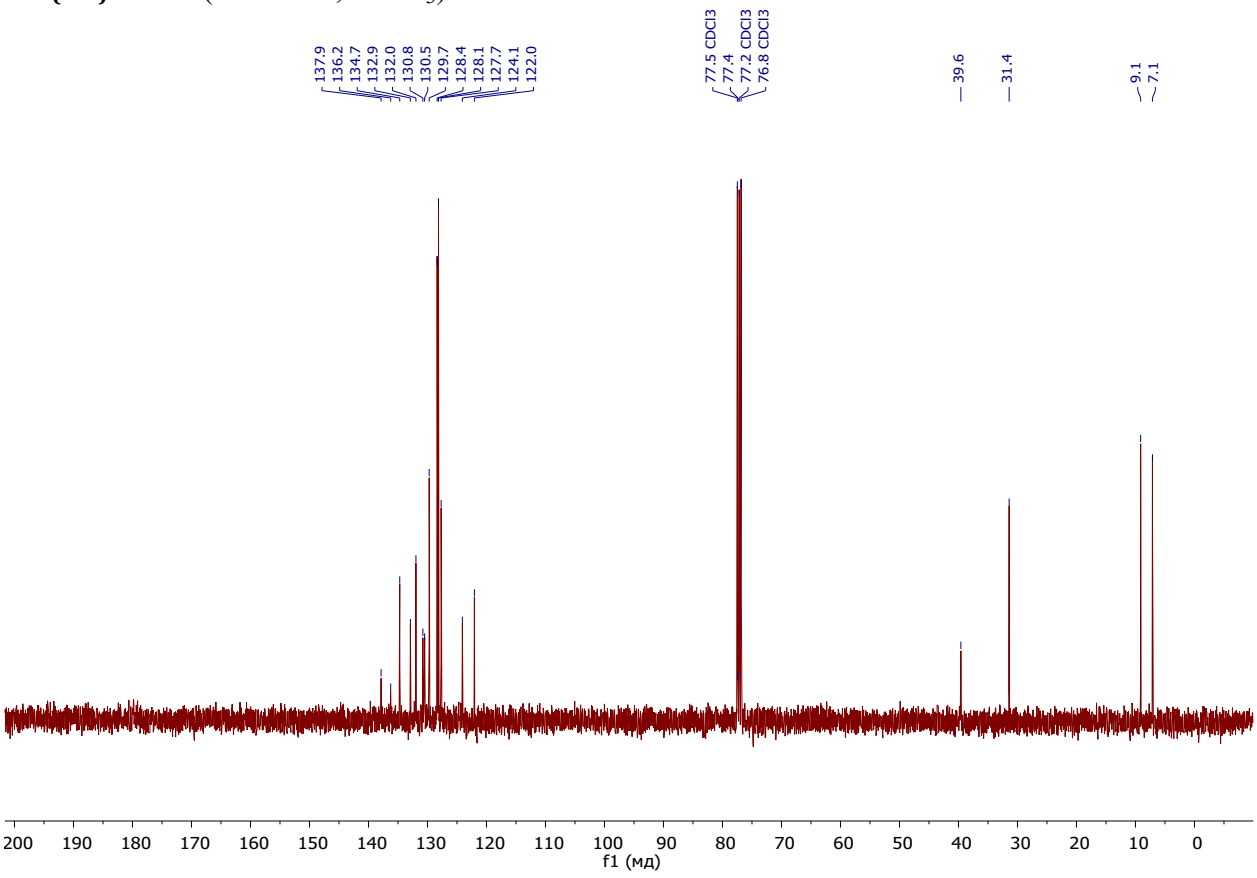
^{1}H NMR (400 MHz, DMSO-d_6) of **4u**



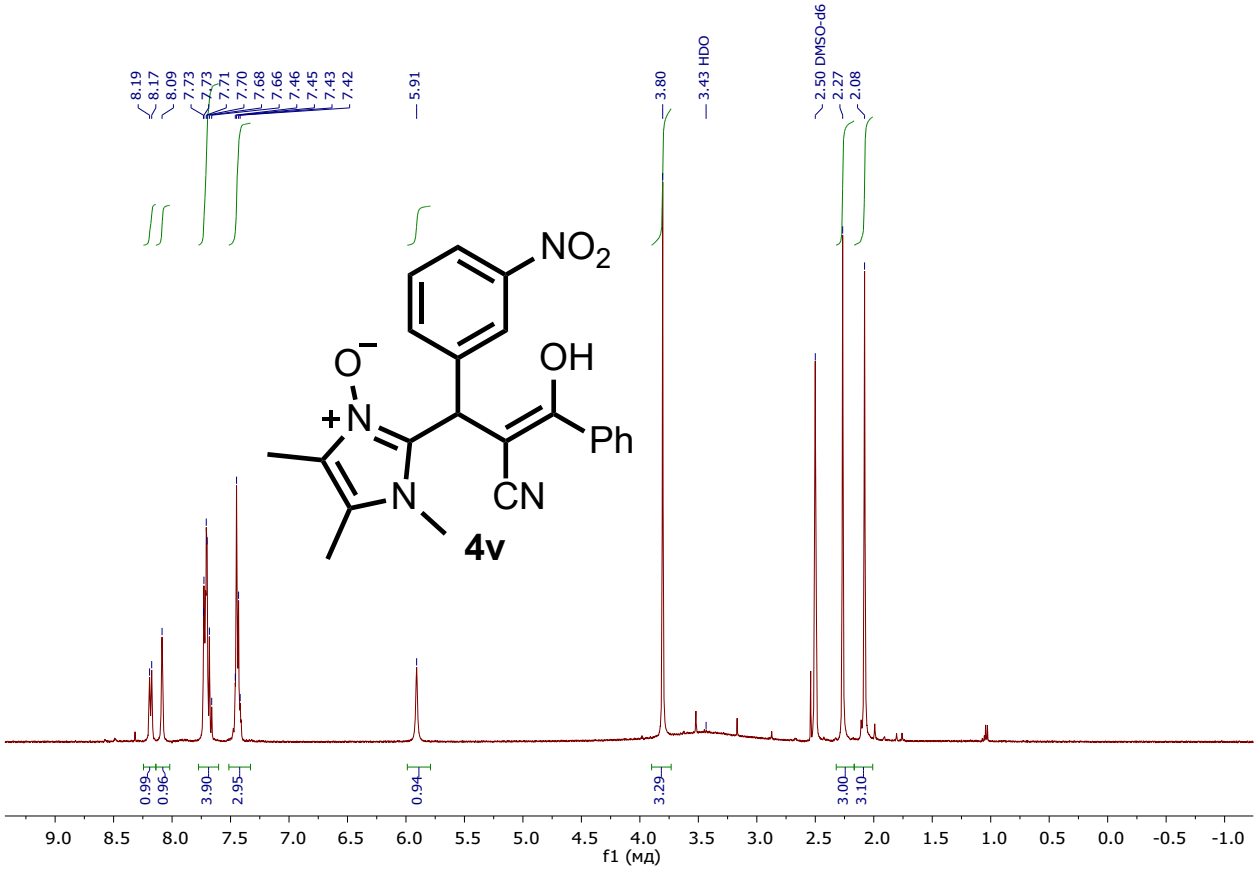
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4u**



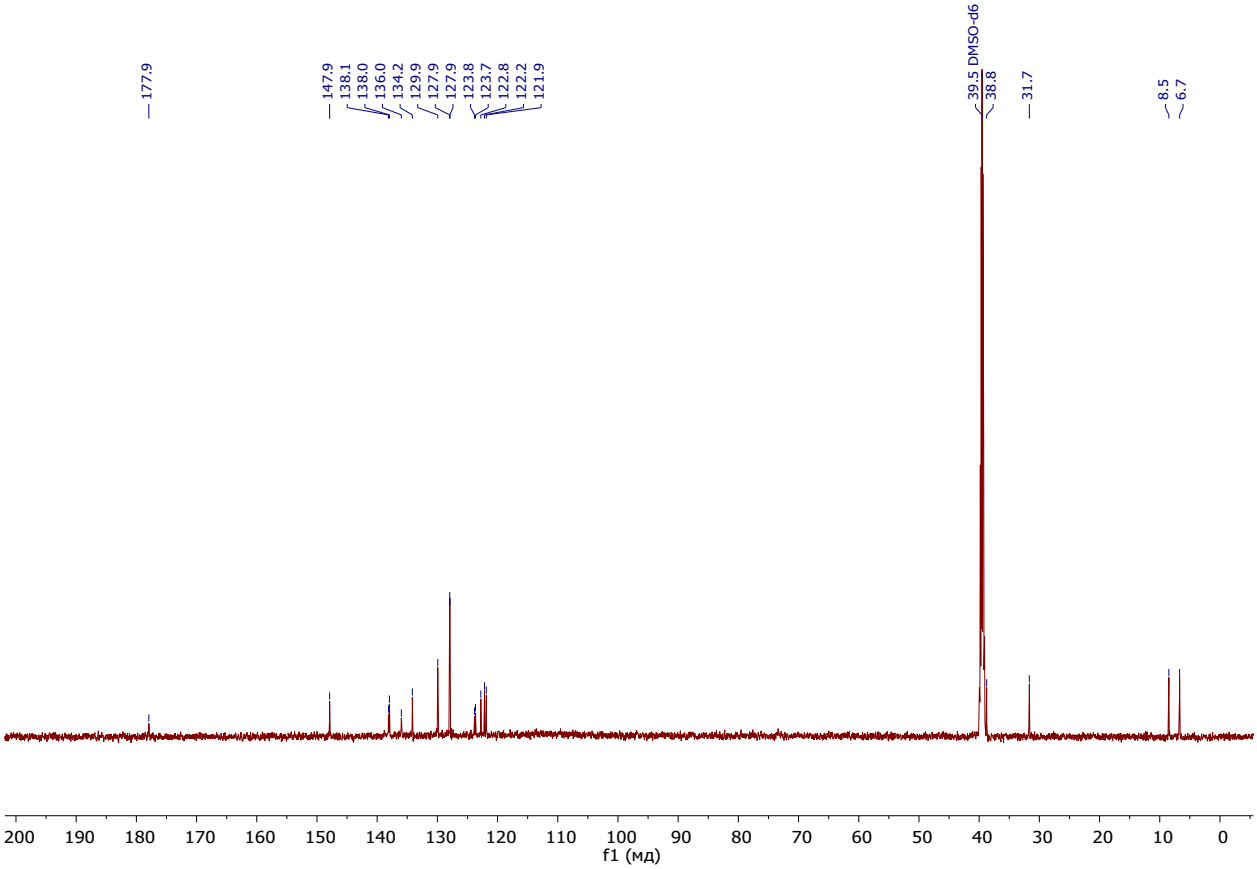
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of **4u**



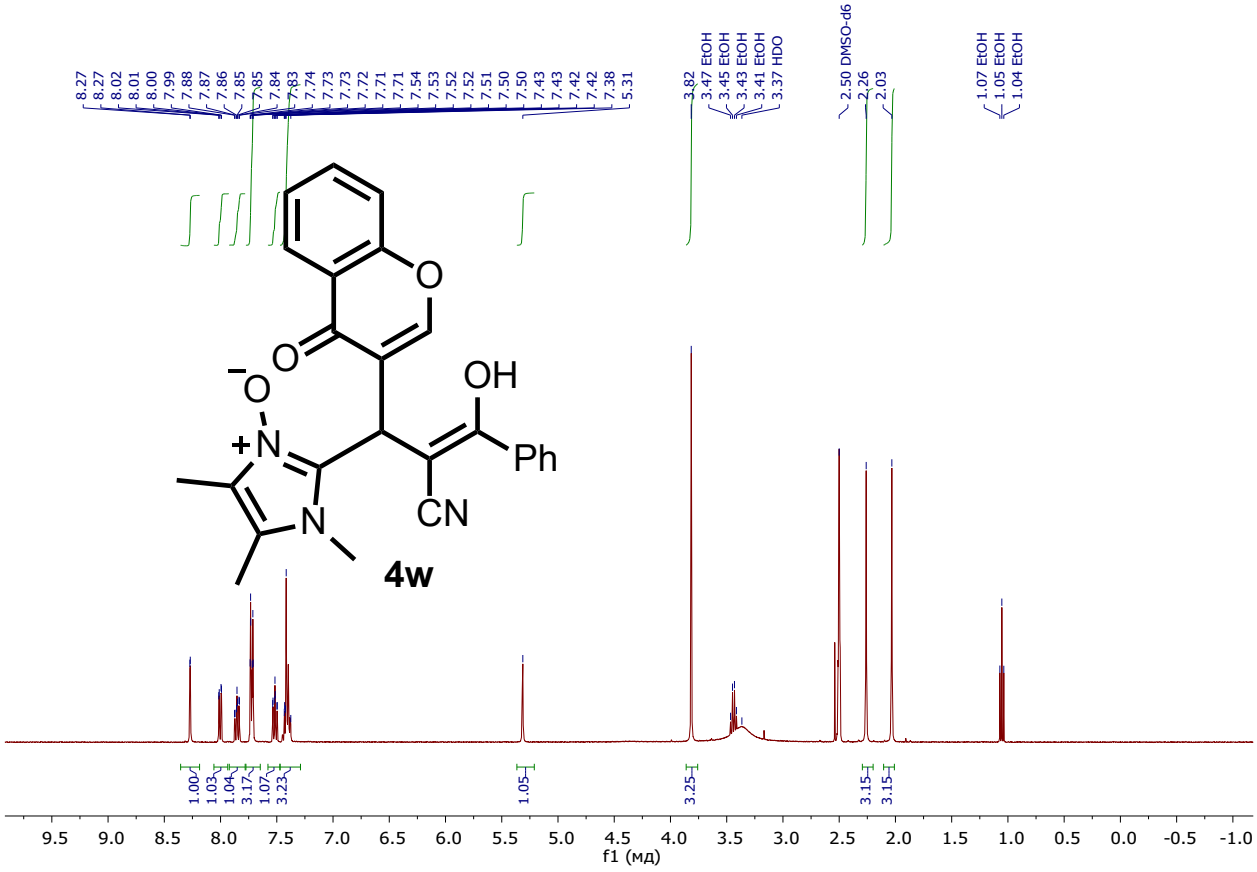
^{1}H NMR (400 MHz, DMSO-d_6) of **4v**



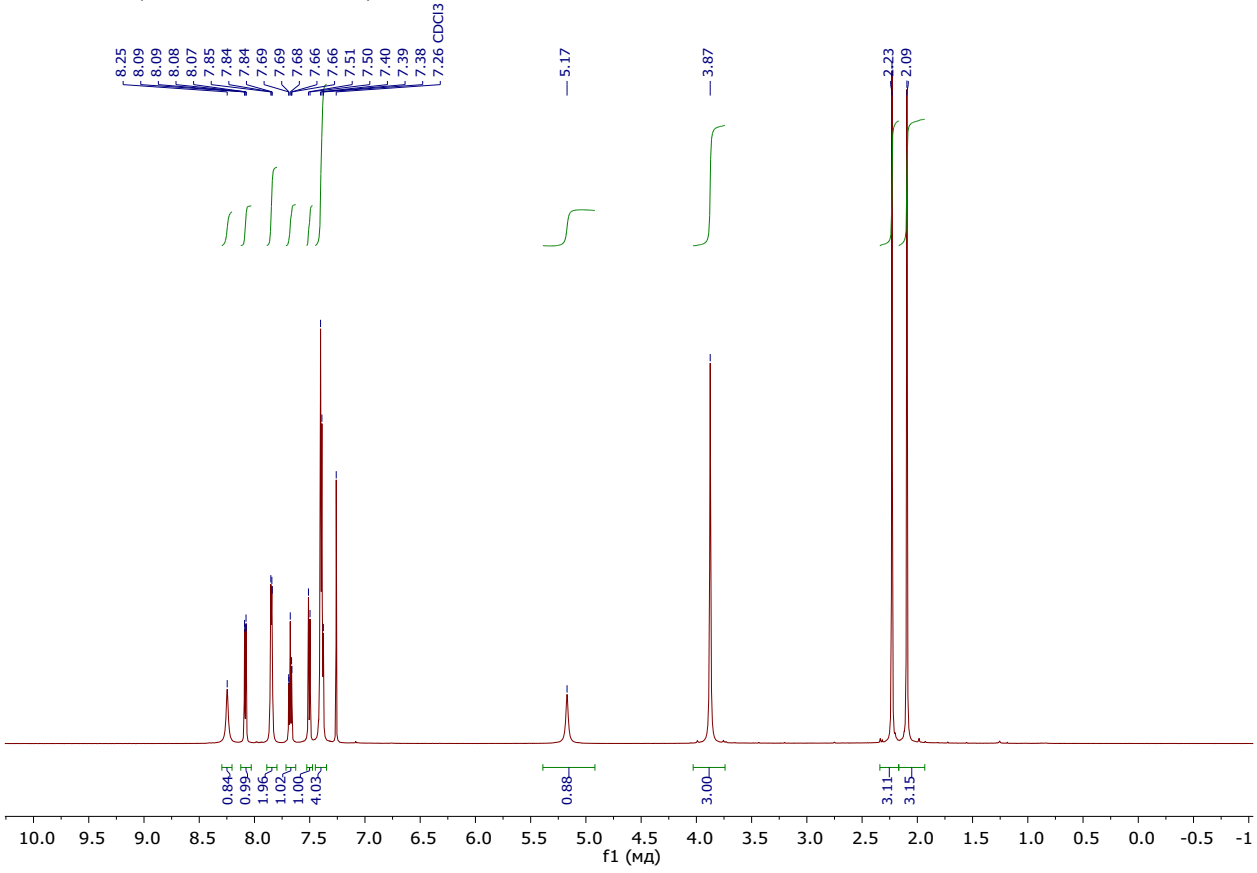
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4v**



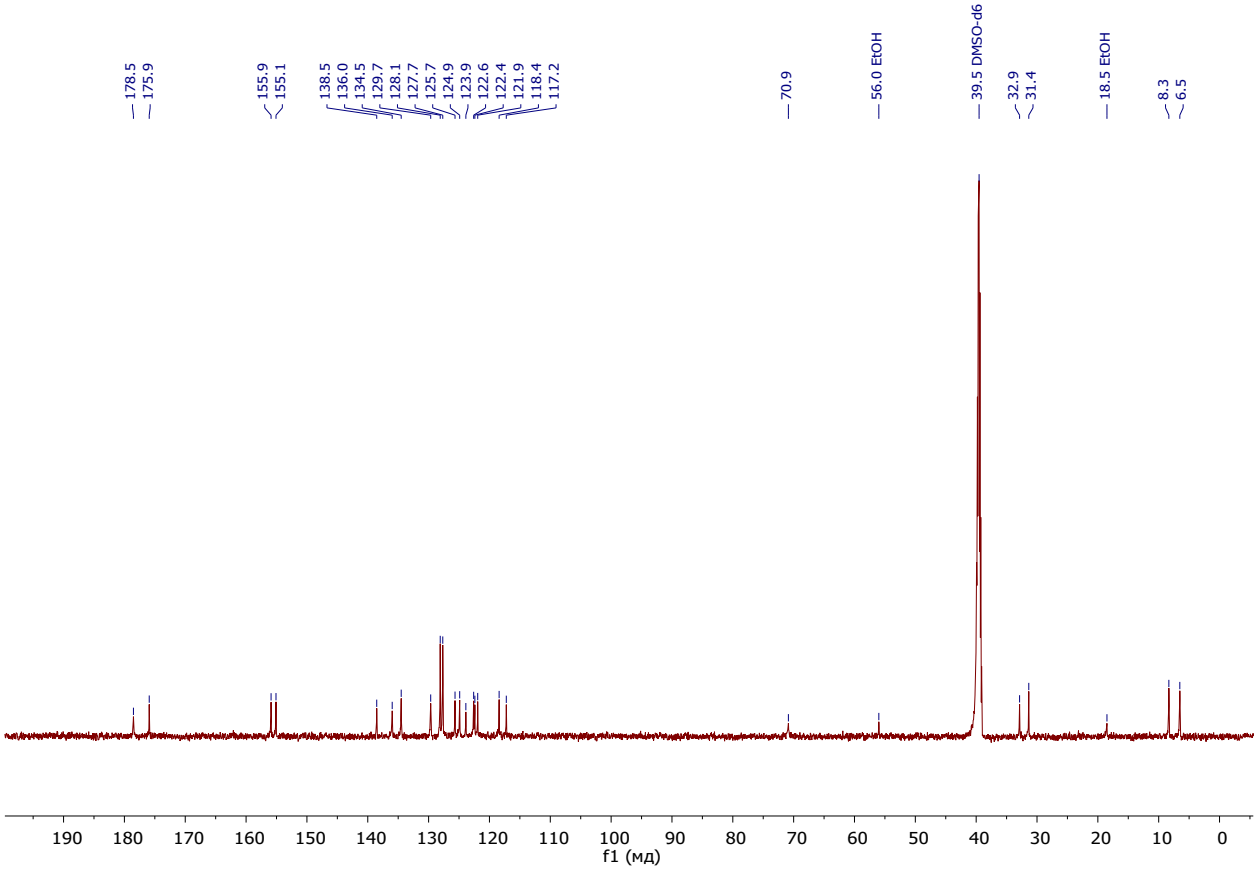
^{1}H NMR (400 MHz, DMSO-d_6) of **4w** solvate with EtOH



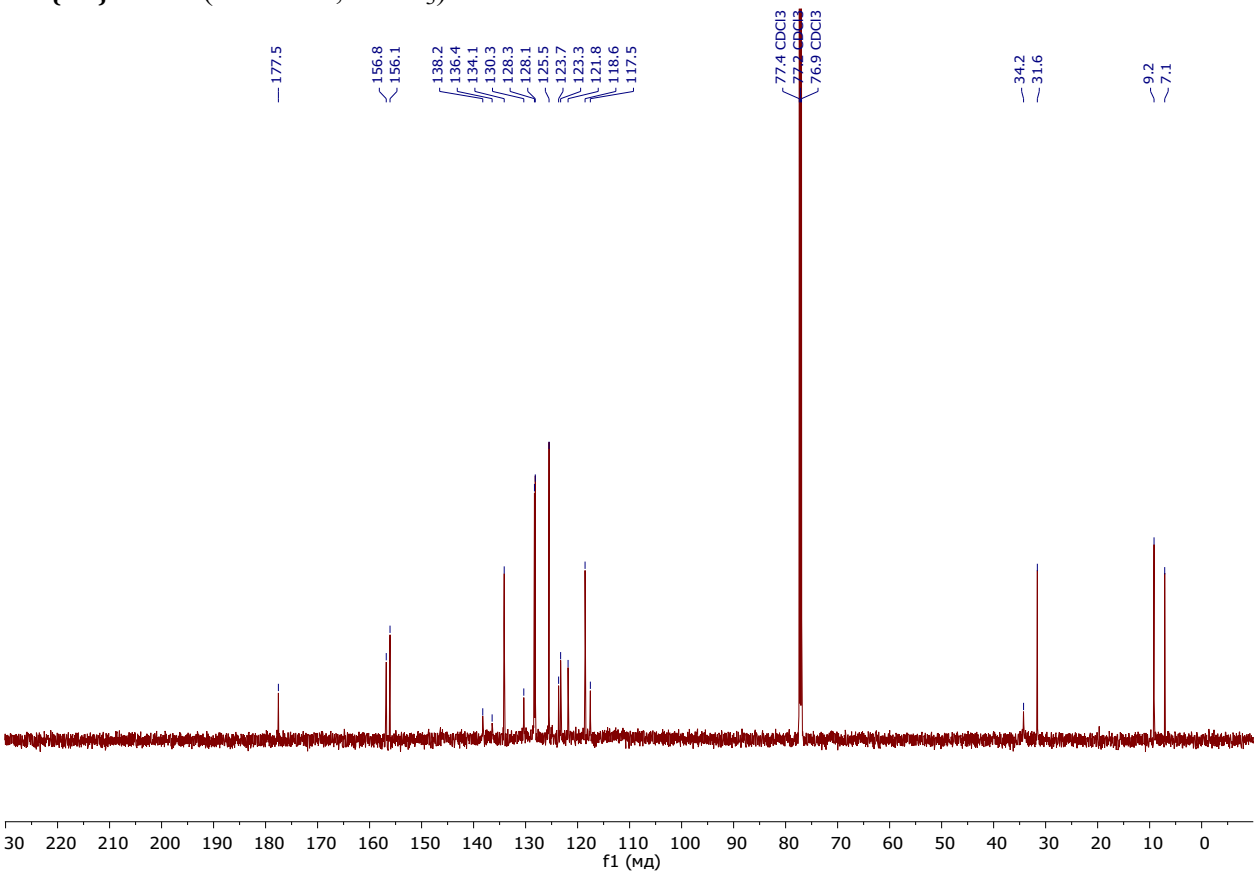
^{1}H NMR (600 MHz, $CDCl_3$) of **4w**



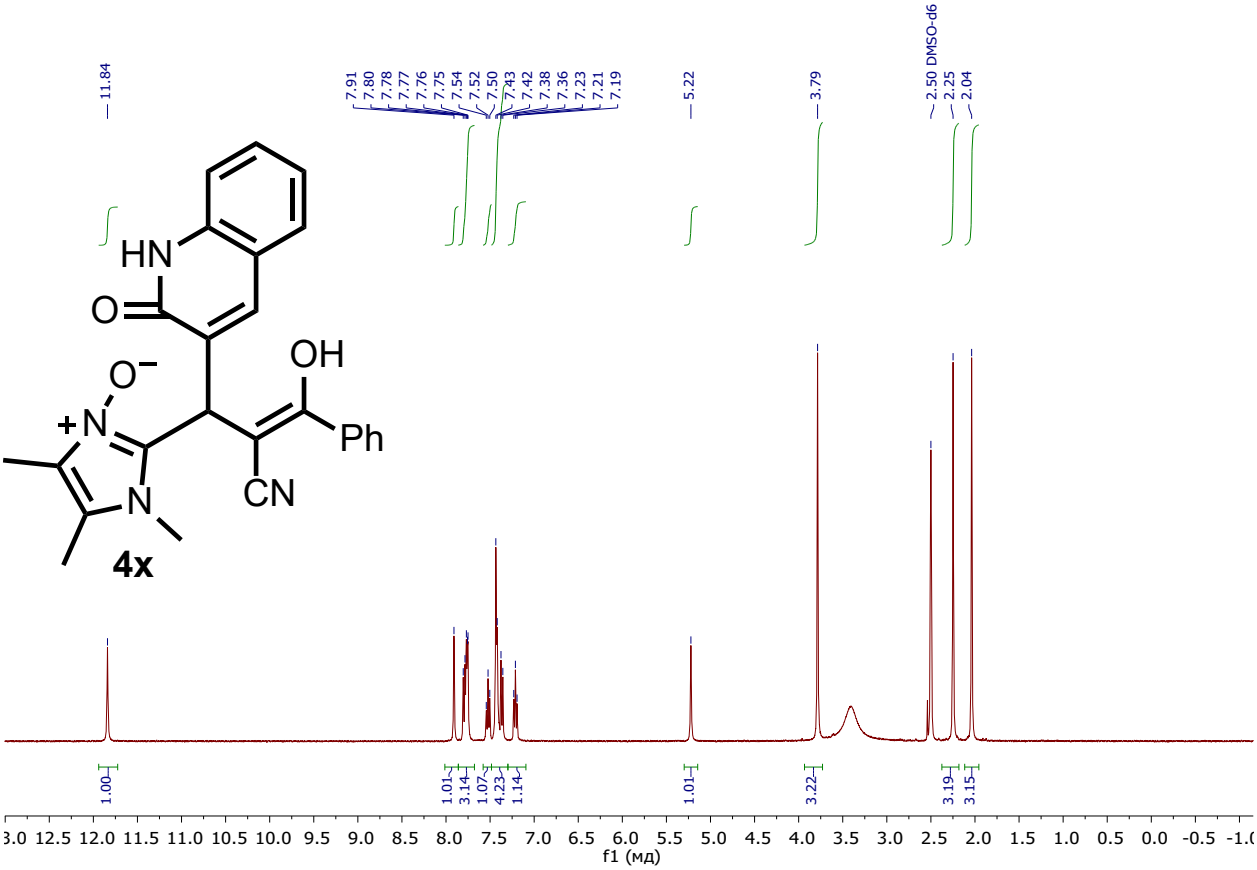
$^{13}C\{^{1}H\}$ NMR (151 MHz, DMSO-d_6) of **4w** solvate with EtOH



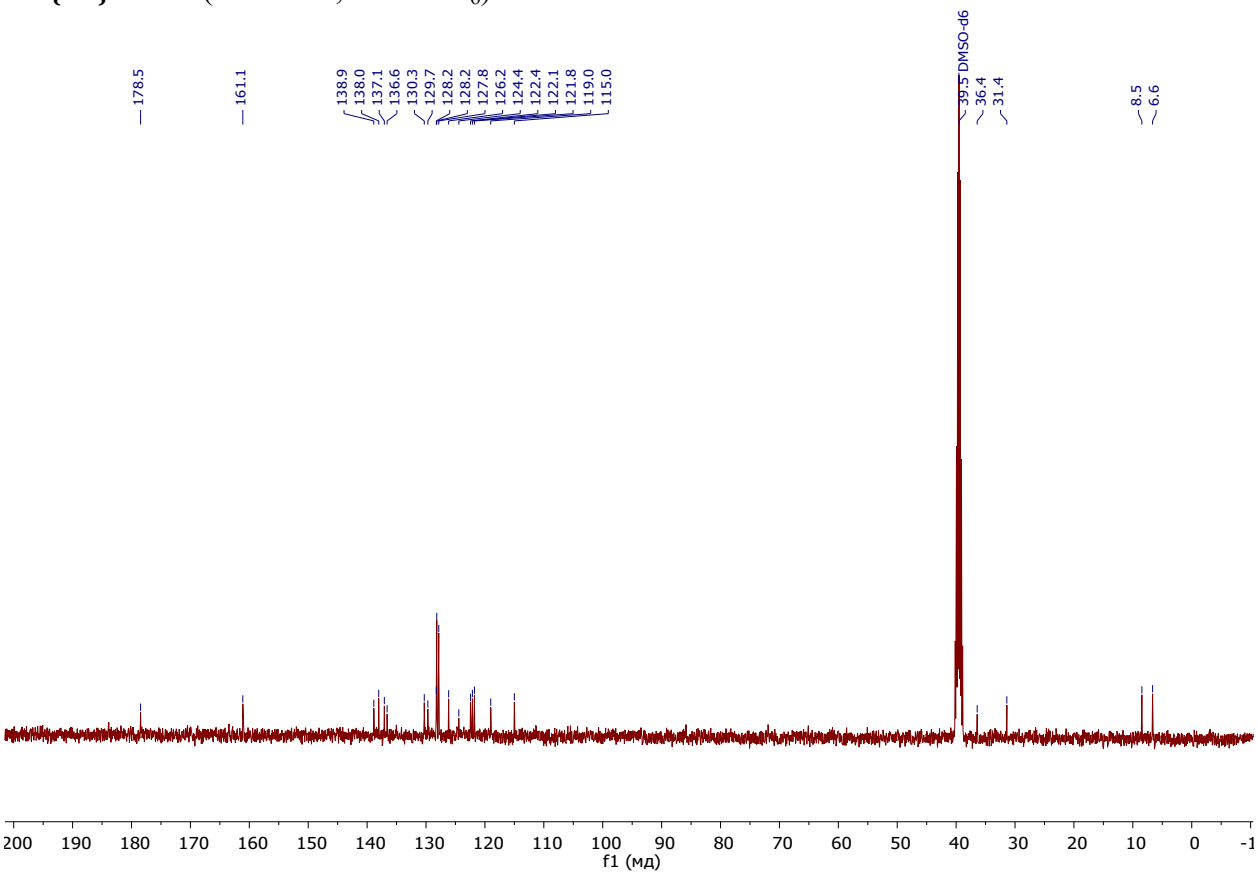
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) of **4w**



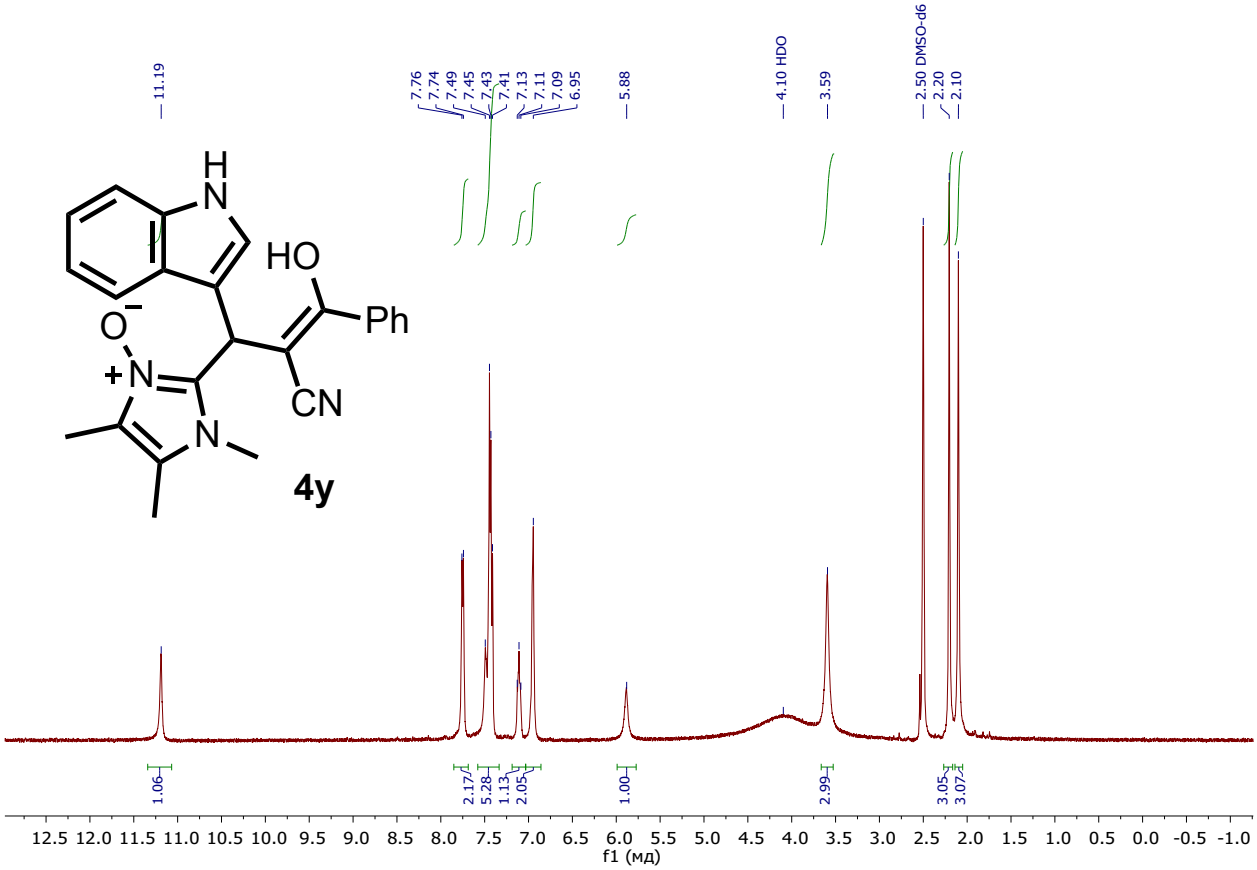
^{1}H NMR (400 MHz, DMSO-d_6) of **4x**



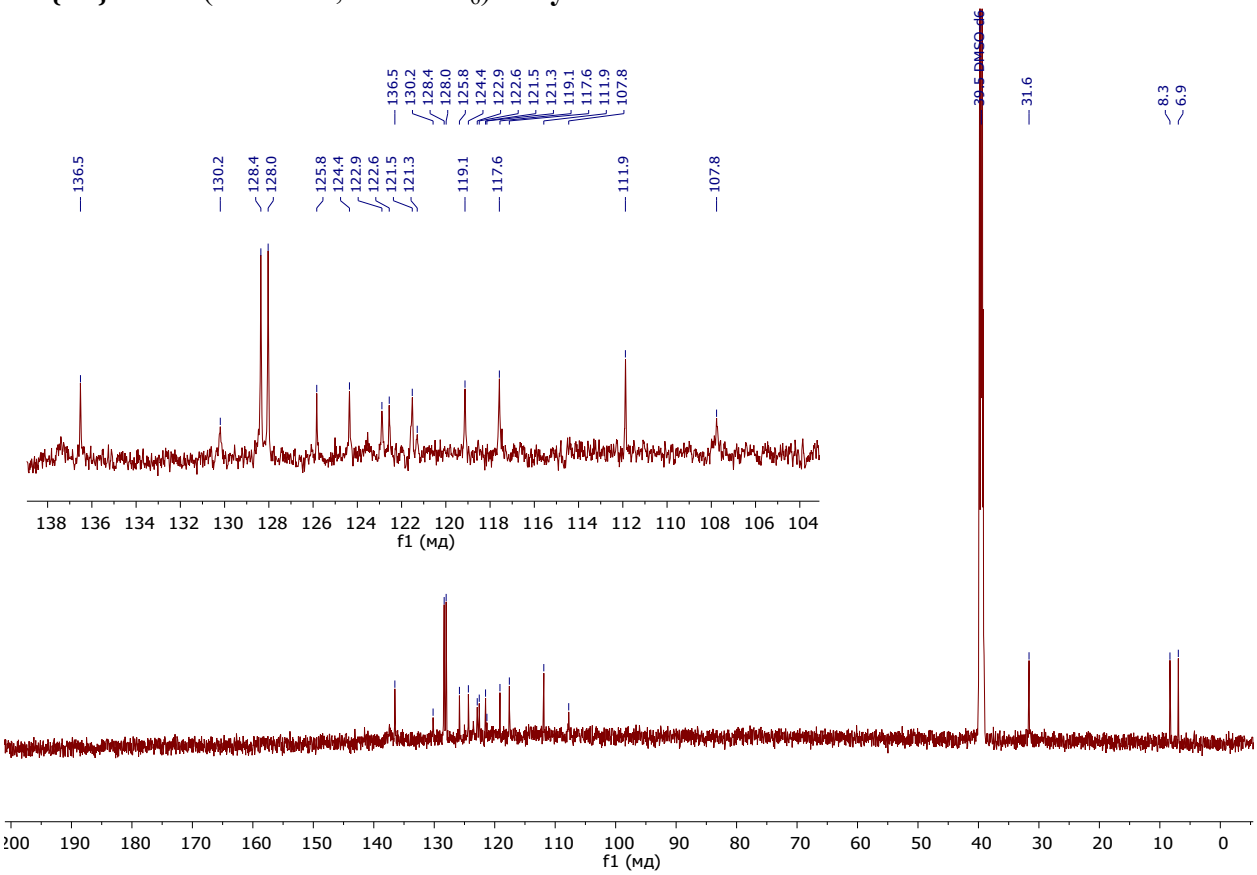
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **4x**



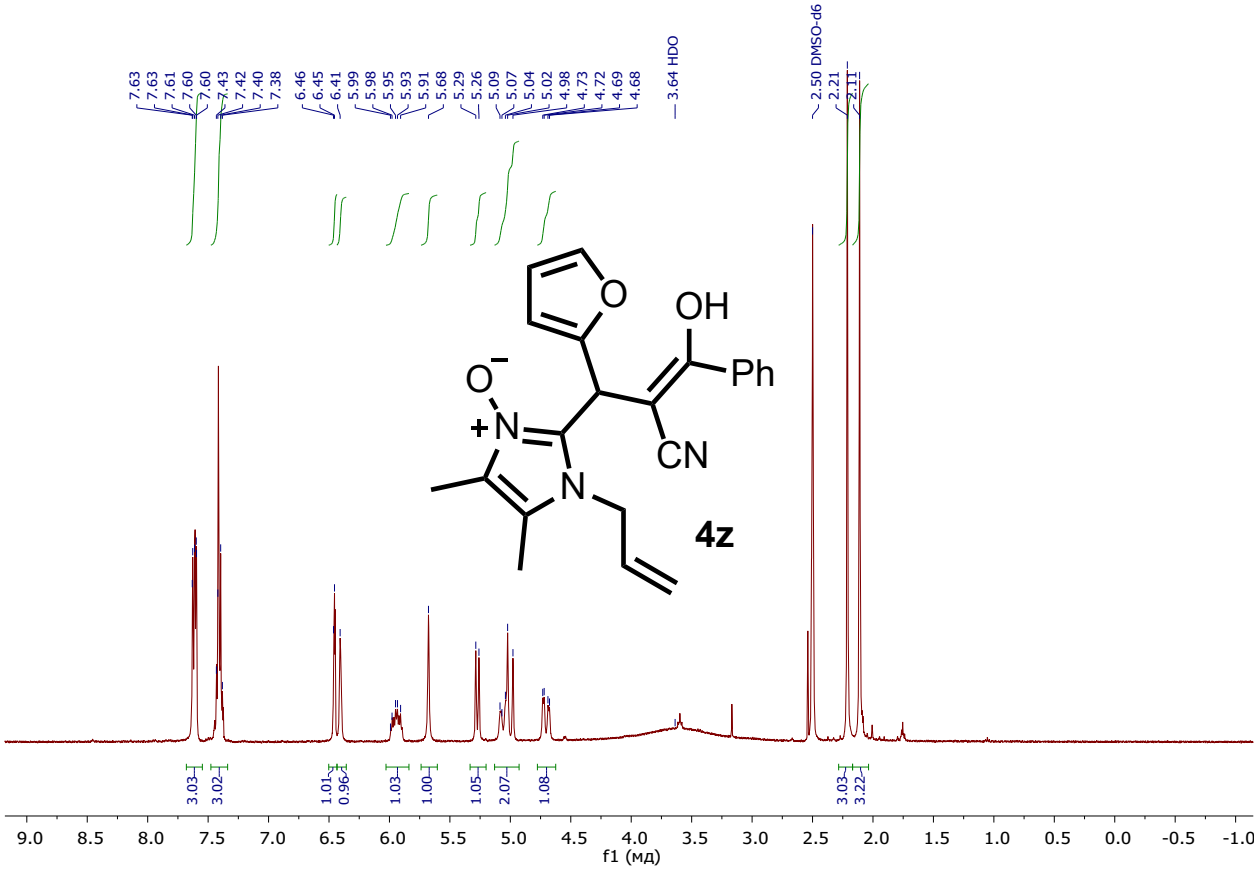
^{1}H NMR (400 MHz, DMSO-d_6) of **4y**



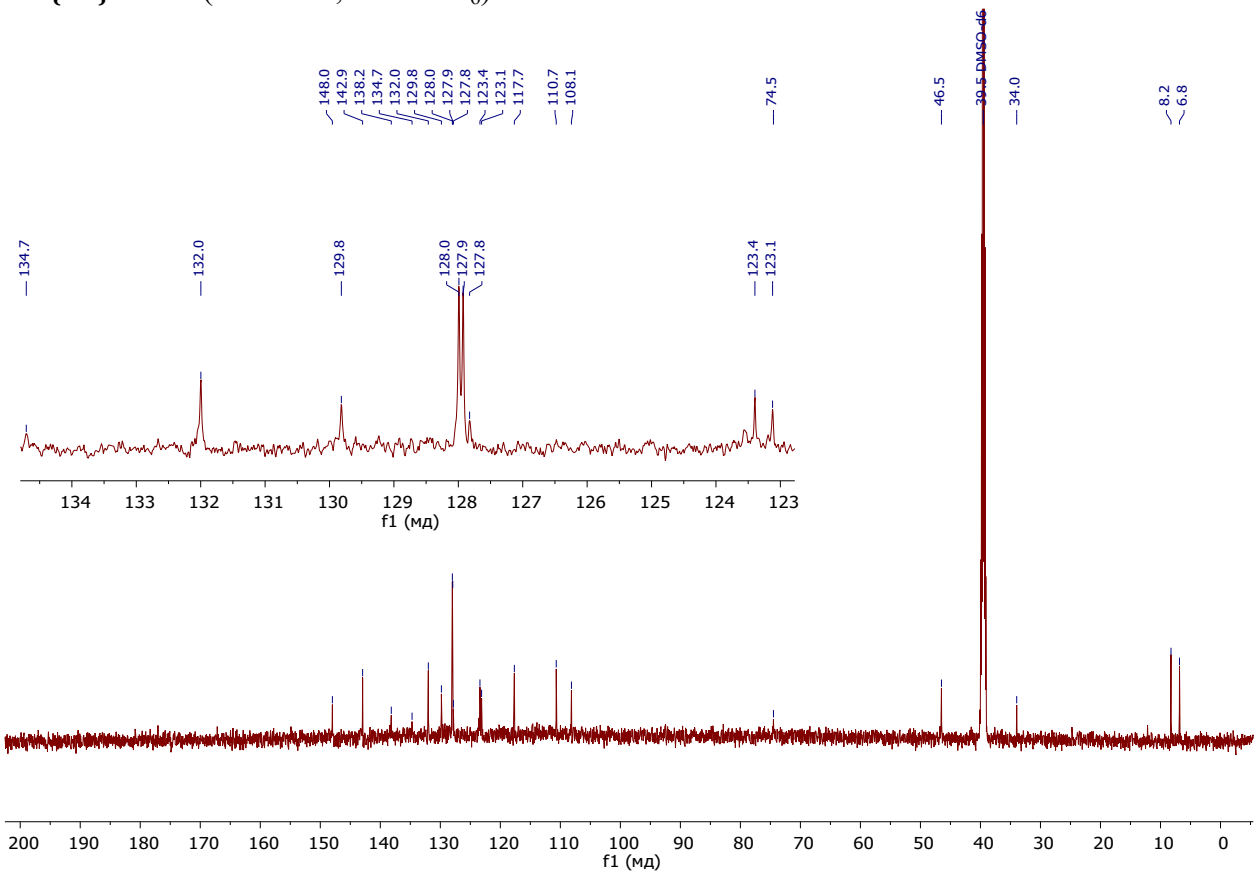
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4y**



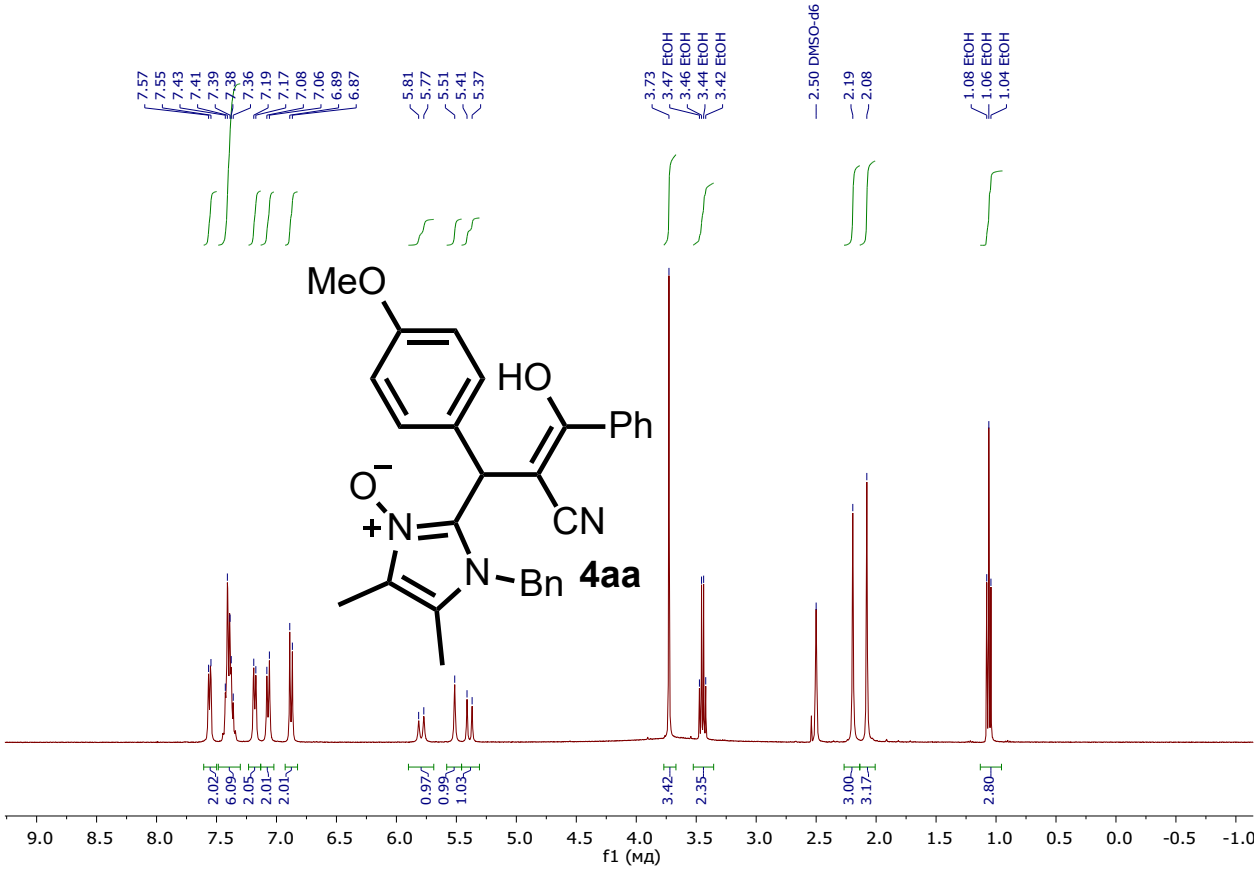
^{1}H NMR (400 MHz, DMSO-d_6) of **4z**



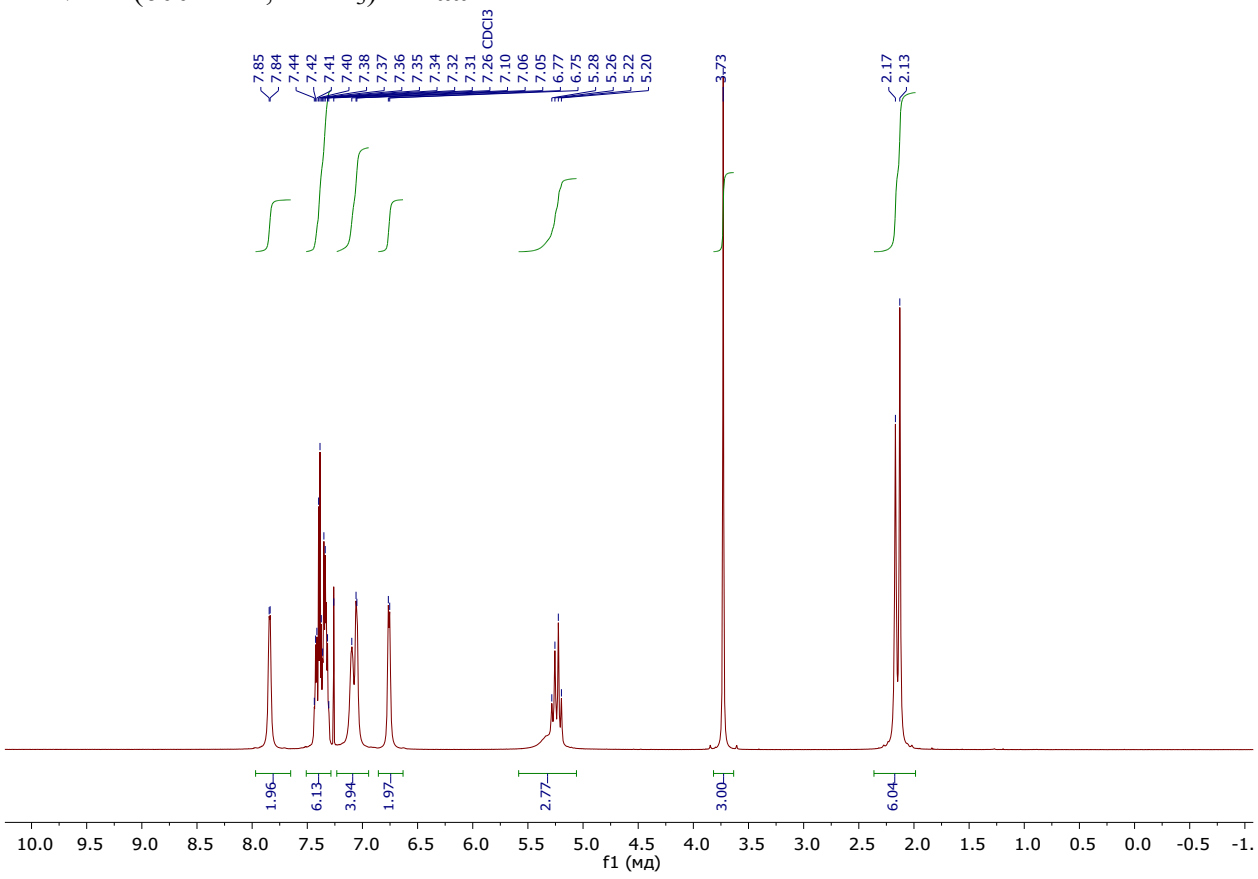
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4z**



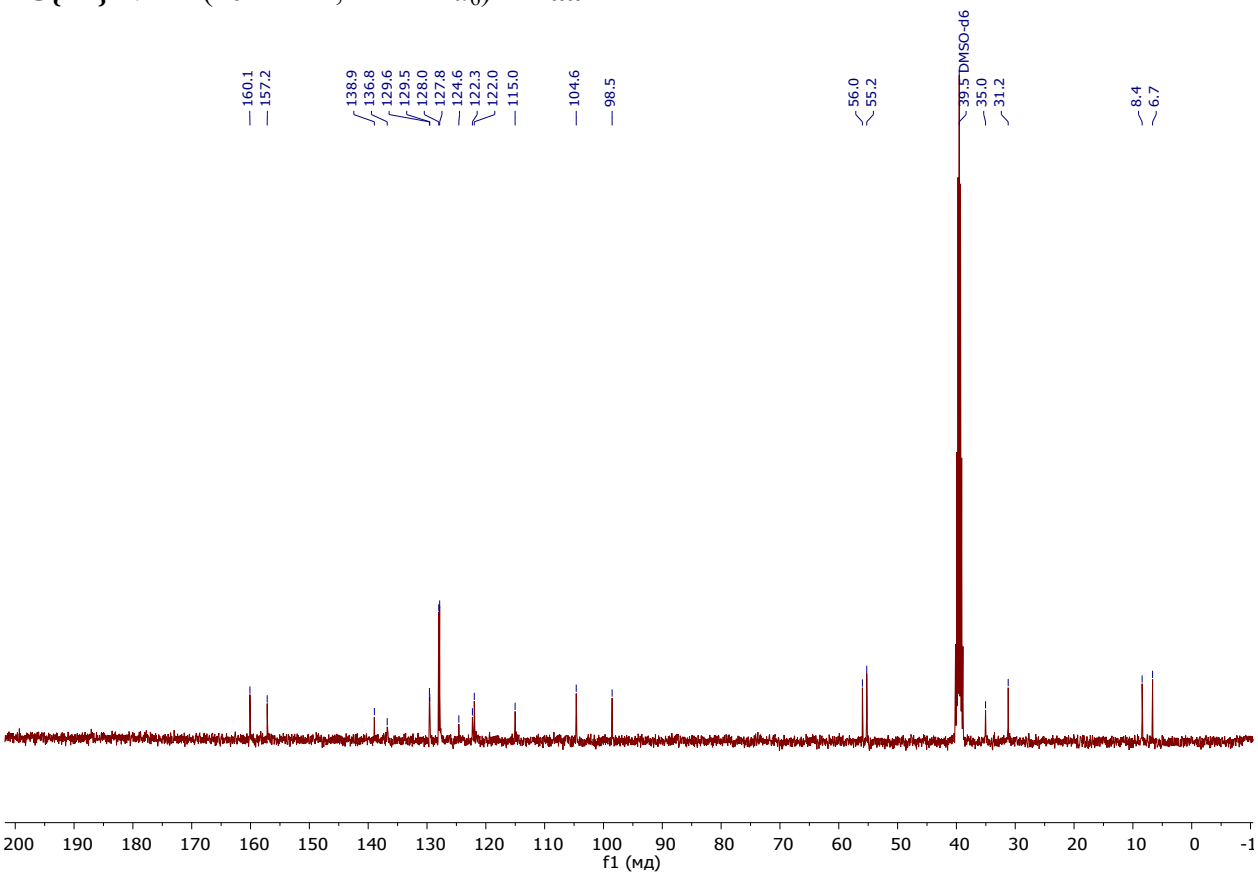
^{1}H NMR (400 MHz, DMSO-d_6) of **4aa** solvate with EtOH



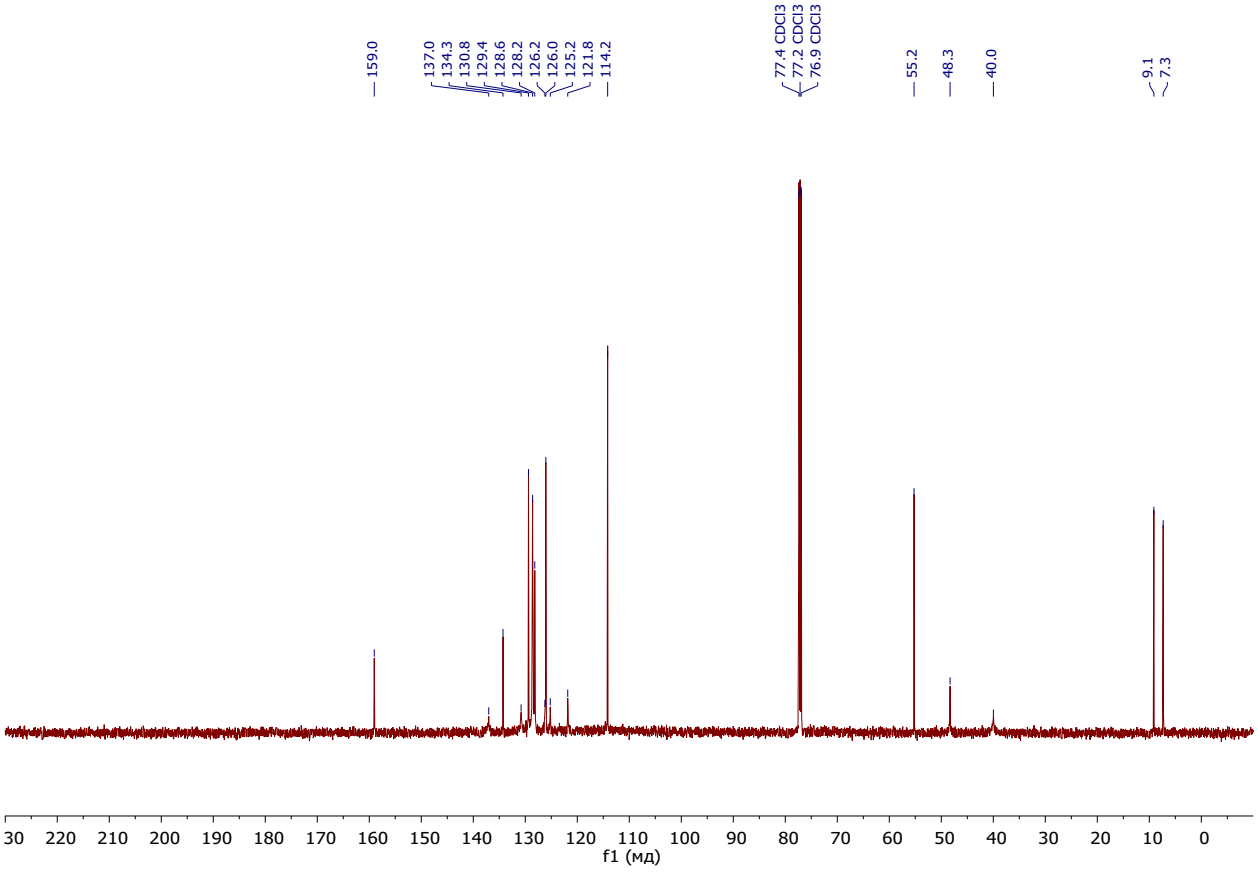
^{1}H NMR (600 MHz, $CDCl_3$) of **4aa**



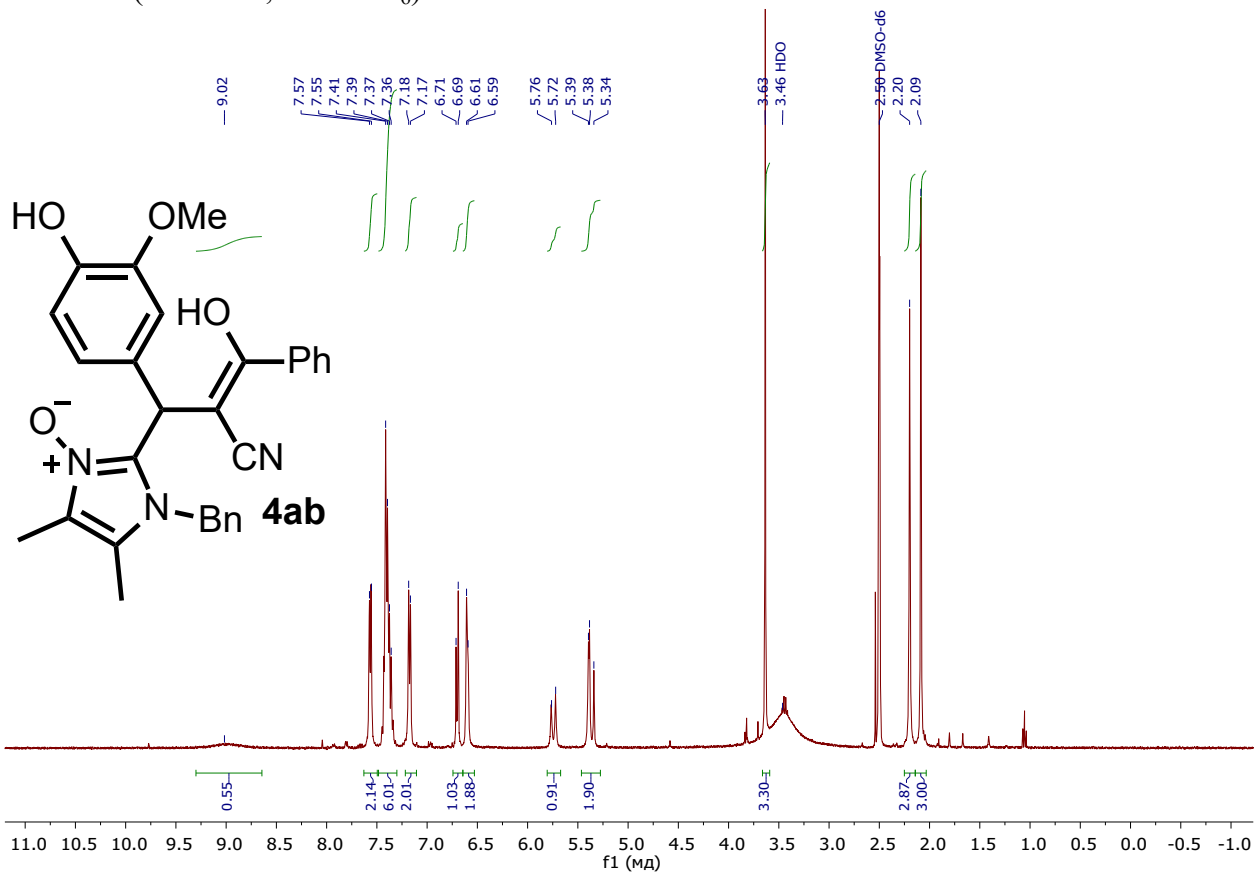
$^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) of **4aa**



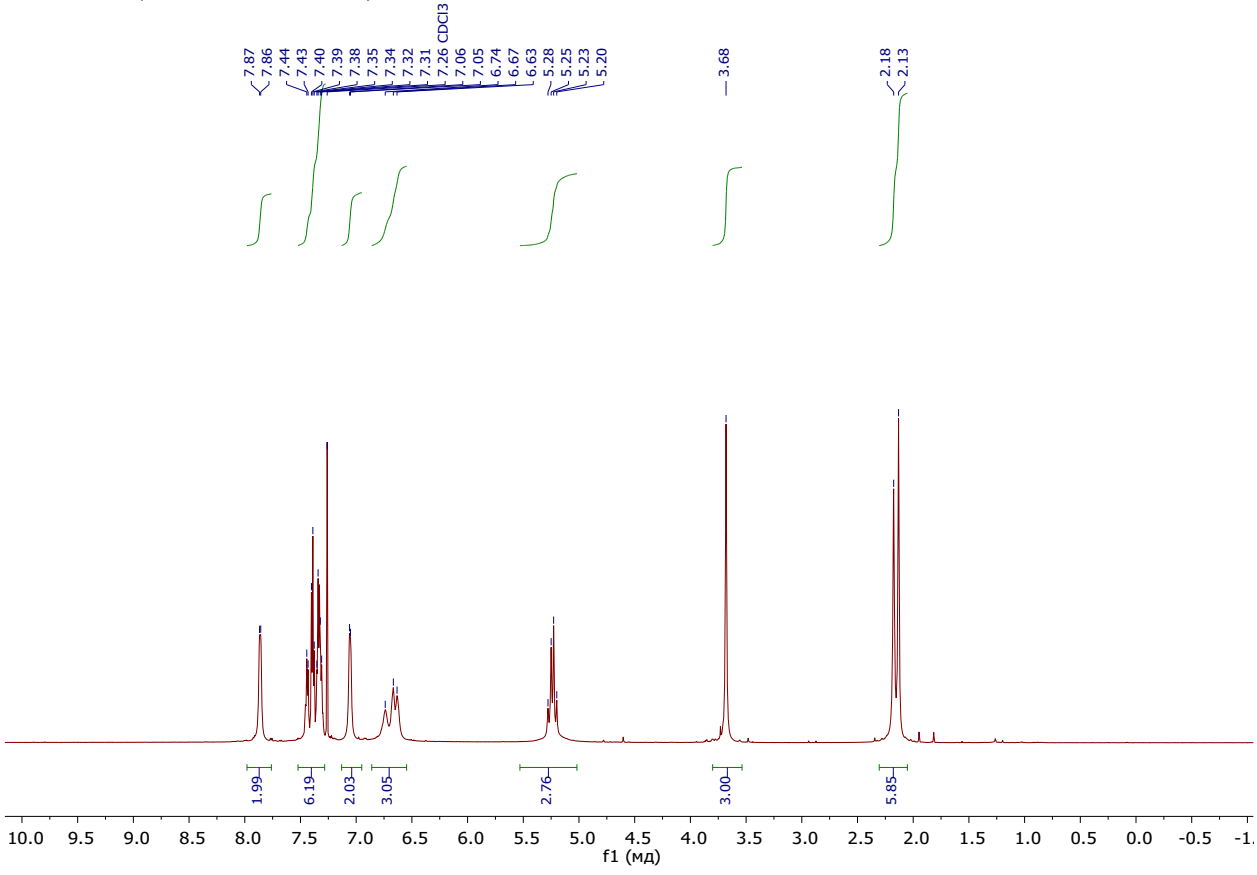
$^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$) of **4aa**



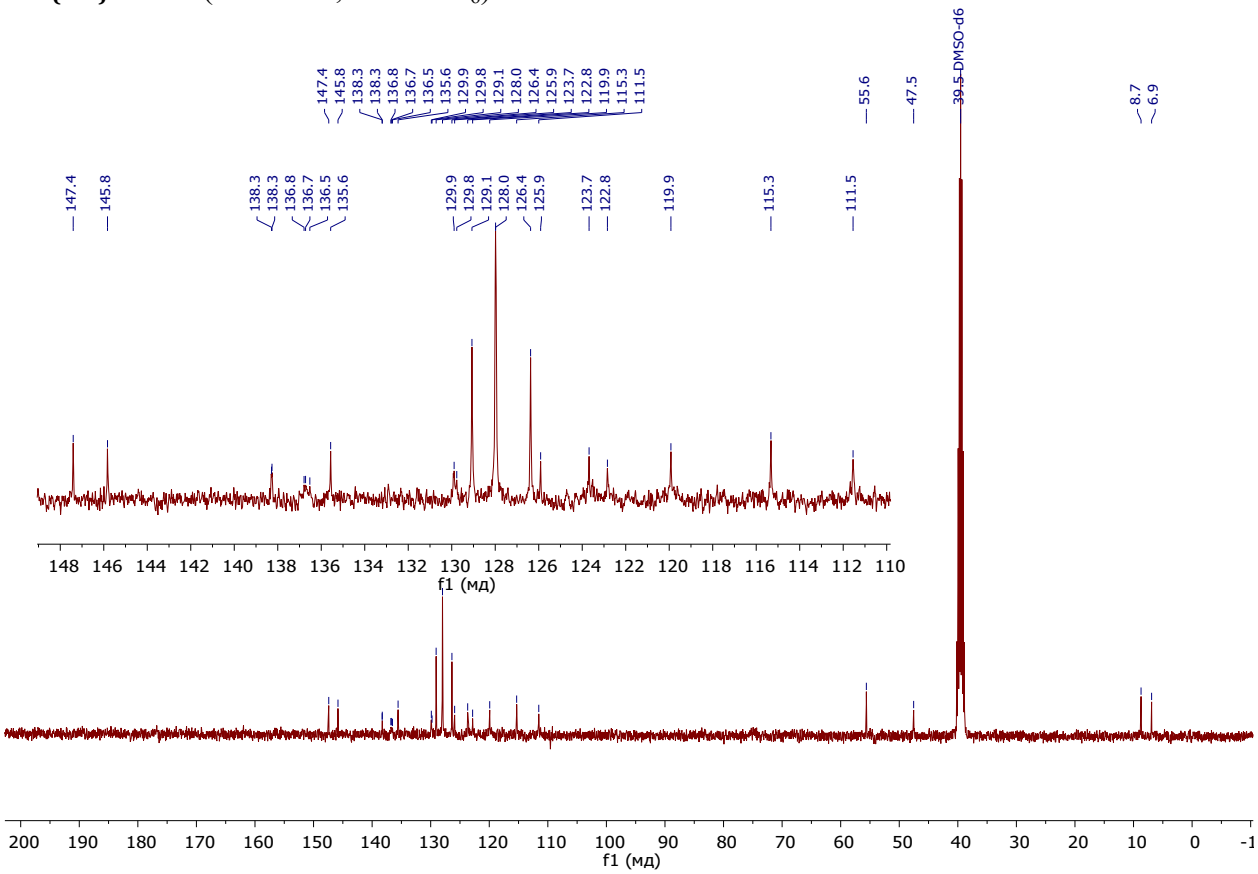
^{1}H NMR (400 MHz, DMSO-d_6) of **4ab**



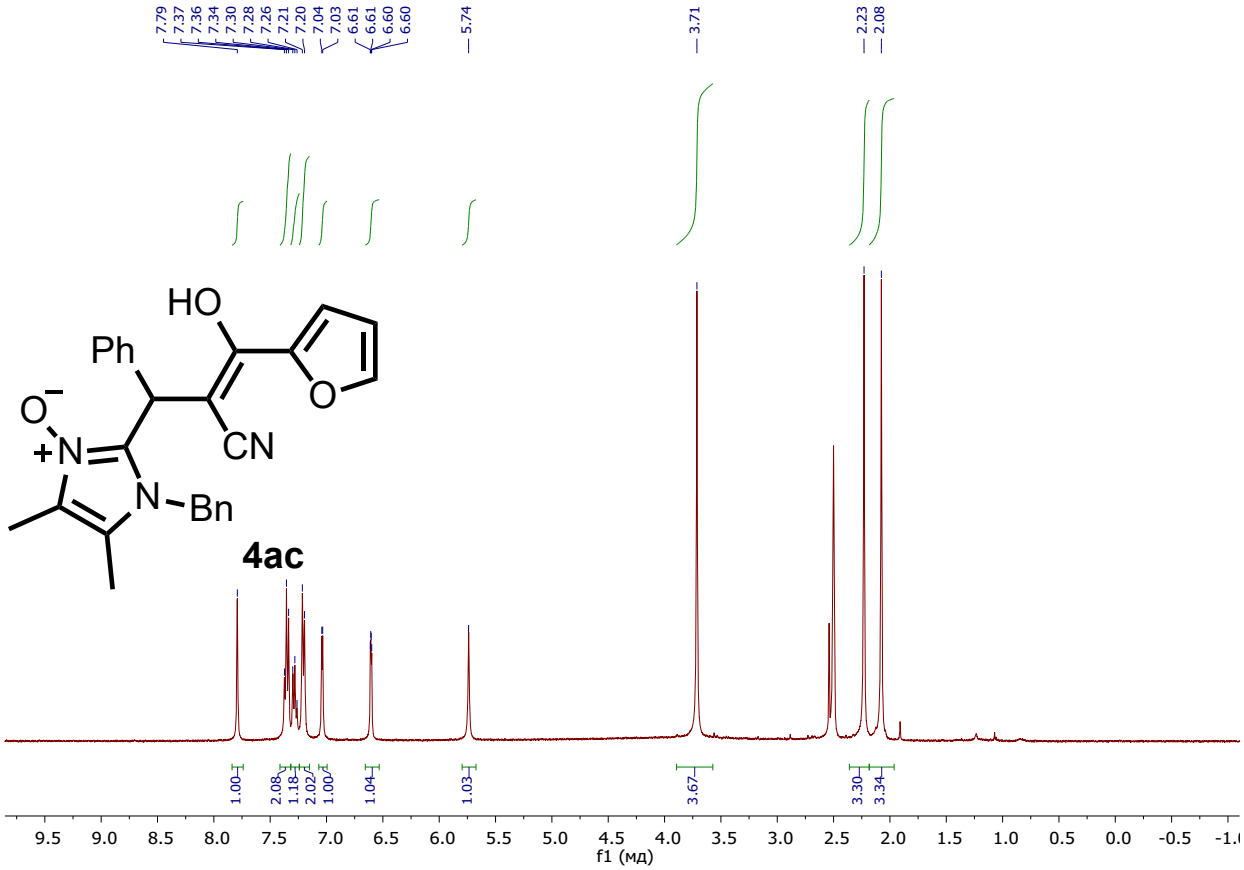
^{1}H NMR (600 MHz, $CDCl_3$) of **4ab**



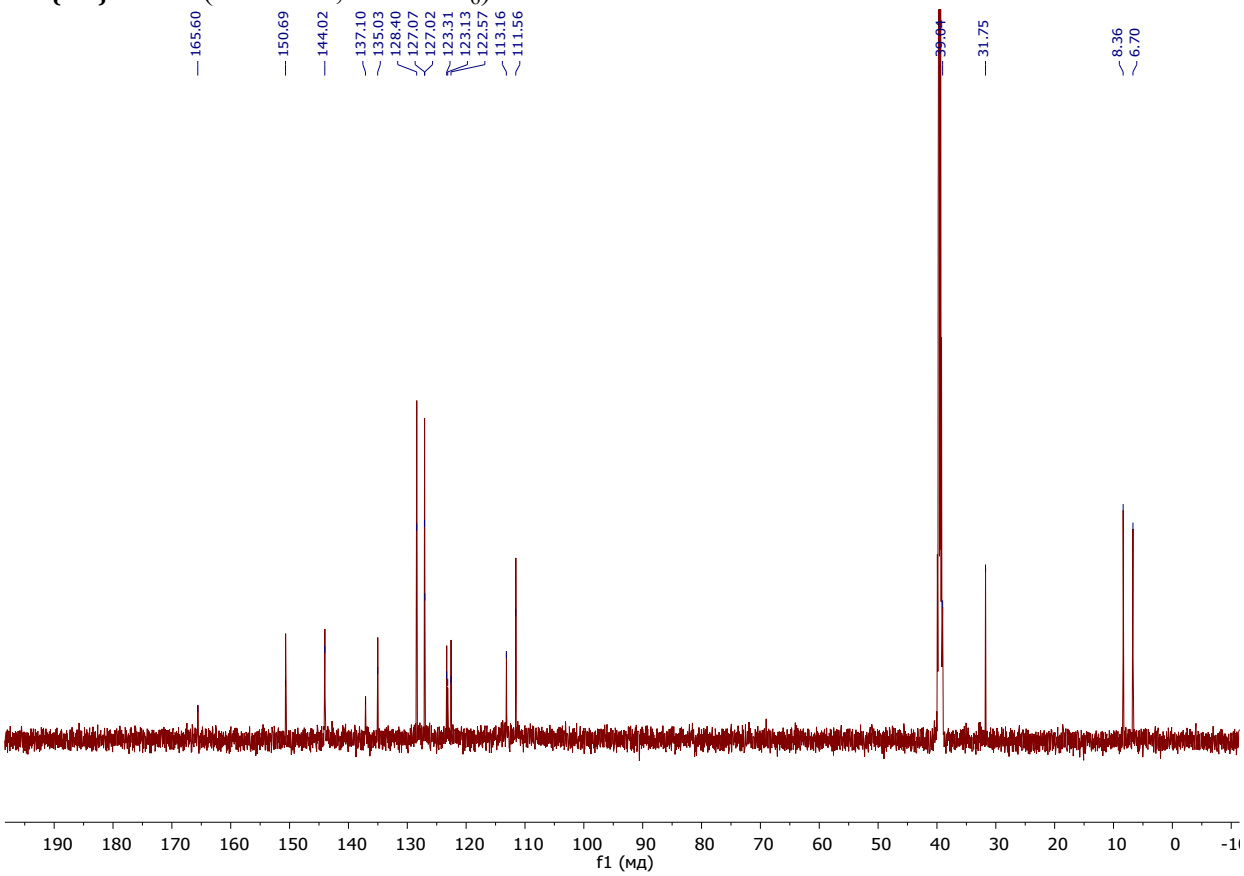
$^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) of **4ab**



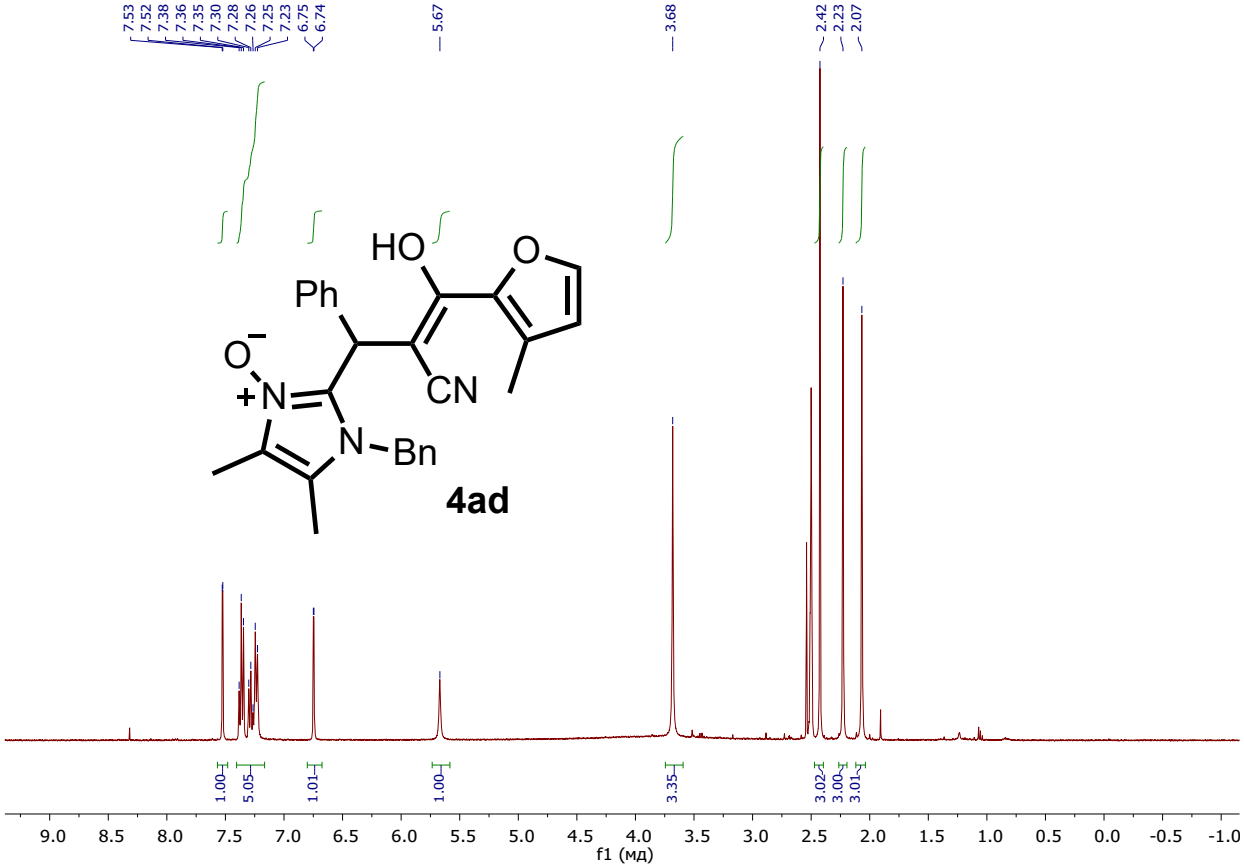
^{1}H NMR (400 MHz, DMSO-d_6) of **4ac**



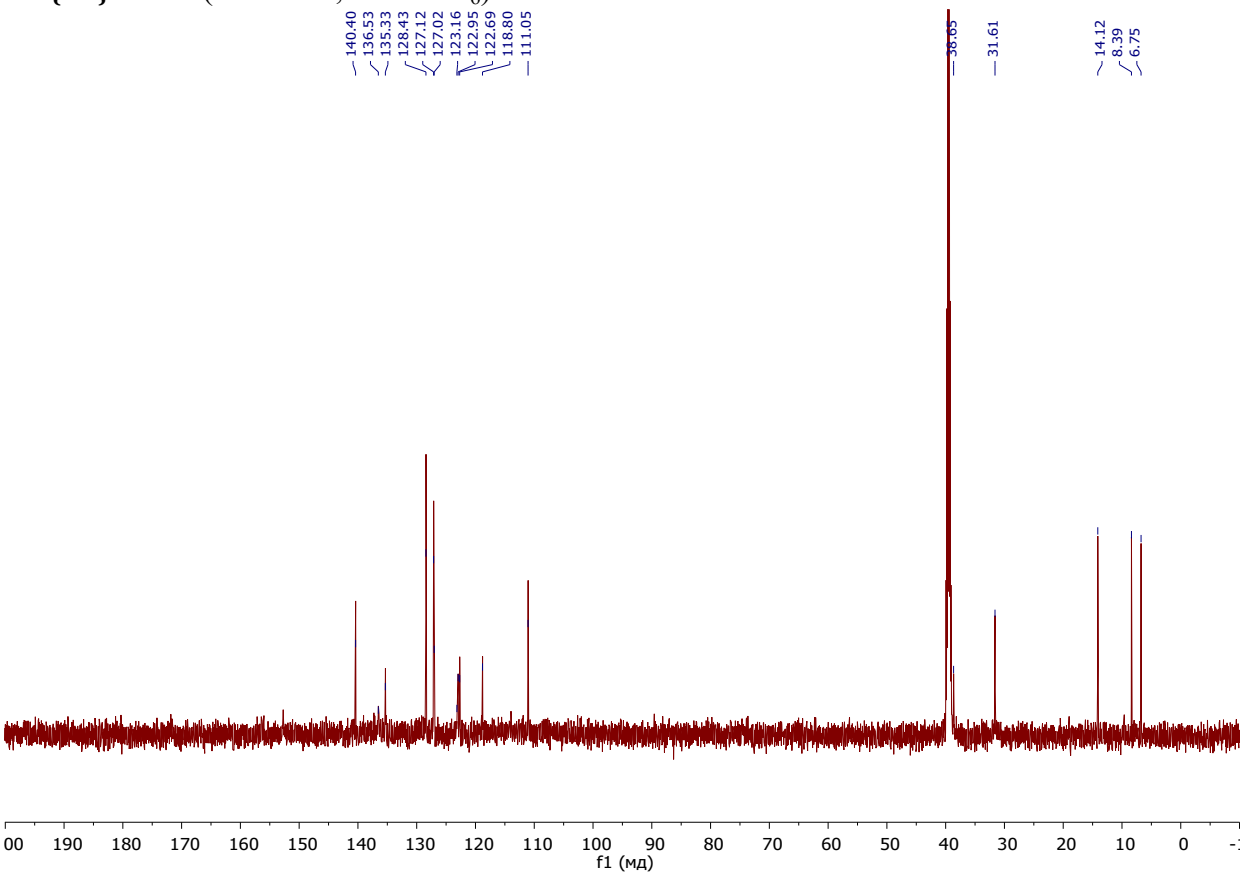
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4ac**



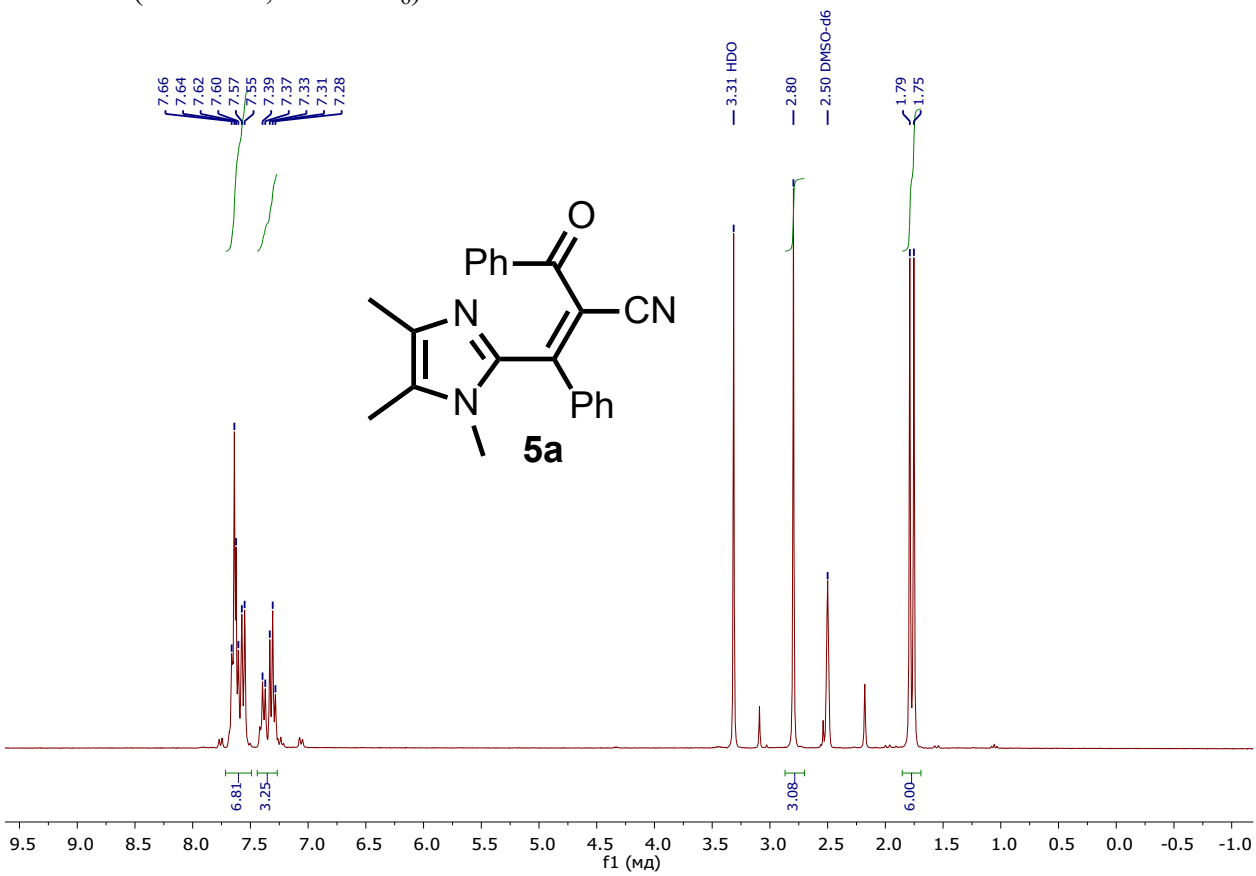
^{1}H NMR (400 MHz, DMSO-d_6) of **4ad**



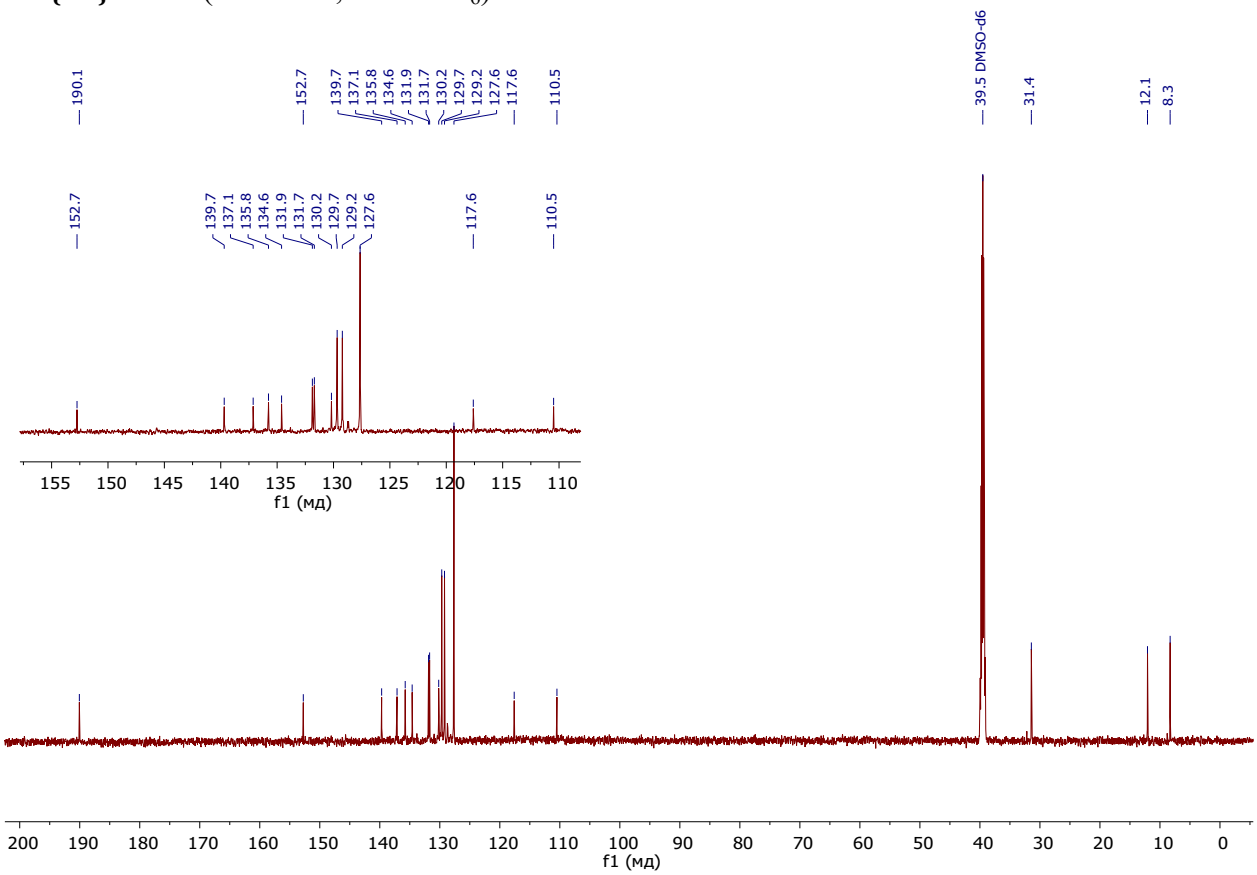
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **4ad**



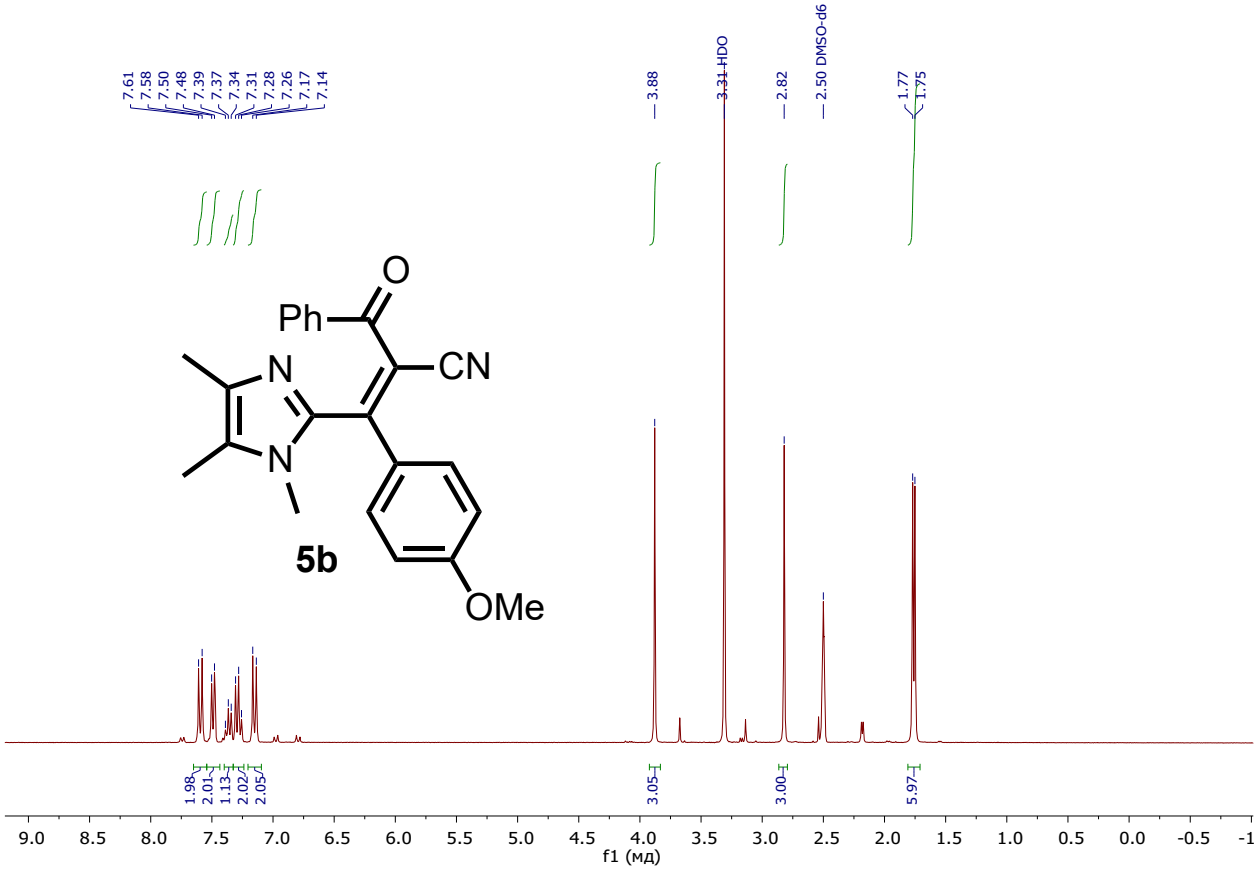
^{1}H NMR (300 MHz, DMSO-d_6) of **5a**



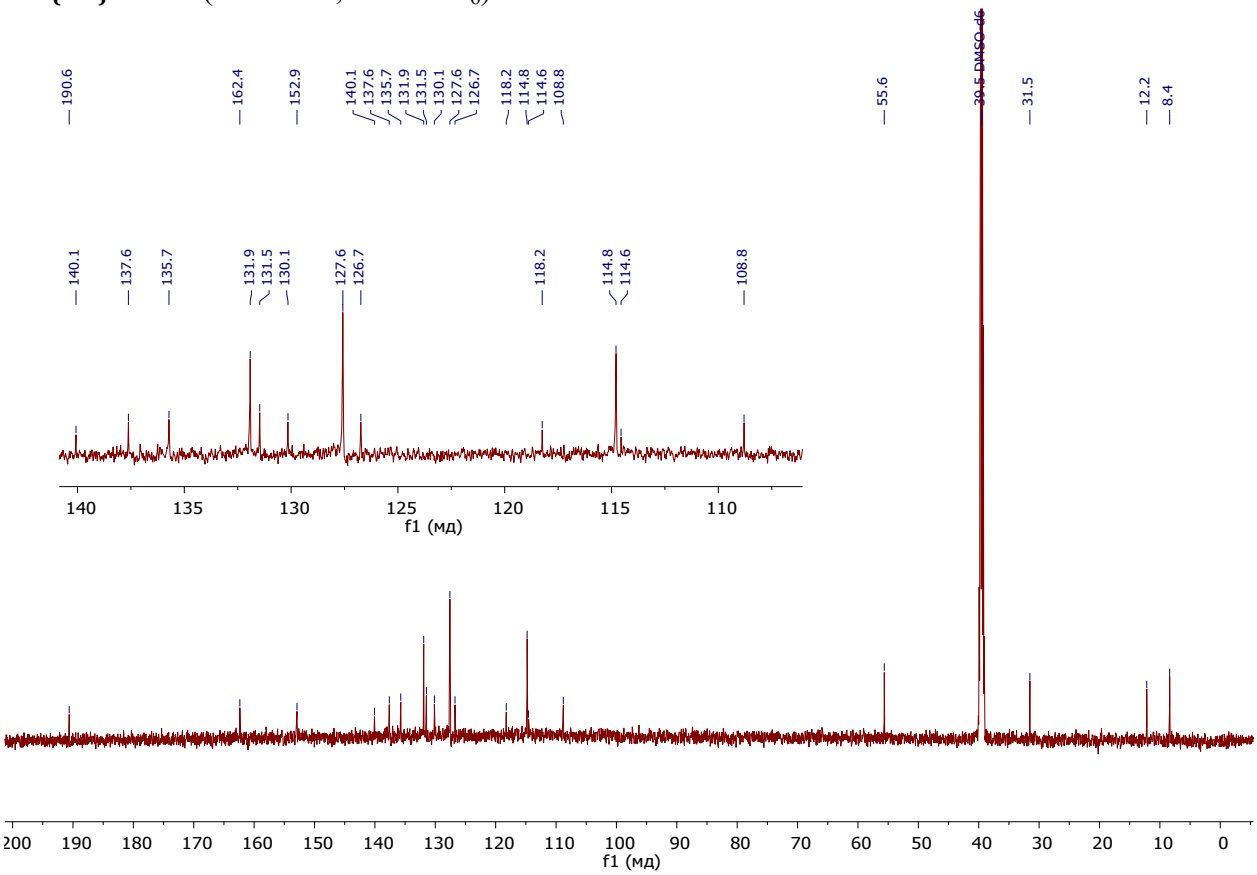
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5a**



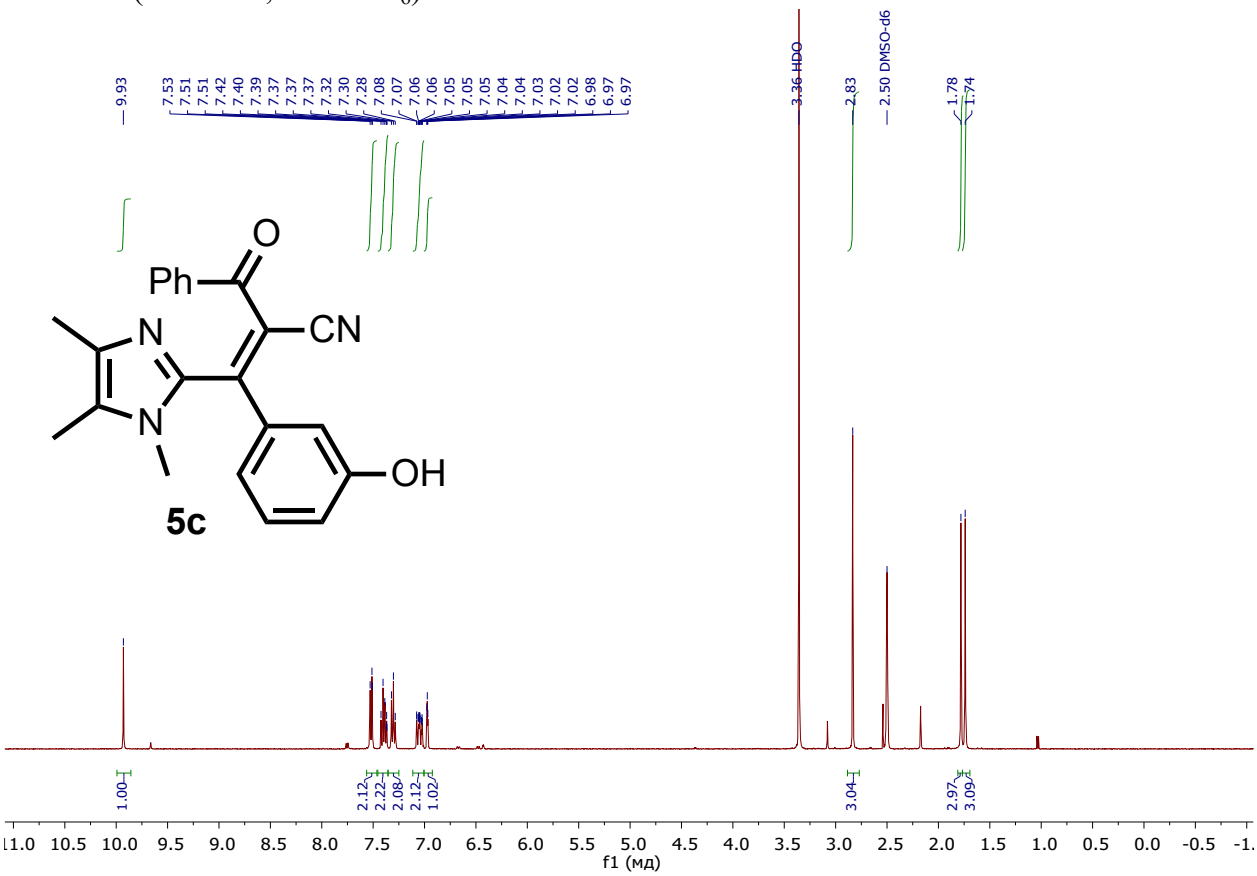
^{1}H NMR (300 MHz, DMSO-d_6) of **5b**



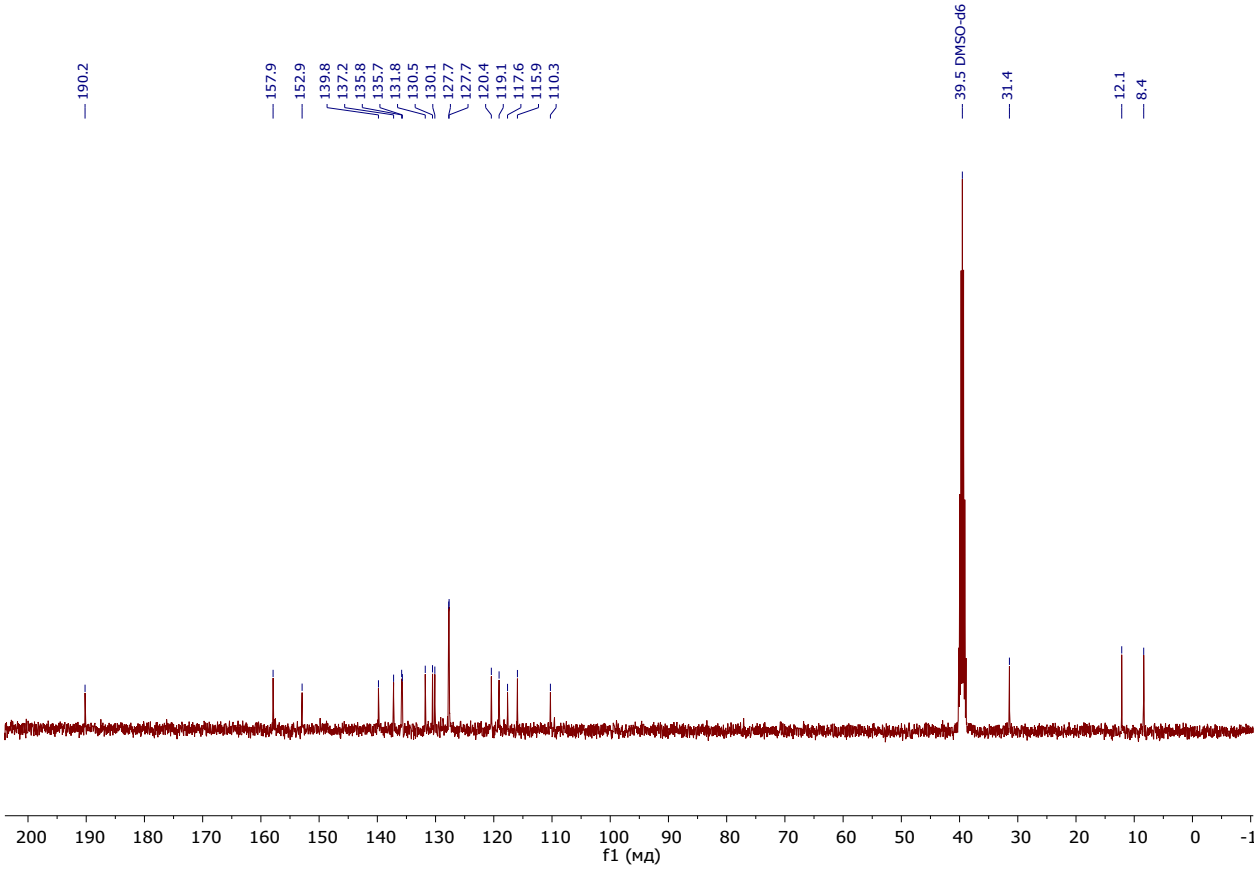
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5b**



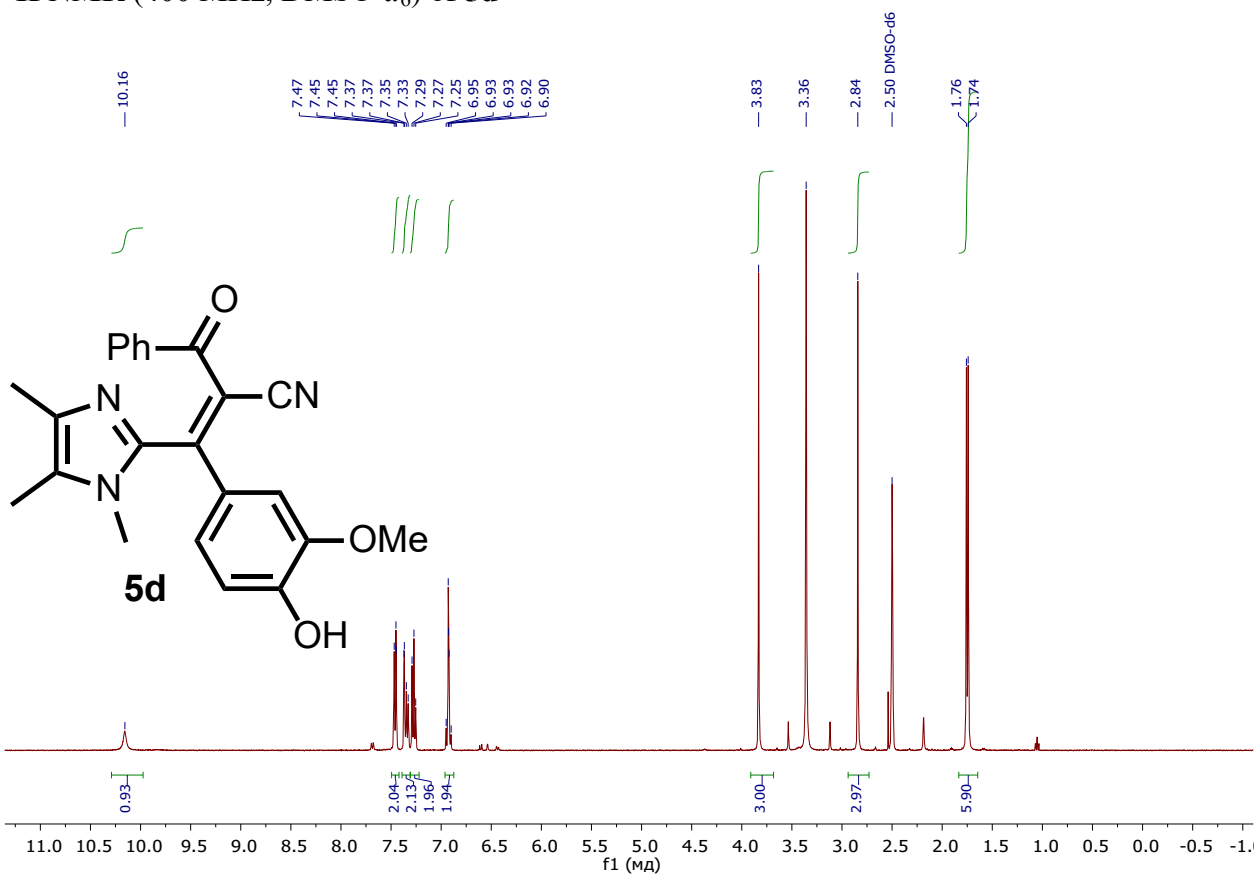
^{1}H NMR (400 MHz, DMSO-d_6) of **5c**



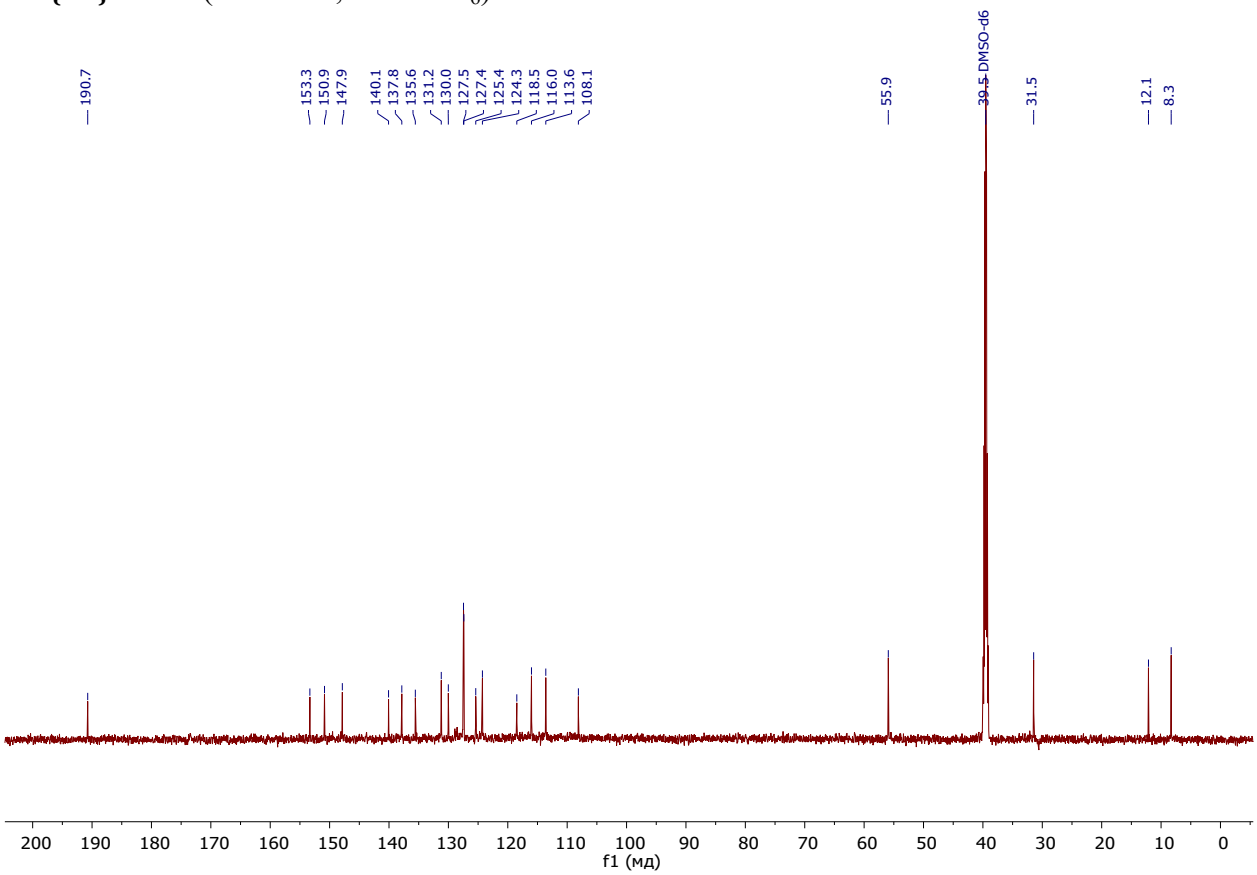
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **5c**



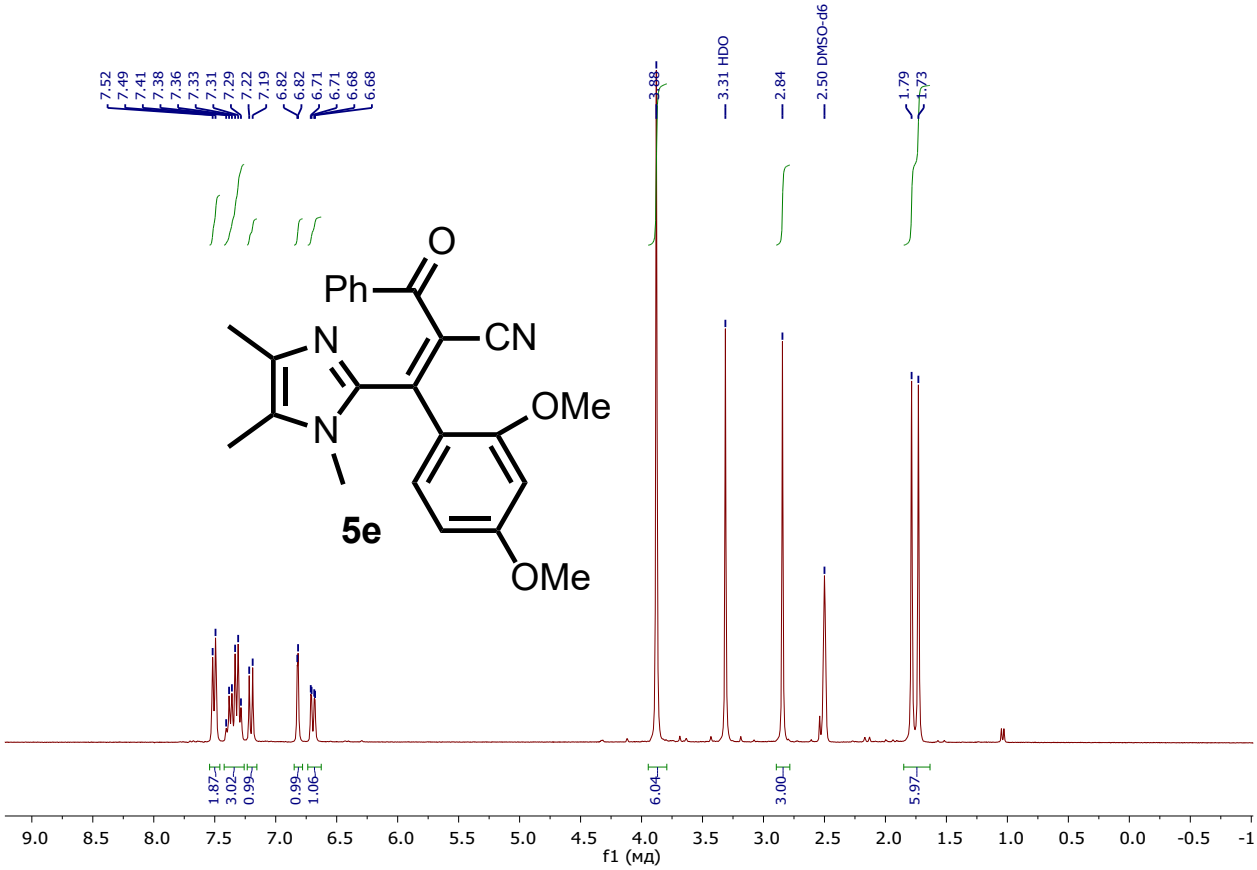
^{1}H NMR (400 MHz, DMSO-d_6) of **5d**



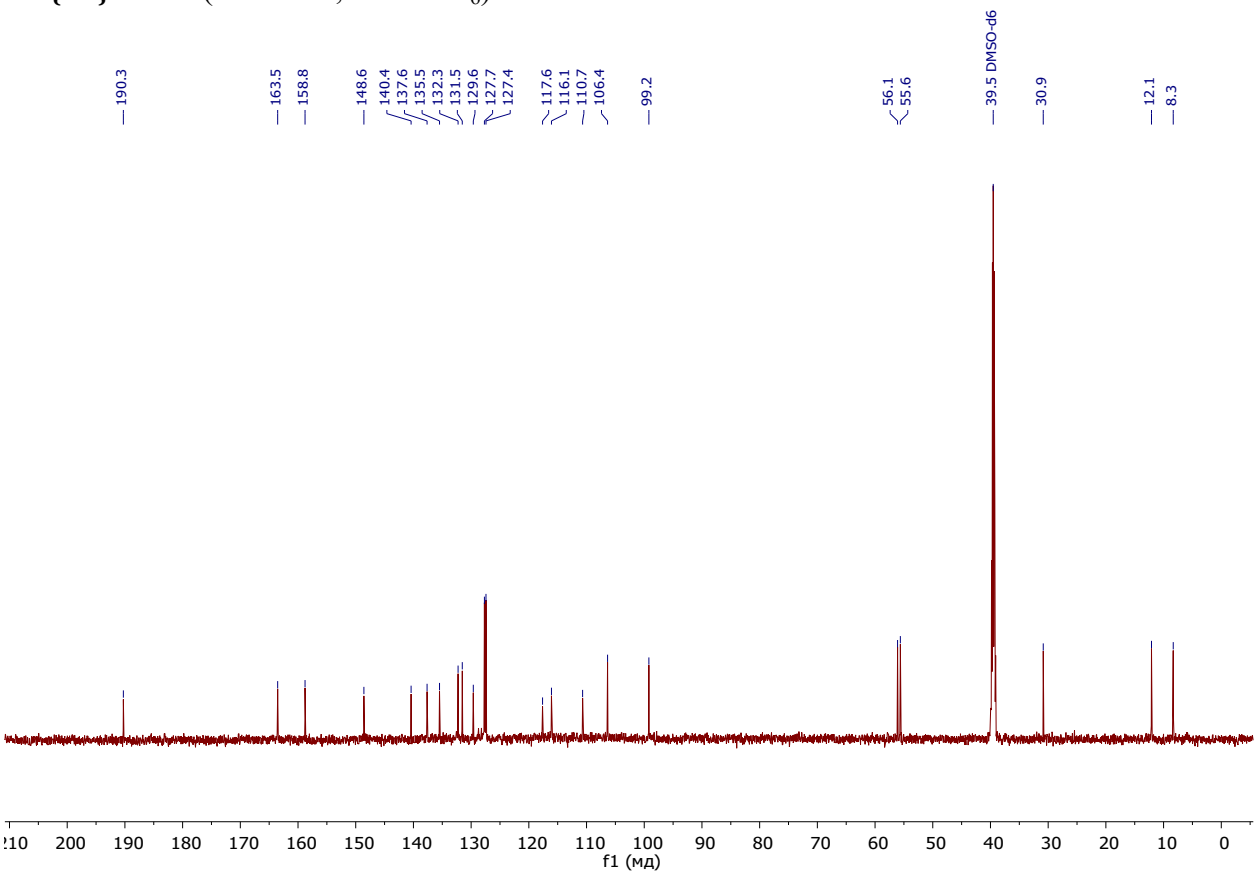
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5d**



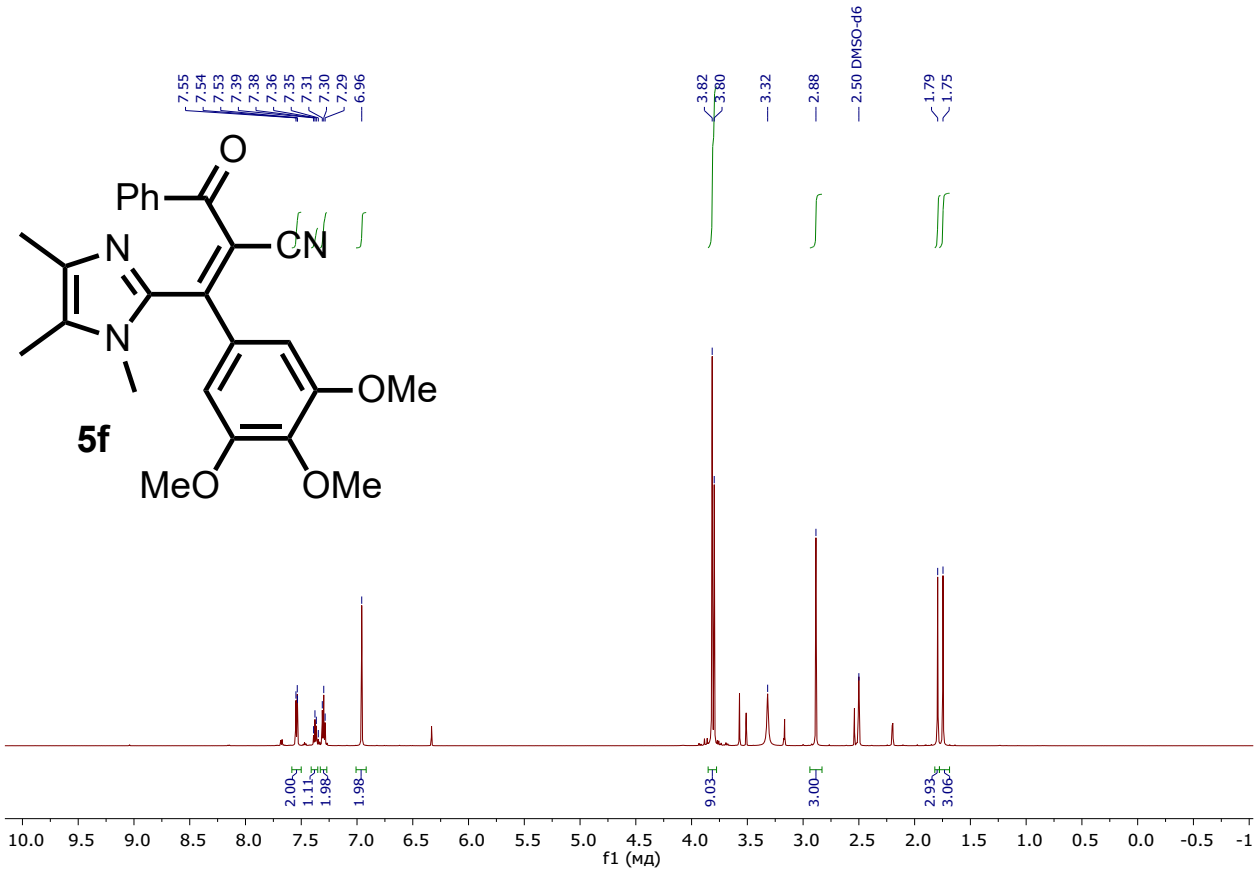
^{1}H NMR (300 MHz, DMSO-d_6) of **5e**



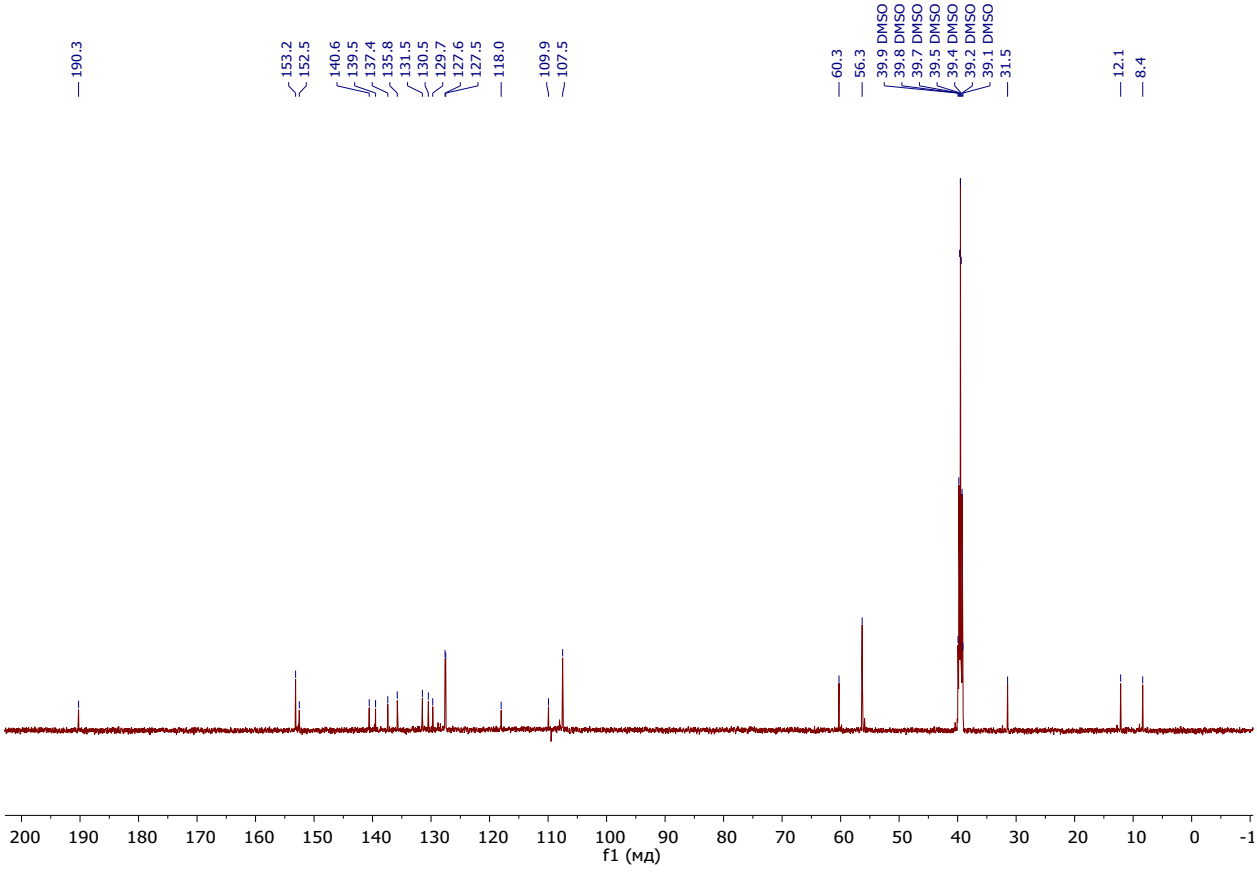
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5e**



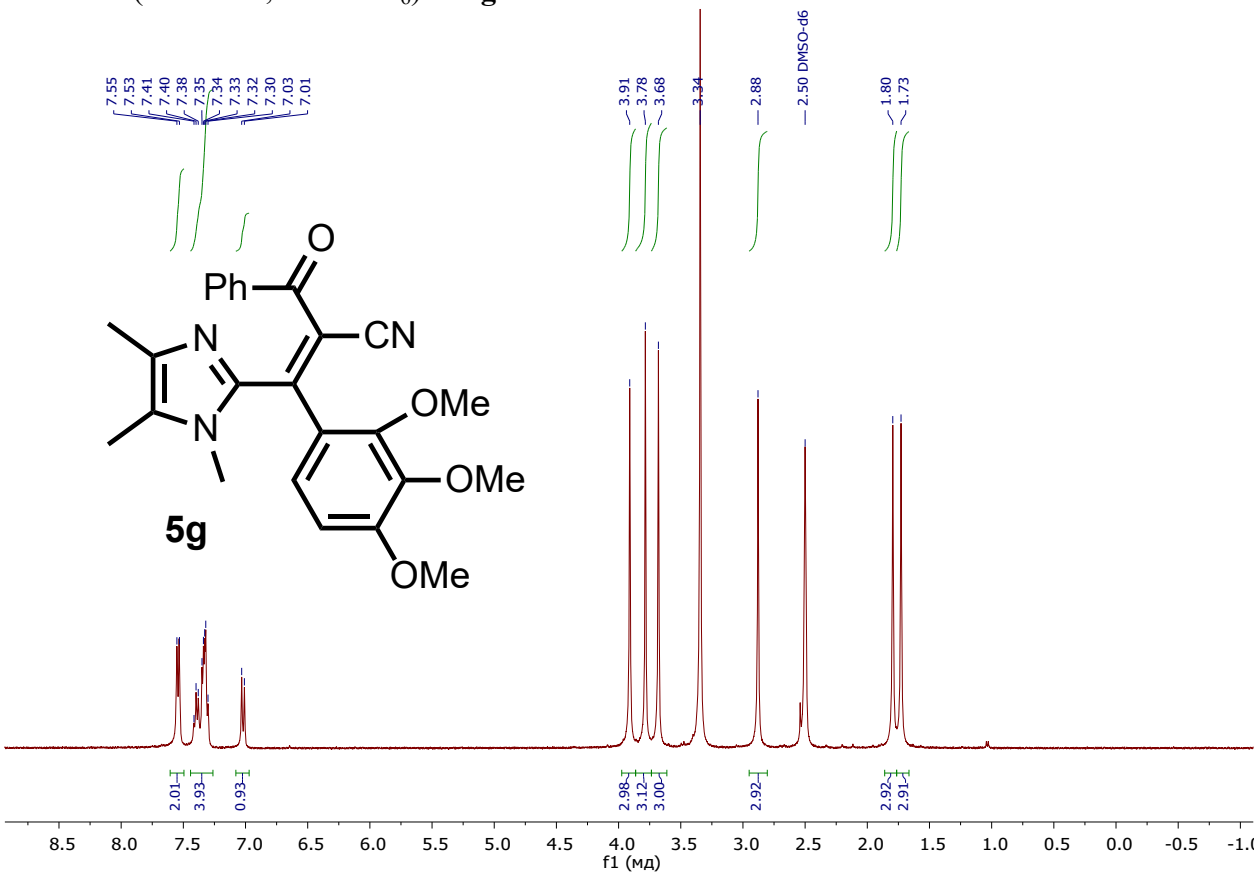
^{1}H NMR (600 MHz, DMSO-d_6) of **5f** (+ ~5 mol. % of (*E*)-isomer)



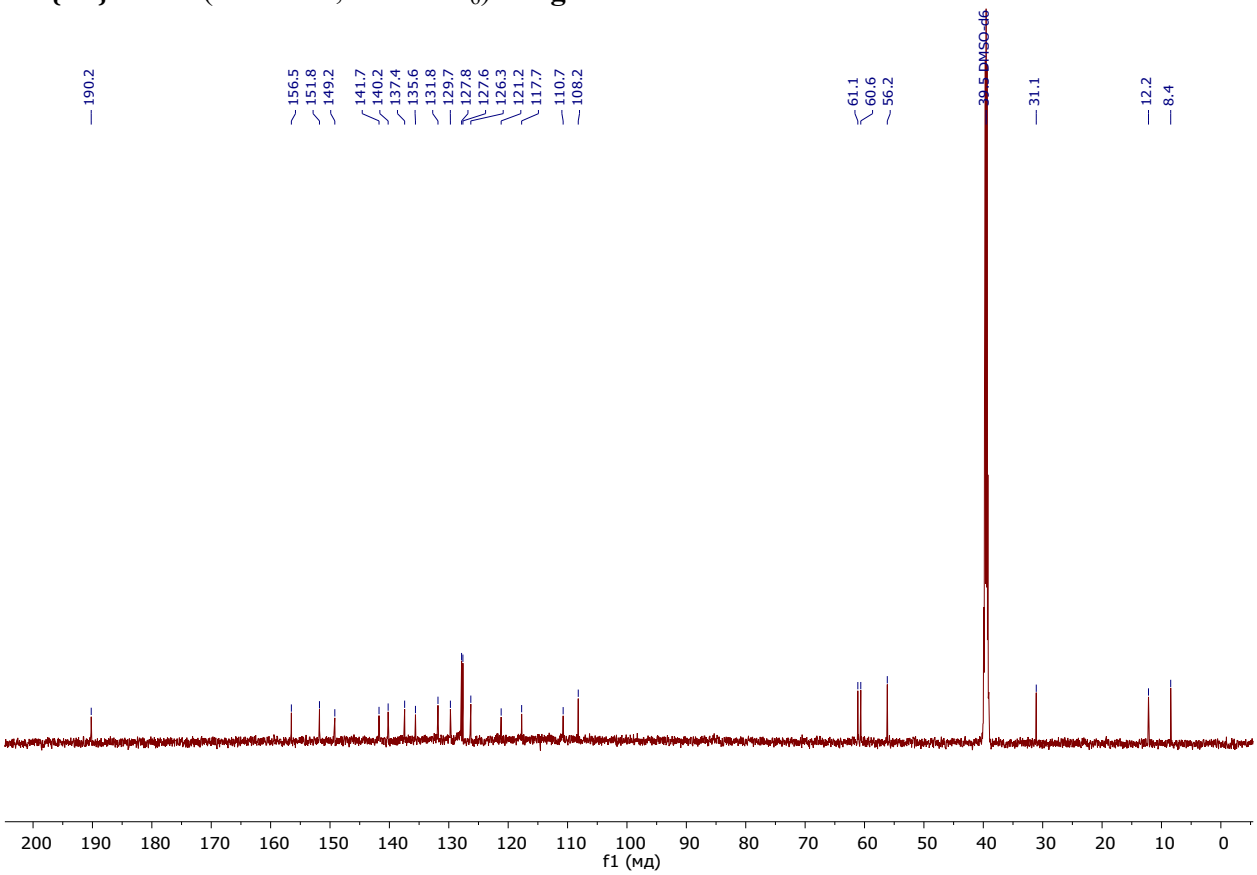
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5f**



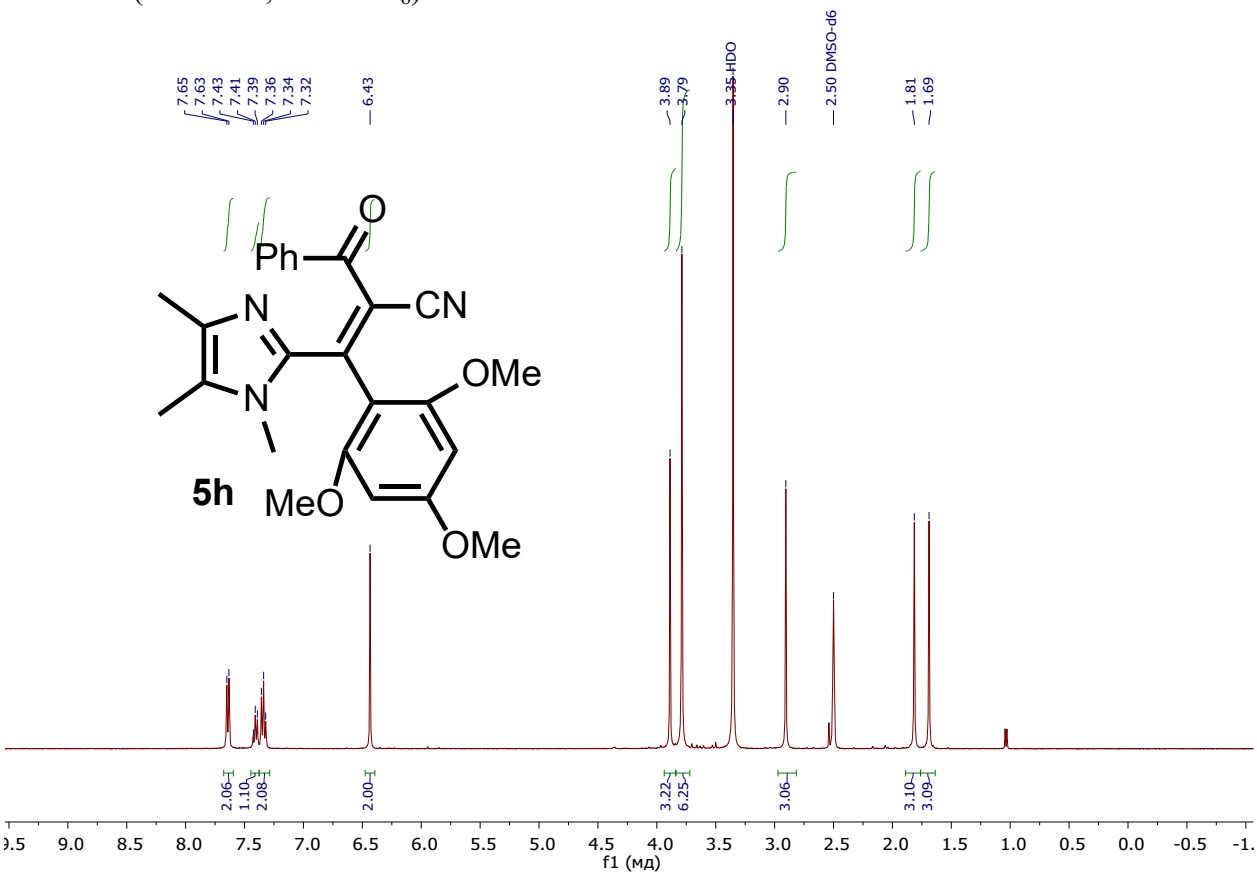
^{1}H NMR (400 MHz, DMSO-d_6) of **5g**



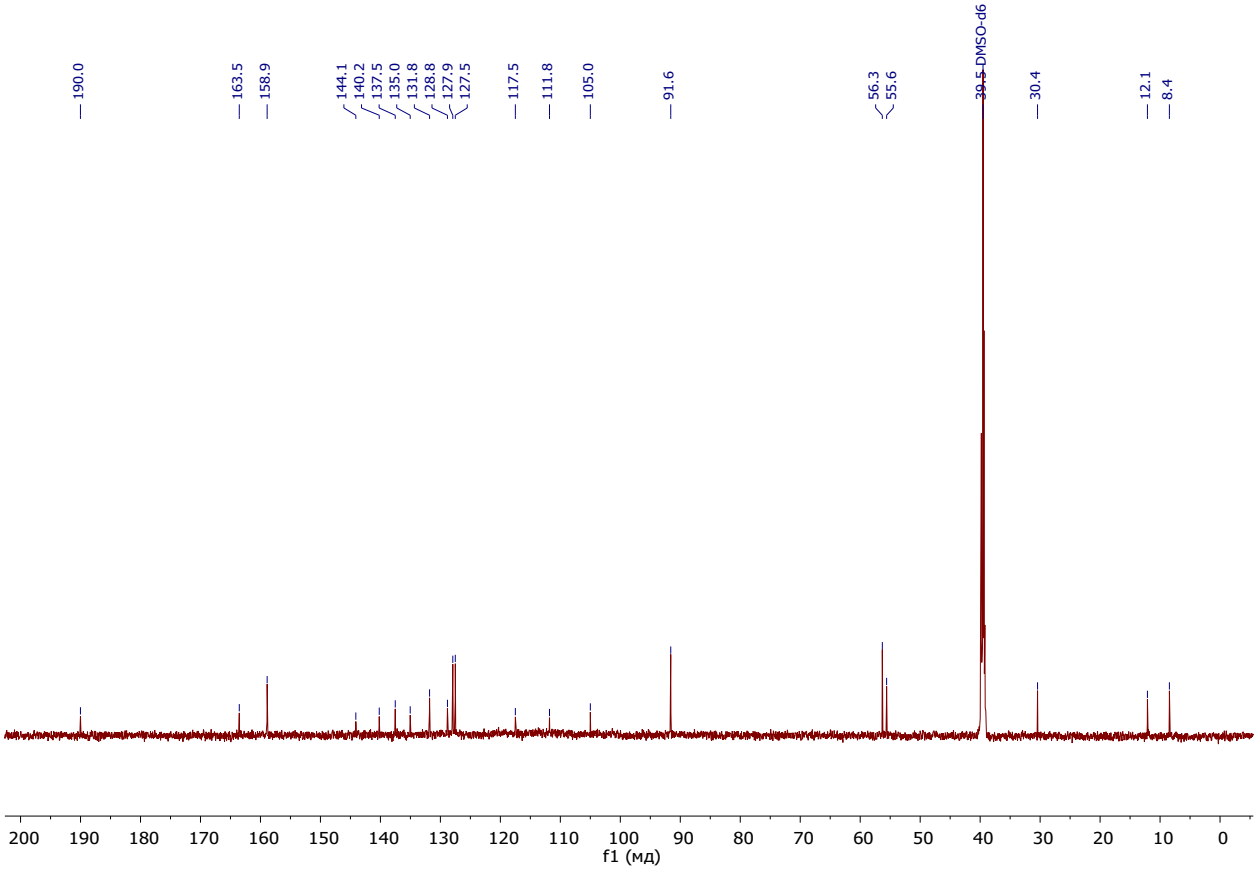
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5g**



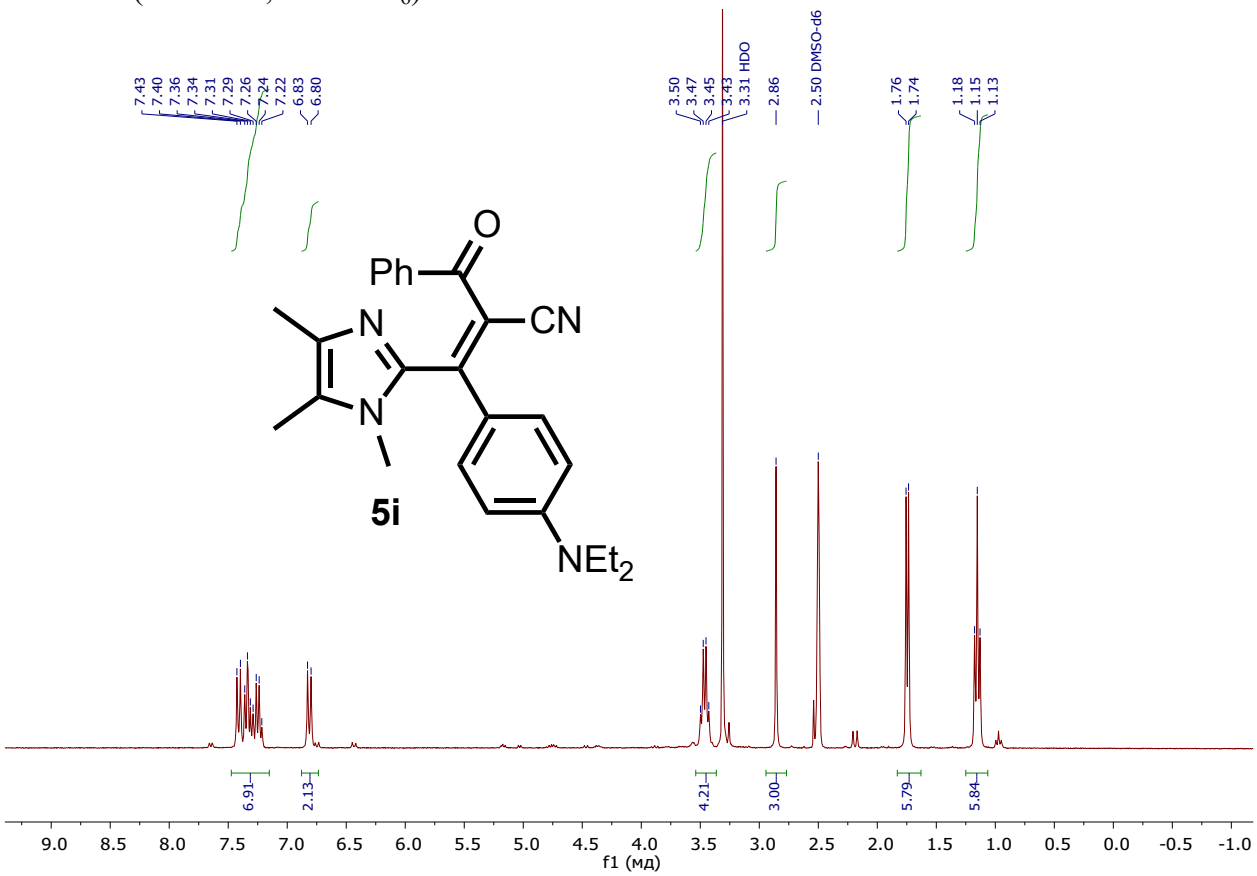
^{1}H NMR (400 MHz, DMSO-d_6) of **5h**



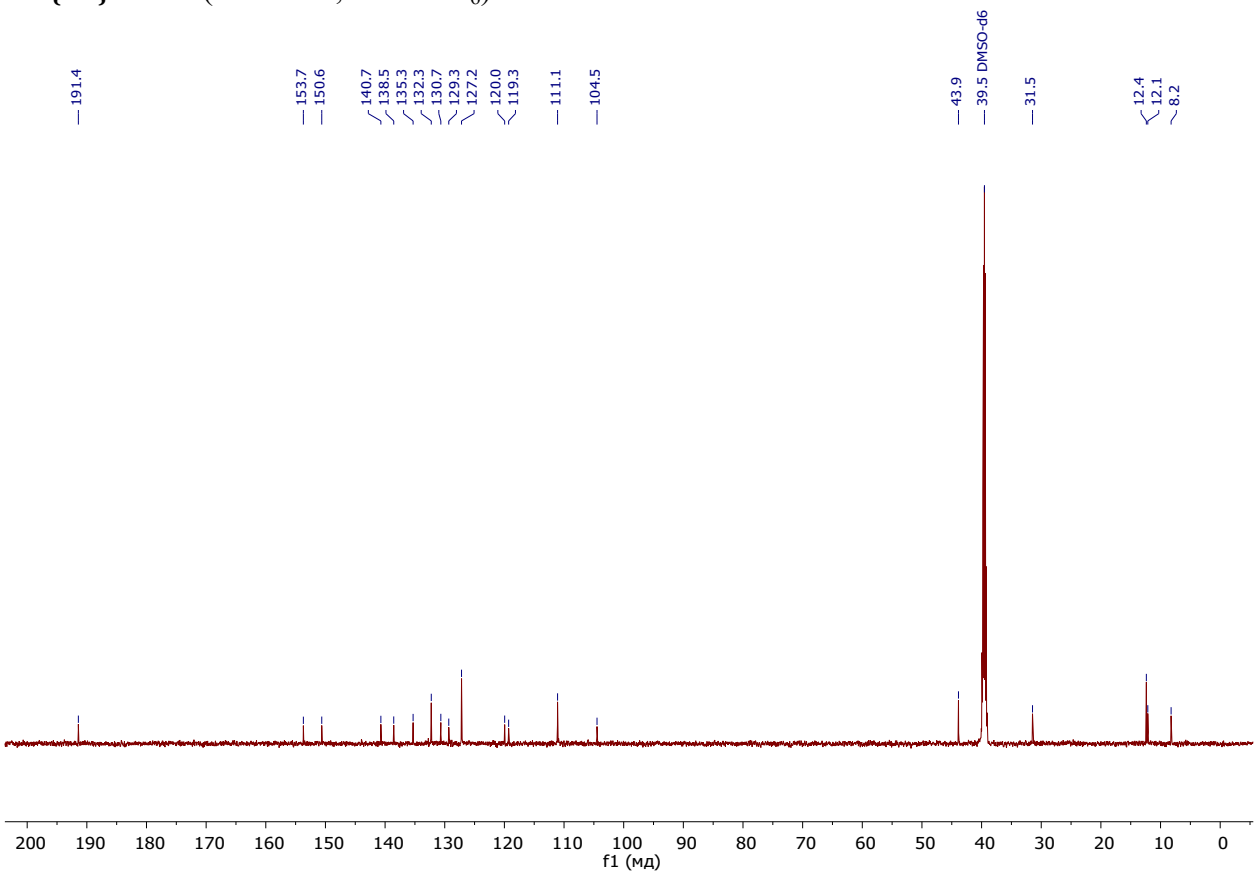
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5h**



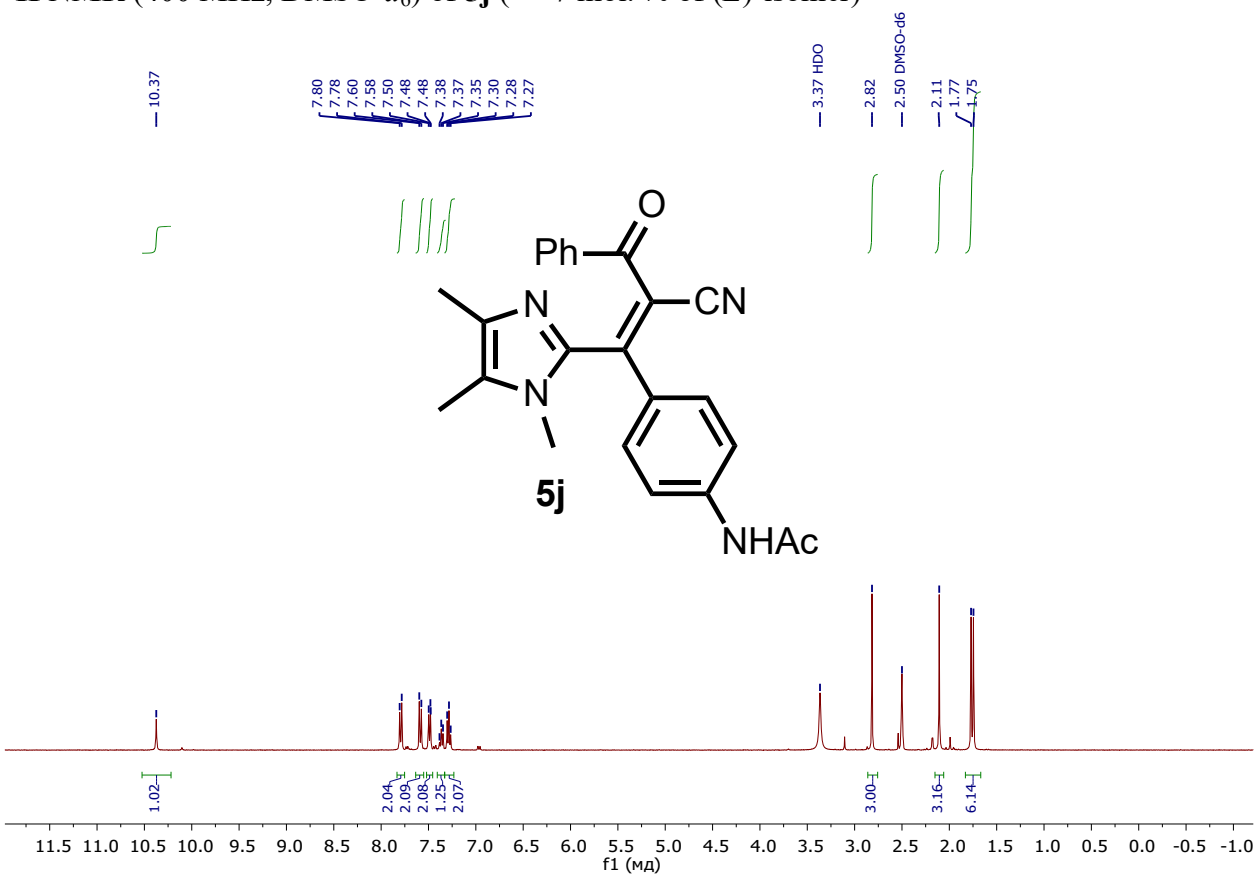
^{1}H NMR (300 MHz, DMSO-d_6) of **5i**



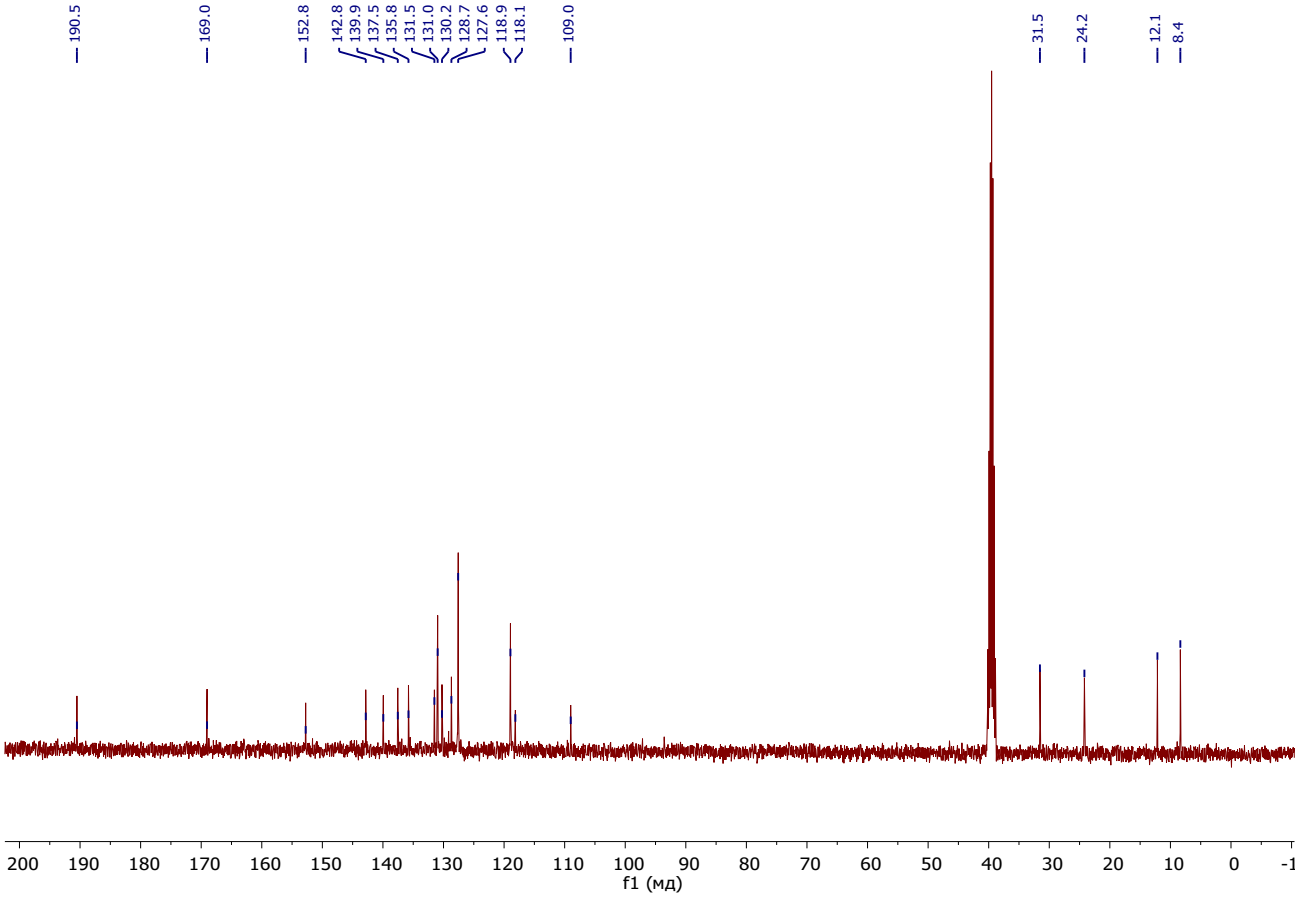
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5i**



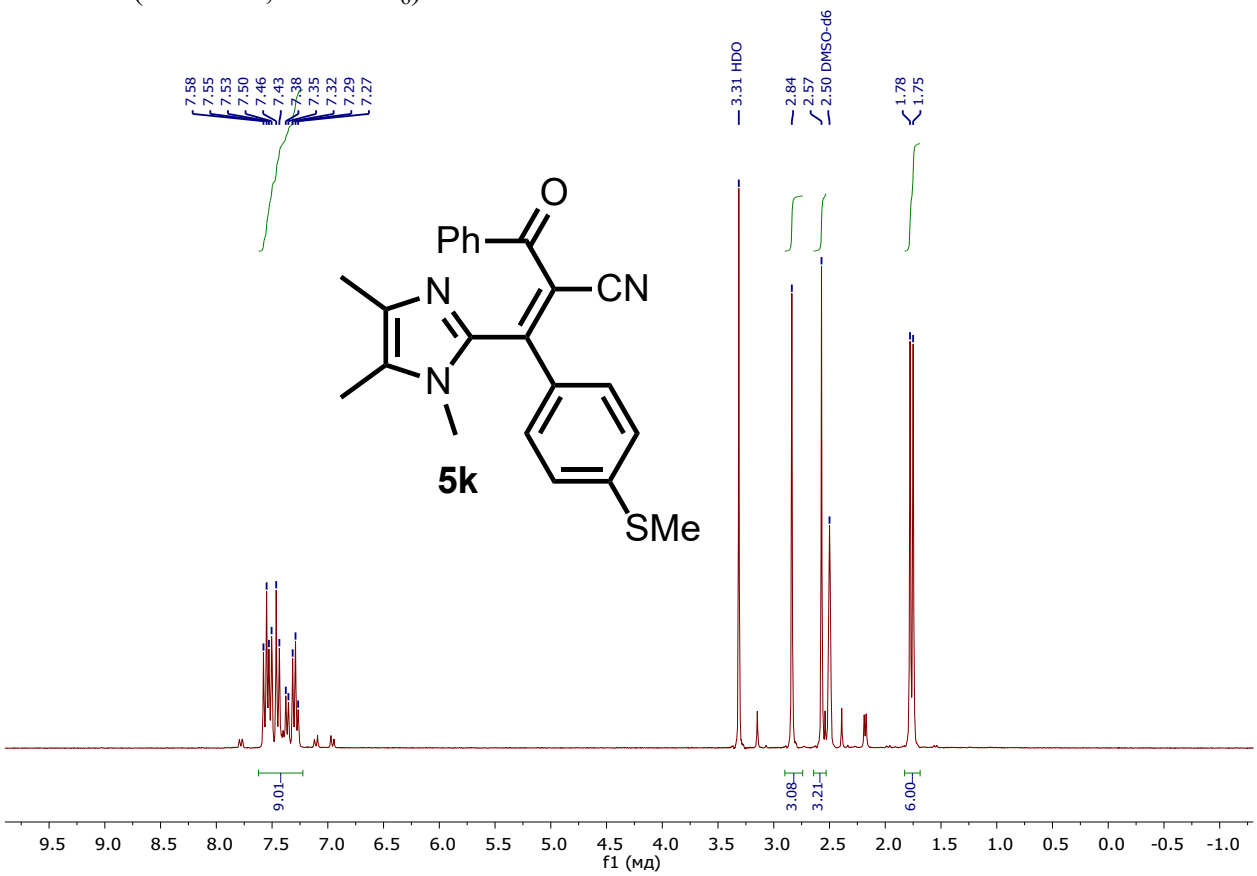
^{1}H NMR (400 MHz, DMSO-d_6) of **5j** (+ ~7 mol. % of (*E*)-isomer)



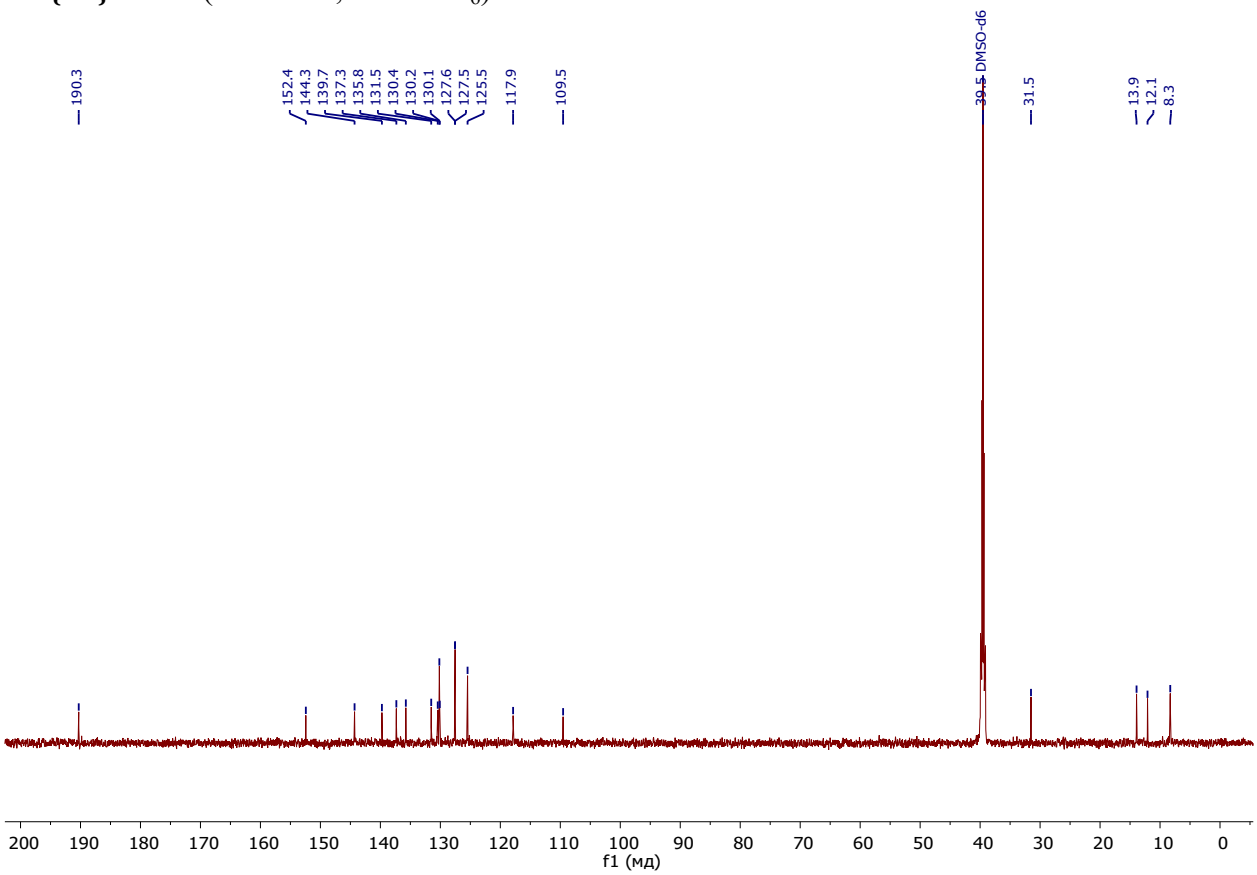
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of **5j**



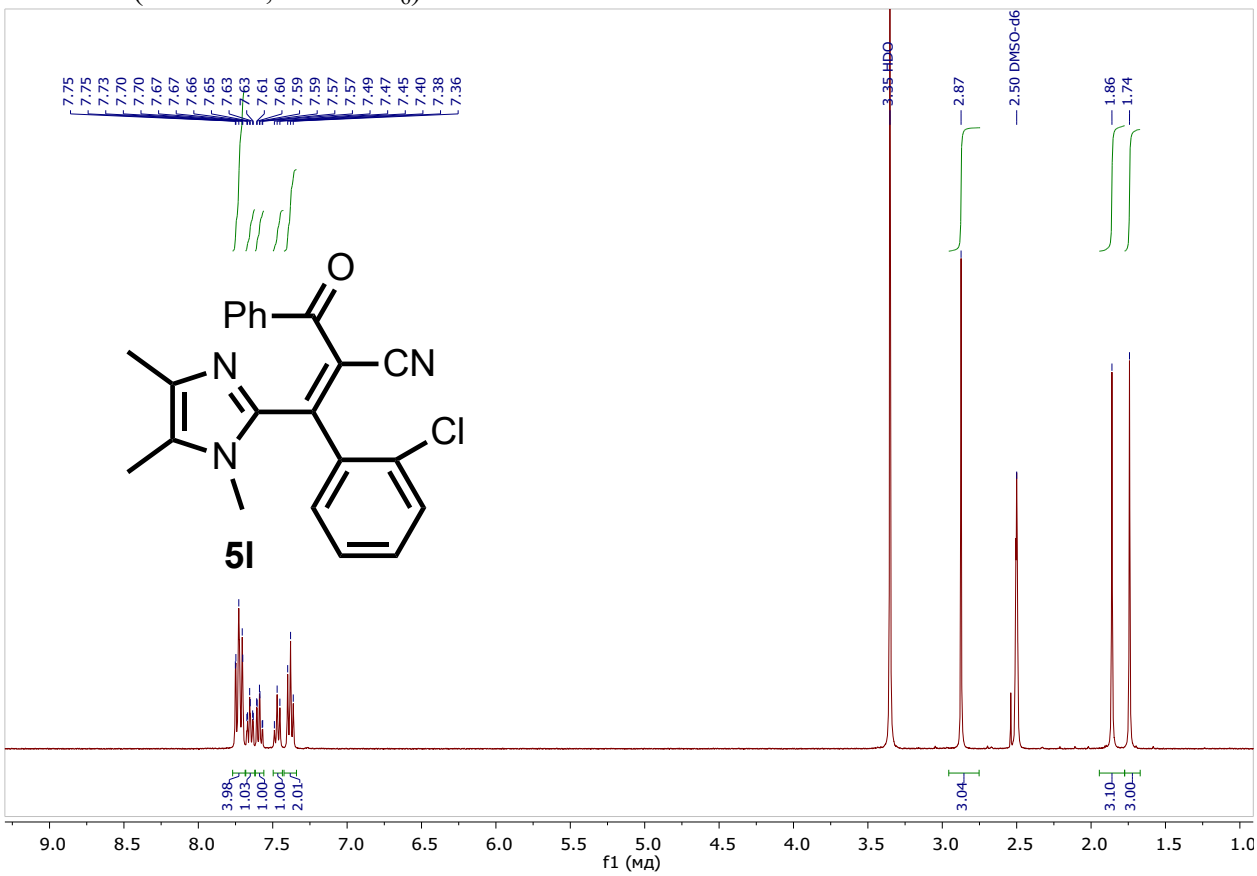
^{1}H NMR (300 MHz, DMSO-d_6) of **5k**



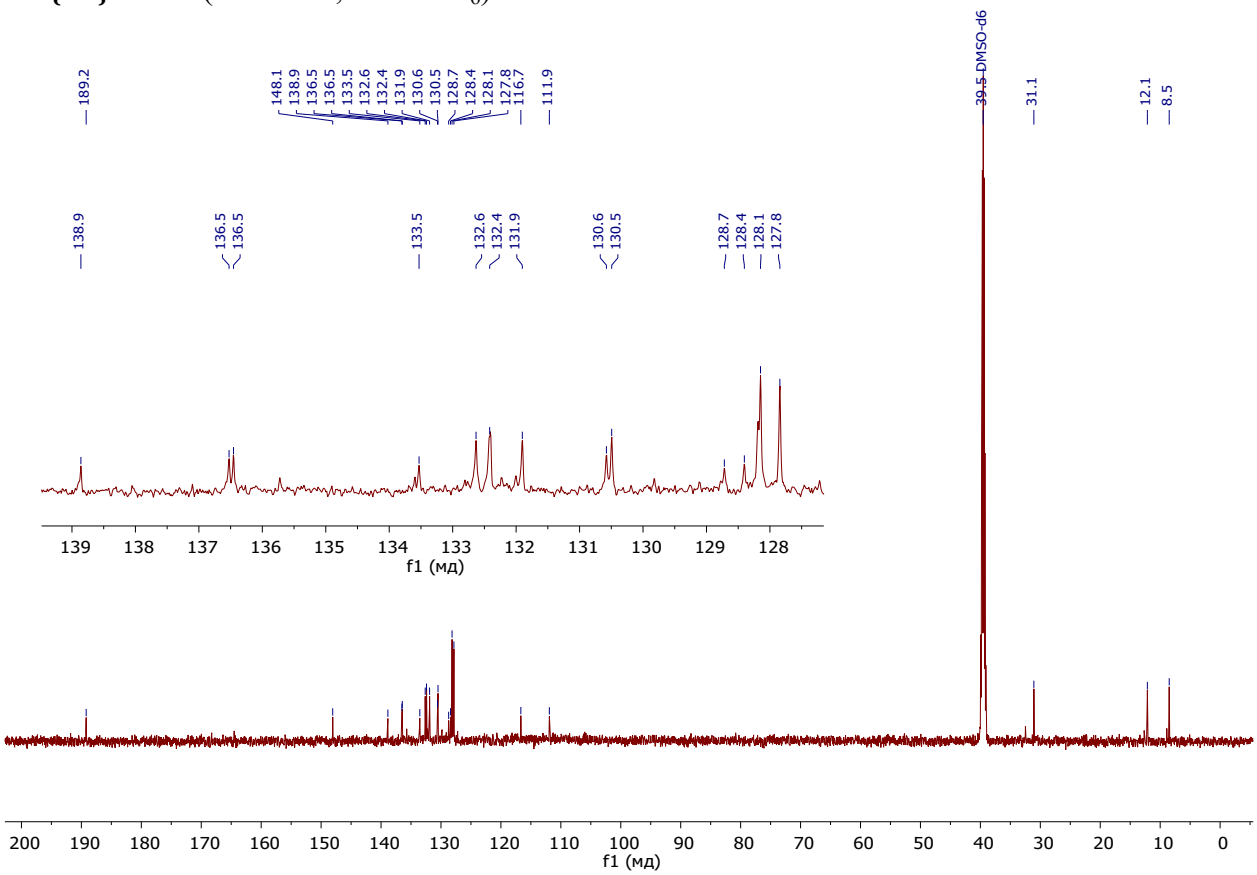
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5k**



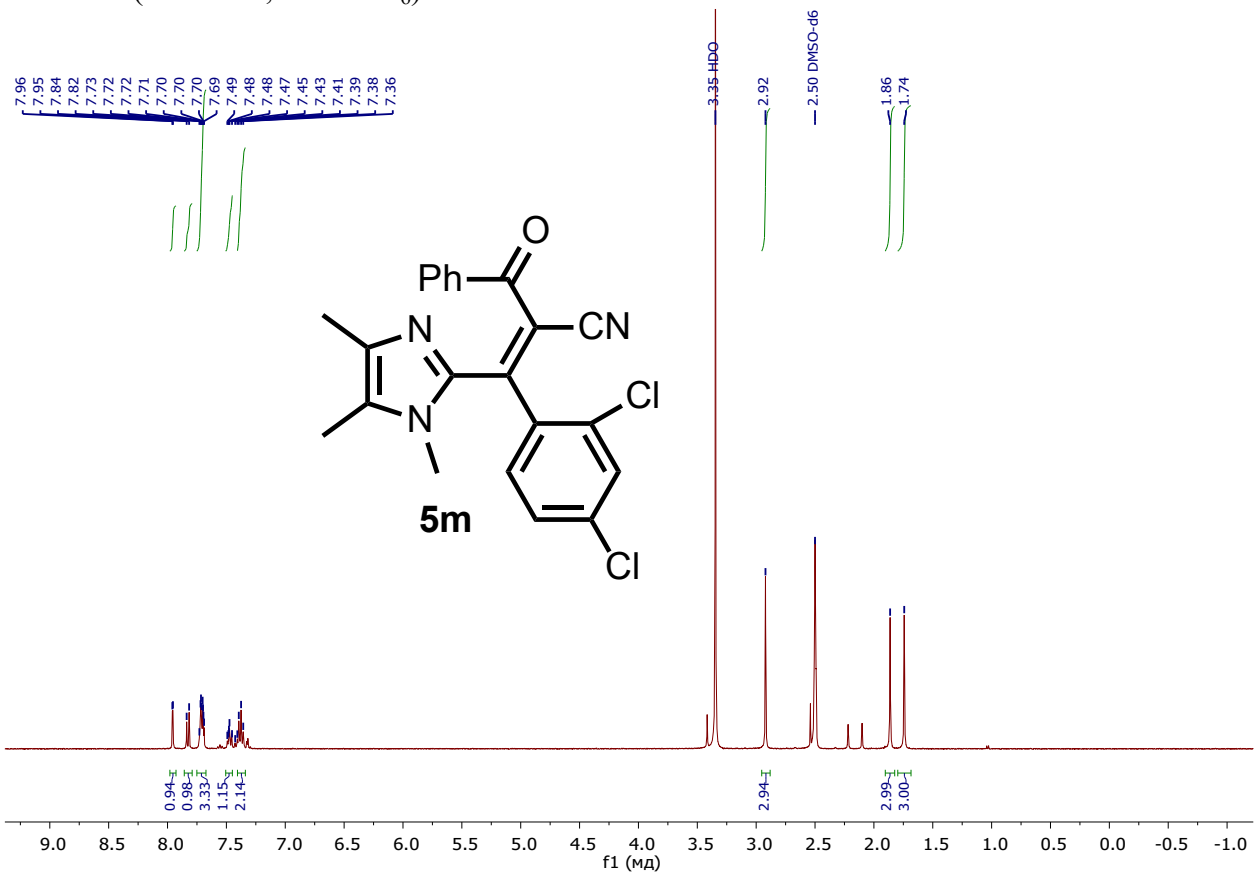
^{1}H NMR (400 MHz, DMSO-d_6) of **5l**



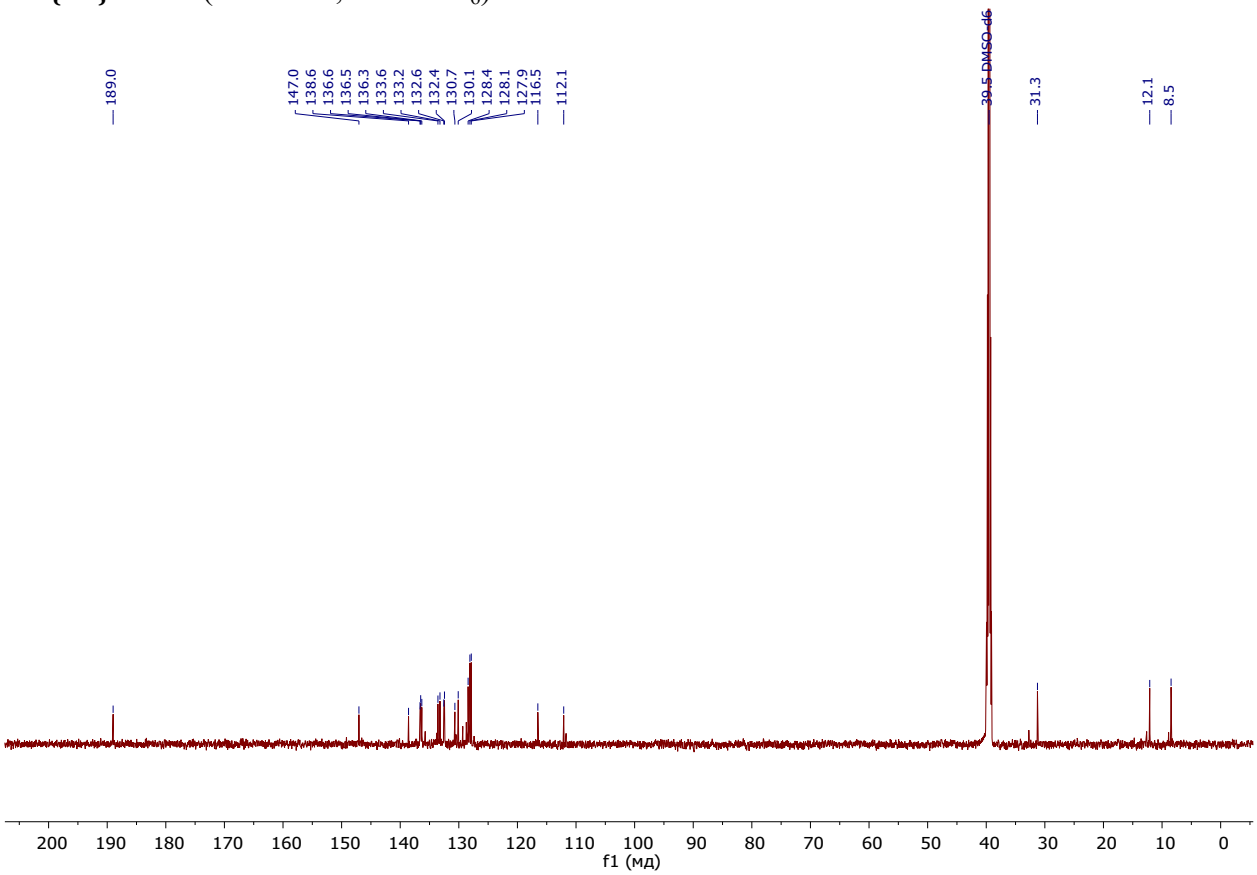
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5l**



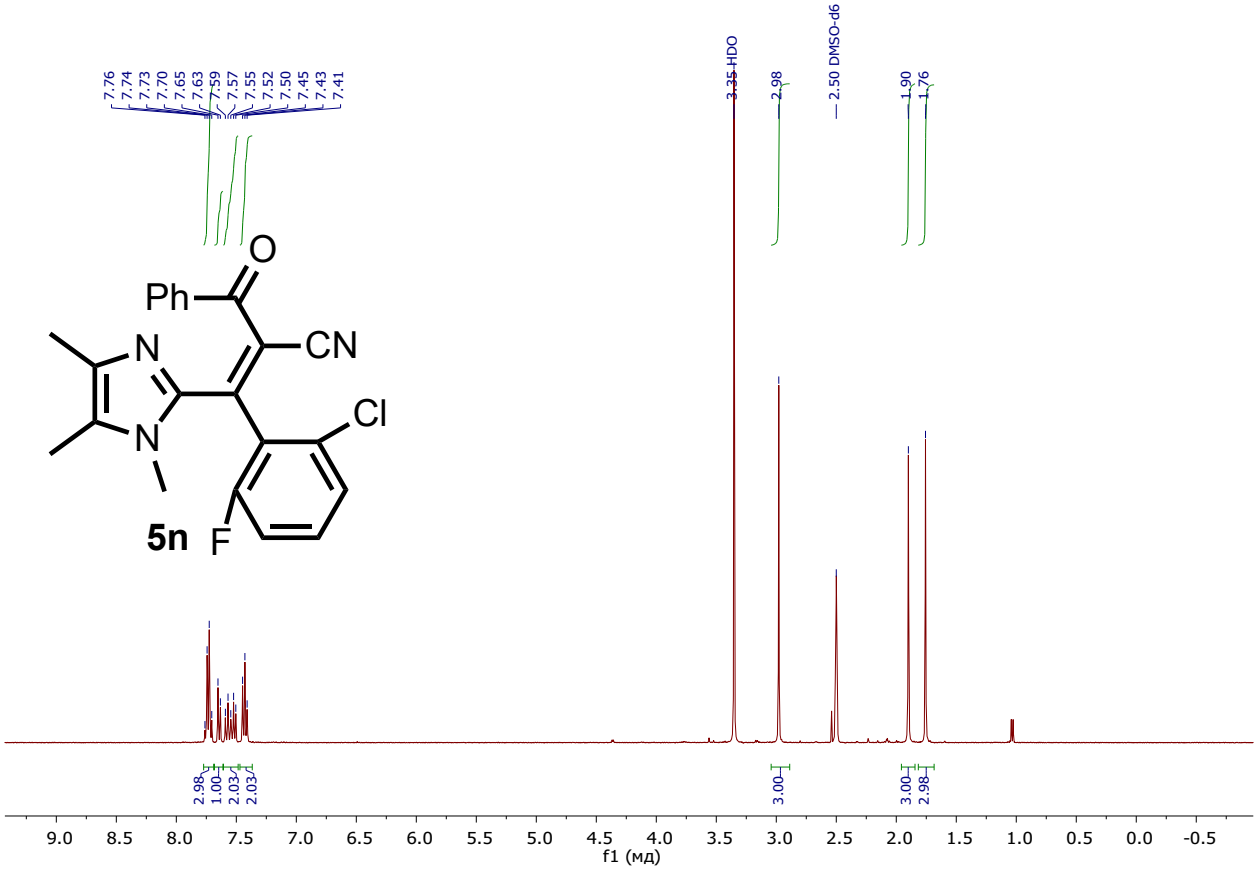
^{1}H NMR (400 MHz, DMSO-d_6) of **5m**



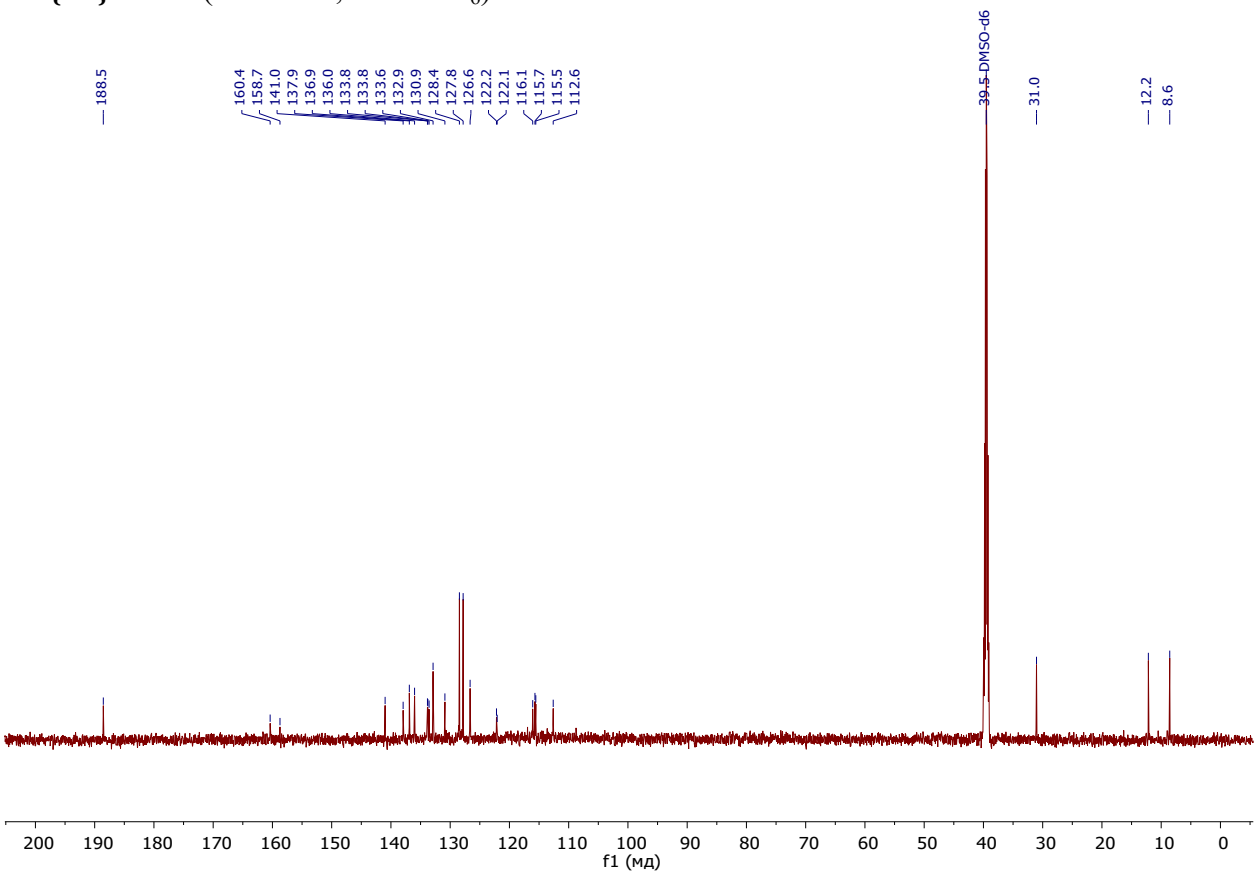
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5m**



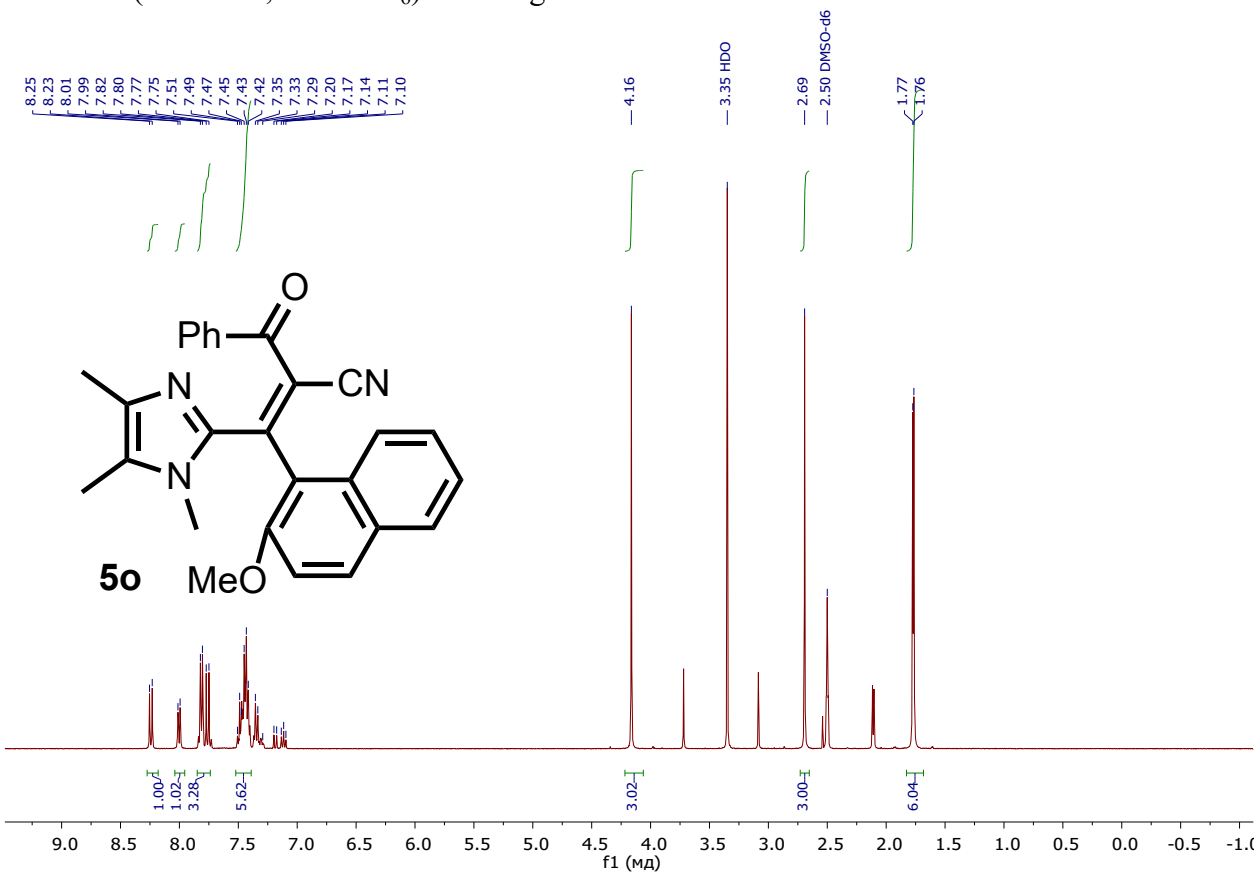
^{1}H NMR (400 MHz, DMSO-d_6) of **5n**



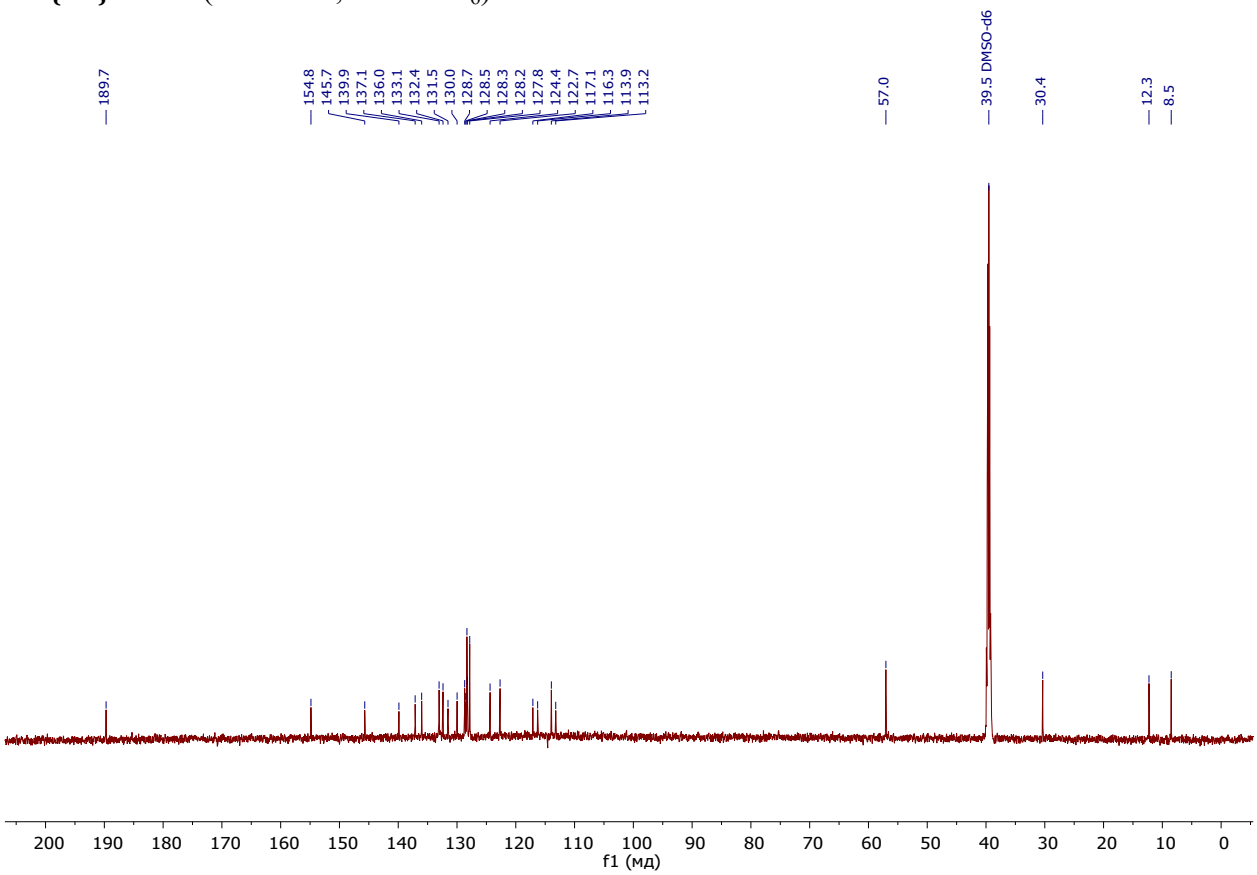
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5n**



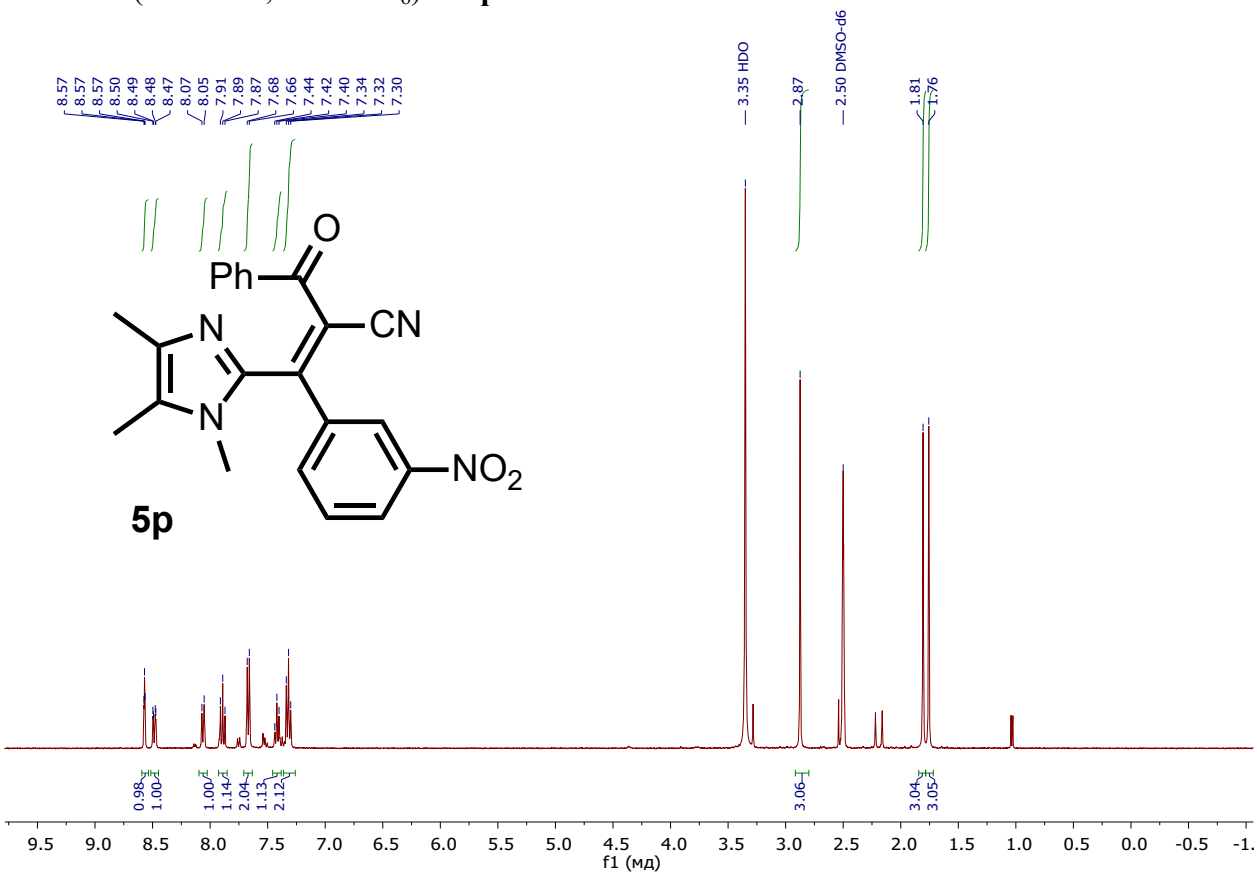
^{1}H NMR (400 MHz, DMSO-d_6) of **5o** regioisomer's mixture



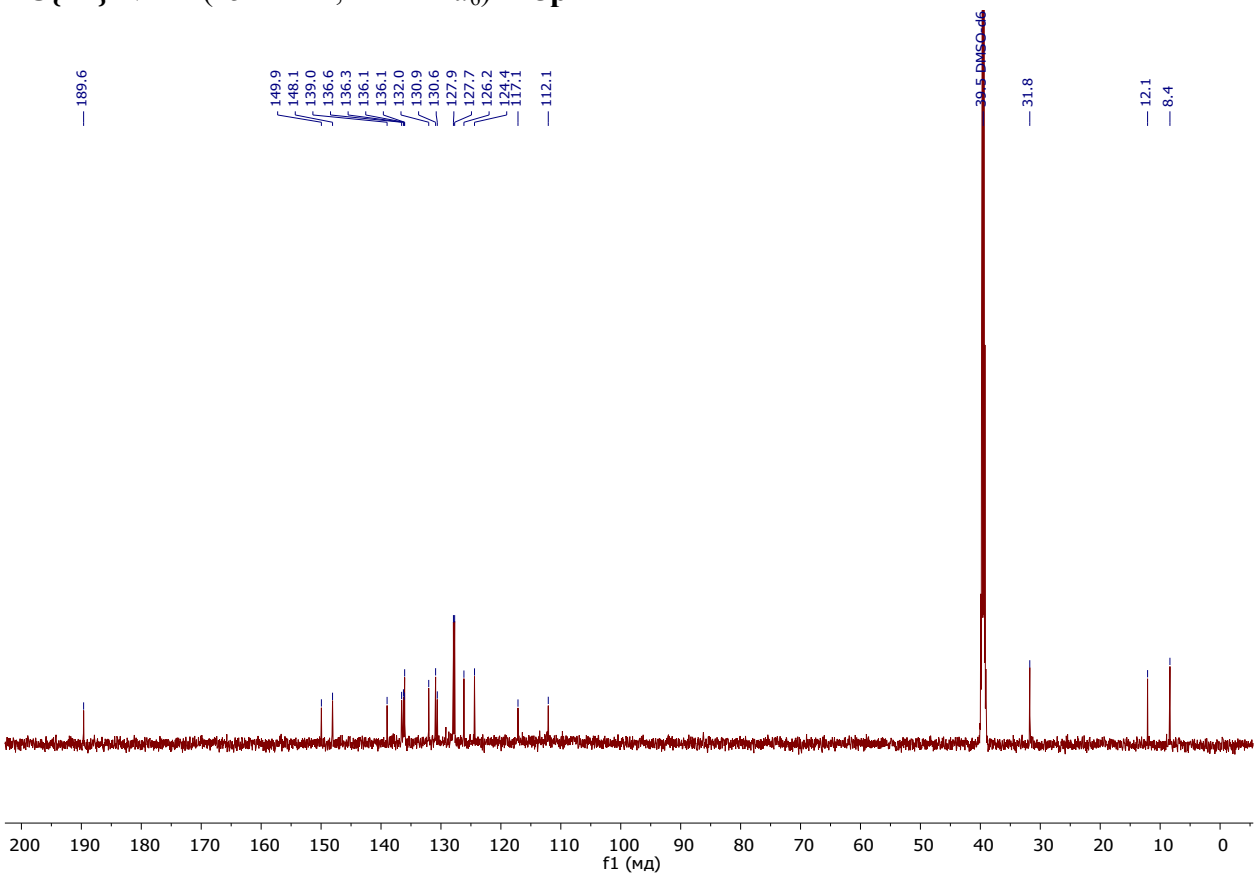
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5o**



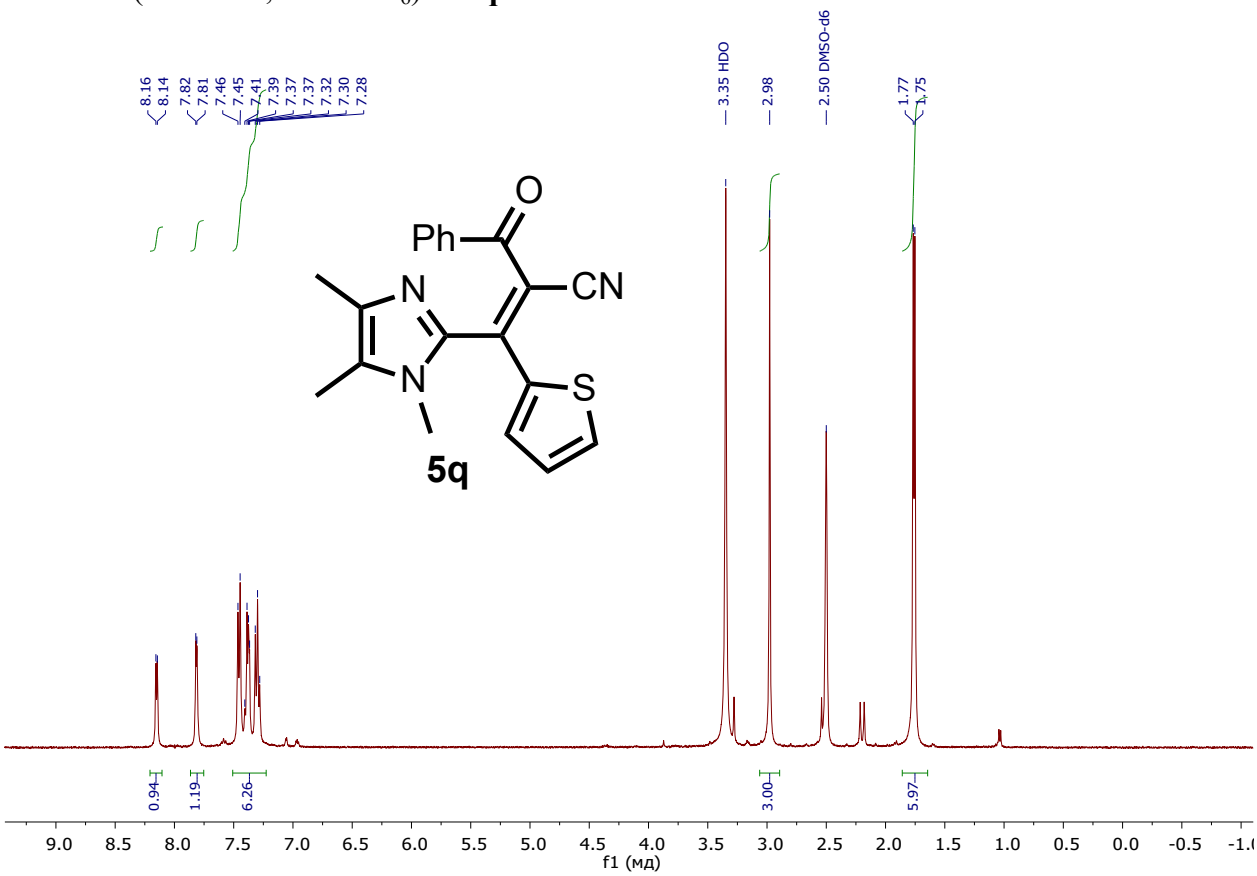
^{1}H NMR (400 MHz, DMSO-d_6) of **5p**



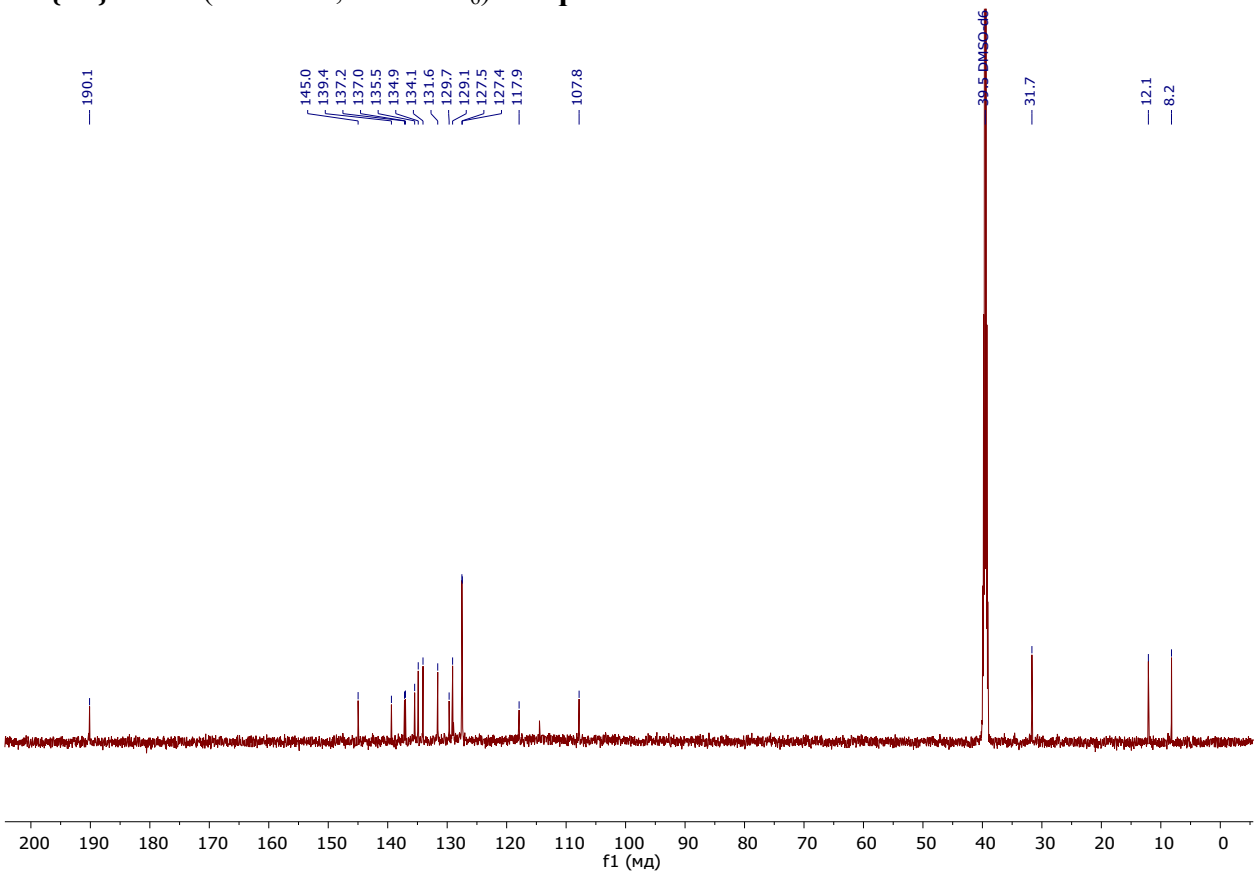
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5p**



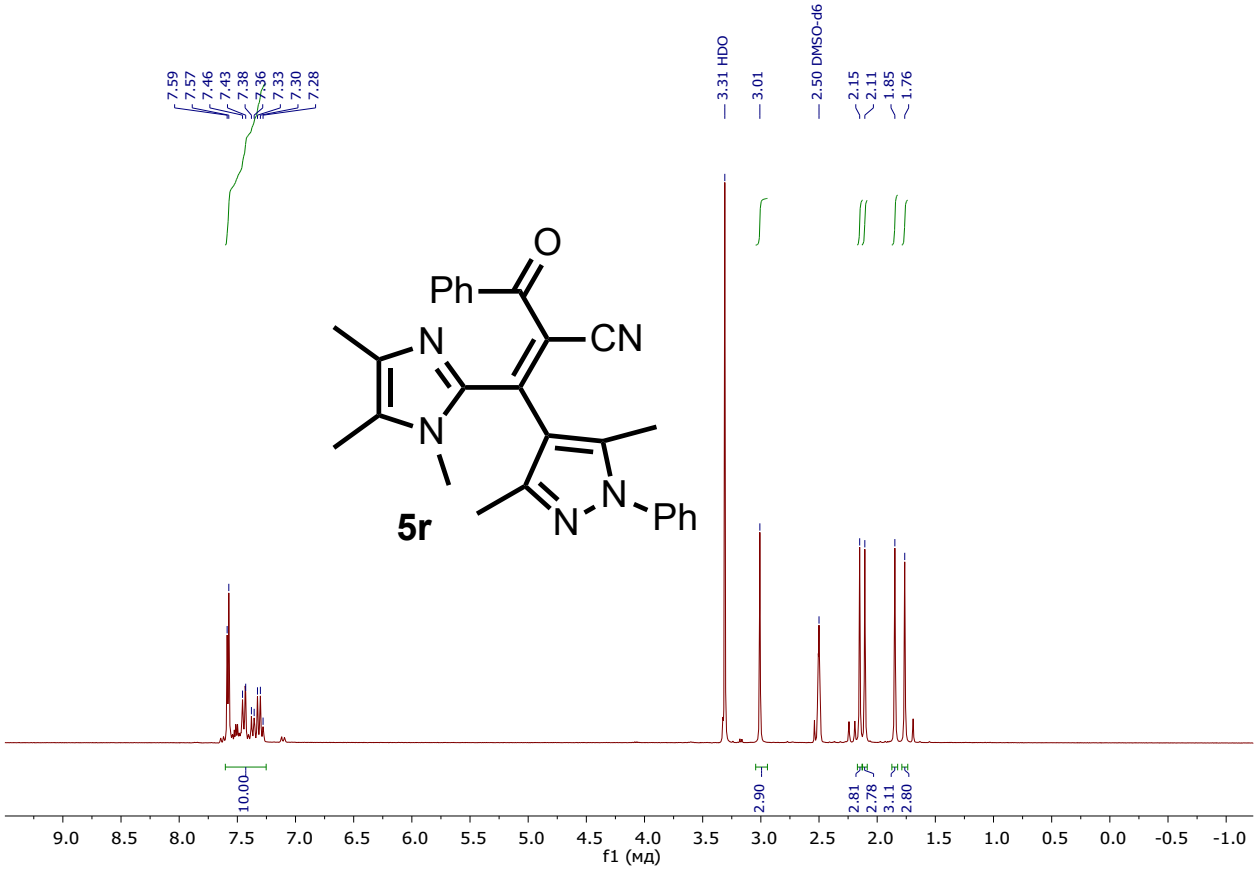
^{1}H NMR (400 MHz, DMSO-d_6) of **5q**



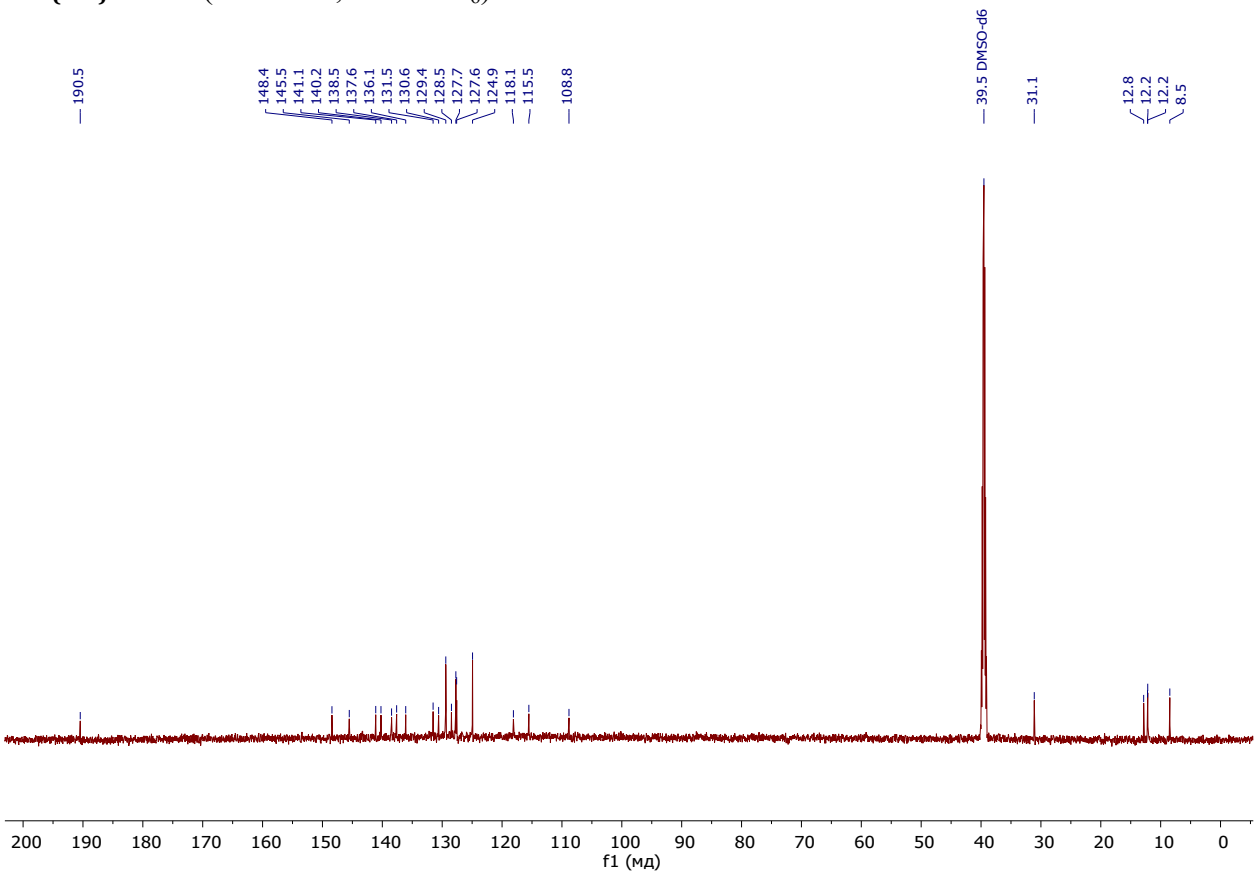
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5q**



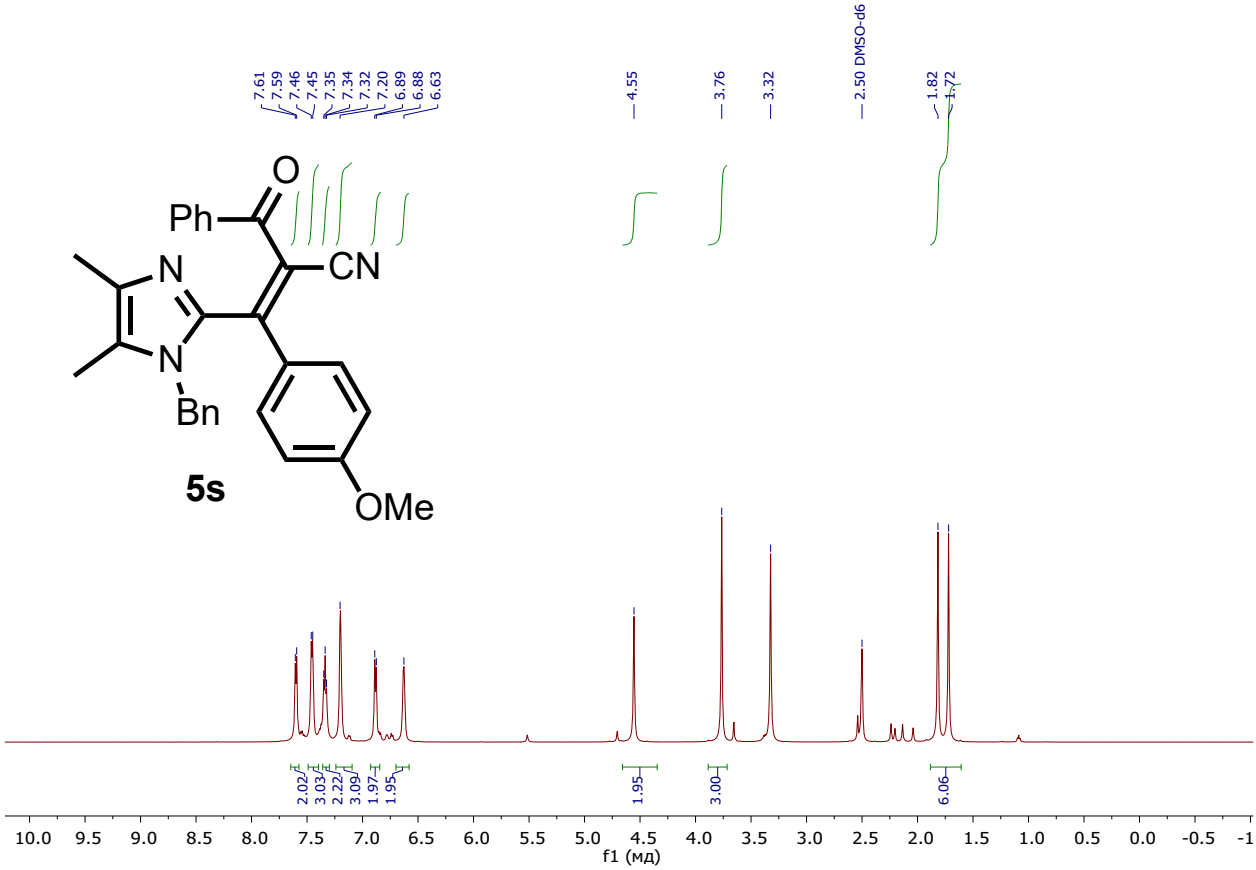
^{1}H NMR (300 MHz, DMSO-d_6) of **5r**



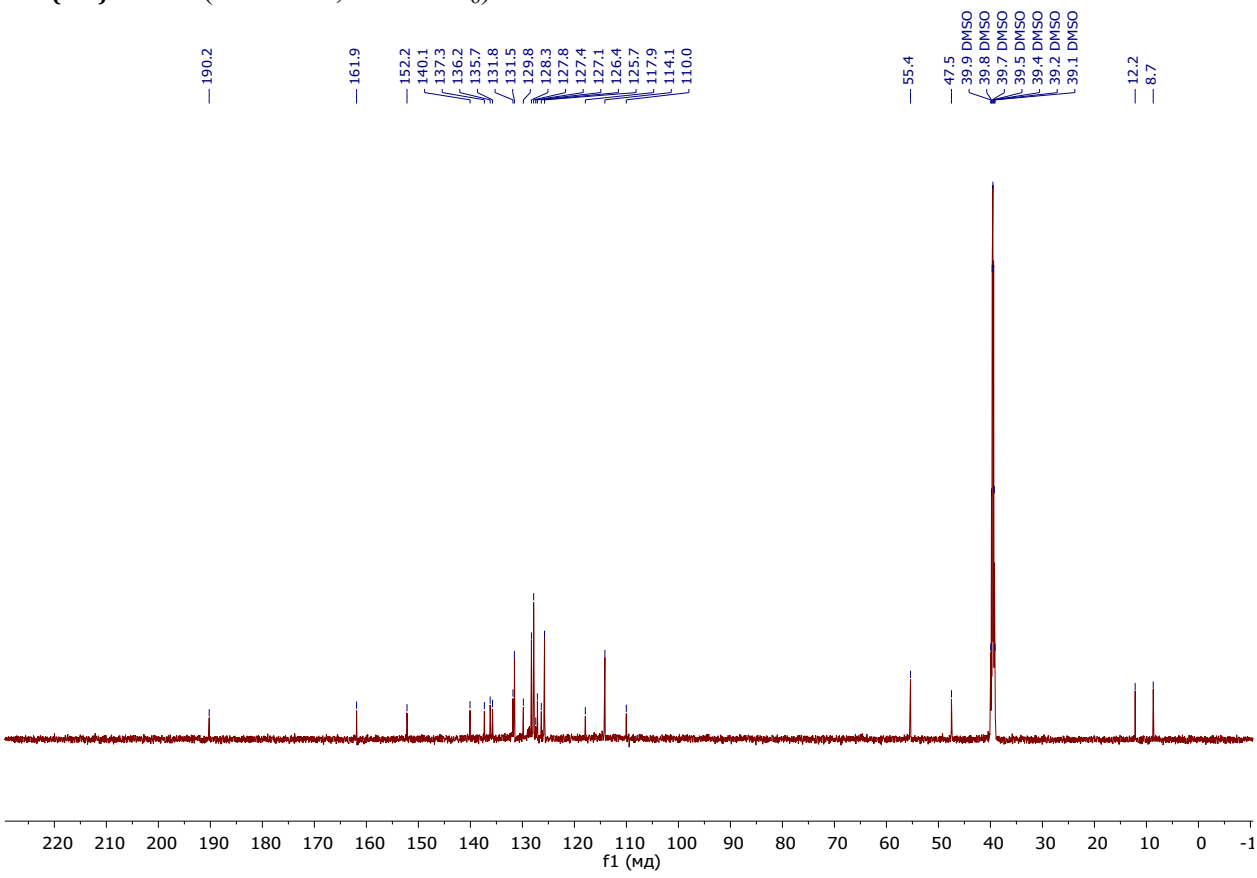
^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5r**



^{1}H NMR (600 MHz, DMSO-d_6) of **5s**

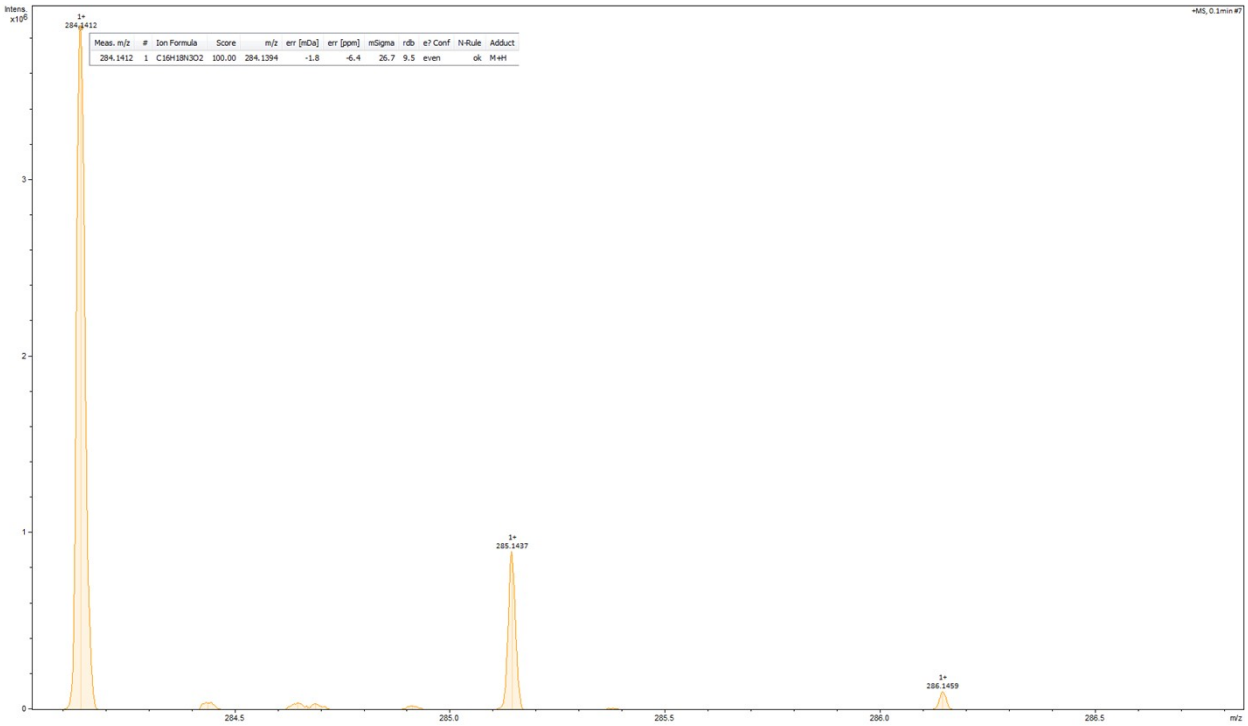


^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) of **5s**

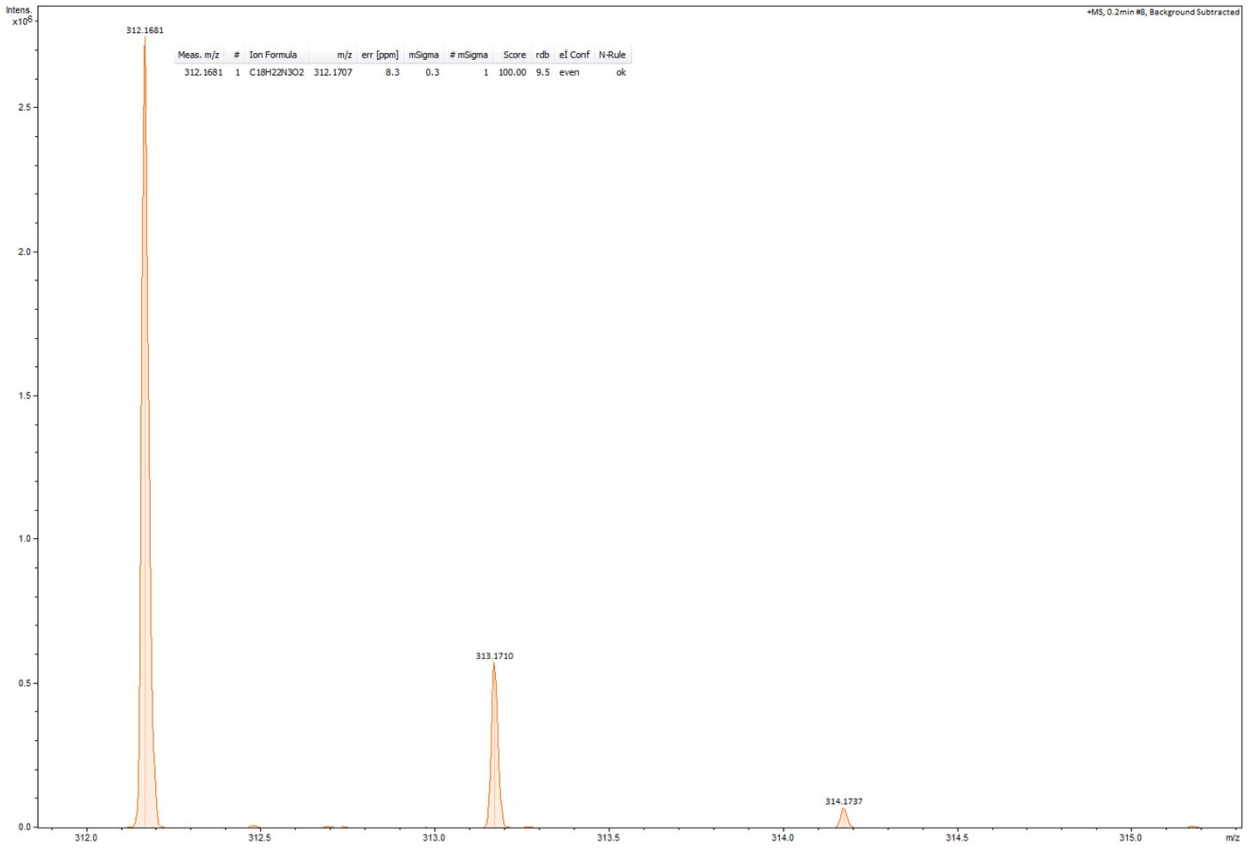


Copies of HRMS

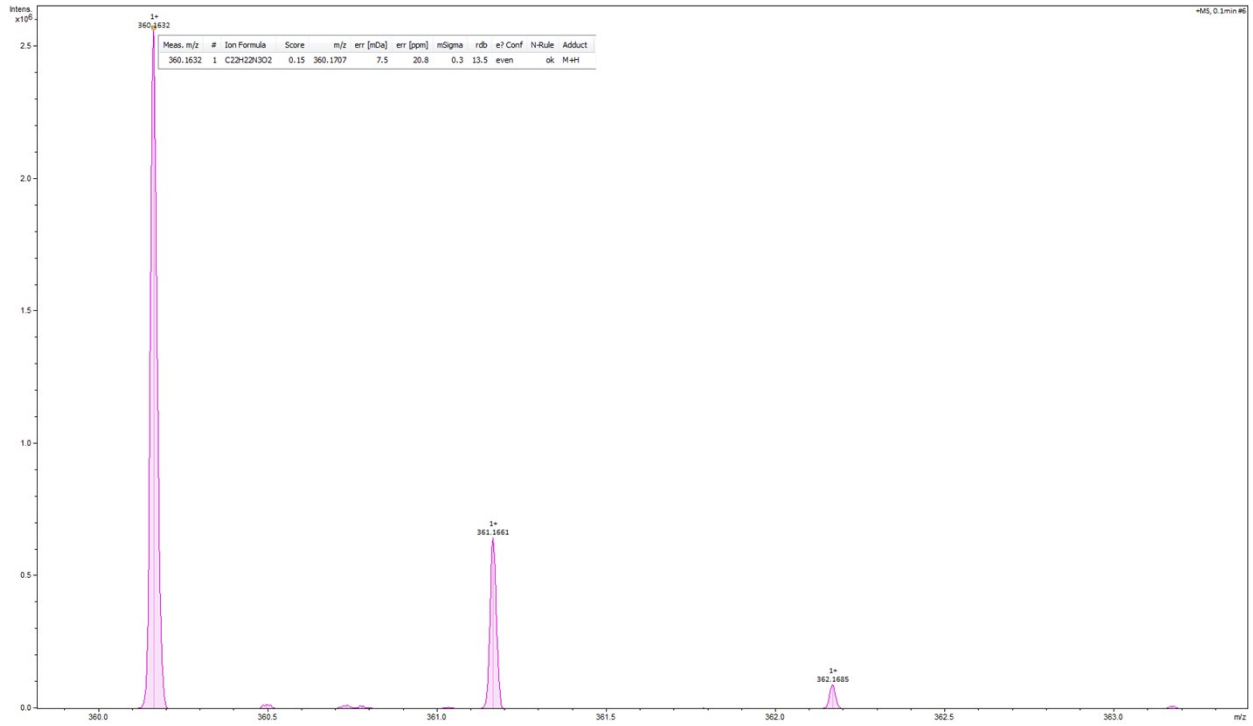
HRMS of **4a**



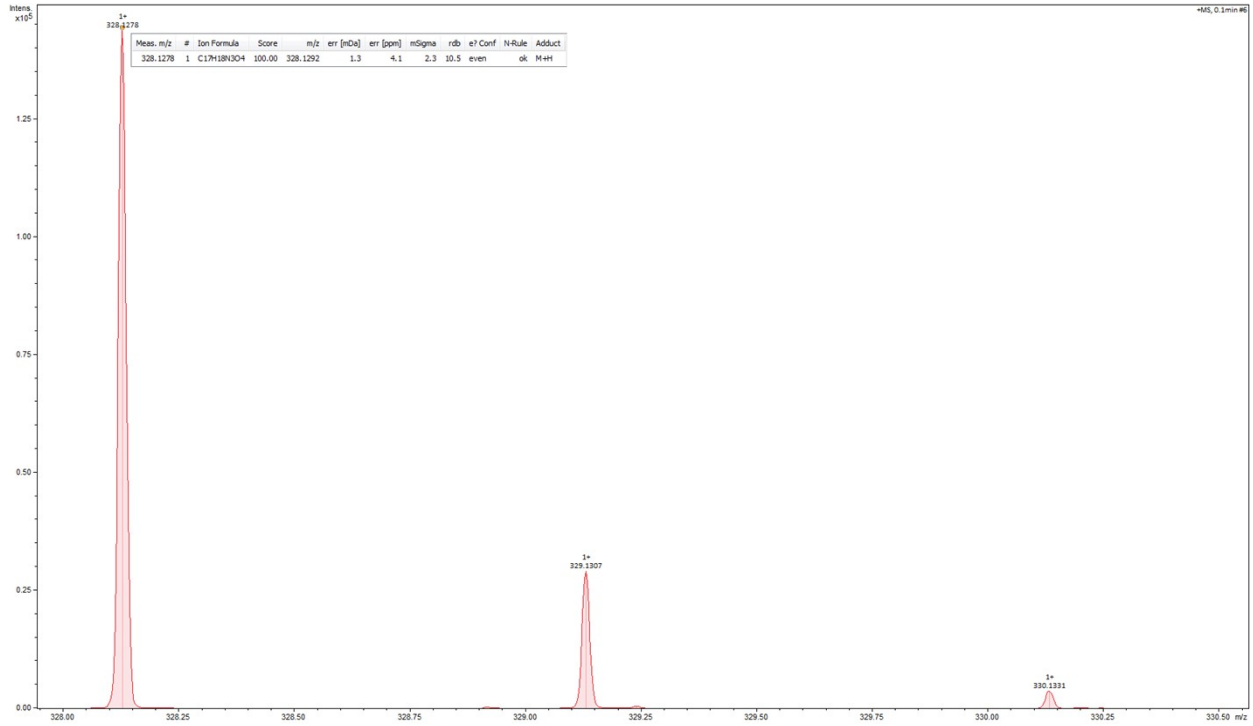
HRMS of **4b**



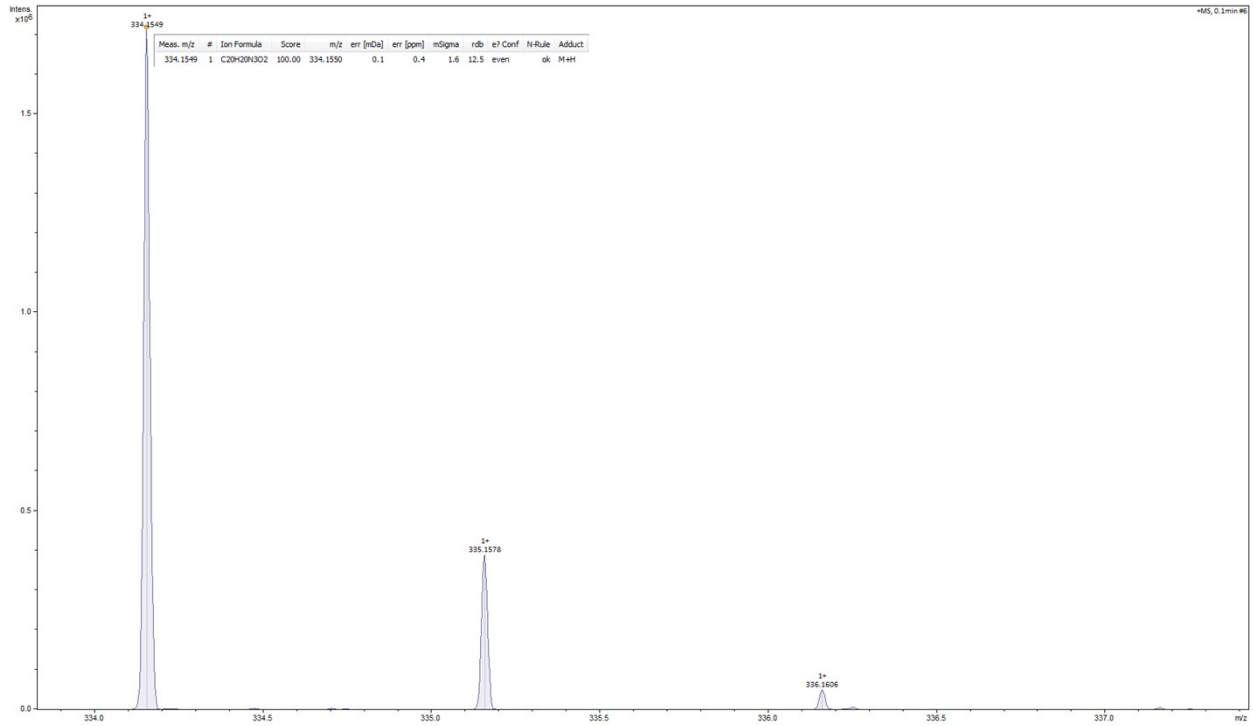
HRMS **4c**



HRMS of **4d**

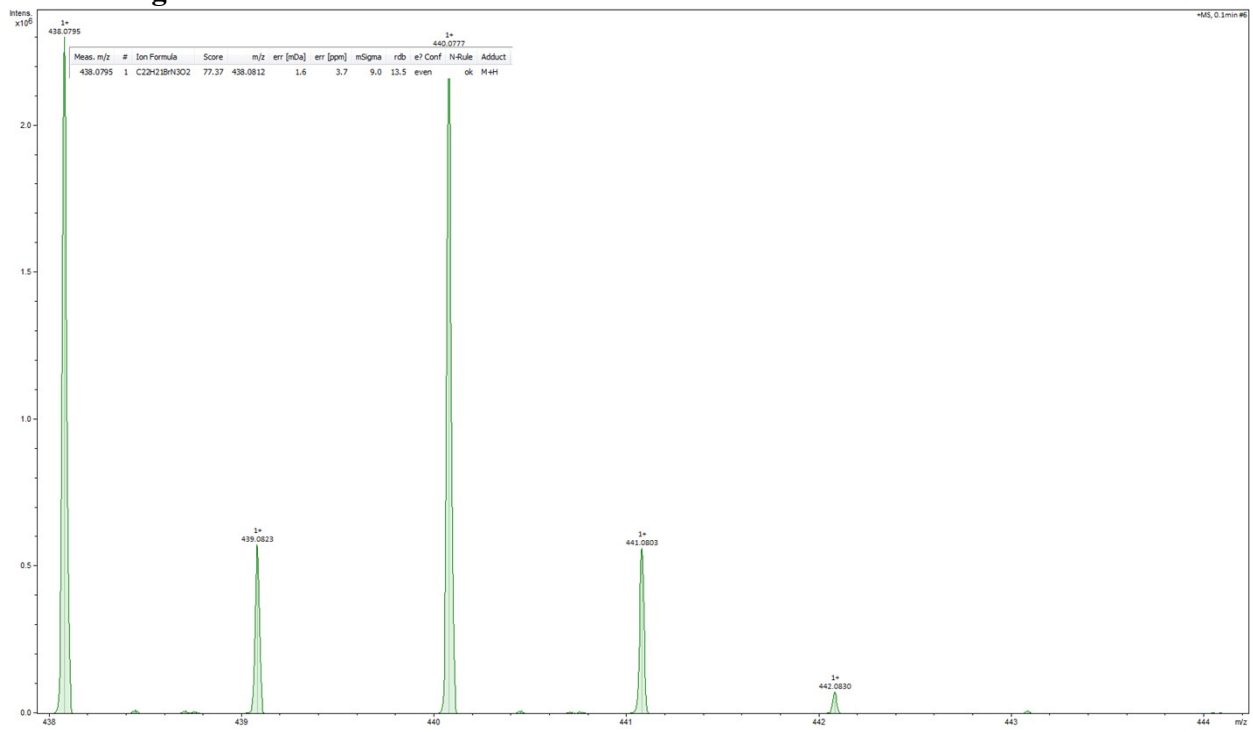


HRMS of **4e**



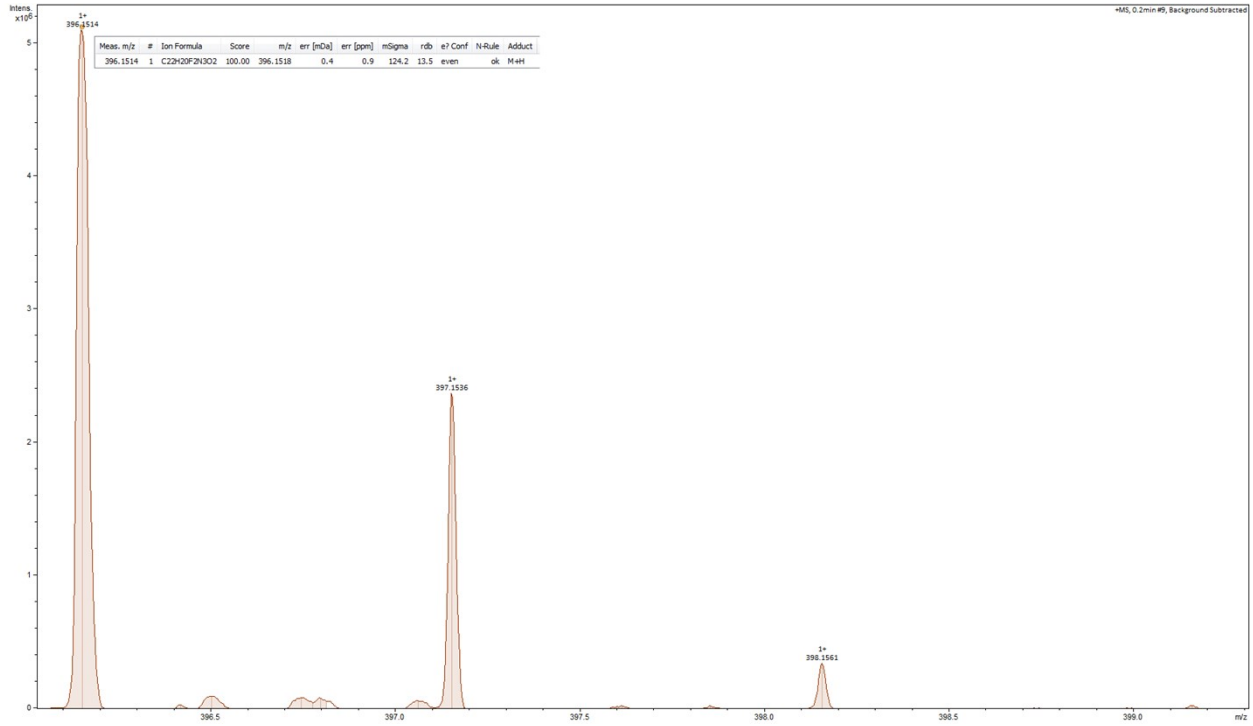
HRMS of **4f**

HRMS of **4g**



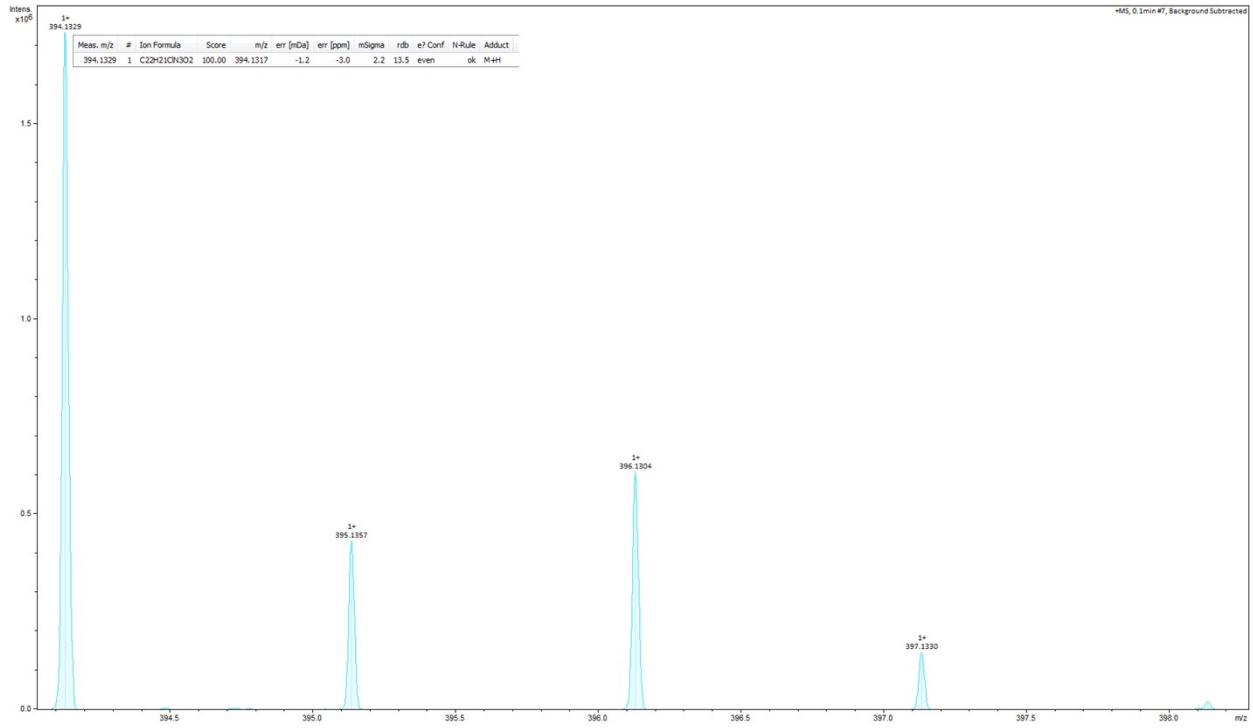
Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e? Conf	N-Rule	Adduct
438.0795	1	C22H21BrN3O2	77.37	438.0812	1.6	3.7	9.0	13.5	even	ok	M+H

HRMS of **4h**

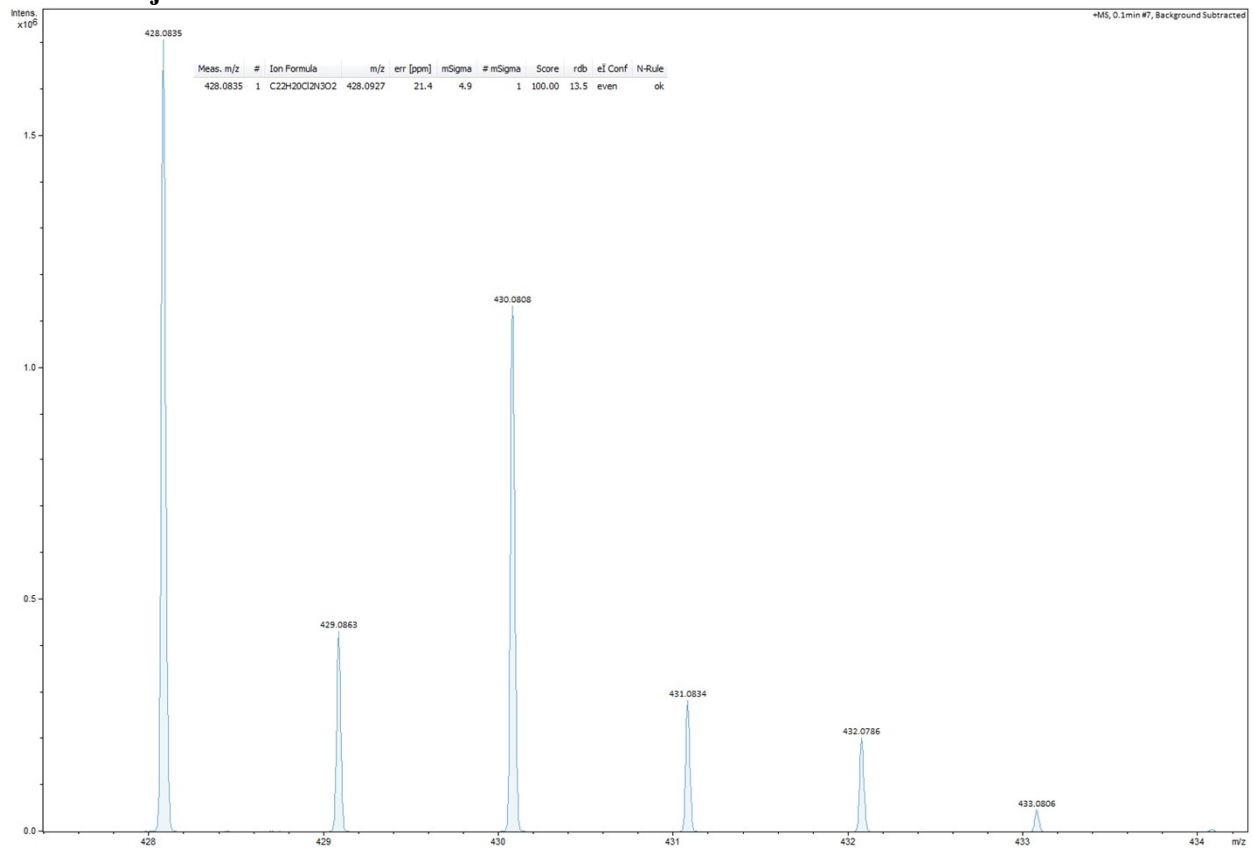


Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e? Conf	N-Rule	Adduct
396.1514	1	C22H20F2N3O2	100.00	396.1518	0.4	0.9	124.2	13.5	even	ok	M+H

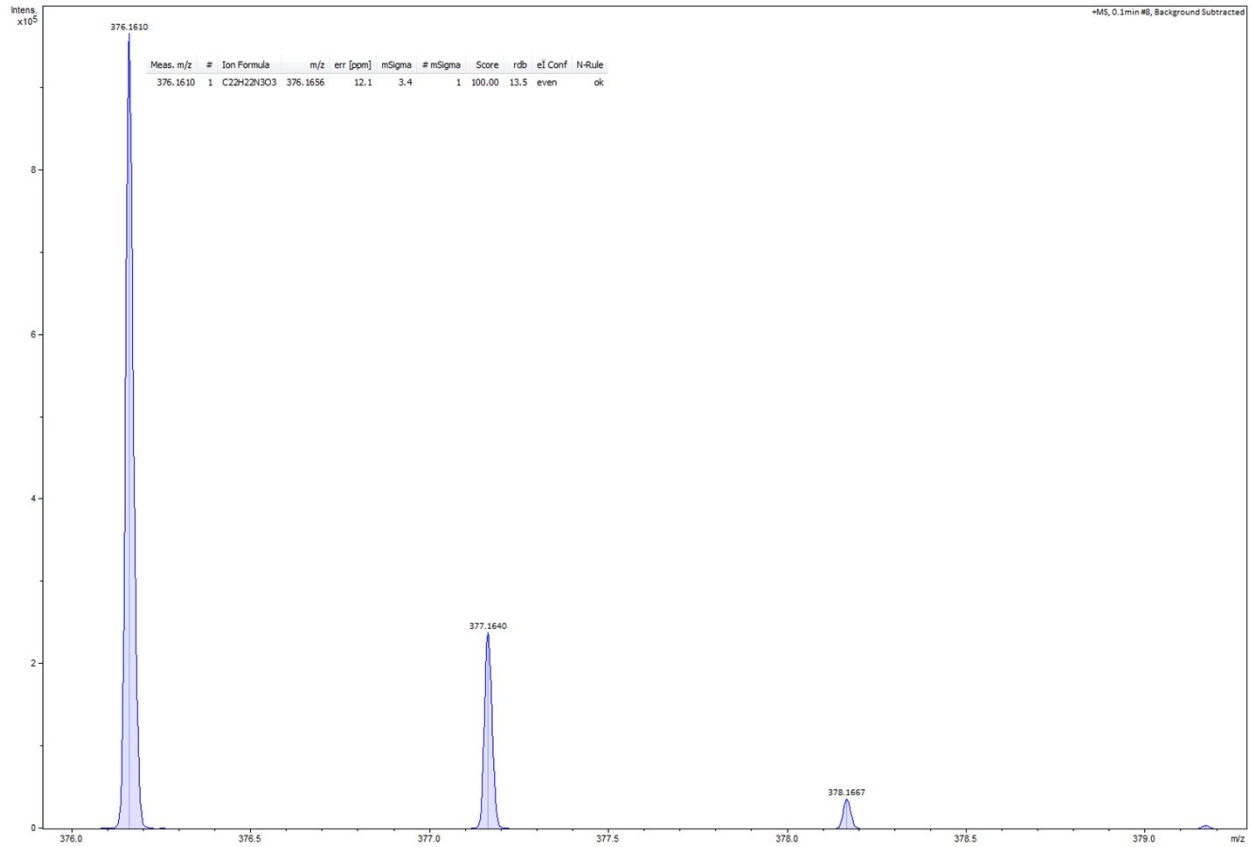
HRMS of **4i**



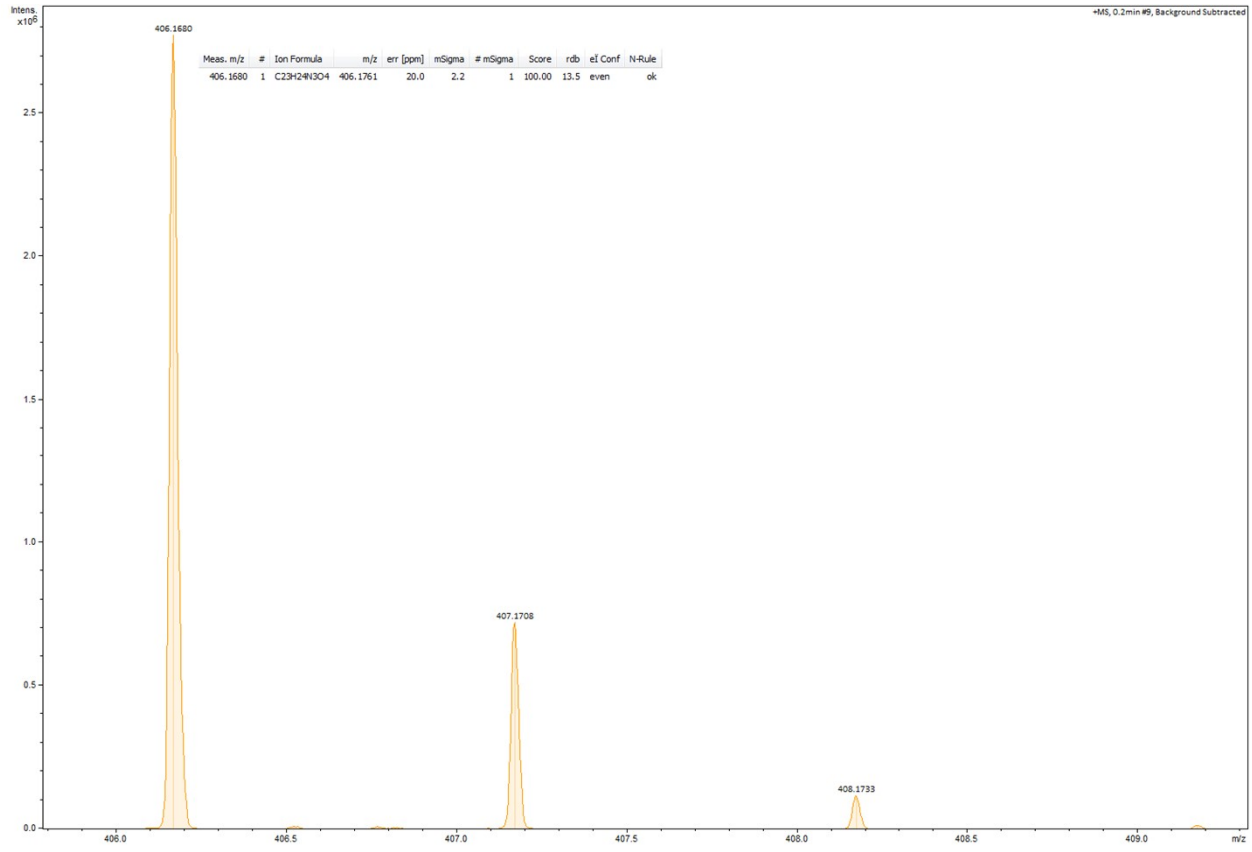
HRMS of **4j**



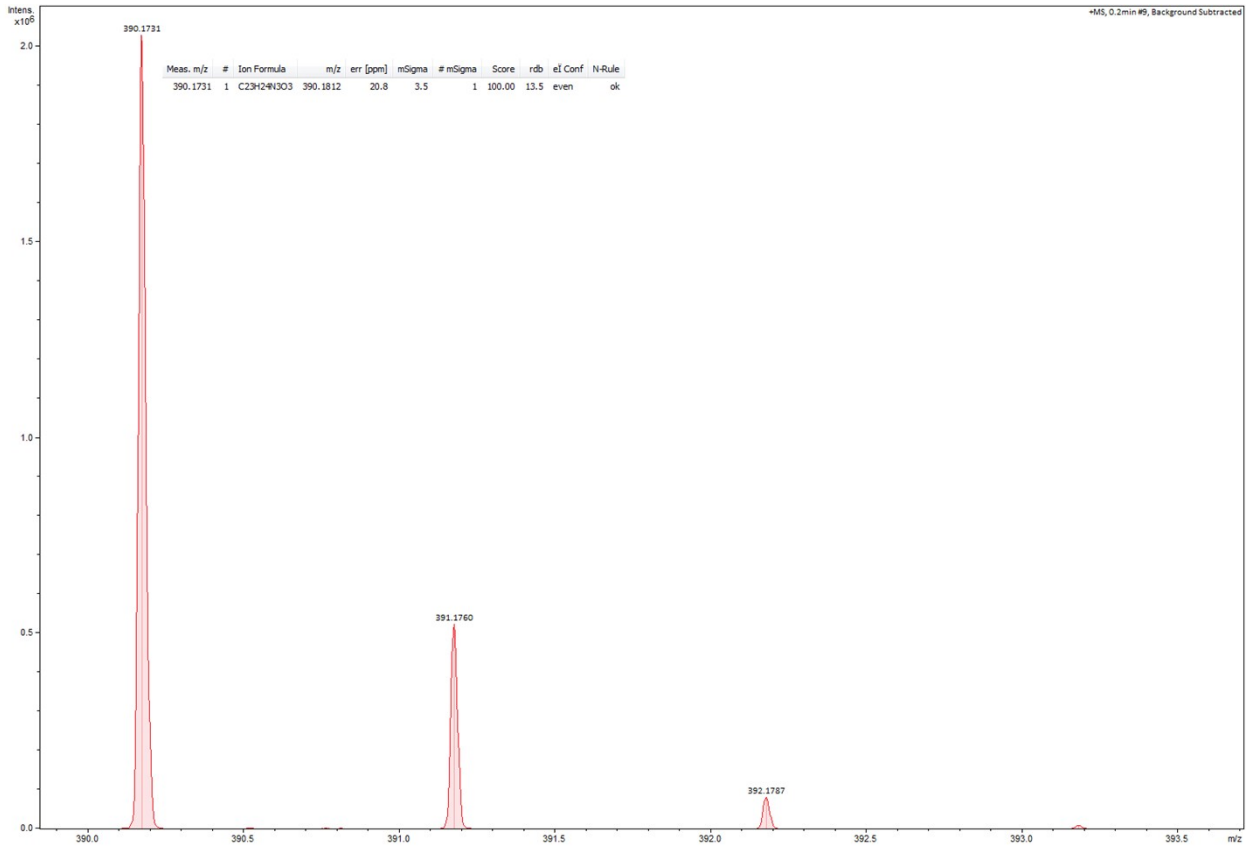
HRMS of **4k**



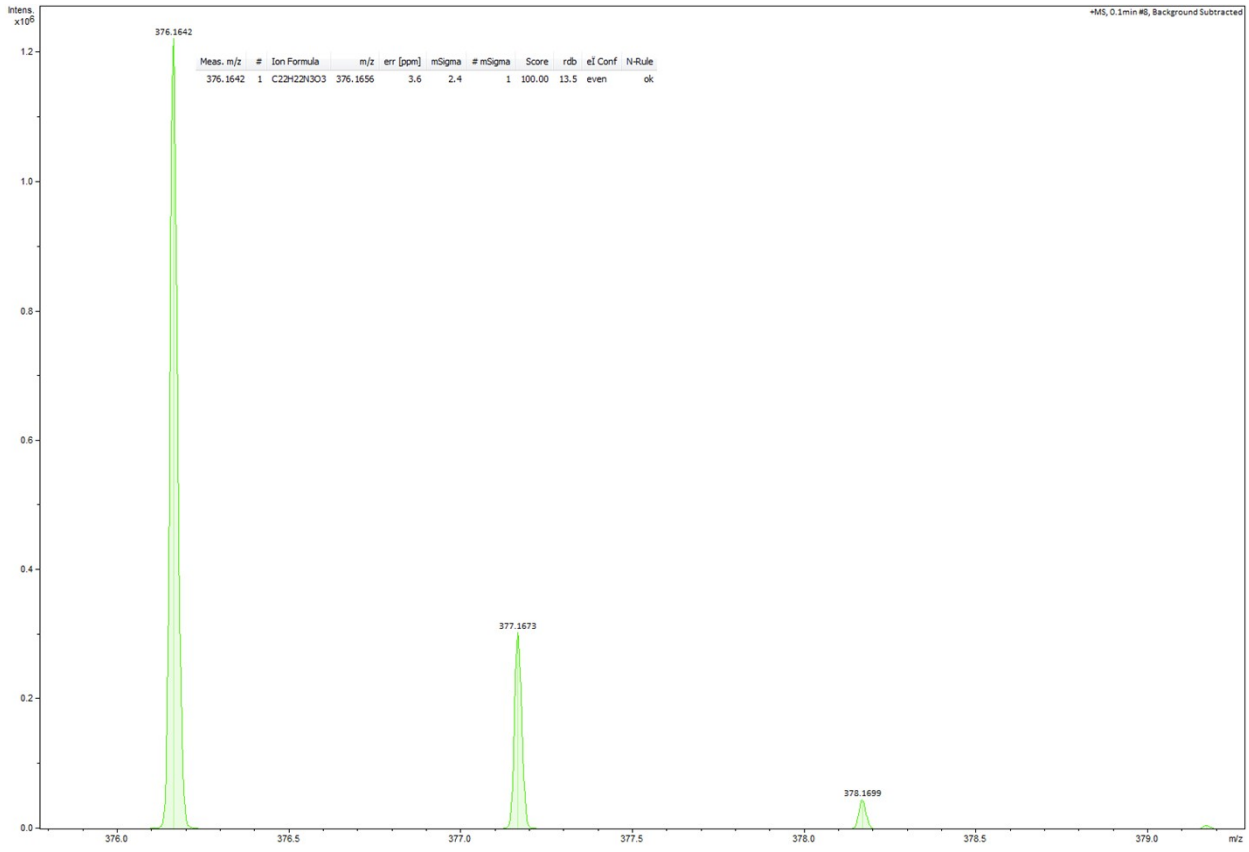
HRMS of **4l**



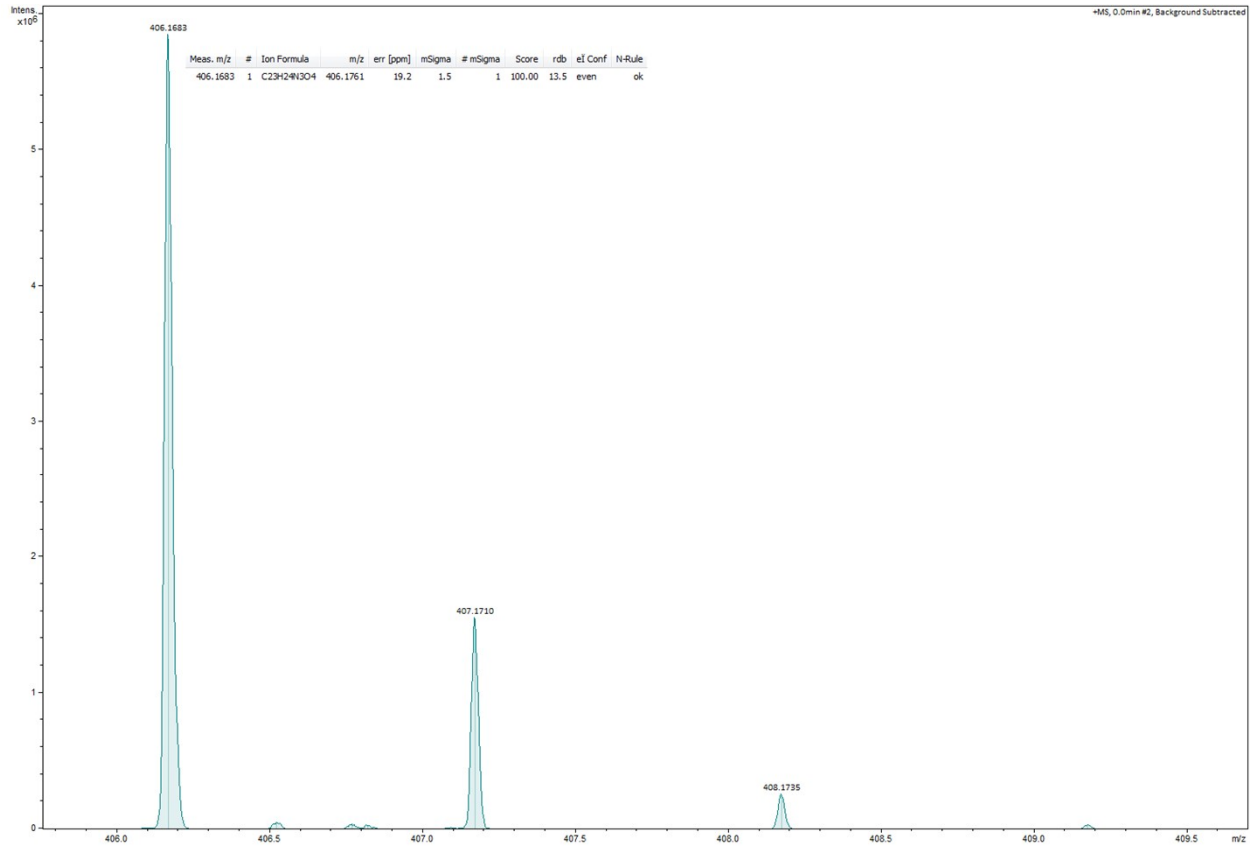
HRMS of **4m**



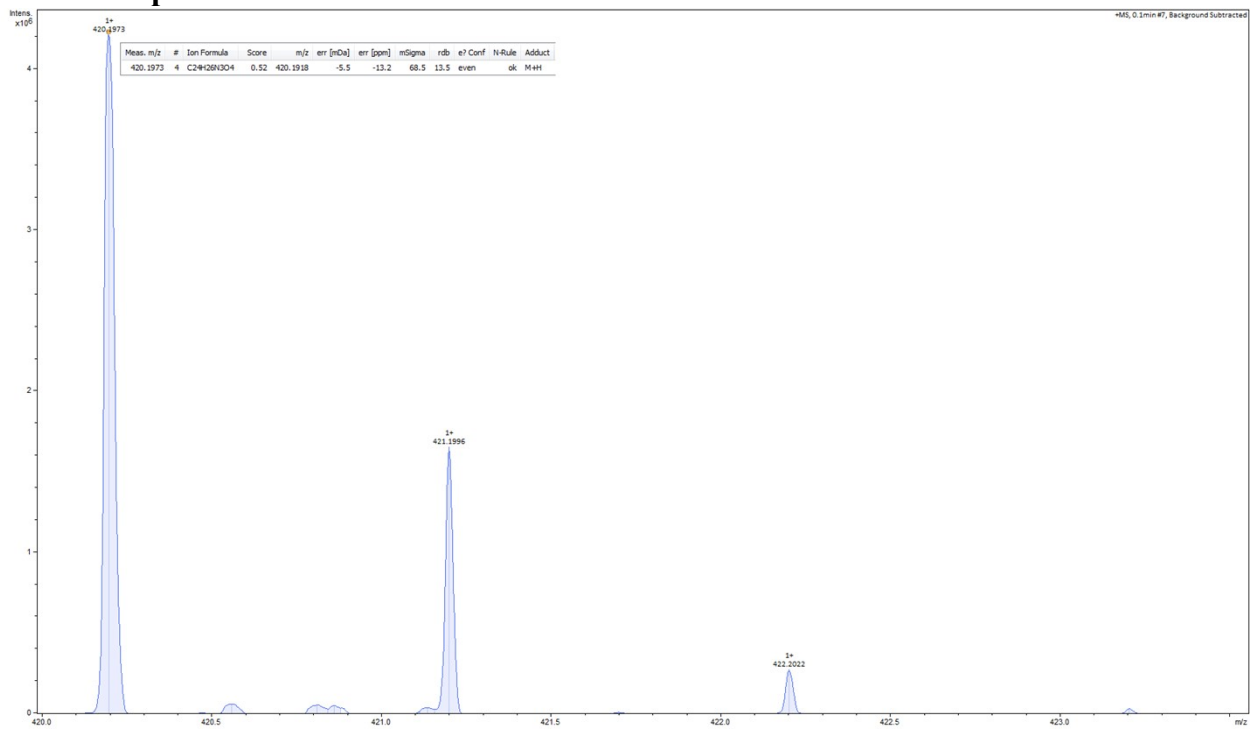
HRMS of **4n**



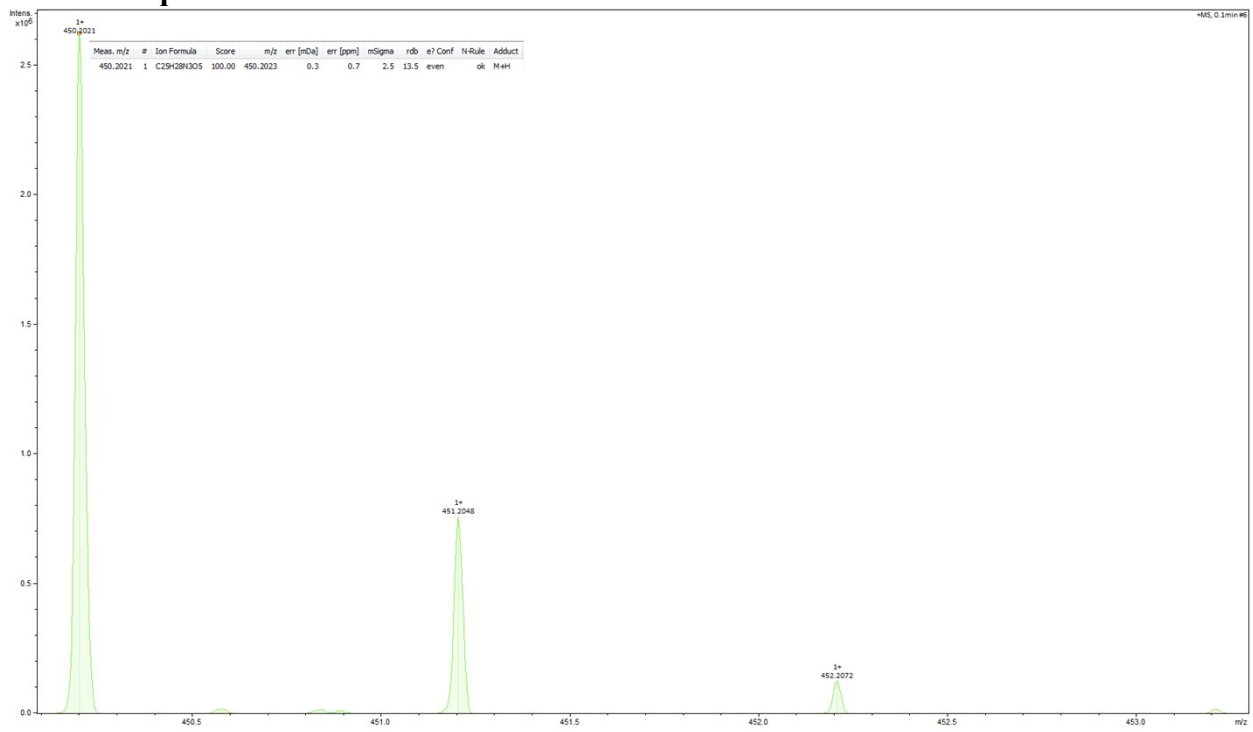
HRMS of **4o**



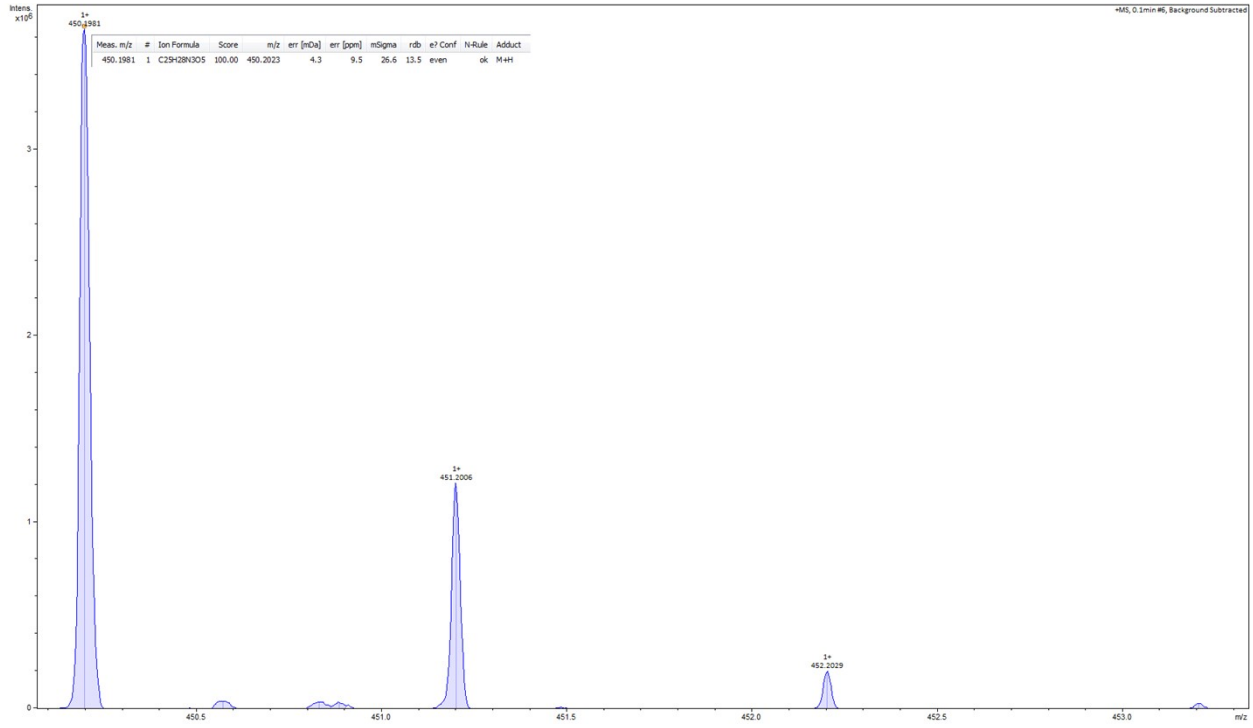
HRMS of **4p**



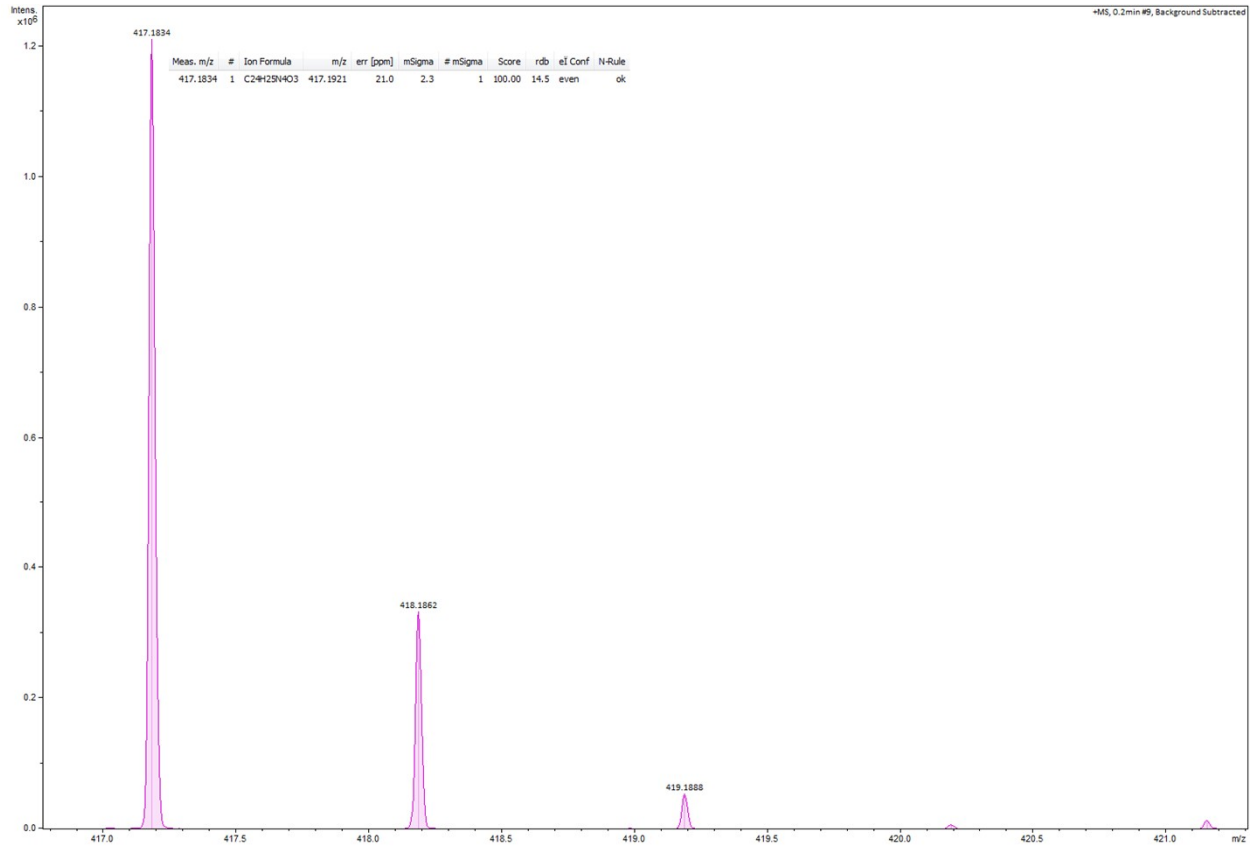
HRMS of **4q**



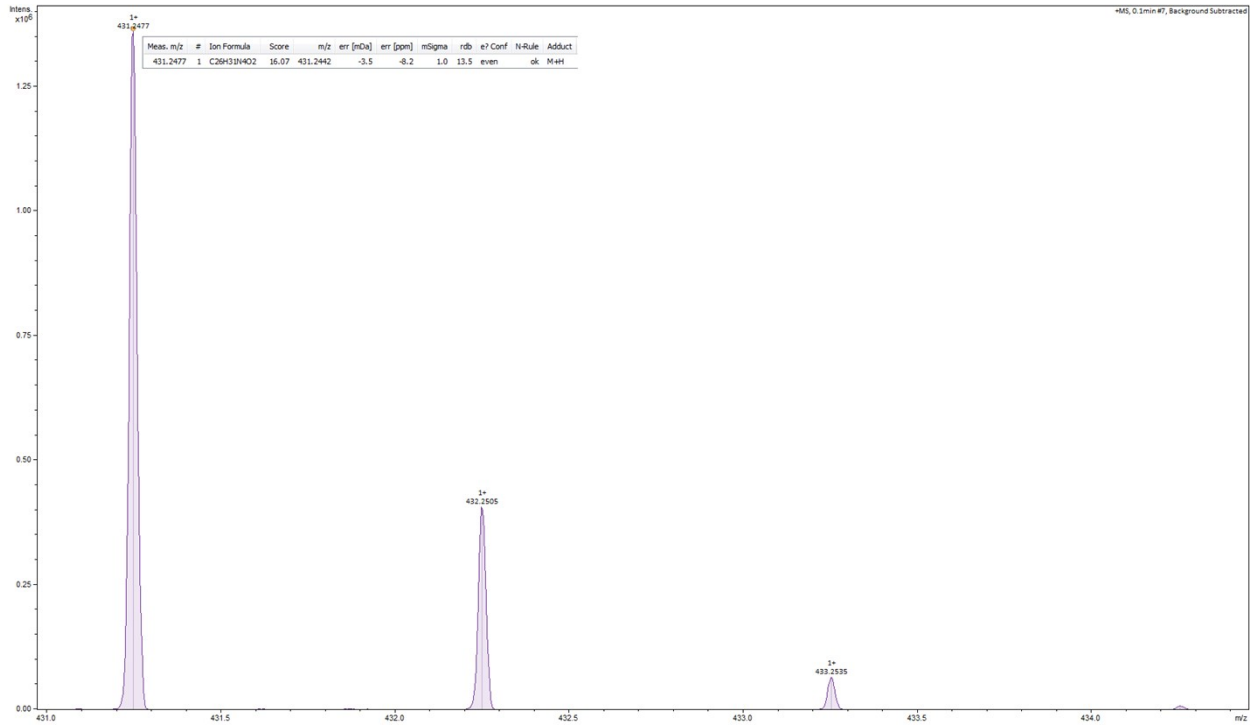
HRMS of **4r**



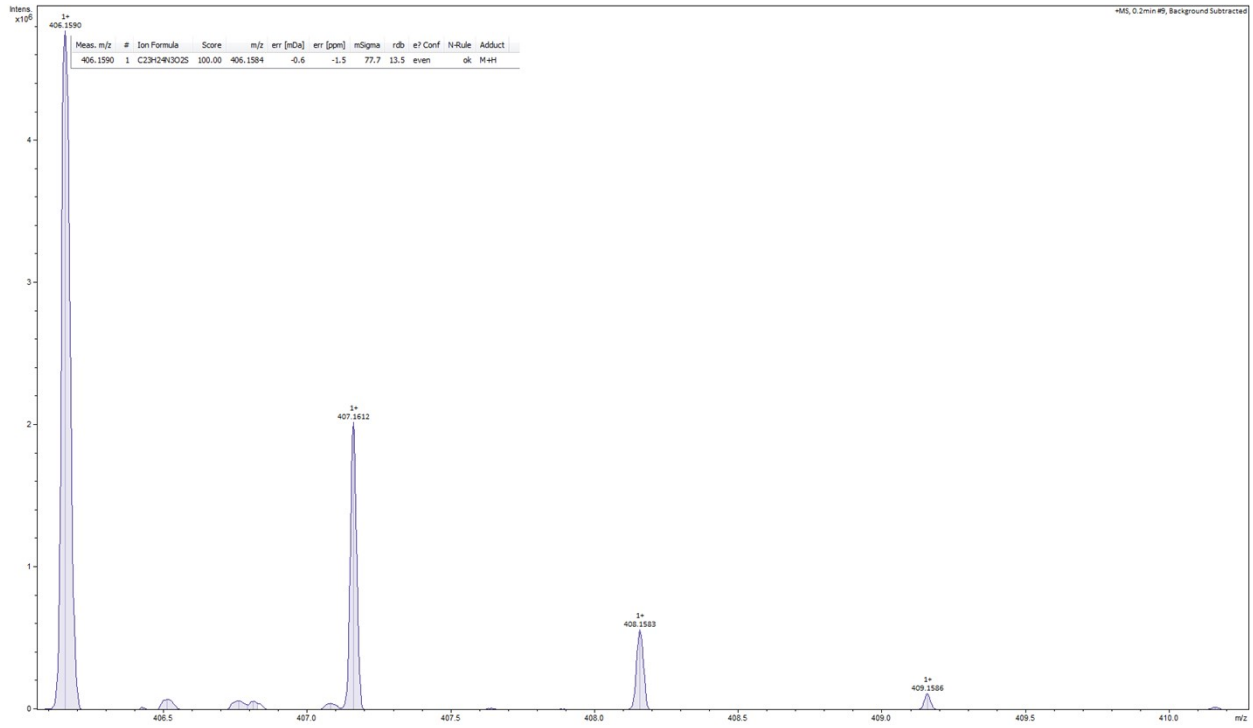
HRMS of **4s**



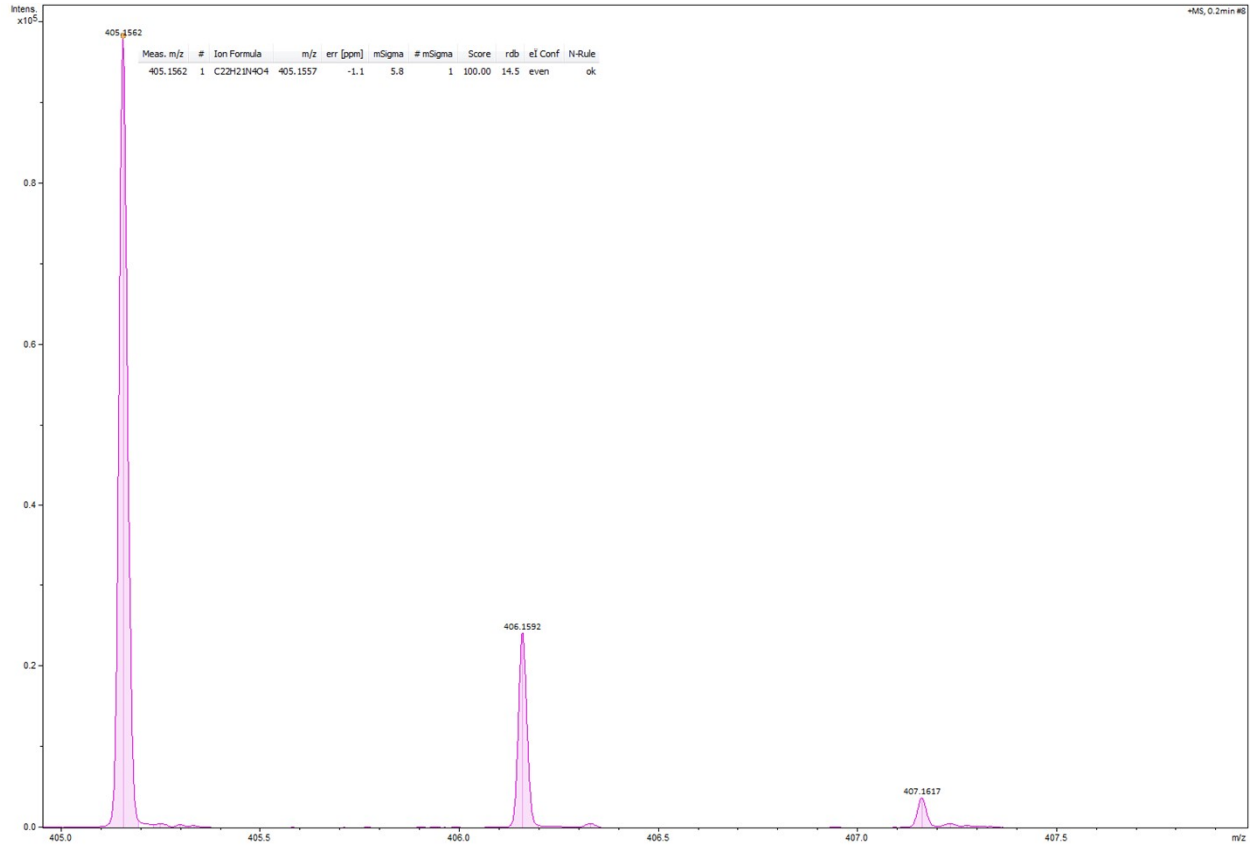
HRMS of **4t**



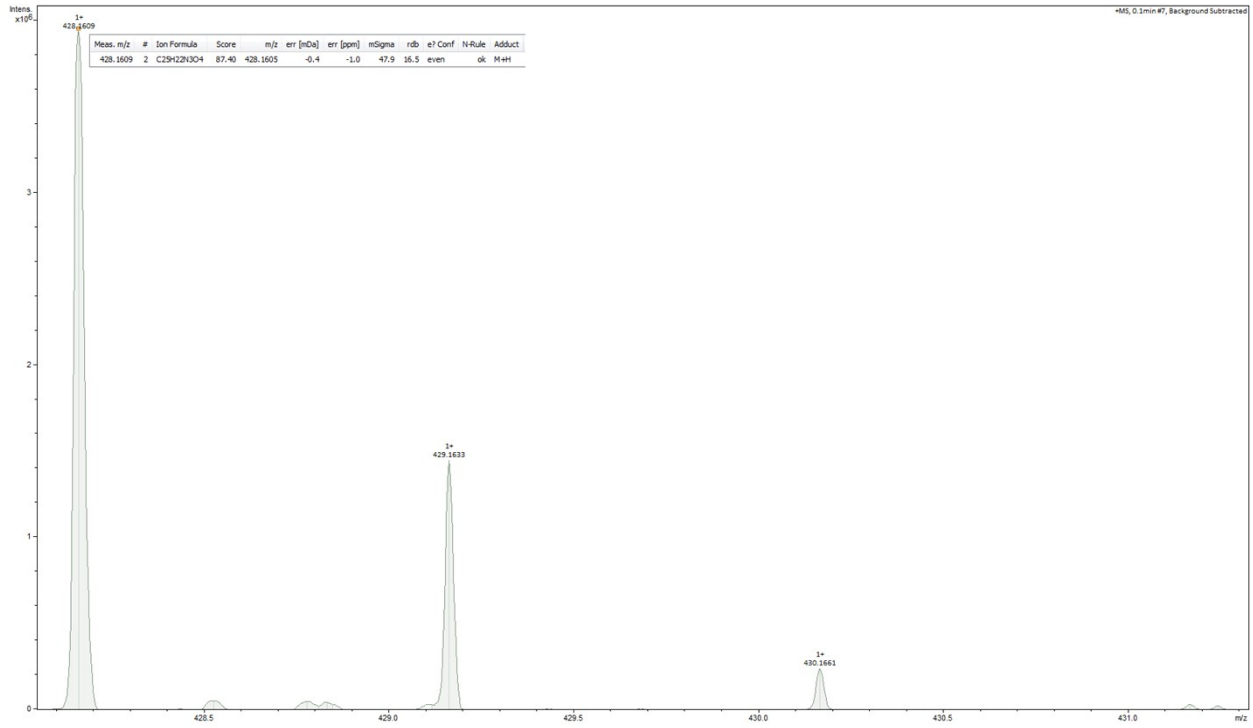
HRMS of **4u**



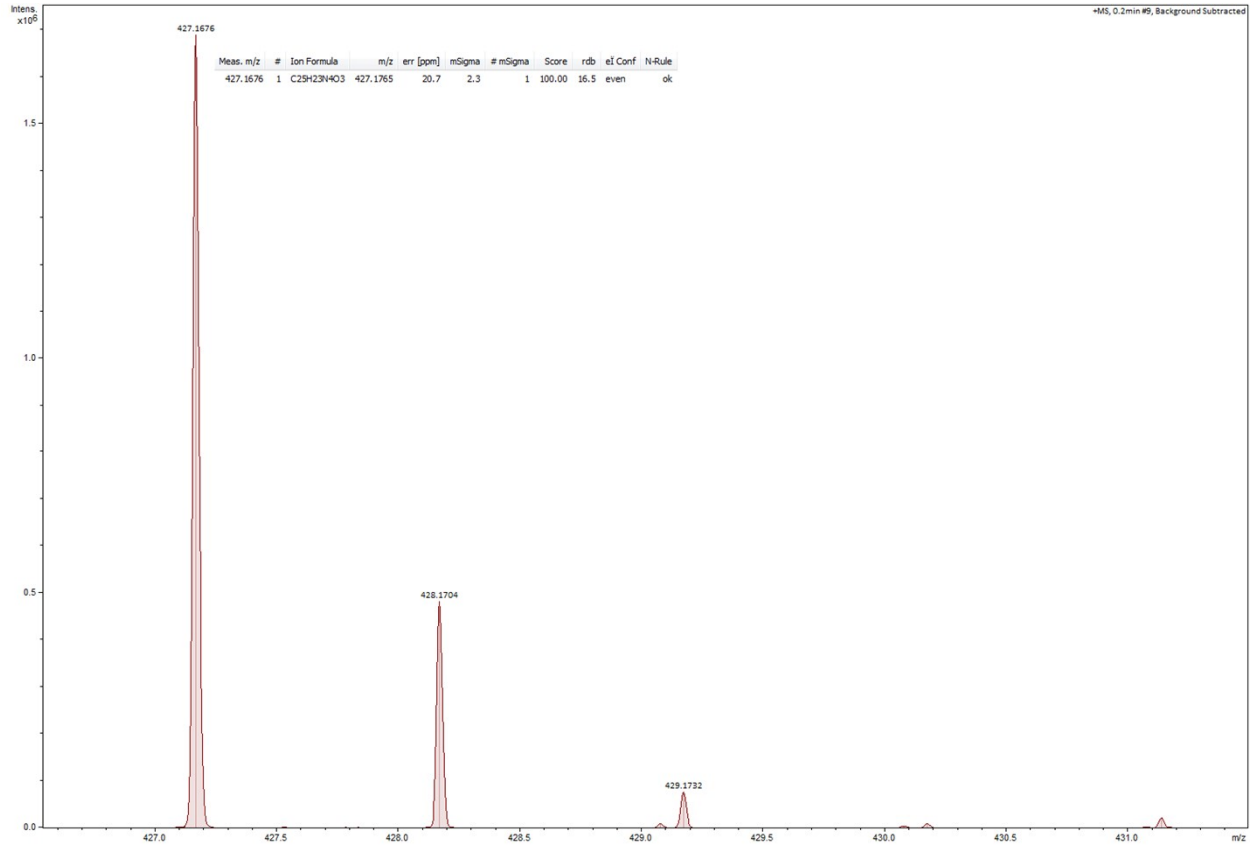
HRMS of **4v**



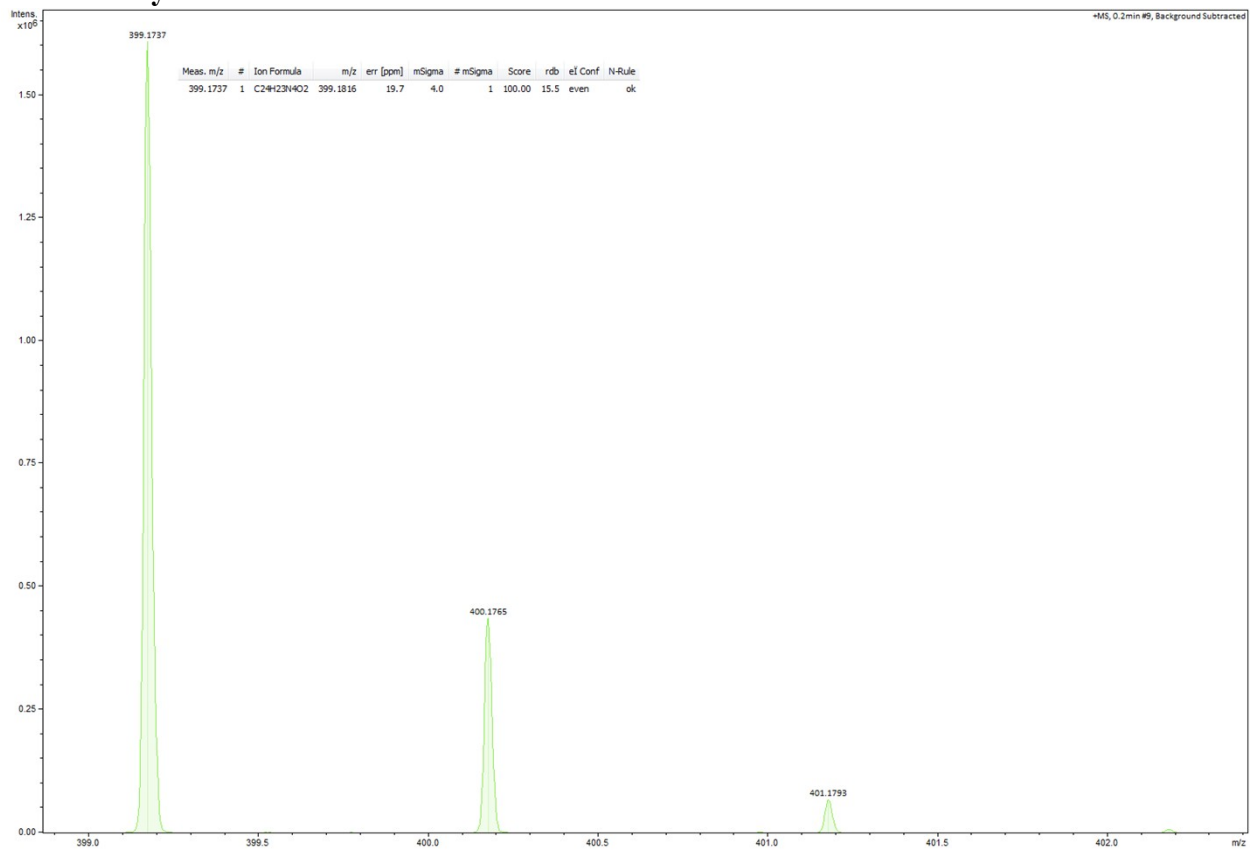
HRMS of **4w**



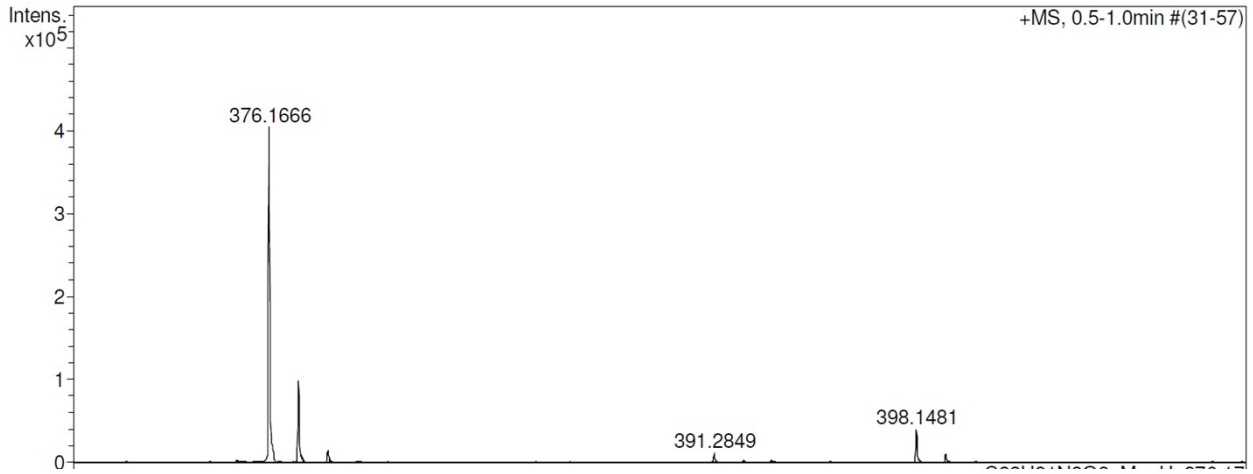
HRMS of **4x**



HRMS of **4y**

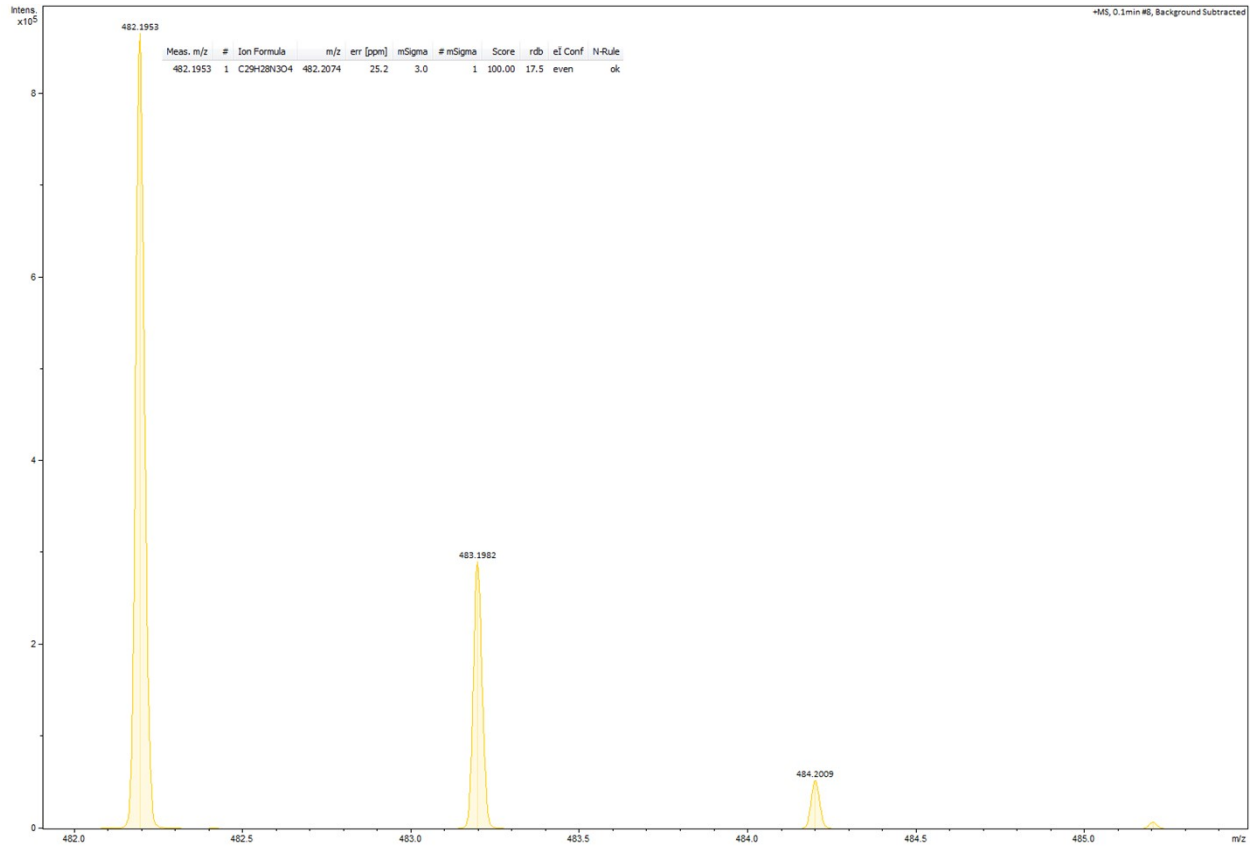


HRMS of **4z**

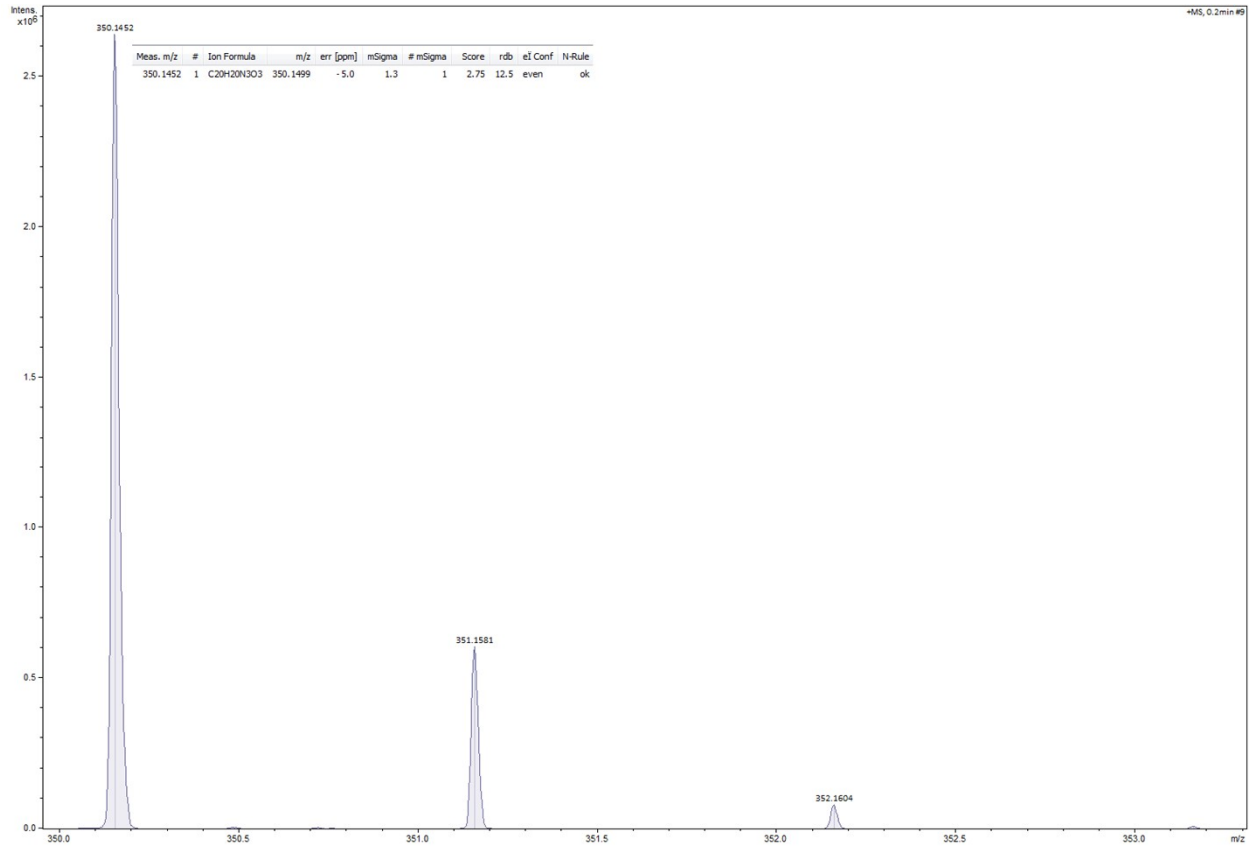


HRMS of **4aa**

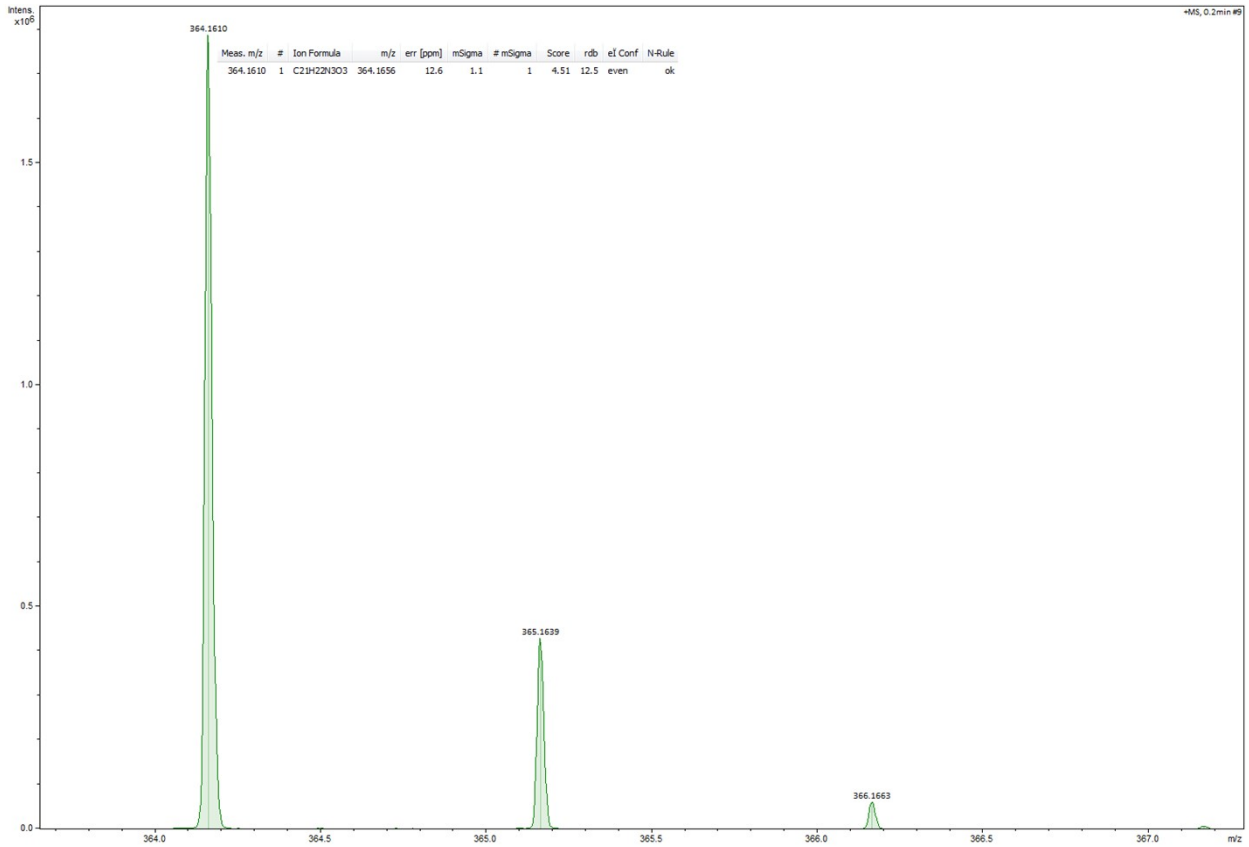
HRMS of **4ab**



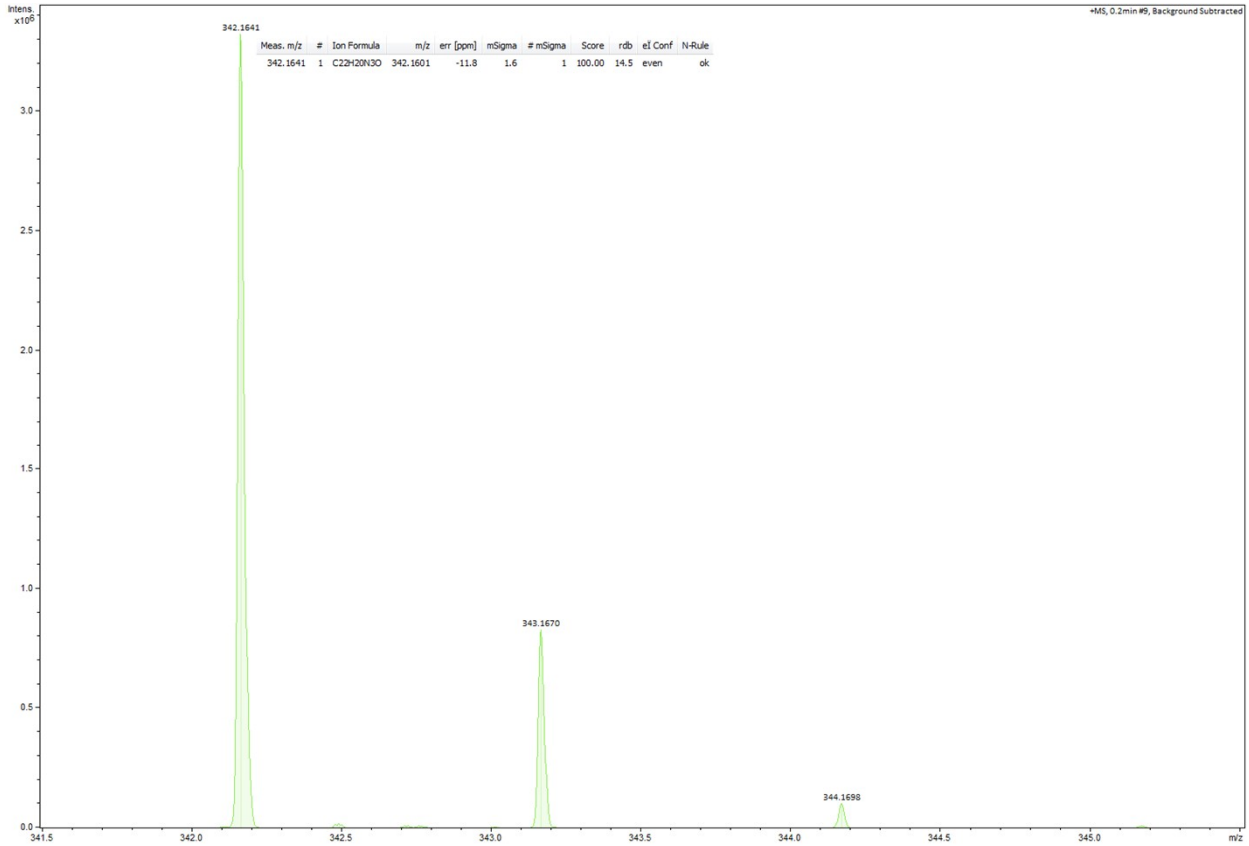
HRMS of **4ac**



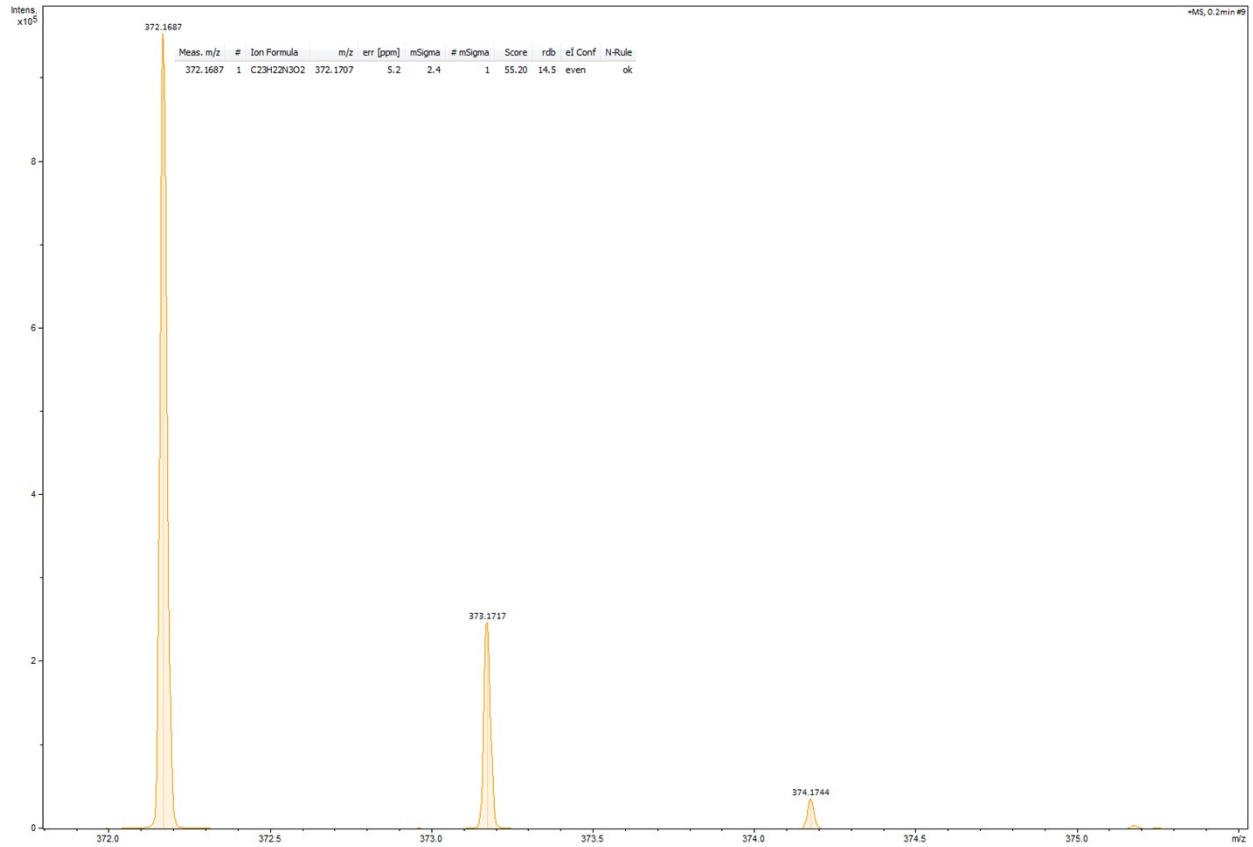
HRMS of **4ad**



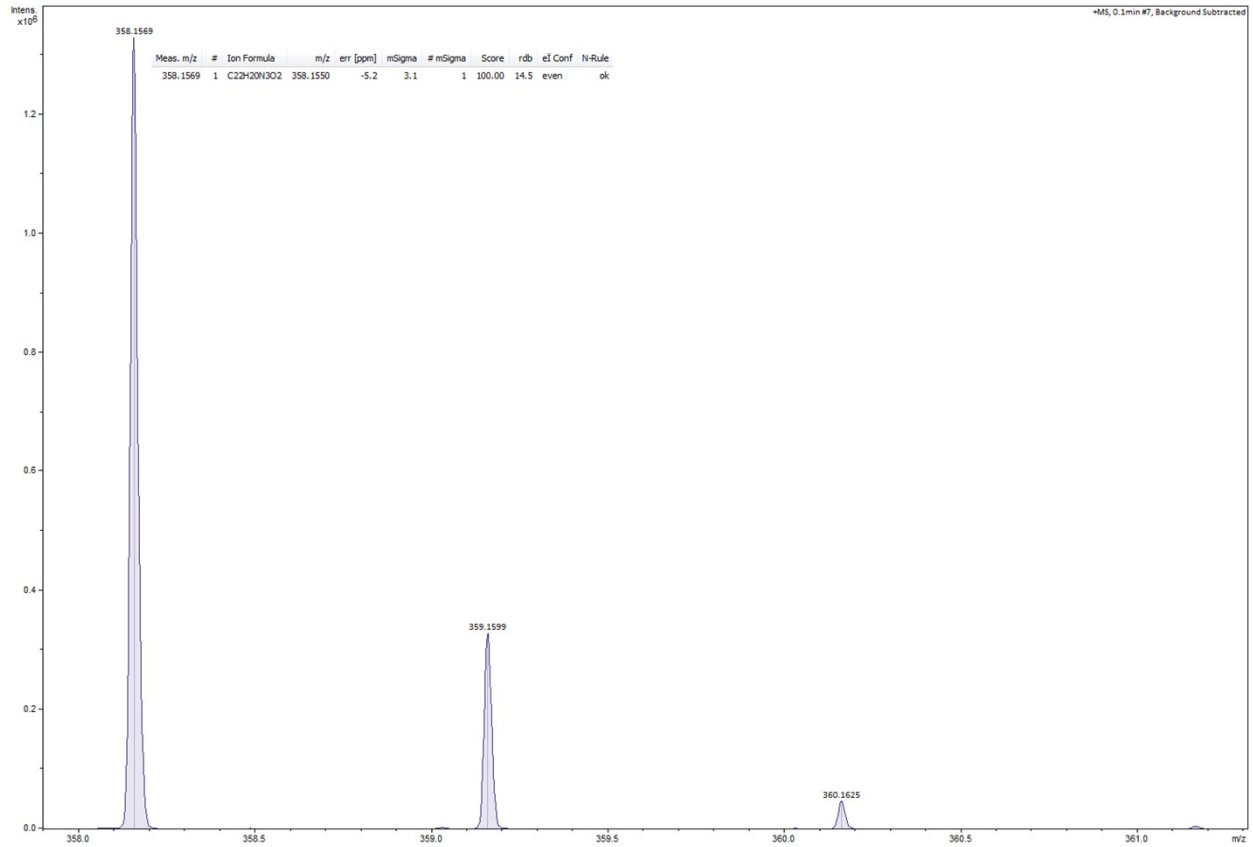
HRMS of **5a**



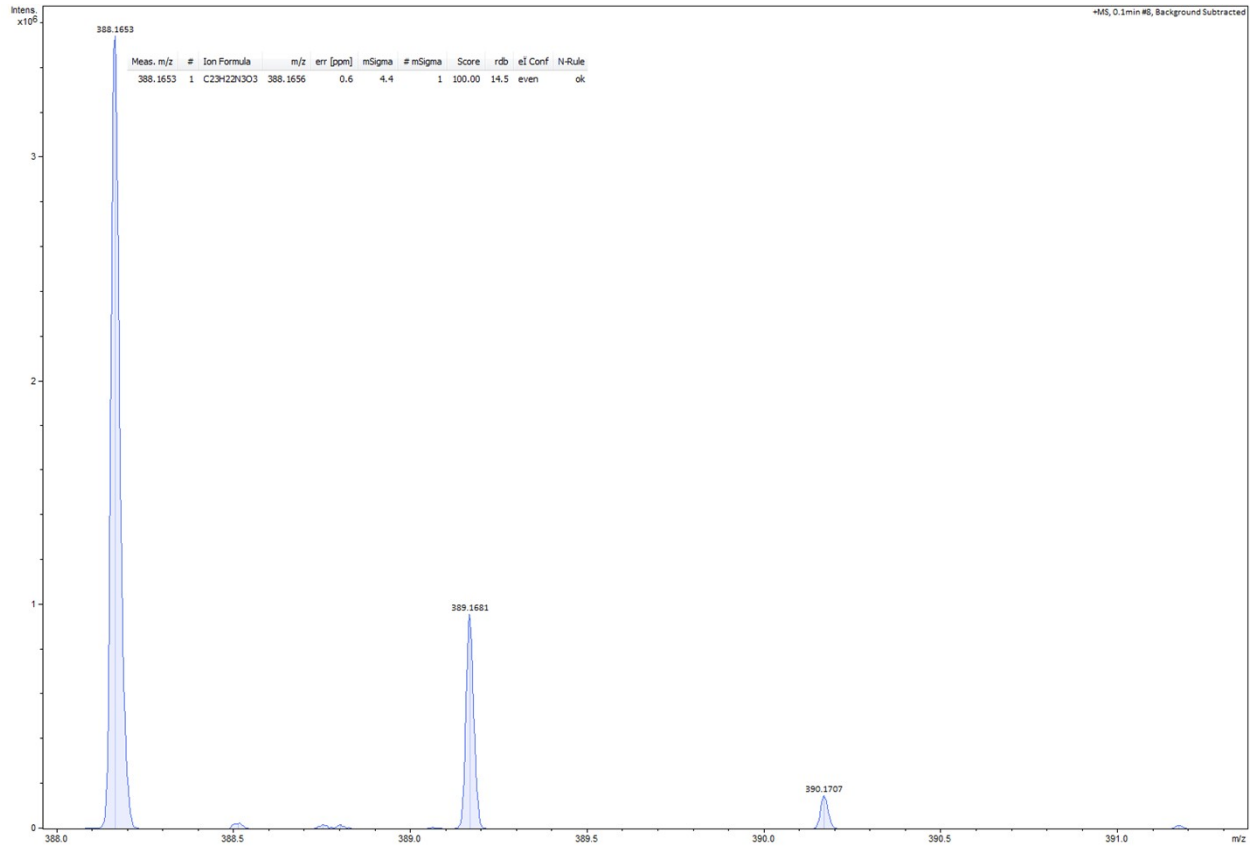
HRMS of **5b**



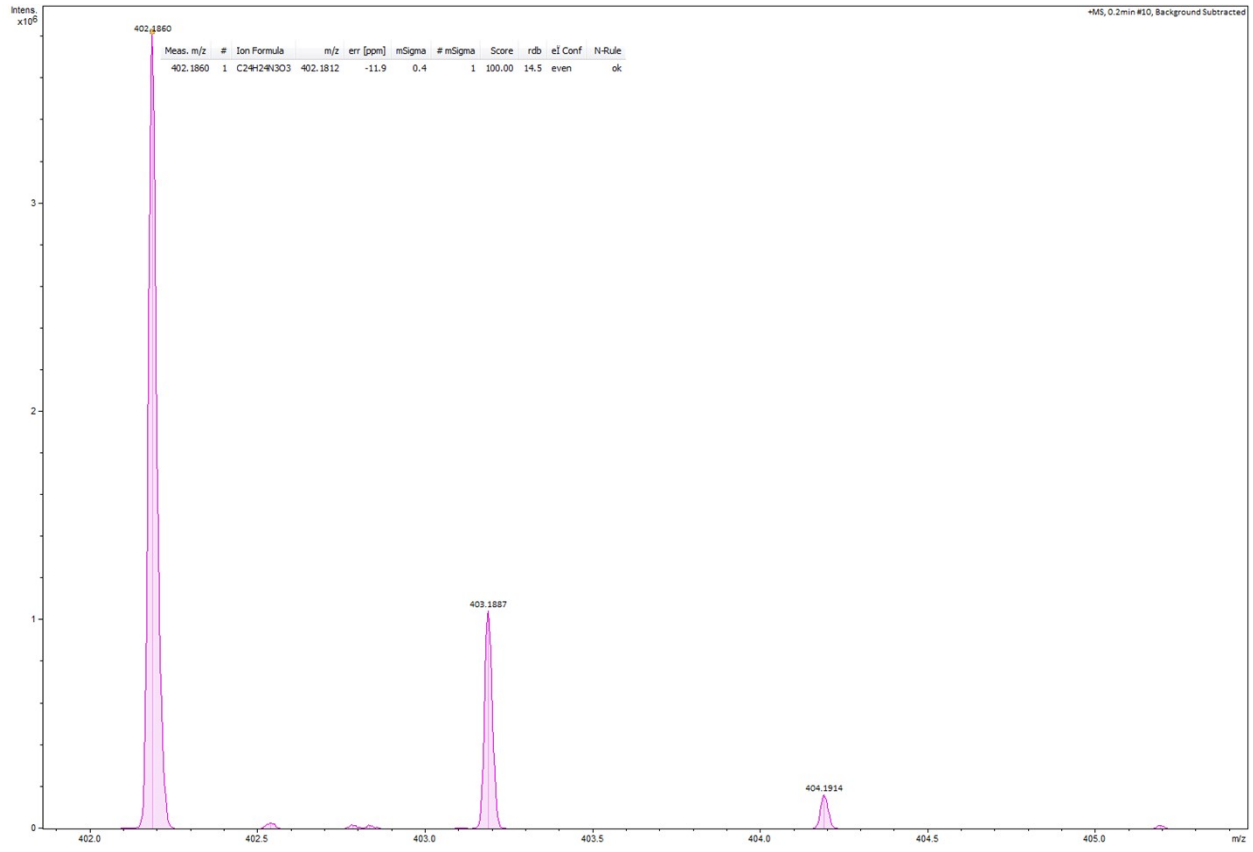
HRMS of **5c**



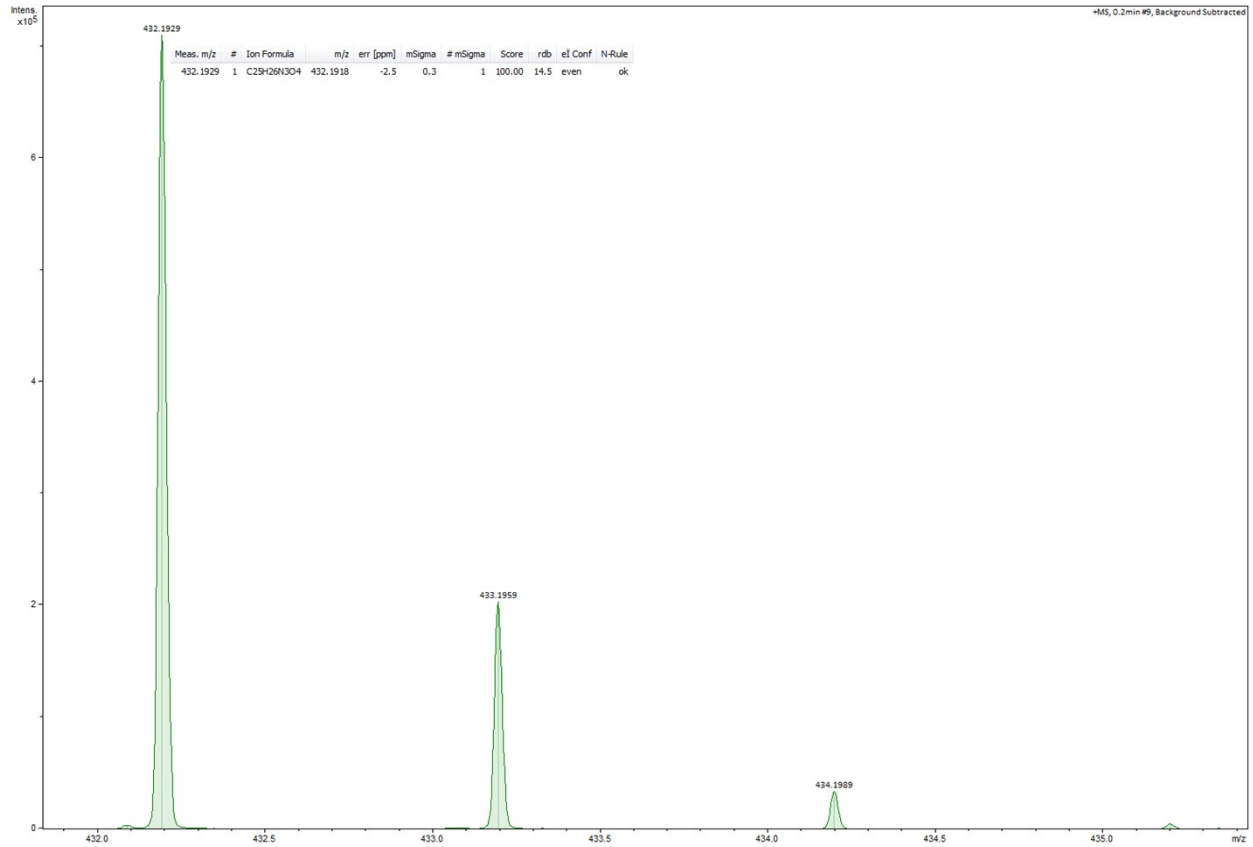
HRMS of **5d**



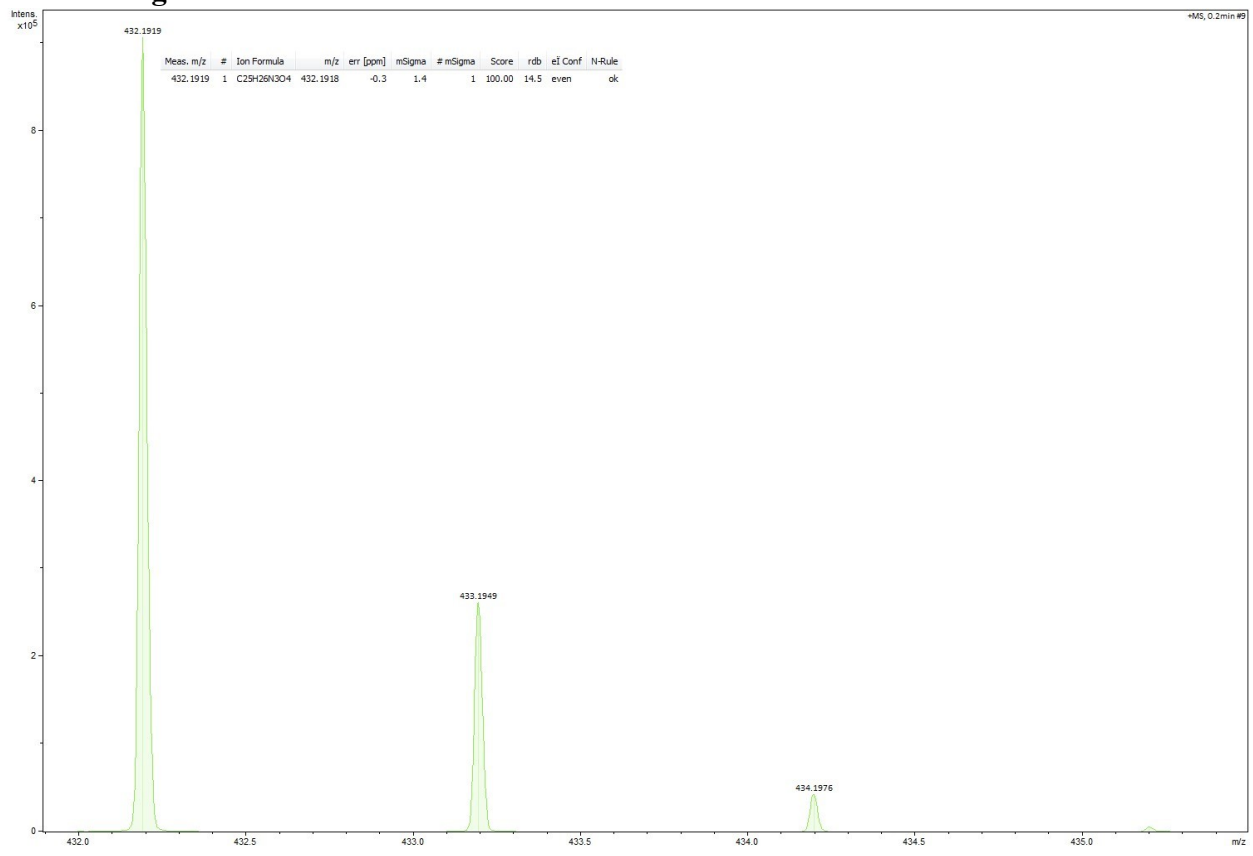
HRMS of **5e**



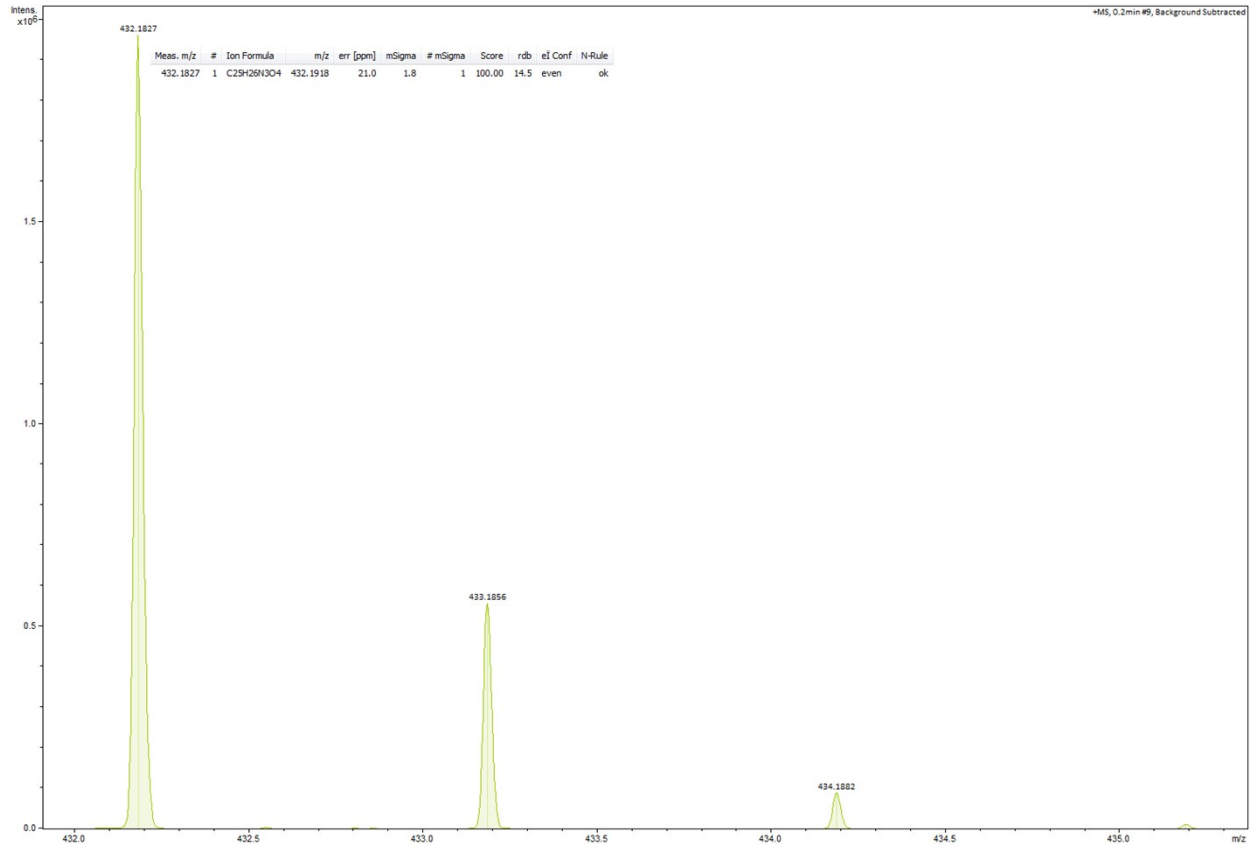
HRMS of **5f**



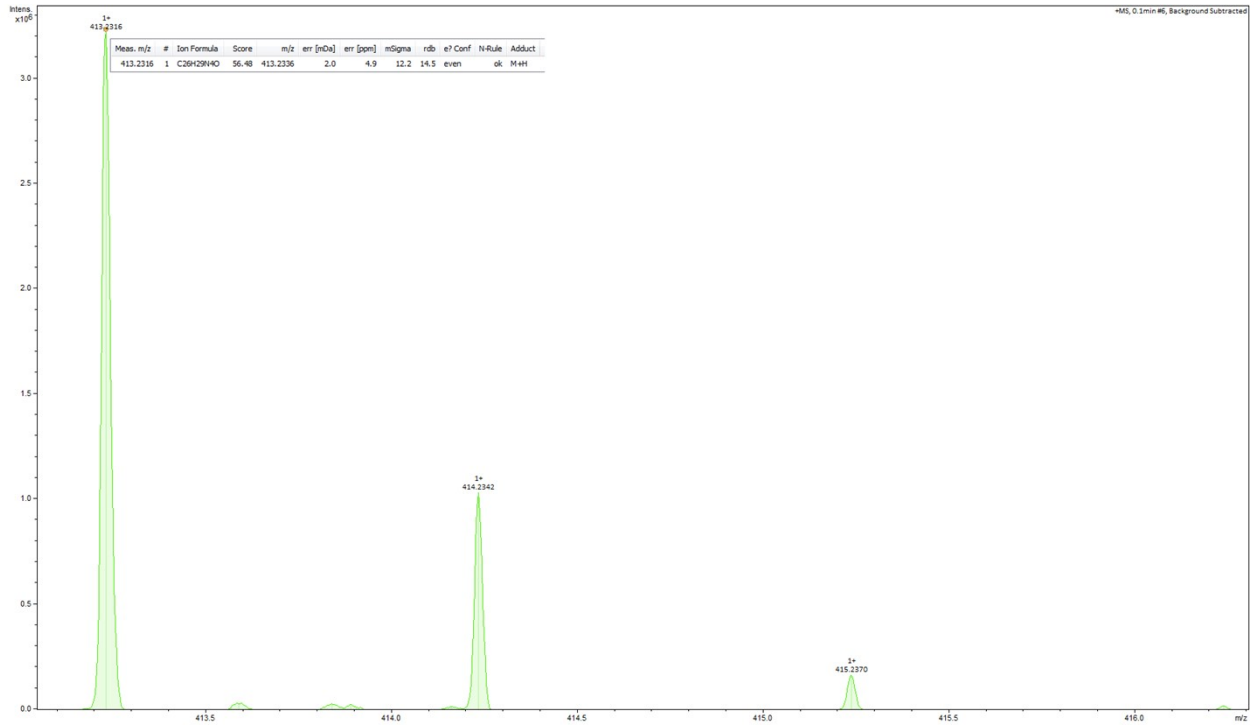
HRMS of **5g**



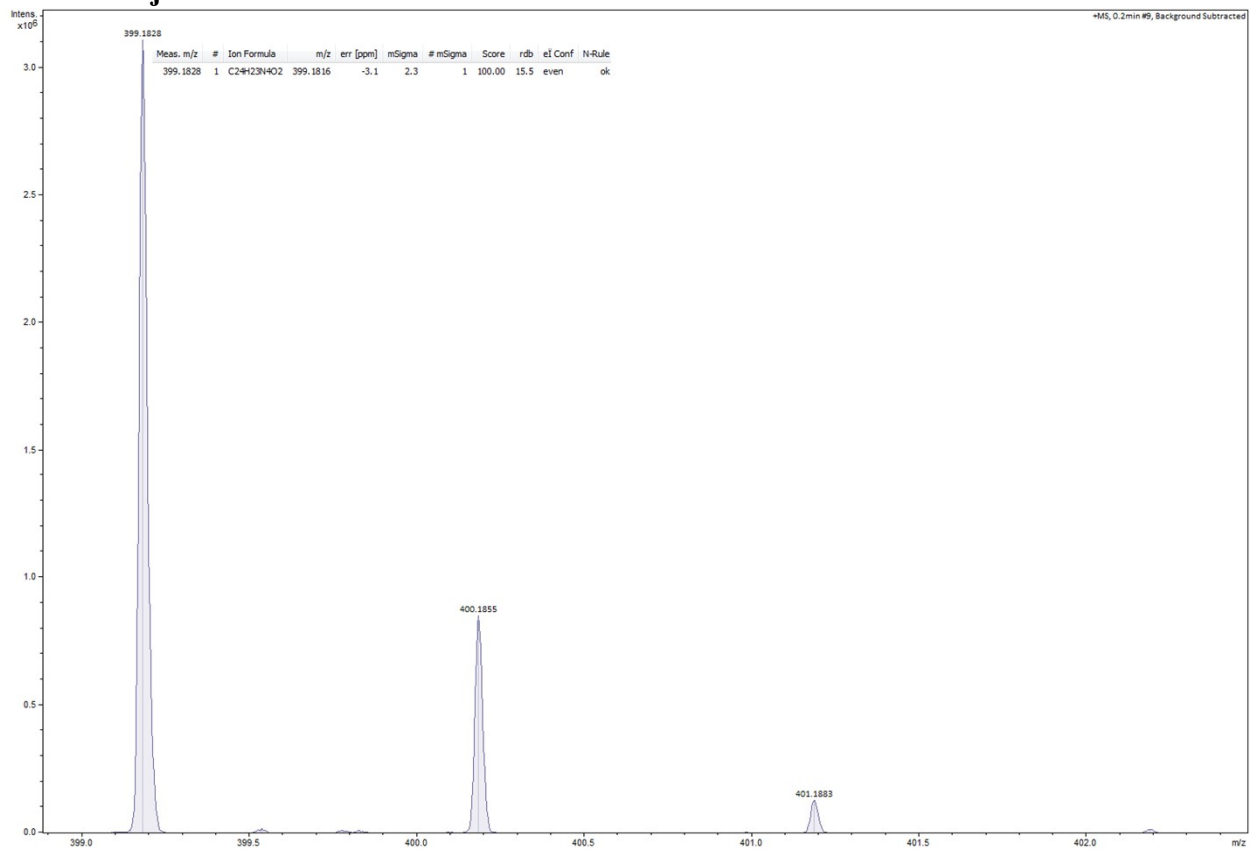
HRMS of **5h**



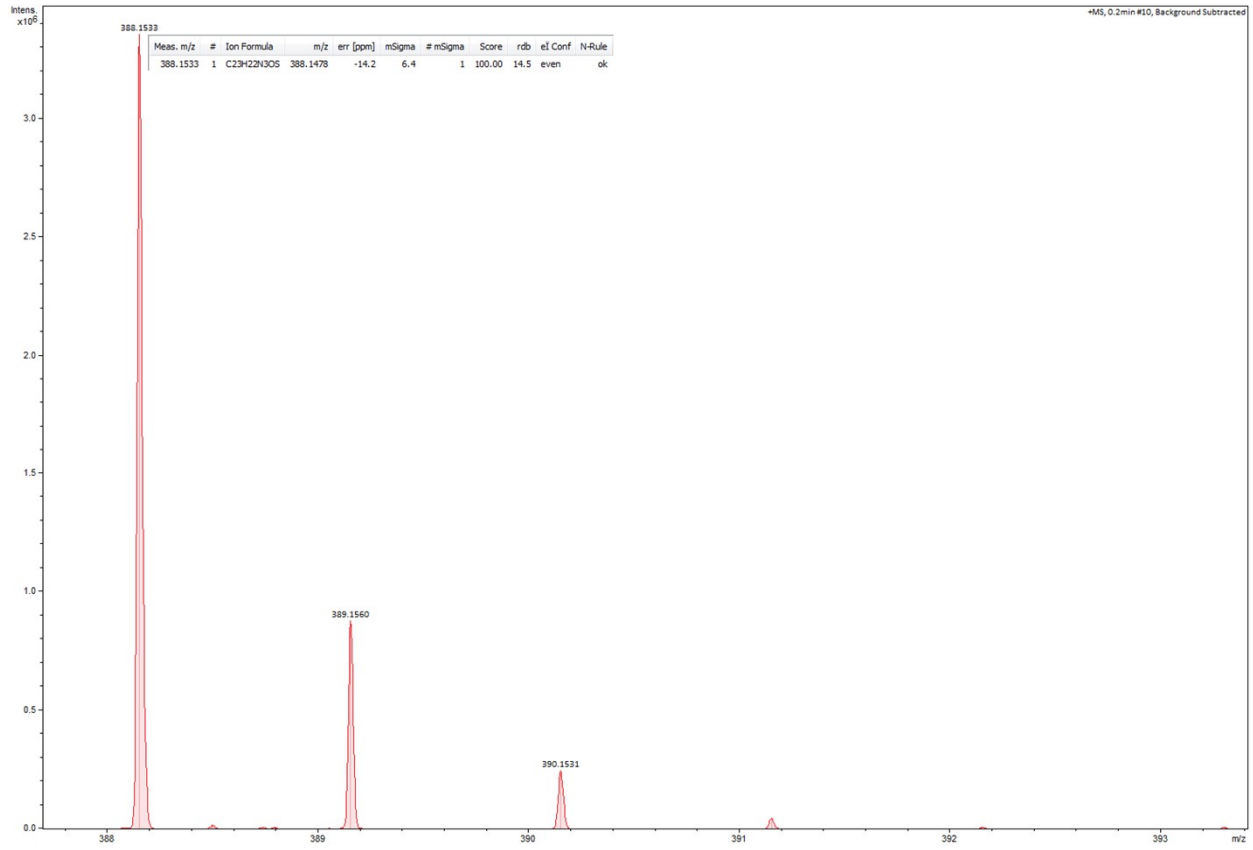
HRMS of **5i**



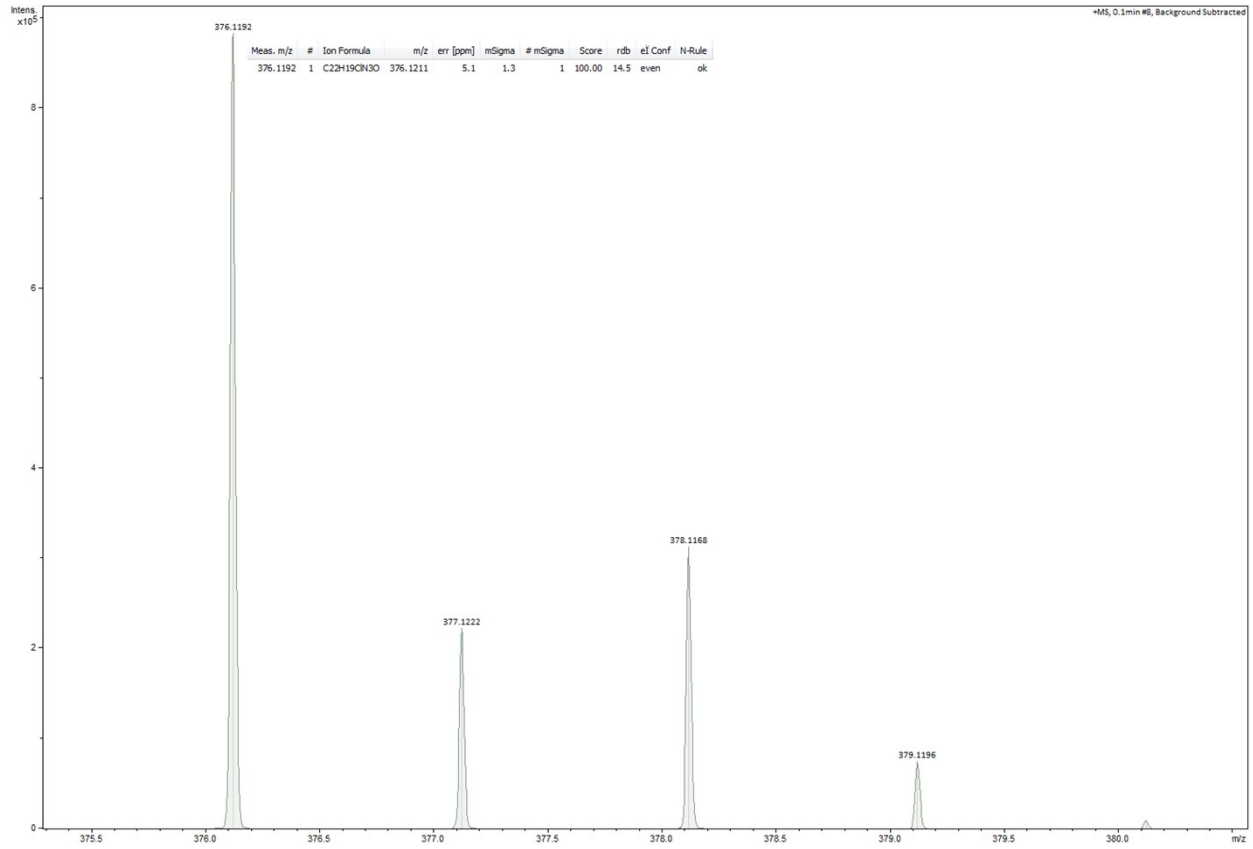
HRMS of **5j**



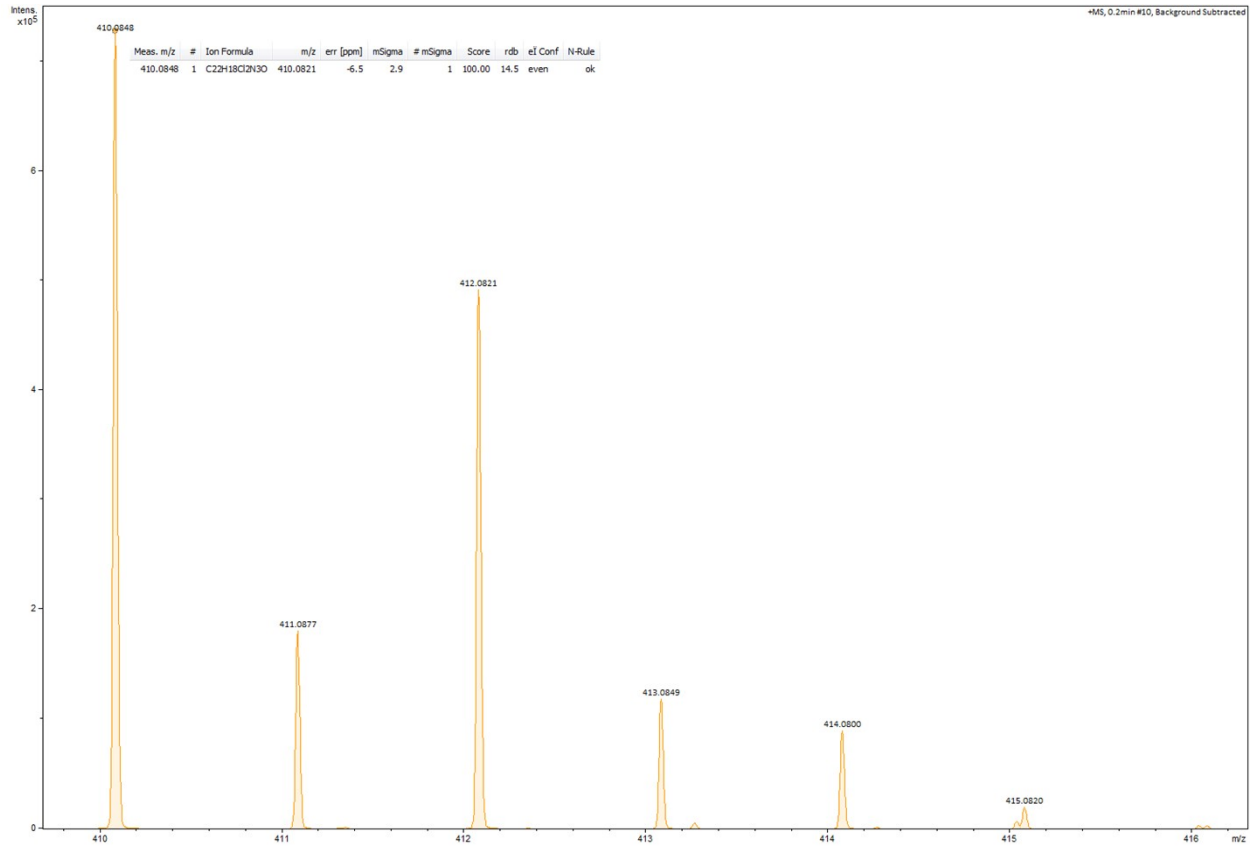
HRMS of **5k**



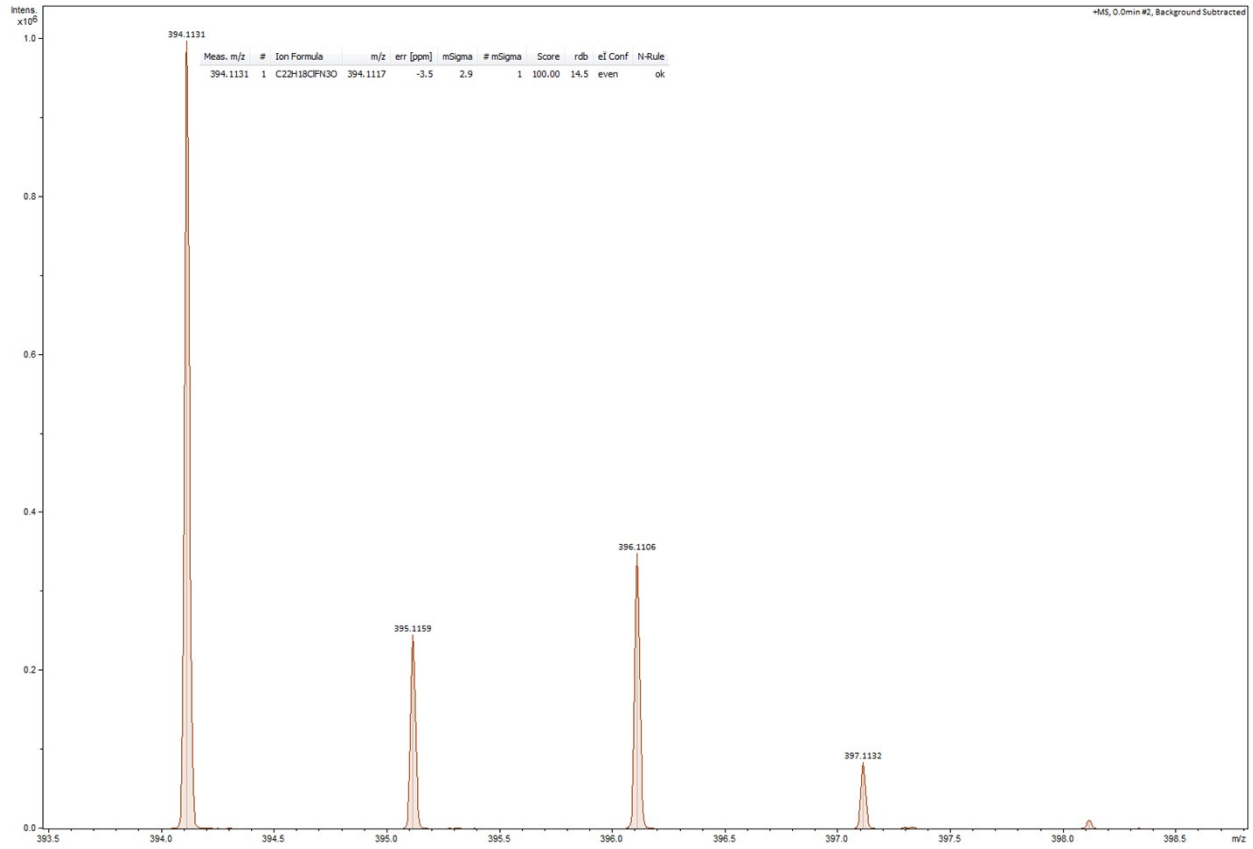
HRMS of **5l**



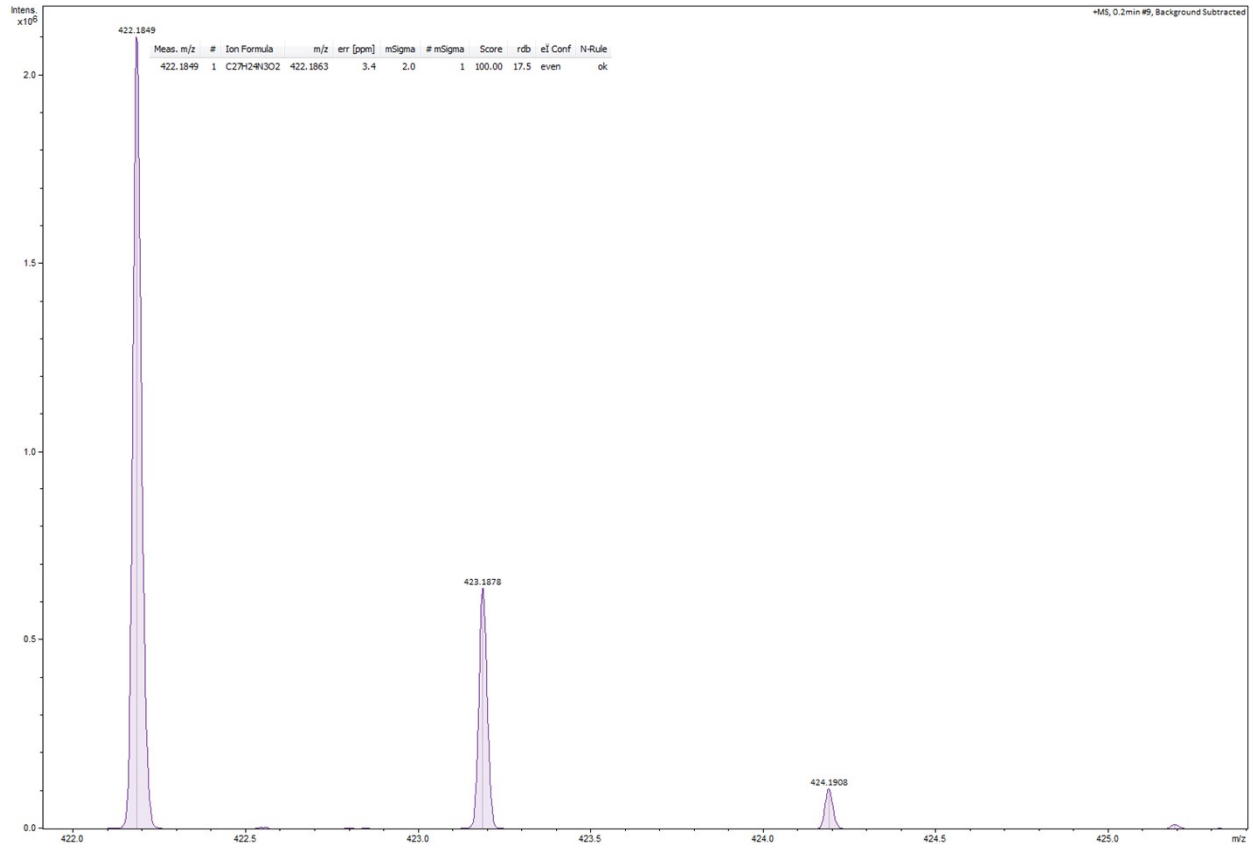
HRMS of **5m**



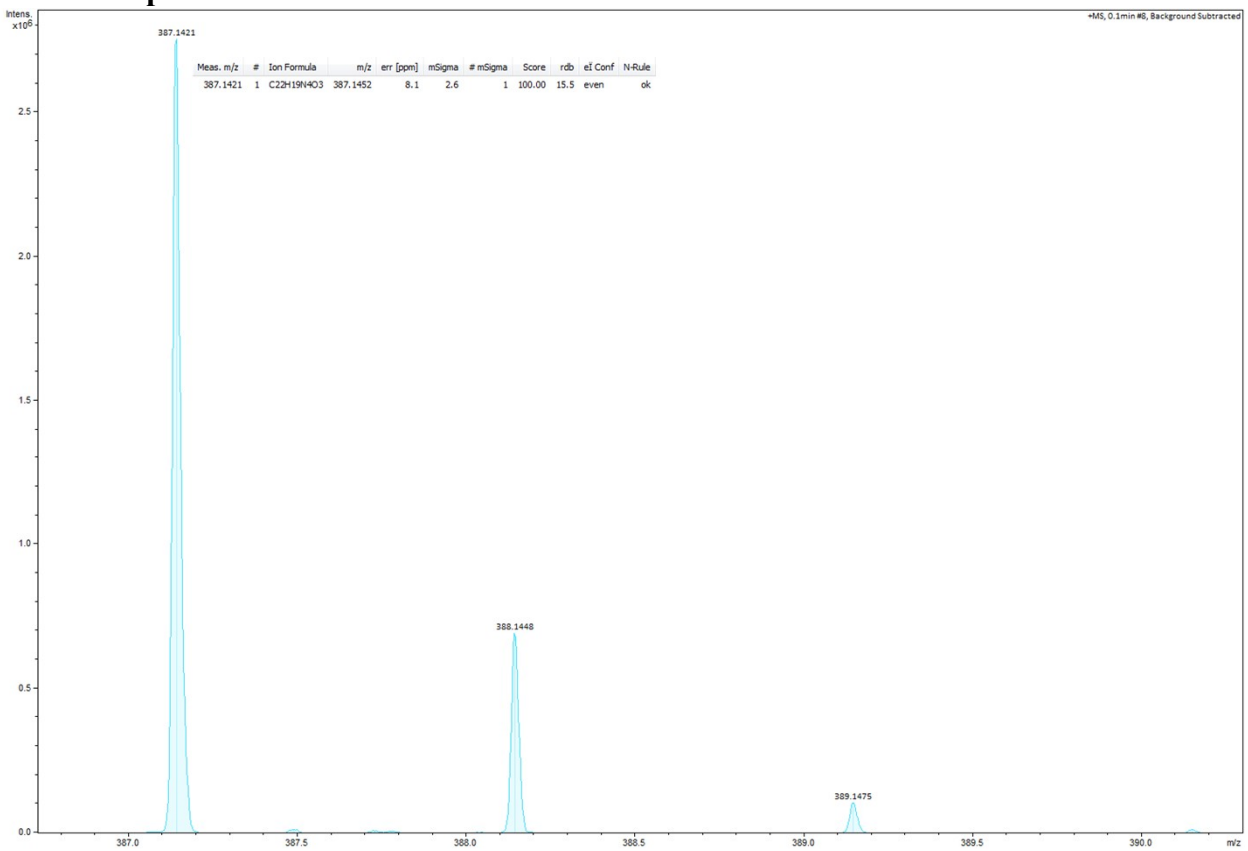
HRMS of **5n**



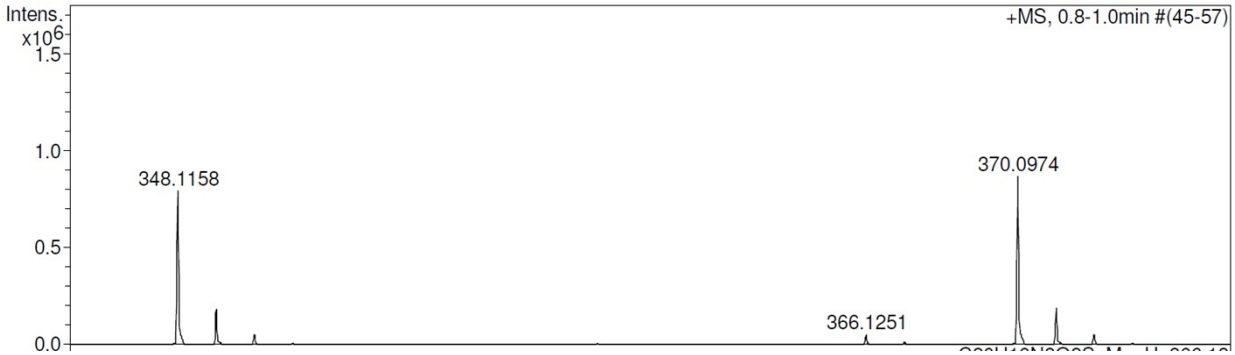
HRMS of **5o**



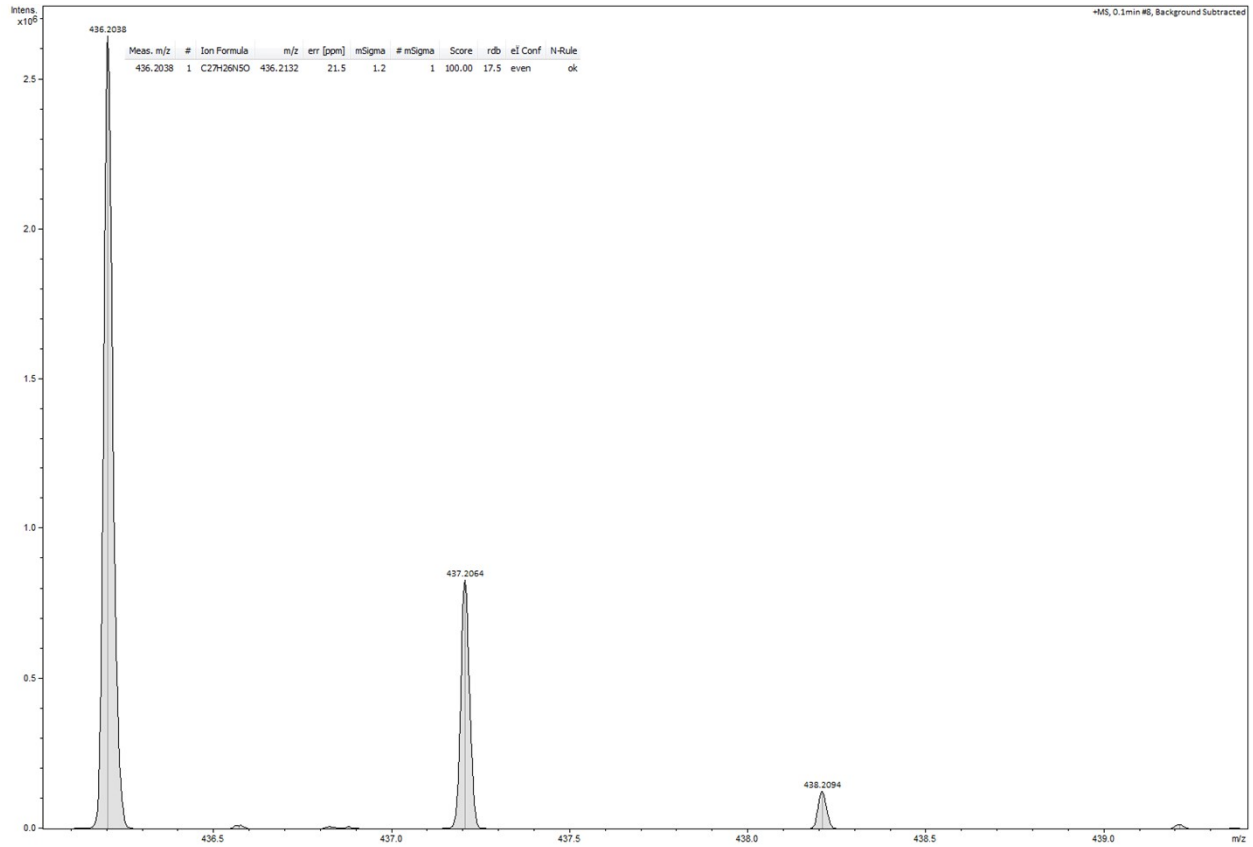
HRMS of **5p**



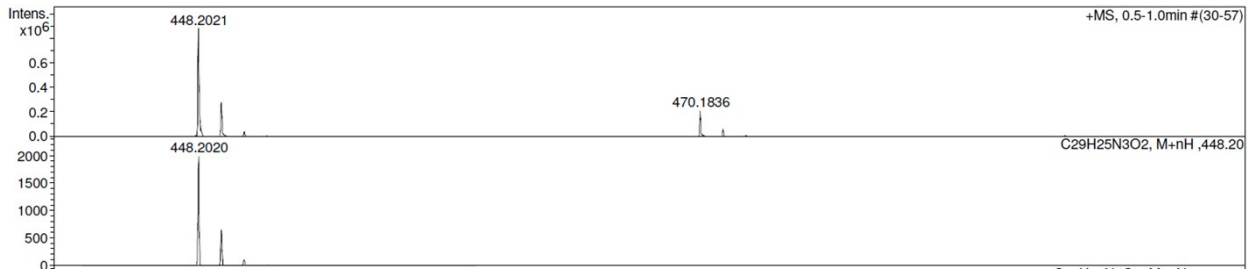
HRMS of **5q**



HRMS of **5r**



HRMS of **5s**



X-Ray Crystallographic Data of products

X-ray crystallography. X-ray diffraction data for **4x**, **4j**, **5b** and **5k** were collected at 100 K with a Bruker Quest D8 CMOS diffractometer, using graphite monochromated Mo-Kα radiation (lλ = 0.71073 Å). Using Olex2,[10] the structures were solved with the ShelXT[11] structure solution program using Intrinsic Phasing and refined with the XL[12] refinement package using Least-Squares minimization against F^2 in anisotropic approximation for non-hydrogen atoms. Hydrogen atom of NH group of **4x** and that of the OH group of its solvate methanol molecule were located from difference Fourier synthesis while the positions of other hydrogen atoms were calculated, and they all were refined in isotropic approximation within the riding model. Crystal data and structure refinement parameters are given in Table S3. CCDC 2215936, 2215935, 2211258 and 2211260 contain the supplementary crystallographic data for **4x**, **4j**, **5b** and **5k**, respectively.

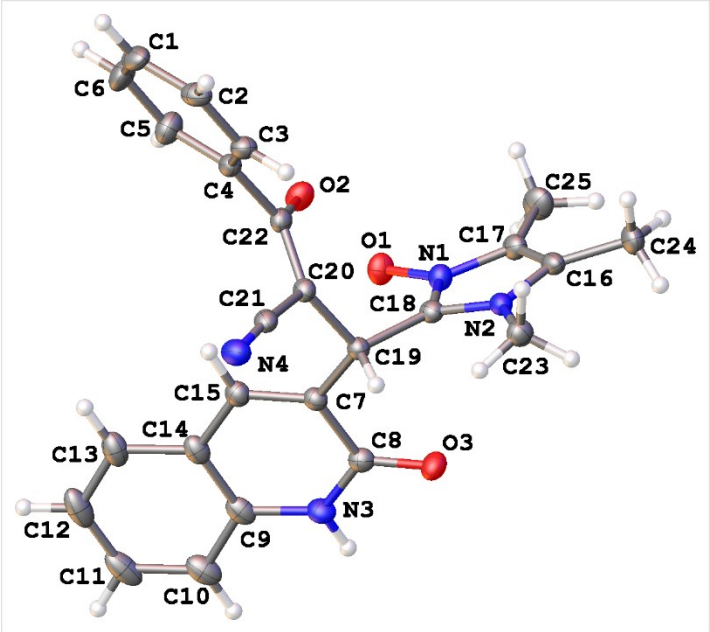


Figure 1. General view of **4x** in representation of atoms *via* thermal ellipsoids at 50% probability level. The solvate molecule of methanol is omitted for clarity.

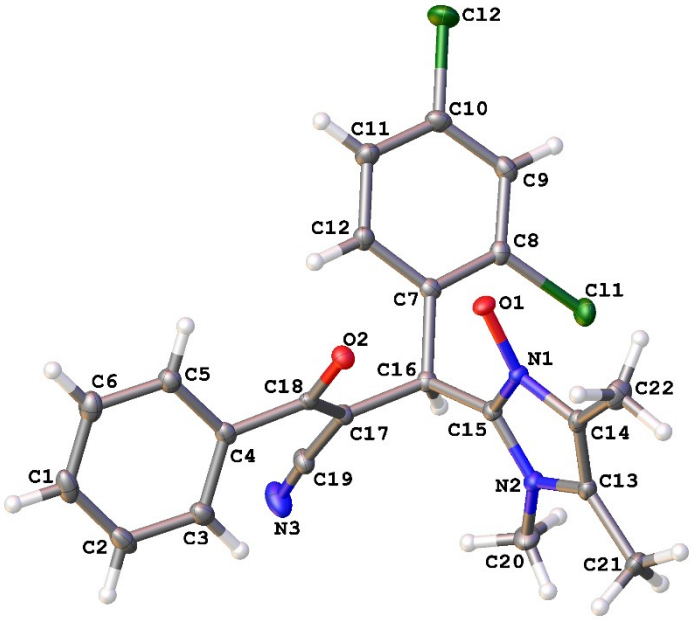


Figure 2. General view of **4j** in representation of atoms *via* thermal ellipsoids at 50% probability level.

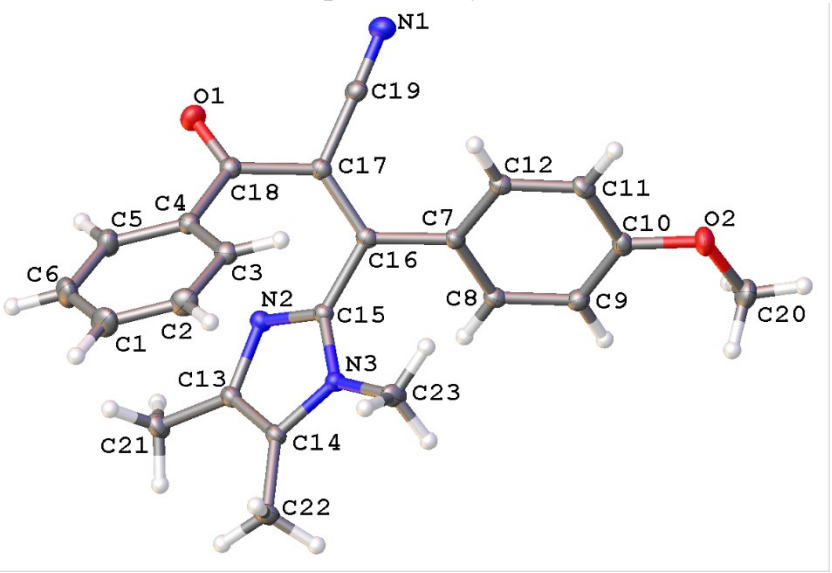


Figure 3. General view of **5b** in representation of atoms *via* thermal ellipsoids at 50% probability level.

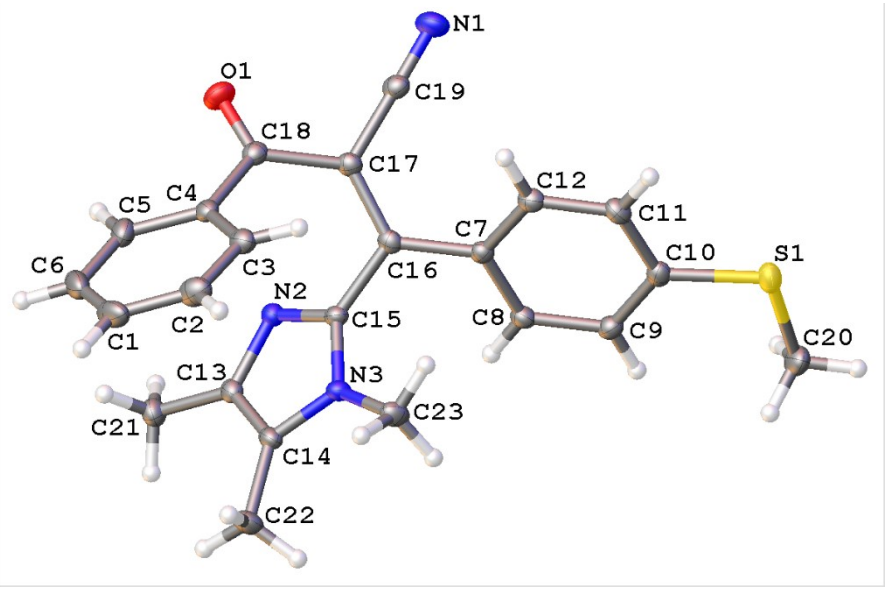


Figure 4. General view of **5k** in representation of atoms *via* thermal ellipsoids at 50% probability level.

Table S3. Crystal data and structure refinement parameters for **4x**, **4j**, **5b** and **5k**.

	4x	**4j**	**5b**	**5k**
Empirical formula	$C_{26}H_{25}N_4O_4$	$C_{22}H_{18}Cl_2N_3O_2$	$C_{23}H_{21}N_3O_2$	$C_{23}H_{21}N_3OS$
Formula weight	457.513	427.312	371.442	387.509
T, K	100	100	100	100
Crystal system	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	$P2_1/n$	Pbca	C2/c	$P2_1/c$
Z	4	8	8	4
a, Å	10.6494(3)	13.8855(2)	28.6642(5)	13.4764(2)
b, Å	10.3451(3)	10.0424(2)	8.5510(2)	8.5980(2)
c, Å	21.0786(6)	29.2647(5)	17.5757(3)	17.6336(3)
α, °	90	90	90	90
β, °	98.471(1)	90	116.701(1)	100.610(1)
γ, °	90	90	90	90
V, Å^3	2296.88(11)	4080.78(12)	3848.55(13)	2008.27(7)
D_{calc} (g cm^{-1})	1.323	1.391	1.282	1.282
μ, см$^{-1}$	0.91	3.42	0.83	1.79
F(000)	964	1768	1568	816
$2\theta_{max}$, °	58	58	58	58
Reflections measured	29945	52179	24875	25188
Independent reflections	6100	5423	5110	5329

Observed reflections [I > 2σ(I)]	4573	4562	4265	4460
Parameters	316	265	257	257
R1	0.0515	0.0354	0.0434	0.0478
wR2	0.1324	0.0951	0.1151	0.1258
GOF	1.053	1.024	1.030	1.048
$\Delta\rho_{max}$/ $\Delta\rho_{min}$ (e Å^{-3})	0.561/-0.259	0.621/-0.310	0.361/-0.234	0.392/-0.474

DFT calculations

Details of calculation and discussion

All of the DFT calculations were performed with the Orca 5.0.1 program package.[13,14] The geometry optimization of all the minima involved were performed at the R2SCAN-3c level of theory.[15] The structures of the reactants, intermediates, transition states, and products were fully optimized without any restriction. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. In order to find the minimum energy reaction path the NEB calculations[16] were carried out to connect the related reactants and products and obtain transition states.

DFT-Computed energies of all stationary points

Table S4. Electronic energy (E, in Hartree), zero point energy correction (ZPE, in Hartree), Thermal correction (T, in Hartree) enthalpies (H, in Hartree), and free energies (G, in Hartree). For transition state structures, one imaginary frequency (Ifreq) was observed and given below. For all minimum structures, no imaginary frequency was observed.

Structure	E	ZPE	T	H	G	Ifreq
1a	-419.22361394	0.15674295	0.00990370	-419.05602308	-419.10124175	
6	-608.51929336	0.16288959	0.01270968	-608.34369409	-608.39501100	
3	-860.61900327	0.25465206	0.01742557	-860.34598144	-860.40849925	
1a+6	-1027.76701221	0.32114795	0.02427453	-1027.42064552	-1027.49687715	
TS1a	-1027.74320160	0.32259739	0.02214881	-1027.39751119	-1027.46891605	-177.46
INT1a	-1027.74424110	0.32335823	0.02240389	-1027.39753478	-1027.46941962	
TS2a	-1027.73765319	0.32112553	0.02227545	-1027.39330800	-1027.46491179	-84.47
INT2a	-1027.77858545	0.32024082	0.02403558	-1027.43336484	-1027.50927119	

TS3a	-1027.76475288	0.31682870	0.02348937	-1027.42349060	-1027.49835469	-316.47
INT3a	-1027.83509293	0.32375879	0.02329959	-1027.48709035	-1027.56083126	
TS4a	-1027.82040611	0.32097076	0.02292819	-1027.47556295	-1027.54878238	-157.42
7	-1027.84098988	0.32184283	0.02358664	-1027.49461620	-1027.56937322	
1a+3	-1279.85709063	0.41299135	0.02868000	-1279.41447507	-1279.49888564	
TS1b	-1279.83624650	0.41309279	0.02680414	-1279.39540536	-1279.47610845	-298.77
INT1b	-1279.84163536	0.41405412	0.02707021	-1279.39956682	-1279.48188405	
TS2b	-1279.83974766	0.41250730	0.02705536	-1279.39924078	-1279.48190624	-69.43
INT2b	-1279.86600552	0.41543189	0.02682843	-1279.42280099	-1279.50350252	
4m	-1279.88952778	0.41499832	0.02743065	-1279.44615461	-1279.52825981	
TS1c	-1279.82801892	0.41408214	0.02677354	-1279.38621903	-1279.46686187	-227.03
INT1c	-1279.83707307	0.41487411	0.02695659	-1279.39429817	-1279.47483669	
TS2c	-1279.83431733	0.41326469	0.02680423	-1279.39330420	-1279.47364773	-218.24
INT3c	-1279.89135742	0.41201844	0.02868614	-1279.44970863	-1279.53420847	

The coordinates of all stationary points (Å)

1a

N	4.64256707180487	2.45356507395820	-7.53815974661250
C	4.64370734886422	3.55338075700890	-6.76476354839007
C	4.58487739369781	1.33061514126353	-6.69909429932096

C	4.55260129678228	1.78489034269207	-5.40400033412382
N	4.60398444601548	3.16153852627703	-5.45522845622871
H	4.68974449872974	4.56616974936817	-7.12945789549079
O	4.69840589547008	2.39951546251955	-8.81676830938276
C	4.58781434780387	-0.02218401235224	-7.29747262747976
H	5.48518947946998	-0.16924425017372	-7.90845477678607
H	4.55342716238754	-0.79141892485498	-6.52256090625043
H	3.73006704208177	-0.14935869841712	-7.96688321115588
C	4.48087415373143	1.04087057558045	-4.11841248521922
H	3.60318933619992	1.32674801954206	-3.52572228790419
H	4.41024636176807	-0.03032814806703	-4.31611327387711
H	5.37061164633808	1.20476091057810	-3.49788534712173
C	4.45788088749927	4.06326021323553	-4.32971452301372
H	3.41760660517891	4.10930825376562	-3.98223392225205
H	5.09421527674472	3.74173236373554	-3.49982482650417
H	4.76981389043178	5.06516948634027	-4.63351224288590

6

C	-3.13351204678328	-1.10072408151760	-5.94347823091705
C	-2.04243469328558	-0.30797360774249	-5.70481004147058
H	-1.14262549629883	-0.62385794271176	-6.22956962698938
C	-4.42498882761144	-0.91366245791046	-5.38258036267762
N	-5.48190465782348	-0.78044329653241	-4.92526440975277
C	-1.88426308234127	0.85934168304798	-4.88530538088808
C	-2.90436146326583	1.46035017831368	-4.12288149998096
C	-0.60000425027459	1.45031689510560	-4.84398827111780
C	-2.65975193691701	2.58744121524947	-3.35940756085244
C	-0.34467299886188	2.57070822592192	-4.08815347528569
C	-1.37616949481744	3.15134590229425	-3.33584356894958
H	-3.90566500474410	1.04732635248295	-4.12161553030935
H	0.20531730452239	1.00692353786332	-5.42394734296335

H	-3.47191171359573	3.01991270982060	-2.78737835144752
H	0.64186487165595	3.02121210963559	-4.05809353048640
O	-1.03408768654962	4.24620668392632	-2.62524508522411
C	-2.04210574201764	4.88520230161788	-1.83562345681843
H	-2.43349656354299	4.20462340425955	-1.06974994916361
H	-1.54601155627824	5.72875435695281	-1.35491234318347
H	-2.86224711849996	5.25196608675608	-2.46486719813872
C	-3.00302430898017	-2.21550171518654	-6.82002626674324
N	-2.88925255568923	-3.12107237464676	-7.53396335463975

3

C	-3.06779445564411	-1.21905352045332	-5.89111566480719
C	-2.02445303822265	-0.36182386444549	-5.68727472200941
H	-1.12935949904120	-0.65076924509581	-6.23814648950478
C	-4.32311466364091	-1.08704088545298	-5.25142442702152
N	-5.34962339543004	-0.99888949470166	-4.71518927071209
C	-2.81143719274568	-2.40882524659519	-6.77976029753965
O	-1.66293083746688	-2.75421872870922	-7.01509571104451
C	-3.95849197124681	-3.15812456922809	-7.35947728274079
C	-5.15876278266119	-2.53707261176697	-7.71963946906155
C	-3.78265909370728	-4.52259116759095	-7.61834536855338
C	-6.16901778613658	-3.27451933993800	-8.32528404836698
C	-4.80329712066081	-5.25990162690254	-8.19903435929028
C	-5.99834892974885	-4.63635001267278	-8.55446287224547
H	-5.30042635387482	-1.47464067318679	-7.55112786698814
H	-2.83743432818500	-4.98506301958515	-7.35211865470168
H	-7.09368114974684	-2.78450073767084	-8.61471402103793
H	-4.66895694816894	-6.32220640920659	-8.38032760307674
H	-6.79578006715088	-5.21287030298021	-9.01469402440805
C	-1.89413981162798	0.82788215628498	-4.89293803535407
C	-2.89934623091705	1.37556166899222	-4.07294584676704

C	-0.64966414161342	1.49831259994017	-4.93619175850686
C	-2.67856887857177	2.52602209976663	-3.33584974101337
C	-0.41782918350551	2.64286407769162	-4.20849204515938
C	-1.43438197029968	3.16810208189242	-3.39819801631731
H	-3.86924148290974	0.89845658143087	-4.00439892808178
H	0.14363659947603	1.09505144820402	-5.56019430056664
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H	0.53909211759904	3.15319901328503	-4.24343841199183
O	-1.11722856447061	4.29222311900605	-2.71843585407443
C	-2.10930613132711	4.86915643896909	-1.86575150453128
H	-2.40262661239302	4.17037175560510	-1.07265031692400
H	-1.63992634024810	5.74789364882094	-1.42227486159985
H	-2.99329739212427	5.17574344438537	-2.43850681083236

1a+6

C	-3.70875807283141	2.04031637227238	-4.07224412632910
C	-3.13657105670128	1.16680527705184	-3.17668843053958
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C	-3.24068292238181	3.35335302031665	-4.34379296975986
N	-2.92744402685639	4.44775084284644	-4.57105942154910
C	-1.87519052589804	1.27895009652695	-2.49039070427651
C	-0.84276655233290	2.14588353095104	-2.87696450675380
C	-1.65436149139484	0.44318731375757	-1.37556862618167
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H	1.13364458427714	2.86836729295344	-2.51855500389095
H	-0.30804898083923	-0.14366142204831	0.19593911401993
O	1.67102406449923	1.33619057581117	-0.31505184348959

C	2.73785352682178	2.21481308088661	-0.67076914762787
H	2.42281468068890	3.26460223258474	-0.61491089224382
H	3.52705097939935	2.03256605778973	0.05986092549301
H	3.11453168376964	1.99462173860879	-1.67789283404810
C	-4.93628352764202	1.71694090125127	-4.71206643034269
N	-5.94805634446023	1.49011070842987	-5.23449009565543
C	-5.67342039574559	3.31728482012116	-2.16775511381667
H	-4.89431919994436	4.06262468277812	-2.14613477573084
O	-4.54999123958980	1.58046754491677	-1.04939223570953
N	-5.59114522936886	2.09273905731984	-1.61975372887605
C	-6.79411124718549	1.42062444973978	-1.84386248059683
N	-6.89844445624991	3.44423470101942	-2.73645575245635
C	-7.29024315645217	4.54339233153119	-3.60380468679526
H	-7.30562951601964	4.21400301573253	-4.64897513997641
H	-8.27887205832914	4.91926938942446	-3.32394073830463
H	-6.56229813054181	5.35049180586347	-3.49986978213062
C	-7.60033456081733	2.26884136215000	-2.55875329352394
C	-6.96922608726991	0.03110560844042	-1.36731030087767
H	-6.72272421790628	-0.04507265900634	-0.30335259218298
H	-7.99820145740674	-0.30041815955241	-1.52048441402191
H	-6.30157003690537	-0.65428129904008	-1.90243211302883
C	-8.94267816944473	2.05543730272251	-3.15511788717290
H	-9.66356762441033	2.81596620759533	-2.83349679889864
H	-8.88850464174582	2.07124296326992	-4.25023000111299
H	-9.32969589317982	1.07970589327829	-2.85662719643655

TS1a

C	-0.30815274171317	0.45554871717481	-1.09776875855043
C	0.08925845209473	-0.38417982235949	0.11898610726428
H	-0.40109378720524	-1.36122092492782	0.01349006646183
C	0.61938761898407	1.44220163740861	-1.55151664766103

N	1.29623815219790	2.33362698629040	-1.85504010484447
C	1.54889487442109	-0.55847857410388	0.38755722286922
C	2.32650747273540	0.48040549219880	0.89355102271349
C	2.16354278422897	-1.78038664103144	0.09750401500455
C	3.69139824107674	0.31667022926030	1.10298208190866
C	3.52124285835855	-1.95718360348958	0.29419830045952
C	4.29418298973139	-0.90605059571431	0.79783933046622
H	1.86508284332286	1.43323785734954	1.13172095052824
H	1.56995657785611	-2.60271421576457	-0.29482328347034
H	4.26694887889846	1.14577935975435	1.49673910559675
H	4.00578876661832	-2.90134003926763	0.06759202942752
O	5.61889340195194	-1.17505582372585	0.95835421760469
C	6.45144733095403	-0.12798605708064	1.44875345402542
H	6.14731134997139	0.18606740990568	2.45616461103458
H	7.45931713905913	-0.54396582996193	1.48869134171475
H	6.44104789271827	0.73873441200037	0.77472470844310
C	-0.94406954439666	-0.28514676301556	-2.14036409042498
N	-1.52944966338035	-0.87784032856618	-2.94855501092942
C	-1.71415211054180	1.50575228510434	-0.23033651655527
H	-1.24529920223190	2.48940190741470	-0.22733736063730
O	-0.49302463174244	0.29782570716767	1.30596754400903
N	-1.76037835030581	0.75664379025586	0.96444916802209
C	-2.78774493005973	-0.22092388550495	0.77339903342490
N	-2.95632442055135	1.35982812478151	-0.80024218445610
C	-3.33878413382272	2.02086907827649	-2.03866087222247
H	-3.01772734533417	1.45862315668913	-2.92306493151453
H	-4.42396630170786	2.15032692162119	-2.06779854045476
H	-2.87610183017696	3.01169216630216	-2.06109684170963
C	-3.53245476516860	0.18240650006256	-0.27961985577800
C	-2.96013667255679	-1.31215069052963	1.76128327910513
H	-3.18202631507055	-0.90797528145560	2.75655362876041

H	-3.77798635946461	-1.97233033930374	1.46527544103320
H	-2.04979532543638	-1.91487343781318	1.85464787086453
C	-4.77643770612707	-0.37921227667099	-0.85856059769326
H	-5.60814958363149	0.33404528293147	-0.81235371443190
H	-4.62031664064986	-0.65349413293907	-1.90908889493615
H	-5.07287526390385	-1.27717775872391	-0.31419632447207

INT1a

C	-3.95211663829457	2.30746264279709	-3.74798352984653
C	-3.56995099973384	1.45594107357271	-2.48303147582590
H	-4.02077422794600	0.46496928324282	-2.63608543218512
C	-2.93512485221263	3.24418615497136	-4.17322099439039
N	-2.18589036785037	4.07061768084092	-4.47960044983369
C	-2.11591475772240	1.33047402869728	-2.16926775948715
C	-1.41294844932871	2.36105970920550	-1.55008029847409
C	-1.42873403710294	0.16983732524387	-2.53843230564147
C	-0.04988619312132	2.24752241892324	-1.30091178443457
C	-0.07129122357400	0.04546846002956	-2.30519980946193
C	0.62660622110582	1.08659022490803	-1.68410734644045
H	-1.93403158267960	3.26556613086045	-1.25301869480344
H	-1.96475966072026	-0.64446598456726	-3.02027592603147
H	0.46772262189689	3.06697553742175	-0.81692005923794
H	0.47074867358817	-0.84989597282681	-2.59154264678021
O	1.95619003601028	0.87045903496491	-1.49446474934419
C	2.71425128426157	1.90630338304841	-0.87527026895794
H	2.35390619522176	2.11165903484299	0.14150759573415
H	3.73936553688340	1.53591329063758	-0.82773845432457
H	2.68757093805632	2.82970717121599	-1.46867422504131
C	-4.34215788565186	1.43058435256639	-4.83241846381757
N	-4.65934052287000	0.70265047503187	-5.67475373427893
C	-5.27080449425558	3.20976549858039	-3.14263188884891

H	-4.92093207007493	4.24429000857046	-3.08060769054928
O	-4.24117113234015	2.12947621203996	-1.38982124108820
N	-5.50022590956916	2.56637210877588	-1.86204215456735
C	-6.43997727556318	1.51415474627815	-2.16665343699850
N	-6.49656533136023	3.03662049481237	-3.82124577945595
C	-6.67892382723796	3.54664749848563	-5.17047827415148
H	-6.13161486157607	2.97816027738291	-5.93437142563788
H	-7.74262723239123	3.53598472462315	-5.42188864863471
H	-6.34017365705555	4.58762394443676	-5.19732649438202
C	-7.05390937819489	1.83587359638019	-3.32453257771408
C	-6.72585662347192	0.48345954894266	-1.14014854783073
H	-7.10292857763006	0.94566238560479	-0.21894811421859
H	-7.47135958838502	-0.22785184217223	-1.50193622802471
H	-5.82283360573359	-0.07654990425308	-0.87065518598530
C	-8.20685431705841	1.19868161299467	-4.00574614111623
H	-9.05677013692442	1.88750173044800	-4.08751473156203
H	-7.93197826291113	0.88038466985122	-5.01892173611893
H	-8.53692082648212	0.31880623258941	-3.45137589021034

TS2a

C	-0.21394841732277	1.05553409455666	-0.83647990697672
C	0.08923167476085	-0.29836192818334	-0.00966136783065
H	-0.25587011031948	-1.09594743142171	-0.70318724866358
C	0.43941940052132	2.20743803900350	-0.21971307617499
N	0.95128308282877	3.12007042915135	0.26814885611332
C	1.57499715954518	-0.46459668363651	0.23667078318941
C	2.16120848648054	0.04117252802432	1.39153953344216
C	2.37684094216307	-1.12291987733343	-0.69934800653128
C	3.52905867233693	-0.08675822266269	1.61312232307107
C	3.73985172823566	-1.25489608074364	-0.49534206451791
C	4.32334410501060	-0.73363716114540	0.66371140062890

H	1.53364449497920	0.53765839859551	2.12456555649189
H	1.93078917664671	-1.53402572384490	-1.60223668729671
H	3.95668592436858	0.31925330895157	2.52229404361248
H	4.37230314251583	-1.76057698951457	-1.21800184360014
O	5.67033782157217	-0.91570669199000	0.77688258838671
C	6.31044465948916	-0.39000388480863	1.93466462005595
H	5.92593709657830	-0.85661664934796	2.85170950905228
H	7.36944971237167	-0.62937301165809	1.82415310178625
H	6.18814798435821	0.69948580205860	1.99964527839107
C	0.21352804243711	0.92811245928583	-2.22122970957813
N	0.55211987588903	0.75055580384744	-3.31214259567361
C	-1.74850951983856	1.21482453381797	-0.66759354395825
H	-2.04696965194179	2.22941850902882	-0.98663055223037
O	-0.63685745279866	-0.20207938778810	1.13266996103889
N	-2.03402820444150	1.07652691075680	0.74134763845702
C	-3.16468958177672	0.32639651918257	0.81680147684863
N	-2.58462618424852	0.22715968475901	-1.35990970124619
C	-2.92182775509478	0.37808647703505	-2.77294813226069
H	-2.01583655203369	0.55375519781627	-3.35334173889746
H	-3.38044821517125	-0.54319703179760	-3.14027215257298
H	-3.62025085140022	1.21342552929416	-2.93583027016366
C	-3.50627660894281	-0.17384143136727	-0.43145589628636
C	-3.75893854856903	0.01818739575114	2.14522424845559
H	-3.81423017136320	0.92616269420410	2.75215307953351
H	-4.76100312289211	-0.40902473007626	2.06325560541738
H	-3.11778708595273	-0.69552428875670	2.67646333802738
C	-4.67853297338822	-0.99864021308924	-0.81447952772154
H	-5.32236139881237	-0.47575494301208	-1.53222437995042
H	-4.35185873836432	-1.93282744917242	-1.28675870763004
H	-5.27377203841615	-1.24891450377012	0.06376416776178

INT2a

C	-0.357170000	1.688759000	-1.245189000
C	-0.169984000	-1.280243000	-0.257840000
H	-0.366228000	-1.383827000	-1.347800000
C	0.596023000	2.029820000	-0.281648000
N	1.413300000	2.300953000	0.504811000
C	1.225584000	-1.107076000	0.082169000
C	1.632624000	-0.909704000	1.407127000
C	2.185348000	-1.075194000	-0.944200000
C	2.961976000	-0.693110000	1.713665000
C	3.512880000	-0.856077000	-0.652923000
C	3.907275000	-0.657954000	0.678513000
H	0.880668000	-0.908638000	2.190079000
H	1.867629000	-1.191608000	-1.977778000
H	3.251745000	-0.518871000	2.742659000
H	4.266041000	-0.807590000	-1.432261000
O	5.228133000	-0.431331000	0.863104000
C	5.682172000	-0.136445000	2.184648000
H	5.511854000	-0.983709000	2.861205000
H	6.753862000	0.045339000	2.093657000
H	5.189038000	0.760743000	2.578489000
C	0.042258000	1.203909000	-2.484941000
N	0.312885000	0.755992000	-3.532261000
C	-1.831149000	1.890627000	-0.970916000
H	-2.301441000	2.750355000	-1.485525000
O	-1.101317000	-1.339634000	0.549591000
N	-2.029147000	1.954941000	0.449621000
C	-2.718998000	0.932924000	0.820843000
N	-2.604242000	0.661130000	-1.388054000
C	-2.778567000	0.229796000	-2.768000000
H	-2.750321000	1.106818000	-3.418802000

H	-1.962043000	-0.432717000	-3.074950000
H	-3.741591000	-0.276253000	-2.873934000
C	-3.081793000	0.082088000	-0.322228000
C	-3.055706000	0.614522000	2.231026000
H	-2.699440000	1.413973000	2.881853000
H	-4.136926000	0.492001000	2.362612000
H	-2.570156000	-0.326039000	2.514286000
C	-3.883843000	-1.161472000	-0.316168000
H	-4.917485000	-0.944103000	-0.619384000
H	-3.467746000	-1.903815000	-1.001542000
H	-3.896002000	-1.589281000	0.686386000

TS3a

C	-0.46299345095872	-0.73404589800096	-1.13741820010027
C	0.38424675088834	-0.23728167332198	1.44933383500575
H	-0.07929191335214	-1.23673825633422	1.51773319746256
C	0.45406685049609	0.25295211515834	-1.50616185251467
N	1.16755293136723	1.13292870453555	-1.79172040327460
C	1.81798285559818	-0.19926993399895	1.41222759949007
C	2.51088580349535	1.00888081631729	1.24231991639788
C	2.53998267946538	-1.40755236895155	1.46084652053466
C	3.88923038940173	1.02251515925478	1.14430762050992
C	3.91199007969502	-1.40550895650448	1.36293638918200
C	4.59484976955211	-0.18827298812967	1.20599169818226
H	1.94329045328218	1.92984935509222	1.16479494706594
H	2.00217056321744	-2.34829228288714	1.54935005943007
H	4.40373402725422	1.96418024950875	0.99612139705384
H	4.48620927873354	-2.32571483736610	1.38392071622558
O	5.94009916075274	-0.28996469938803	1.11180086477935
C	6.69461796930639	0.90404495333464	0.89723345131533
H	6.57584979114764	1.60411091410823	1.73378168977793

H	7.73600192311704	0.58594024093762	0.83441127688627
H	6.40261372432368	1.39176109020916	-0.04092899872048
C	-0.15197307799836	-2.09137434161718	-1.27232046179734
N	0.12154973131473	-3.22191474297794	-1.35109306809345
C	-1.74310648698243	-0.31252515880172	-0.51125606056454
H	-1.35415173242789	0.35220281657512	0.45069063160454
O	-0.34826553235081	0.78430738184841	1.43138200134688
N	-2.55256395554495	-1.27191219250649	0.10609343573957
C	-3.80387837179836	-0.95412042552498	-0.12145858020103
N	-2.64919591705331	0.57200867437920	-1.23430003382171
C	-2.20377289272786	1.66247303726089	-2.08771417806405
H	-3.06602701732582	2.21365593581224	-2.46621080953069
H	-1.54730147144524	2.33276708119564	-1.52655763624662
H	-1.62461688026798	1.24563080400884	-2.91841501234315
C	-3.89113024019671	0.21734945863973	-0.95096606332023
C	-4.95778007363745	-1.70024375358134	0.45591734739850
H	-4.58599016262616	-2.56965733995978	1.00013858775616
H	-5.53160628965682	-1.07310700740192	1.14814683049884
H	-5.64171223183234	-2.04219202302909	-0.32853003544965
C	-5.10510999045170	0.96240031001646	-1.37222336948628
H	-5.08781042229457	1.99225724672006	-0.99698280444047
H	-5.19049170252213	1.00557431759077	-2.46397417425725
H	-5.99815491895724	0.47189821777956	-0.98124827141744

INT3a

C	-0.30680601961765	-0.02757567534732	-0.42443688286475
C	0.33725572488430	-0.57526896388597	0.95358269309199
H	0.01660585015949	-1.62804060071804	0.98869211251591
C	0.08567798806922	1.37126567762442	-0.63124164770996
N	0.34090935383144	2.48600626091091	-0.79347268970697
C	1.83629603393962	-0.48720605729566	0.91694626177365

C	2.49141535674189	0.66552520183197	1.34135551290844
C	2.59671899133829	-1.55895480973073	0.43957741229692
C	3.87823275606706	0.76206332527810	1.28662208286749
C	3.97594704532807	-1.47694668912890	0.37501185069230
C	4.62467897046942	-0.31217262269089	0.79709862642255
H	1.91242849390049	1.49740309397070	1.72811993741418
H	2.10391381754021	-2.47090643714966	0.11220103834243
H	4.35695409844222	1.67269081329606	1.62651475823163
H	4.57249279188904	-2.30476111245288	0.00601919300356
O	5.98267845720968	-0.32769774261347	0.69839737628440
C	6.68921541941771	0.83785473709528	1.11255864697934
H	6.52363901303866	1.04817277438641	2.17760570766159
H	7.74534690960822	0.61955929142419	0.94687539711379
H	6.39991608585790	1.71317940944195	0.51603437746111
C	0.18516105761982	-0.85720464797639	-1.53006253712021
N	0.52752947538642	-1.55565491129189	-2.38468328345972
C	-1.81891501254824	-0.12522047322144	-0.35450268540198
H	-1.12081193808264	-0.03235697763598	2.05441701875650
O	-0.16614972855306	0.16687638313430	2.02240341982495
N	-2.47628350234042	-0.57694778413503	0.69360483812457
C	-3.81280916353920	-0.48113812351757	0.37698846259311
N	-2.66374457105053	0.26038983700837	-1.35202699090105
C	-2.32141055067901	0.89017443471479	-2.62182863959878
H	-3.04496711909950	0.58770240703442	-3.38223336251246
H	-2.32446764796556	1.98194939644147	-2.52700995571883
H	-1.33169957323309	0.56640104142724	-2.94903608662270
C	-3.95274065146947	0.04113794168304	-0.88895695151803
C	-4.86050384449203	-0.91814051701809	1.34194395854655
H	-4.75605970159104	-0.38712841447580	2.29394194486356
H	-5.86450778546274	-0.72877590183937	0.95507967332828
H	-4.77401845001578	-1.98960473389643	1.55244168246787

C	-5.15210171801314	0.35303407325069	-1.71002078788969
H	-5.17105685496902	1.40278696313908	-2.02627457209319
H	-5.20846801467655	-0.26941793983469	-2.61176769505525
H	-6.05549284334047	0.16694907276451	-1.12647721539320

TS4a

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H	-0.07113730590546	-1.59044319232944	0.51292968986867
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C	1.83073337548041	-0.63245179942422	0.96986403468677
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C	2.57107011314188	-1.47768573371770	0.12075475136981
C	3.87473483735602	0.49460074574421	1.61315730994574
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H	2.05820121037323	-2.22992097345566	-0.47123057229664
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N	0.71430220322662	-0.84395559146669	-2.66015890416650
C	-1.79950755119141	0.29670288079559	-0.52850873118566
H	-1.25415919632107	-0.11214528196675	1.69957341073338
O	-0.24824485018104	-0.17159044147048	2.00483864863383

N	-2.36387847663772	0.09527934273405	0.65780156732692
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H	-6.04655239509772	-0.41536815756351	-1.01235380484258

7

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C	2.91812947426014	-1.39407303149254	1.63809132824022
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H	8.03614125725150	-1.24873263678096	0.44359122852820
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H	-5.35292016497628	-0.64941667065762	-1.21209183145942

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H	-0.87098416729953	1.54468245757602	-4.35740356184511
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H	2.87131287709749	-0.66418165449259	-2.70349513565497
H	2.96457963317405	-2.05098435761302	-1.58065720722818
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H	-2.70958577063948	3.09146313352402	-7.45496480370273
H	-7.23595631263319	4.91838539618525	-6.64663676077845
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TS1b

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C	2.23314348099328	0.05887634228715	1.64429511043534
C	3.38523378779710	-1.43532671801305	-0.38356484296110
C	3.48839358133854	-0.48850728235634	1.83308798270788
C	4.07553193309798	-1.24690169541837	0.81566842652627

H	1.59909541682603	-1.01578254162525	-1.49814868875077
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H	3.81369256075549	-2.01600344272806	-1.19246069530533
H	4.03550206465214	-0.33718839556817	2.75838007894811
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C	5.95462263570886	-2.51050900736523	0.07089707959835
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H	6.91991827582596	-2.80457518304446	0.48555690266924
H	5.37926057957651	-3.40977404428734	-0.18642016921362
C	-1.17027177762756	2.41152934081624	-0.00798676396329
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C	-0.43402815296550	1.05931059865825	-1.99427321943780

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C	-1.08398065110369	2.00275181173146	-2.95422694848030
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C	-0.42533438977994	2.24728568692364	-4.16378206020695
C	-2.91087639088100	3.39752725648633	-3.69197500201707
C	-0.99079401726721	3.08633253219653	-5.11377891418003
C	-2.23658338870752	3.66461208366209	-4.87923440005769
H	-2.87873877052104	2.35696836516485	-1.81339724334101
H	0.53341848544476	1.76982827892518	-4.34235158541044
H	-3.89177696093882	3.82865357097633	-3.51379896203133
H	-0.46354785378421	3.28607631577288	-6.04235248031228
H	-2.68437704201571	4.31521085464233	-5.62531277679798

INT1b

C	-3.34507243869763	2.77571004784463	-3.73478590219062
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C	2.88060735508812	-0.99320167549326	-3.19947676304364
H	2.97915870925022	-0.37528951020688	-4.10173615692877
H	3.87293153191765	-1.26775660277416	-2.83827798430322

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O	-5.87728451340373	1.98159906083150	-3.12809210183903
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C	-2.85715722589597	-1.17255666933918	-1.14135192603707
H	-2.34293572839577	-1.31380054317511	-2.09282750036127
H	-2.10389084272749	-0.89369291006846	-0.39637367855175
H	-3.33593879451883	-2.11337658687927	-0.84603099859031
C	-4.84304266563971	0.15430564322571	-0.41461003730303
C	-6.97976610306209	1.68821976771982	-0.48187193934373
H	-7.85219841764693	1.38234253933072	-1.07014499690506
H	-7.15481538642883	1.43664316826435	0.56534356661724
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C	-4.88366531128171	-0.46139089748484	0.93438581929634
H	-5.08599040553182	-1.53805249523964	0.87169425360500
H	-3.92570870724251	-0.33746252818853	1.45120169864630
H	-5.66680234482068	-0.00647705281714	1.54187811292877
C	-3.62265535748358	2.25165834488673	-5.03205160291185
O	-3.48107280062816	1.02778087670031	-5.27457235520225
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C	-5.03930765230058	4.16645876227230	-5.91682518302232
C	-3.70091497264893	2.85036952112183	-7.43232766155789
C	-5.50690728664762	4.91578646776952	-6.99124176155463
C	-4.15439494436864	3.61239684609868	-8.49995203909119
C	-5.05906538840234	4.64959962020644	-8.28146102312924
H	-5.40626849467452	4.37093582331859	-4.91708612992234

H	-3.01365717724383	2.02447526230937	-7.58822139897340
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H	-5.41997636897858	5.24335296775185	-9.11678810453341

TS2b

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C	2.01019555467673	-0.02275725291268	1.91377419258327
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C	3.23918743996918	-0.64874942340577	2.03406696160701
C	3.89594720117026	-1.11455908266462	0.89000980739765
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H	1.51220463451415	0.34667088185699	2.80853688405356
H	3.80779194818495	-1.26133286469609	-1.27052165322560
H	3.72102569788497	-0.76929087065980	2.99943079206631
O	5.09781284455195	-1.71840109110442	1.10562989678407
C	5.82767871937779	-2.16268538815118	-0.03477295416837
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H	-0.65888552770054	-3.35676807636291	1.21811839887954
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H	-4.02553936643508	-0.34156090492210	4.14209080377784
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INT2b

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4m

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H	-7.49516735629781	-0.06603312567389	0.22458109913671
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C	-5.45253773732969	-2.02700562437241	-0.81545420970081
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C	-0.48310551614198	-1.64854364096568	1.95916004289325
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C	0.29323351022828	3.03102846400608	0.28504534663514
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H	-0.58398044020647	3.59497317609124	-0.01005179644513
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H	-0.04239532847203	5.81407034107847	0.41975960707665
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C	0.55606320645486	-1.99572919972694	-2.01525791472417
N	1.09760130956682	-0.87178375417290	-2.67398253023444
N	-0.77022854149386	-2.02053748809751	-2.40212377659428
C	-1.11645763221140	-0.76373690118427	-2.92974326680186
C	0.01283327416052	-0.03563662225813	-3.06213306066371
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C	-2.52243264842748	-0.43675731775518	-3.26450452121042
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H	-2.94181349968769	-1.12066932915024	-4.01308500962441
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INT1c

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C	-5.19880216966425	-1.05755702541644	-9.74812977259016
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INT3c

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References

(1) Mlostoń, G.; Gendek, T.; Heimgartner, H. First Examples of Reactions of AzoleN-Oxides with Thioketones: A Novel Type of Sulfur-Transfer Reaction. *Helvetica Chimica Acta* **1998**, *81* (9), 1585–1595. https://doi.org/10.1002/(SICI)1522-2675(19980909)81:9<1585::AID-HLCA1585>3.0.CO;2-N.

(2) Kutasevich, A. V.; Niktarov, A. S.; Uvarova, E. S.; Karnoukhova, V. A.; Mityanov, V. S. A Novel Approach to Bis(1,3-Azol-2-Yl)Acetonitriles and Bis(1,3-Azol-2-Yl)Methanes via the [3 + 2]-Dipolar Cycloaddition of Imidazole N -Oxides and 2-Heteroaryl-3,3-Dimethylacrylonitriles. *Organic & Biomolecular Chemistry* **2021**, *19* (41), 8988–8998. https://doi.org/10.1039/D1OB01441B.

(3) Jasiński, M.; Mlostoń, G.; Heimgartner, H. Synthesis of 2,3-Dihydroimidazo[2,1-b]Thiazole Derivatives via Cyclization of N-Allylimidazoline-2-Thiones. *Journal of Heterocyclic Chemistry* **2010**, *47* (6), 1287–1293. https://doi.org/10.1002/jhet.469.

(4) Perevalov, V. P.; Mityanov, V. S.; Lichitsky, B. V.; Komogortsev, A. N.; Kuz'mina, L. G.; Koldaeva, T. Yu.; Miroshnikov, V. S.; Kutasevich, A. V. Synthesis of Highly Functional Imidazole Derivatives via Assembly of 2-Unsubstituted Imidazole N-Oxides with CH-Acids and Arylglyoxals. *Tetrahedron* **2020**, *76* (8), 130947. https://doi.org/10.1016/j.tet.2020.130947.

(5) Shen, J.; Yang, D.; Liu, Y.; Qin, S.; Zhang, J.; Sun, J.; Liu, C.; Liu, C.; Zhao, X.; Chu, C.; Liu, R. Copper-Catalyzed Aerobic Oxidative Coupling of Aromatic Alcohols and Acetonitrile to β-Ketonitriles. *Org. Lett.* **2014**, *16* (2), 350–353. https://doi.org/10.1021/ol403555n.

(6) Yang, Z.; Son, K.-I.; Li, S.; Zhou, B.; Xu, J. Specific 1,2-Hydride Shift in the Boron Trifluoride Catalyzed Reactions of Aromatic Aldehydes with Diazoacetonitrile: Simple Synthesis of β-Ketonitriles. *European Journal of Organic Chemistry* **2014**, *2014* (29), 6380–6384. https://doi.org/10.1002/ejoc.201402901.

(7) Katritzky, A. R.; Abdel-Fattah, A. A. A.; Wang, M. Expedient Acylations of Primary and Secondary Alkyl Cyanides to α-Substituted β-Ketonitriles. *The Journal of Organic Chemistry* **2003**, *68* (12), 4932–4934. https://doi.org/10.1021/jo026796x.

(8) Bedjeguelal, K.; Rabot, R.; Kaloun, E. B.; Mayer, P.; Marchand, A.; Rahier, R.; Schambel, P.; Bienayme, H. Preparation of Pyrazolopyridine Derivatives as ALK Kinase Inhibitors for Treating Cancer. WO2011045344, 2009.

(9) Kolosov, M. A.; Orlov, V. D.; Kolos, N. N.; Shishkin, O. V.; Zubatyuk, R. I. Reactions of α-Cyanochalcones with Phenylhydrazine. *Arkivoc* **2007**, *2007* (16), 187–194. https://doi.org/10.3998/ark.5550190.0008.g19.

(10) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2 : A Complete Structure Solution, Refinement and Analysis Program. *Journal of Applied Crystallography* **2009**, *42* (2), 339–341. https://doi.org/10.1107/S0021889808042726.

(11) Sheldrick, G. M. SHELXT – Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallographica Section A Foundations and Advances* **2015**, *71* (1), 3–8. https://doi.org/10.1107/S2053273314026370.

(12) Sheldrick, G. M. A Short History of SHELX. *Acta Crystallographica Section A Foundations of Crystallography* **2008**, *64* (1), 112–122. https://doi.org/10.1107/S0108767307043930.

(13) Neese, F. The ORCA Program System. *WIREs Comput Mol Sci* **2012**, *2* (1), 73–78. https://doi.org/10.1002/wcms.81.

(14) Neese, F. Software Update: The ORCA Program System, Version 4.0. *WIREs Comput Mol Sci* **2018**, *8* (1), e1327. https://doi.org/10.1002/wcms.1327.

(15) Grimme, S.; Hansen, A.; Ehlert, S.; Mewes, J.-M. *r2SCAN-3c: An Efficient "Swiss Army Knife" Composite Electronic-Structure Method*; preprint; Chemistry, 2020. https://doi.org/10.26434/chemrxiv.13333520.v2.
(16) Ásgeirsson, V.; Birgisson, B. O.; Bjornsson, R.; Becker, U.; Neese, F.; Riplinger, C.; Jónsson, H. Nudged Elastic Band Method for Molecular Reactions Using Energy-Weighted Springs Combined with Eigenvector Following. *J. Chem. Theory Comput.* **2021**, *17* (8), 4929–4945. https://doi.org/10.1021/acs.jctc.1c00462.