Supporting Information

Synthesis, structure investigation and evaluation of anti-orthopoxvirus activity of 2-(2-arylethenyl)imidazoles

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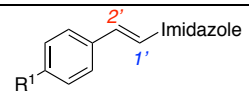
Content

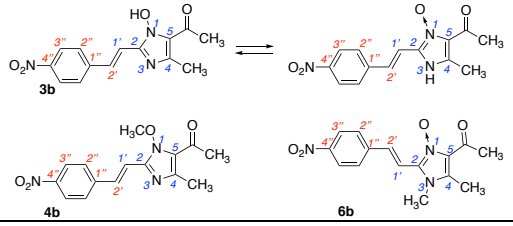
SI 1. Comparison of NMR spectroscopy data

Table S1. ^{1}H chemical shift values (δ, ppm) and spin-spin coupling constants (*J*, Hz) of the doublets of the ethylene bond protons of the compounds **3a-h, 4a-h, 6a-d** in ^{1}H NMR spectra in DMSO-d_6.



№	R^1	R^2	R^3	H1'		H2'	
				δ, ppm	*J*, Hz	δ, ppm	*J*, Hz
3a	NO_2	$CH_2C(CH_3)_3CH_2CO$		7.31	16.2	7.70	16.2
3b	NO_2	CH_3	$COCH_3$	7.34	16.3	7.68	16.3
3c	NO_2	CH_3	$COOC_2H_5$	7.31	16.3	7.65	16.3
3d	NO_2	CH_3	CH_3	7.22	16.4	7.46	16.4
3e	H	$CH_2C(CH_3)_3CH_2CO$		7.09	16.3	7.62	16.3
3f	H	CH_3	$COCH_3$	7.11	16.3	7.59	16.3
3g	H	CH_3	$COOC_2H_5$	7.07	16.3	7.55	16.3
3h	H	CH_3	CH_3	6.95	16.5	7.32	16.5
4a	NO_2	$CH_2C(CH_3)_3CH_2CO$		7.40	16.2	7.78	16.2
4b	NO_2	CH_3	$COCH_3$	7.36	16.2	7.73	16.2
4c	NO_2	CH_3	$COOC_2H_5$	7.36	16.2	7.71	16.2
4d	NO_2	CH_3	CH_3	7.27	16.2	7.42	16.2
4e	H	$CH_2C(CH_3)_3CH_2CO$		7.16	16.2	7.69	16.2
4f	H	CH_3	$COCH_3$	7.13	16.2	7.64	16.2
4g	H	CH_3	$COOC_2H_5$	7.12	16.2	7.62	16.2
4h	H	CH_3	CH_3	7.01	16.3	7.32	16.3
6a	NO_2	$CH_2C(CH_3)_3CH_2CO$		7.36	15.8	8.85	15.8
6b	NO_2	CH_3	$COCH_3$	7.35	15.8	8.88	15.8
6c	NO_2	CH_3	CH_3	7.34	15.7	8.73	15.7
6d	H	CH_3	CH_3	7.10	15.8	8.67	15.8

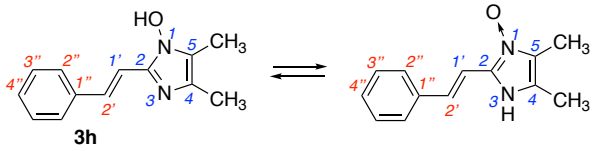
Table S2. ^{13}C NMR chemical shift values (δ, ppm) for 5-acetylsubstituted imidazole derivatives **3b, 4b, 6b**.

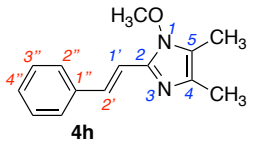


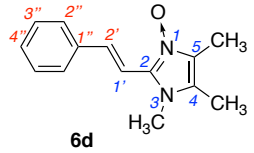
	δ_C, ppm					
	3b		**4b**		**6b**	
	DMSO-d_6	acetone-d_6	DMSO-d_6	acetone-d_6	DMSO-d_6	acetone-d_6
C2 (Im)	**141.3**	**140.3**	**141.1**	**142.3**	**132.0**	**133.4**
C4 (Im)	**143.4**	**145.1**	**144.0**	**145.2**	**133.2**	**134.0**
C5 (Im)	126.0	124.5	124.2	125.5	128.9	130.5
4-CH_3	**16.3**	**16.9**	**16.8**	**17.4**	**10.1**	**10.4**
C=O (5-Ac)	187.3	191.3	186.1	186.7	190.1	191.0
CH_3 (5-Ac)	29.7	28.9	29.5	29.8	30.4	30.9
C1'	116.3	116.5	115.6	116.7	113.1	113.7
C2'	131.3	133.1	132.9	133.8	128.6	129.8
C1'' (Ph)	142.6	143.6	142.2	143.6	144.1	145.5
C2'' (Ph)	128.0	129.0	128.4	129.1	127.8	128.5
C3'' (Ph)	124.1	125.0	123.9	124.9	123.9	124.9
C4'' (Ph)	146.8	148.5	147.0	148.6	146.5	148.0
OCH_3/NCH_3	--	--	68.2	68.8	30.5	31.0

Note: For the convenience, the numeration of the atoms in N-oxide cycle is the same as in N-methoxy- and N-hydroxy- derivatives.

Table S3. ^{13}C and ^{15}N NMR chemical shift values (δ, ppm) for 4,5-dimethylsubstituted imidazole derivatives **3h, 4h, 6d**.







	3h		**4h**		**6d**	
	DMSO-d_6	acetone-d_6	DMSO-d_6	acetone-d_6	DMSO-d_6	acetone-d_6
δ_C, ppm						
C2 (Im)	**135.5** (br.)	**136.7** (br.)	**136.9**	**138.1**	**131.0**	**132.5**
C4 (Im)	**125.6** (br.)	**125.6** (br.)	**129.8**	**131.2**	**121.5**	**122.1**
C5 (Im)	123.0	124.9	120.0	120.7	125.4	126.9
4-CH_3	**11.7**	**11.4**	**13.0**	**13.4**	**8.7**	**9.0**
5-CH_3	7.3	7.6	7.2	7.6	7.2	7.4
C1'	111.9	112.2	112.9	114.1	109.8	110.3
C2'	128.3	130.7	129.4	130.4	129.1	130.7
C1'' (Ph)	136.5	137.7	136.5	138.0	137.5	139.1
C2'' (Ph)	126.3	127.4	128.0	127.5	126.6	127.5
C3'' (Ph)	128.9	129.7	128.8	129.6	128.8	129.6
C4'' (Ph)	127.9	128.9	126.7	128.8	127.8	128.6
OCH_3/ NCH_3	--	--	67.1	67.4	30.2	30.6
δ_N, ppm						
N1		226.7		221.2		261.6
N3		190.7		250.2		132.5

Notes: (br.) – broadened signal. For the convenience, the numeration of the atoms in N-oxide cycle is the same as in N-methoxy- and N-hydroxy- derivatives.

SI 2. Single crystal X-ray analysis

Table S4. Crystallographic characteristics, details of the experiment and structure refinement for compounds **3a,c**.

Parameter	**3a**	**3c**
Chemical formula	$C_{17}H_{17}N_3O_4 \cdot C_3H_7NO$	$C_{15}H_{15}N_3O_5 \cdot C_{15}H_{14}N_3O_5$
Mr	400.43	633.59
Crystal system, space group	Monoclinic, P21/c	Triclinic, P-1
Temperature (K)	293(2)	293(2)
a, b, c (Å)	7.4075 (5), 13.1203 (11), 21.0062 (15)	7.3738 (5), 14.1463 (10), 15.4463 (10)
α, β, γ (°)	90, 92.715 (6), 90	66.399 (6), 88.379 (5), 86.836 (5)
V (Å^3)	2039.3 (3)	1474.18 (18)
Z	4	2
Radiation type	Mo Kα	Mo Kα
μ (mm^{-1})	0.10	0.11
Crystal size (mm)	0.48 × 0.4 × 0.08 × 0.40	0.96 × 0.17 × 0.06
Data collection		
Diffractometer	TD-5000	TD-5000
Absorption correction	For a cylinder mounted on the φ axis CrysAlis PRO 1.171.43.143a (Rigaku Oxford Diffraction, 2024) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan CrysAlis PRO 1.171.42.49 (Rigaku Oxford Diffraction, 2022) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.630, 1.000	0.697, 1.000
No. of measured, independent and observed [I >2σ(I)] reflections	12599, 5367, 3387	29468, 9515, 4312
R_{int}	0.082	0.107
(sin θ/λ)max (Å^{-1})	0.694	0.781
Refinement		
R[F2 > 2σ(F2)], wR(F2), S	0.059, 0.187, 1.04	0.088, 0.294, 0.98
No. of reflections	5367	9515
No. of parameters	274	420
No. of restraints	7	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
Δρmax, Δρmin (e Å^{-3})	0.17, −0.26	0.36, −0.27
CCDC deposition number	2469646	2469647

Table S5. Crystallographic characteristics, details of the experiment and structure refinement for compounds **4c,f**.

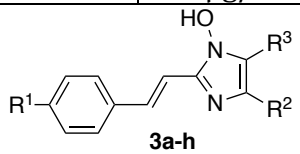
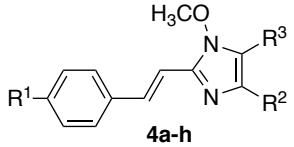
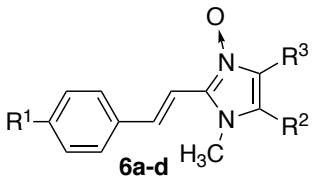
Parameter	**4c**	**4f**
Chemical formula	$C_{16}H_{18}N_3O_5$	$C_{15}H_{16}N_2O_2$
Mr	332.33	256.30
Crystal system, space group	Monoclinic, P21/c	Triclinic, P-1
Temperature (K)	293(2)	293(2)
a, b, c (Å)	4.7308 (9), 38.246 (3), 9.089 (2)	7.5492 (8), 7.7057 (9), 13.4133 (14)
α, β, γ (°)	90, 96.796 (17), 90	96.792 (9), 99.738 (9), 114.016 (11)
V (Å^3)	1632.9 (5)	687.12 (14)
Z	4	4
Radiation type	Mo Kα	Mo Kα
μ (mm^{-1})	0.10	0.08
Crystal size (mm)	0.84 × 0.09 × 0.06	0.9 × 0.64 × 0.04
Data collection		
Diffractometer	TD-5000	TD-5000
Absorption correction	For a sphere CrysAlis PRO 1.171.43.143a (Rigaku Oxford Diffraction, 2024) Spherical absorption correction using equivalent radius and absorption coefficient. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan CrysAlis PRO 1.171.42.49 (Rigaku Oxford Diffraction, 2022) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.937, 0.937	0.413, 1.000
No. of measured, independent and observed [I >2σ(I)] reflections	11371, 2799, 1581	7588, 2317, 1846
R_{int}	0.117	0.113
(sin θ/λ)max (Å^{-1})	0.595	0.595
Refinement		
R[F2 > 2σ(F2)], wR(F2), S	0.080, 0.274, 1.01	0.077, 0.224, 1.03
No. of reflections	2799	2317
No. of parameters	220	175
No. of restraints	2	-
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
Δρmax, Δρmin (e Å^{-3})	0.37, −0.28	0.23, −0.22
CCDC deposition number	2469648	2469649

Table S6. Crystallographic characteristics, details of the experiment and structure refinement for compounds **6b,d**.

Parameter	**6d**	**6b**
Chemical formula	$C_{14}H_{16}N_2O \cdot H_2O$	$C_{14}H_{15}N_3O_3 \cdot H_2O$
Mr	246.30	291.30
Crystal system, space group	Monoclinic, C2/c	Monoclinic, P21/n
Temperature (K)	293(2)	293(2)
a, b, c (Å)	13.398 (2), 9.5481 (13), 20.887 (4)	12.9411 (8), 8.0804 (6), 14.2750 (11)
α, β, γ (°)	90, 97.339 (17), 90	90, 105.129 (8), 90
V (Å^3)	2650.1 (8)	1440.99 (19)
Z	8	4
Radiation type	Mo Kα	Mo Kα
μ (mm^{-1})	0.08	0.10
Crystal size (mm)	0.5 × 0.48 × 0.08 × 0.40 (radius)	0.7 × 0.12 × 0.12 × 0.40 (radius)
Data collection		
Diffractometer	TD-5000	TD-5000
Absorption correction	For a sphere CrysAlis PRO 1.171.43.143a (Rigaku Oxford Diffraction, 2024) Spherical absorption correction using equivalent radius and absorption coefficient. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	For a sphere CrysAlis PRO 1.171.43.143a (Rigaku Oxford Diffraction, 2024) Spherical absorption correction using equivalent radius and absorption coefficient. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.993, 0.993	0.940, 0.940
No. of measured, independent and observed [I >2σ(I)] reflections	8198, 2291, 1491	10865, 2482, 1968
R_{int}	0.071	0.072
(sin θ/λ)max (Å^{-1})	0.595	0.595
Refinement		
R[F2 > 2σ(F2)], wR(F2), S	0.093, 0.294, 1.10	0.050, 0.149, 1.07
No. of reflections	2291	2482
No. of parameters	139	223
No. of restraints	1	-
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
Δρmax, Δρmin (e Å^{-3})	0.65, −0.23	0.20, −0.16
CCDC deposition number	2469650	2469651

SI 3.1. Evaluation of anti-orthopoxvirus activity

Table S7. Cytotoxicity and antiviral activity of compounds **3a-h, 4a-h, 6a-d** against Vaccinia virus (VACV, Copenhagen strain) in Vero cell culture.

№	R^1	R^2	R^3	CC_{50}, μg/mL	IC_{50}, μg/mL	SI
 **3a-h**						
3a	NO_2	$CH_2C(CH_3)_3CH_2CO$		8.8	2.1	4*
3b	NO_2	CH_3	$COCH_3$	6.3	2.4	3*
3c	NO_2	CH_3	$COOC_2H_5$	4.2	N/A	--
3d	NO_2	CH_3	CH_3	4.6	N/A	--
3e	H	$CH_2C(CH_3)_3CH_2CO$		47.5±13.1	3.27±1.96	15
3f	H	CH_3	$COCH_3$	19.4±4.7	1.16±0.71	17
3g	H	CH_3	$COOC_2H_5$	23.3±5.6	2.85±1.70	8
3h	H	CH_3	CH_3	0.85	N/A	--
 **4a-h**						
4a	NO_2	$CH_2C(CH_3)_3CH_2CO$		>100	N/A	--
4b	NO_2	CH_3	$COCH_3$	238.7±58.4	0.77±0.40	305
4c	NO_2	CH_3	$COOC_2H_5$	181.0±42.2	0.95±0.22	188
4d	NO_2	CH_3	CH_3	115.7±9.45	0.57±0.16	202
4e	H	$CH_2C(CH_3)_3CH_2CO$		>100	N/A	--
4f	H	CH_3	$COCH_3$	27.47±6.8	0.67±0.32	41
4g	H	CH_3	$COOC_2H_5$	12.96±0.25	0.17±0.03	76
4h	H	CH_3	CH_3	0.80	N/A	--
 **6a-d**						
6a	NO_2	$CH_2C(CH_3)_3CH_2CO$		>100	32.437	>3*
6b	NO_2	CH_3	$COCH_3$	>100	33.4	3*
6c	NO_2	CH_3	CH_3	2.393	N/A	--
6d	H	CH_3	CH_3	1.248	0.41	3*
Reference substances						
Cidofovir				290.0±65.6	8.97±1.99	32
NIOCH-14				455.2±82.4	0.003±0.002	151882

Note: CC_{50} – 50% cytotoxicity concentration at which 50% of cells in uninfected monolayers are destroyed; IC_{50} – 50% virus inhibiting concentration at which 50% of cells in infected monolayers are preserved; for certain compounds expanded testing was performed in 3 repeats; M±SD; M – mean value; SD – standard deviation; n=3 – the number of repeats of measurement of CC_{50} and IC_{50}; SI – selectivity index of the compound, ratio CC_{50}/IC_{50}. * - chemical compounds with SI<8 are considered as non-perspective for further investigation as antiviral chemicals. N/A – not active.

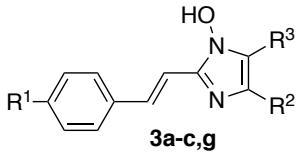
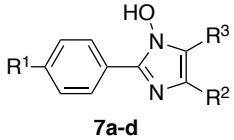
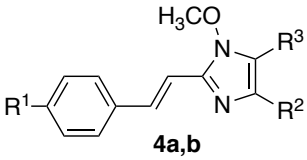
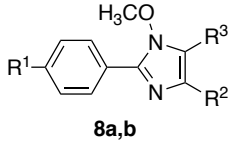
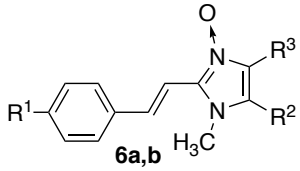
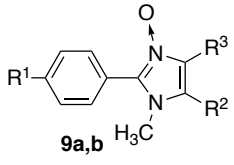
Table S8. Cytotoxicity and antiviral activity of 2-(2-arylethenyl)-1-methoxyimidazoles **4b-d,f,g** against Cowpox virus (CPXV, Grishak strain) and Ectromelia virus (ECTV, K-1 strain) in Vero cell culture.

№	CC_{50}, μg/mL	IC_{50}(CPXV), μg/mL	SI (CPXV)	IC_{50}(ECTV), μg/mL	SI(ECTV)
4b	238.7±58.4	6.5±0.5	37	3.2±0.4	74
4c	181.0±42.2	76.0±20.7	2*	64.7±5.7	3*
4d	115.7±9.45	10.4±1.1	11	2.3±0.2	50
4f	27.47±6.8	4.12±0.17	7*	4.13±0.13	7*
4g	12.96±0.25	1.7±0.1	8	1.4±0.1	9
Cidofovir	290.0±65.6	10.88±2.64	27	10.37±1.87	28
NIOCH-14	455.2±82.4	0.036±0.006	12685	0.006±0.003	76953

Note: CC_{50} – 50% cytotoxicity concentration at which 50% of cells in uninfected monolayers are destroyed; IC_{50} – 50% virus inhibiting concentration at which 50% of cells in infected monolayers are preserved; M±SD; M – mean value; SD – standard deviation; n=3 – the number of repeats of measurement of CC_{50} and IC_{50}; SI – selectivity index of the compound, ratio CC_{50}/IC_{50}. * - chemical compounds with SI<8 are considered as non-perspective for further investigation as antiviral chemicals.

SI 3.2. Comparison of anti-orthopoxvirus activities of novel 2-(2-arylethenyl)imidazoles with previously described [10.1016/j.bmcl.2022.129080; 10.1039/d4md00181h**] 2-arylimidazoles similarly substituted at positions 1,4,5 of heterocycle and position 4 of aryl moiety**

Table S9. Cytotoxicity and antiviral activity of compounds **3a-c,g, 4a,b, 6a,b, 7a-d, 8a,b, 9a,b** against Vaccinia virus (VACV, Copenhagen strain) in Vero cell culture.

№	R^1	R^2	R^3	CC_{50}, μM	IC_{50}, μM	SI	№	CC_{50}, μM	IC_{50}, μM	SI
 **3a-c,g**							 **7a-d**			
3a	NO_2	$CH_2C(CH_3)_2CH_2CO$		26.8	6.4	4*	**7a**	142.38±48.45	0.133±0.03	1072
3b	NO_2	CH_3	$COCH_3$	22.0	8.4	3*	**7b**	28.33±6.89	0.651±0.19	44
3c	NO_2	CH_3	$COOC_2H_5$	13.4	N/A	--	**7c**	45.70±8.93	0.45±0.03	102
3g	H	CH_3	$COOC_2H_5$	85.6±20.6	10.5±6.2	8	**7d**	171.54±55.28	N/A	
 **4a,b**							 **8a,b**			
4a	NO_2	$CH_2C(CH_3)_2CH_2CO$		>292.9	N/A	--	**8a**	1154.34±272.41	3.96±0.22	291
4b	NO_2	CH_3	$COCH_3$	792.2±193.8	2.6±1.3	305	**8b**	443.58±102.02	4.76±0.11	93
 **6a,b**							 **9a,b**			
6a	NO_2	$CH_2C(CH_3)_2CH_2CO$		>292.9	95.0	>3*	**9a**	2440.93±610.23	183.4±42.2	13
6b	NO_2	CH_3	$COCH_3$	>331.9	110.9	>3*	**9b**	2979.00±655.38	N/A	

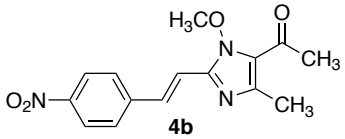
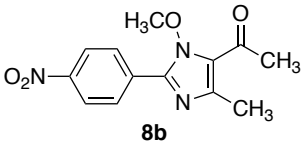
Note: CC_{50} – 50% cytotoxicity concentration at which 50% of cells in uninfected monolayers are destroyed; IC_{50} – 50% virus inhibiting concentration at which 50% of cells in infected monolayers are preserved; for certain compounds expanded testing was performed in 3 repeats; M±SD; M – mean value; SD – standard deviation; n=3 – the number of repeats of measurement of CC_{50} and IC_{50}; SI – selectivity index of the compound, ratio CC_{50}/IC_{50}. * - chemical compounds with SI<8 are considered as non-perspective for further investigation as antiviral chemicals. N/A – not active. Data for compounds **7a,b, 8a,b, 9a,b** were obtained from [10.1039/d4md00181h]; data for compounds **7c,d** – from [10.1016/j.bmcl.2022.129080].

Commentary. For now, the influence of the presence of ethenyl linker between heterocyclic and aryl moieties of imidazole derivatives under study is not evident enough. Nevertheless, it is clear that in most cases methylation of 1-hydroxyimidazoles led to less toxic

compounds. Obviously, 2-(2-arylethenyl)-1-hydroxyimidazoles **3a-c,g** exhibited poorer virus-inhibiting activities than the ones of similarly substituted 2-aryl-1-hydroxyimidazoles **7a-d**. Strangely enough, while methylation of 2-aryl-1-hydroxyimidazoles **7a,b** resulted in the decrease of virus-inhibiting activity in case of 2-aryl-1-methoxyimidazoles **8a,b**; 2-(2-arylethenyl)-1-methoxyimidazoles could demonstrate more promising virus-inhibiting concentrations as in the case of compound **4b**. The activities of 1-methylimidazole 3-oxides **6a,b, 9a,b** were poor regardless of the character of substituent in position 2 of imidazole.

It may also be of interest to compare the activities against various orthopoxviruses of the lead compound of 2-(arylethenyl)imidazole series (**4b**) and of similarly substituted at positions 1,4,5 of heterocycle 2-(4-nitrophenyl)imidazole **8b** [10.1039/d4md00181h] (Table S10).

Table S10. Cytotoxicity and antiviral activity of compounds **4b** and **8b** against Vaccinia virus (VACV, Copenhagen strain), Cowpox virus (CPXV, Grishak strain) and Ectromelia virus (ECTV, K-1 strain) in Vero cell culture.

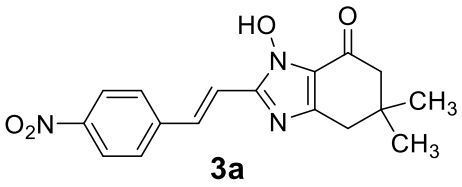
 **4b**				 **8b**			
CC_{50}, µM	Virus	IC_{50}, µM	SI	CC_{50}, µM	Virus	IC_{50}, µM	SI
792.2±193.8	VACV	2.6±1.3	305	443.58±102.02	VACV	4.76±0.11	93
	CPXV	21.6±1.6	37		CPXV	22.27±4.89	20
	ECTV	10.7±1.4	74		ECTV	13.88±1.13	32

Note: CC_{50} – 50% cytotoxicity concentration at which 50% of cells in uninfected monolayers are destroyed; IC_{50} – 50% virus inhibiting concentration at which 50% of cells in infected monolayers are preserved; M±SD; M – mean value; SD – standard deviation; n=3 – the number of repeats of measurement of CC_{50} and IC_{50}; SI – selectivity index of the compound, ratio CC_{50}/IC_{50}.

Strictly speaking, the virus-inhibiting concentrations of compounds **4b** and **8b** against all the three orthopoxviruses are comparable. Due to its lower cytotoxicity, 1-methoxy-2-(2-(4-nitrophenyl)ethenyl)imidazole **4b** obtained higher selectivity indices than the ones of 1-methoxy-2-(4-nitrophenyl)imidazole **8b**.

SI 4. Copies of NMR spectra of compounds 3a-h, 4a-h, 5, 6a-d.

S4.1. 3-Hydroxy-6,6-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-3,5,6,7-tetrahydro-*4H*-benzimidazol-4-one (**3a**).



3a

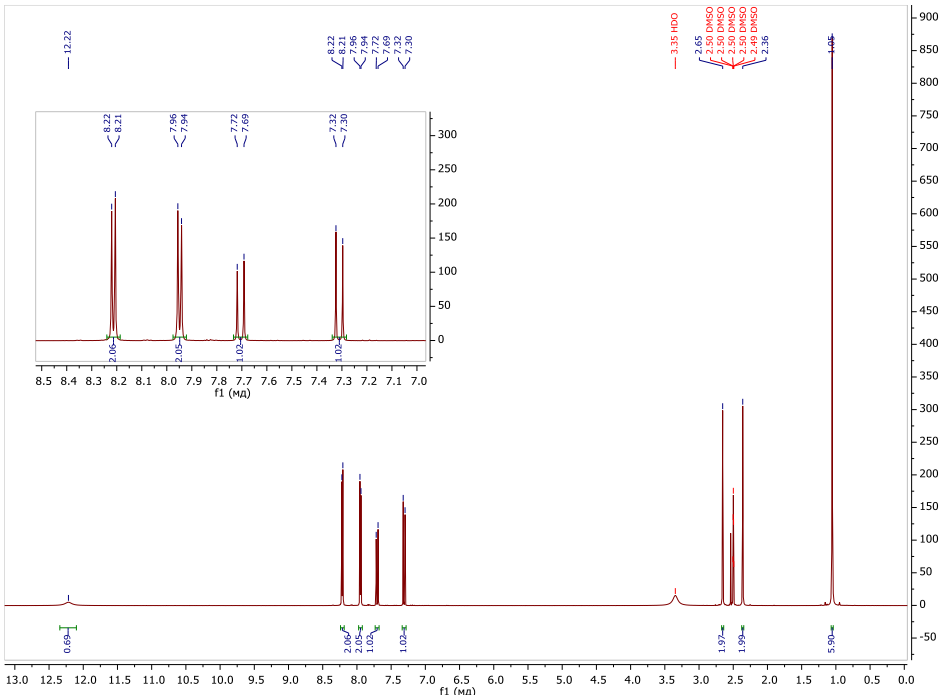


Fig. S 1. ^{1}H NMR spectrum of compound 3a (600 MHz, DMSO-d_6).

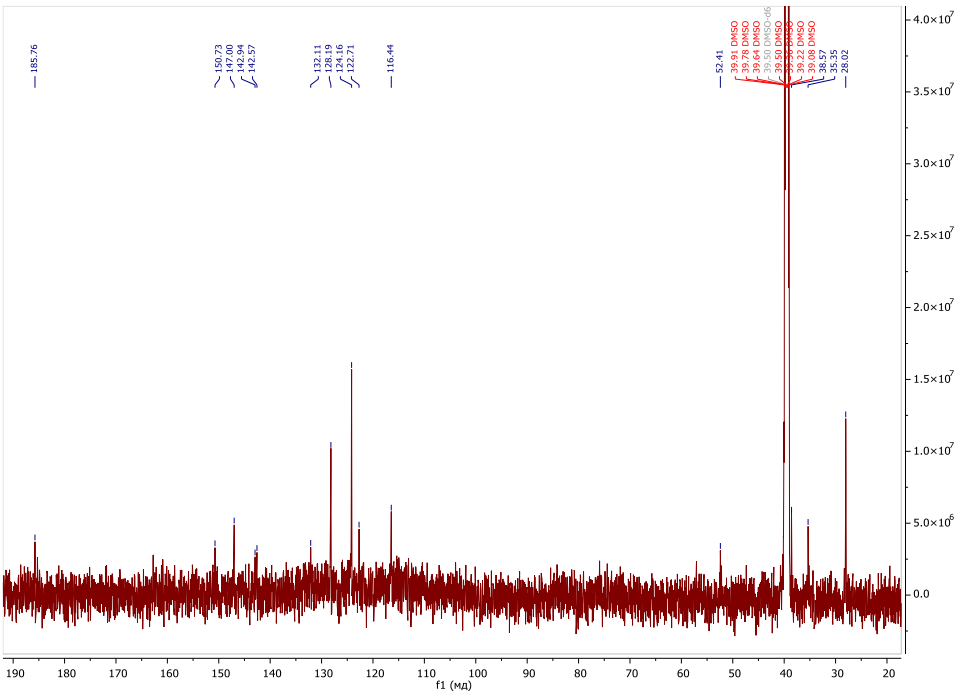
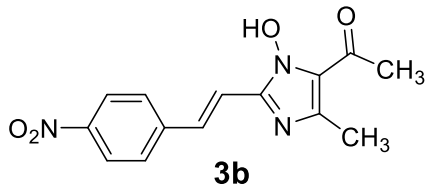


Fig. S 2. ^{13}C NMR spectrum of compound 3a (151 MHz, DMSO-d_6).

S4.2. 1-(1-Hydroxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazol-5-yl)ethanone (**3b**).



3b

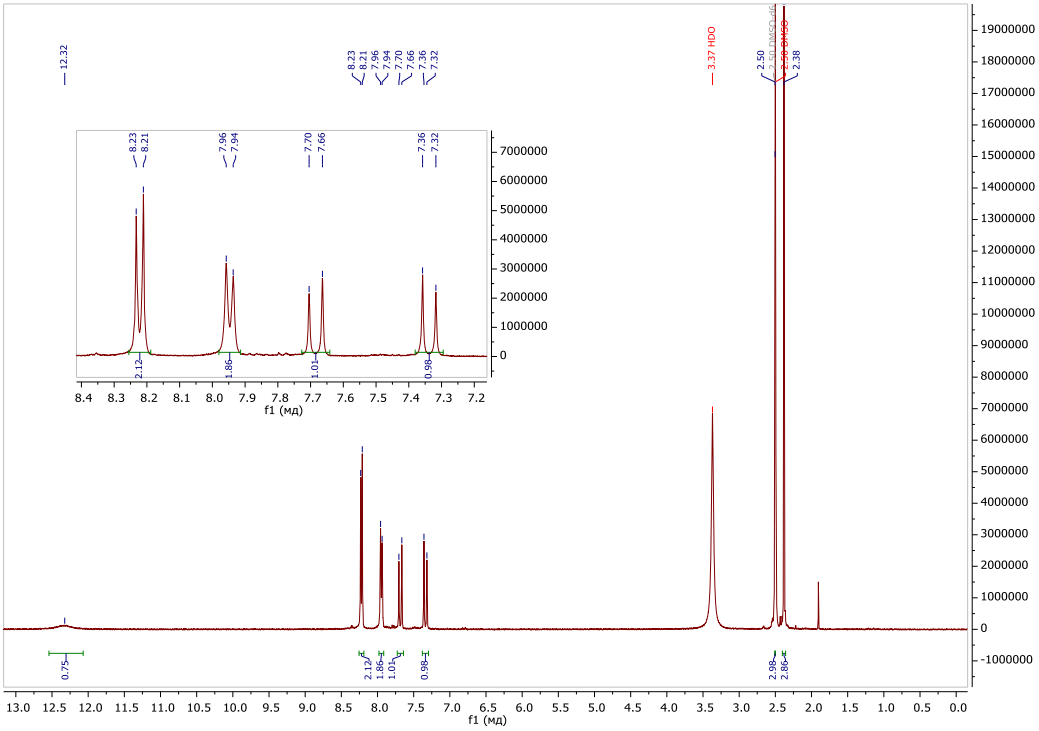


Fig. S 3. ^{1}H NMR spectrum of compound 3b (400 MHz, DMSO-d_6).

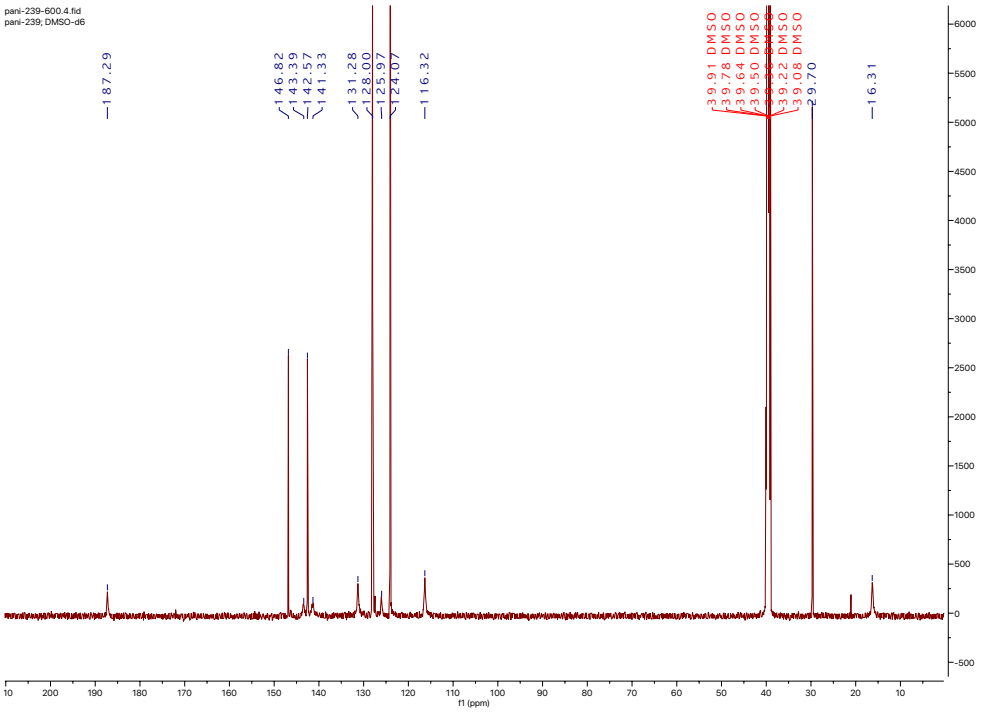


Fig. S 4. ^{13}C NMR spectrum of compound 3b (151 MHz, DMSO-d_6).

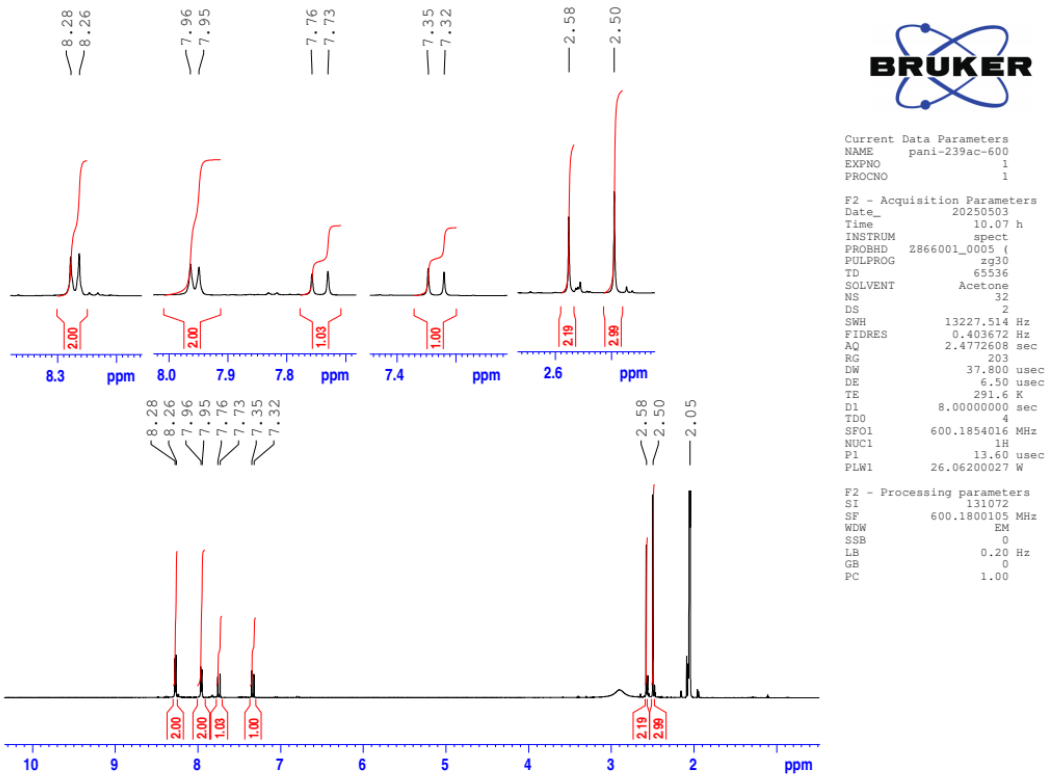


Fig. S 5. ^{1}H NMR spectrum of compound 3b (600 MHz, acetone-d_6). The integral intensity of 2.58 ppm signal of methyl group is lowered due to the partial exchange of hydrogen for deuterium from the solvent.

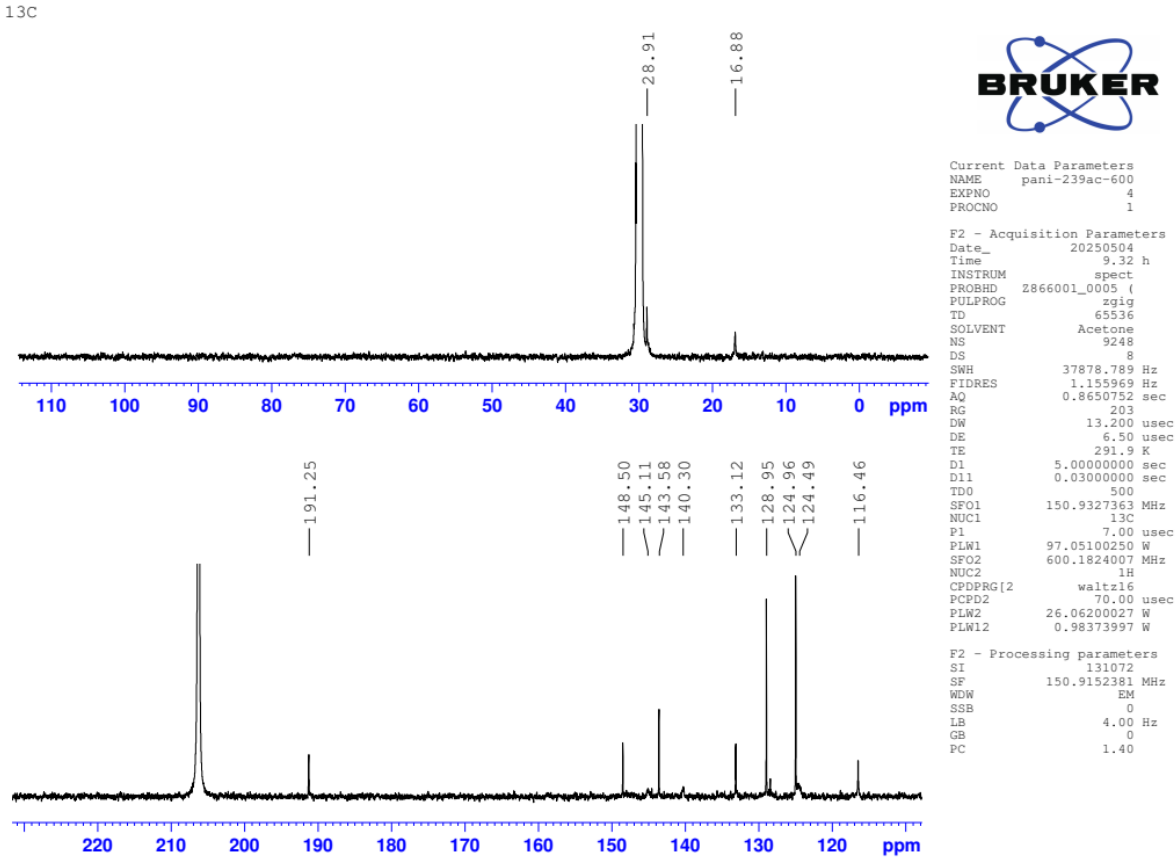


Fig. S 6. ^{13}C NMR spectrum of compound 3b (151 MHz, acetone-d_6).

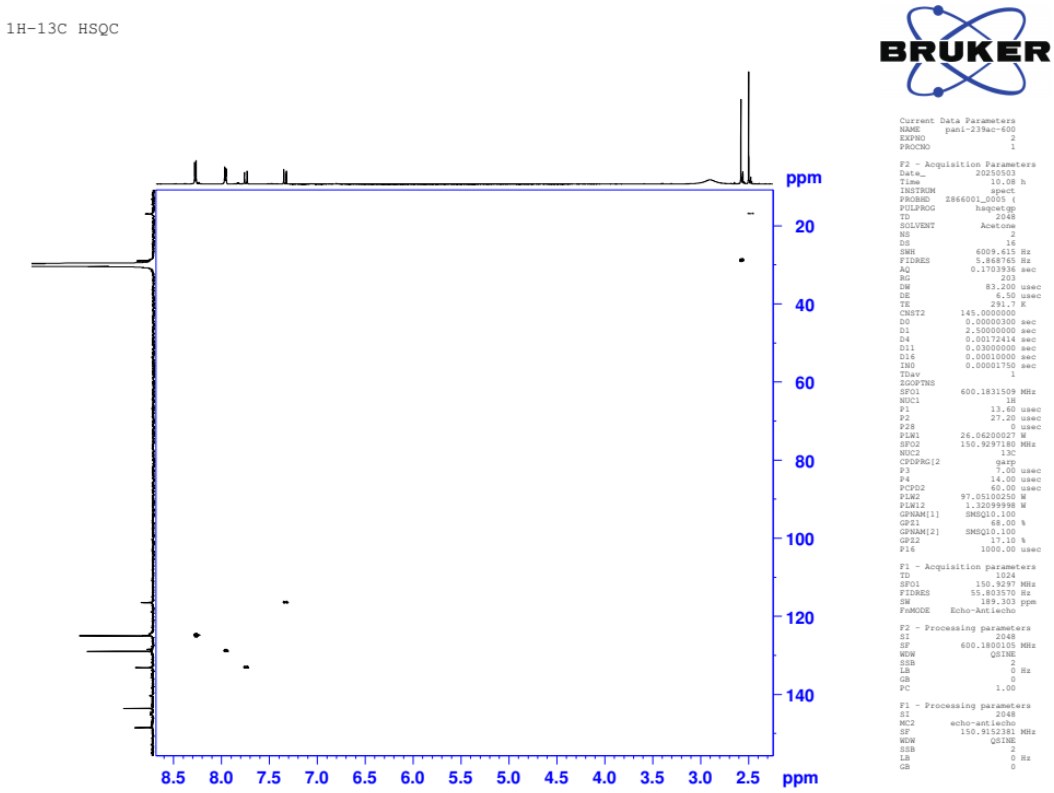


Fig. S 7. ^{1}H-^{13}C HSQC spectrum of compound 3b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

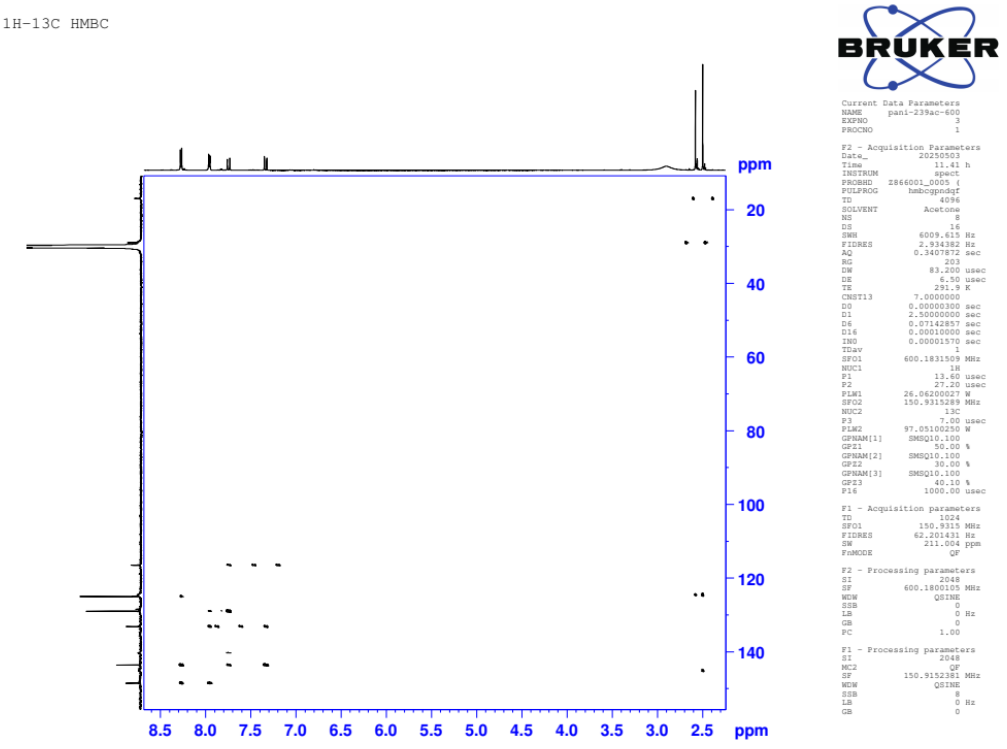


Fig. S 8. ^{1}H-^{13}C HMBC spectrum of compound 3b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

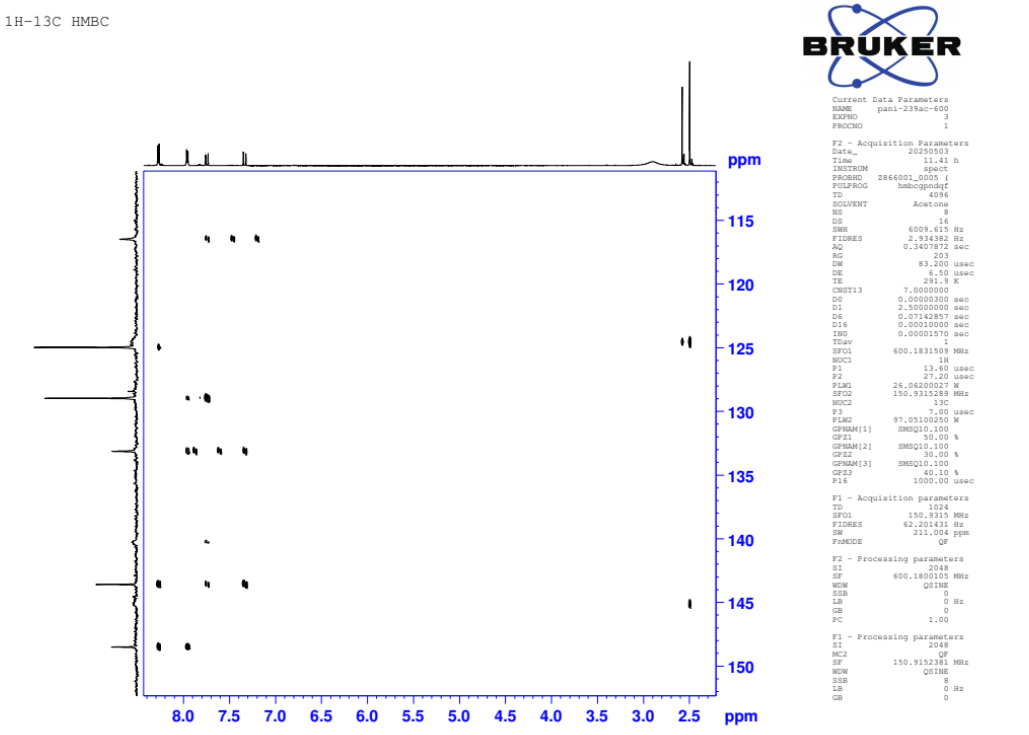


Fig. S 9. Part of ^{1}H-^{13}C HMBC spectrum of compound 3b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

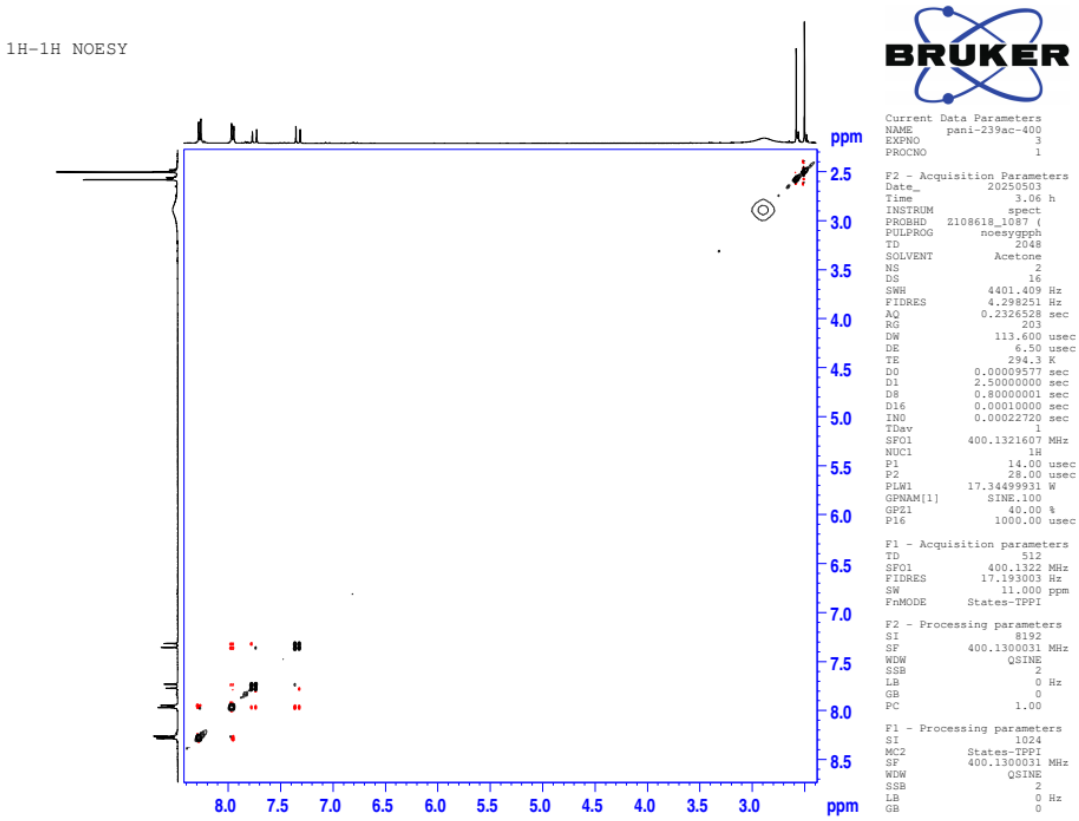


Fig. S 10. ^{1}H-^{1}H NOESY spectrum of compound 3b (400 MHz, acetone-d_6).

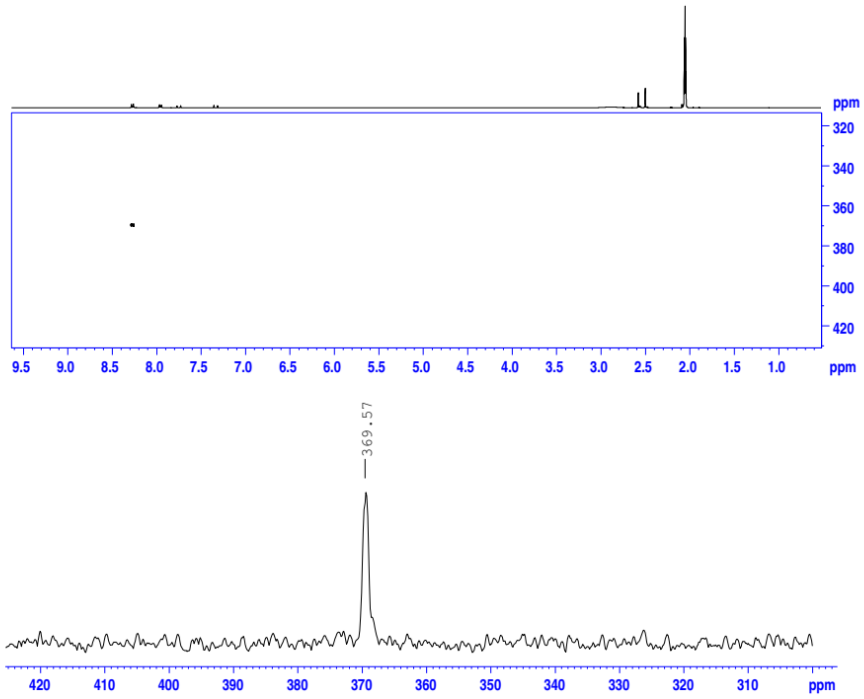
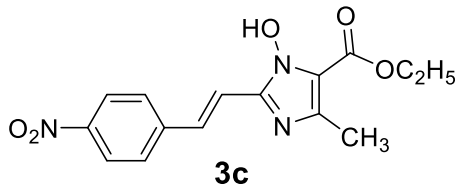


Fig. S 11. ^{1}H-^{15}N HMBC spectrum of compound 3b (400 MHz – ^{1}H, 41 MHz – ^{15}N, acetone-d_6).

S4.3. Ethyl 1-hydroxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole-5-carboxylate (**3c**).



3c

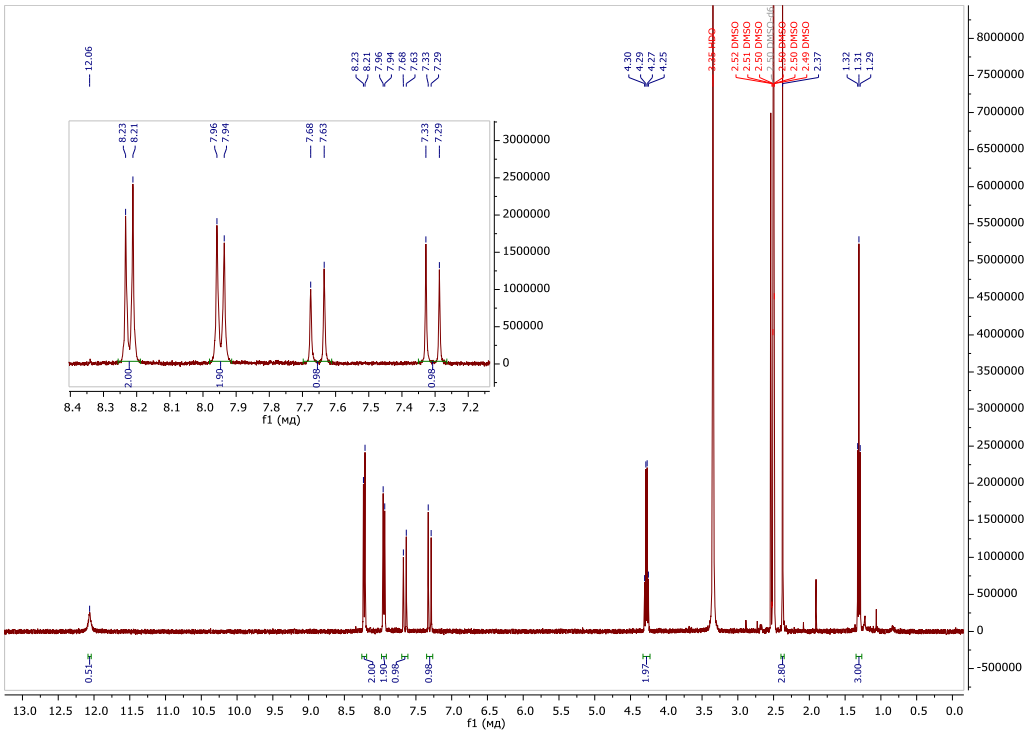


Fig. S 12. ^{1}**H NMR spectrum of compound 3c (400 MHz, DMSO-*d*$_6$).**

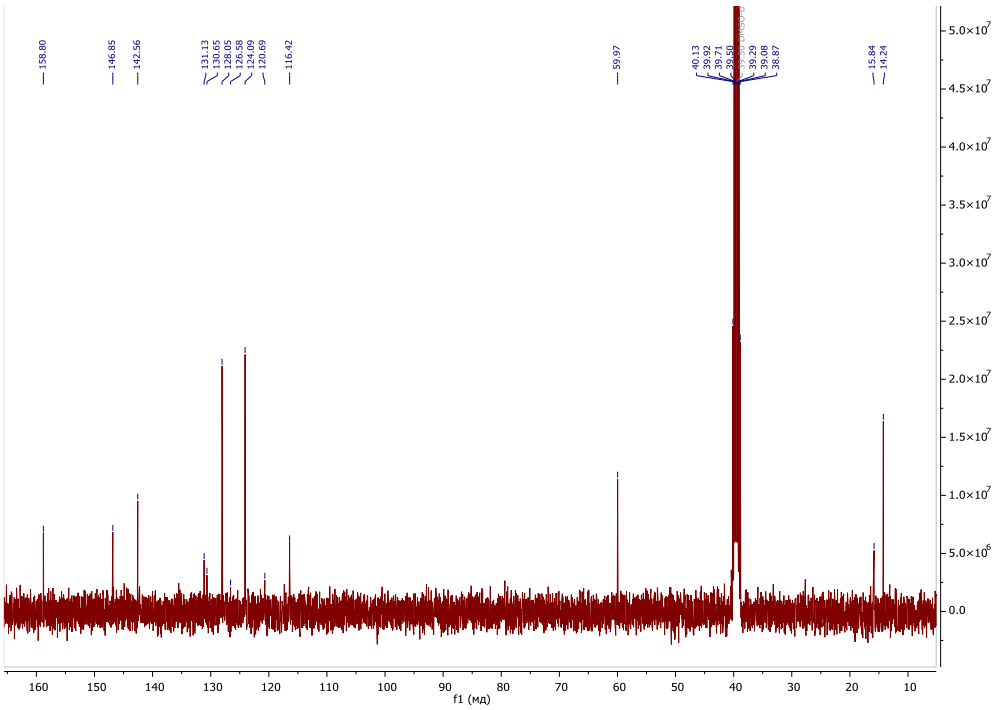
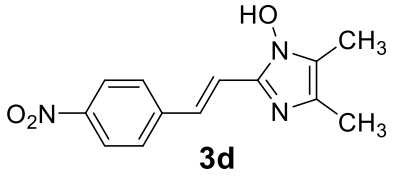


Fig. S 13. ^{13}**C NMR spectrum of compound 3c (101 MHz, DMSO-*d*$_6$).**

S4.4. 4,5-Dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazol-1-ol (**3d**).



3d

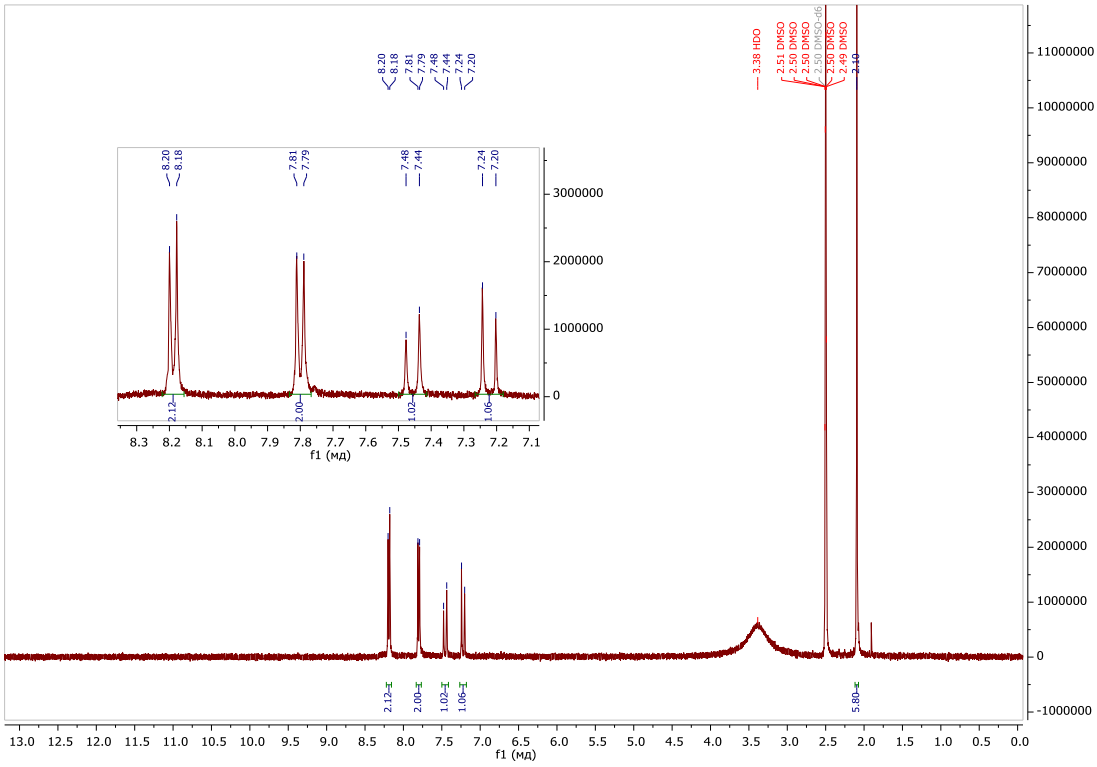


Fig. S 14. ^{1}H NMR spectrum of compound 3d (400 MHz, DMSO-d_6).

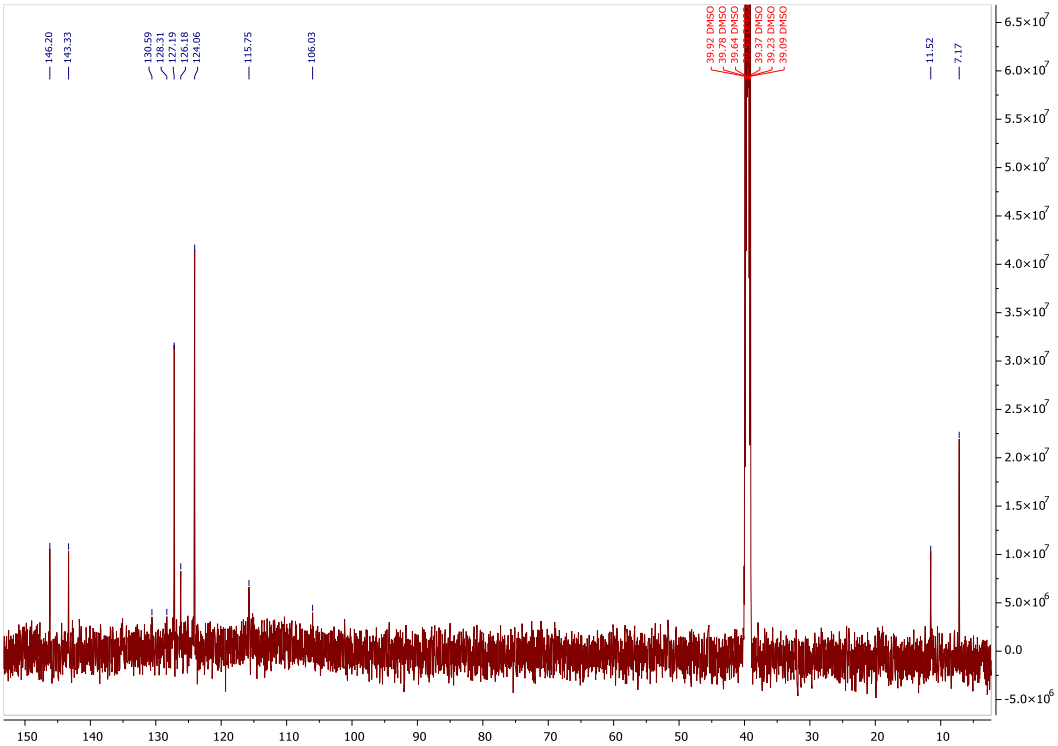
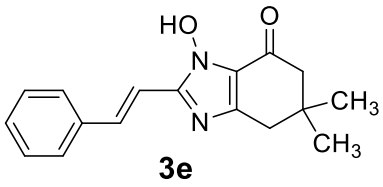


Fig. S 15. ^{13}C NMR spectrum of compound 3d (151 MHz, DMSO-d_6).

S4.5. 3-Hydroxy-6,6-dimethyl-2-((*E*)-2-phenylethenyl)-3,5,6,7-tetrahydro-*4H*-benzimidazol-4-one (**3e**).



3e

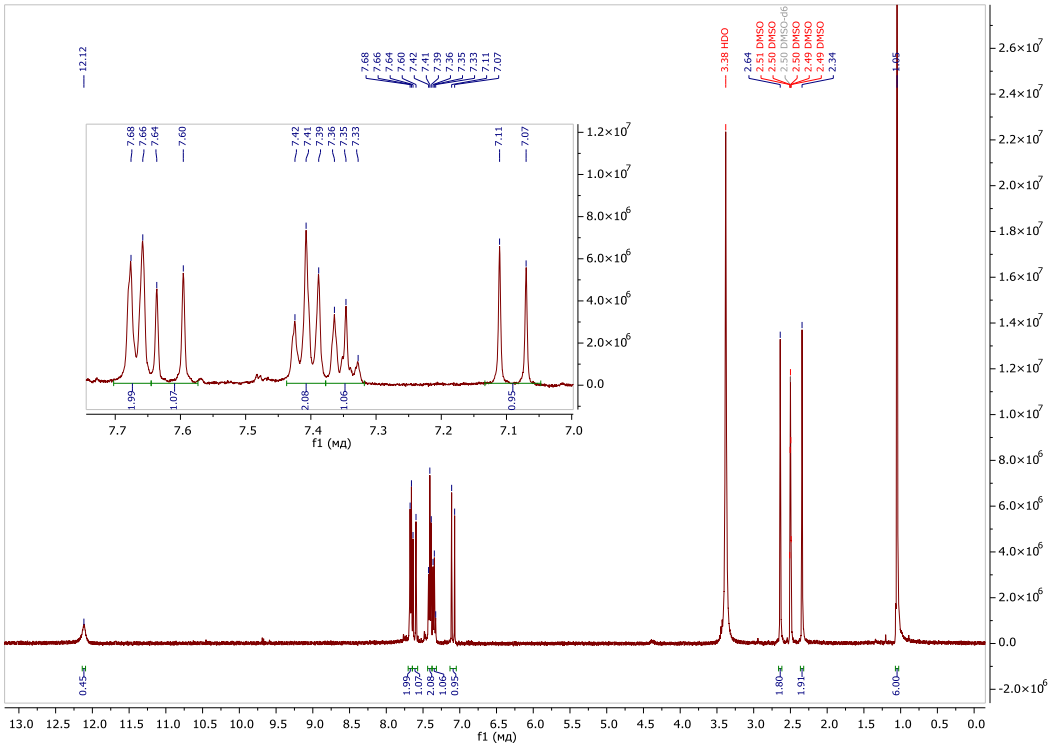


Fig. S 16. ^{1}H NMR spectrum of compound 3e (400 MHz, DMSO-*d*$_6$).

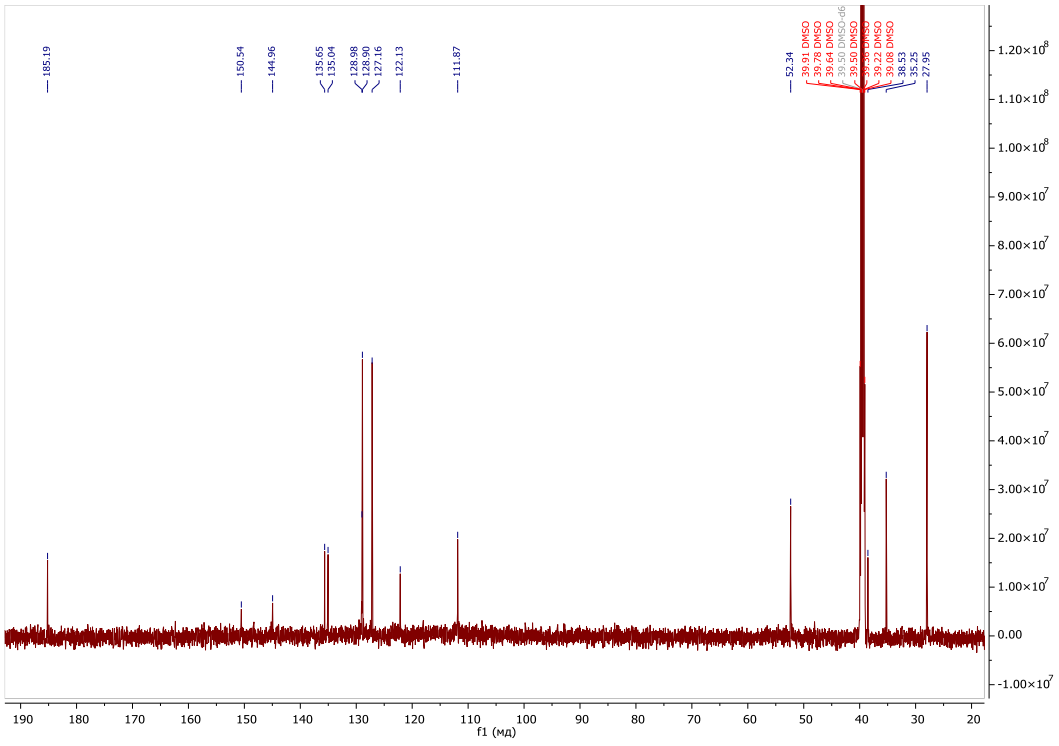
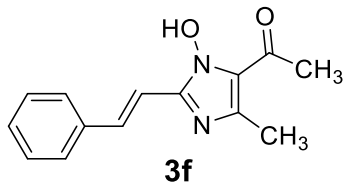


Fig. S 17. ^{13}C NMR spectrum of compound 3e (151 MHz, DMSO-*d*$_6$).

3.6. 1-(1-Hydroxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazol-5-yl)ethanone (**3f**).



3f

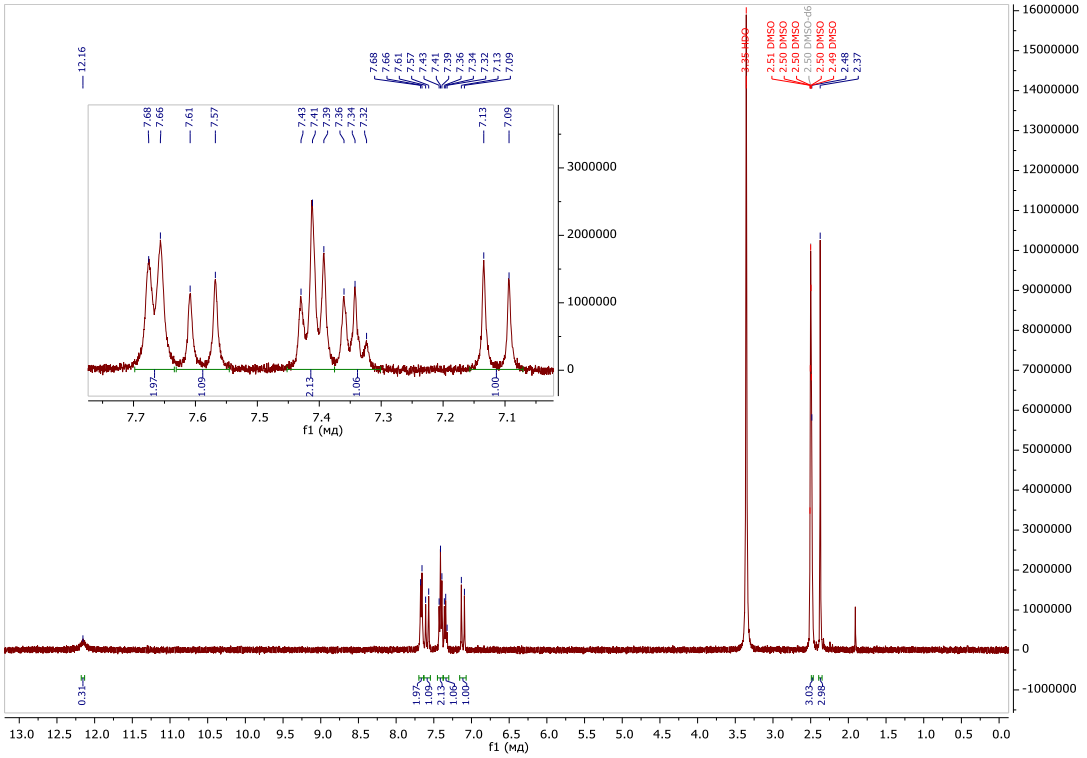


Fig. S 18. ^{1}H NMR spectrum of compound 3f (400 MHz, DMSO-*d*$_6$).

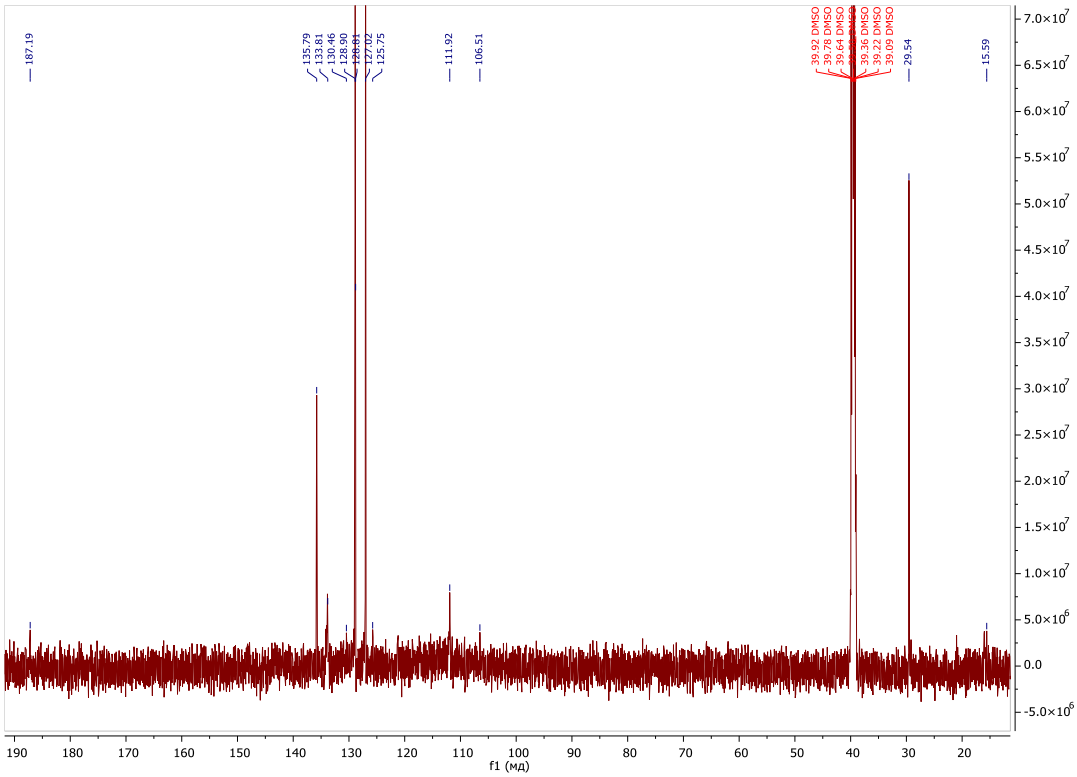
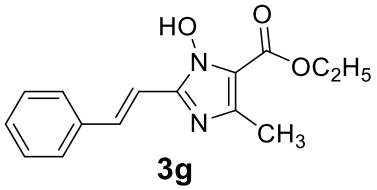


Fig. S 19. ^{13}C NMR spectrum of compound 3f (151 MHz, DMSO-*d*$_6$).

S4.7. Ethyl 1-hydroxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole-5-carboxylate (**3g**).



3g

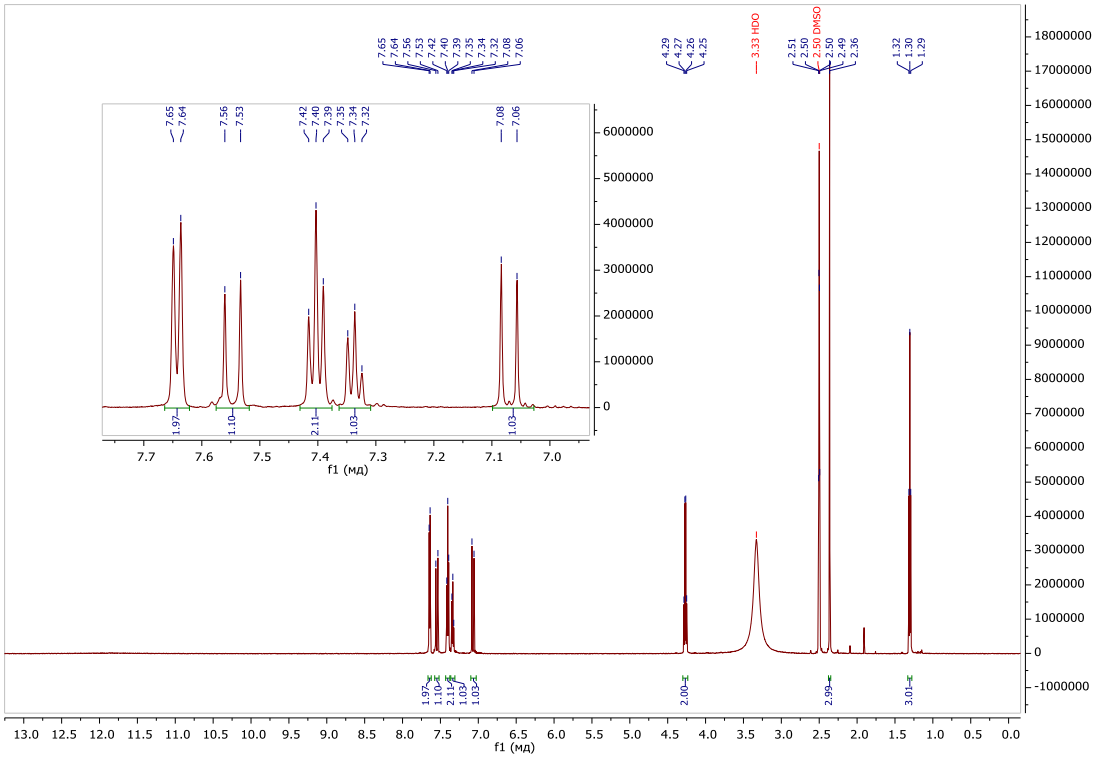


Fig. S 20. ^{1}H NMR spectrum of compound 3g (600 MHz, DMSO-d_6).

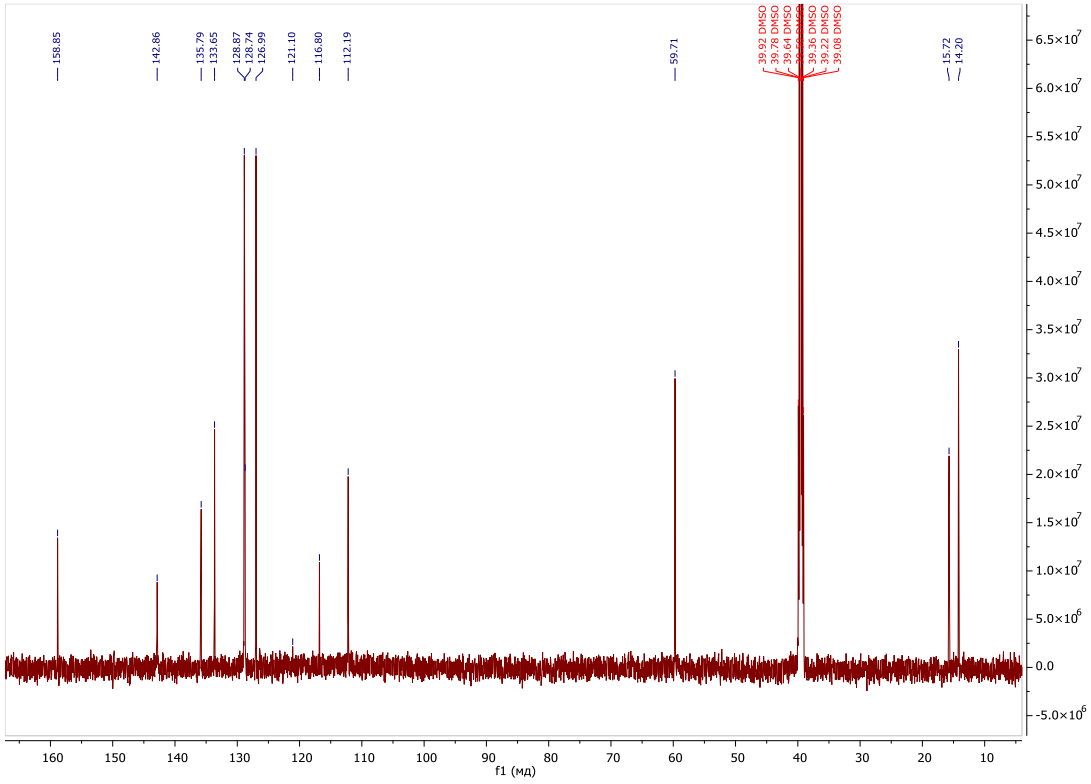


Fig. S 21. ^{13}C NMR spectrum of compound 3g (151 MHz, DMSO-d_6).

S4.8. 4,5-Dimethyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazol-1-ol (**3h**).

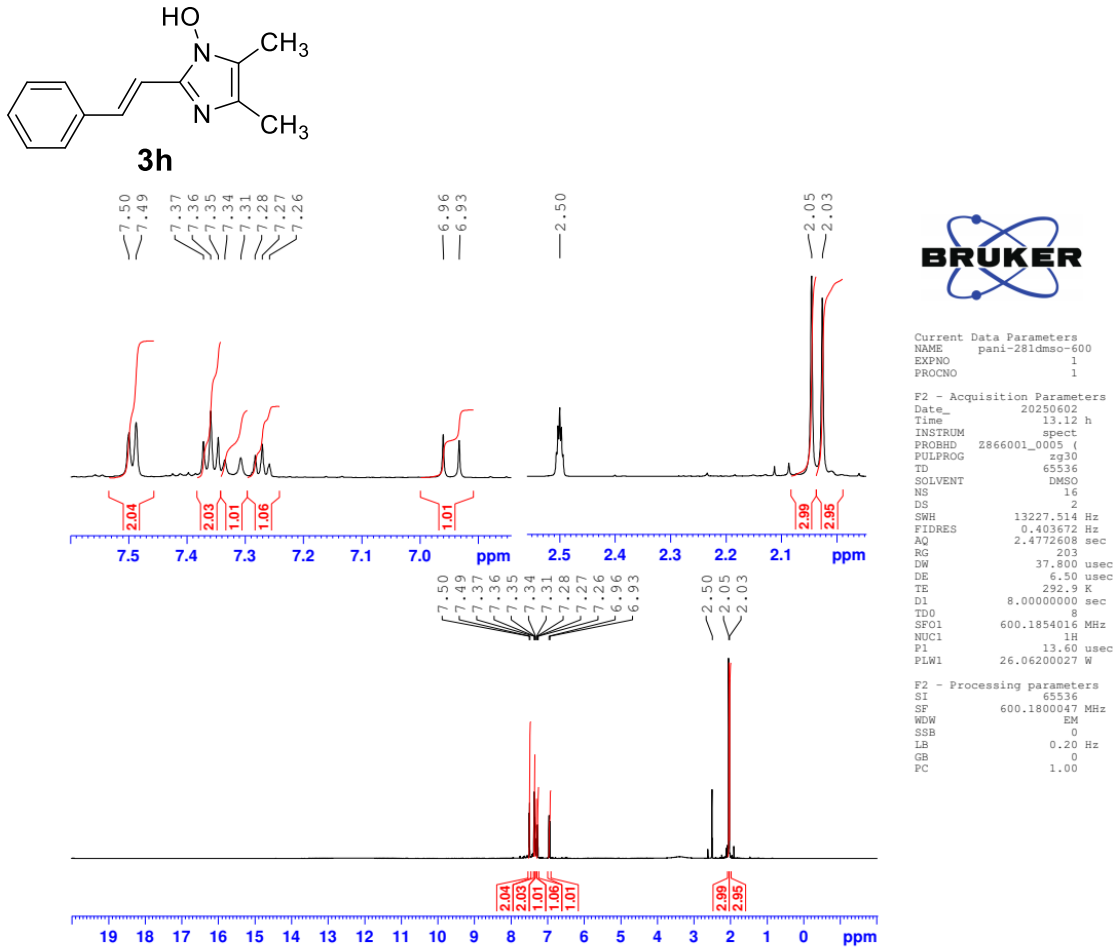


Fig. S 22. ^{1}H NMR spectrum of compound 3h (600 MHz, DMSO-d_6, 23.4°C).

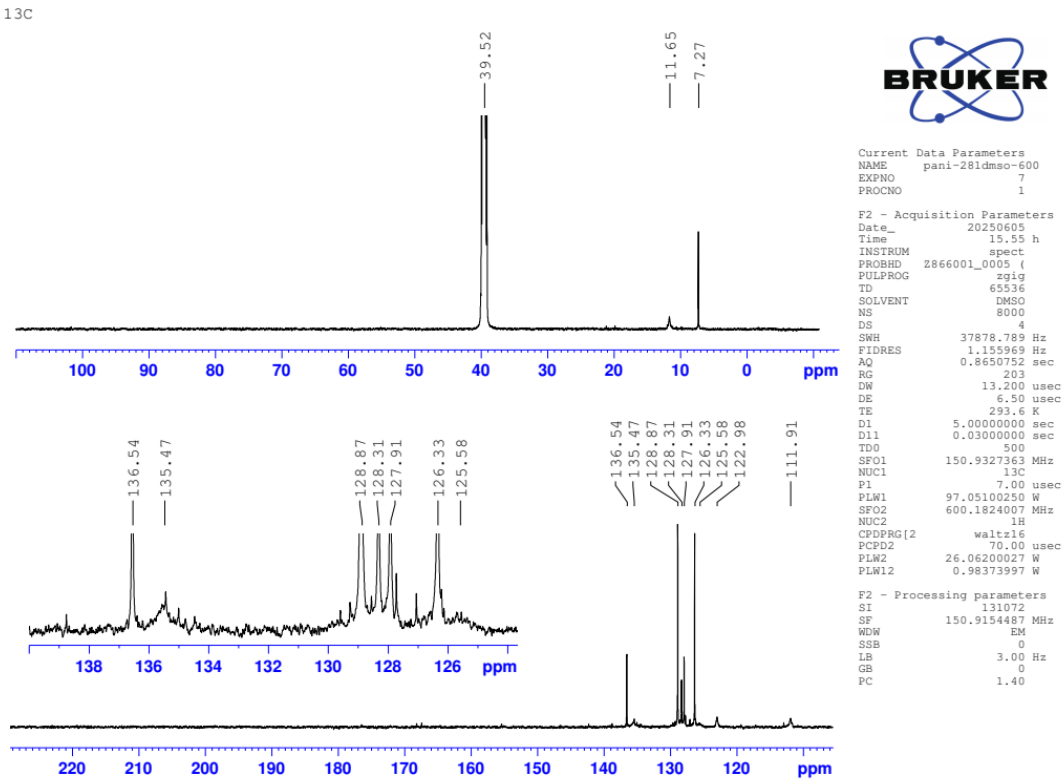


Fig. S 23. ^{13}C NMR spectrum of compound 3h (151 MHz, DMSO-d_6, 23.4°C).

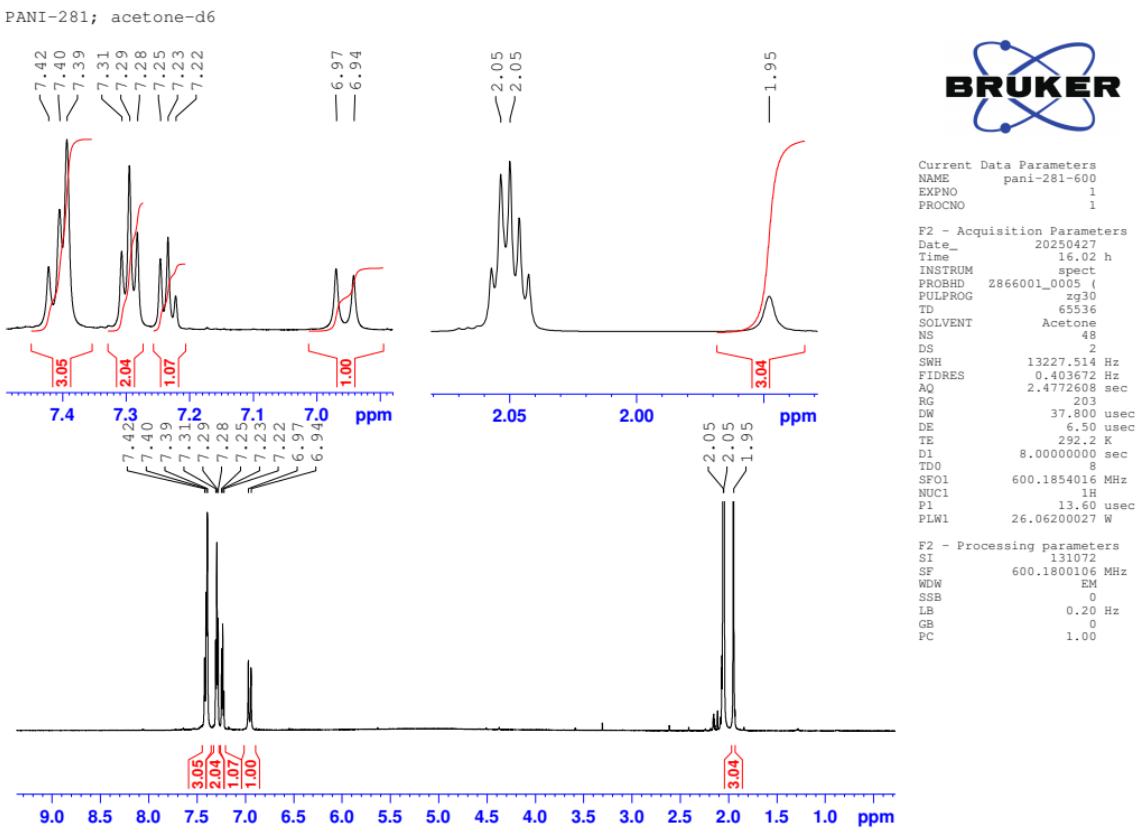


Fig. S 24. ^{1}H NMR spectrum of compound 3h (600 MHz, acetone-d_6).

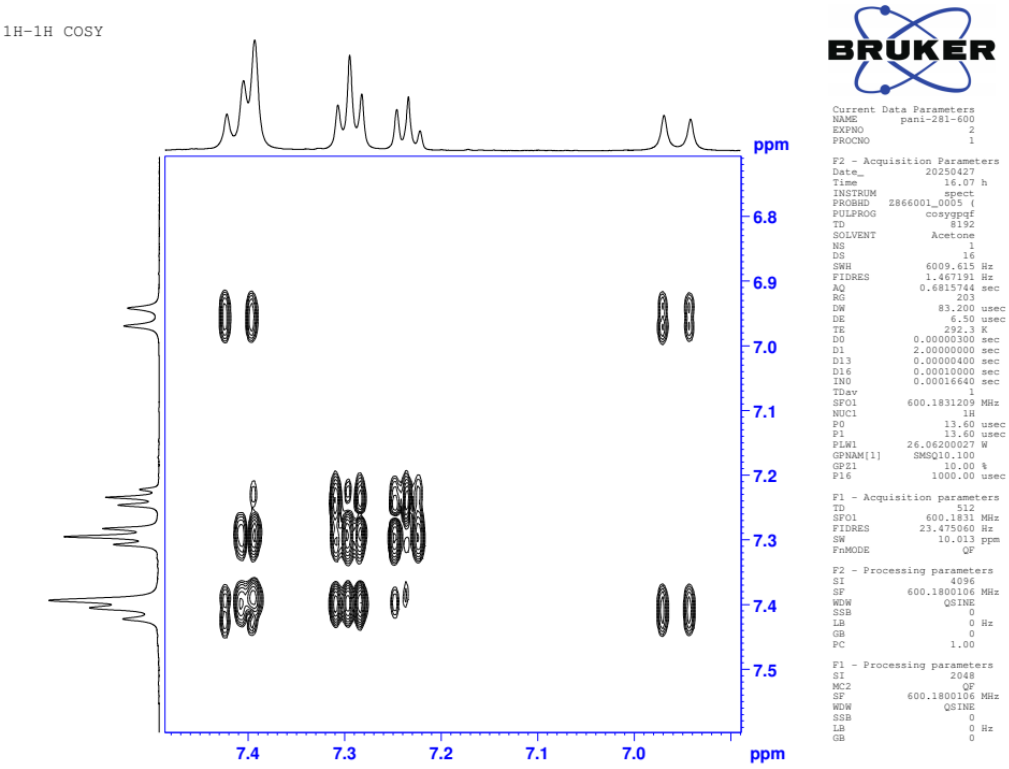


Fig. S 25. ^{1}H-^{1}H COSY spectrum of compound 3h (600 MHz, acetone-d_6).

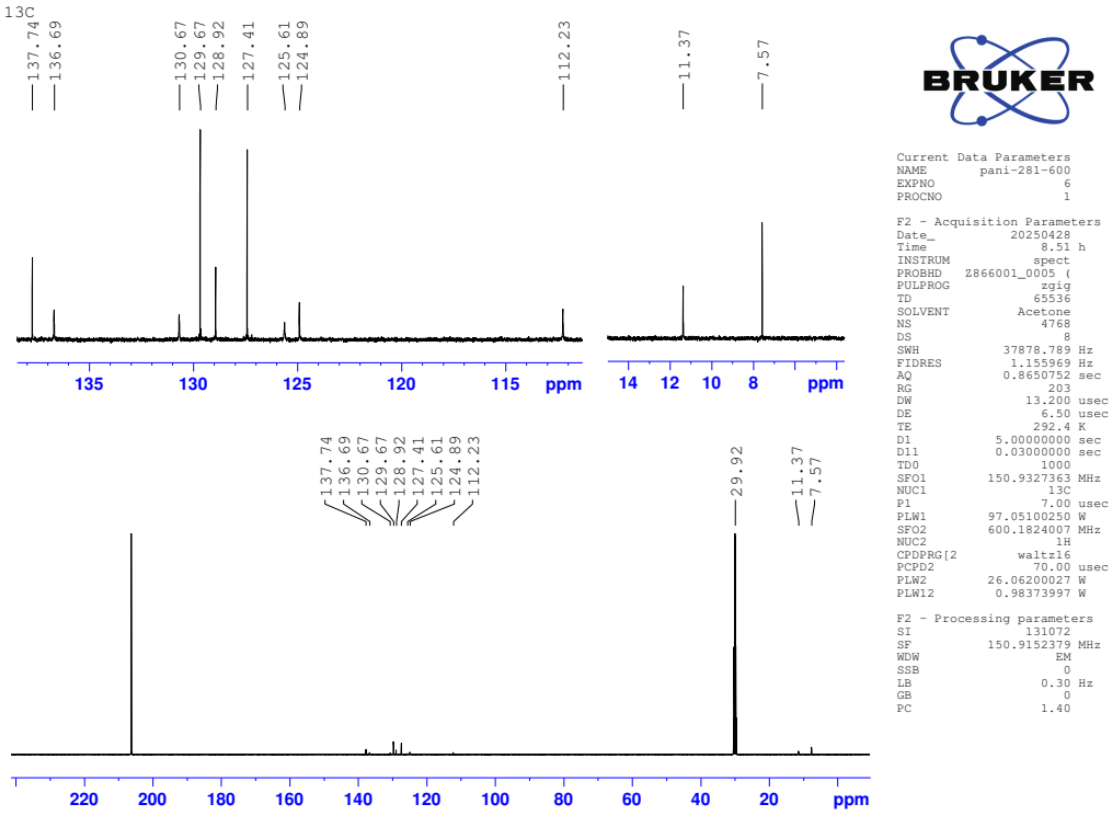


Fig. S 26. ^{13}C NMR spectrum of compound 3h (151 MHz, acetone-d_6).

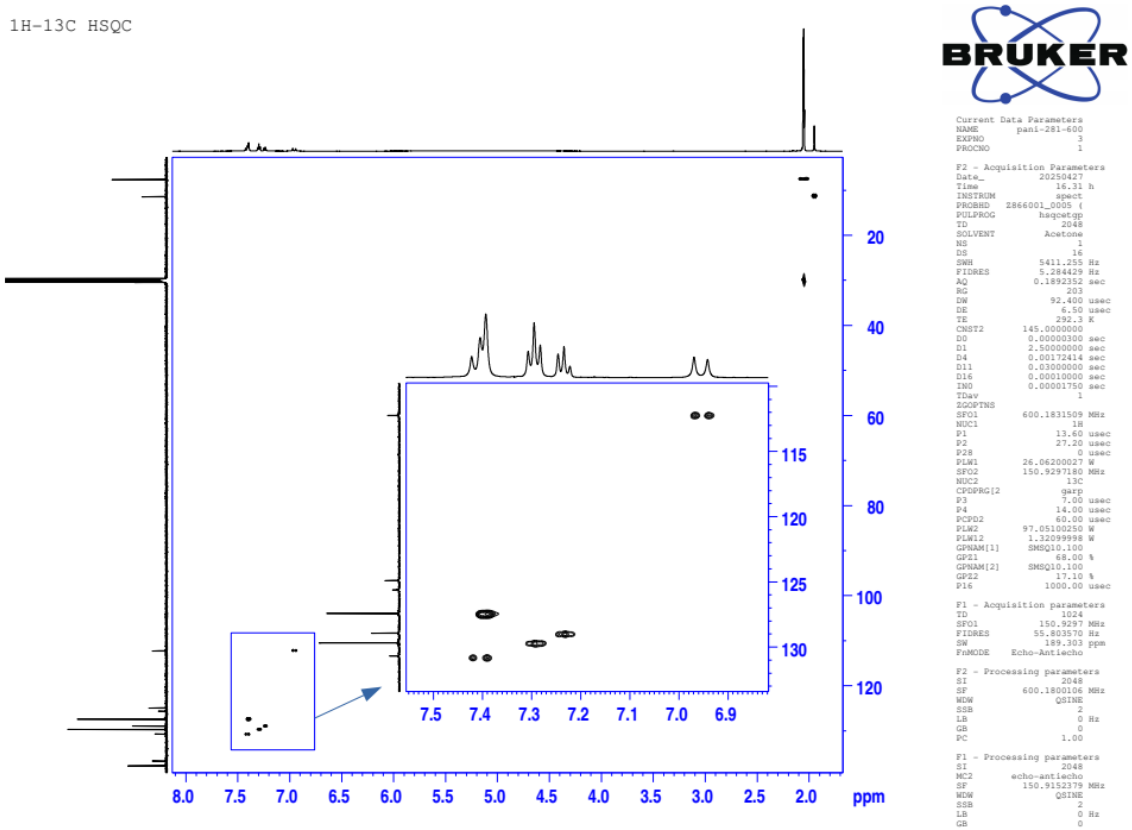


Fig. S 27. ^{1}H-^{13}C HSQC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

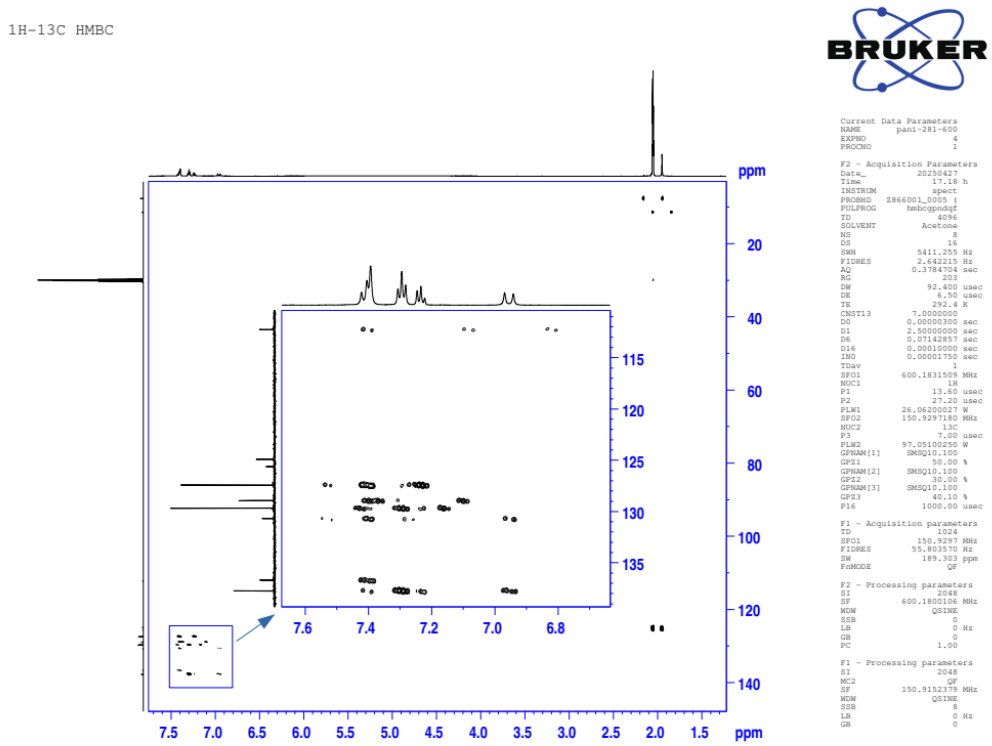


Fig. S 28. ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

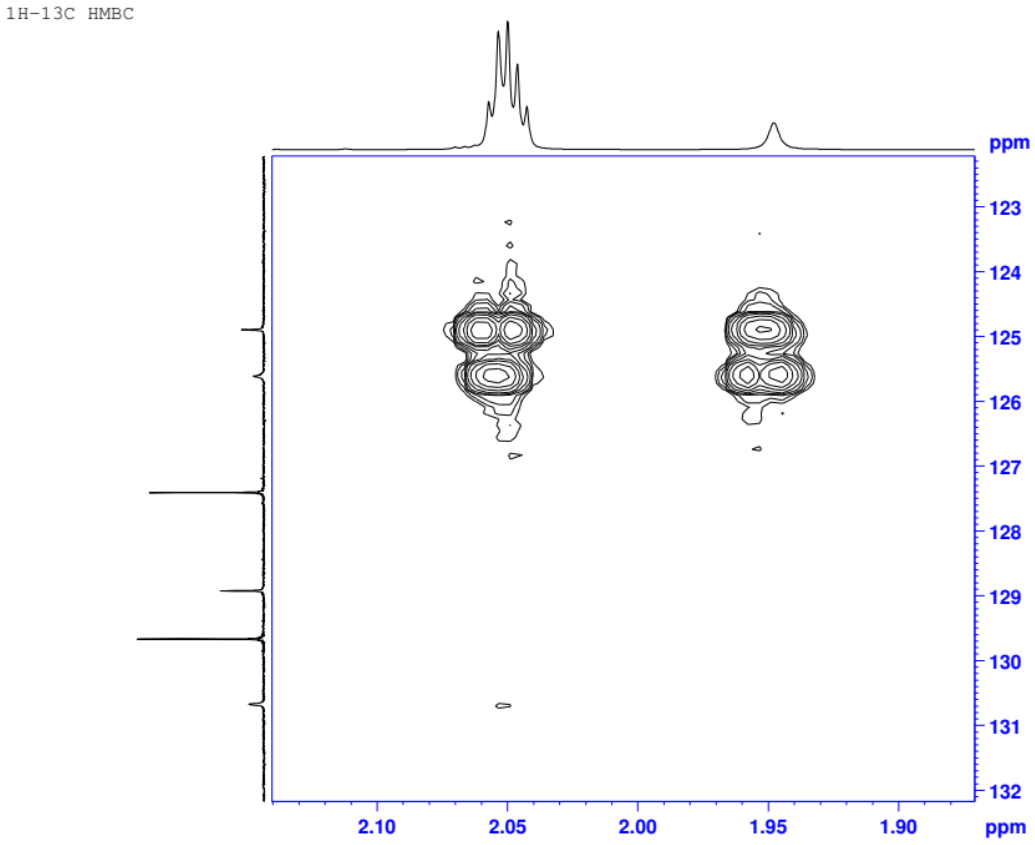


Fig. S 29. Part of ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

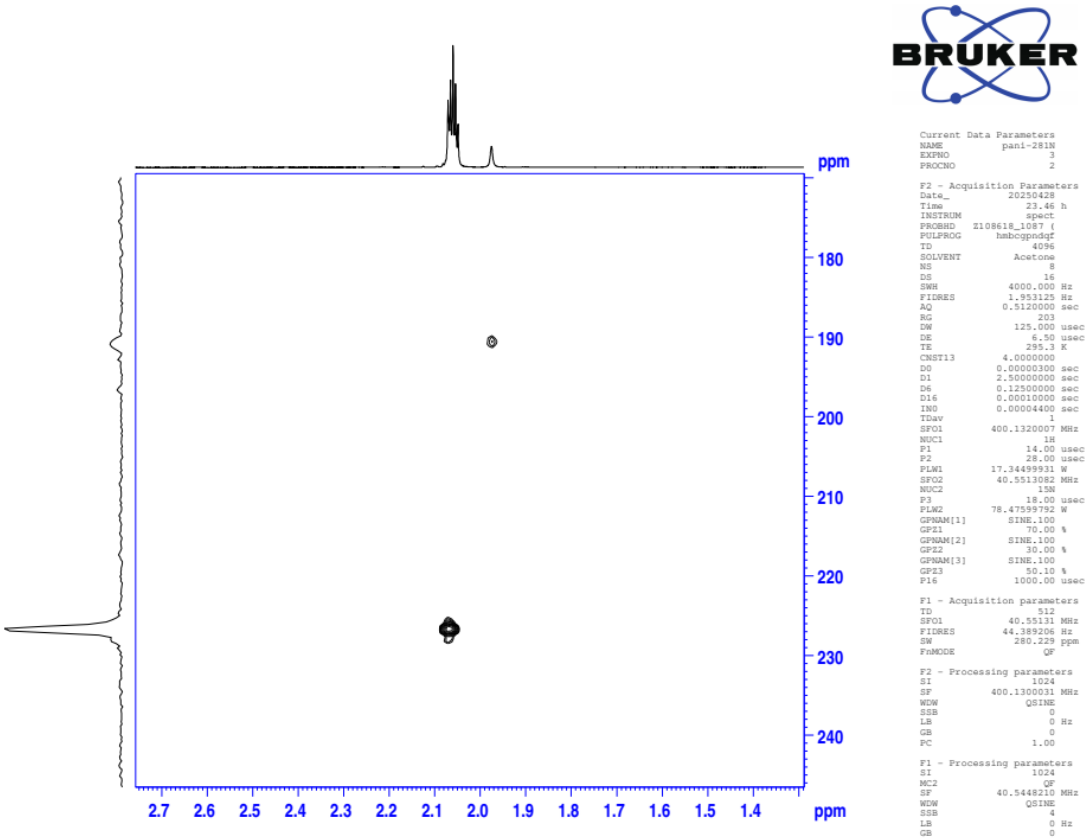


Fig. S 30. ^{1}H-^{15}N HMBC spectrum of compound 3h (400 MHz – ^{1}H, 41 MHz – ^{15}N, acetone-d_6).

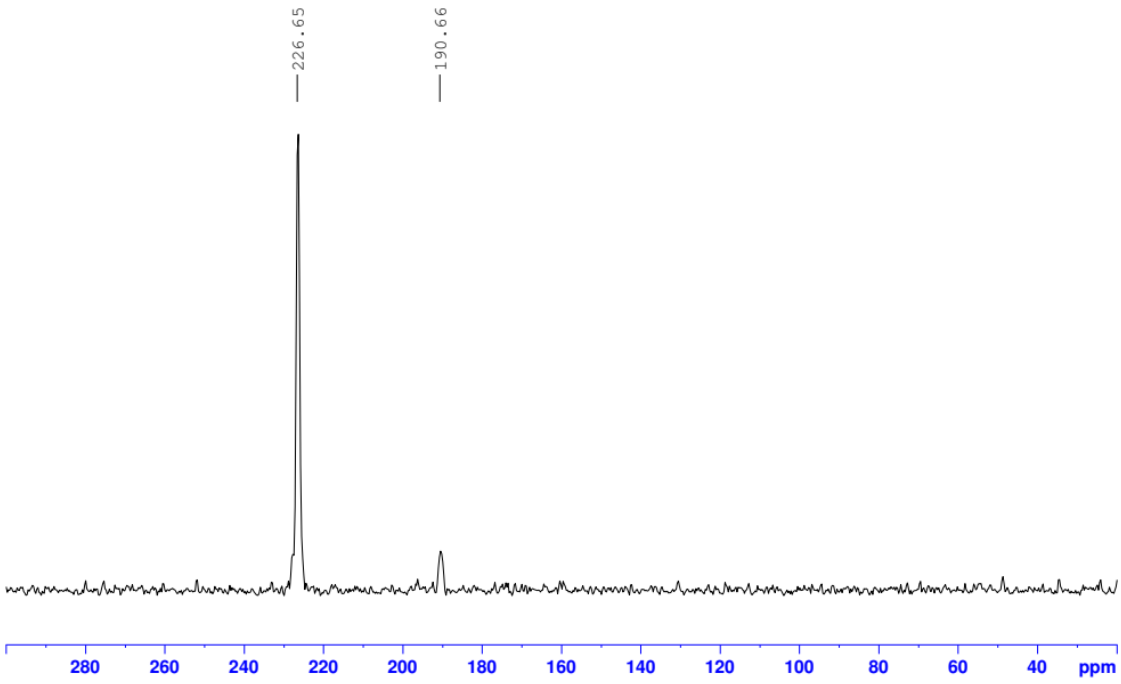


Fig. S 31. ^{15}N NMR spectrum of compound 3h (41 MHz, acetone-d_6), obtained by projection from ^{1}H-^{15}N HMBC spectrum.

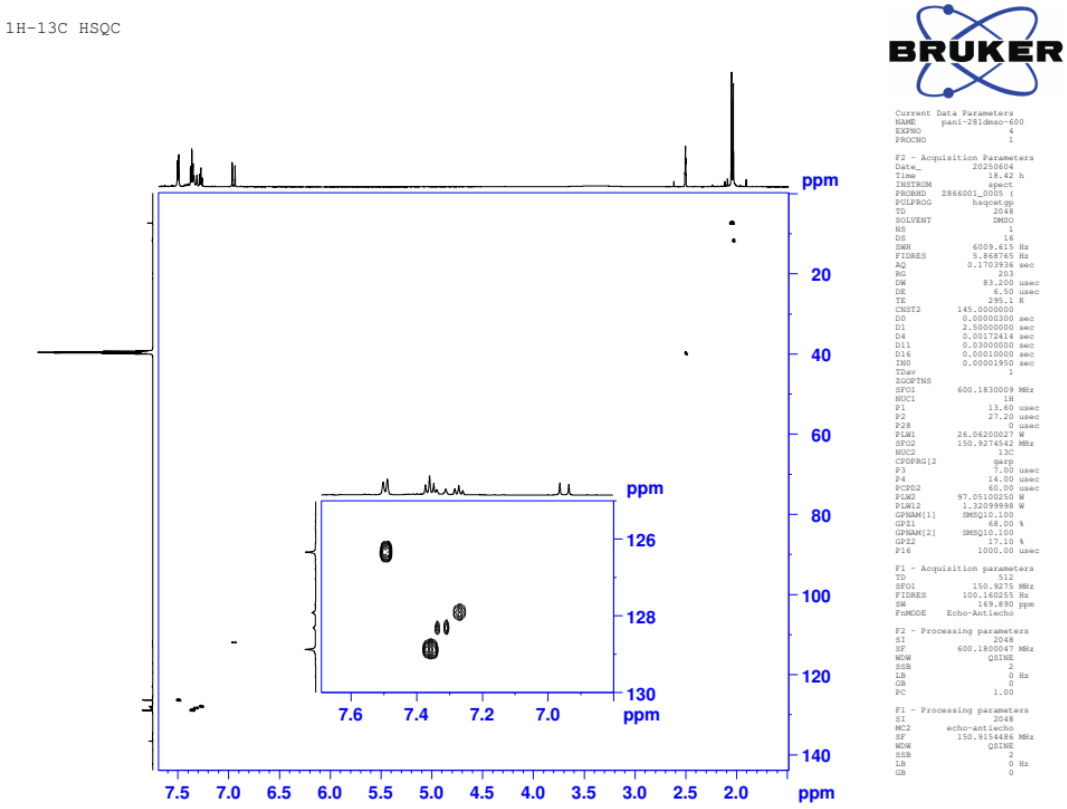


Fig. S 32. ^{1}H-^{13}C HSQC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-d_6, 23.4°C).

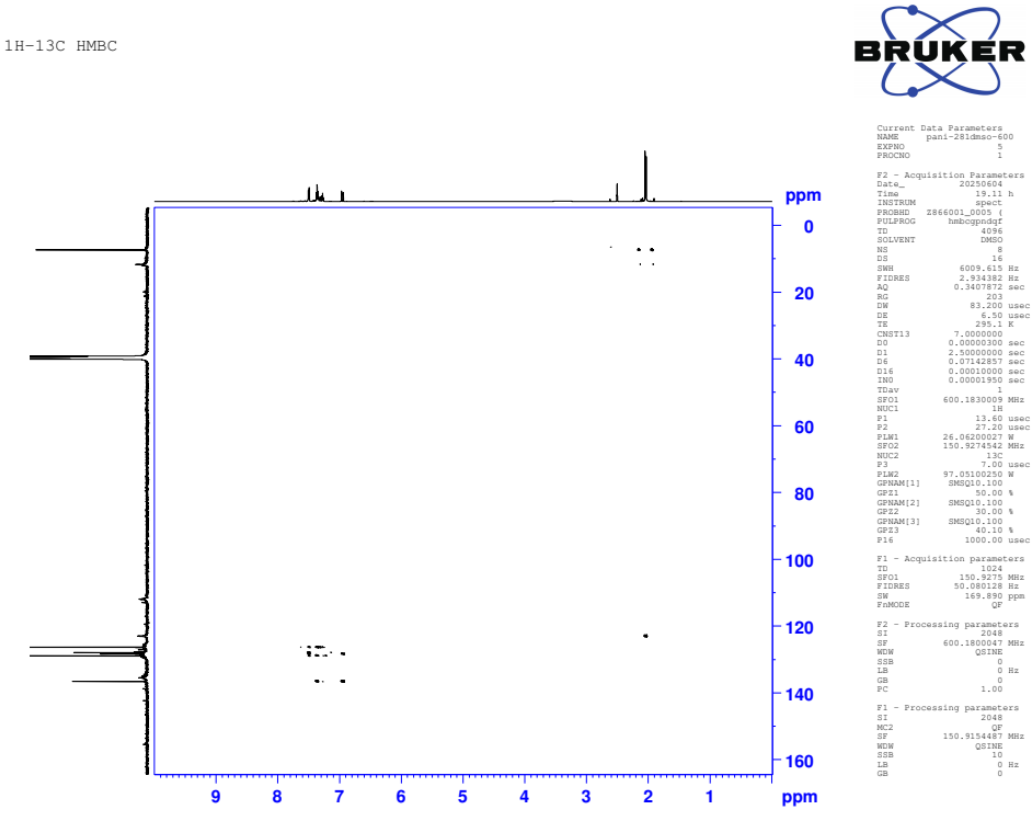


Fig. S 33. ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-d_6, 23.4°C).

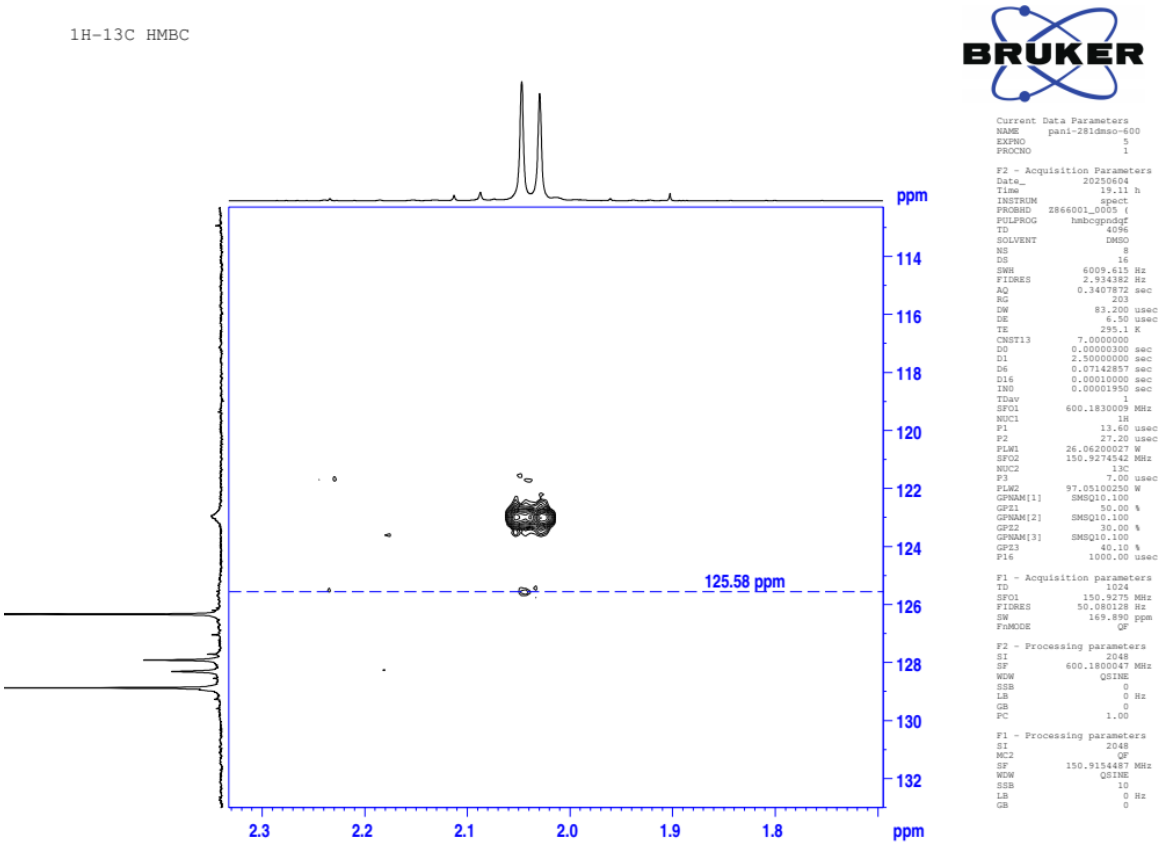


Fig. S 34. Part of ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-*d*$_6$, 23.4°C).

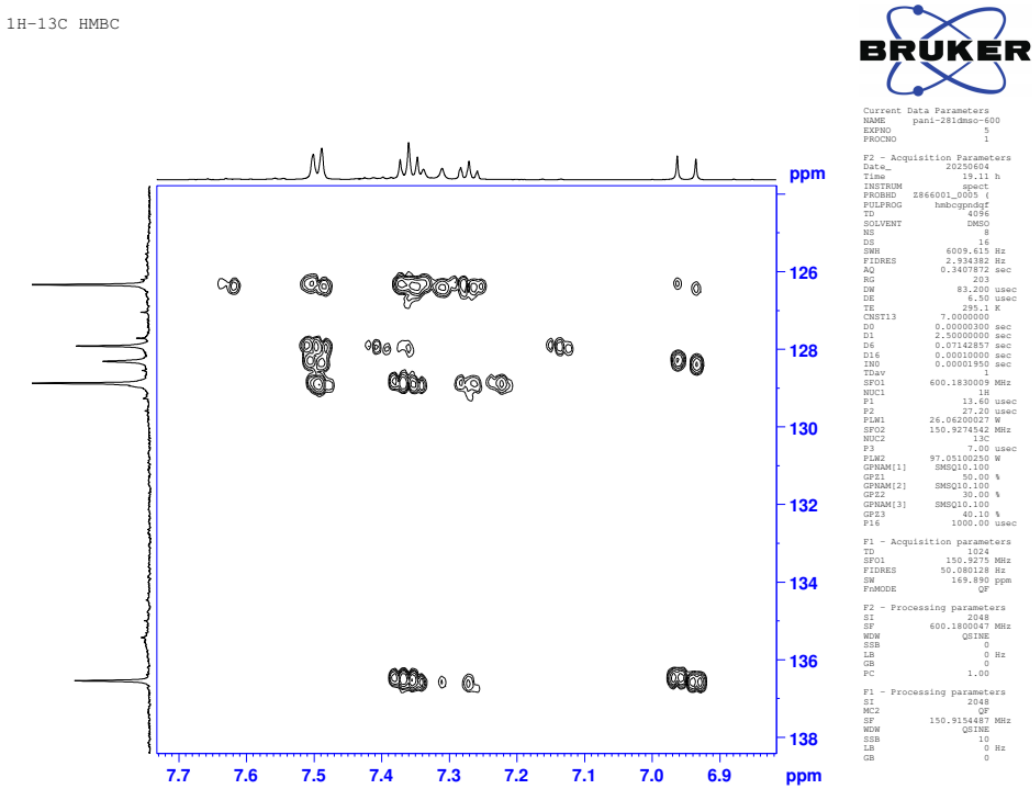


Fig. S 32. Part of ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-*d*$_6$, 23.4°C).

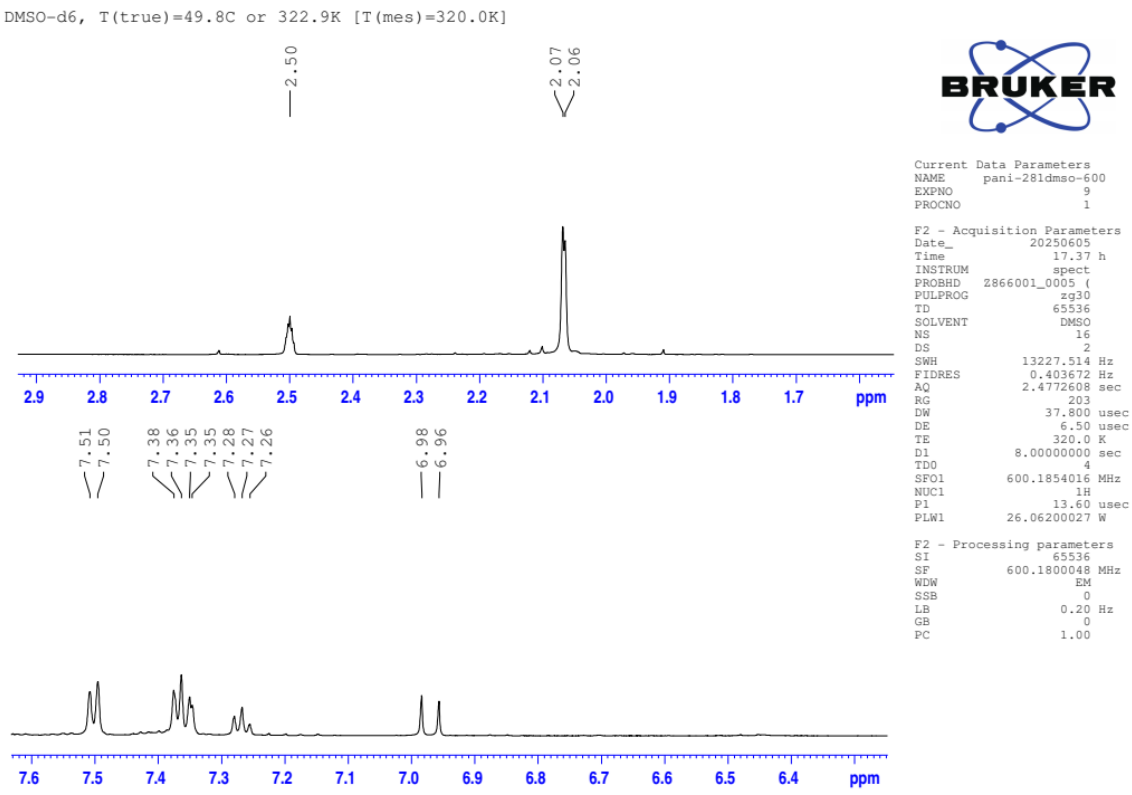


Fig. S 33. ^{1}H NMR spectrum of compound 3h (600 MHz, DMSO-d_6, 49.8°C).

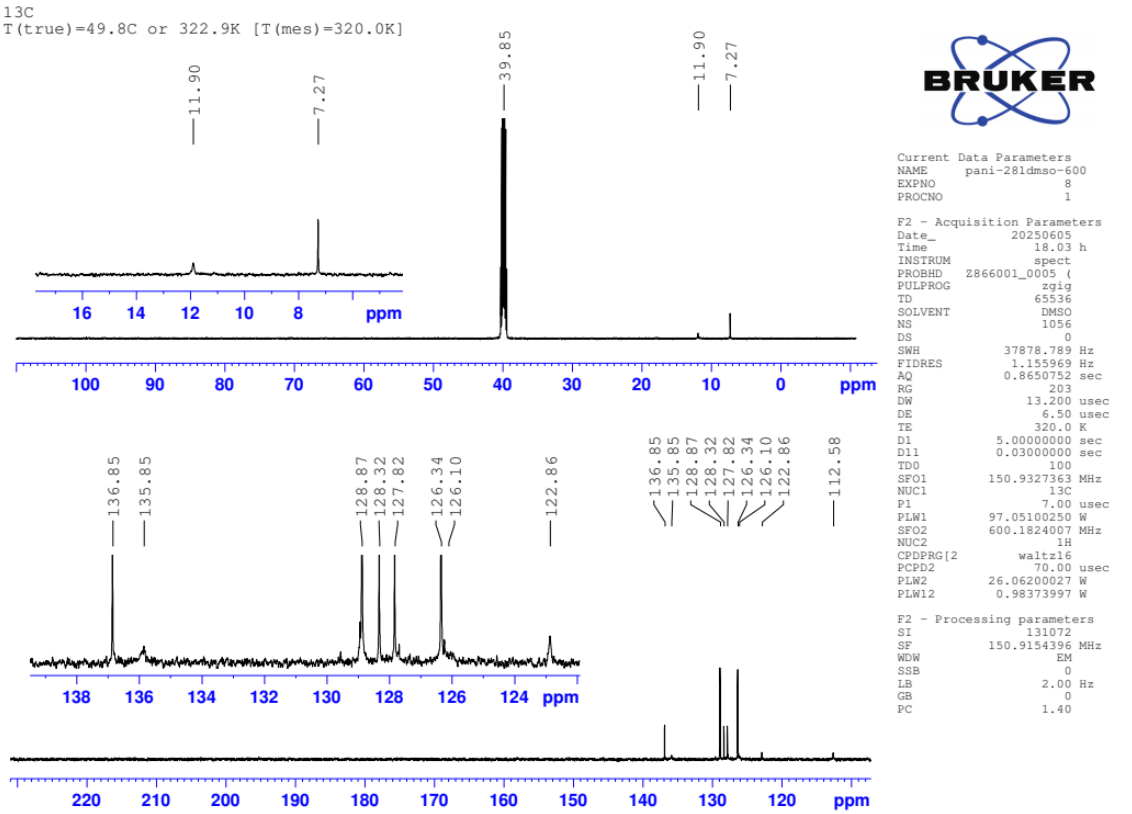


Fig. S 34. ^{13}C NMR spectrum of compound 3h (151 MHz, DMSO-d_6, 49.8°C) calibrated by 3" signal of phenyl moiety, its chemical shift taken equal to 128.97 ppm as at 22.4°C.

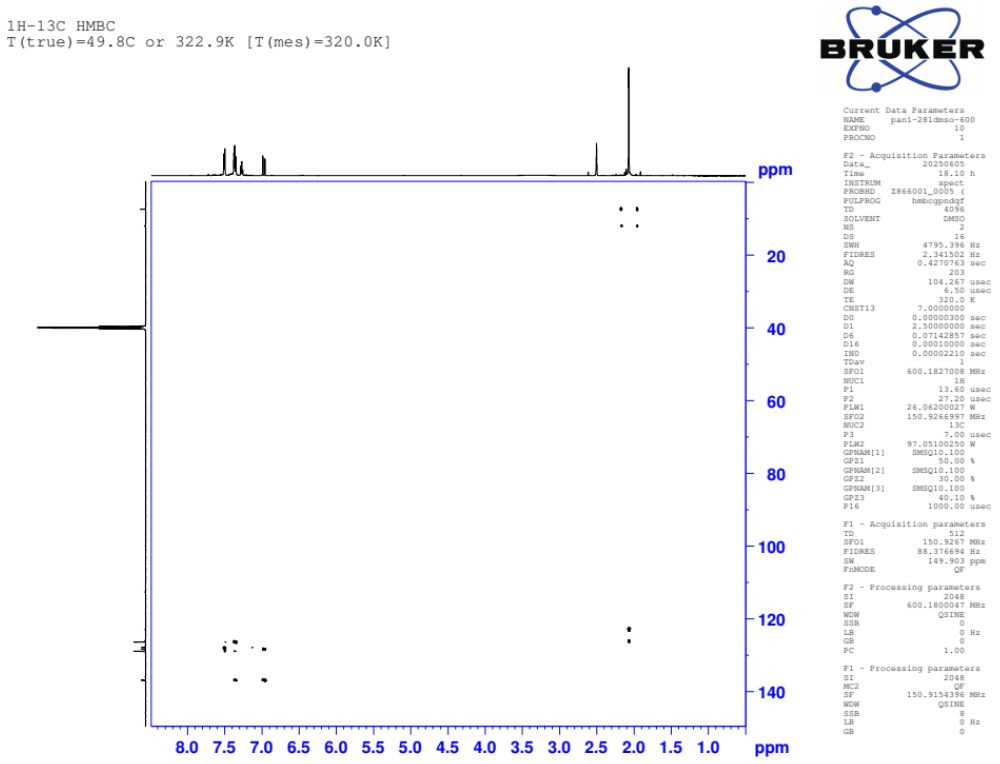


Fig. S 35. ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-*d*$_6$, 49.8°C).

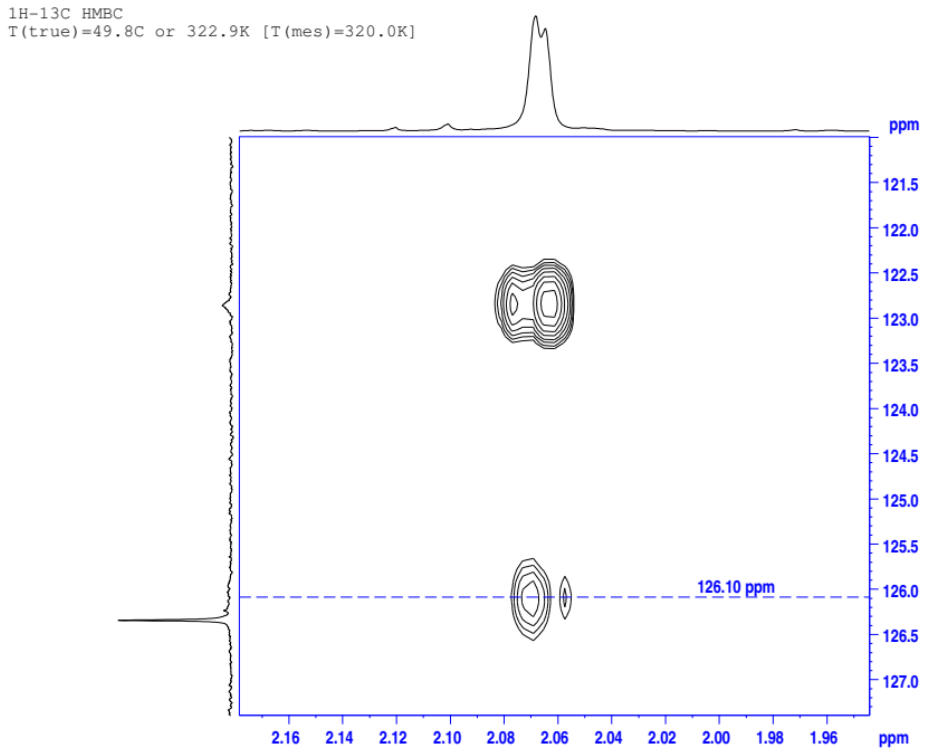


Fig. S 36. Part of ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-*d*$_6$, 49.8°C).

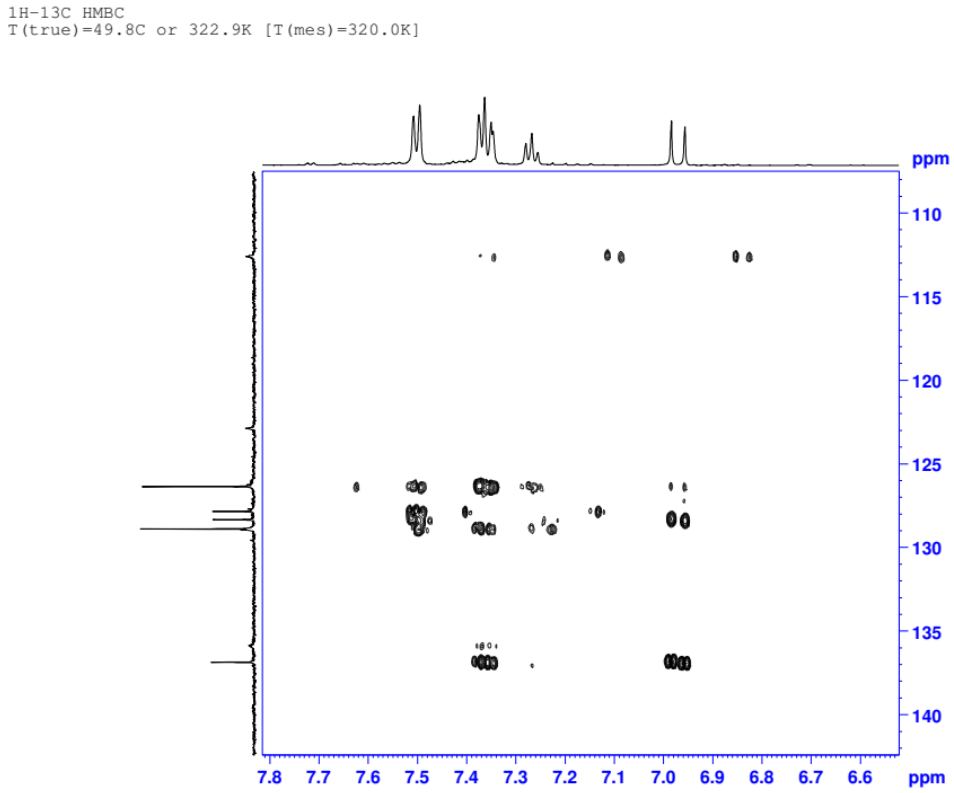
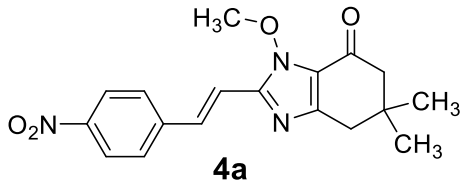


Fig. S 37. Part of ^{1}H-^{13}C HMBC spectrum of compound 3h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-*d*$_6$, 49.8°C).

S4.9. 3-Methoxy-6,6-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-3,5,6,7-tetrahydro-**4H**-benzimidazol-4-one (**4a**).



4a

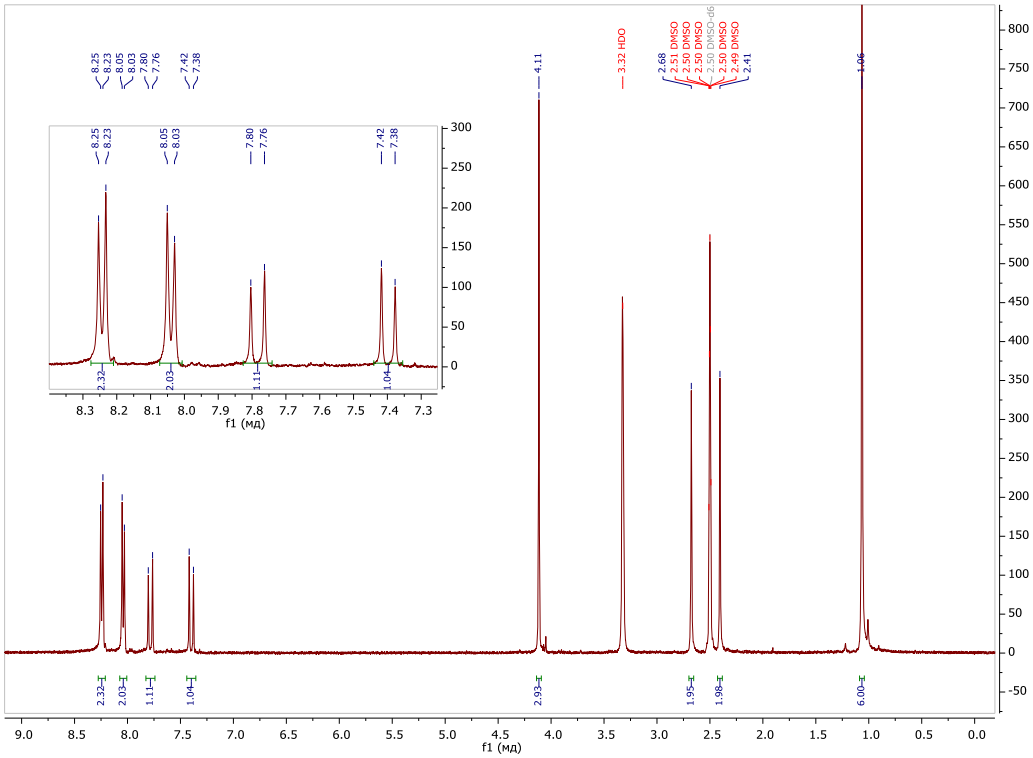


Fig. S 38. ^{1}H NMR spectrum of compound 4a (400 MHz, DMSO-*d*$_6$).

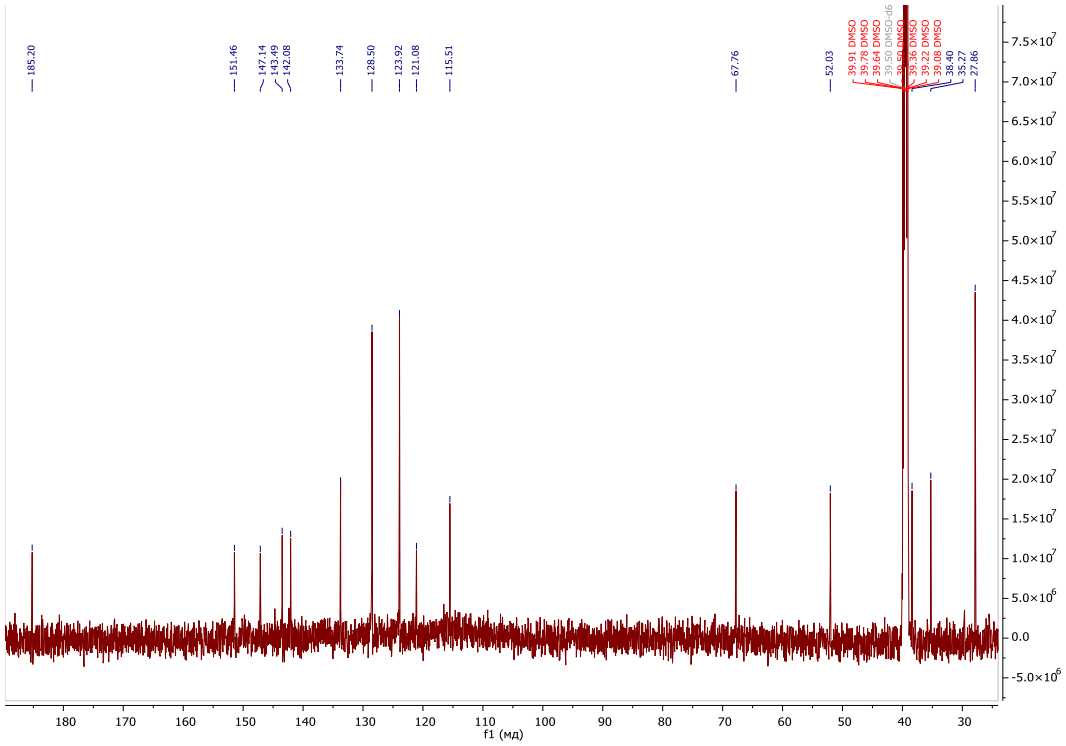
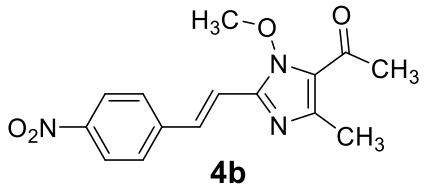


Fig. S 39. ^{13}C NMR spectrum of compound 4a (151 MHz, DMSO-*d*$_6$).

S4.10. 1-(1-Methoxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazol-5-yl)ethanone (**4b**).



4b

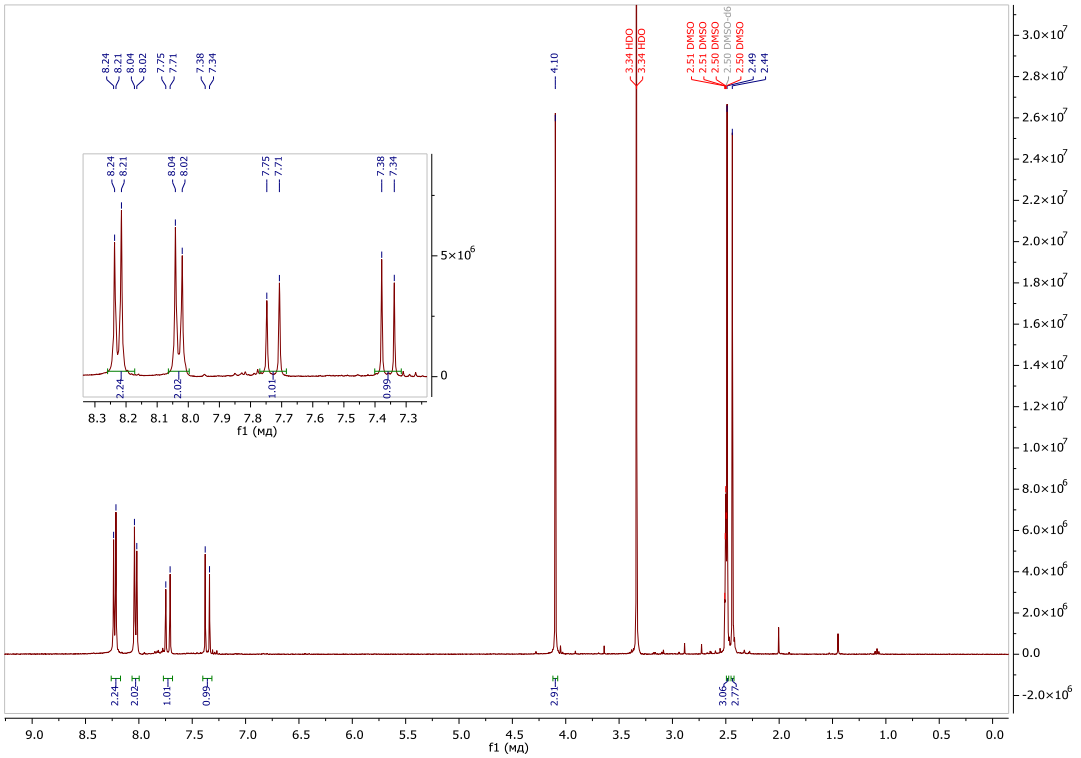


Fig. S 40. ^{1}H NMR spectrum of compound 4b (400 MHz, DMSO-*d*$_6$).

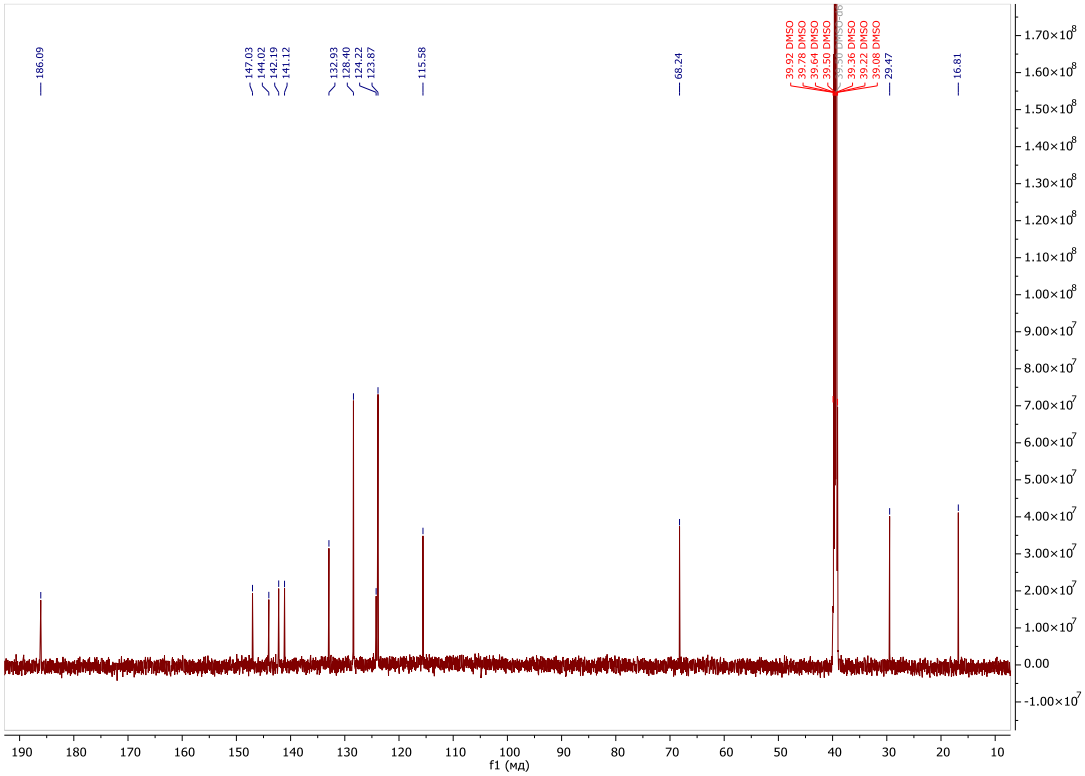


Fig. S 41. ^{13}C NMR spectrum of compound 4b (151 MHz, DMSO-*d*$_6$).

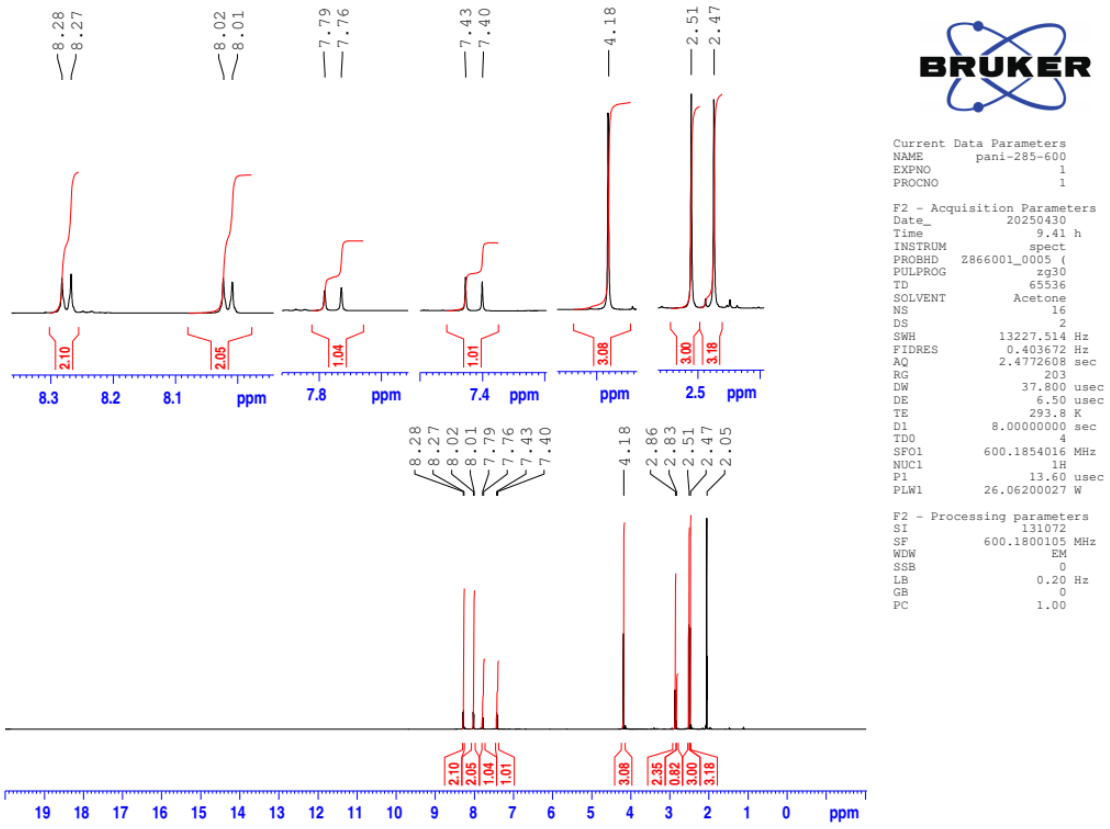


Fig. S 42. ^{1}H NMR spectrum of compound 4b (600 MHz, acetone-d_6).

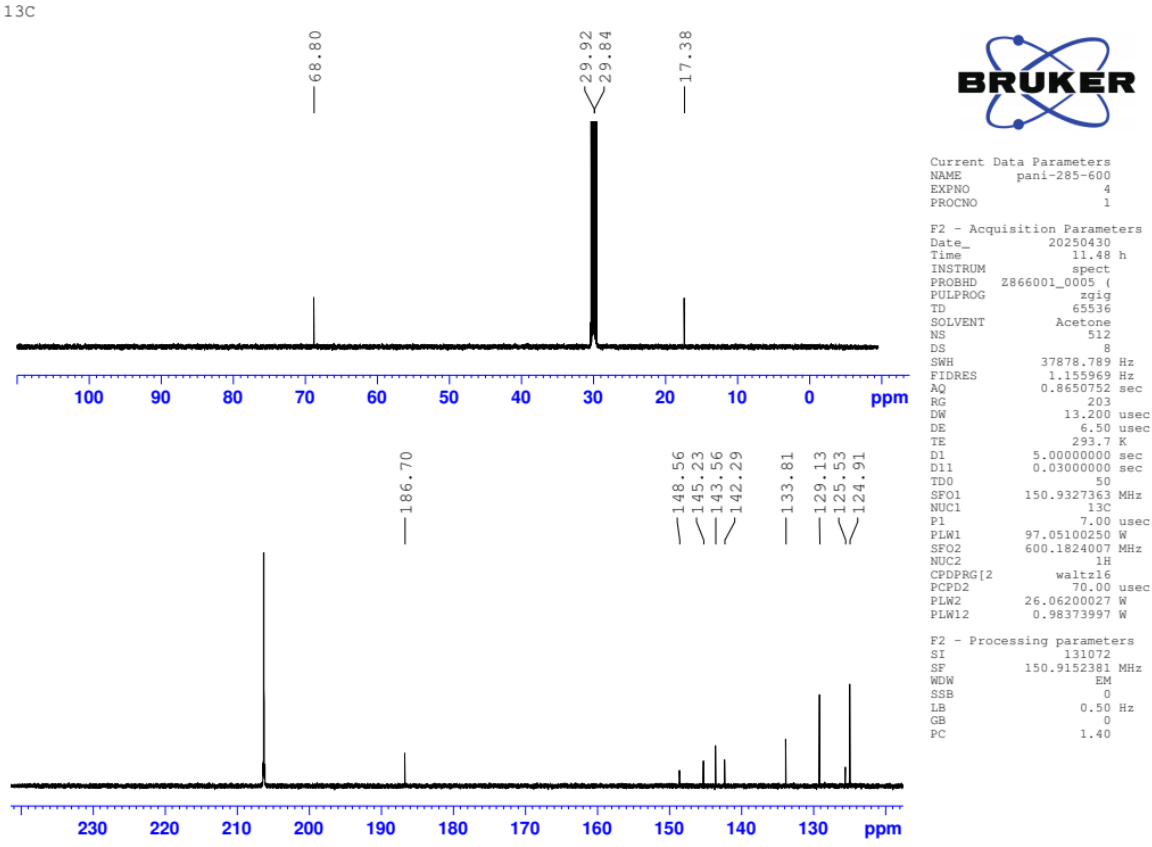


Fig. S 43. ^{13}C NMR spectrum of compound 4b (151 MHz, acetone-d_6).

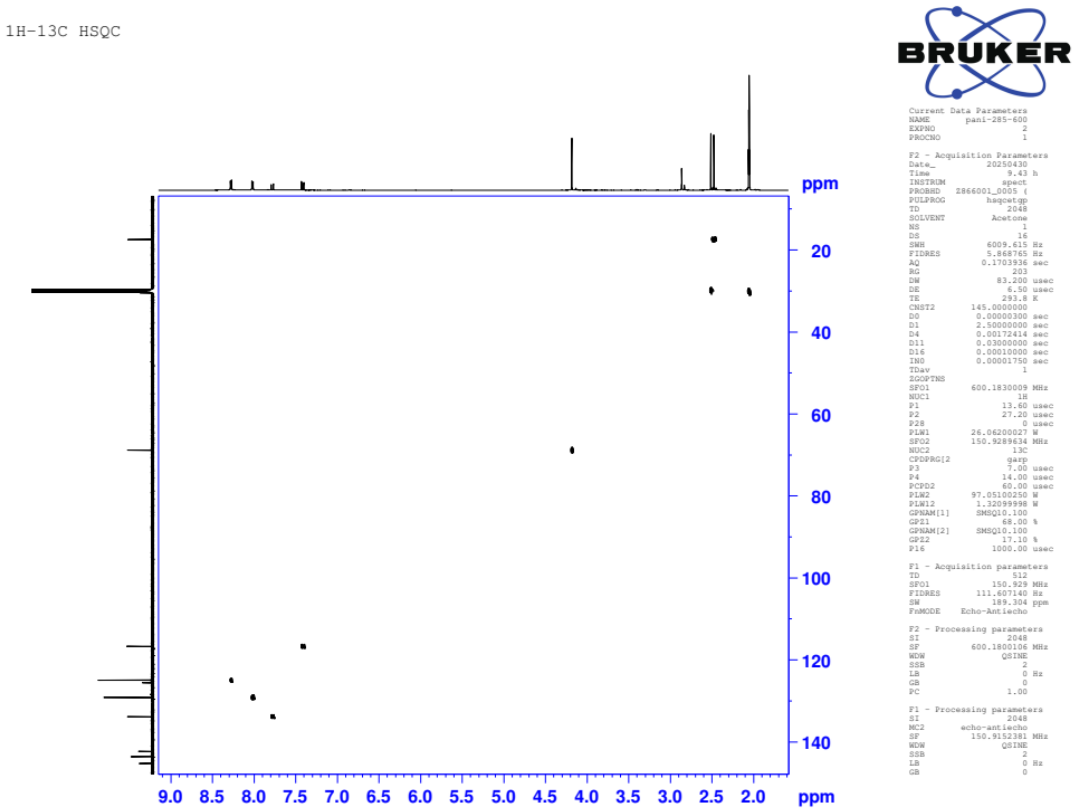


Fig. S 44. ^{1}H-^{13}C HSQC spectrum of compound 4b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

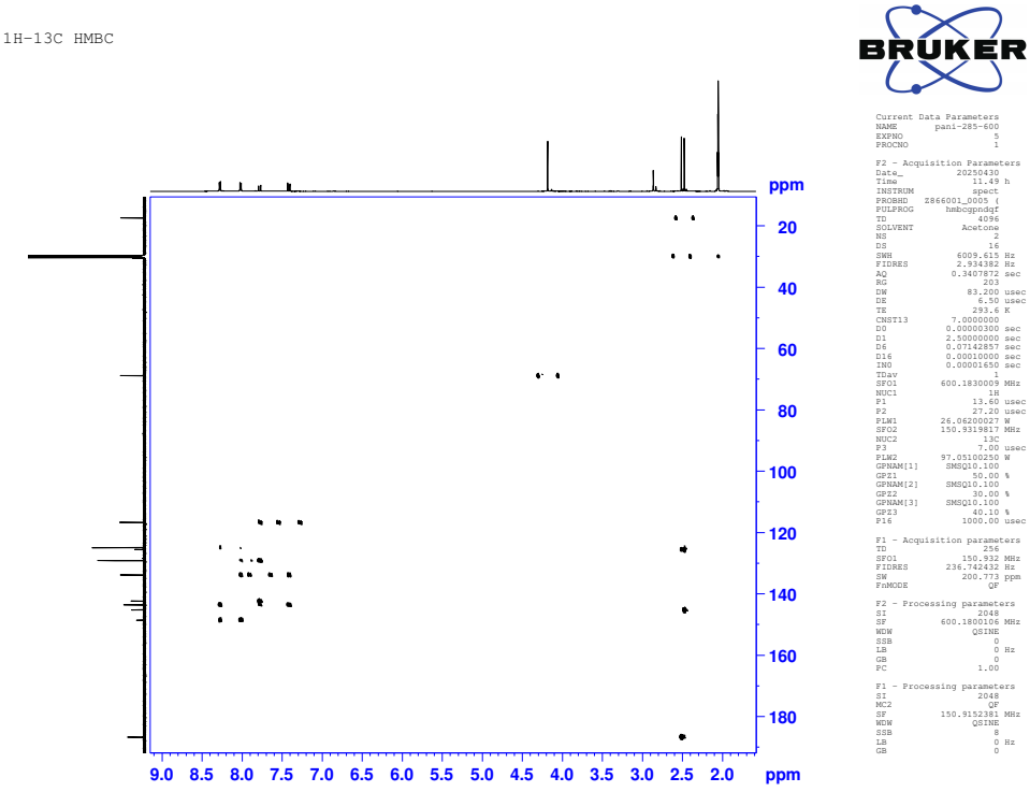


Fig. S 48. ^{1}H-^{13}C HMBC spectrum of compound 4b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

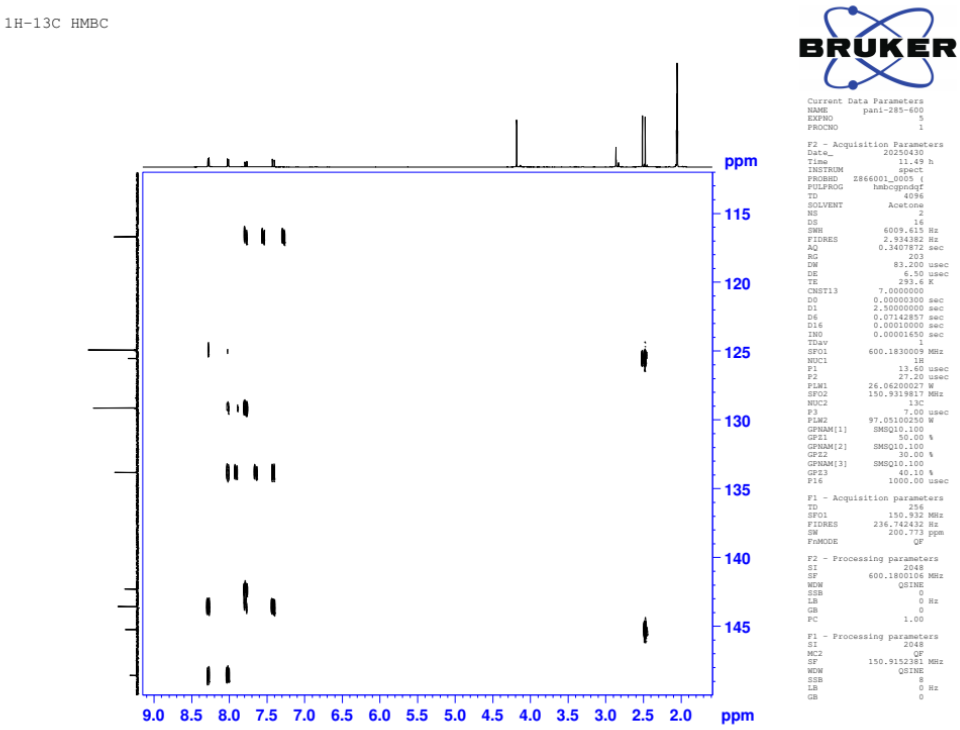


Fig. S 45. Part of ^{1}H-^{13}C HMBC spectrum of compound 4b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

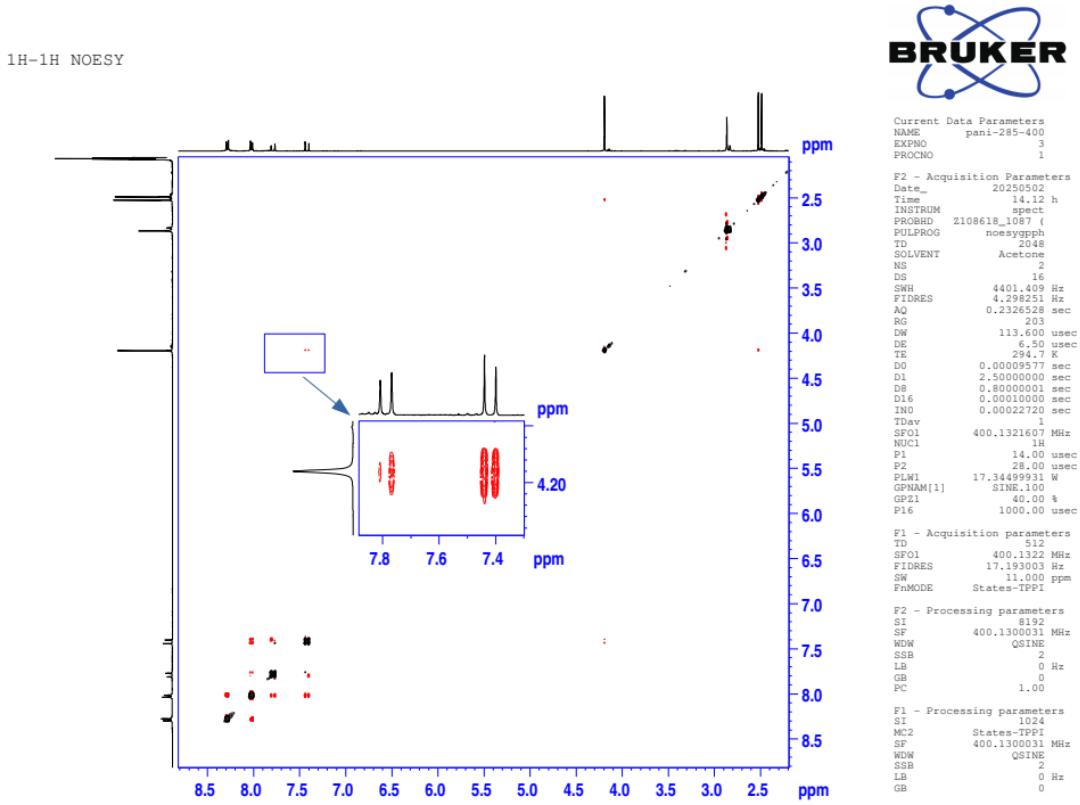


Fig. S 46. ^{1}H-^{1}H NOESY spectrum of compound 4b (400 MHz, acetone-d_6).

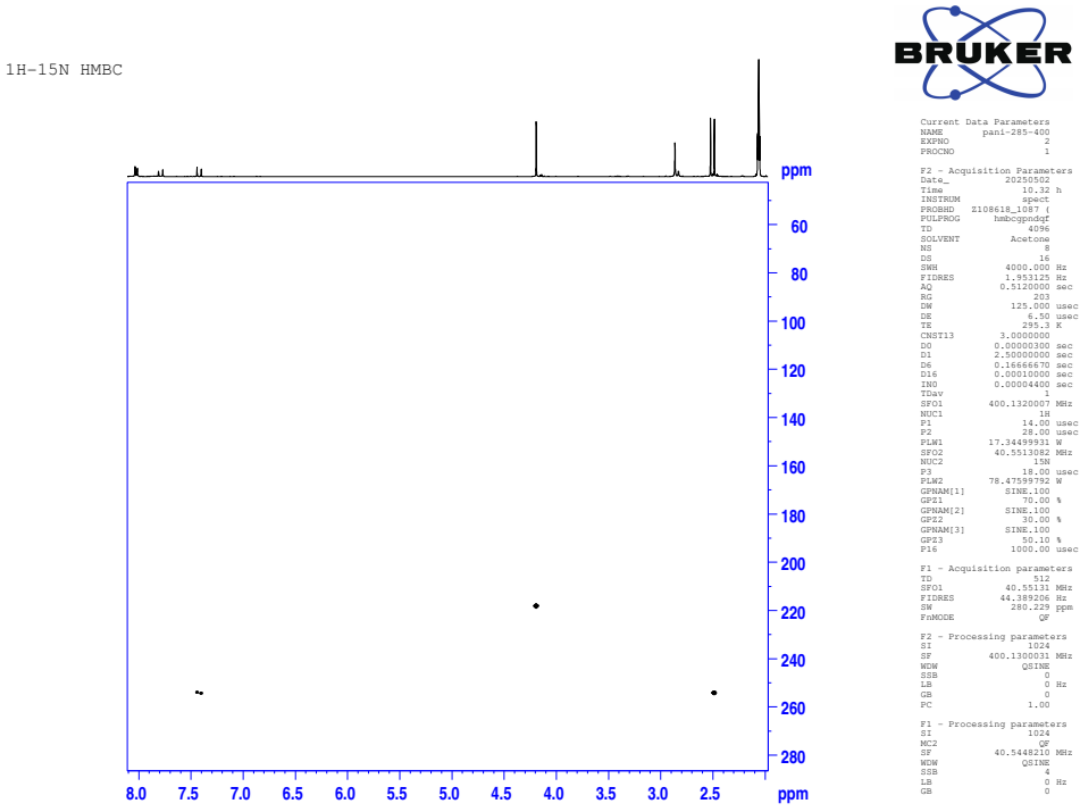


Fig. S 47. ^{1}H-^{15}N HMBC spectrum of compound 4b (400 MHz – ^{1}H, 41 MHz – ^{15}N, acetone-d_6).

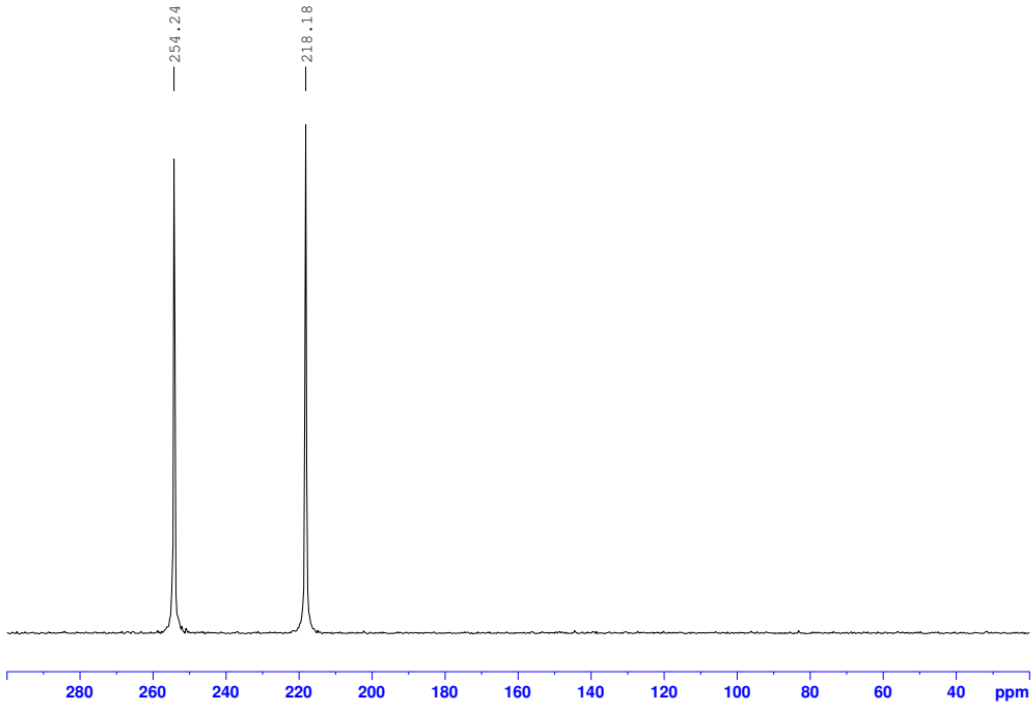
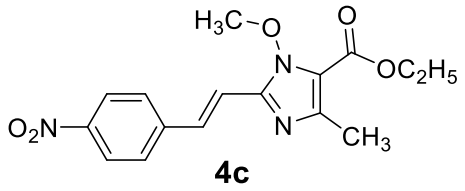


Fig. S 48. ^{15}N NMR spectrum of compound 4b (41 MHz, acetone-d_6), obtained by projection from ^{1}H-^{15}N HMBC spectrum.

S4.11. Ethyl 1-methoxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole-5-carboxylate (**4c**).



4c

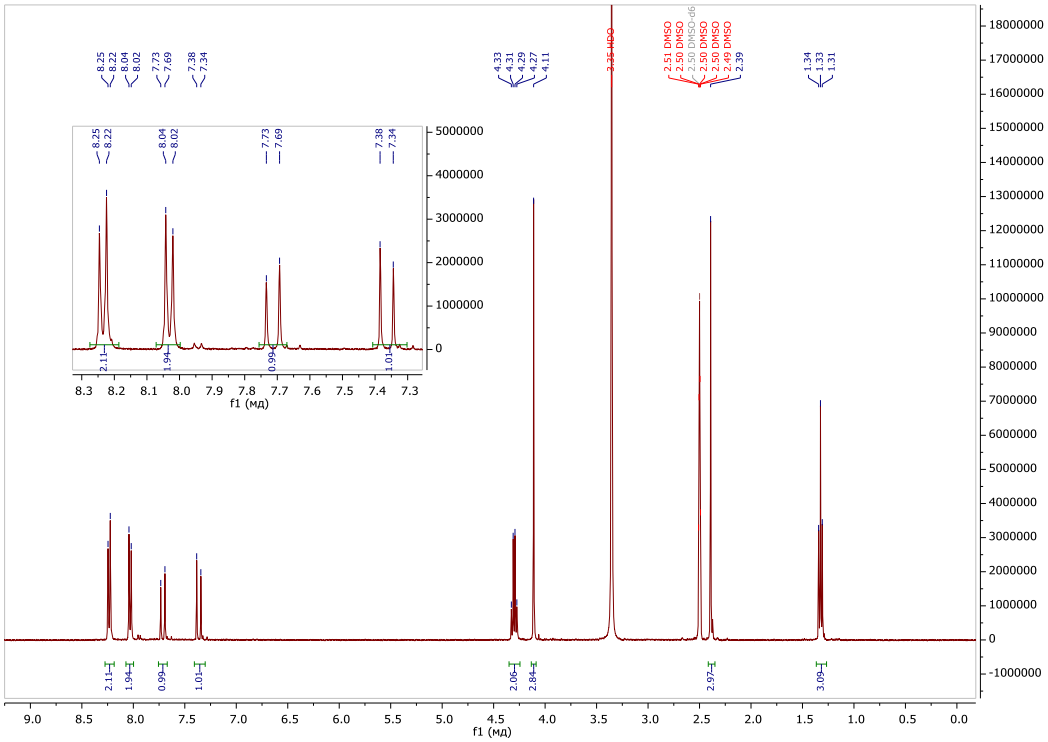


Fig. S 49. ^{1}H NMR spectrum of compound 4c (400 MHz, DMSO-d_6).

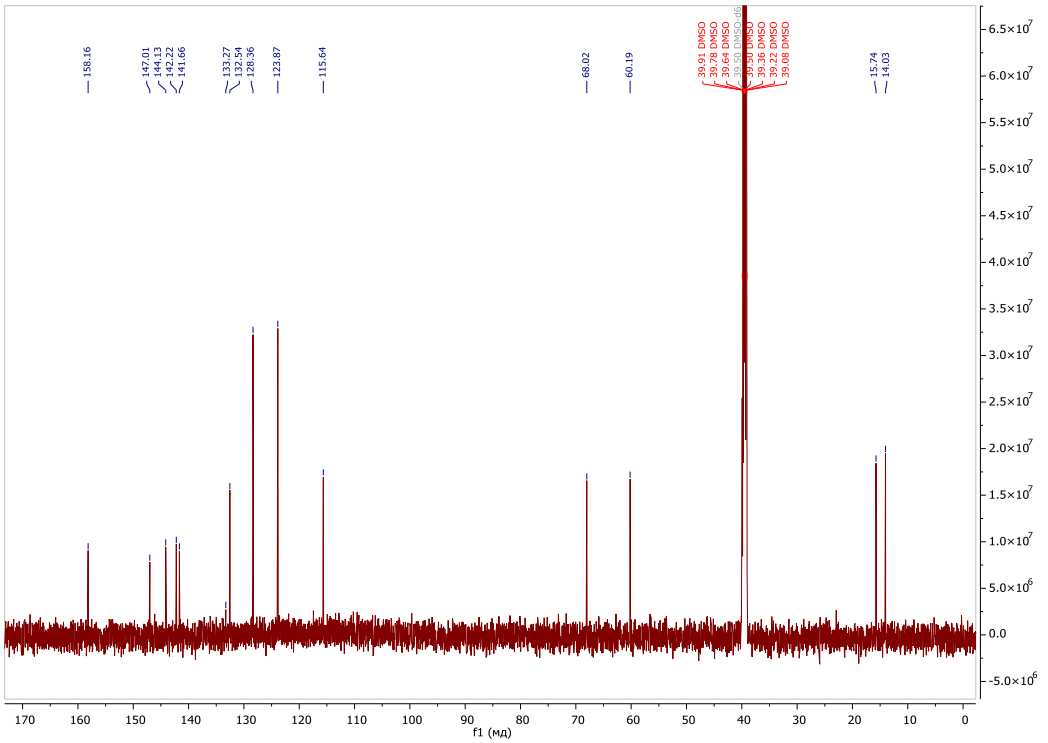
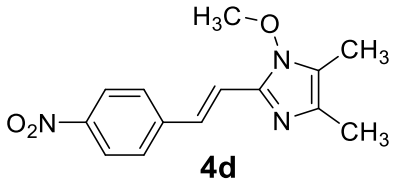


Fig. S 50. ^{13}C NMR spectrum of compound 4c (151 MHz, DMSO-d_6).

S4.12. 1-Methoxy-4,5-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole (**4d**).



4d

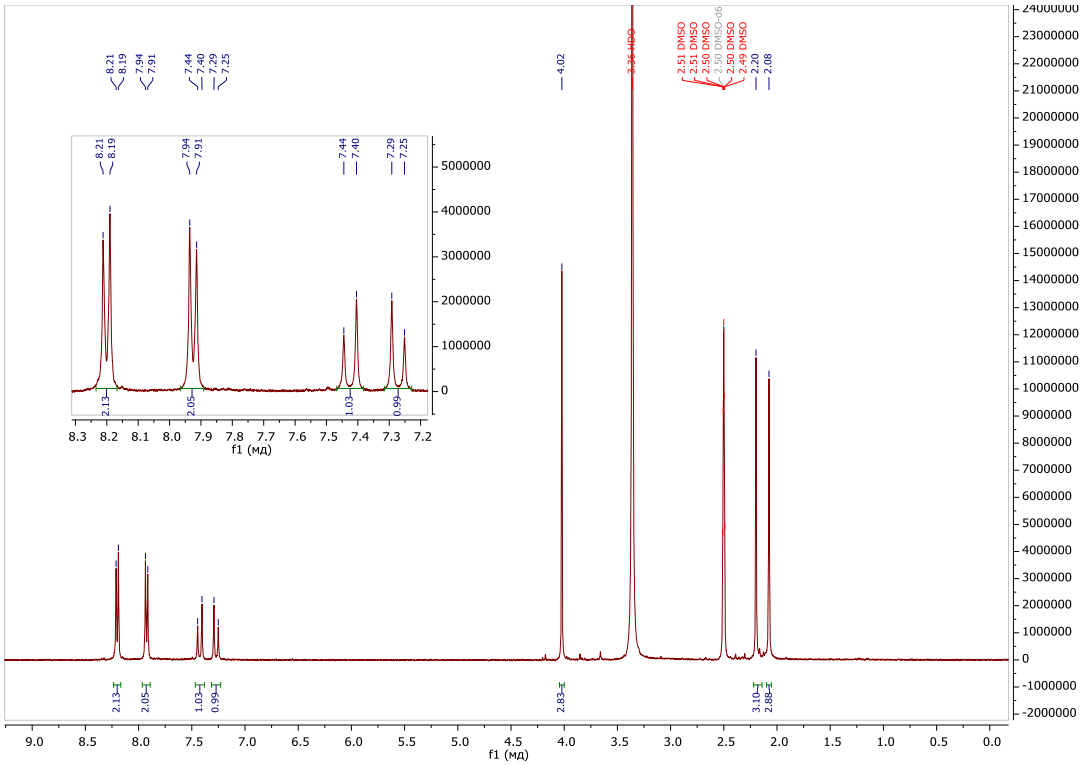


Fig. S 51. ^{1}H NMR spectrum of compound 4d (400 MHz, DMSO-d_6).

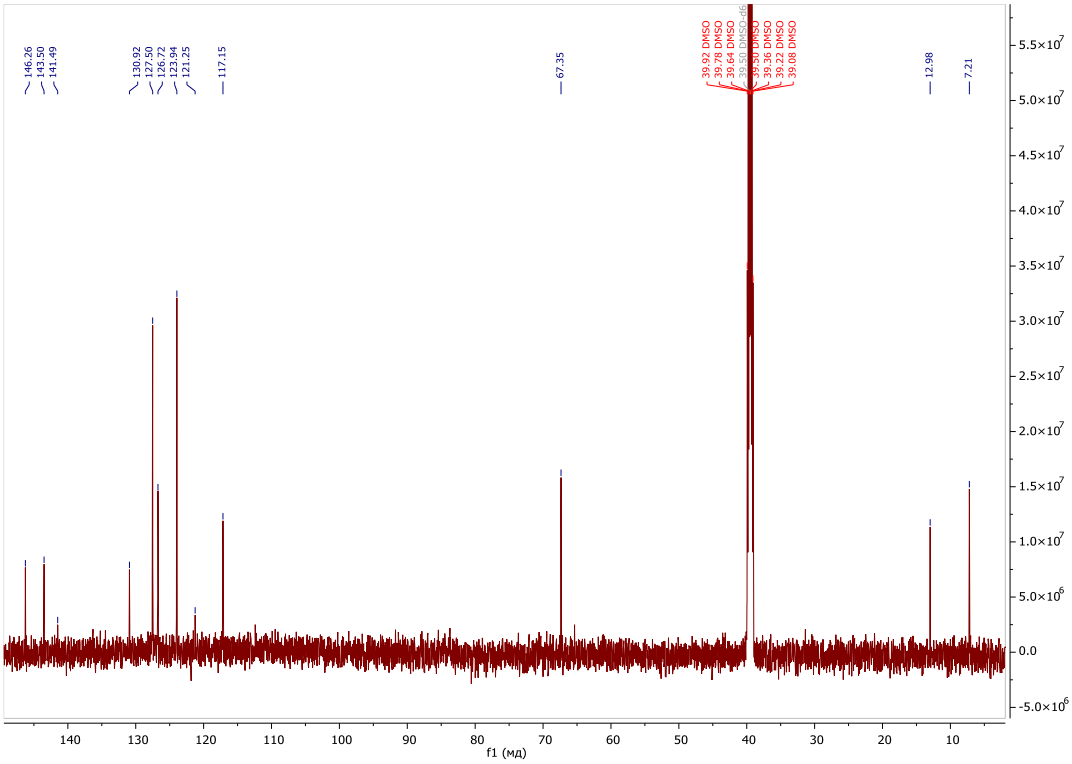
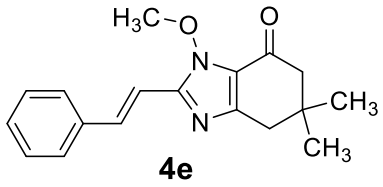


Fig. S 52. ^{13}C NMR spectrum of compound 4d (151 MHz, DMSO-d_6).

S4.13. 3-Methoxy-6,6-dimethyl-2-((*E*)-2-phenylethenyl)-3,5,6,7-tetrahydro-*4H*-benzimidazol-4-one (**4e**).



4e

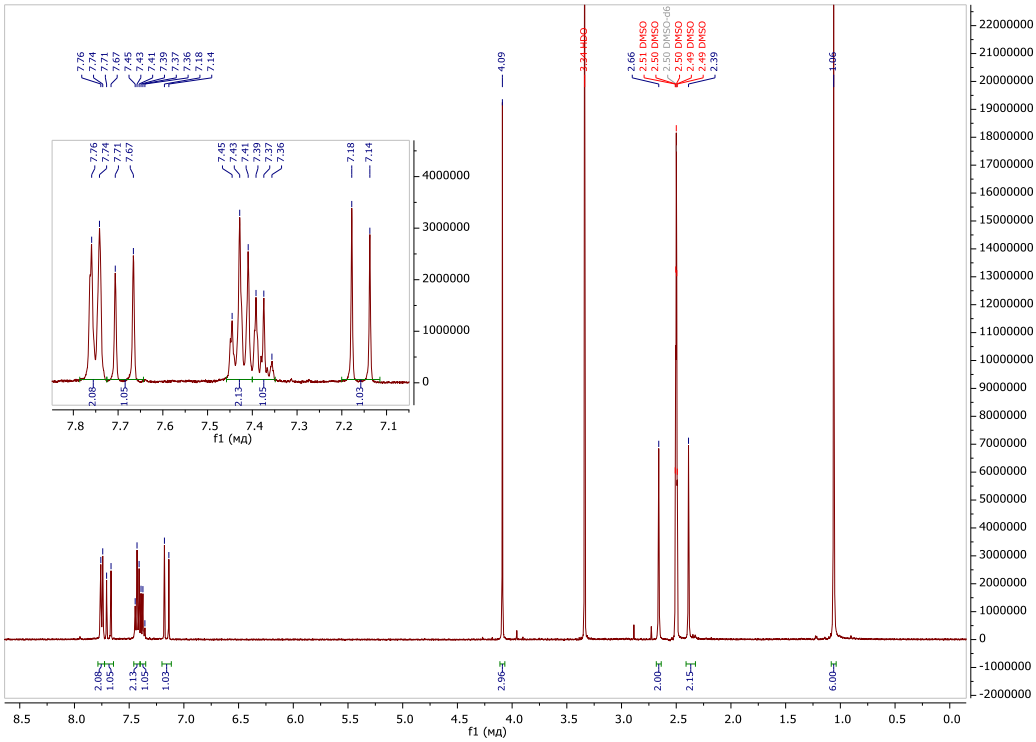


Fig. S 53. ^{1}H NMR spectrum of compound 4e (400 MHz, DMSO-*d*$_6$).

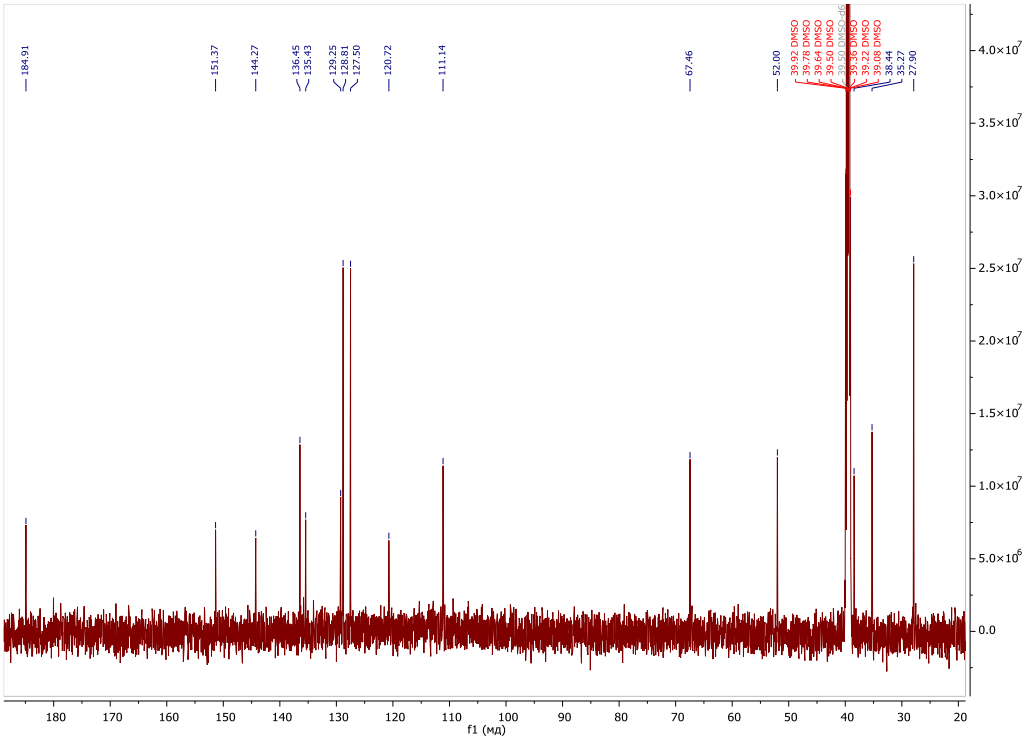
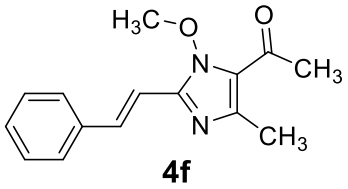


Fig. S 58. ^{13}C NMR spectrum of compound 4e (151 MHz, DMSO-*d*$_6$).

S4.14. 1-(1-Methoxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazol-5-yl)ethanone (**4f**).



4f

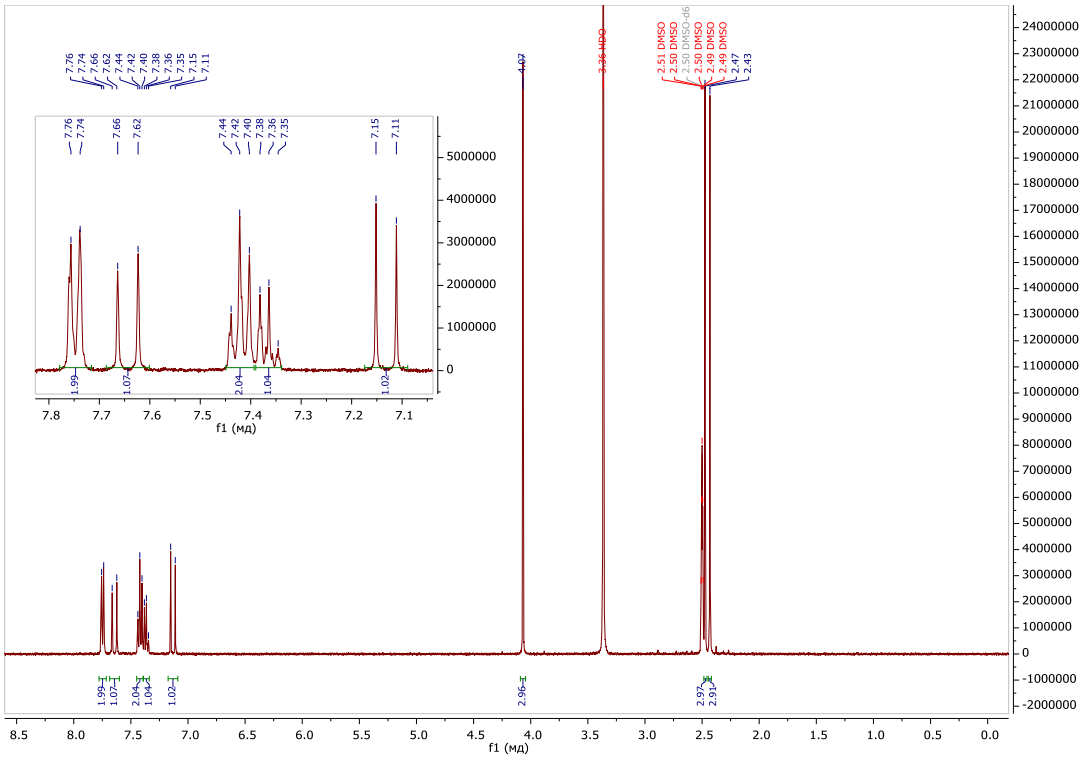


Fig. S 59. ^{1}H NMR spectrum of compound 4f (400 MHz, DMSO-d_6).

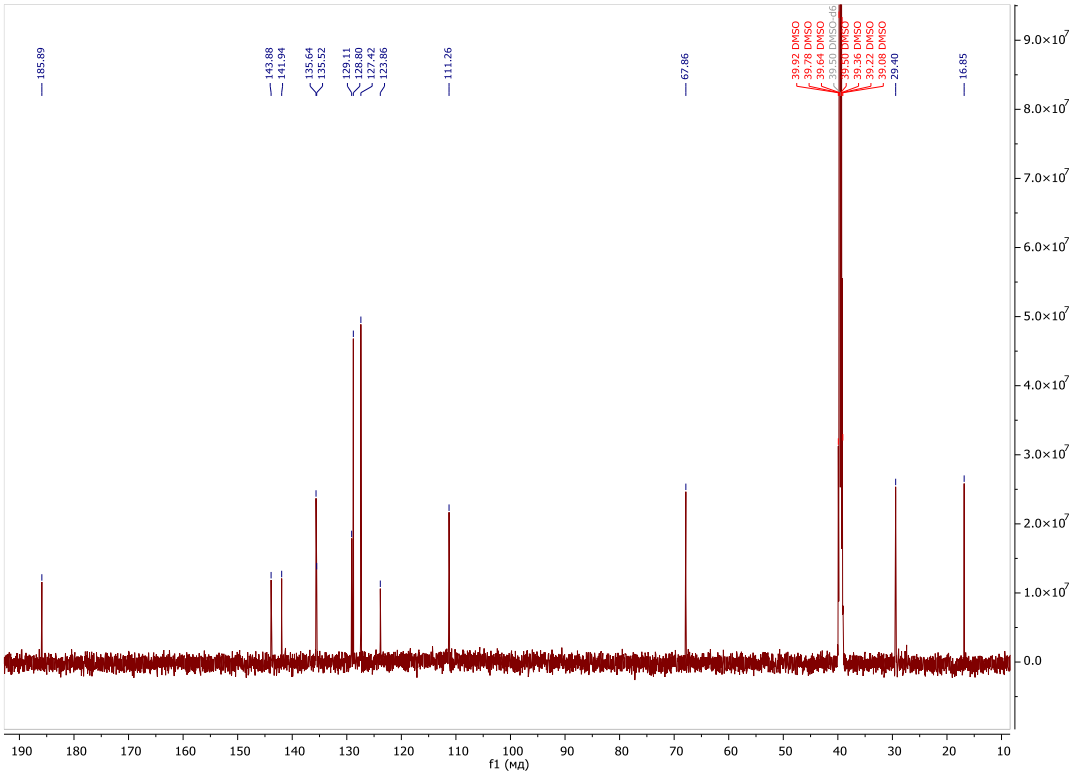
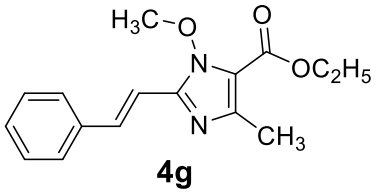


Fig. S 54. ^{13}C NMR spectrum of compound 4f (151 MHz, DMSO-d_6).

S4.15. Ethyl 1-methoxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole-5-carboxylate (**4g**).



4g

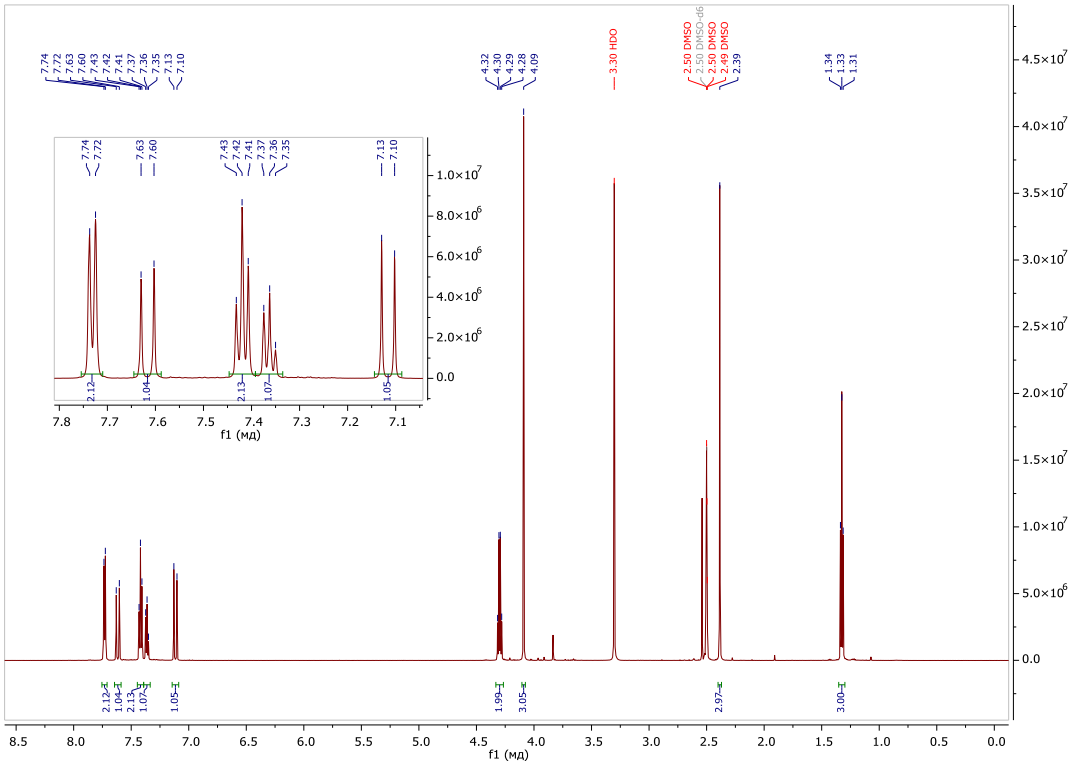


Fig. S 55. ^{1}H NMR spectrum of compound 4g (600 MHz, DMSO-*d*$_6$).

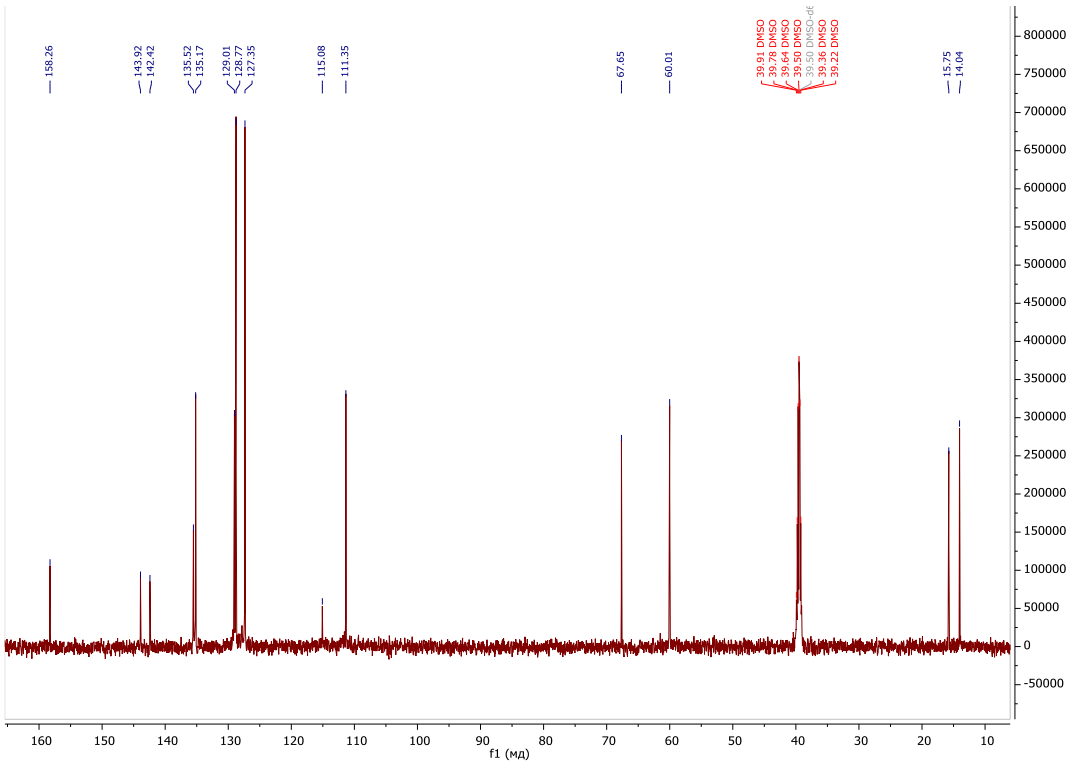
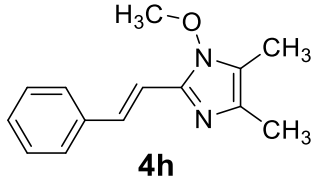


Fig. S 56. ^{13}C NMR spectrum of compound 4g (151 MHz, DMSO-*d*$_6$).

S4.16. 1-Methoxy-4,5-dimethyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole (**4h**).



4h

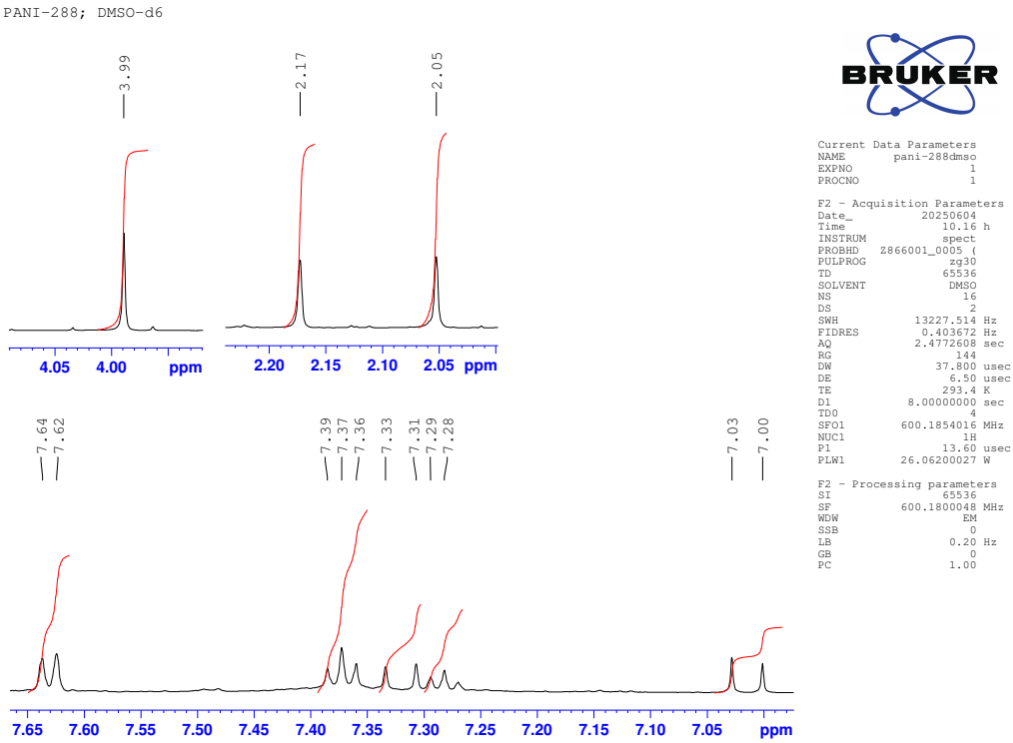


Fig. S 63. ^{1}H NMR spectrum of compound 4h (600 MHz, DMSO-d_6).

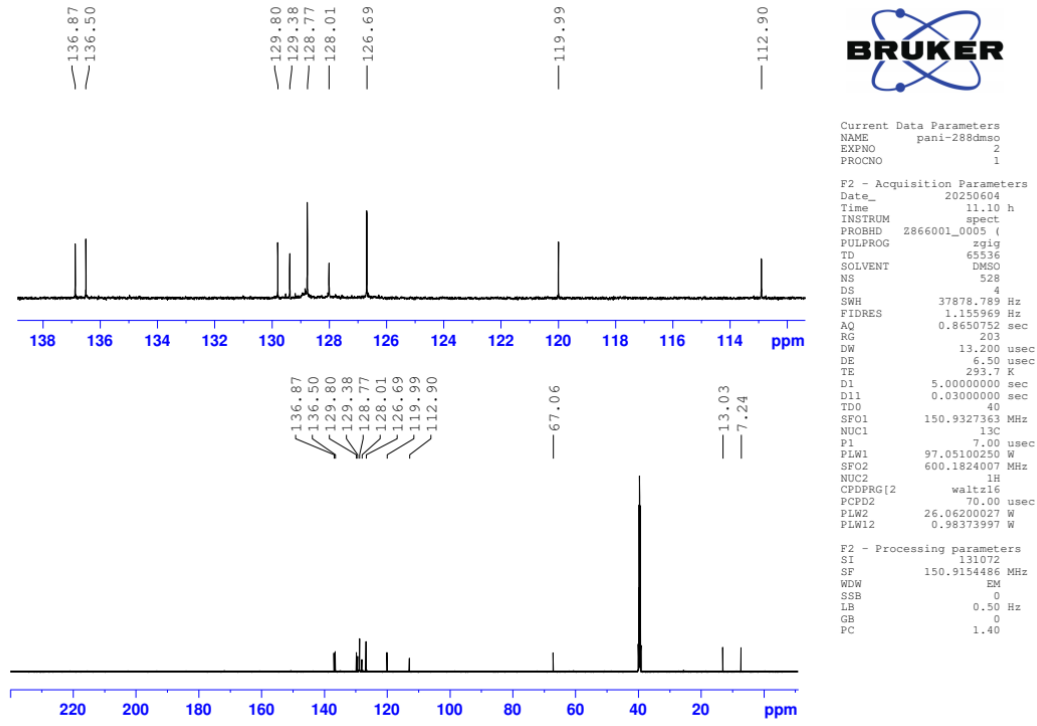


Fig. S 64. ^{13}C NMR spectrum of compound 4h (151 MHz, DMSO-d_6).

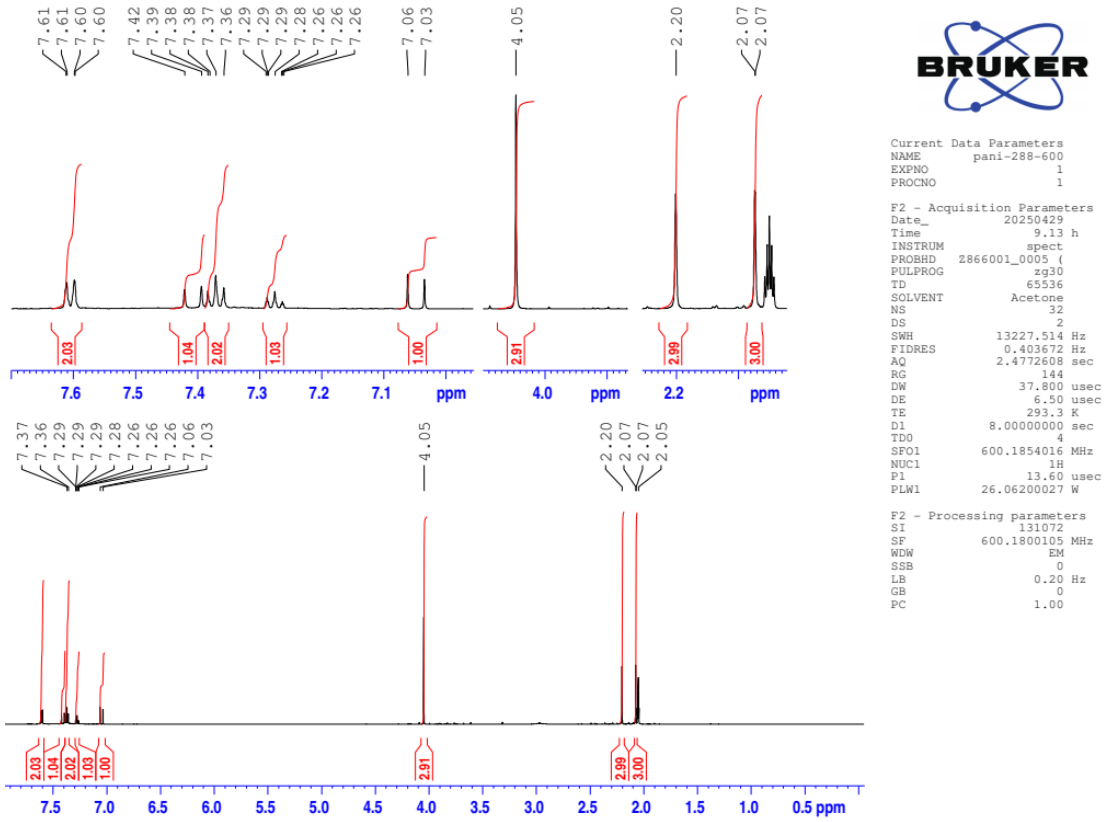


Fig. S 57. ^{1}H NMR spectrum of compound 4h (600 MHz, acetone-d_6).

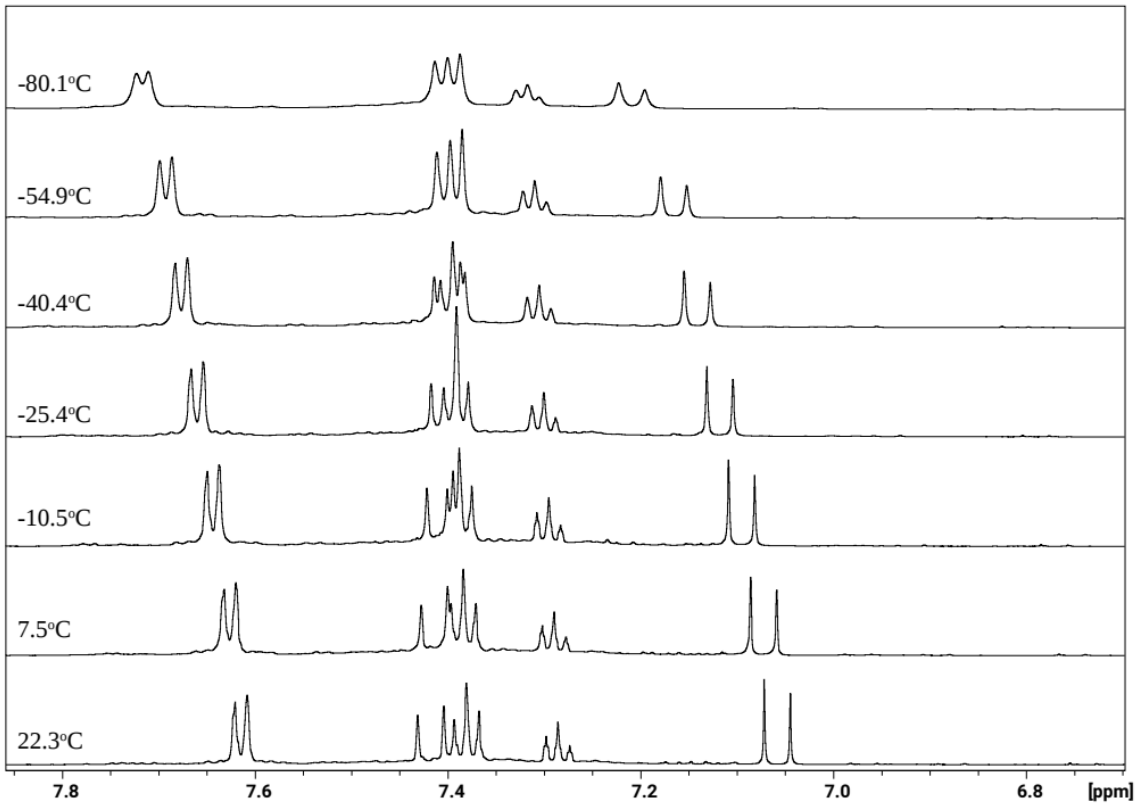


Fig. S 58. ^{1}H NMR spectra of compound 4h registered at different temperatures (600 MHz, acetone-d_6, range 7.0-9.0 ppm).

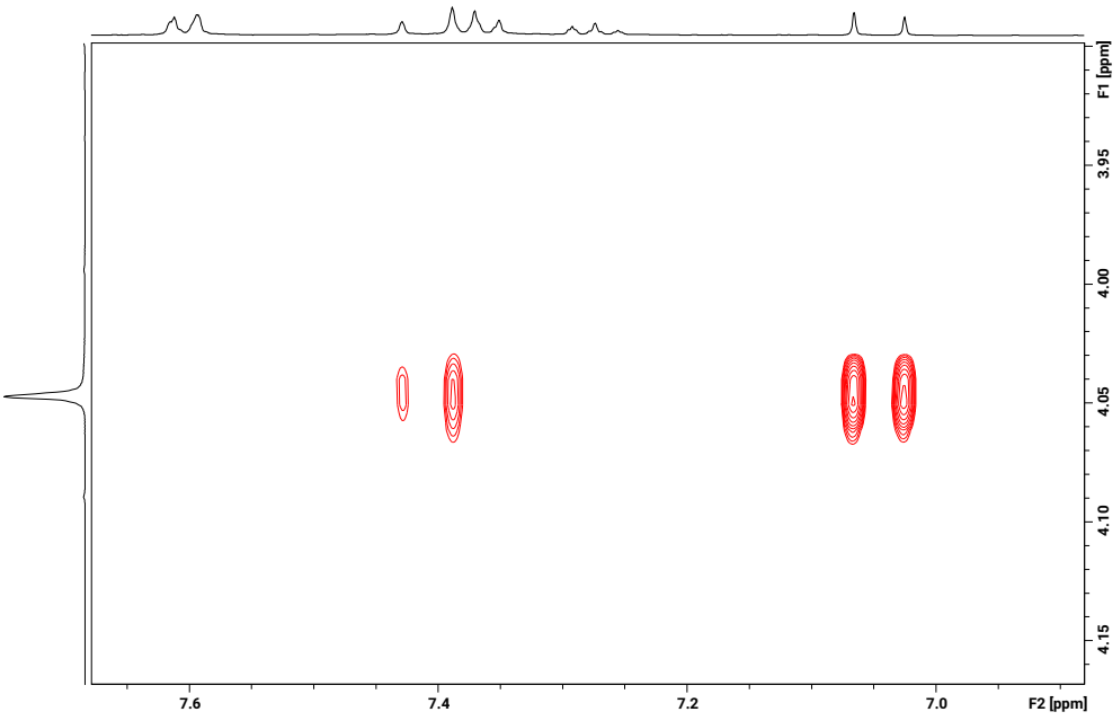


Fig. S 59. Part of ^{1}H-^{1}H NOESY spectrum of compound 4h (400 MHz, acetone-d_6, mixing time – 0.8 s).

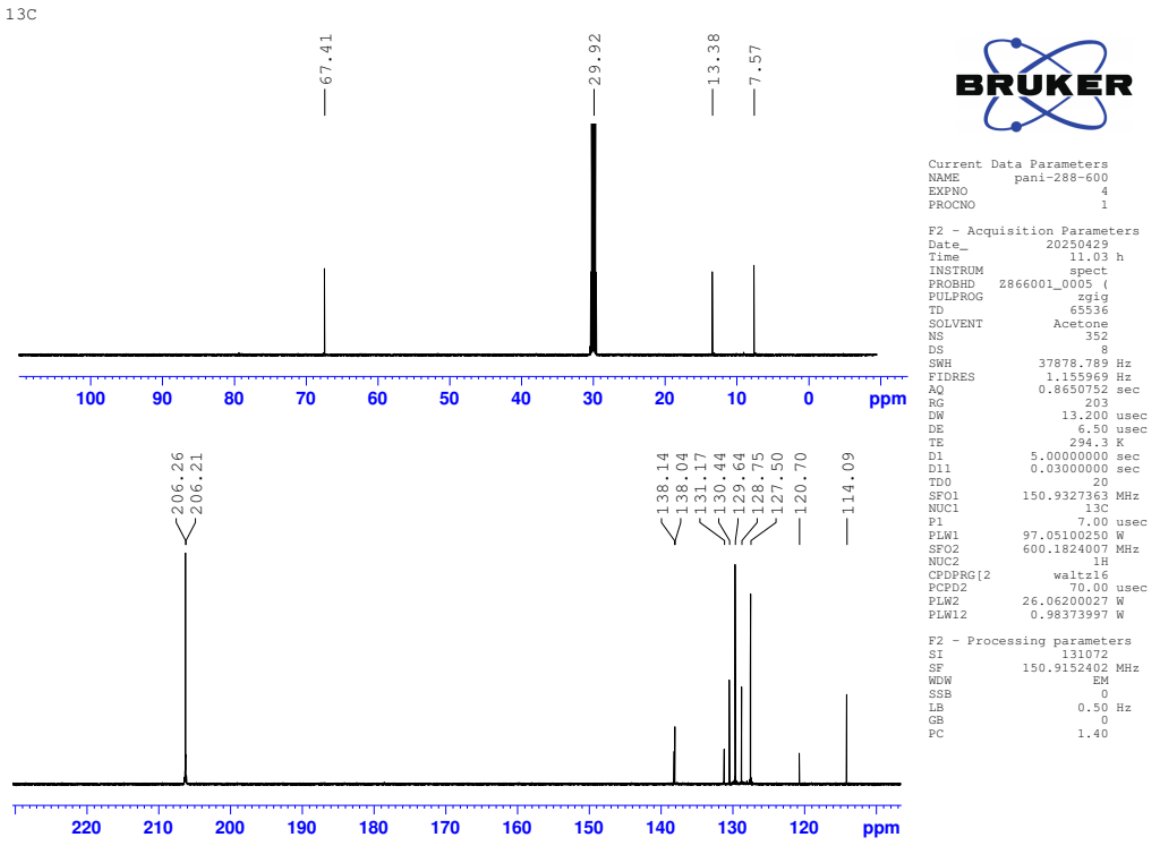


Fig. S 68. ^{13}C NMR spectrum of compound 4h (151 MHz, acetone-d_6).

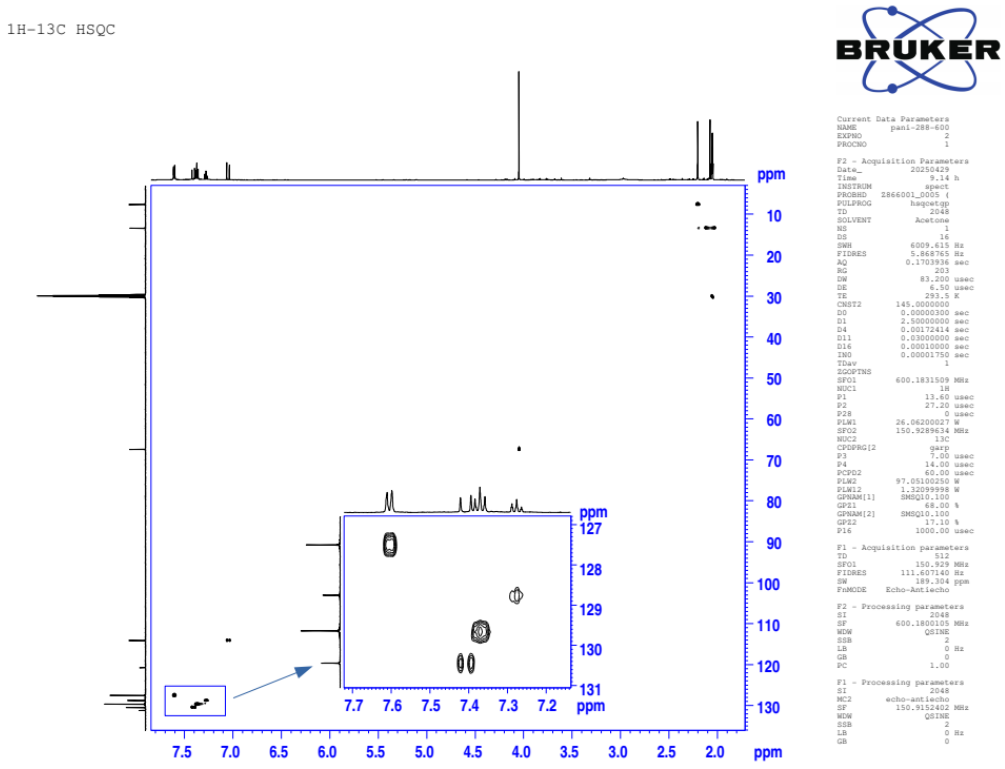


Fig. S 69. ^{1}H-^{13}C HSQC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

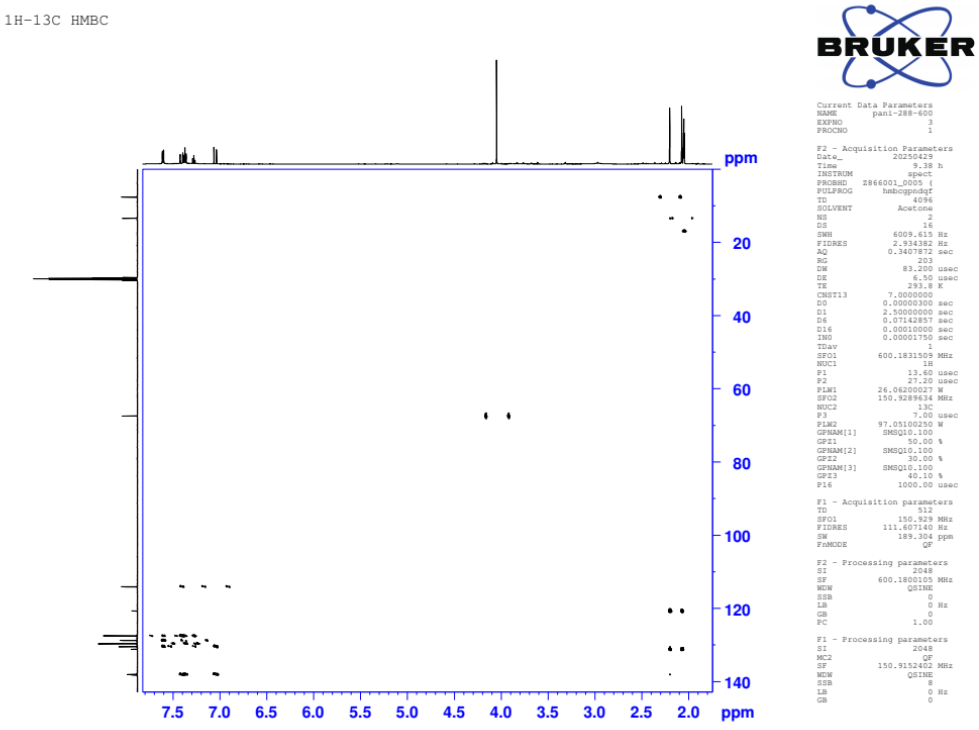


Fig. S 60. ^{1}H-^{13}C HMBC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

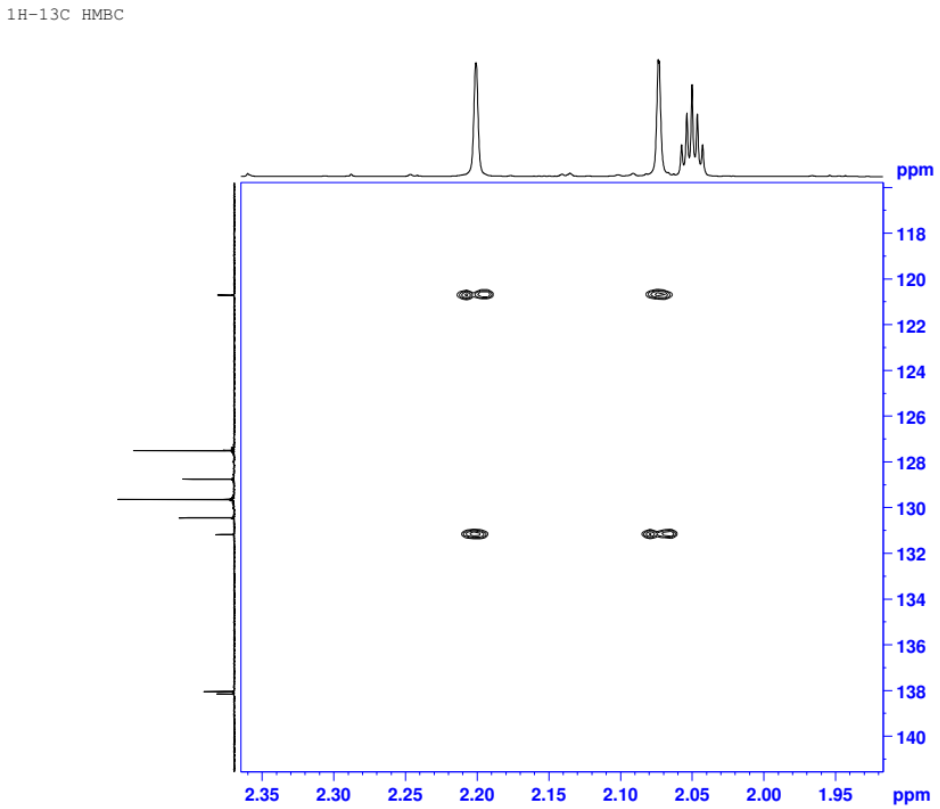


Fig. S 61. Part of ^{1}H-^{13}C HMBC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

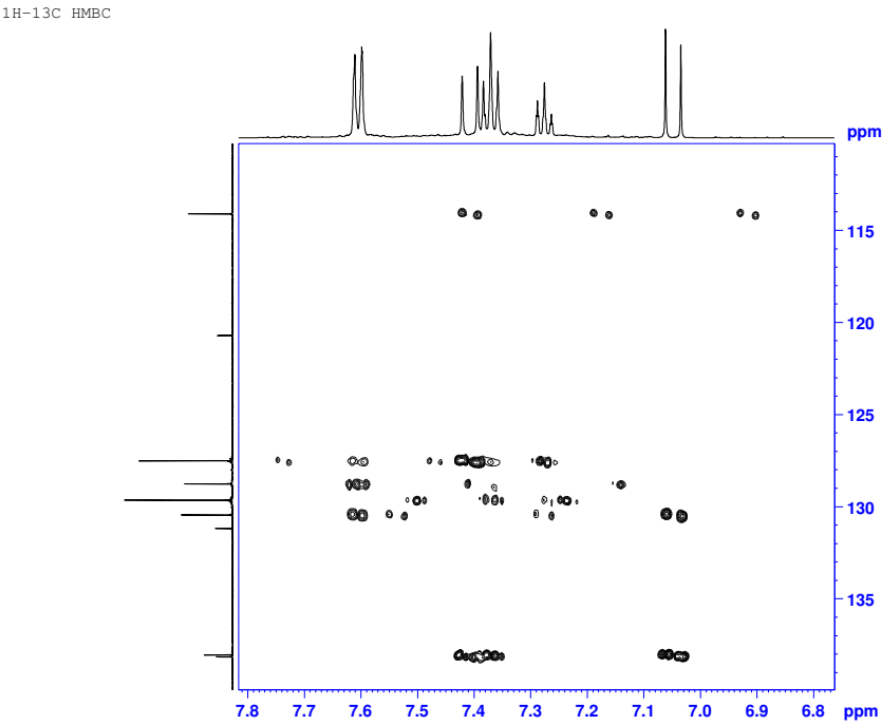


Fig. S 62. Part of ^{1}H-^{13}C HMBC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

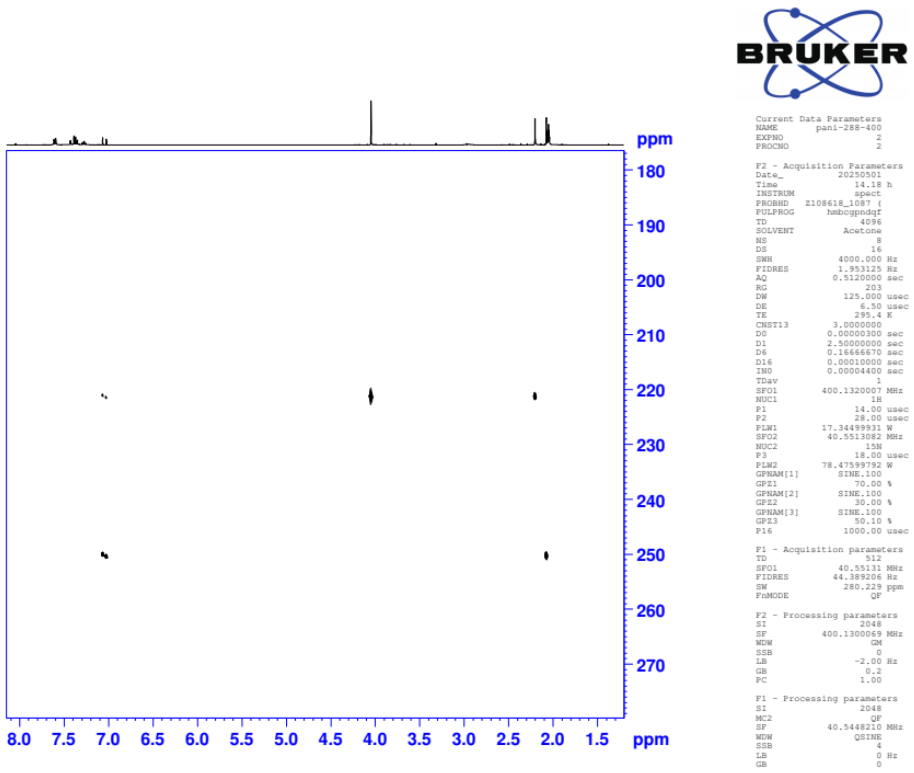


Fig. S 63. ^{1}H-^{15}N HMBC spectrum of compound 4h (400 MHz – ^{1}H, 41 MHz – ^{15}N, acetone-d_6).

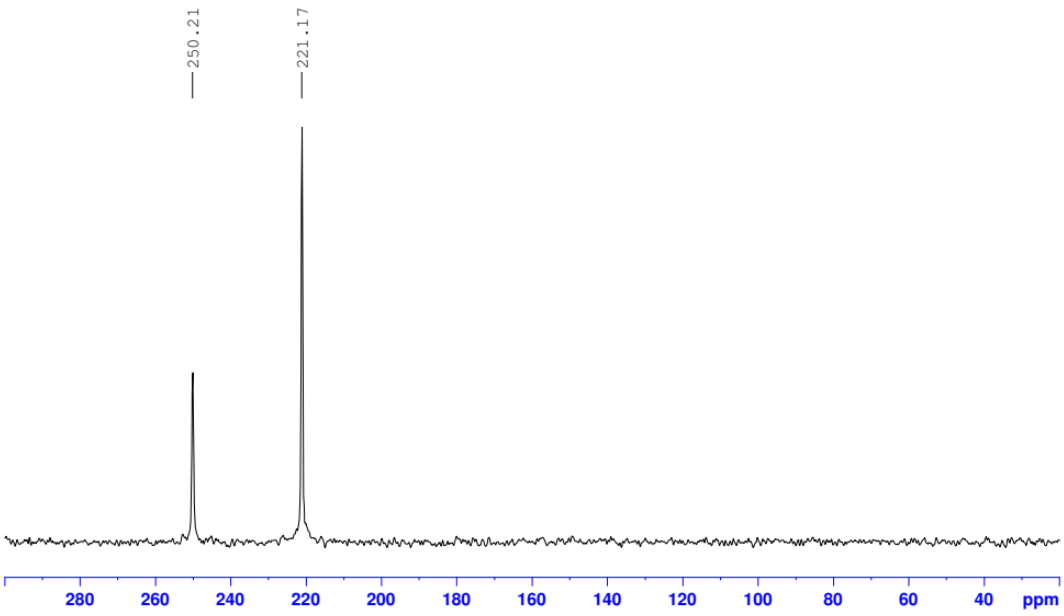


Fig. S 64. ^{15}N NMR spectrum of compound 4h (41 MHz, acetone-d_6), obtained by projection from ^{1}H-^{15}N HMBC spectrum.

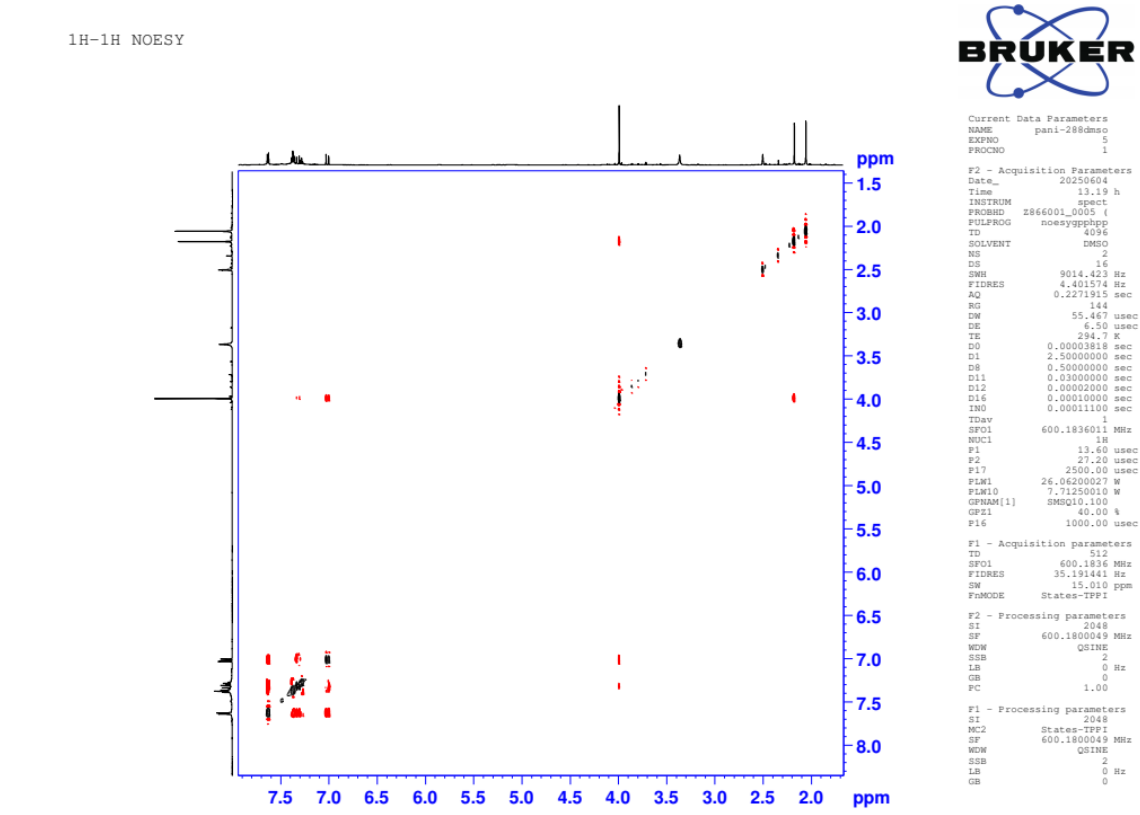


Fig. S 65. ^{1}H-^{1}H NOESY spectrum of compound 4h (600 MHz, DMSO-d_6, mixing time – 0.5 s).

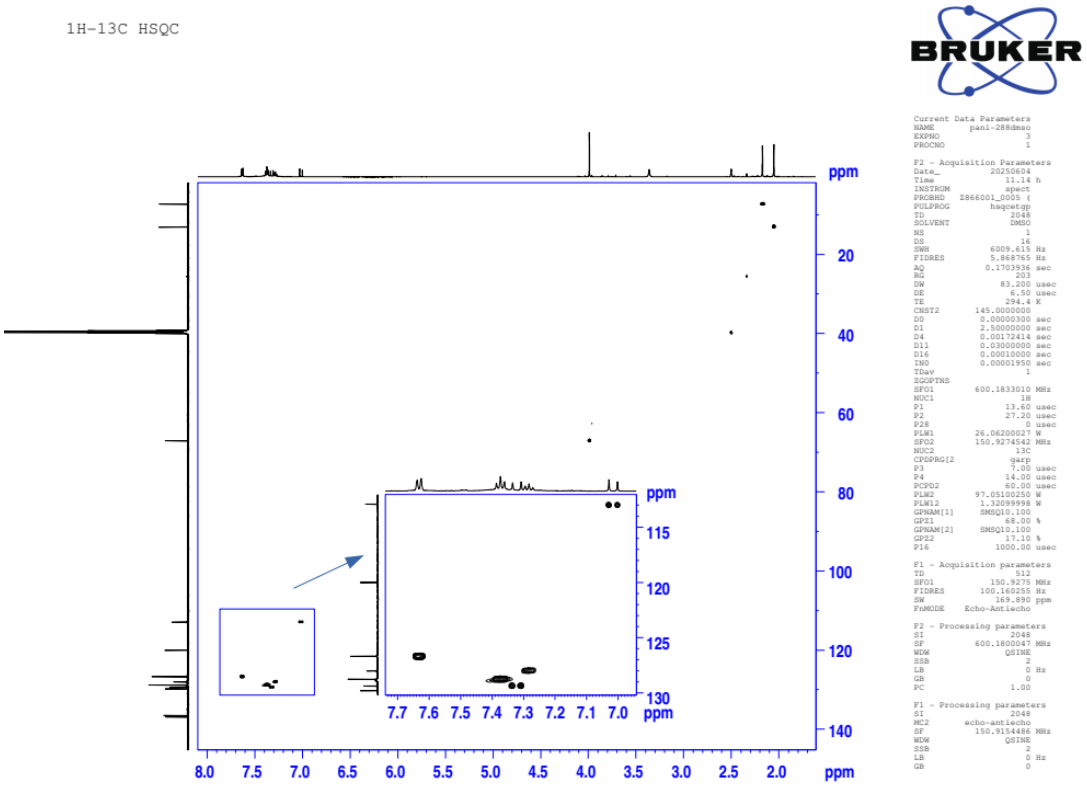


Fig. S 76. ^{1}H-^{13}C HSQC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-d_6).

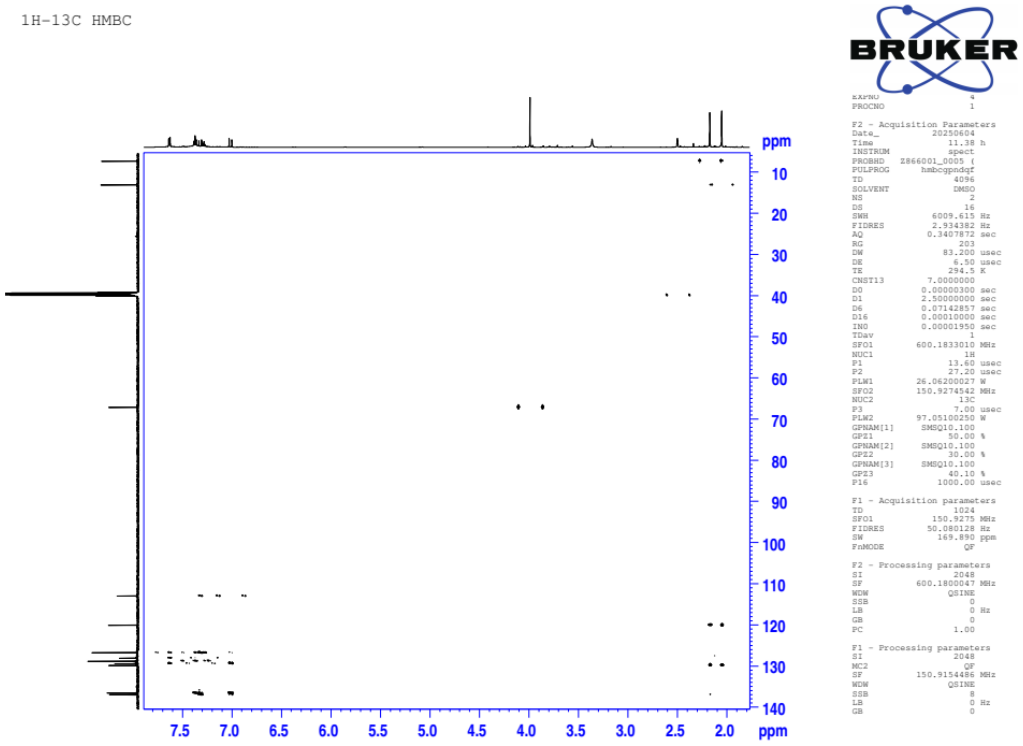


Fig. S 77. ^{1}H-^{13}C HMBC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-*d*$_6$).

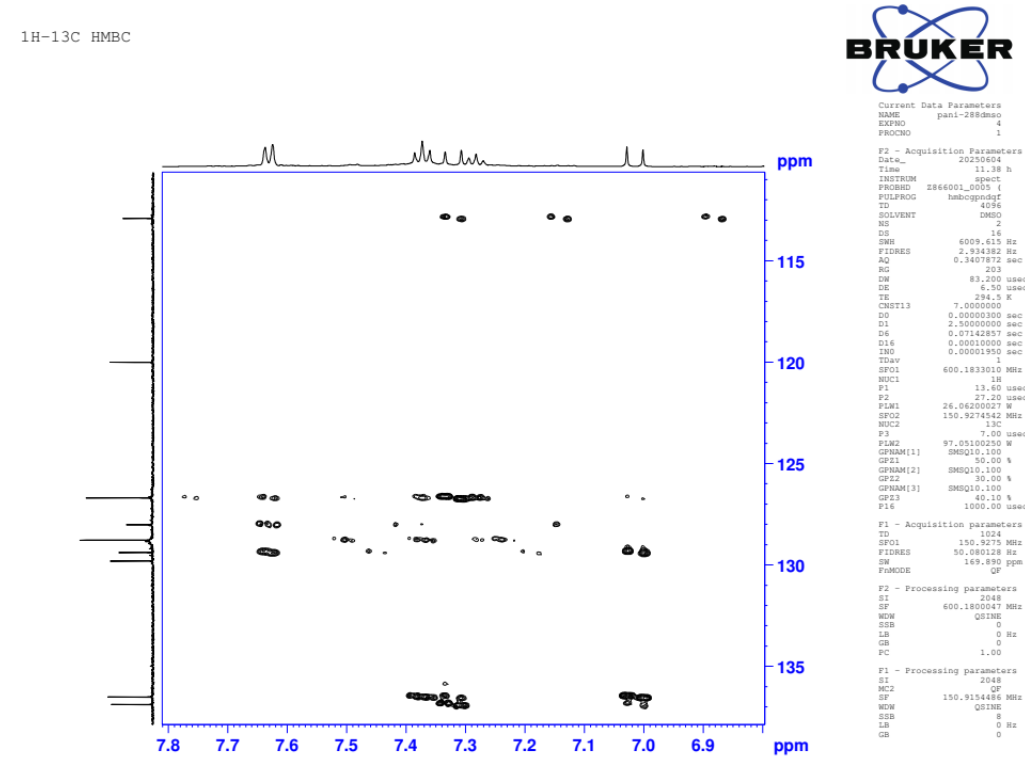


Fig. S 78. Part of ^{1}H-^{13}C HMBC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-*d*$_6$).

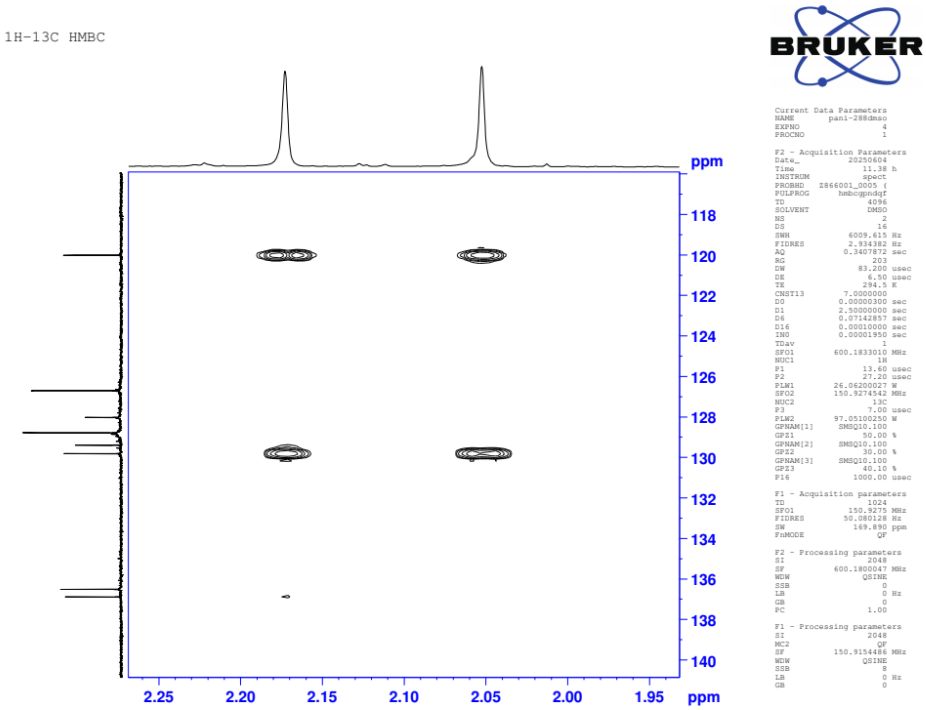
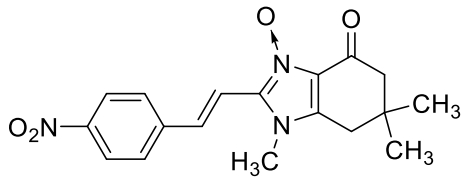


Fig. S 79. Part of ^{1}H-^{13}C HMBC spectrum of compound 4h (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-d_6).

S4.17. 1,6,6-Trimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-4-oxo-4,5,6,7-tetrahydro-*1H*-benzimidazole 3-oxide (**6a**).



6a

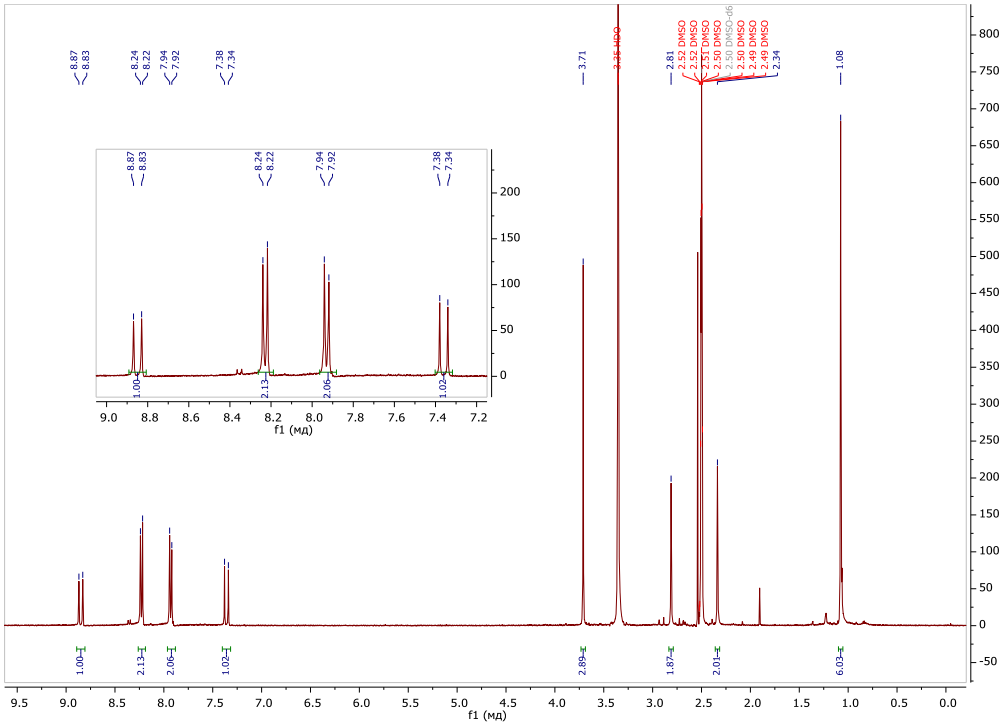


Fig. S 66. ^{1}H NMR spectrum of compound 6a (400 MHz, DMSO-d_6).

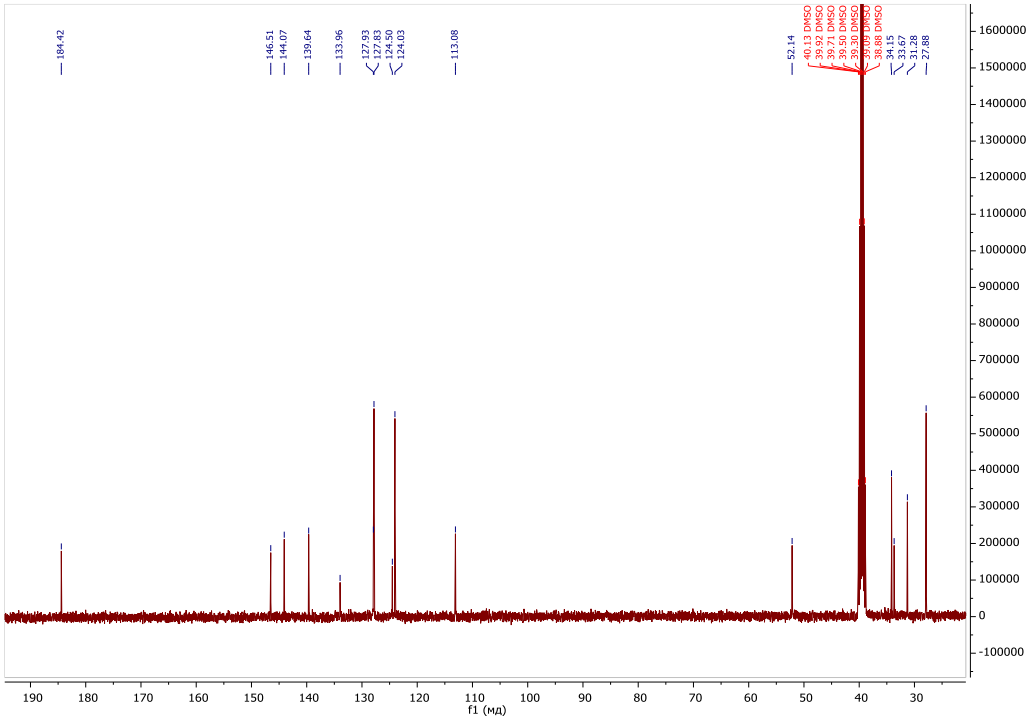
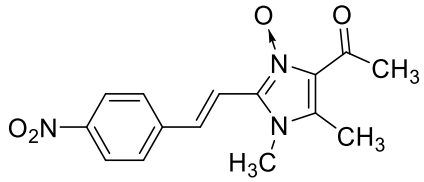


Fig. S 67. ^{13}C NMR spectrum of compound 6a (101 MHz, DMSO-d_6).

S4.18. 4-Acetyl-1,5-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole 3-oxide (**6b**).



6b

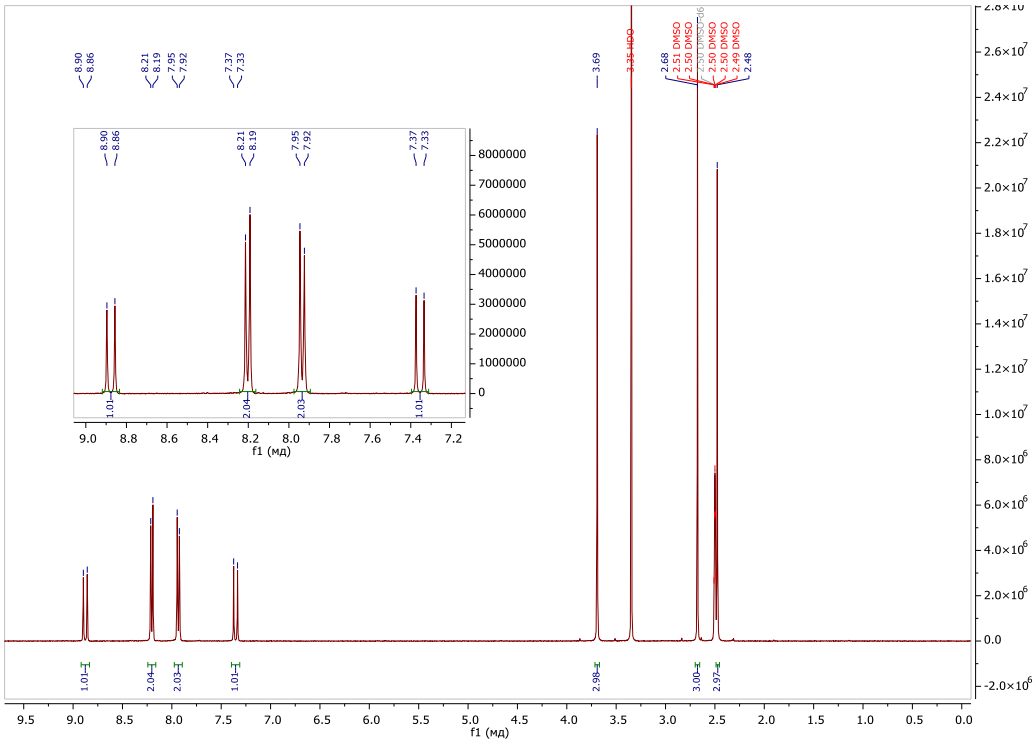


Fig. S 68. ^{1}H NMR spectrum of compound 6b (400 MHz, DMSO-d_6).

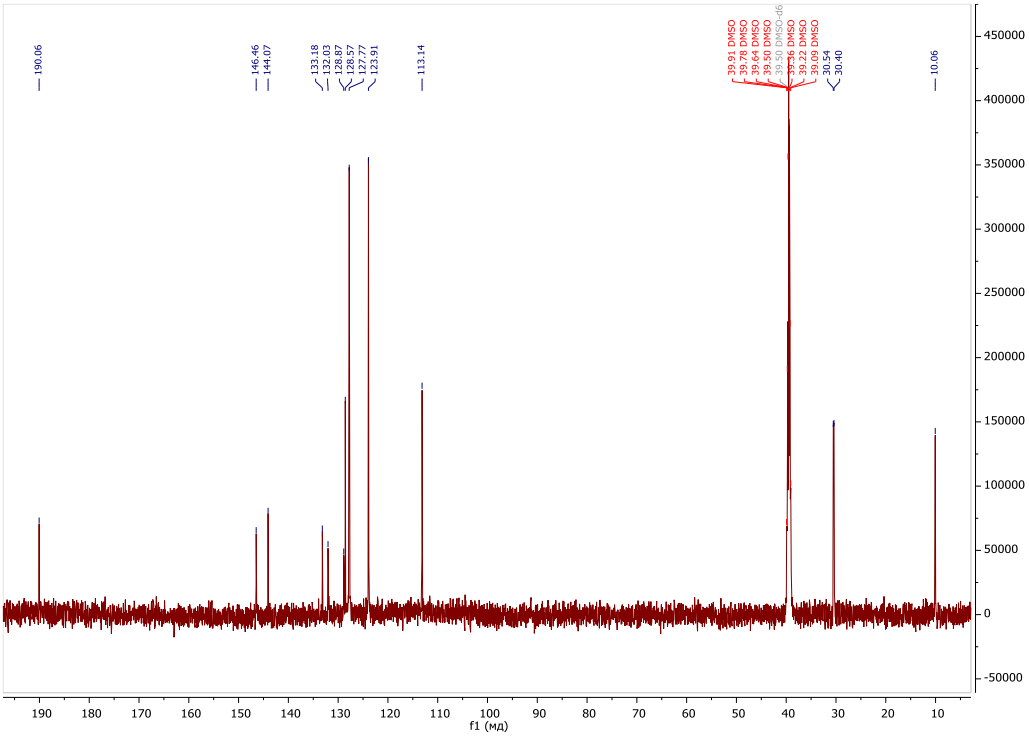


Fig. S 69. ^{13}C NMR spectrum of compounds 6b (151 MHz, DMSO-d_6).

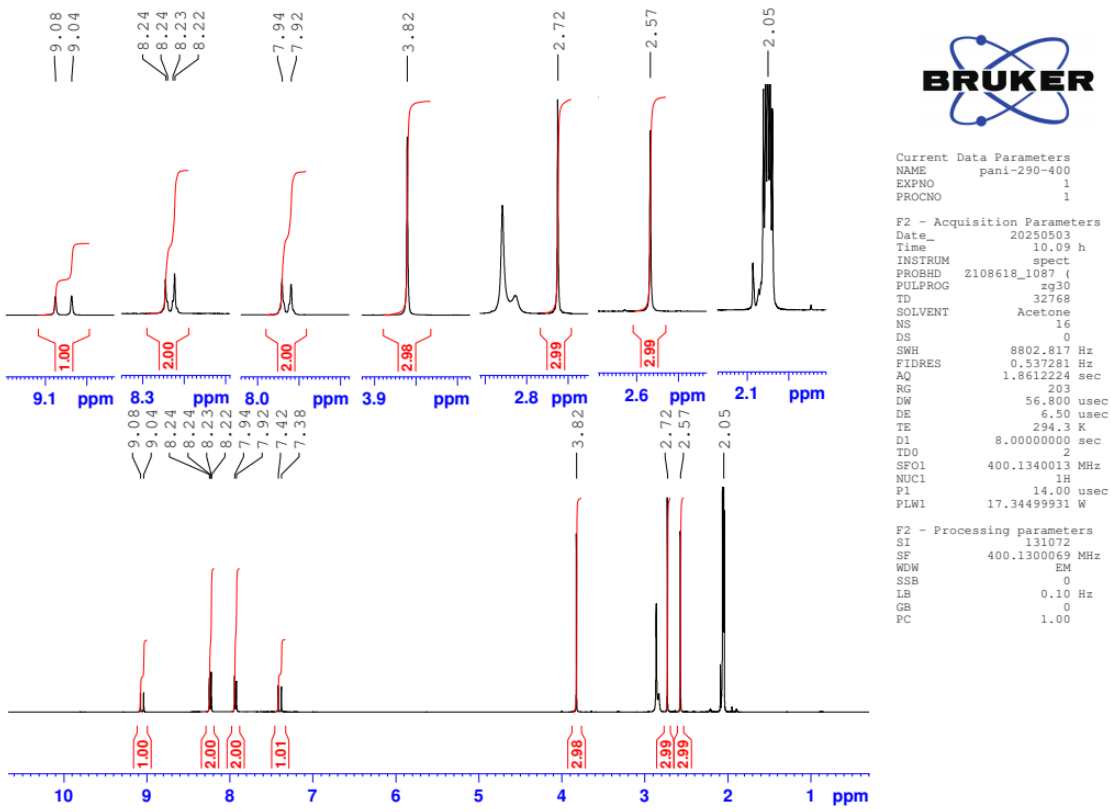


Fig. S 70. ^{1}H NMR spectrum of compound 6b (400 MHz, acetone-d_6).

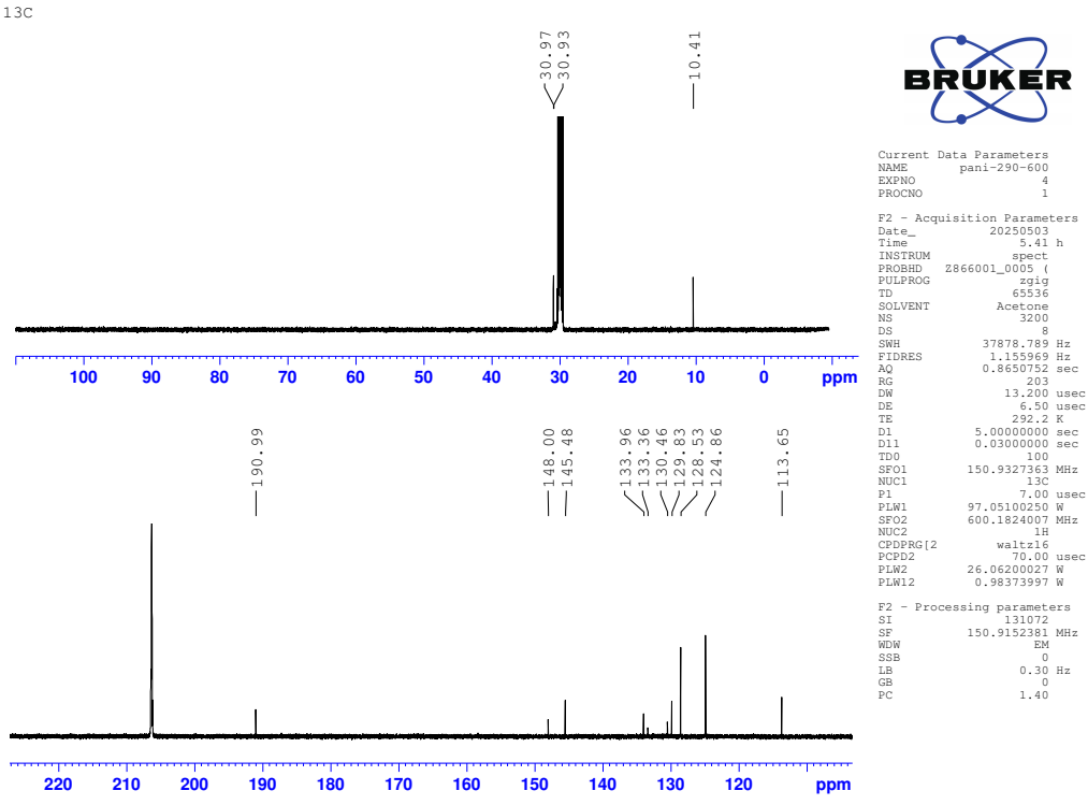


Fig. S 85. ^{13}C NMR spectrum of compound 6b (151 MHz, acetone-d_6).

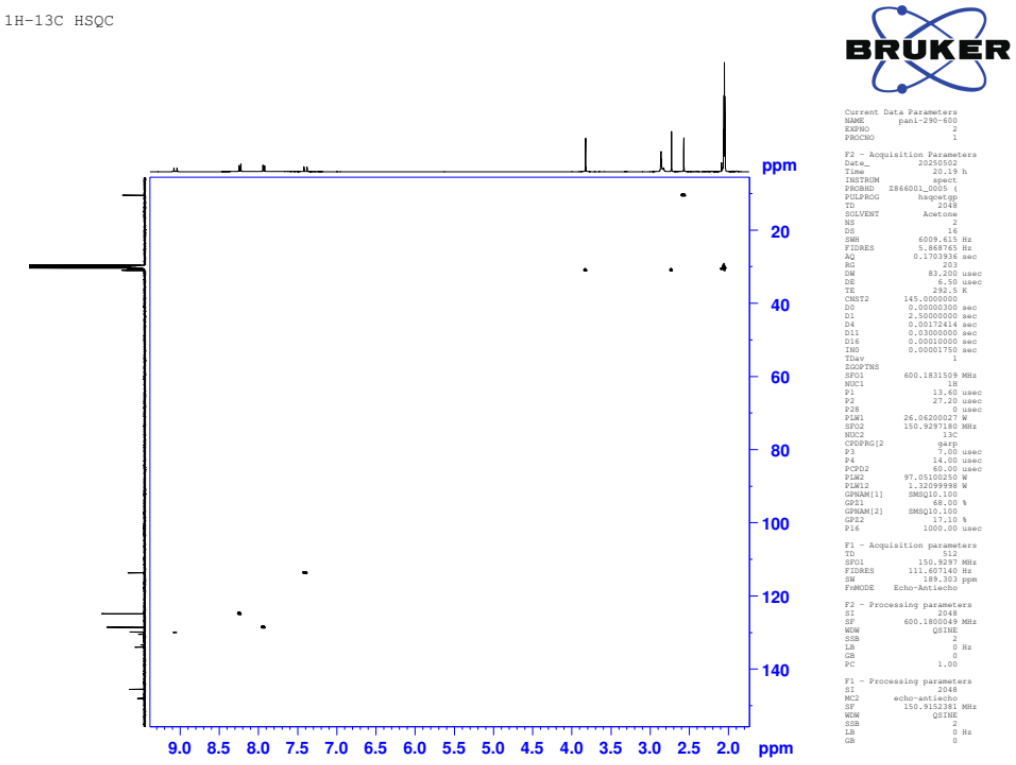


Fig. S 86. ^{1}H-^{13}C HSQC spectrum of compound 6b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

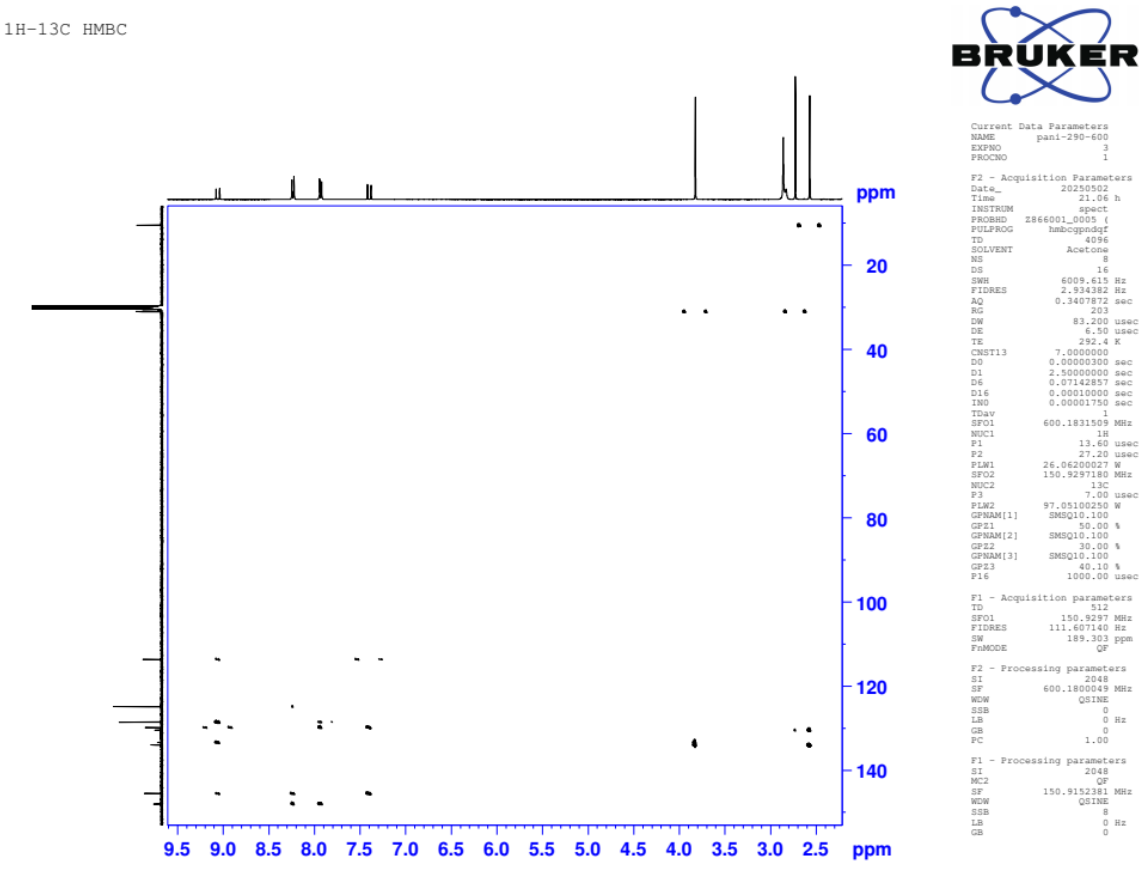


Fig. S 87. ^{1}H-^{13}C HMBC spectrum of compound 6b (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

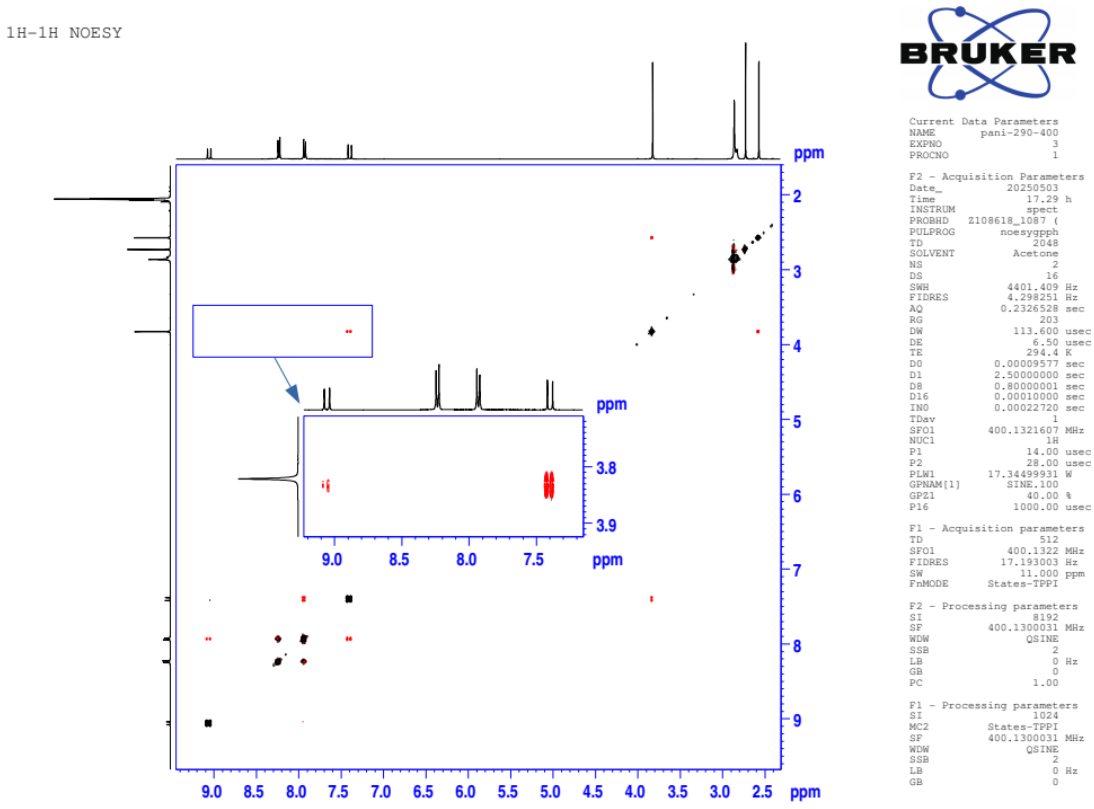


Fig. S 71. ^{1}H-^{1}H NOESY spectrum of compound 6b (400 MHz, acetone-d_6).

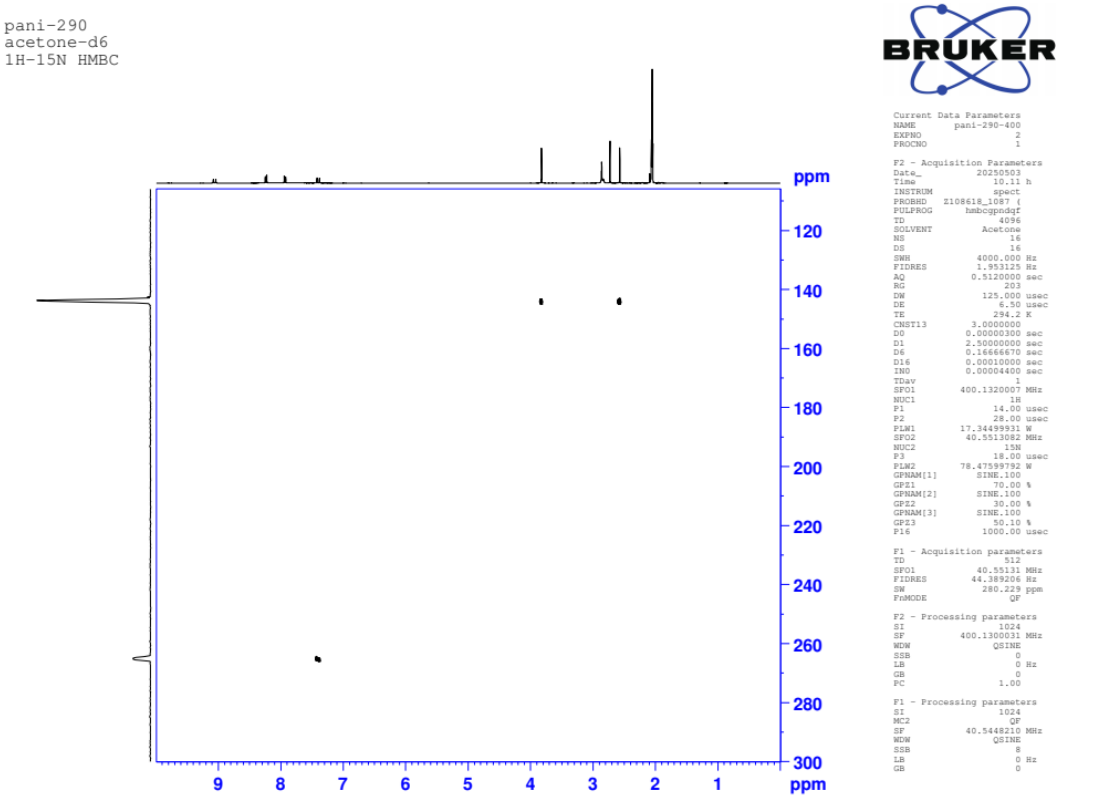
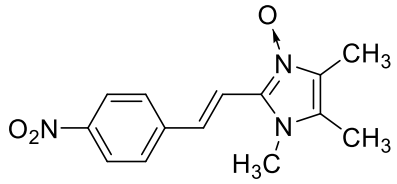


Fig. S 72. ^{1}H-^{15}N HMBC spectrum of compound 6b (400 MHz -^{1}H, 41 MHz – ^{15}N, acetone-d_6).

S4.19. 1,4,5-Trimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole 3-oxide (**6c**).



6c

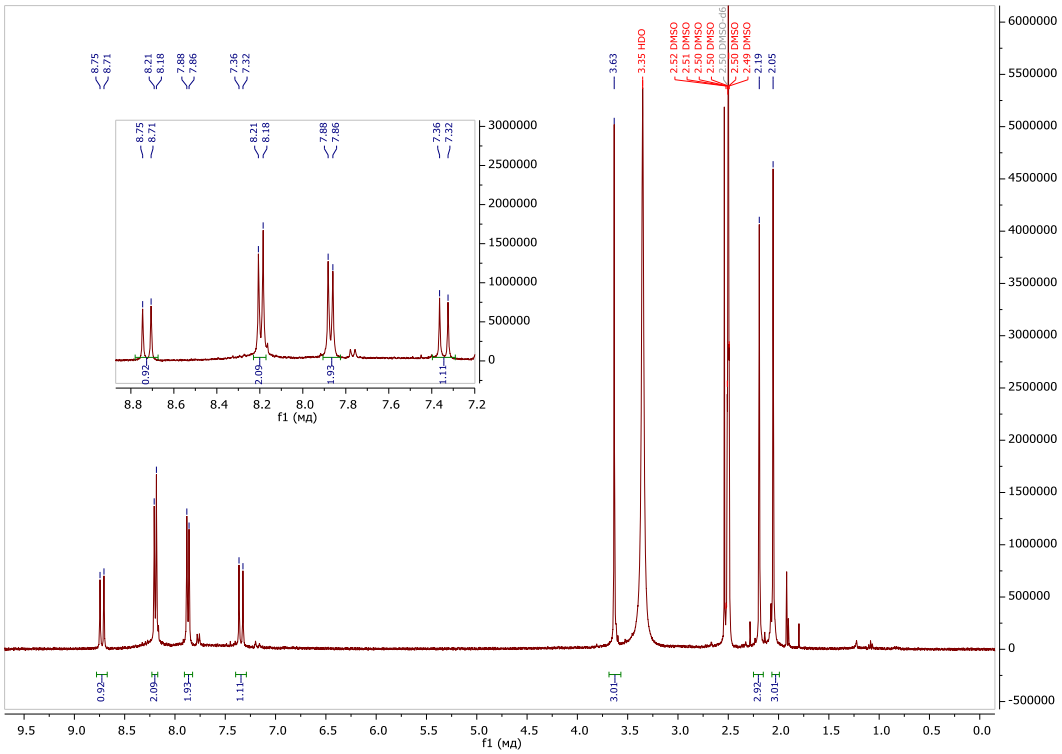


Fig. S 73. ^{1}H NMR spectrum of compound 6c (400 MHz, DMSO-*d*$_6$).

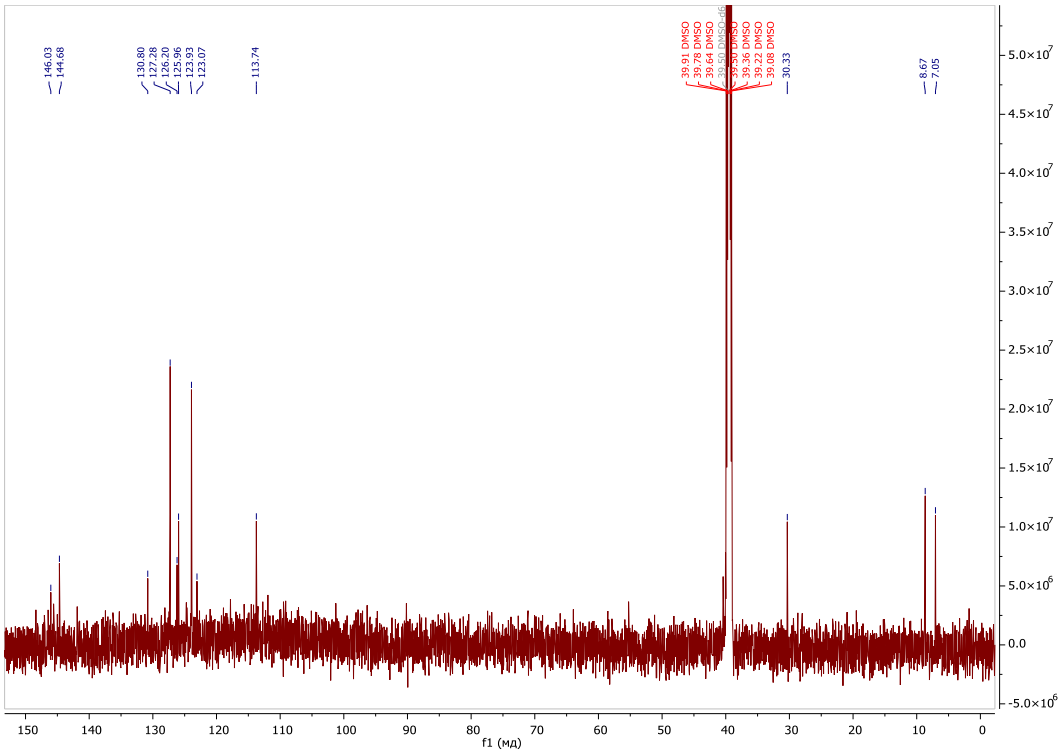
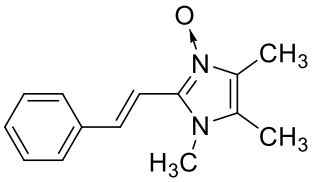


Fig. S 74. ^{13}C NMR spectrum of compound 6c (151 MHz, DMSO-*d*$_6$).

S4.20. 1,4,5-Trimethyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole 3-oxide (**6d**).



6d

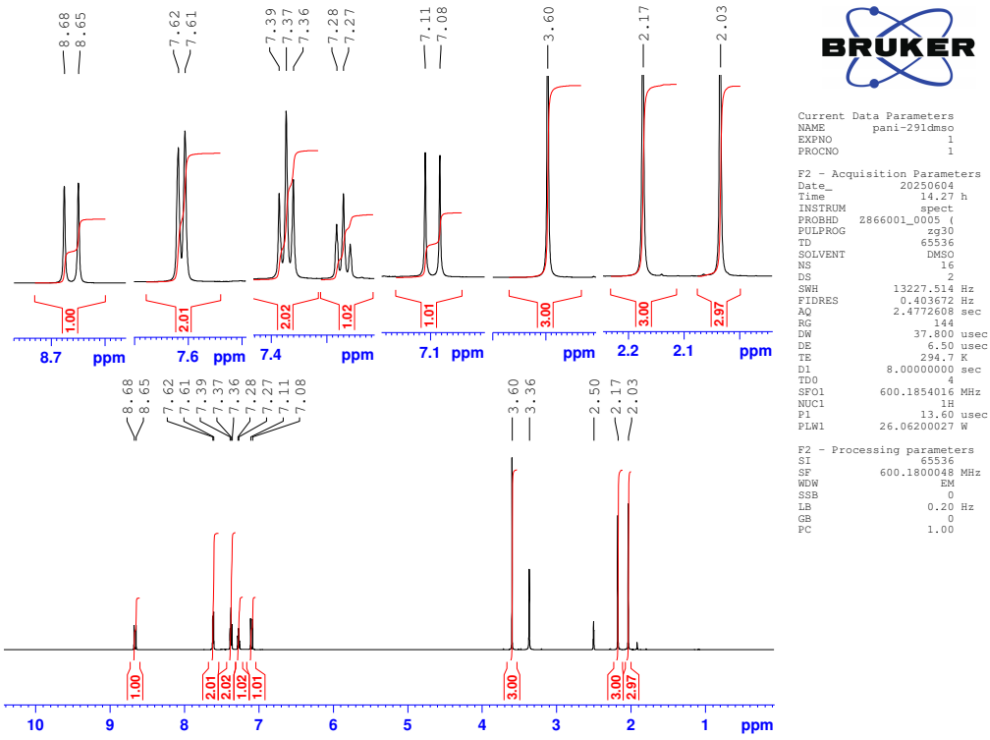


Fig. S 75. ^{1}H NMR spectrum of compound 6d (600 MHz, DMSO-d_6).

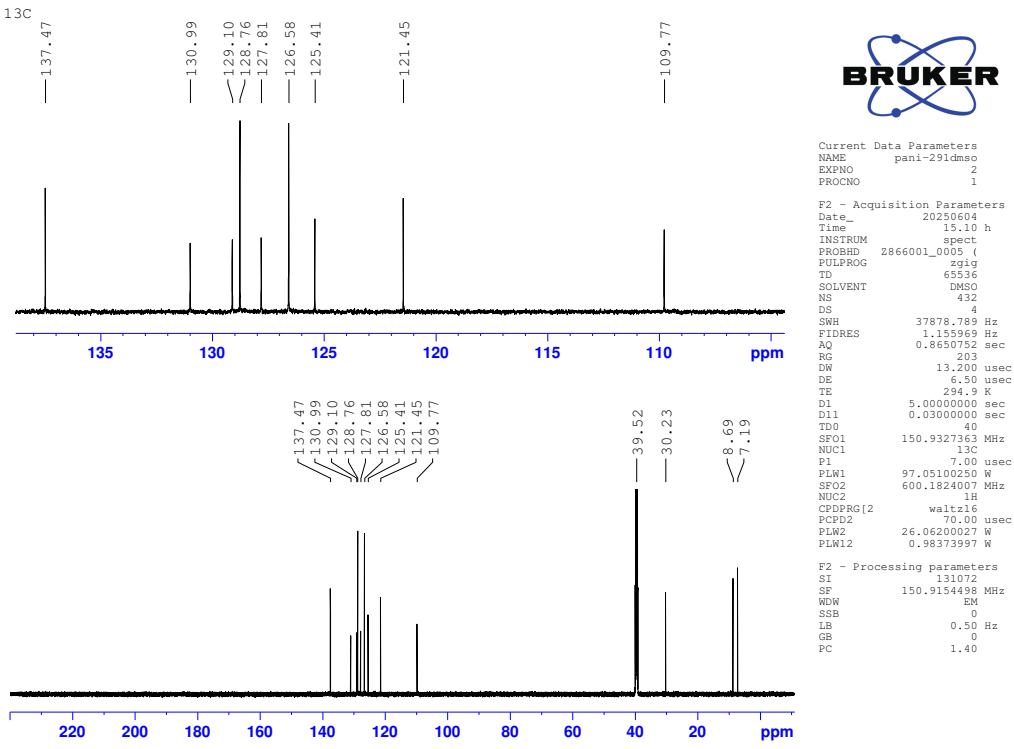


Fig. S 76. ^{13}C NMR spectrum of compound 6d (151 MHz, DMSO-d_6).

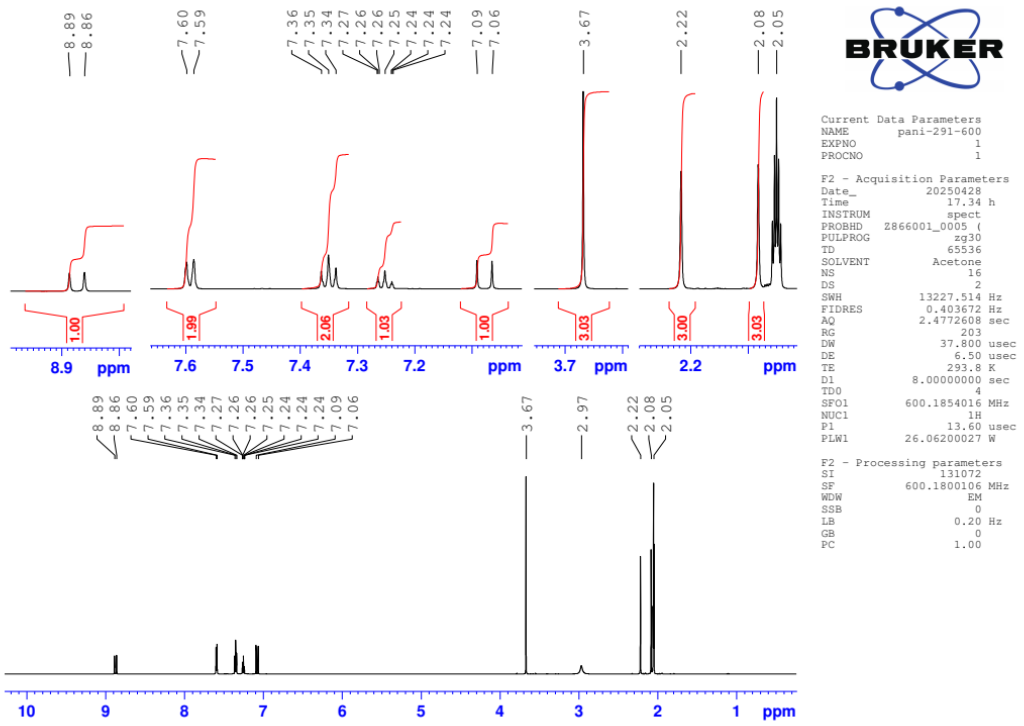


Fig. S 77. ^{1}H NMR spectrum of compounds 6d (600 MHz, acetone-d_6).

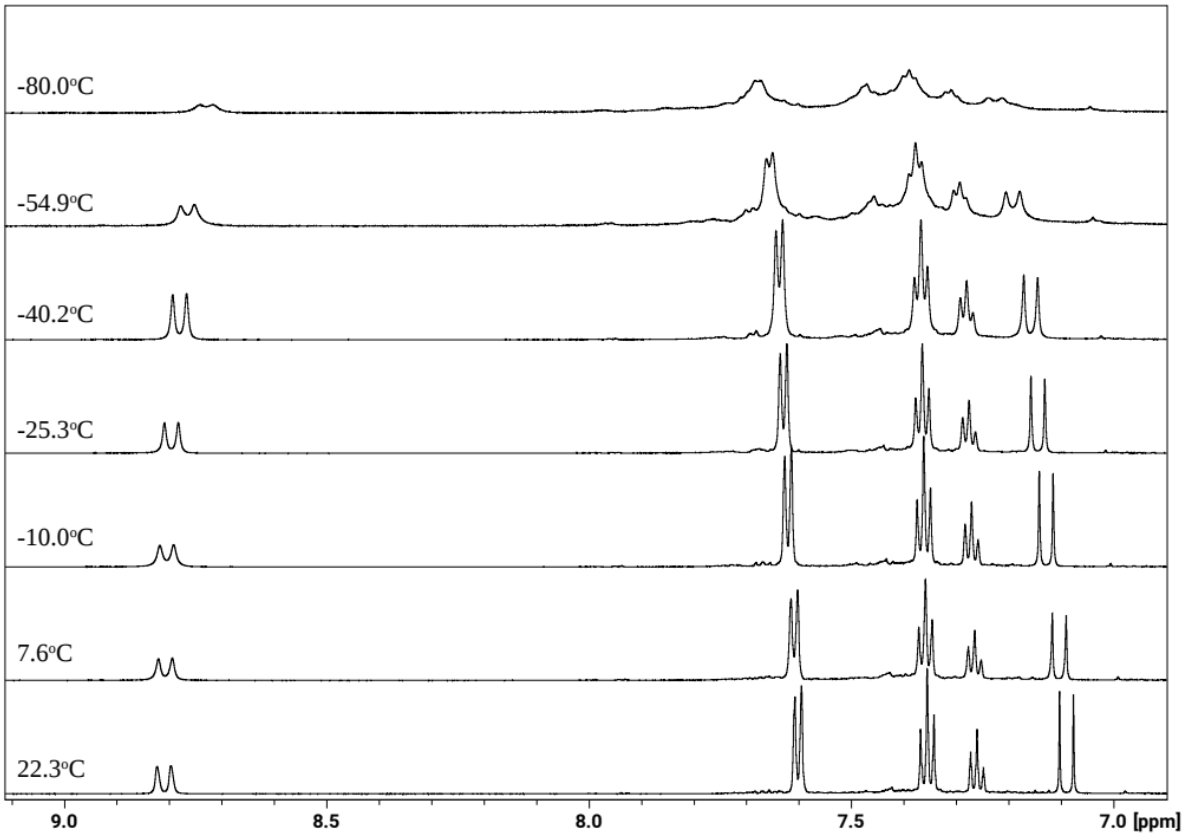


Fig. S 78. ^{1}H NMR spectra of compound 6d at different temperatures (600 MHz, acetone-d_6, range 7.0-9.0 ppm).

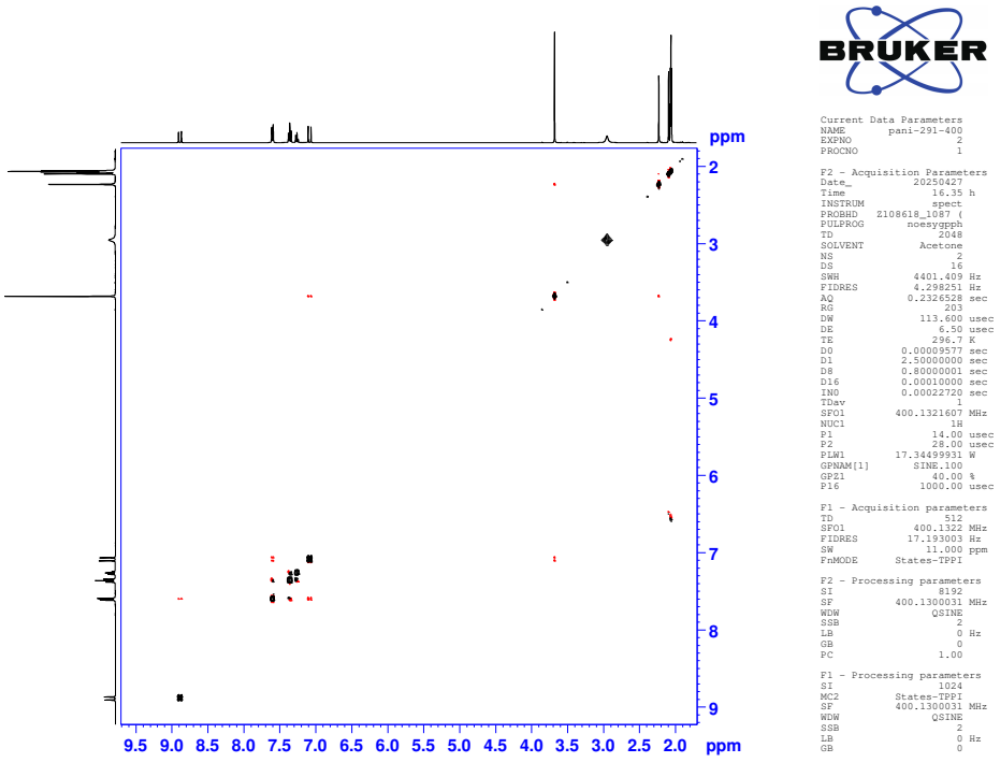


Fig. S 79. ^{1}H-^{1}H NOESY spectrum of compound 6d (400 MHz, acetone-*d*$_6$, mixing time – 0.8 s).

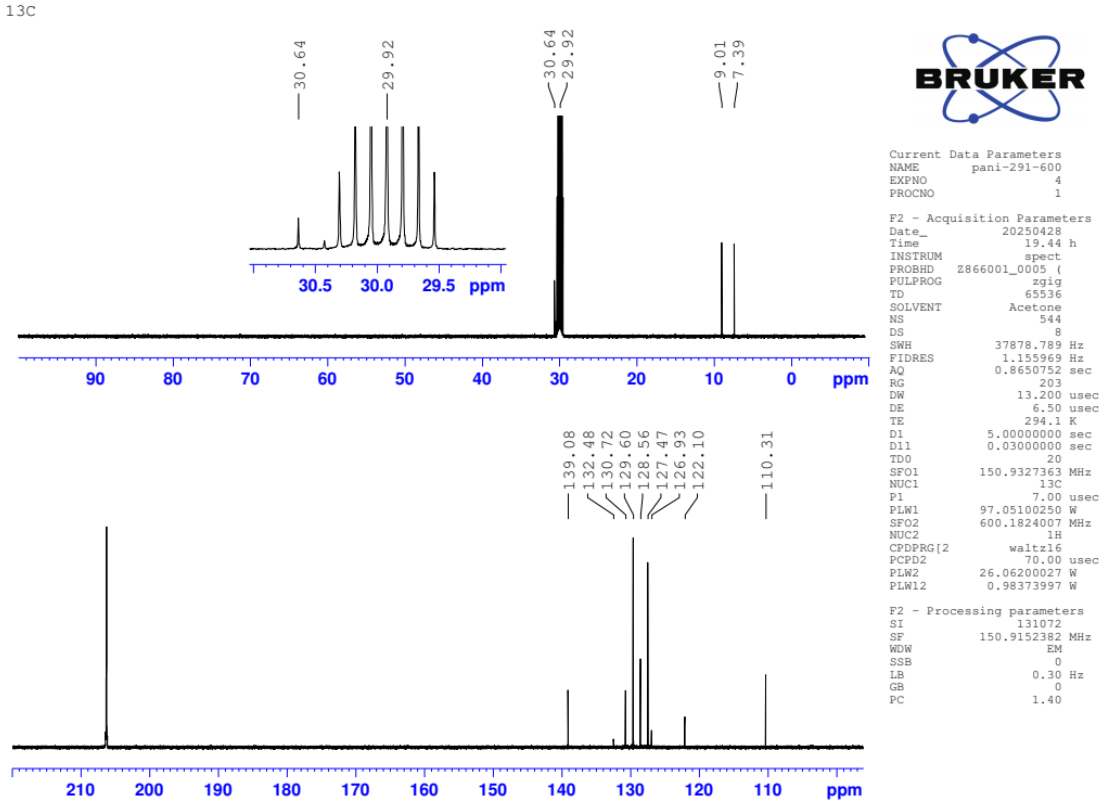


Fig. S 80. ^{13}C NMR spectrum of compound 6d (151 MHz, acetone-*d*$_6$).

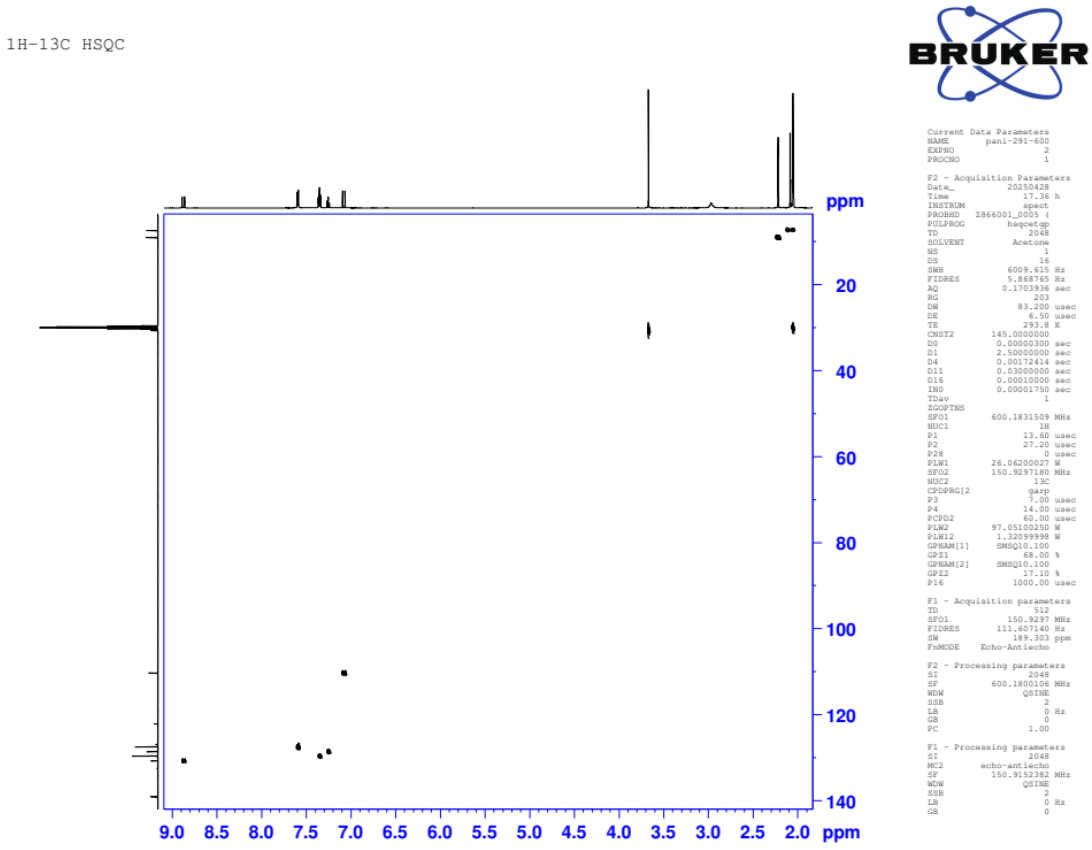


Fig. S 818. ^{1}H-^{13}C HSQC spectrum of compound 6d (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

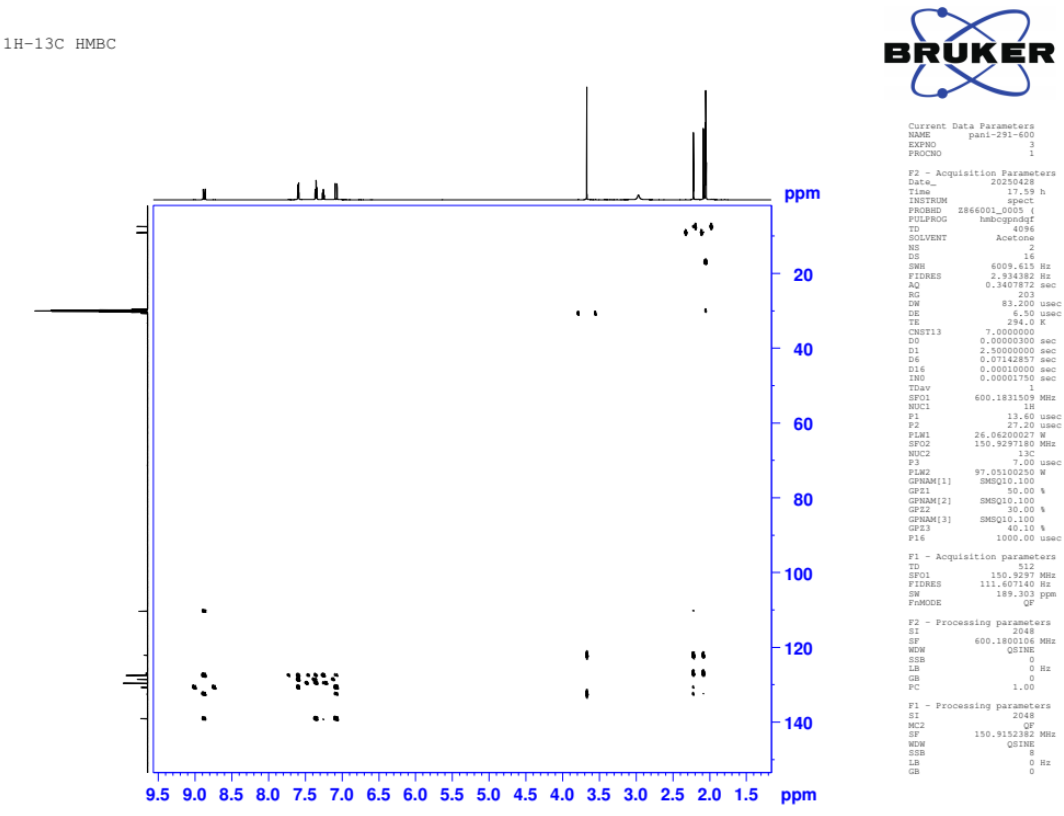


Fig. S 82. ^{1}H-^{13}C HMBC spectrum of compound 6d (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

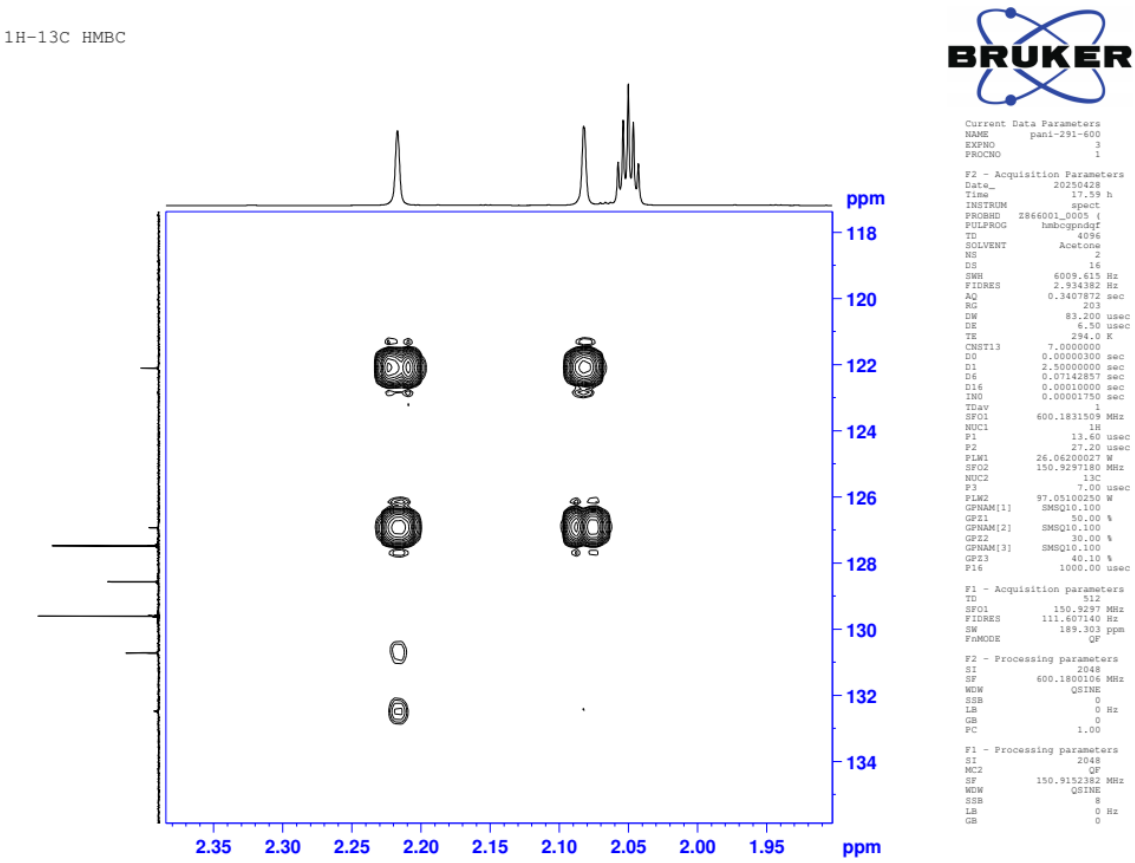


Fig. S 83. Part of ^{1}H-^{13}C HMBC spectrum of compound 6d (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

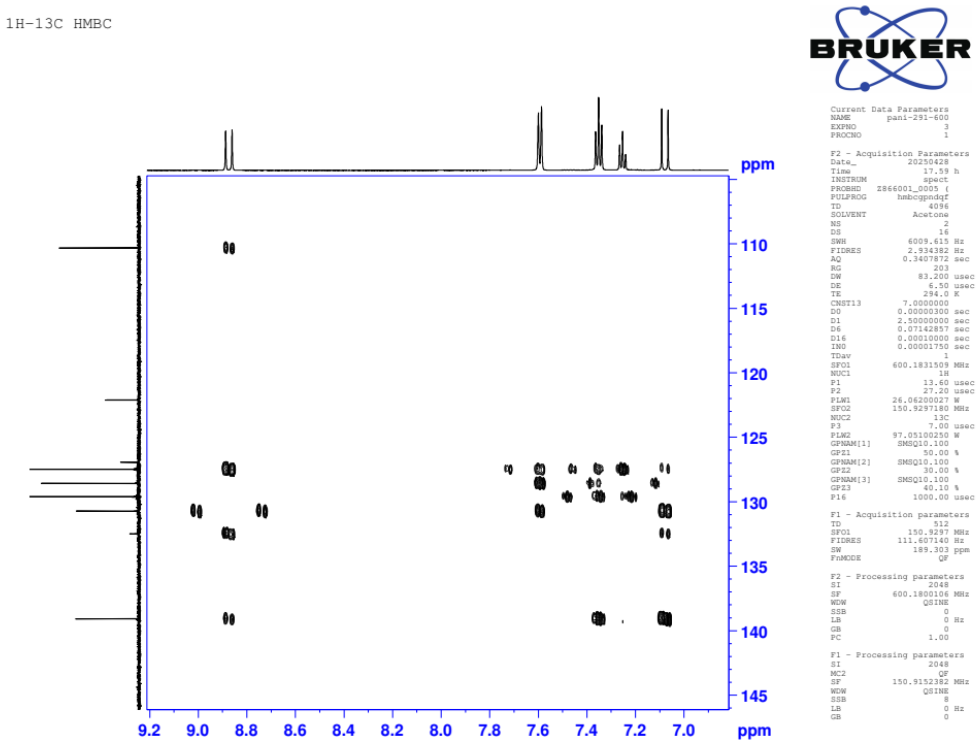


Fig. S 84. Part of ^{1}H-^{13}C HMBC spectrum of compound 6d (600 MHz – ^{1}H, 151 MHz – ^{13}C, acetone-d_6).

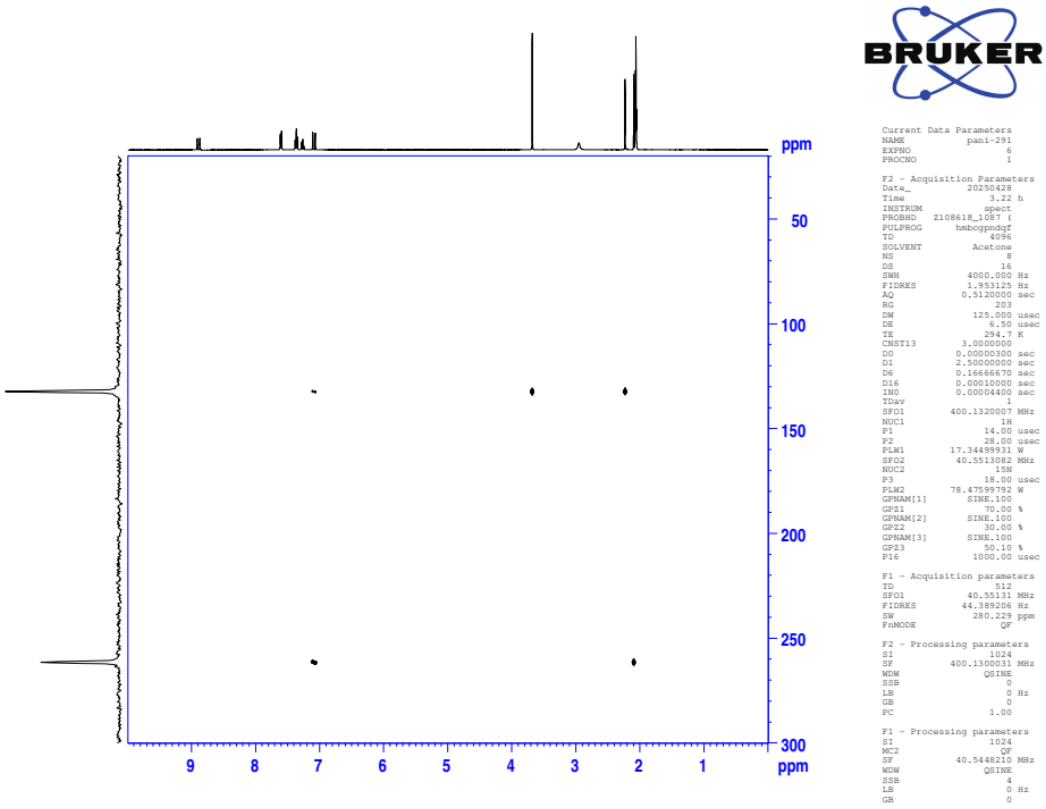


Fig. S 85. ^{1}H-^{15}N HMBC spectrum of compound 6d (400 MHz – ^{1}H, 41 MHz – ^{15}N, acetone-d_6).

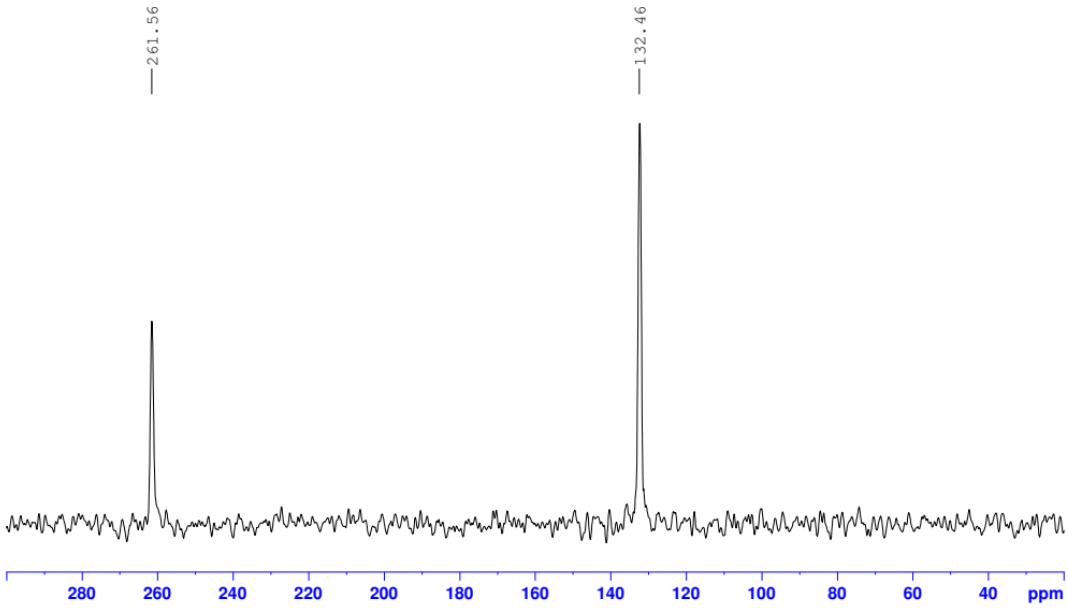


Fig. S 86. ^{15}N NMR spectrum of compound 6d (41 MHz, acetone-d_6), obtained from projection of ^{1}H-^{15}N HMBC spectrum.

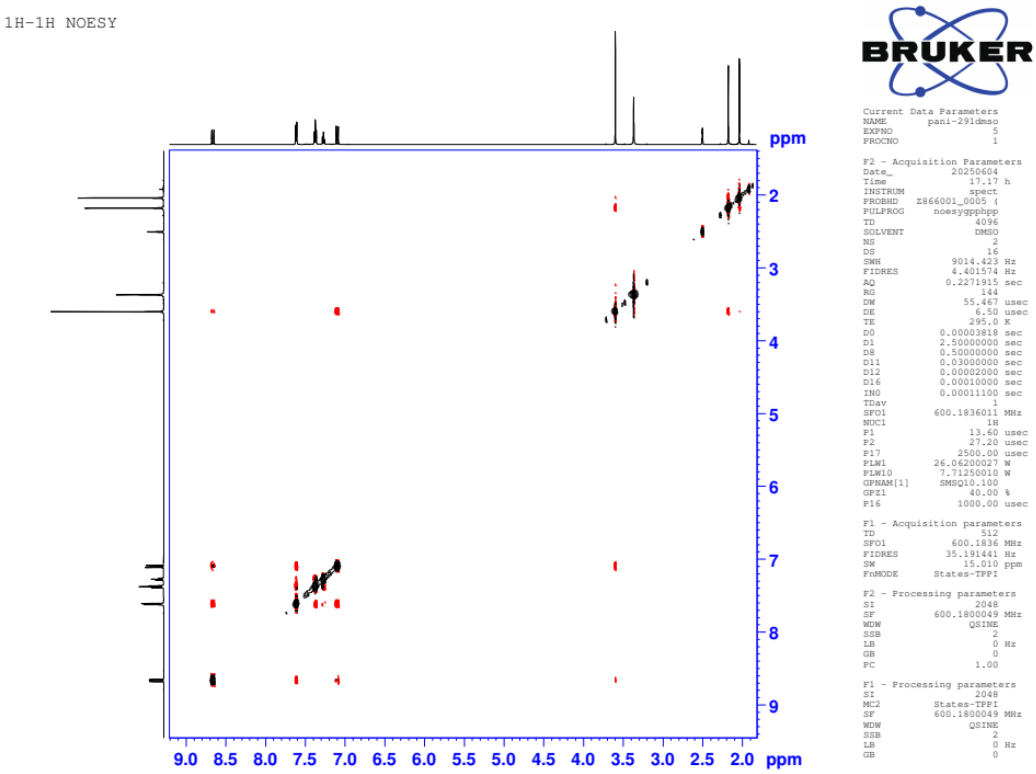


Fig. S 87. ^{1}H-^{1}H NOESY spectrum of compound 6d (600 MHz, DMSO-d_6, mixing time – 0.5 s).

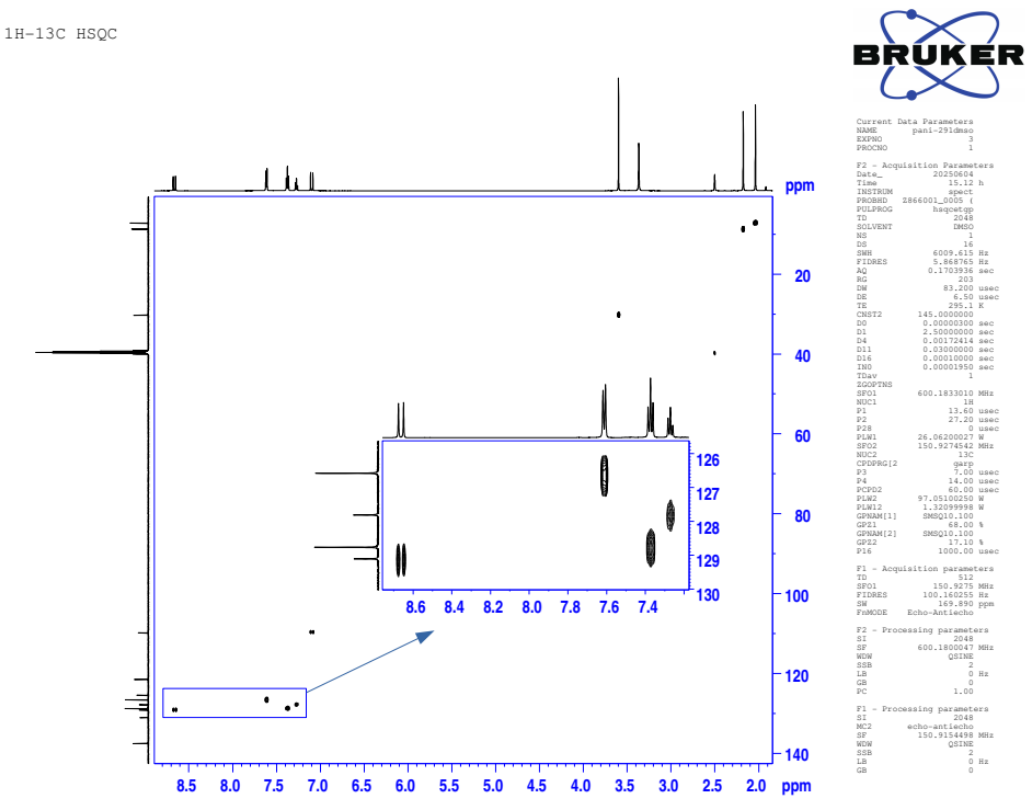


Fig. S 88. ^{1}H-^{13}C HSQC spectrum of compound 6d (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-d_6).

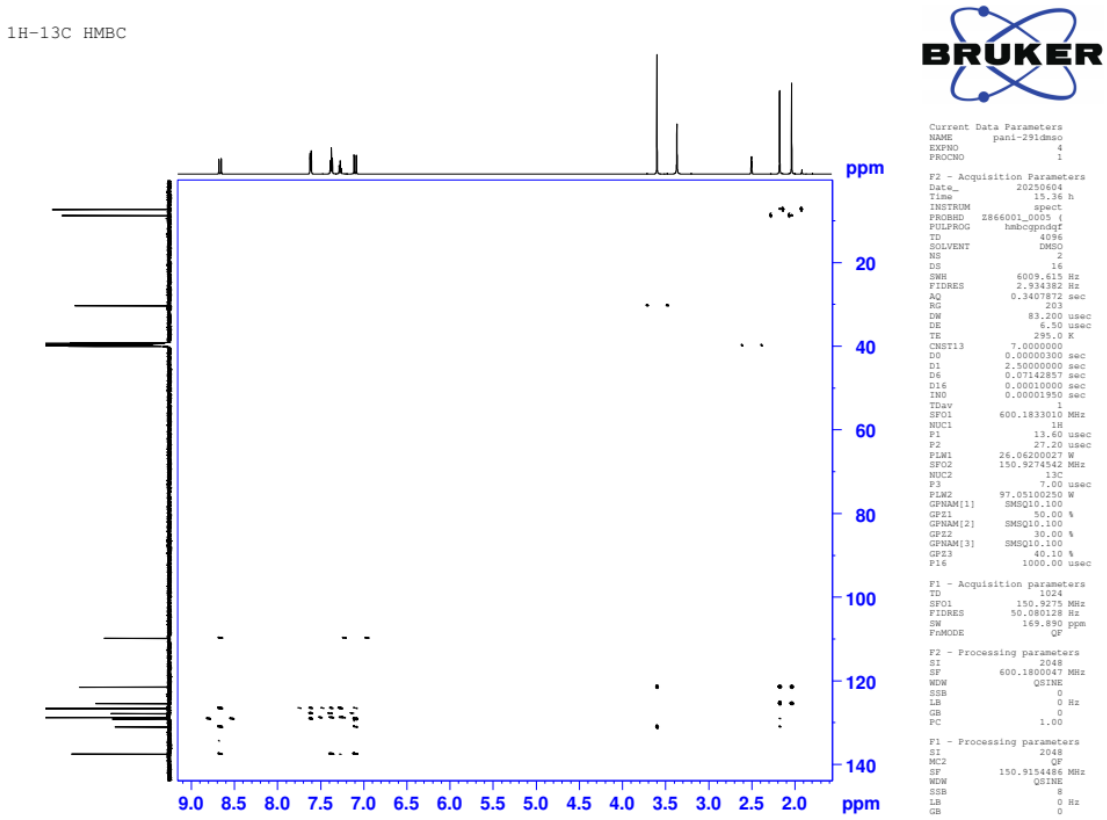


Fig. S 89. ^{1}H-^{13}C HMBC spectrum of compound 6d (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-d_6).

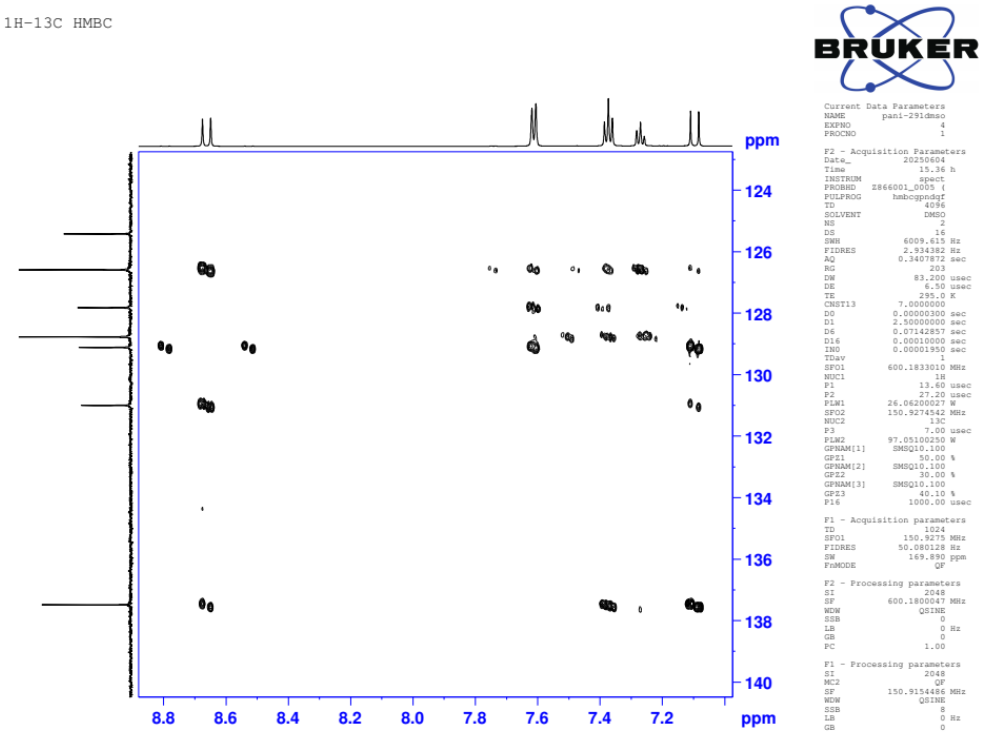
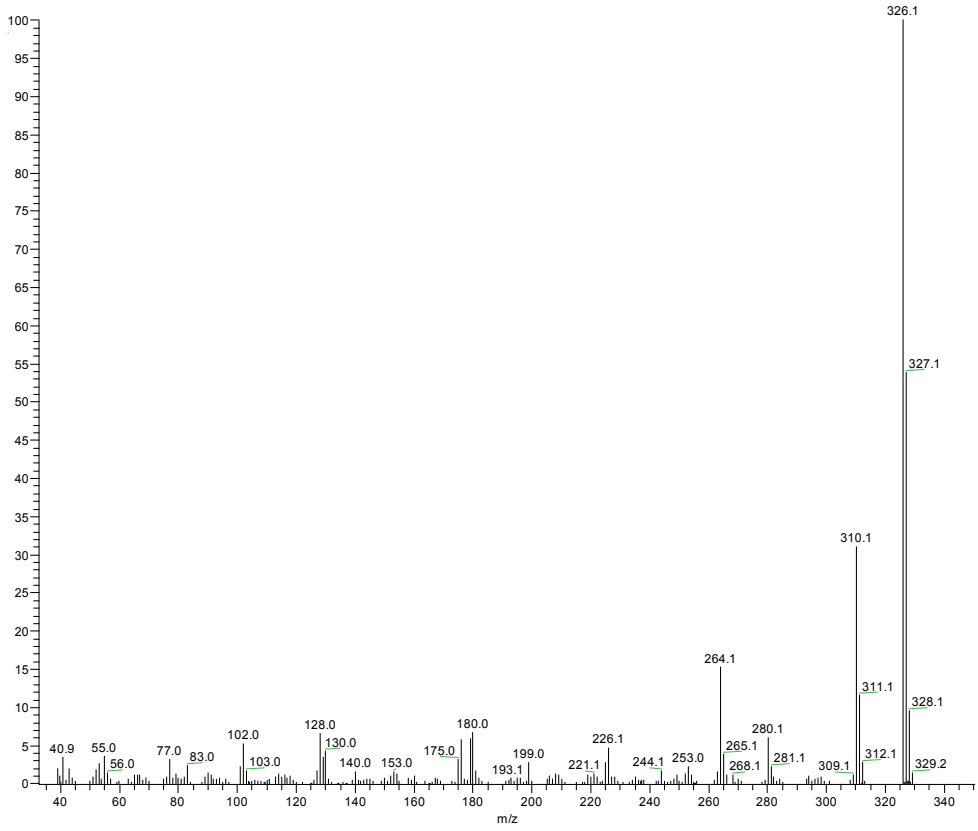


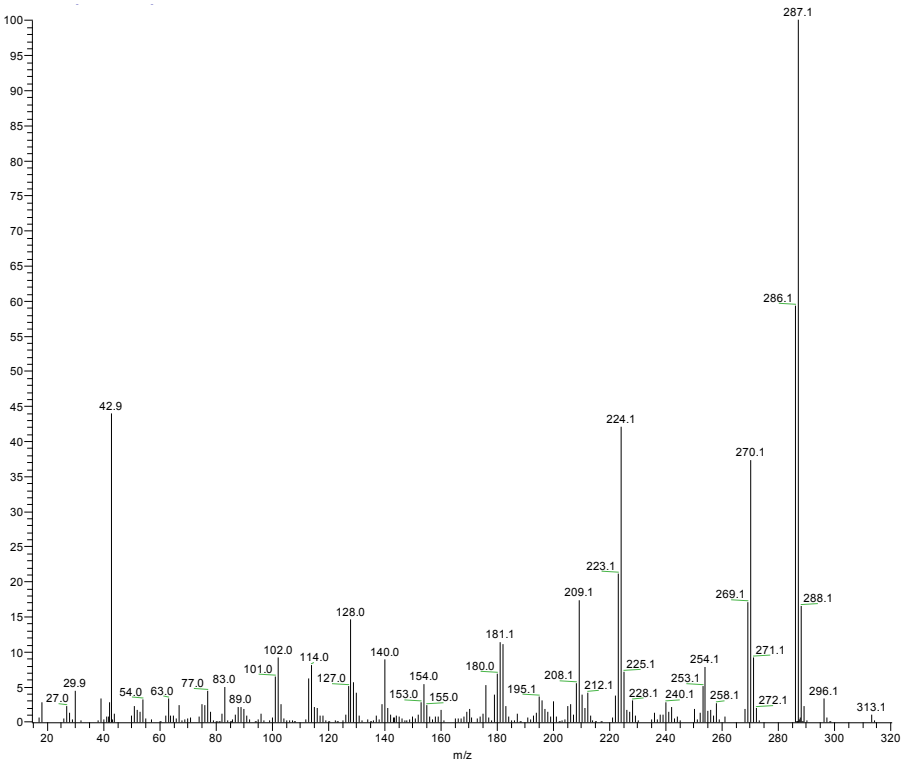
Fig. S 90. Part of ^{1}H-^{13}C HMBC spectrum of compound 4d (600 MHz – ^{1}H, 151 MHz – ^{13}C, DMSO-d_6).

SI 5. Copies of HRMS spectra of compounds 3a-h, 4a-h, 5, 6a-d.

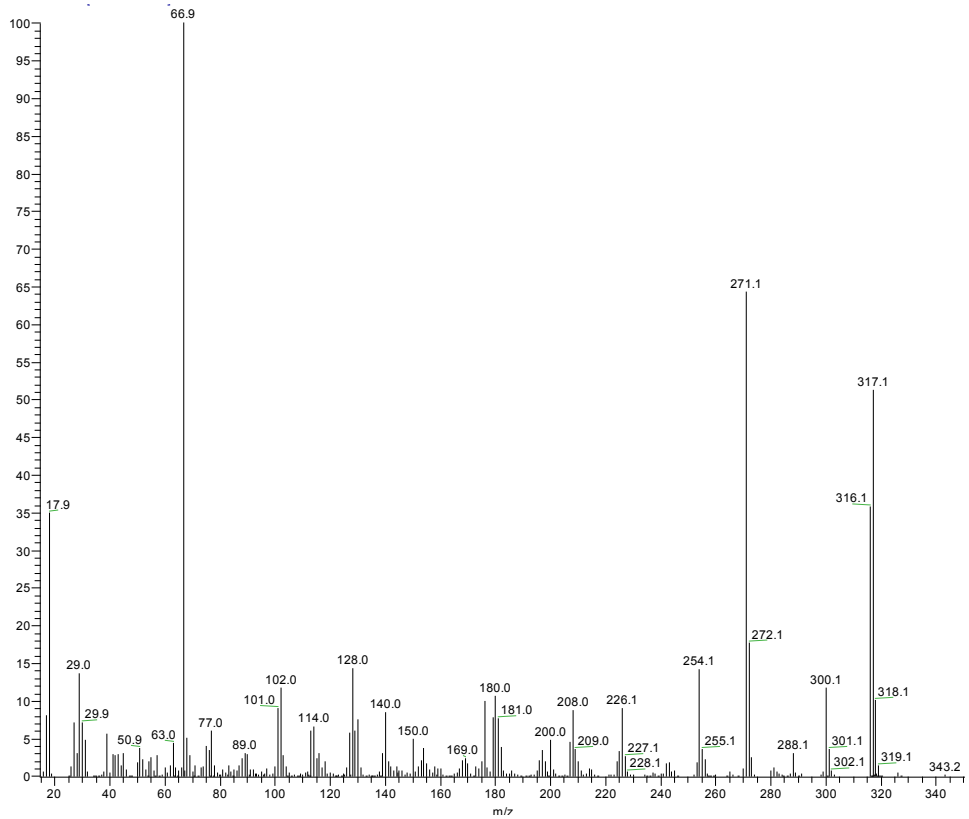
S5.1. 3-Hydroxy-6,6-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-3,5,6,7-tetrahydro-*4H*-benzimidazol-4-one (**3a**).



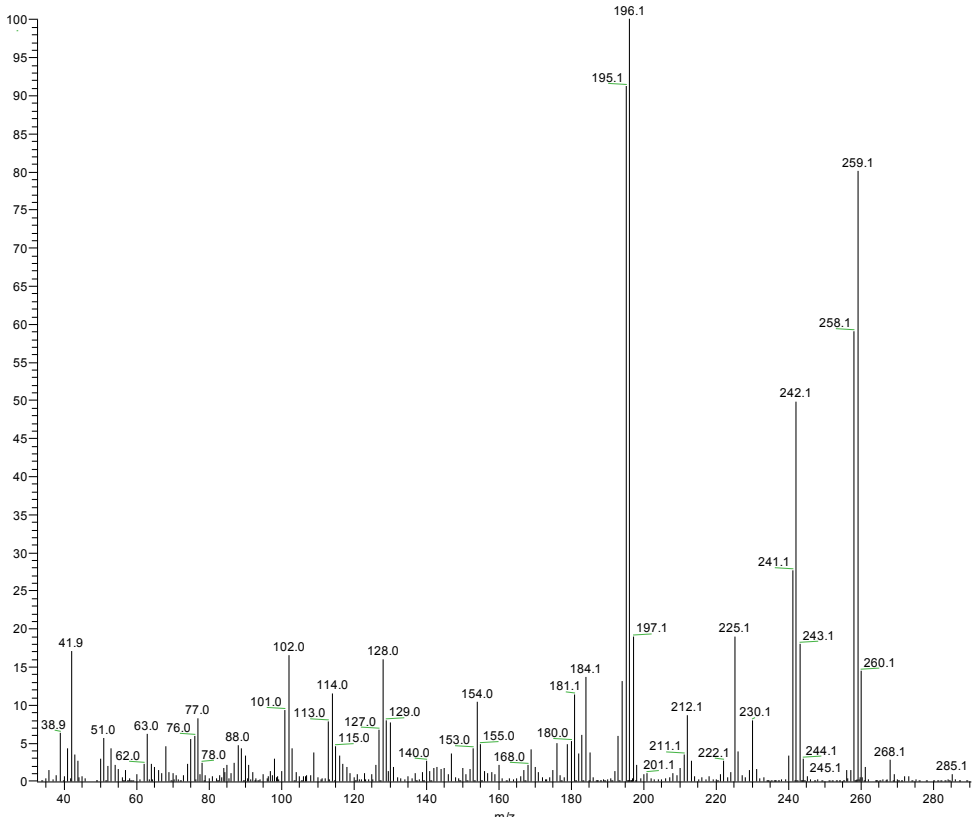
S5.2. 1-(1-Hydroxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazol-5-yl)ethanone (**3b**).



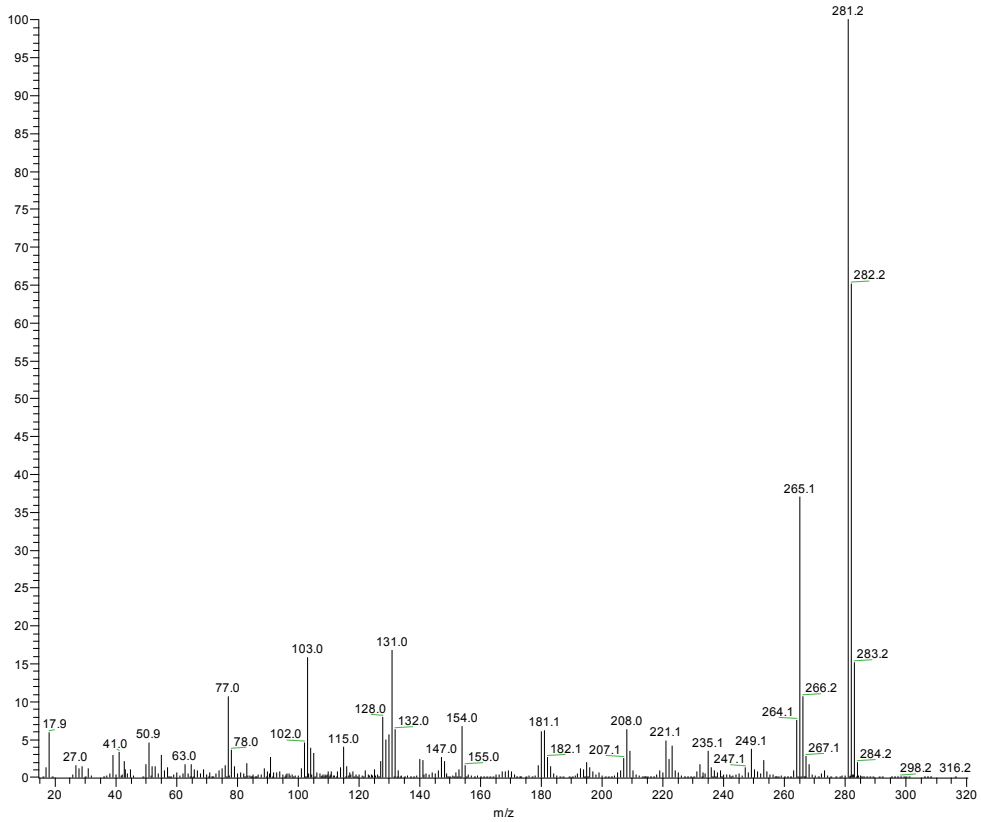
S5.3. Ethyl 1-hydroxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole-5-carboxylate (**3c**).



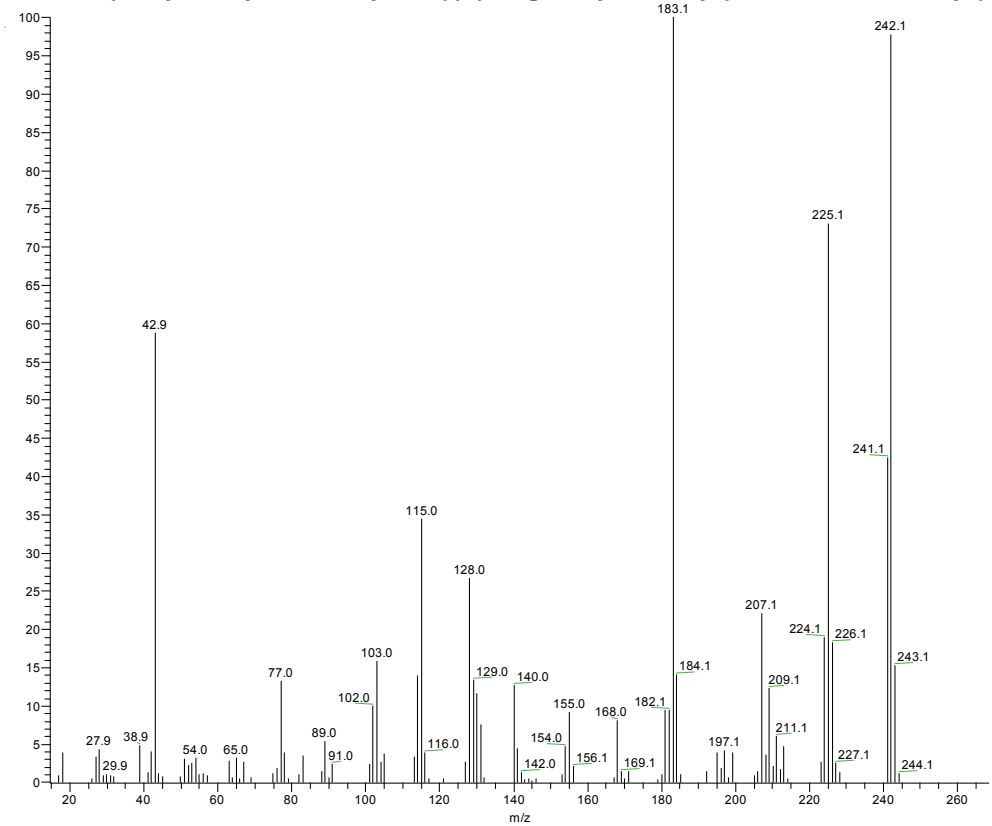
S5.4. 4,5-Dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazol-1-ol (**3d**).



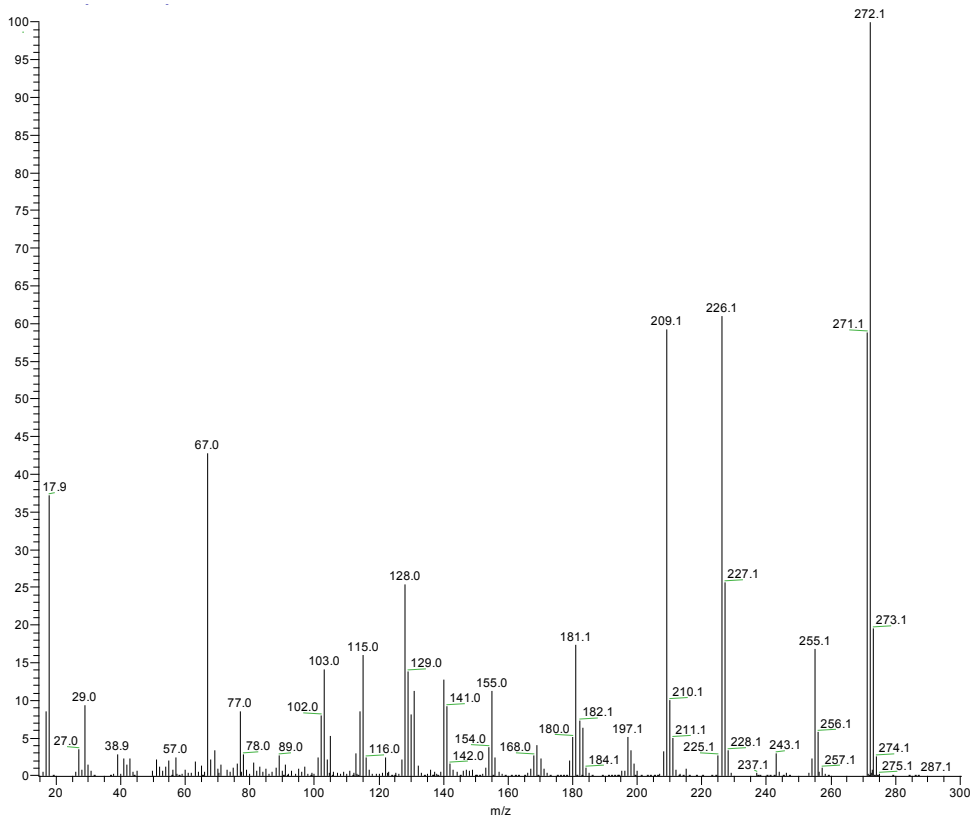
S5.5. 3-Hydroxy-6,6-dimethyl-2-((*E*)-2-phenylethenyl)-3,5,6,7-tetrahydro-*4H*-benzimidazol-4-one (**3e**).



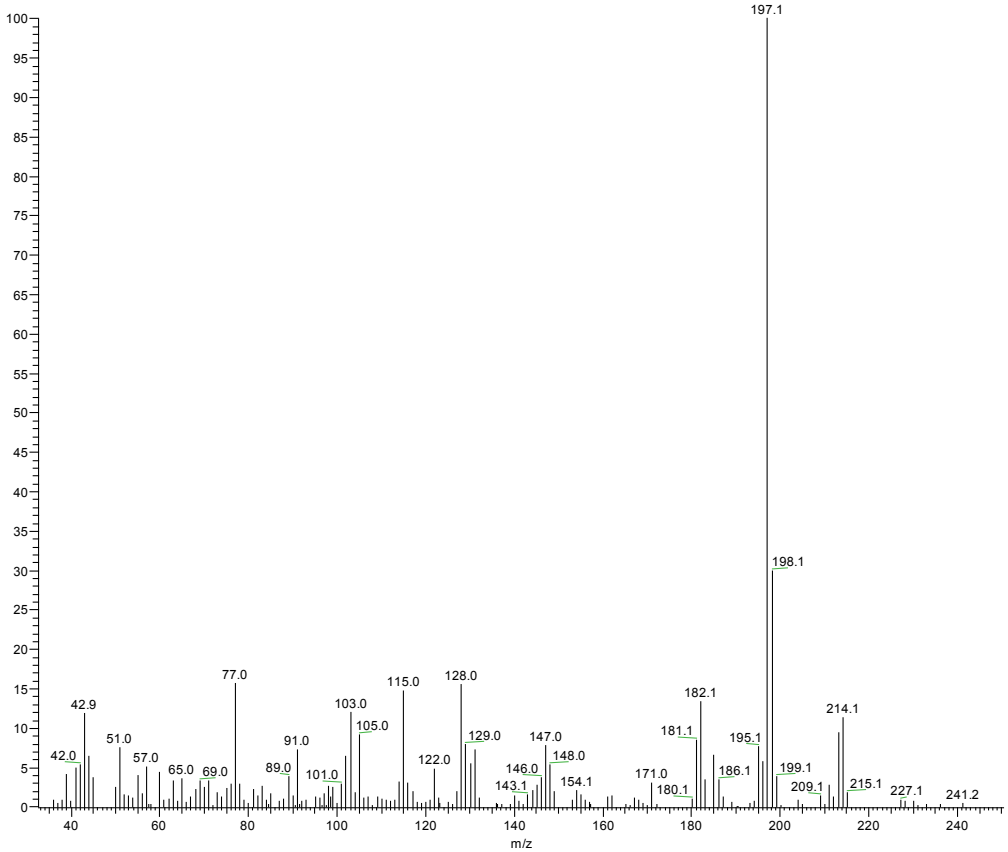
S5.6. 1-(1-Hydroxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazol-5-yl)ethanone (**3f**).



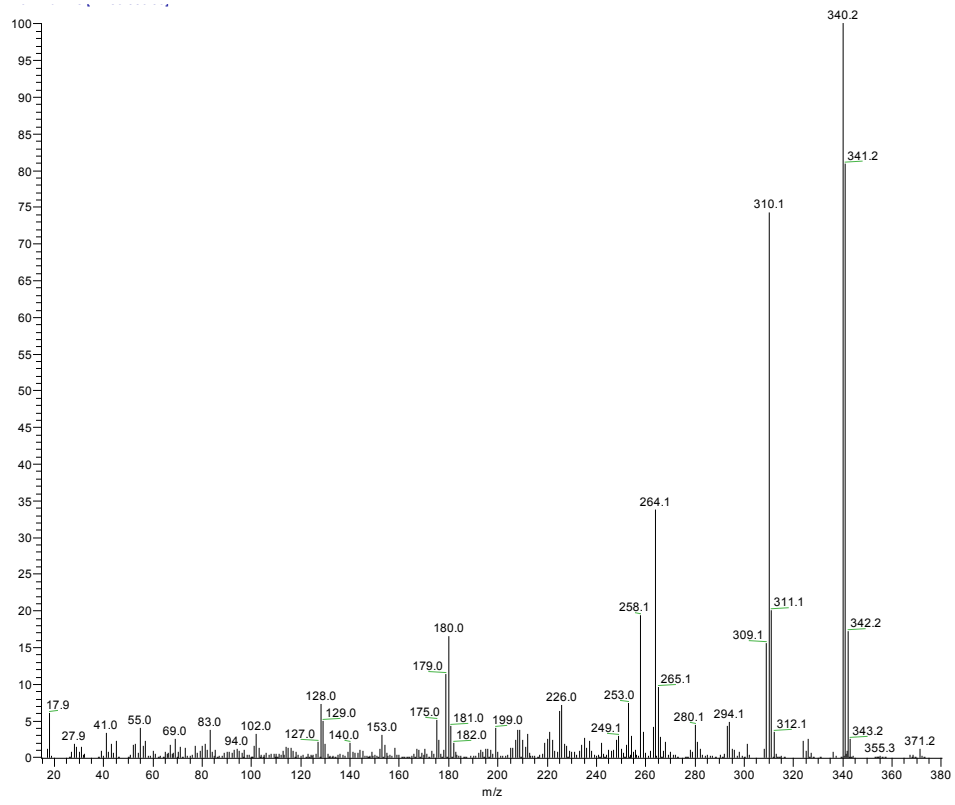
S5.7. Ethyl 1-hydroxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole-5-carboxylate (**3g**).



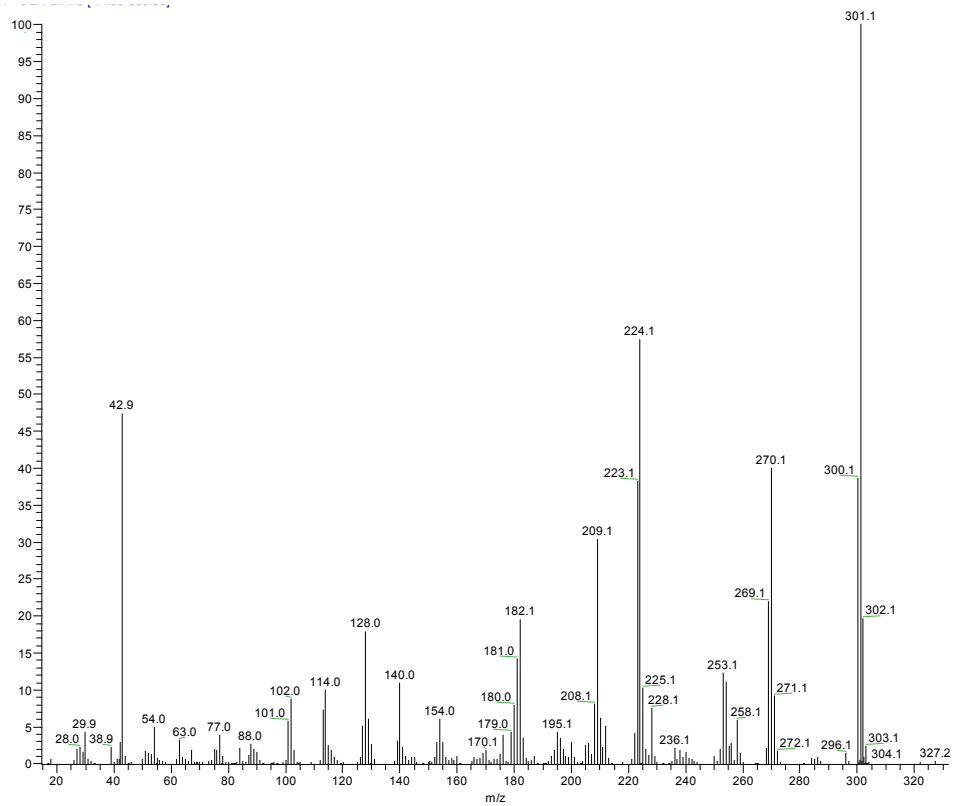
S5.8. 4,5-Dimethyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazol-1-ol (**3h**).



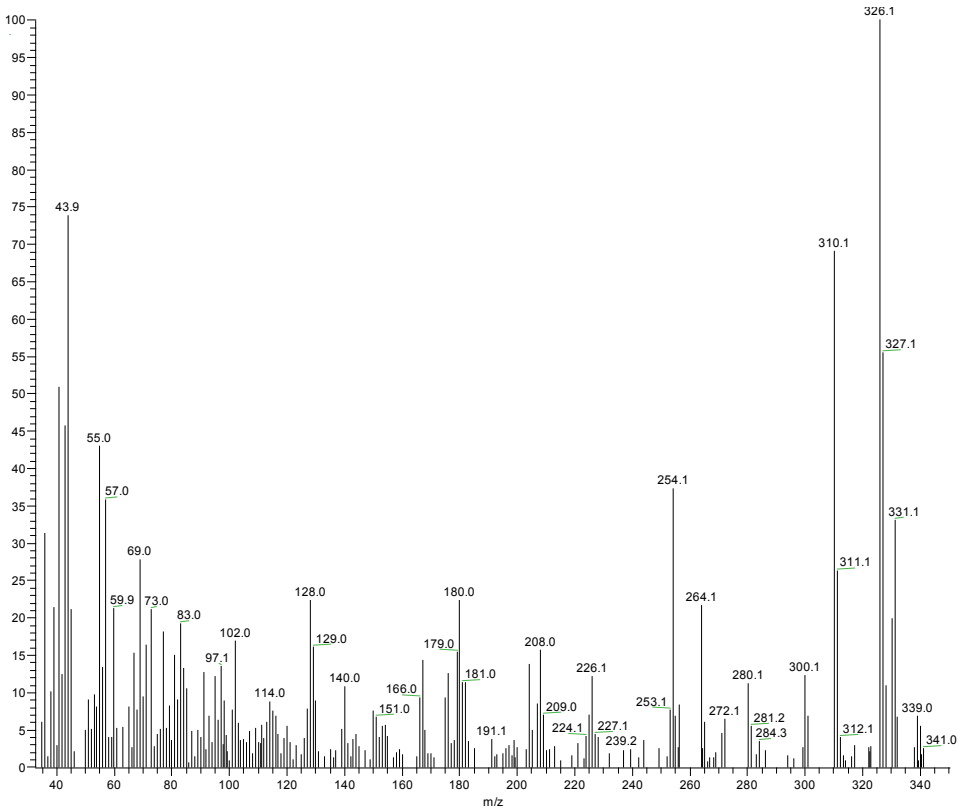
S5.9. 3-Methoxy-6,6-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-3,5,6,7-tetrahydro-*4H*-benzimidazol-4-one (**4a**).



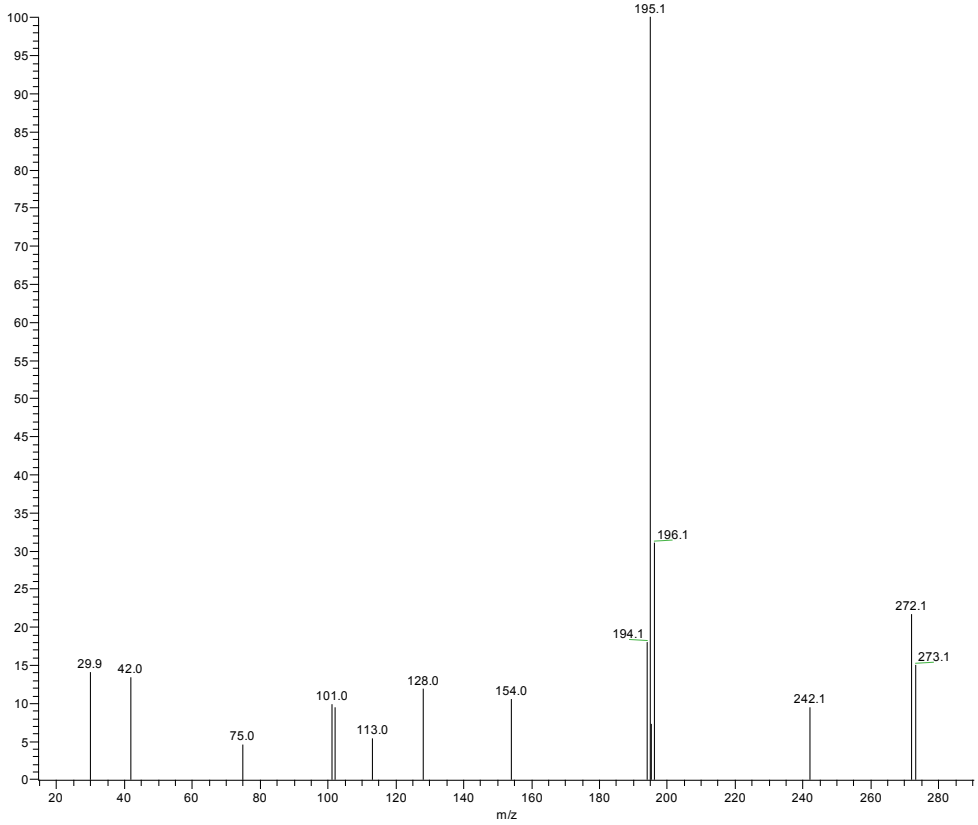
S.5.10. 1-(1-Methoxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazol-5-yl)ethanone (**4b**).



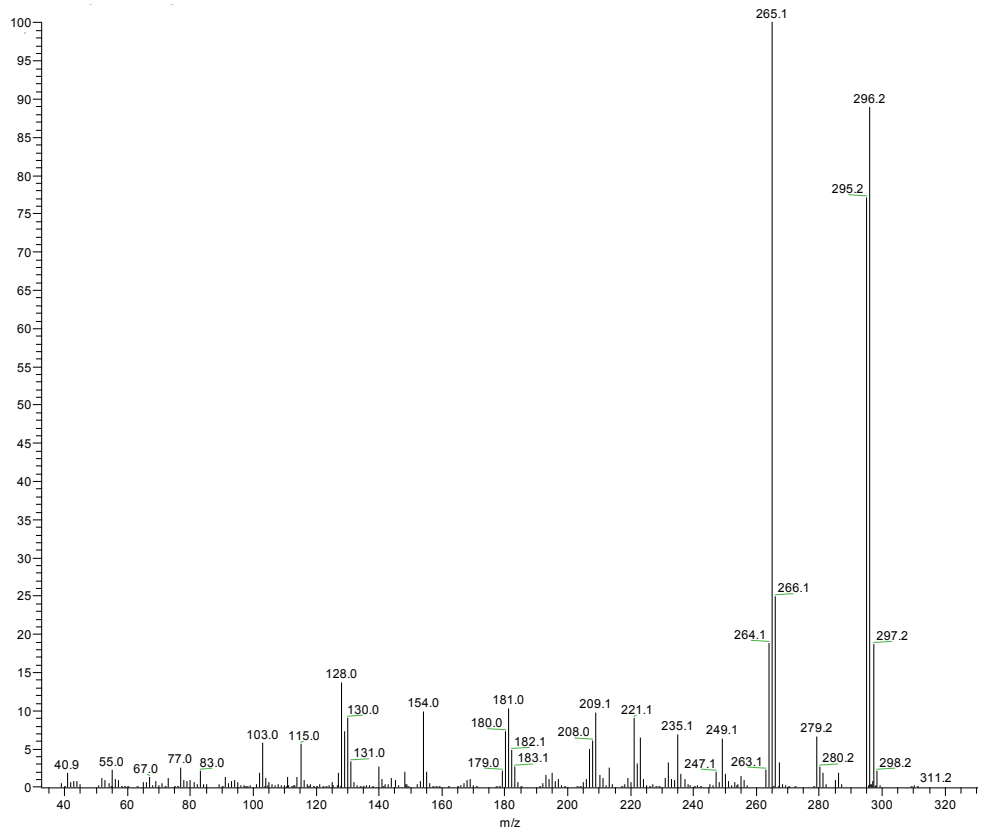
S.5.11. Ethyl 1-methoxy-4-methyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole-5-carboxylate (**4c**).



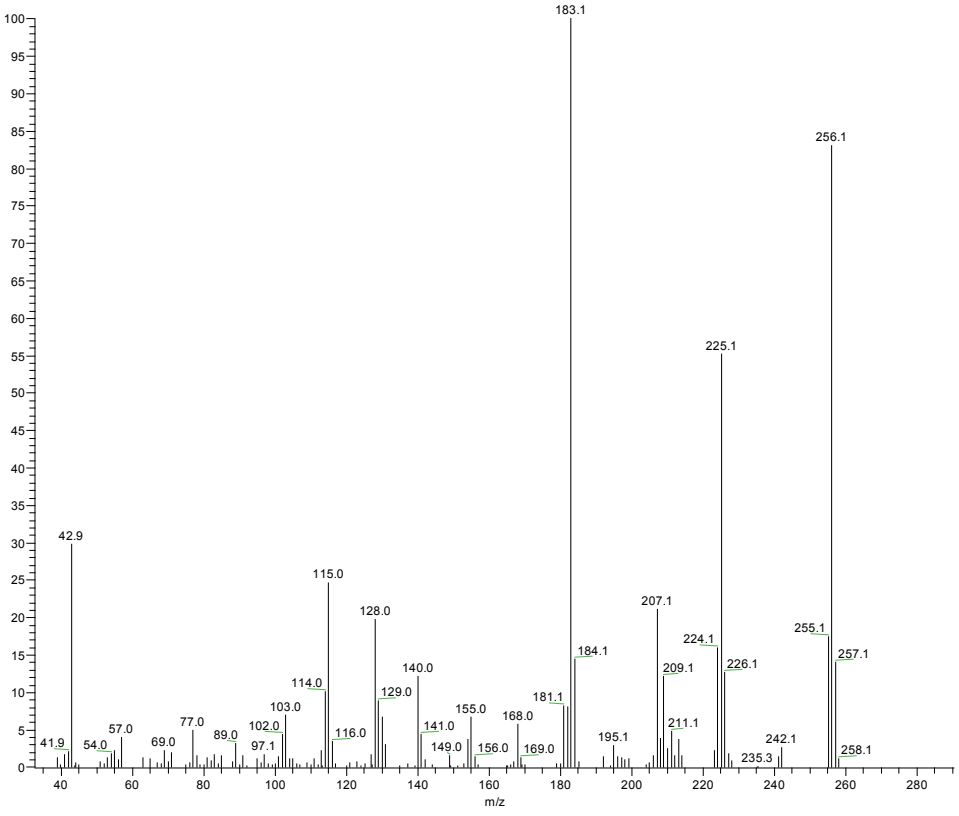
S.5.12. 1-Methoxy-4,5-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole (**4d**).



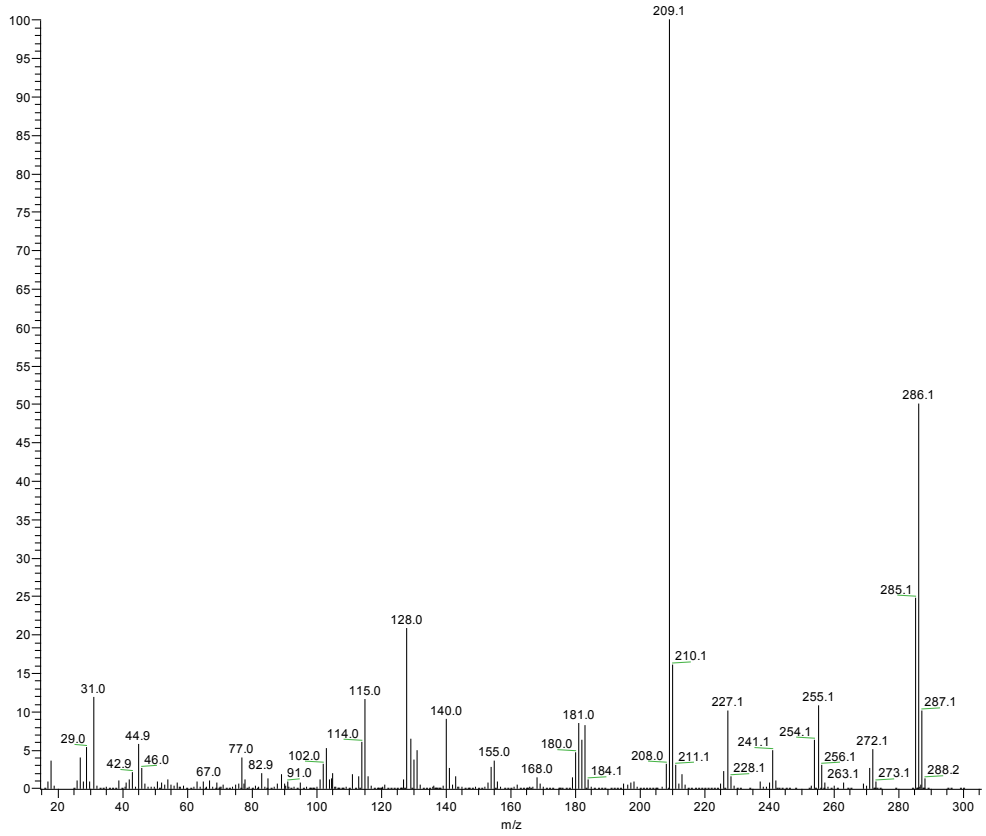
S.5.13. 3-Methoxy-6,6-dimethyl-2-((*E*)-2-phenylethenyl)-3,5,6,7-tetrahydro-*4H*-benzimidazol-4-one (**4e**).



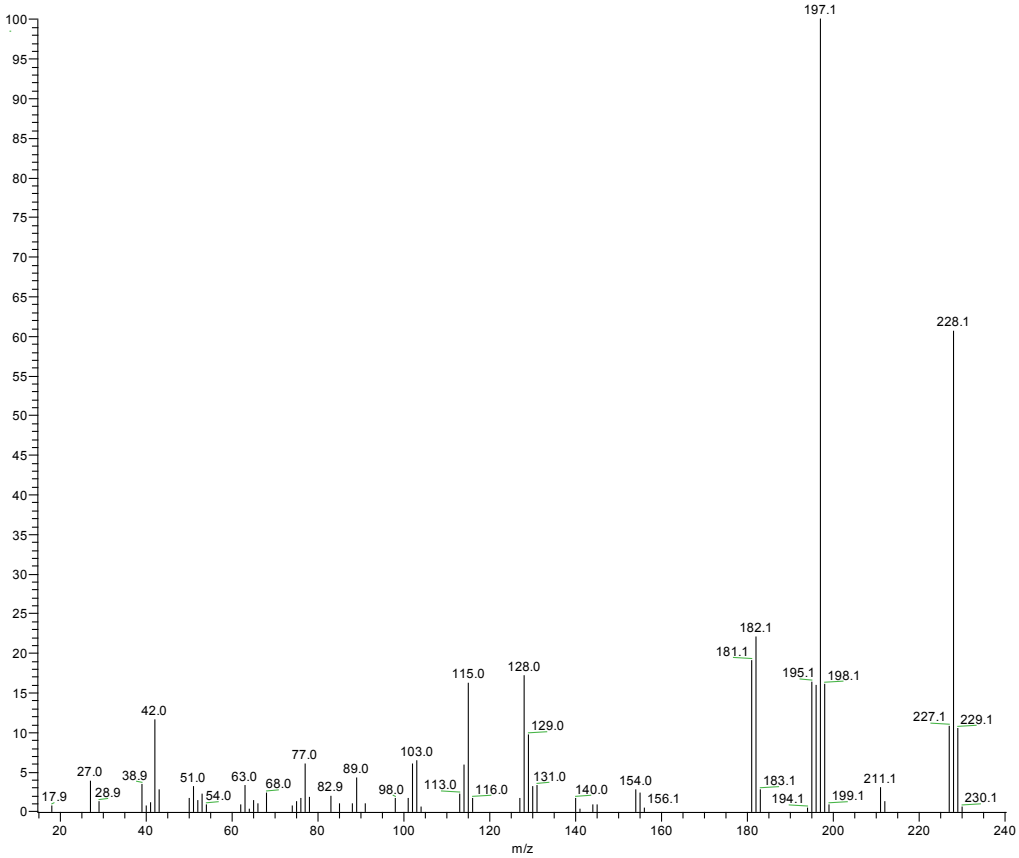
S.5.14. 1-(1-Methoxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazol-5-yl)ethanone (**4f**).



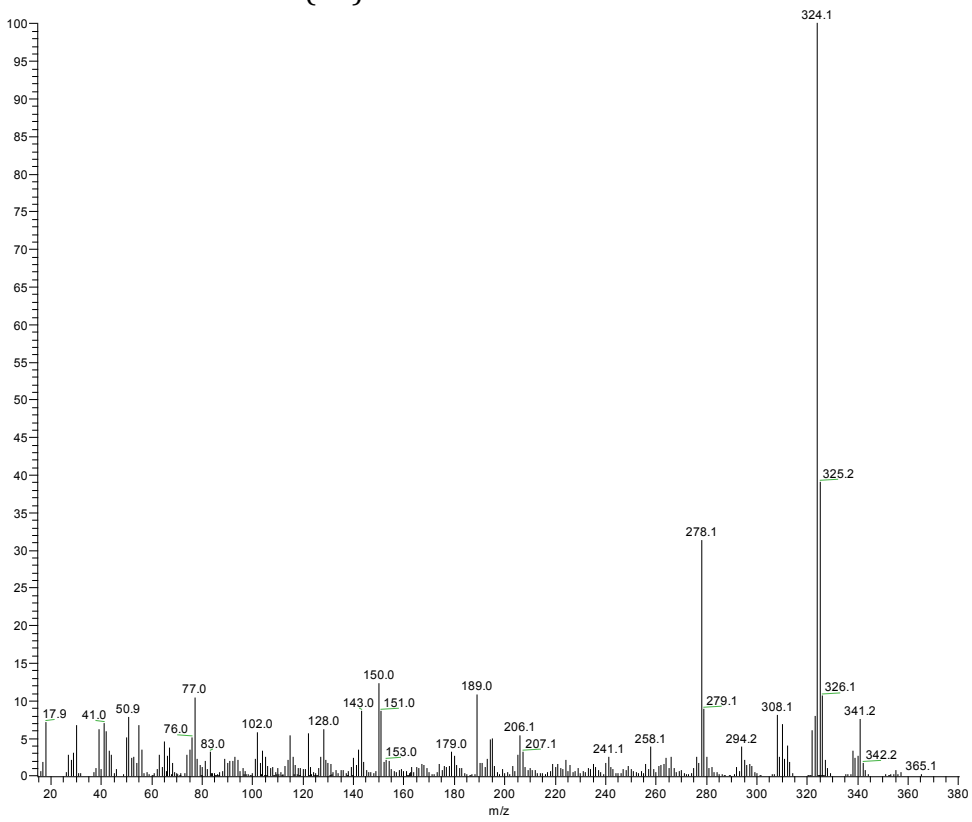
S.5.15. Ethyl 1-methoxy-4-methyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole-5-carboxylate (**4g**).



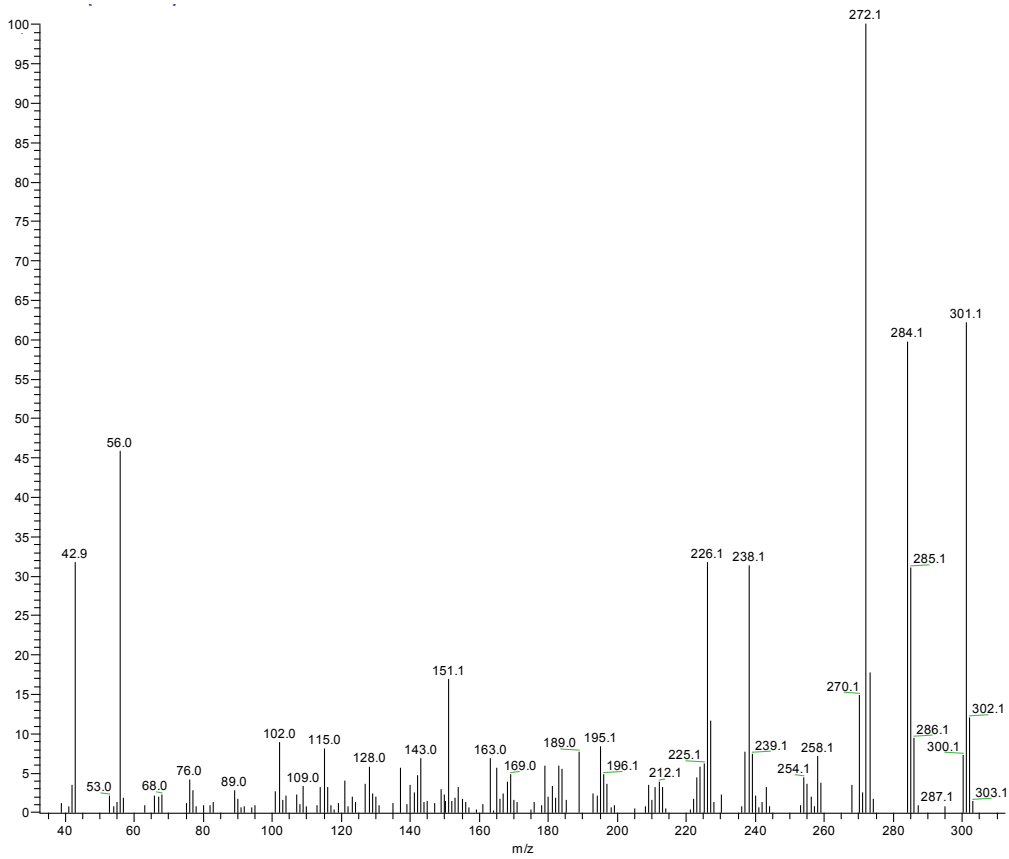
S.5.16. 1-Methoxy-4,5-dimethyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole (**4h**).



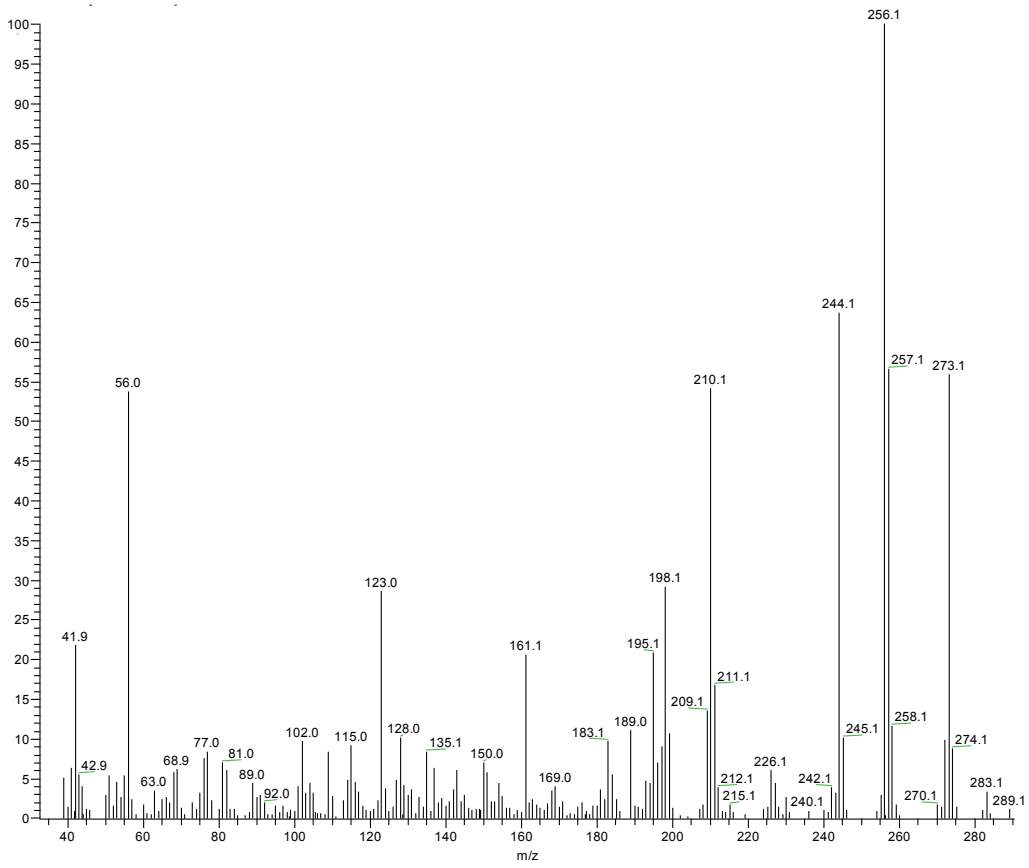
S.5.17. 1,6,6-Trimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-4-oxo-4,5,6,7-tetrahydro-*1H*-benzimidazole 3-oxide (**6a**).



S.5.18. 4-Acetyl-1,5-dimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole 3-oxide (**6b**).



S.5.19. 1,4,5-Trimethyl-2-((*E*)-2-(4-nitrophenyl)ethenyl)-*1H*-imidazole 3-oxide (**6c**).



S.5.20. 1,4,5-Trimethyl-2-((*E*)-2-phenylethenyl)-*1H*-imidazole 3-oxide (**6d**).