Electronic supplementary Materials for the article

Synthesis of antiviral drug tecovirimat and its key maleimide intermediates using organocatalytic Mumm rearrangement at ambient conditions

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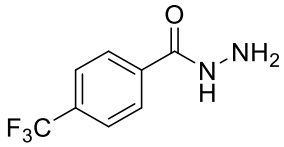
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S2. NMR spectra and UPLC/MS datasets, pp. 5-61

S3. Computational results, pp. 62-78

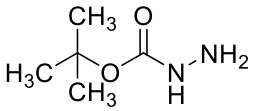
1. SYNTHETIC PROCEDURES AND PHYSICOCHEMICAL DATA FOR HYDRAZIDES 1a-1h

1.1. 4-trifluoromethylbenzohydrazide (1a)



White solid; 783 mg, (72.6% yield); $C_8H_7F_3N_2O$; MW 204.15; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 4.12 (br. s., 2H, -NH_2), 7.68 (d, *J*=8.2 Hz, 2H, Ar-H), 7.86 (d, *J*=8.1 Hz, 2H, Ar-H), 7.93 (br. s., 1H, -NH-); HPLC 99.6%, t_R=1.23 min.

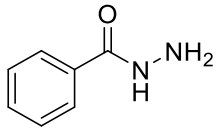
1.2. *Tert*-butyl hydrazinecarboxylate (1b)



Hydrazine monohydrate (3.44 g, 0.0687 mole, 3 eq.) was dissolved in isopropanol (13 mL) in a 100 mL round-bottom flask. Di-tert-butyl dicarbonate (5 g, 0.0229 mole, 1 eq.) in isopropanol (5 mL) was added dropwise to the prepared solution. After the entire volume was added, the reaction mixture was left at room temperature on a magnetic stirrer for 2 hours. After this time, the reaction mixture was evaporated to dryness. The residue was dissolved in CH_2Cl_2 and dried over $MgSO_{4(anh)}$. After filtration and distillation of the solvent, the crude product was obtained and used in further stages of the synthesis.

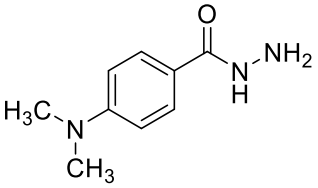
White solid; 2400 mg (79% yield); $C_5H_{12}N_2O_2$; MW 132.16; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 1.36 - 1.5 (s, 9H, $(-CH_3)_3$), 3.17 - 3.48 (br. s., 2H, -NH_2), 5.70 - 5.98 (br. s., 1H, -NH-).

1.3. Benzohydrazide (1c)



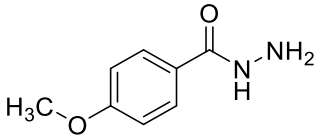
White solid; 760 mg (68% yield); $C_7H_8N_2O$; MW 136.15; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 3.40 (br. s., 2H, NH_2) 7.40 - 7.47 (m, 2H, Ar-H) 7.48 - 7.54 (m, 1H, Ar-H) 7.70 - 7.77 (m, 2H, Ar-H).

1.4. 4-(Dimethylamino)benzohydrazide (1d)



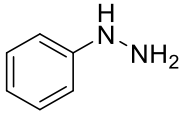
White solid; 640 mg (59% yield); $C_9H_{13}N_3O$; MW 179.22; ^{1}H NMR (500 MHz, DMSO-d_3) δ (ppm) 2.86 - 2.96 (m, 6H, $(CH_3)_2$), 4.20 - 4.38 (m, 2H, NH_2), 6.58 - 6.70 (m, 2H, Ar-H), 7.58 - 7.70 (m, 2H, Ar-H), 9.25 - 9.43 (m, 1H, NH); HPLC 99.53%, t_R=0.853 min.

1.5. 4-Methoxybenzohydrazide (1e)



White solid; 680 mg (62% yield); $C_8H_{10}N_2O_2$; MW 166.18; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 3.83 - 3.84 (m, 3H, $-OCH_3$), 6.89 - 6.93 (m, 2H, Ar-H) 7.70 - 7.74 (m, 2H, Ar-H).

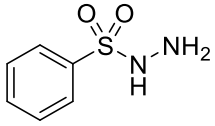
1.6. Phyenylhydrazine (1f)



Phenylhydrazine hydrochloride (3 g, 0.0207 mole) was dissolved in a minimum volume of distilled water and treated with 40% NaOH(aq). The resulting base was extracted into CH_2Cl_2, dried over $Na_2SO_{4(anh)}$ and the solvent was distilled off. The crude product was used in isomaleimide synthesis.

Yellow oil; 1953 mg (87% yield); $C_6H_8N_2$; MW 108.14; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 3.00 - 4.13 (m, 2H, NH_2), 6.79 - 6.84 (m, 2H, Ar-H(3,5)), 7.21 - 7.27 (m, 3H, Ar-H(2,4,6)).

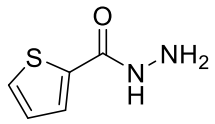
1.7. Benzenesulfonohydrazide (1g)



Sulfonyl chloride (1,77 g, 0.0100 mole, 1 eq.) was added dropwise to a stirring solution of hydrazine monohydrate in CH_2Cl_2 in a 100 mL round-bottom flask. After the entire volume was added, the reaction mixture was stirred for another 15 minutes at room temperature, and then alkalized with 10% $Na_2CO_{3(aq)}$ to pH=11. The reaction mixture was diluted with CH_2Cl_2. After phase separation, the organic layer was dried over $Na_2SO_{4(anh)}$ and the solvent was distilled off. The crude product was crystallized from EtOH and used in the next step of the synthesis.

White solid; 1498 mg (87% yield); $C_6H_8N_2O_2S$; MW 172.20; ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 4.07 (d, J=2.3 Hz, 2H, NH_2), 7.53 - 7.59 (m, 2H, Ar-H(3,5)), 7.59 - 7.64 (m, 1H, Ar-H(4)), 7.74 - 7.79 (m, 2H, Ar-H(2,6)), 8.36 (br. s., 1H, NH); HPLC 99.33% (MaxPlot, 200-800 nm), t_R=0.861 min.

1.8 thiophene-2-carbohydrazide 1h

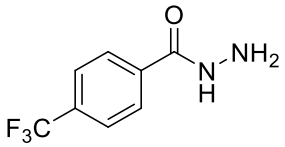


Tiophenecarbonyl chloride (1 g, 0.0068 mol, 1 eq) dissolved in CH_2Cl_2 (10 mL) was added dropwise over one hour to a mixture of hydrazine hydrate (4.5 mL, 13 equiv) and dichloromethane (10 mL), at 0°C. After the addition was completed, the stirring continued overnight. After that, the reaction mixture was diluted with CH_2Cl_2 (20 mL). The aqueous phase was separated and extracted with ethyl acetate (3x20 mL). Both organic phases were then extracted with 5% aqueous hydrochloric acid (3x20 mL). The combined acidic aqueous phase was neutralized with $NaHCO_3$ to slightly basic pH and extracted with ethyl acetate (4x15 mL). The combined organic phase was dried with anhydrous Na_2SO_4 and evaporated to yield the product, which was used without further purification.

White solid; 360 mg (37%), ^{1}H NMR (500 MHz, DMSO-d_6) d ppm 4.42 (br. s., 2 H) 7.09 (dd, *J*=4.98, 3.76 Hz, 1 H) 7.67 (dd, *J*=3.72, 1.07 Hz, 1 H) 7.70 (dd, *J*=5.01, 1.07 Hz, 1 H) 9.72 (s, 1 H);

2. SPECTRA

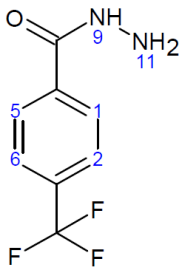
2.1. 4-(Trifluoromethyl)benzohydrazide (1a)

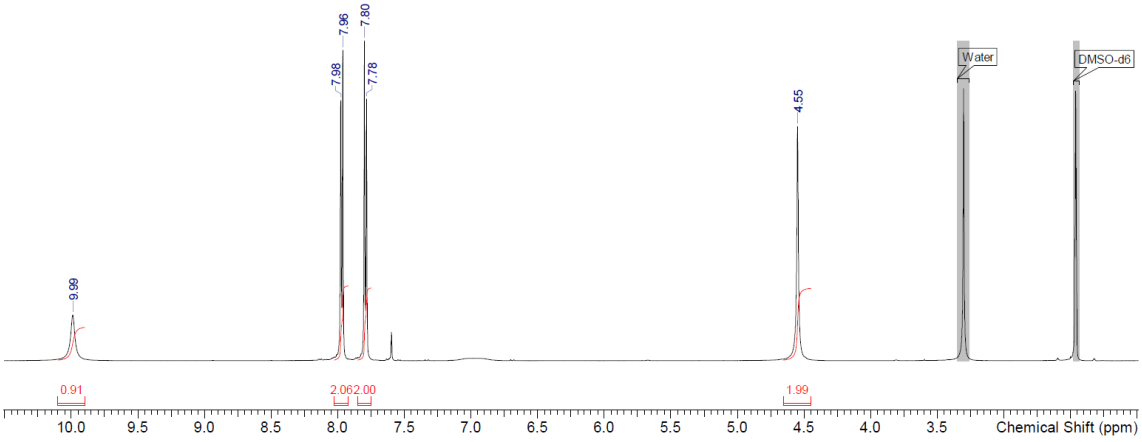


2.1.1. ^{1}H NMR

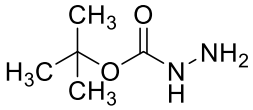
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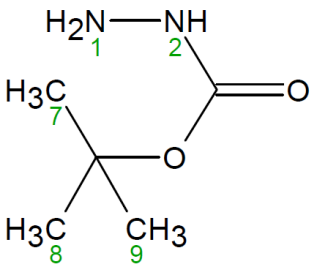
2.2. *Tert*-butyl hydrazinecarboxylate (1b)

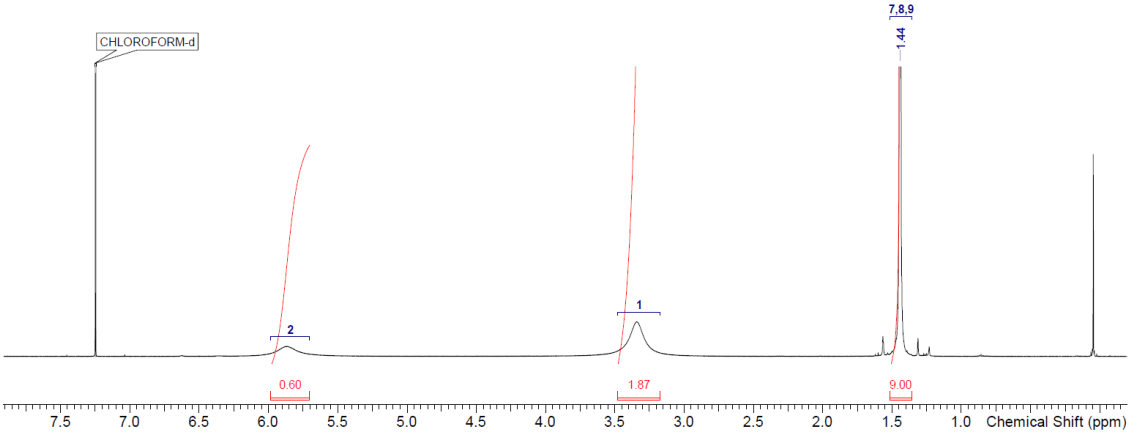


2.2.1. ^{1}H NMR

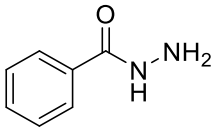
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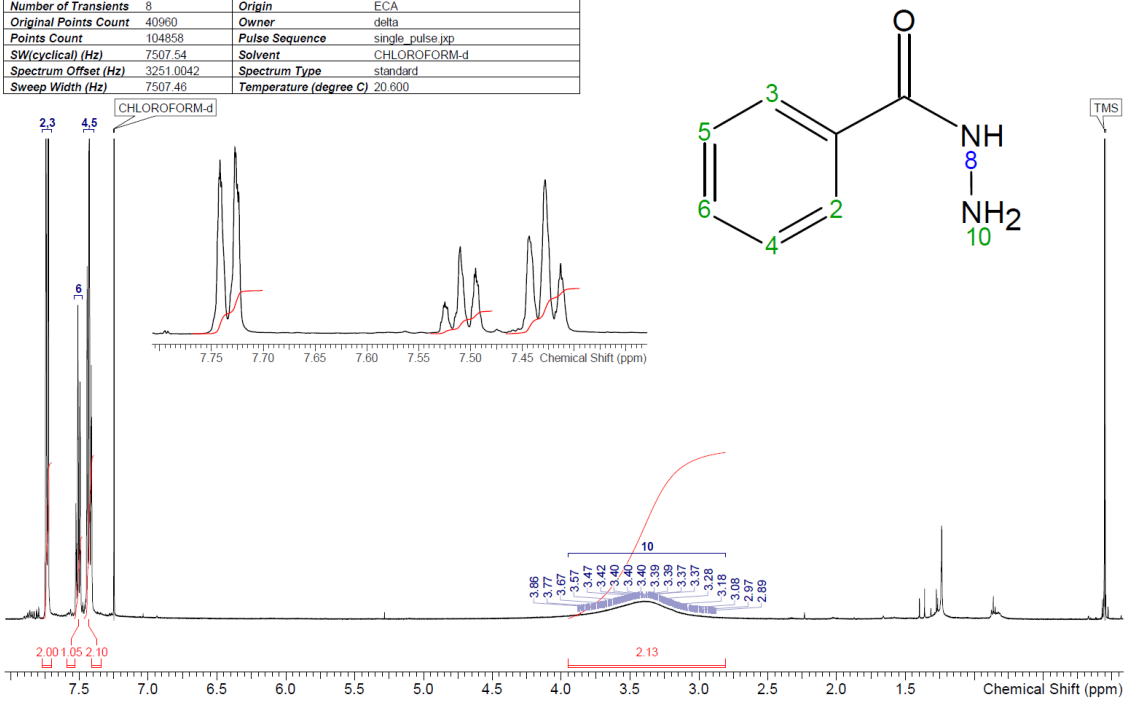
2.3. Benzohydrazide (1c)



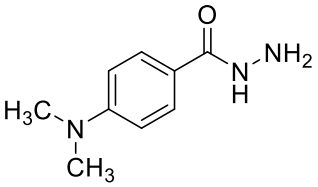
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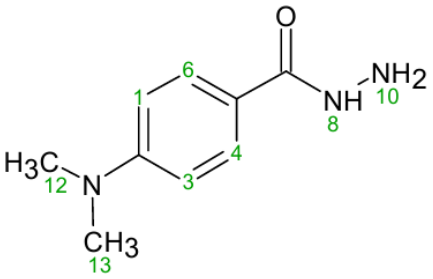
2.4. 4-(Dimethylamino)benzohydrazide (1d)

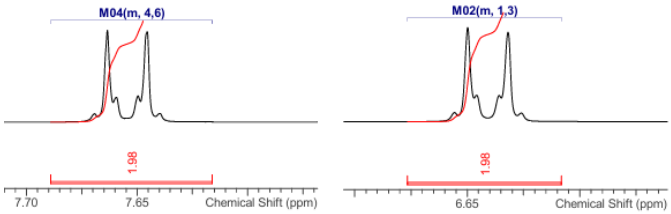


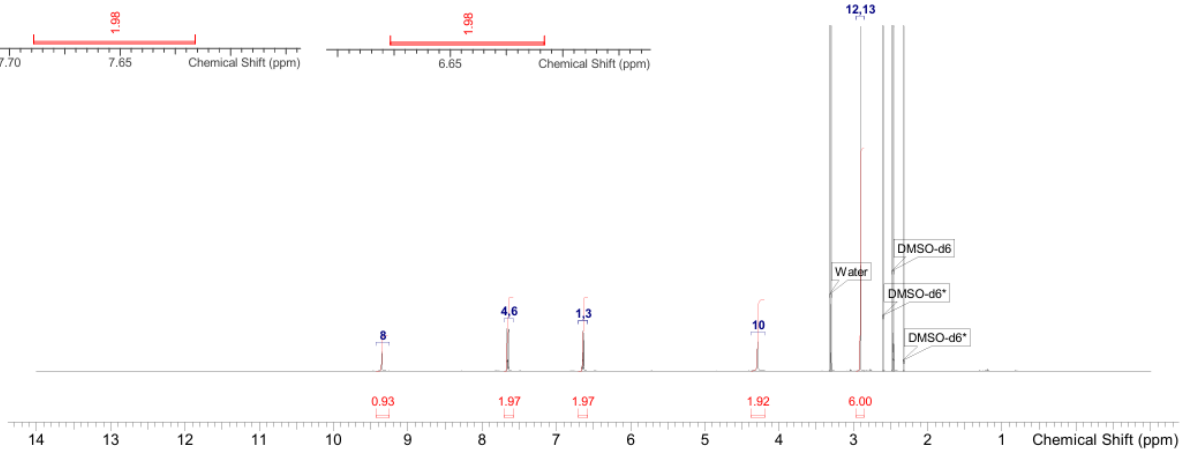
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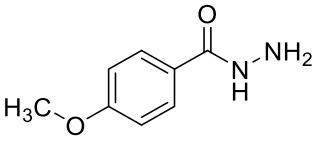
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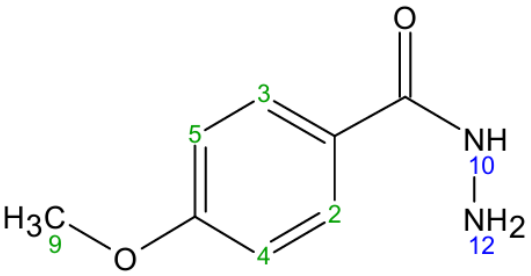
2.5. 4-Methoxybenzohydrazide (1e)

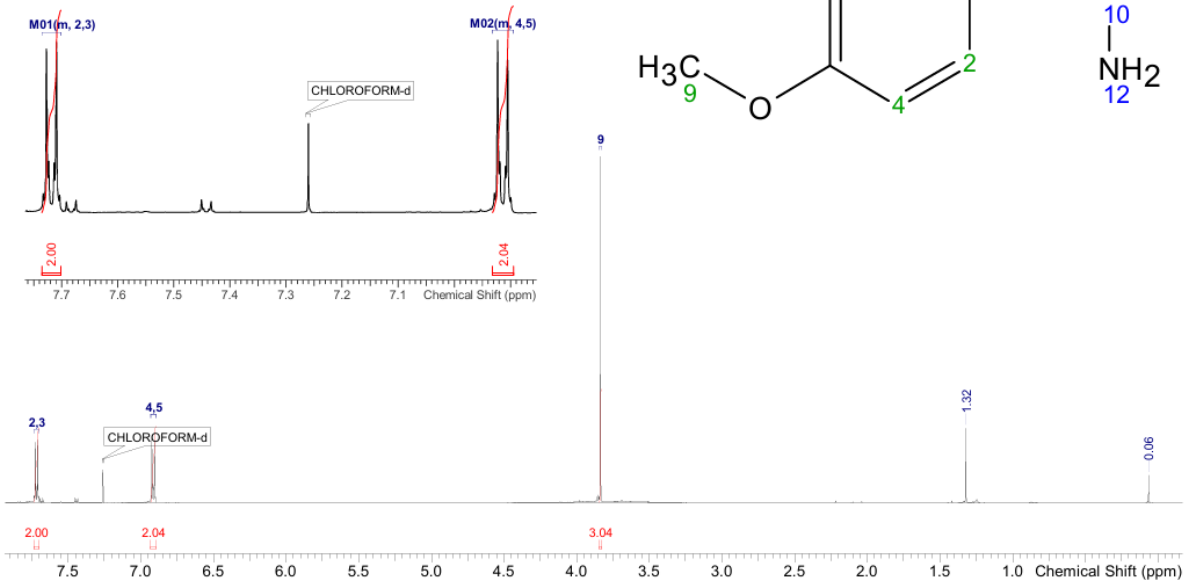


2.5.1. ^{1}H NMR

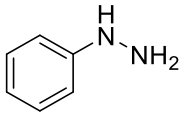
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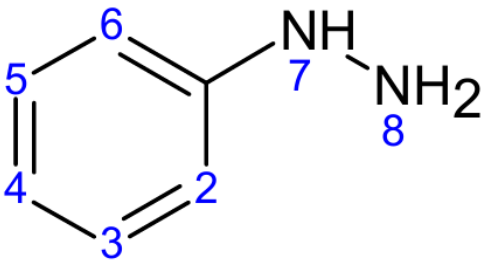
2.6. Phenylhydrazine (1f)

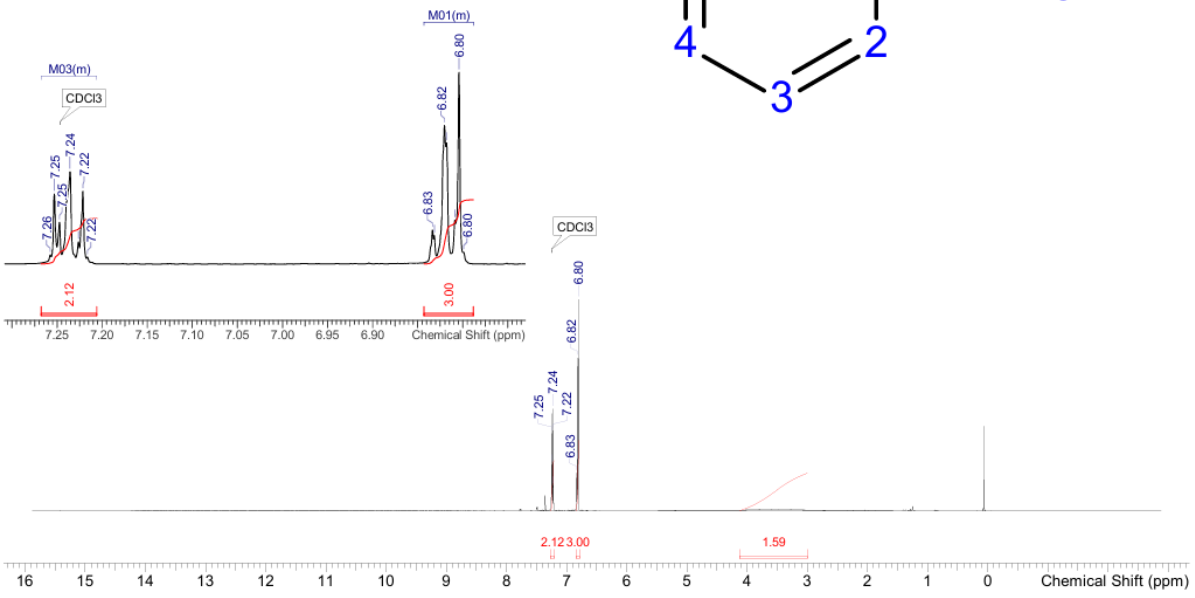


2.6.1. ^{1}H NMR

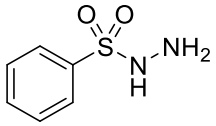
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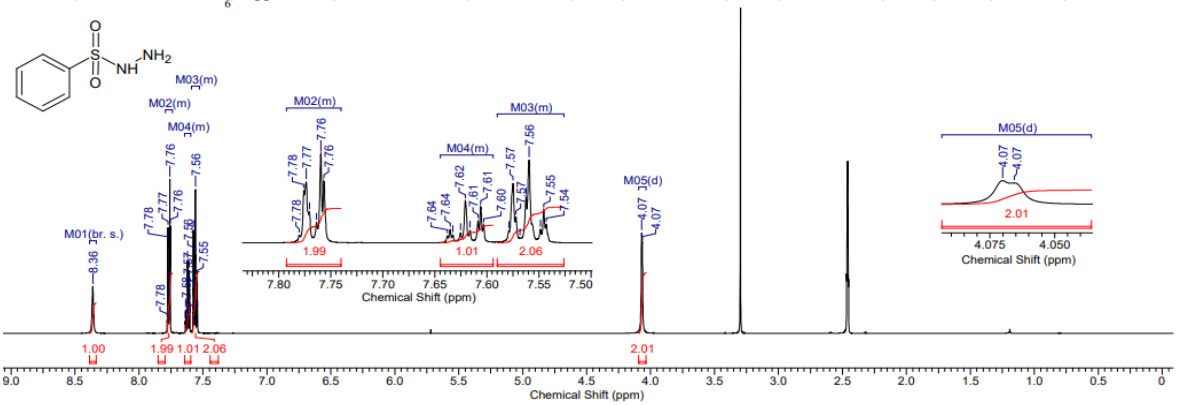
2.7. Benzenesulfonohydrazide (1g)



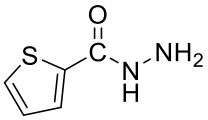
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^{1}H NMR (500 MHz, DMSO-d_6) δ ppm 4.07 (d, J=2.29 Hz, 1 H), 7.53 - 7.59 (m, 2 H), 7.59 - 7.64 (m, 1 H), 7.74 - 7.79 (m, 2 H), 8.36 (br. s., 1 H)



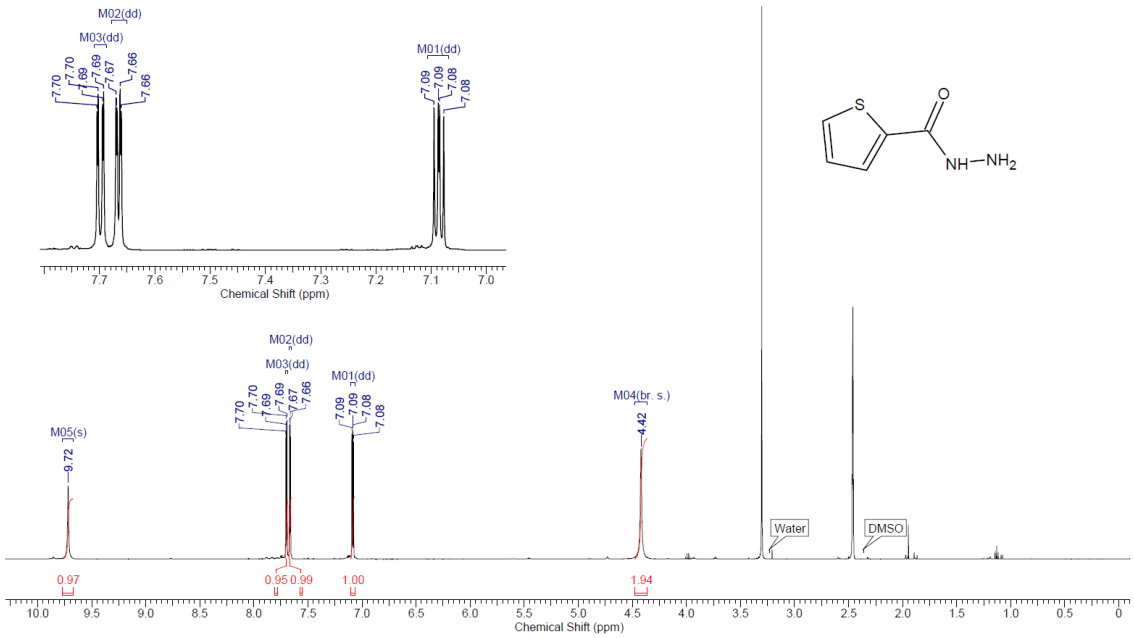
2.8. Thiophenecarbonylhydrazide (1h)



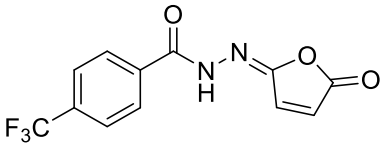
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05.12.2025 01:20:53

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File Name	C:\Users\Admin\OneDrive - Uniwersytet Jagielloński\nmr\2025\Tiof-hydrazyd_935_03_PROTON-1-1.jdf					**Frequency (MHz)**	500.16
Nucleus	1H	**Number of Transients**	8	**Origin**	ECA	**Original Points Count**	19225
Owner	delta	**Points Count**	131072	**Pulse Sequence**	single_pulse.jxp	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	3251.0396	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	9387.80	**Temperature (degree C)**	20.800



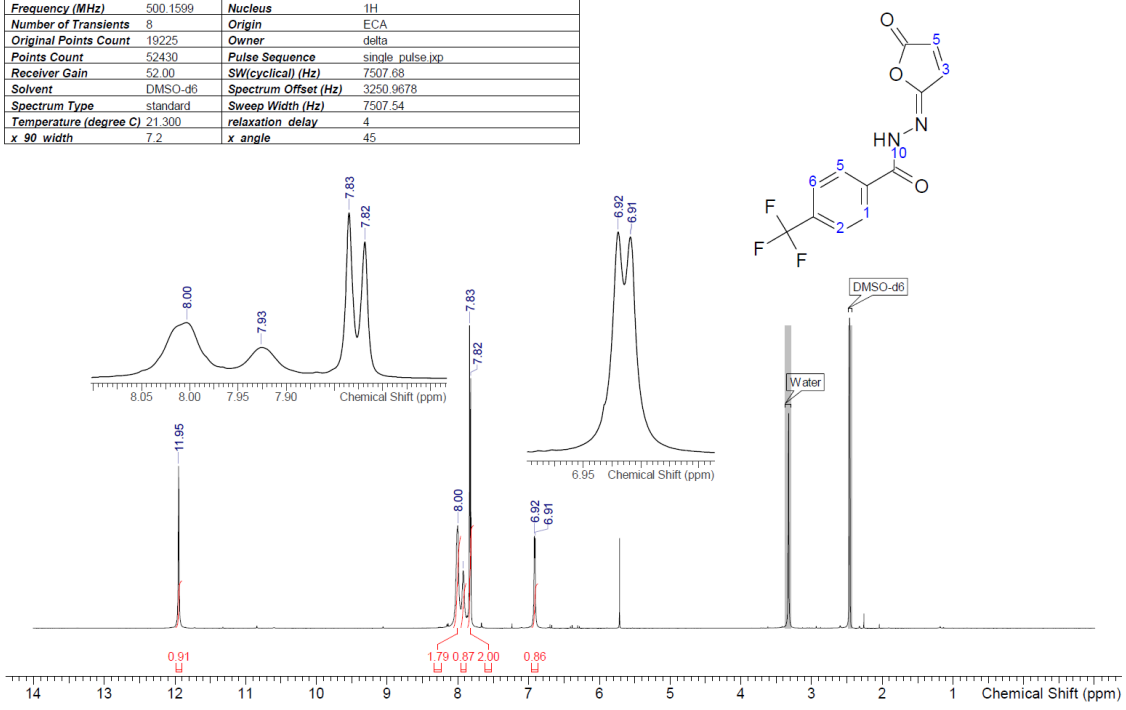
2.9. *N*'-(5-Oxofuran-2(5H)-ylidene)-4-(trifluoromethyl)benzohydrazide (2a)



2.9.1. ^{1}H NMR

Acquisition Time (sec)	2.0486	*Date*	21 Oct 2025 08:08:14
Date Stamp	21 Oct 2025 08:07:23		
File Name	E:\tekowirymat_LCMS\widma_brakujące\CFizomal-DMSO_935_03_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	*Nucleus*	1H
Number of Transients	8	*Origin*	ECA
Original Points Count	19225	*Owner*	delta
Points Count	52430	*Pulse Sequence*	single_pulse.jxp
Receiver Gain	52.00	*SW(cyclical) (Hz)*	7507.68
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	3250.9678
Spectrum Type	standard	*Sweep Width (Hz)*	7507.54
Temperature (degree C)	21.300	*relaxation_delay*	4
x_90_width	7.2	*x_angle*	45

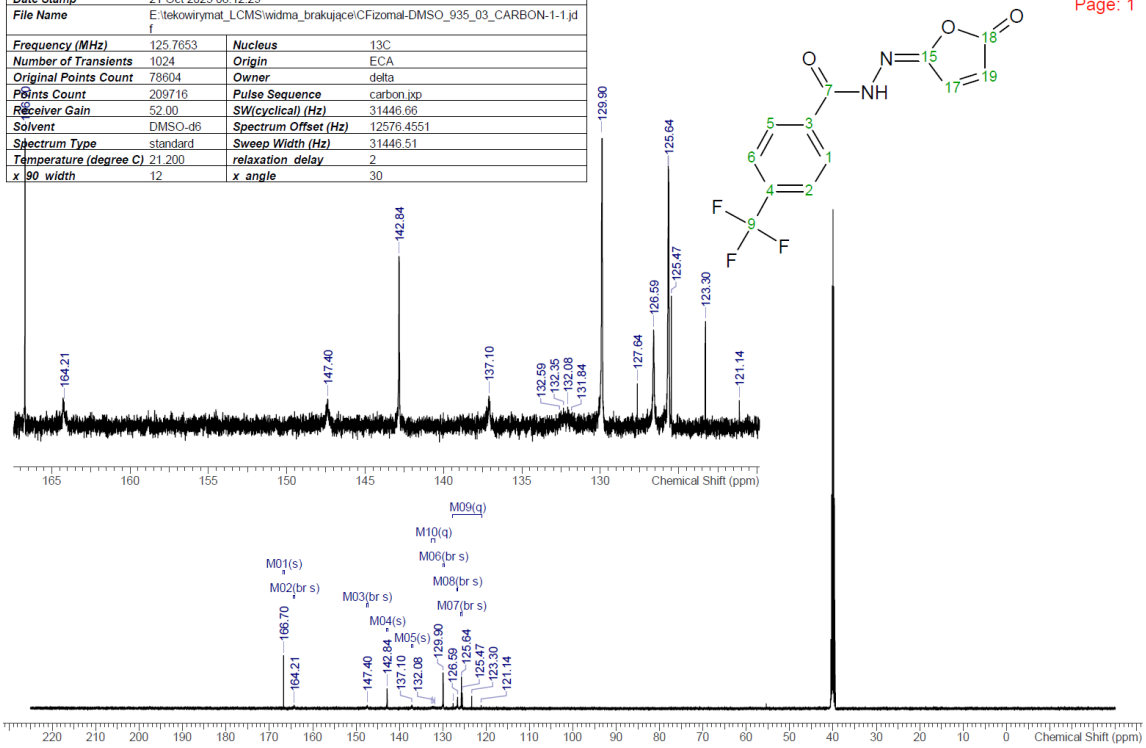
Date (dd/mm/yyyy): 19 11 2025
Page: 1



2.9.2. ^{13}C NMR

Acquisition Time (sec)	1.9997	*Date*	21 Oct 2025 09:21:05
Date Stamp	21 Oct 2025 08:12:29		
File Name	E:\tekowirymat_LCMS\widma_brakujące\CFizomal-DMSO_935_03_CARBON-1-1.jdf		
Frequency (MHz)	125.7653	*Nucleus*	13C
Number of Transients	1024	*Origin*	ECA
Original Points Count	78604	*Owner*	delta
Points Count	209716	*Pulse Sequence*	carbon.jxp
Receiver Gain	52.00	*SW(cyclical) (Hz)*	31446.66
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	12576.4551
Spectrum Type	standard	*Sweep Width (Hz)*	31446.51
Temperature (degree C)	21.200	*relaxation_delay*	2
x_90_width	12	*x_angle*	30

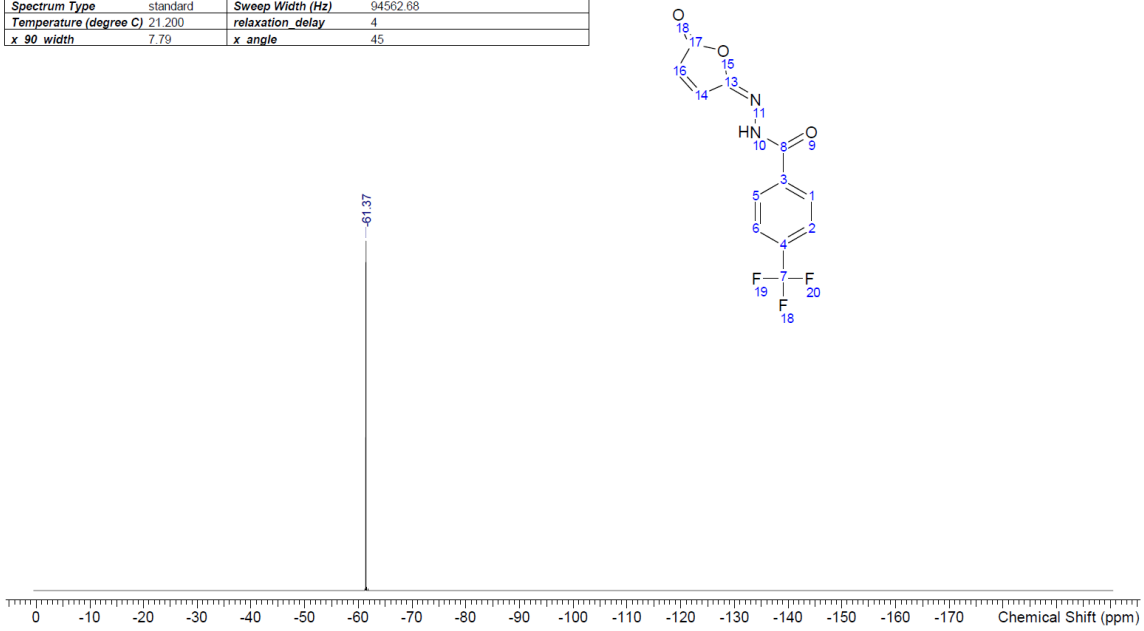
Date (dd/mm/yyyy): 20 11 2025
Page: 1



2.9.3. ^{19}F NMR

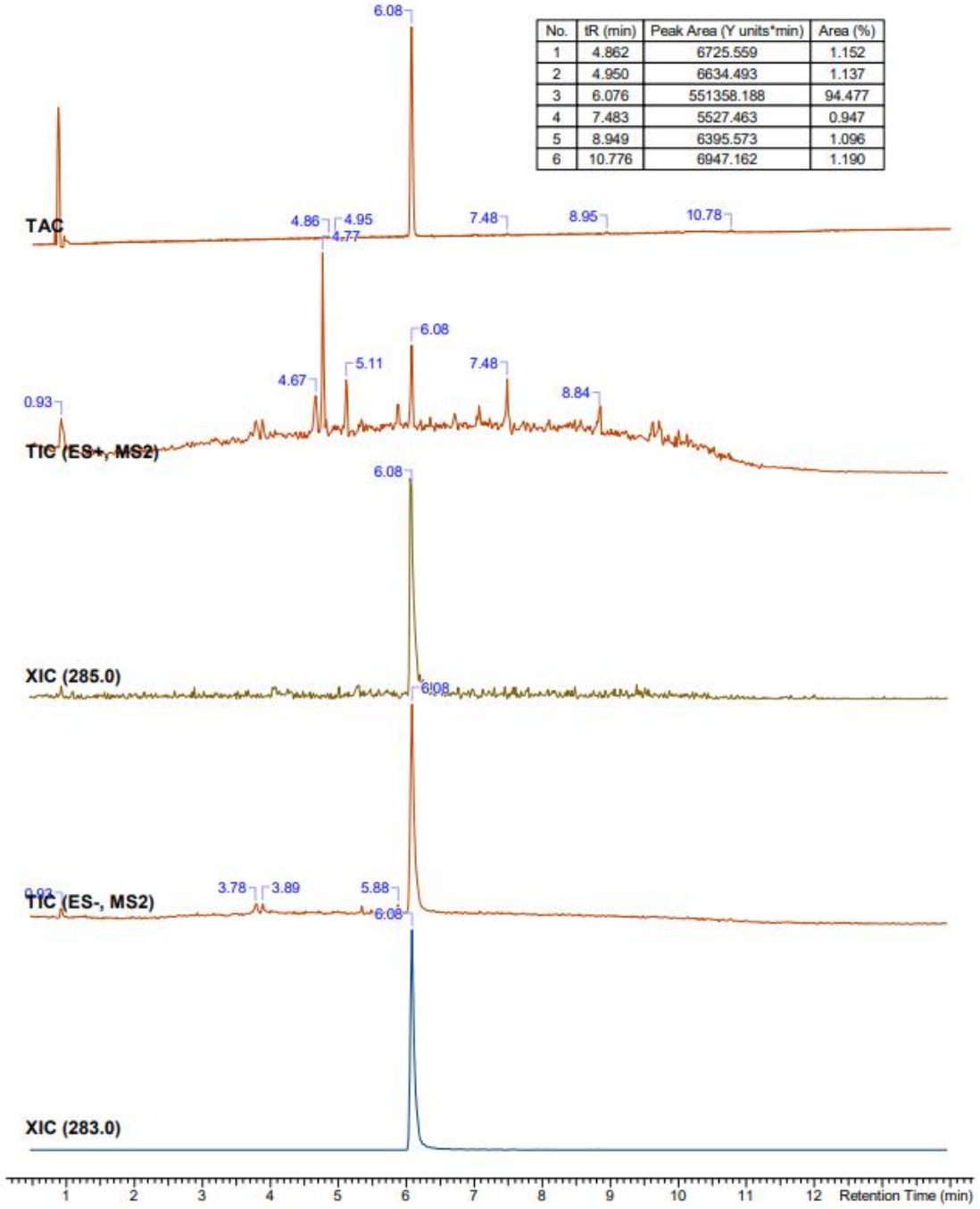
Acquisition Time (sec)	2.9861	*Date*	21 Oct 2025 08:10:54
Date Stamp	21 Oct 2025 08:09:52		
File Name	E:\tekowirymat_LCMS\widma_brakujące\CFizomal-DMSO_935_03_Fluorine-1-1.jdf		
Frequency (MHz)	470.6205	*Nucleus*	19F
Number of Transients	8	*Origin*	ECA
Original Points Count	352967	*Owner*	delta
Points Count	838862	*Pulse Sequence*	single_pulse.jxp
Receiver Gain	62.00	*SW(cyclical) (Hz)*	94562.79
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	-47062.1016
Spectrum Type	standard	*Sweep Width (Hz)*	94562.68
Temperature (degree C)	21.200	*relaxation_delay*	4
x_90_width	7.79	*x_angle*	45

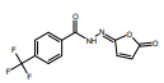
Date (dd/mm/yyyy): 19 11 2025
Page: 1

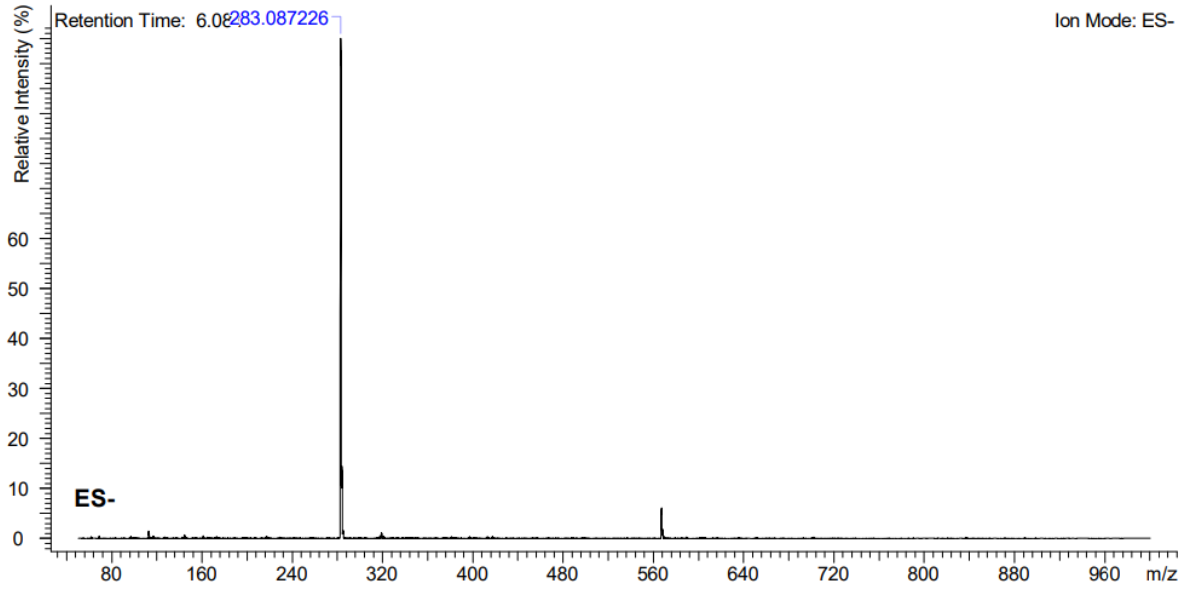


2.9.4. LCMS

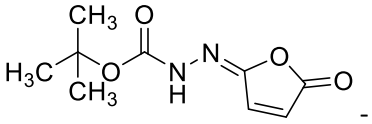
No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	4.862	6725.559	1.152
2	4.950	6634.493	1.137
3	6.076	551358.188	94.477
4	7.483	5527.463	0.947
5	8.949	6395.573	1.096
6	10.776	6947.162	1.190



Compor	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	M+·	M-·	MF	Structure	Area (%)
1	6.076	284.041	285.048	283.034	284.040	284.041	$C_{12}H_7F_3N_2O_3$		TIC (ES-, MS2) = 89.94 Single XIC = 100.00 TIC (ES+, MS2) = 15.54 Single XIC = 100.00 TAC = 94.48


Retention Time: 6.0
283.087226
Ion Mode: ES-
Relative Intensity (%)
60
50
40
30
20
10
0
ES-
80
160
240
320
400
480
560
640
720
800
880
960
m/z

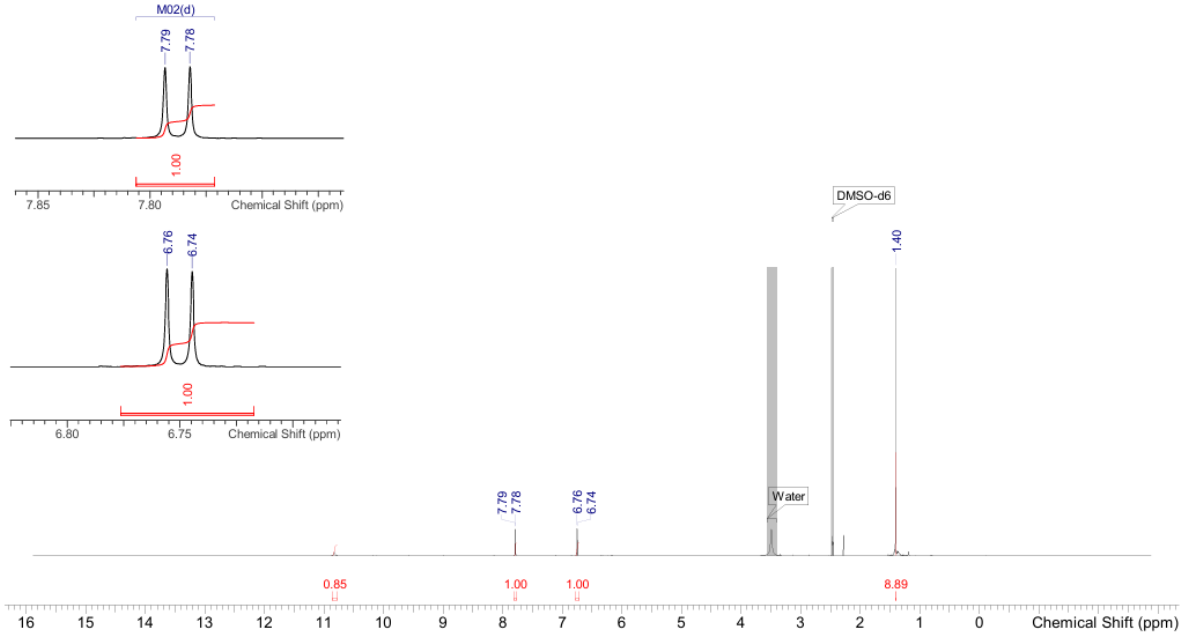
2.10. *Tert*-butyl 2-(5-oxofuran-2(*5H*)-ylidene)hydrazine-1-carboxylate (2b)



2.10.1. ^{1}H NMR

Acquisition Time (sec)	1.9984	*Date*	15 Nov 2023 09:18:09
Date Stamp	15 Nov 2023 09:17:30		
File Name	\\AppServerM9\Wyniki_NMR_43_\2023\KPS23-5_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	*Nucleus*	1H
Number of Transients	8	*Origin*	ECA
Original Points Count	18757	*Owner*	delta
Points Count	131072	*Pulse Sequence*	single_pulse.jxp
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	3251.0396
Spectrum Type	STANDARD	*Sweep Width (Hz)*	9385.89
Temperature (degree C)	20.700		

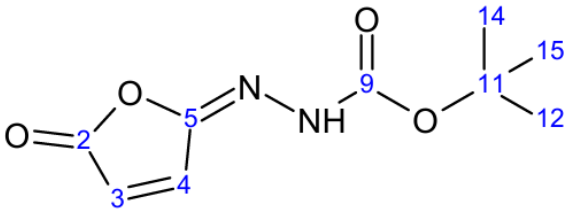
Date (dd/mm/yyyy): 28 10 2025
Page: 1

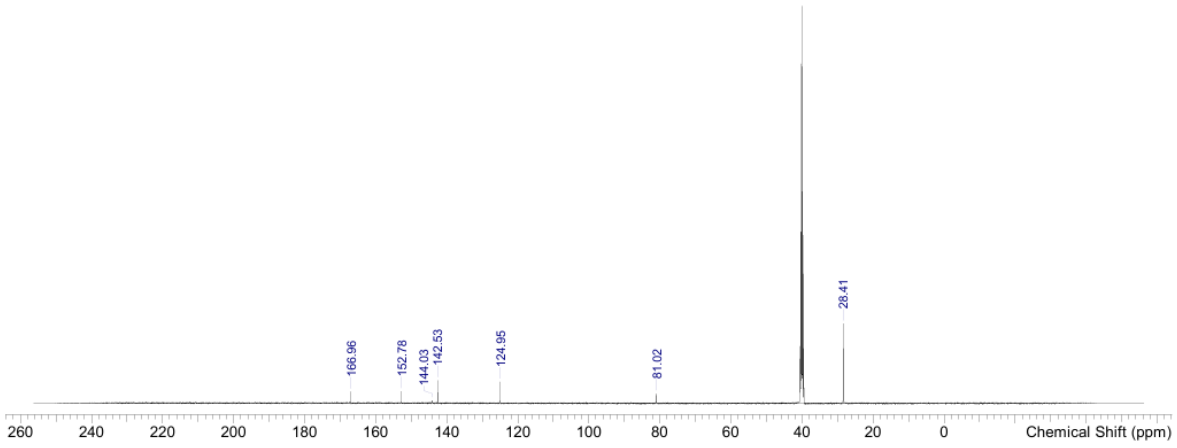


2.10.2. ^{13}C NMR

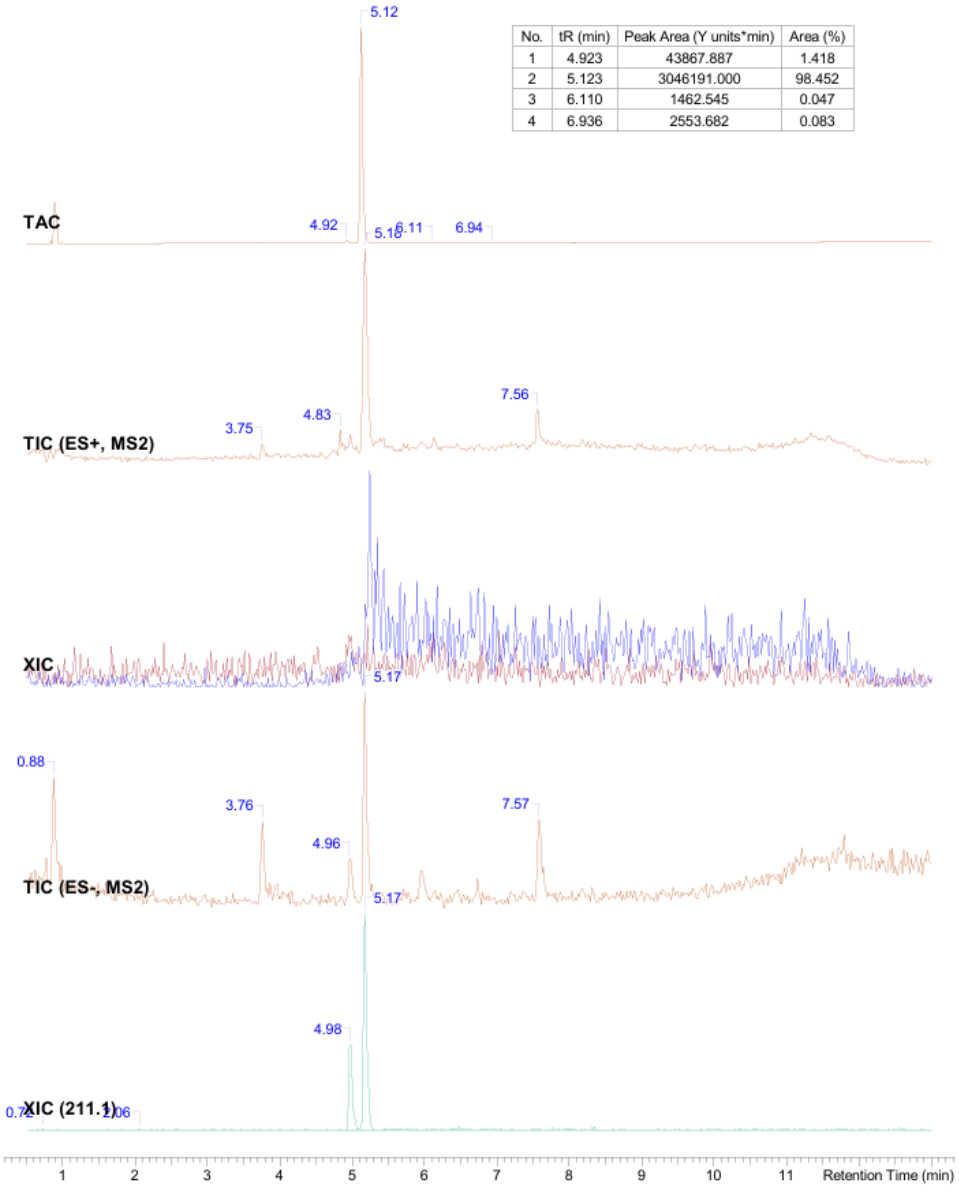
Acquisition Time (sec)	1.9996	***Date***	15 Nov 2023 10:10:44
Date Stamp	15 Nov 2023 09:18:41		
File Name	\\AppServerM9\Wyniki_NMR_43_\2023\KPS23-5_935_43_CARBON-1-1.jdf		
Frequency (MHz)	125.7653	***Nucleus***	13C
Number of Transients	1024	***Origin***	ECA
Original Points Count	78604	***Owner***	delta
Points Count	131072	***Pulse Sequence***	carbon.jxp
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	12576.5293
Sweep Width (Hz)	39310.18	***Temperature (degree C)***	20.800

Date (dd/mm/yyyy): 28 10 2025
Page: 1

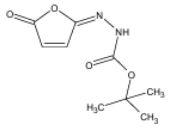


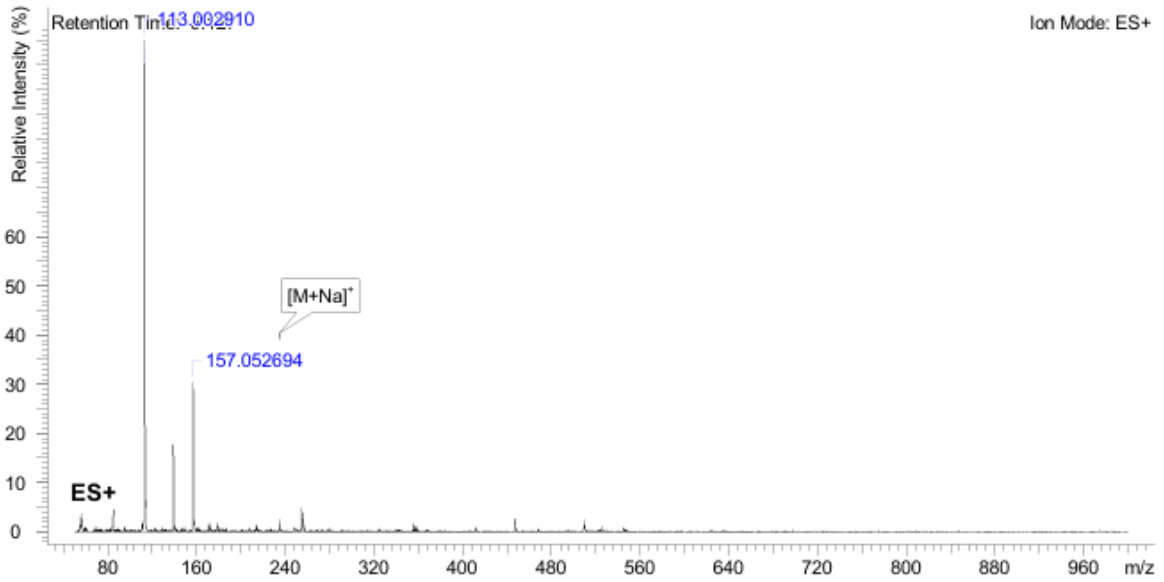


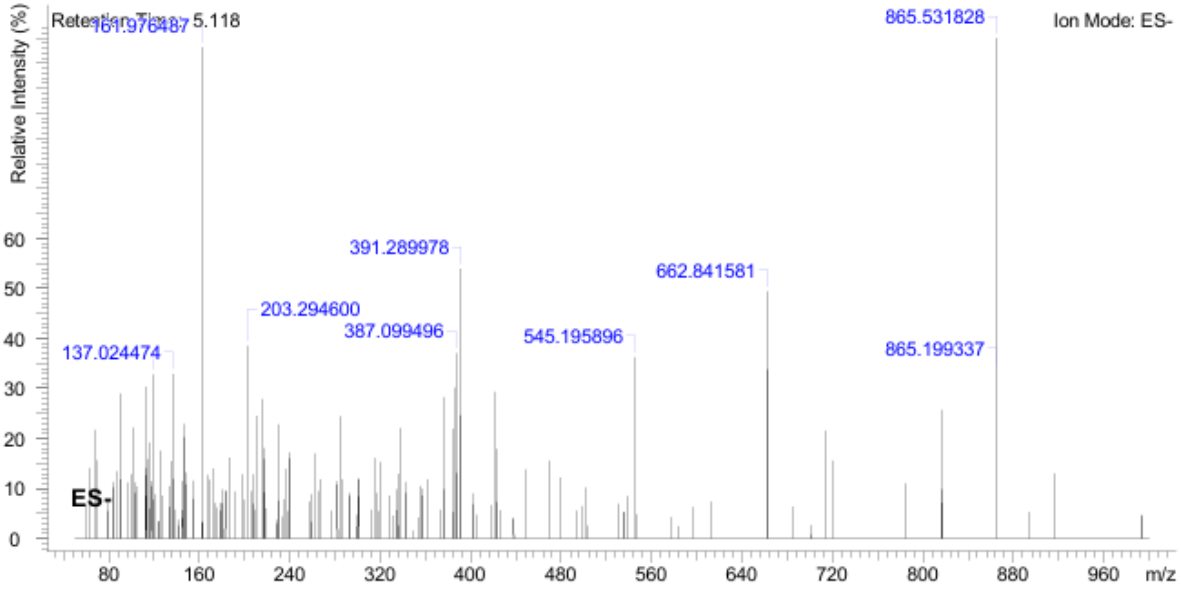
2.10.3. LCMS



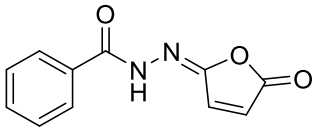
No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	4.923	43867.887	1.418
2	5.123	3046191.000	98.452
3	6.110	1462.545	0.047
4	6.936	2553.682	0.083

Compor	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	M+·	M-·	MF	Structure	Area (%)
1	5.123	212.080	213.087	211.072	212.079	212.080	$C_9H_{12}N_2O_4$		TIC (ES-, MS2) = 37.19 Single XIC = 70.05 TIC (ES+, MS2) = 72.48 TAC = 98.45


Retention Time: 0.122
113.092910
Ion Mode: ES+
Relative Intensity (%)
[M+Na]+
157.052694
ES+
m/z


Retention Time: 5.118
161.976487
865.531828
Ion Mode: ES-
Relative Intensity (%)
391.289978
662.841581
203.294600
387.099496
545.195896
137.024474
865.199337
ES-
m/z

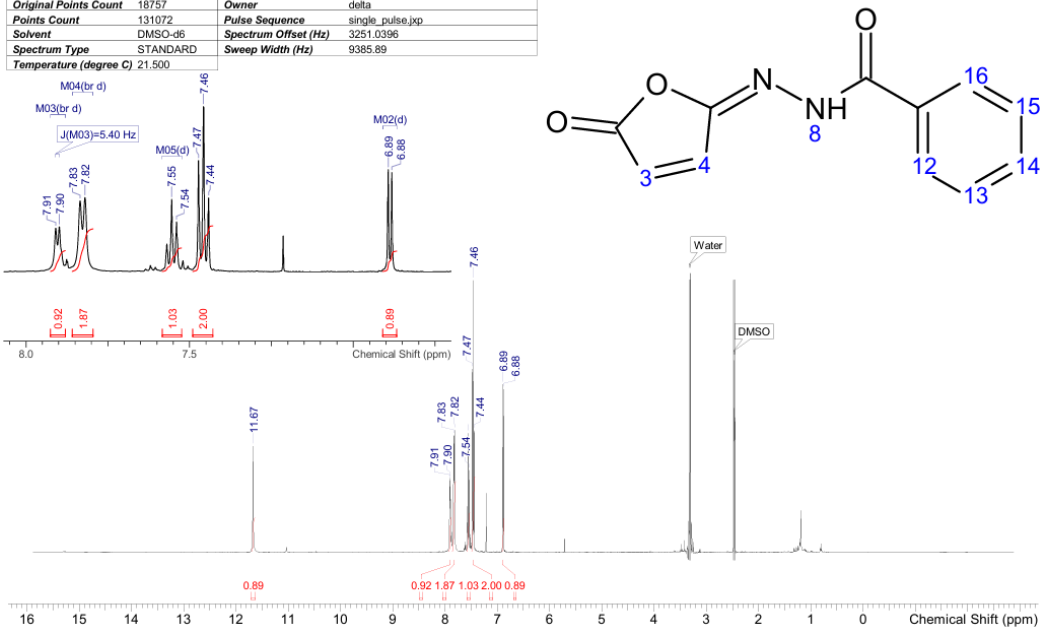
2.11.*N*'-(5-Oxofuran-2(5*H*)-ylidene)benzohydrazide (2c)



2.11.1. ^{1}H NMR

Acquisition Time (sec)	1.9984	*Date*	15 Nov 2023 08:22:18
Date Stamp	15 Nov 2023 08:21:39		
File Name	\\AppServerM9\Wyniki_NMR_43_\2023\KPS-15_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	*Nucleus*	1H
Number of Transients	8	*Origin*	ECA
Original Points Count	18757	*Owner*	delta
Points Count	131072	*Pulse Sequence*	single_pulse.jxp
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	3251.0396
Spectrum Type	STANDARD	*Sweep Width (Hz)*	9385.89
Temperature (degree C)	21.500		

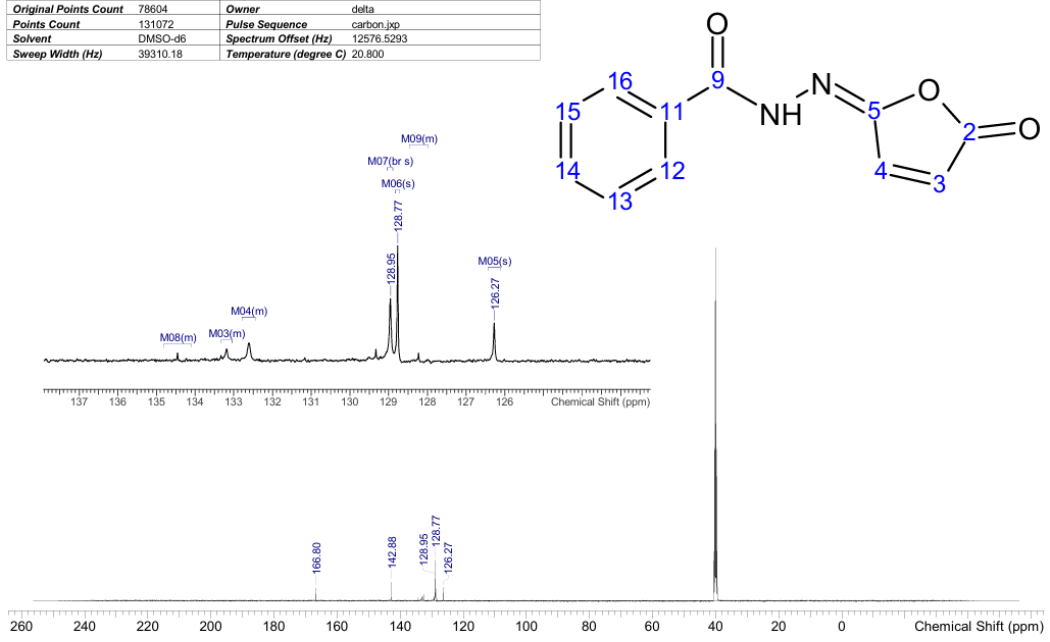
Date (dd/mm/yyyy): 29 10 2025
Page: 1



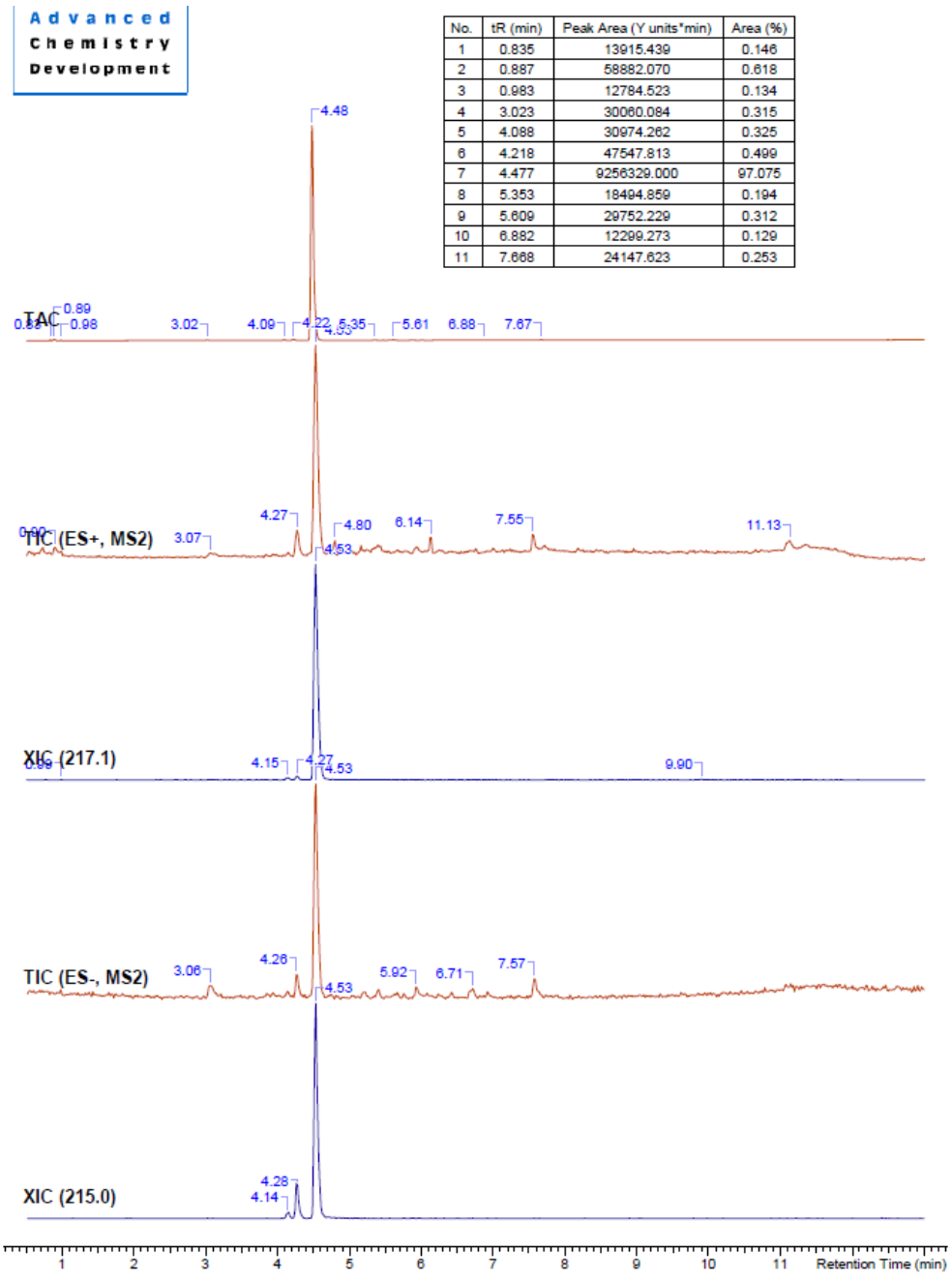
2.11.2. ^{13}C NMR

Acquisition Time (sec)	1.9996	*Date*	15 Nov 2023 09:14:52
Date Stamp	15 Nov 2023 08:22:49		
File Name	\\AppServerM9\Wyniki_NMR_43_\2023\KPS-15_935_43_CARBON-1-1.jdf		
Frequency (MHz)	125.7653	*Nucleus*	13C
Number of Transients	1024	*Origin*	ECA
Original Points Count	78604	*Owner*	delta
Points Count	131072	*Pulse Sequence*	carbon.jxp
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	12576.5293
Sweep Width (Hz)	39310.18	*Temperature (degree C)*	20.800

Date (dd/mm/yyyy): 29 10 2025
Page: 1

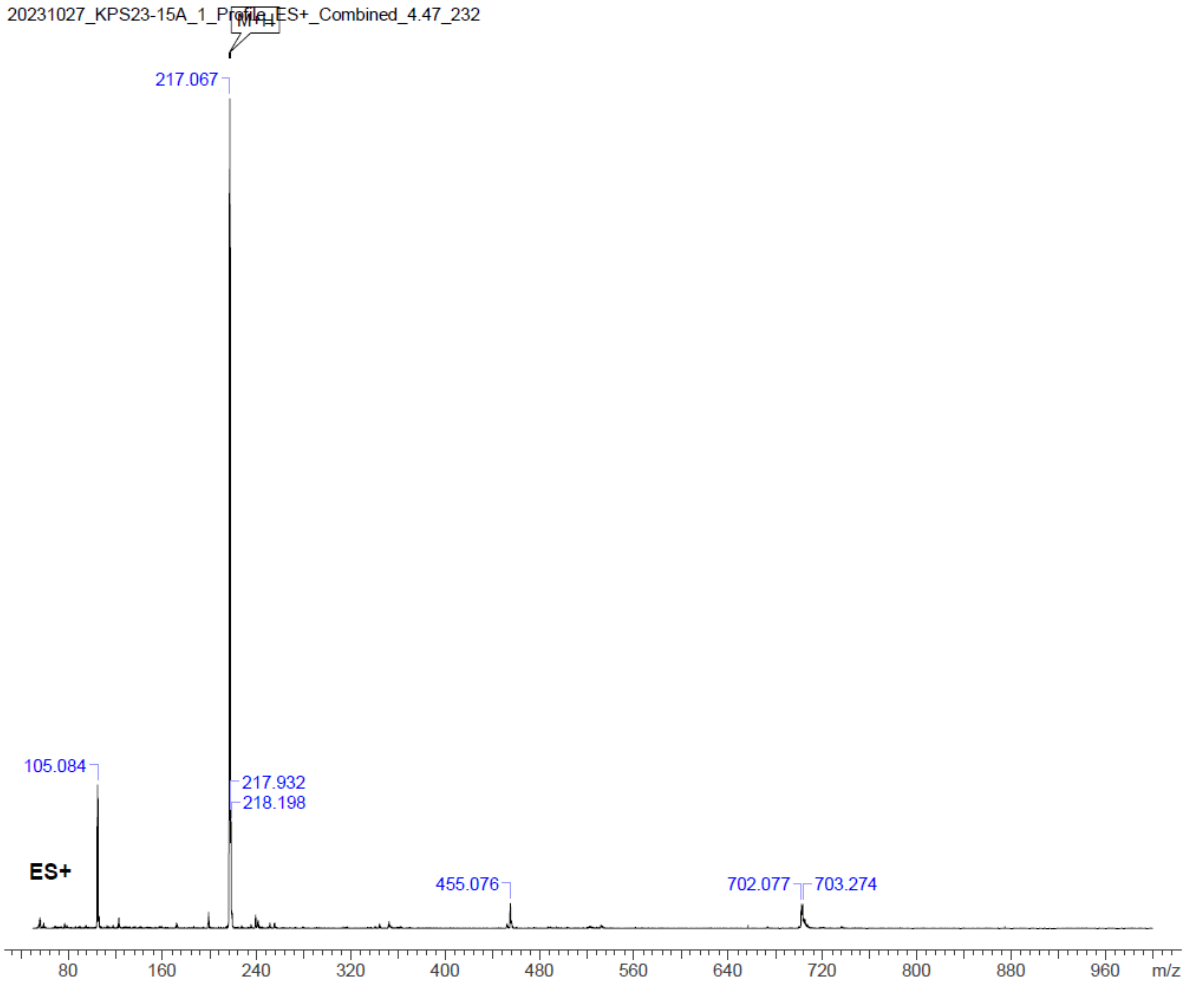


2.11.3. LCMS

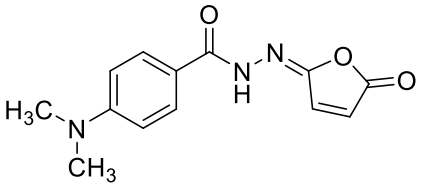


No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	0.835	13915.439	0.146
2	0.887	58882.070	0.618
3	0.983	12784.523	0.134
4	3.023	30060.084	0.315
5	4.088	30974.262	0.325
6	4.218	47547.813	0.499
7	4.477	9256329.000	97.075
8	5.353	18494.859	0.194
9	5.609	29752.229	0.312
10	6.882	12299.273	0.129
11	7.668	24147.623	0.253

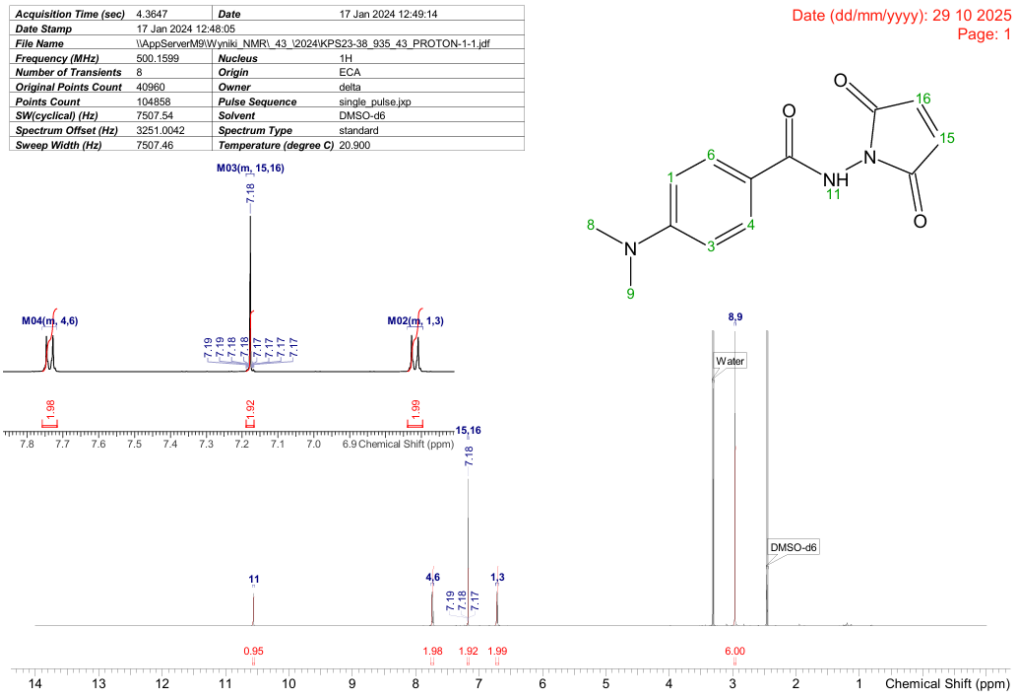
tR (min)	Mass (Ao)	[M+H]+	[M-H]-	Area (%)
4.477	216.053	217.061	215.046	TIC (ES-, MS2) = 69.94 XIC = 76.88 TIC (ES+, MS2) = 70.06 XIC = 89.10 TAC = 97.08


20231027_KPS23-15A_1_Profile_ES+_Combined_4.47_232
[M+H]+
217.067
105.084
217.932
218.198
ES+
455.076
702.077
703.274
80
160
240
320
400
480
560
640
720
800
880
960
m/z

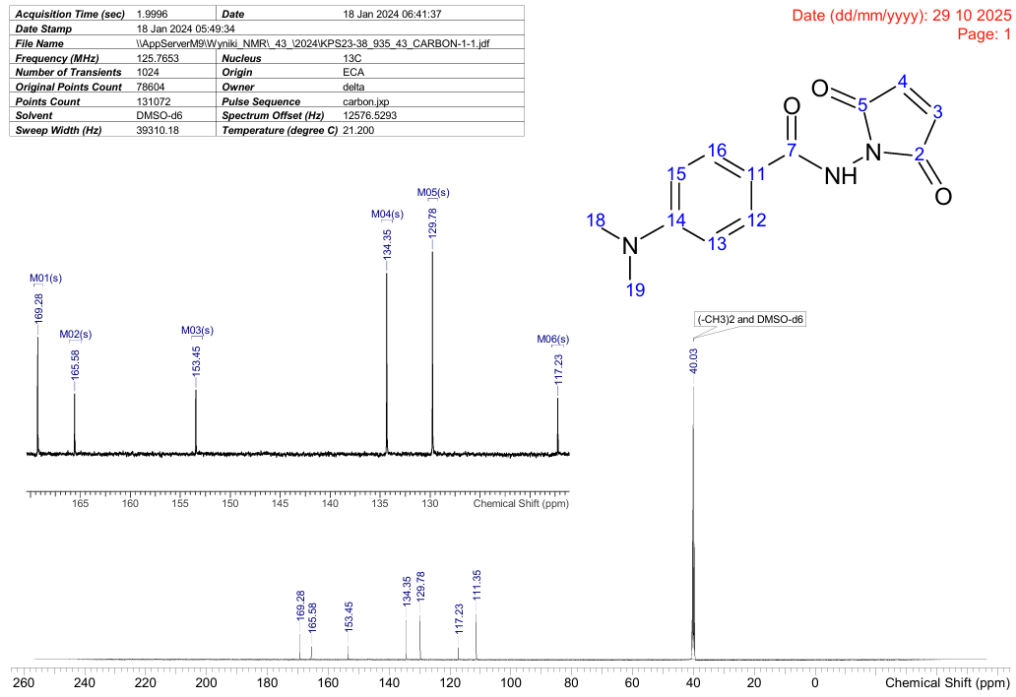
2.12.4-(Dimethylamino)-N'-(5-oxofuran-2(*5H*)-ylidene)benzohydrazide (2d)



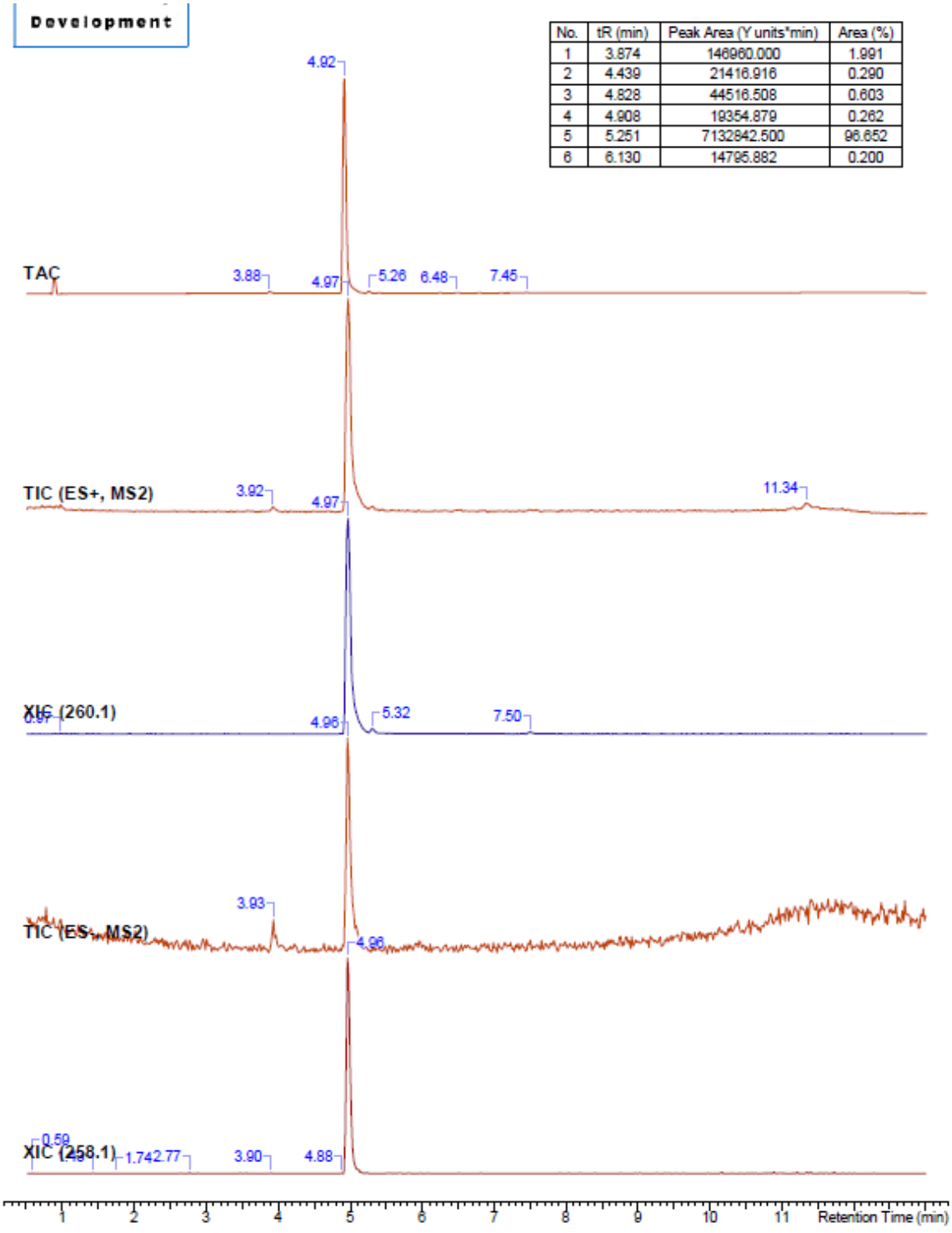
2.12.1. ^{1}H NMR



2.12.2. ^{13}C NMR

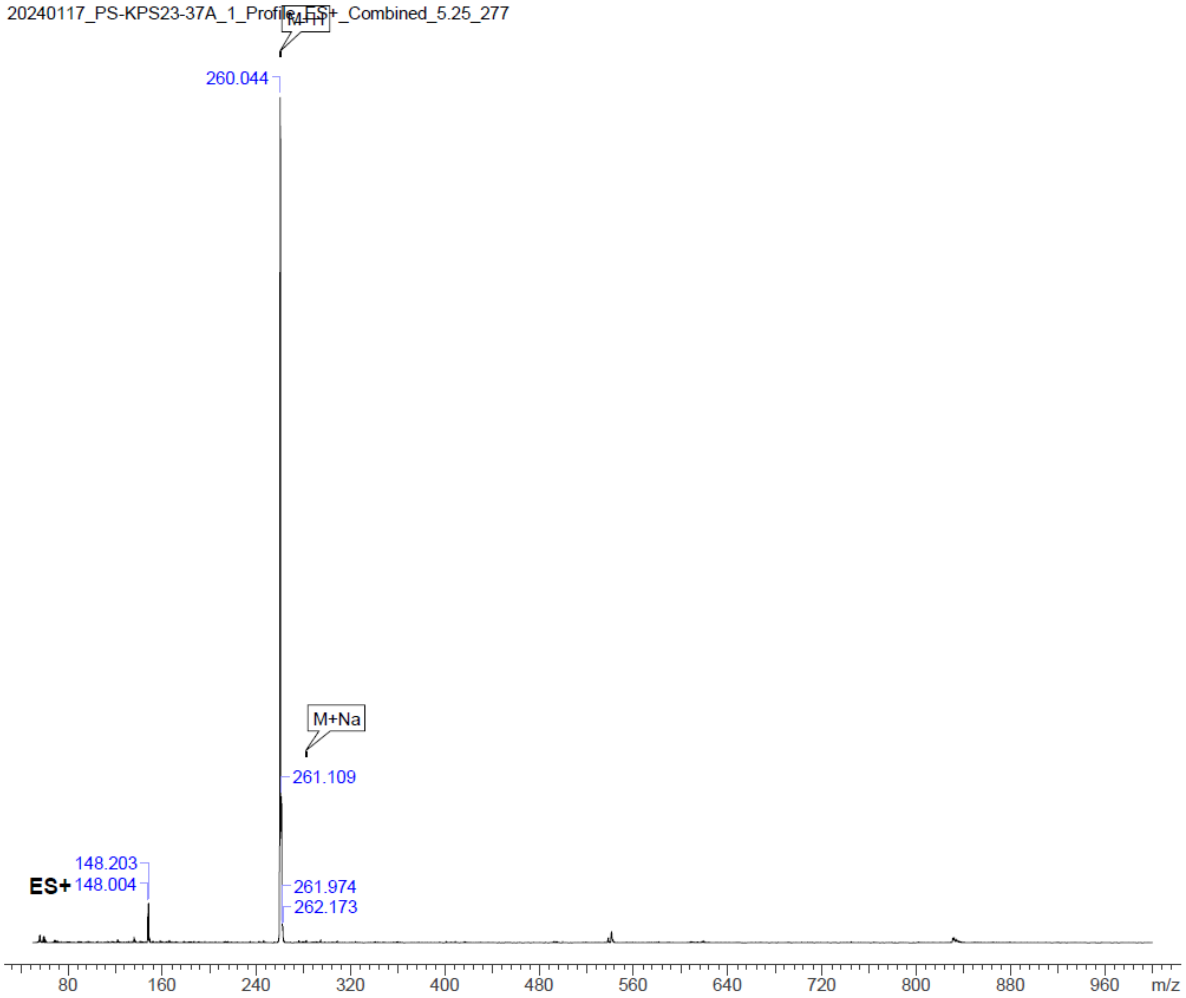


2.12.3. LCMS

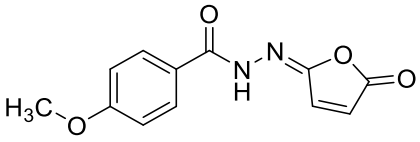


No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	3.874	146960.000	1.991
2	4.439	21416.916	0.290
3	4.828	44516.508	0.603
4	4.908	19354.879	0.262
5	5.251	7132842.500	96.652
6	6.130	14795.882	0.200

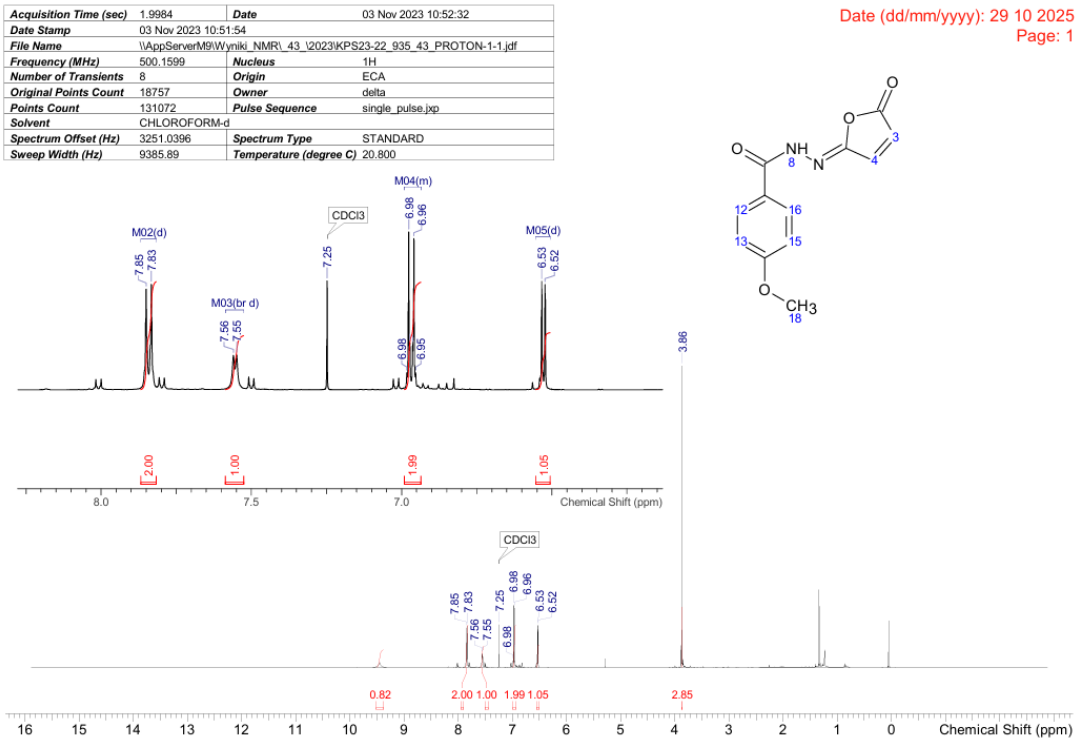
tR (min)	Mass (Ao)	[M+H]+	[M-H]-	Area (%)
5.251	259.096	260.103	258.088	TIC (ES-, MS2) = 82.72 XIC = 55.17 TIC (ES+, MS2) = 86.09 XIC = 75.98 TAC = 96.65


20240117_PS-KPS23-37A_1_Profile_ES+_Combined_5.25_277
M+H
260.044
M+Na
261.109
148.203
ES+ 148.004
261.974
262.173
80
160
240
320
400
480
560
640
720
800
880
960
m/z

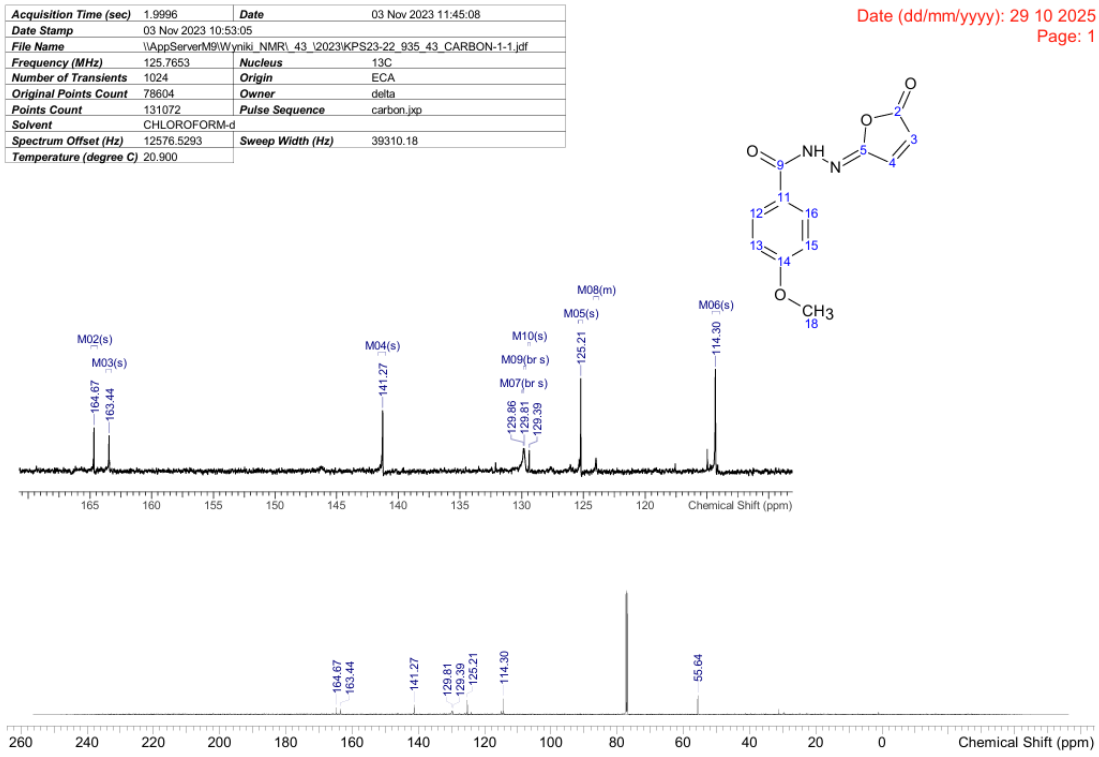
2.13.4-Methoxy-*N*'-(5-oxofuran-2(*5H*)-ylidene)benzohydrazide (2e)



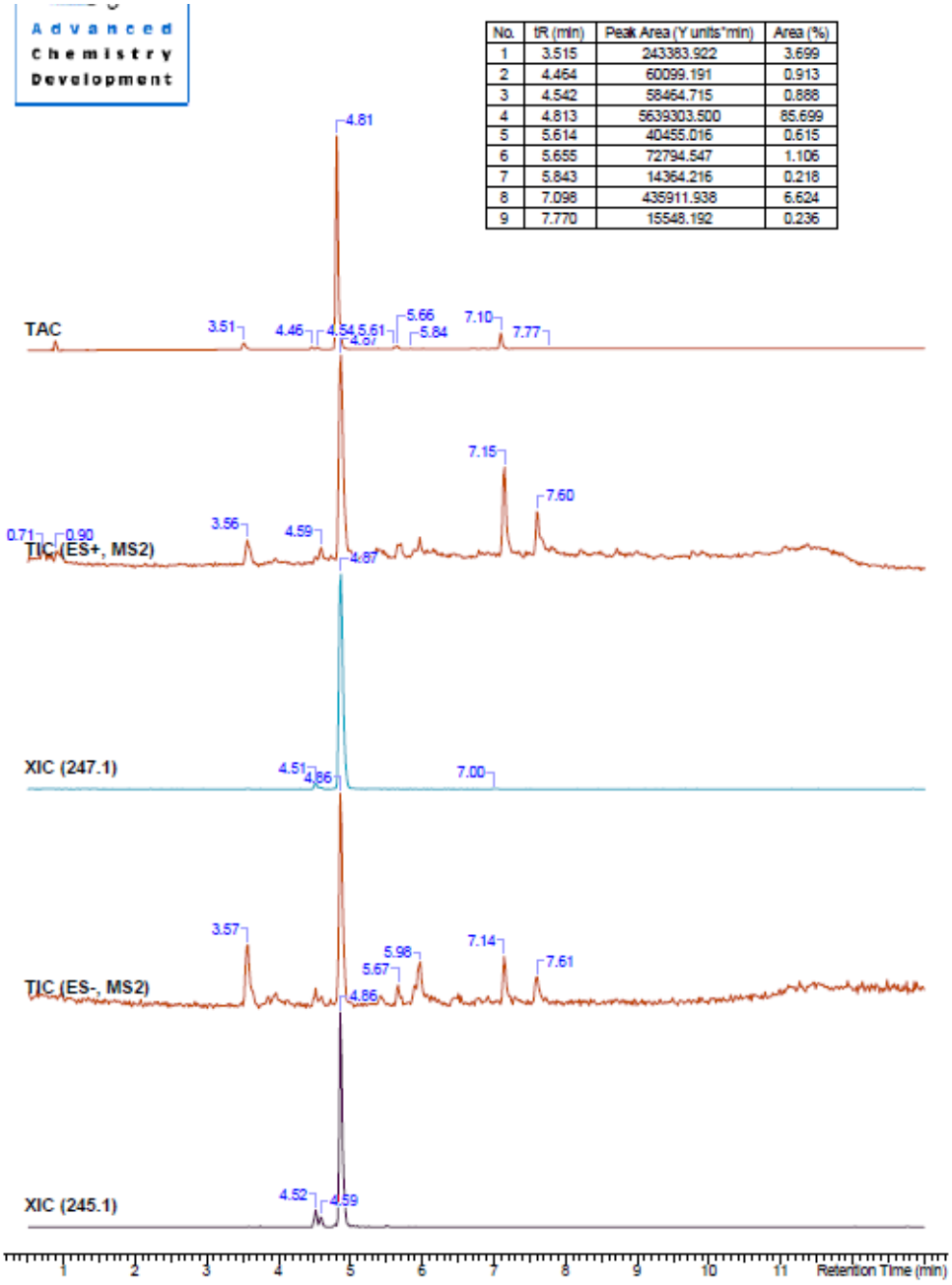
2.13.1. ^{1}H NMR



2.13.2. ^{13}C NMR

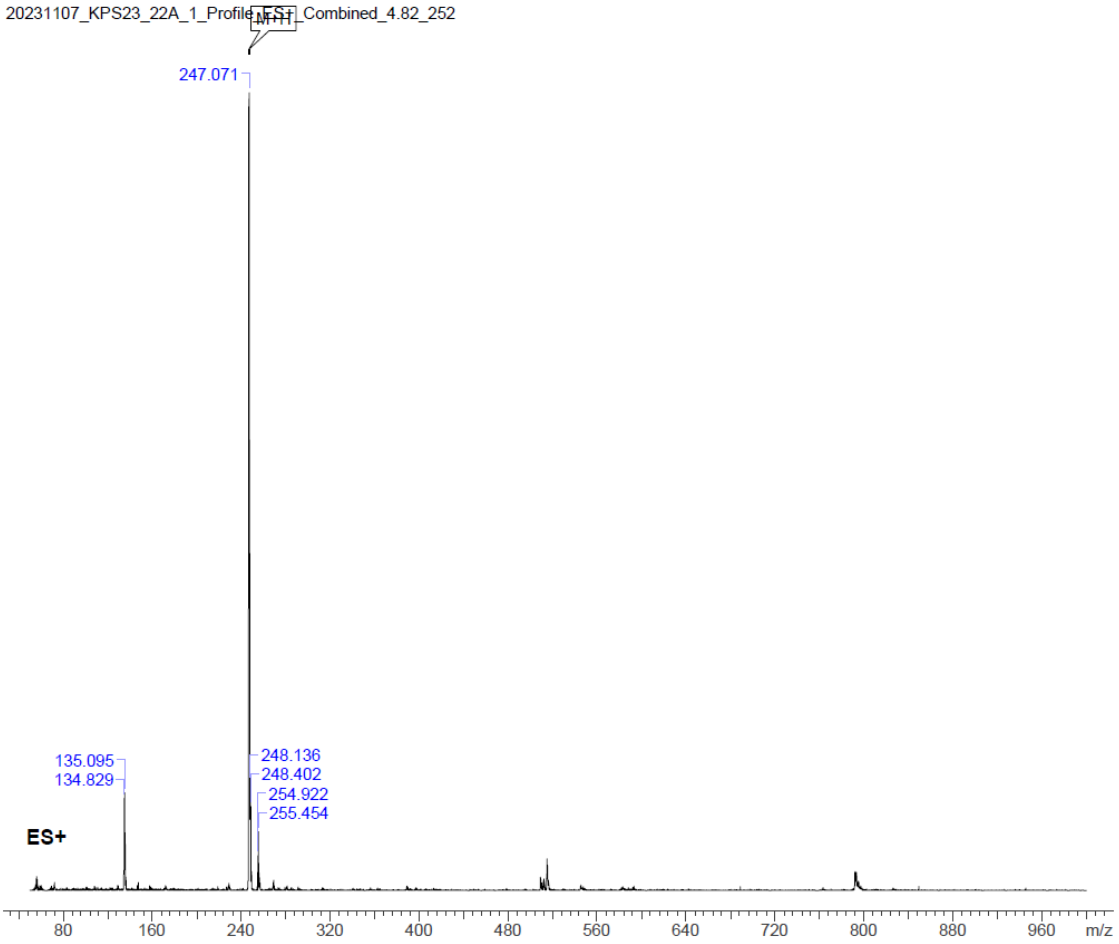


2.13.3. LCMS

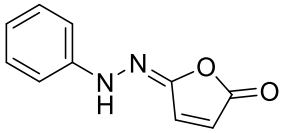


No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	3.515	243383.922	3.699
2	4.464	60099.191	0.913
3	4.542	58464.715	0.888
4	4.813	5639303.500	85.699
5	5.614	40455.016	0.615
6	5.655	72794.547	1.106
7	5.843	14364.216	0.218
8	7.098	435911.938	6.624
9	7.770	15548.192	0.236

tR (min)	Mass (Ao)	[M+H]+	[M-H]-	Area (%)
4.813	246.064	247.071	245.057	TIC (ES-, MS2) = 44.57 XIC = 79.58 TIC (ES+, MS2) = 49.85 XIC = 90.98 TAC = 85.70


20231107_KPS23_22A_1_Profile_ES+_Combined_4.82_252
MH+
247.071
135.095
134.829
248.136
248.402
254.922
255.454
ES+
80
160
240
320
400
480
560
640
720
800
880
960
m/z

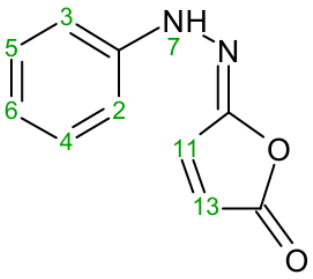
2.14.5-(2-Phenylhydrazineylidene)furan-2(*5H*)-one (2f)



2.14.1. ^{1}H NMR

Acquisition Time (sec)	4.3647	***Date***	09 Feb 2024 13:32:57
Date Stamp	09 Feb 2024 13:31:47		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS24-7-fr14-25_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	***Nucleus***	1H
Number of Transients	8	***Origin***	ECA
Original Points Count	40960	***Owner***	delta
Points Count	104858	***Pulse Sequence***	single_pulse.jxp
SW(cyclical) (Hz)	7507.54	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	3251.0042	***Spectrum Type***	standard
Sweep Width (Hz)	7507.46	***Temperature (degree C)***	20.200

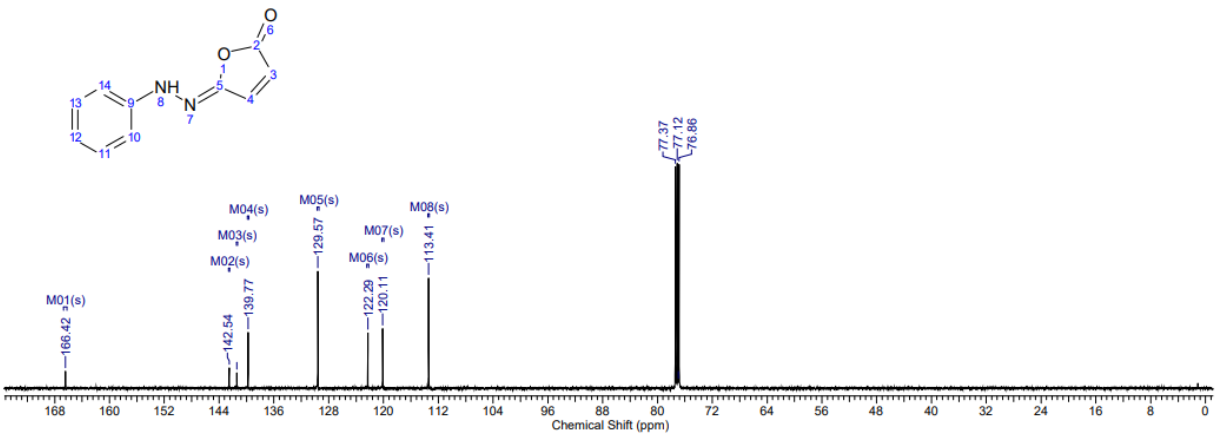
Date (dd/mm/yyyy): 29 10 2025
Page: 2



2.14.2. ^{13}C NMR

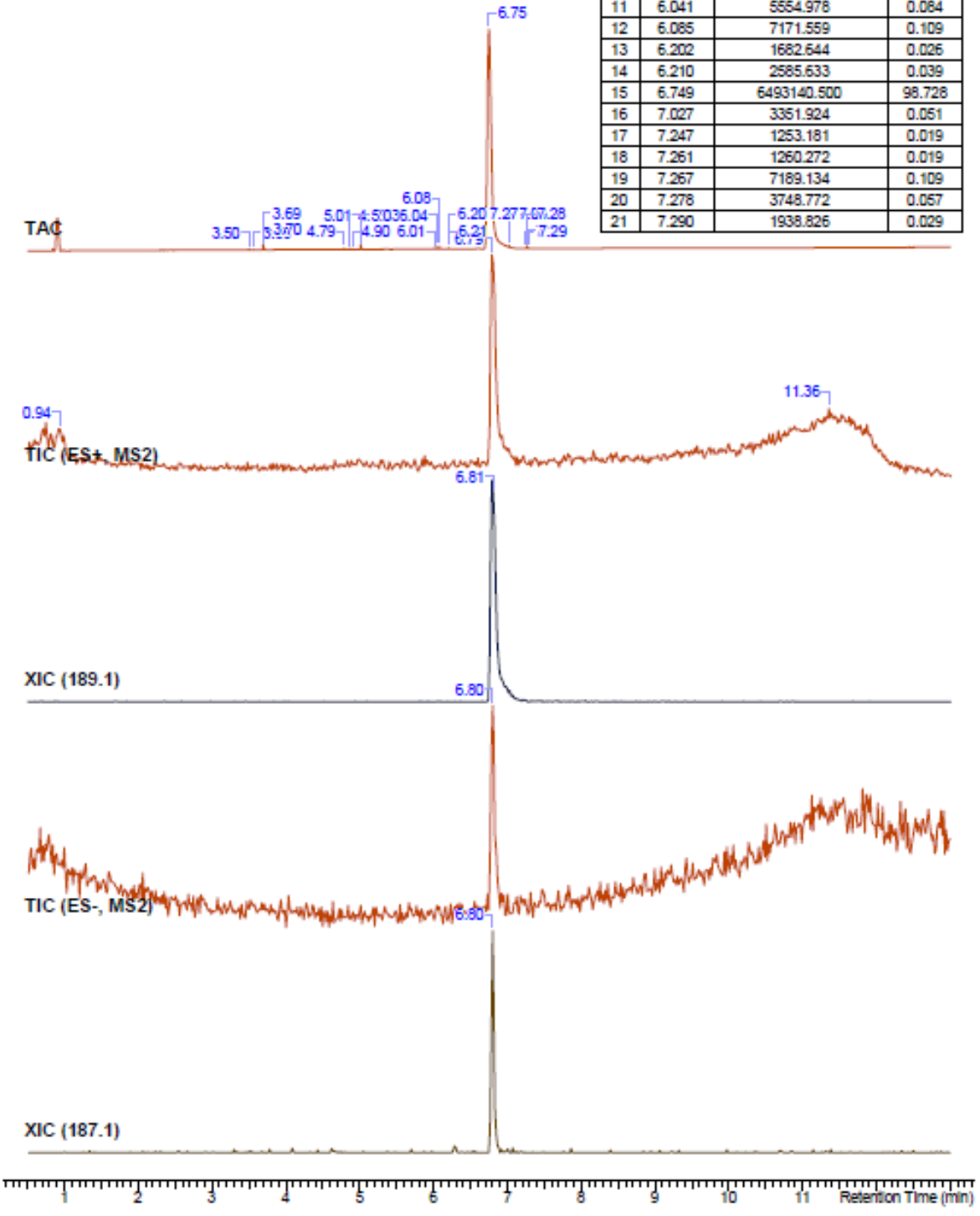
Acquisition Time (sec)	1.9996	***Date***	09 Feb 2024 12:20:12			***Date Stamp***	09 Feb 2024 11:28:09
File Name	C:\Users\panczykk\Desktop\Widma_KPS_PZ\NMR\2024\KPS24-7-fr14-25_935_43_CARBON-1-1.jdf					***Frequency (MHz)***	125.77
Nucleus	13C	***Number of Transients***	1024	***Origin***	ECA	***Original Points Count***	78604
Owner	delta	***Points Count***	131072	***Pulse Sequence***	carbon.jxp	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	12576.5293	***Sweep Width (Hz)***	39310.18	***Temperature (degree C)***	20.100		

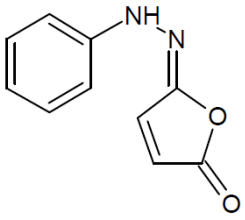
^{13}C NMR (126 MHz, CHLOROFORM-*d*) δ ppm 113.41 (s, 1 C), 120.11 (s, 1 C), 122.29 (s, 1 C), 129.57 (s, 1 C), 139.77 (s, 1 C), 141.41 (s, 1 C), 142.54 (s, 1 C), 166.42 (s, 1 C)

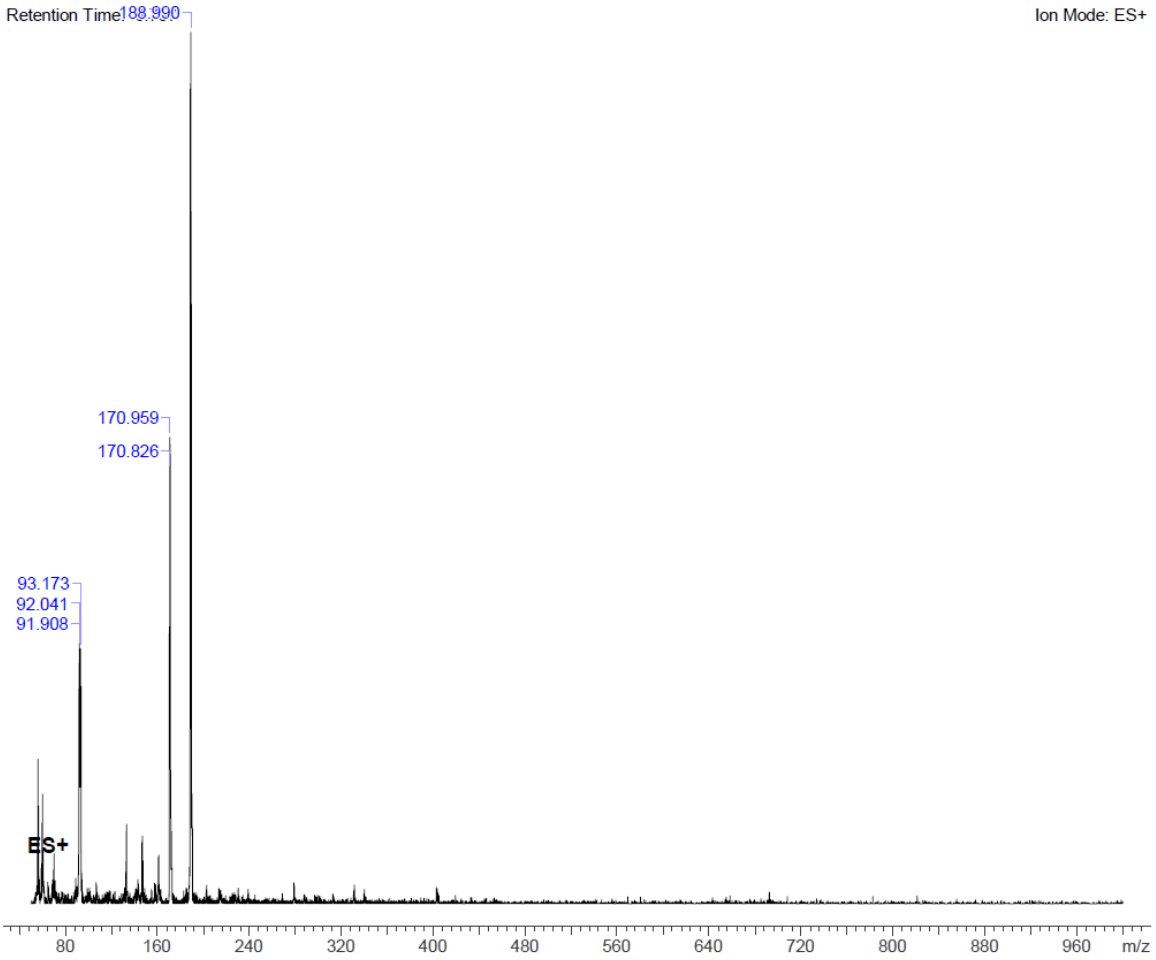


2.14.3. LCMS

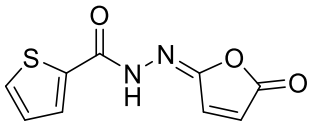
No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	3.501	3752.794	0.057
2	3.558	985.523	0.015
3	3.692	12786.192	0.194
4	3.701	6817.278	0.104
5	4.791	2193.344	0.033
6	4.850	1708.168	0.026
7	4.898	1646.208	0.025
8	5.014	15022.431	0.228
9	5.026	2008.124	0.031
10	6.011	1015.560	0.015
11	6.041	5554.978	0.084
12	6.085	7171.559	0.109
13	6.202	1682.644	0.026
14	6.210	2585.633	0.039
15	6.749	6493140.500	98.728
16	7.027	3351.924	0.051
17	7.247	1253.181	0.019
18	7.261	1260.272	0.019
19	7.267	7189.134	0.109
20	7.278	3748.772	0.057
21	7.290	1938.826	0.029



tR (min)	Mass (Ao)	[M+H]+	[M-H]-	Structure	Area (%)
6.749	188.059	189.066	187.051		TIC (ES-, MS2) = 100.00 XIC = 72.61 TIC (ES+, MS2) = 80.71 XIC = 69.61 TAC = 98.73



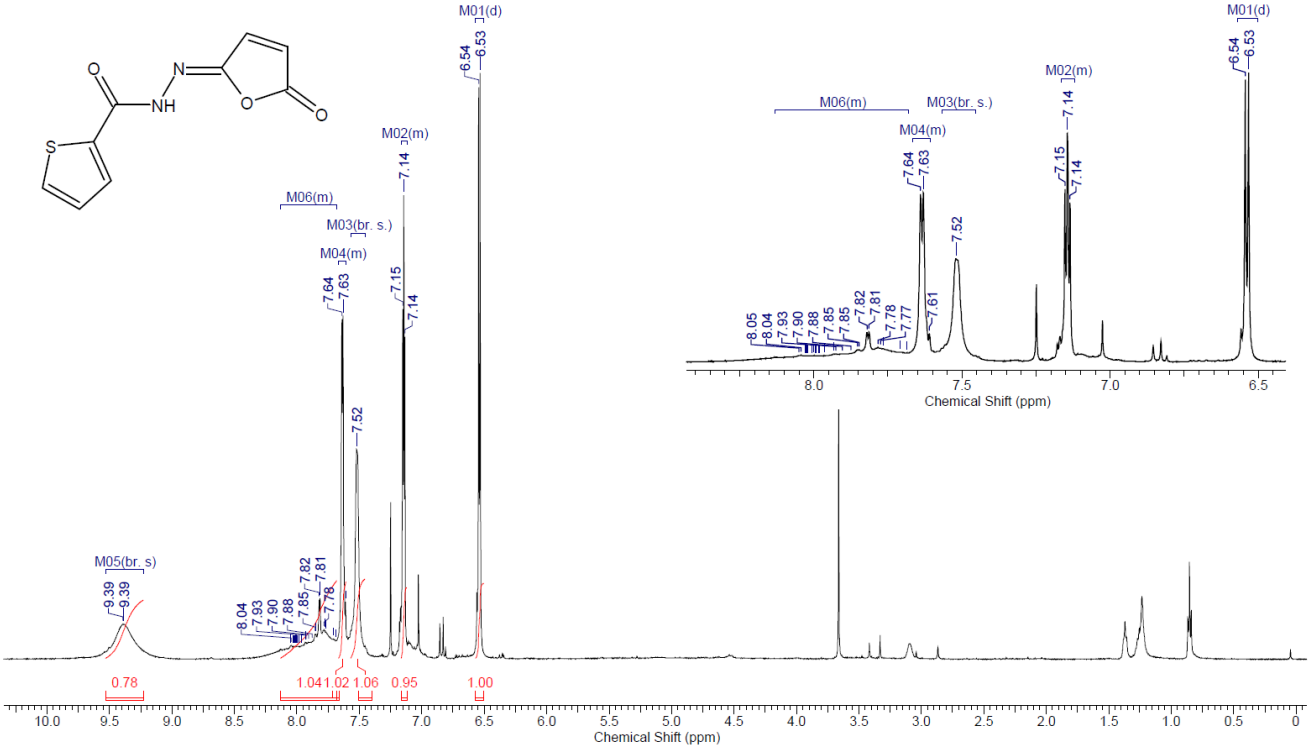
2.15. N'-[5-oxo-2,5-dihydrofuran-2-ylidene]thiophene-2-carbohydrazide (2h)



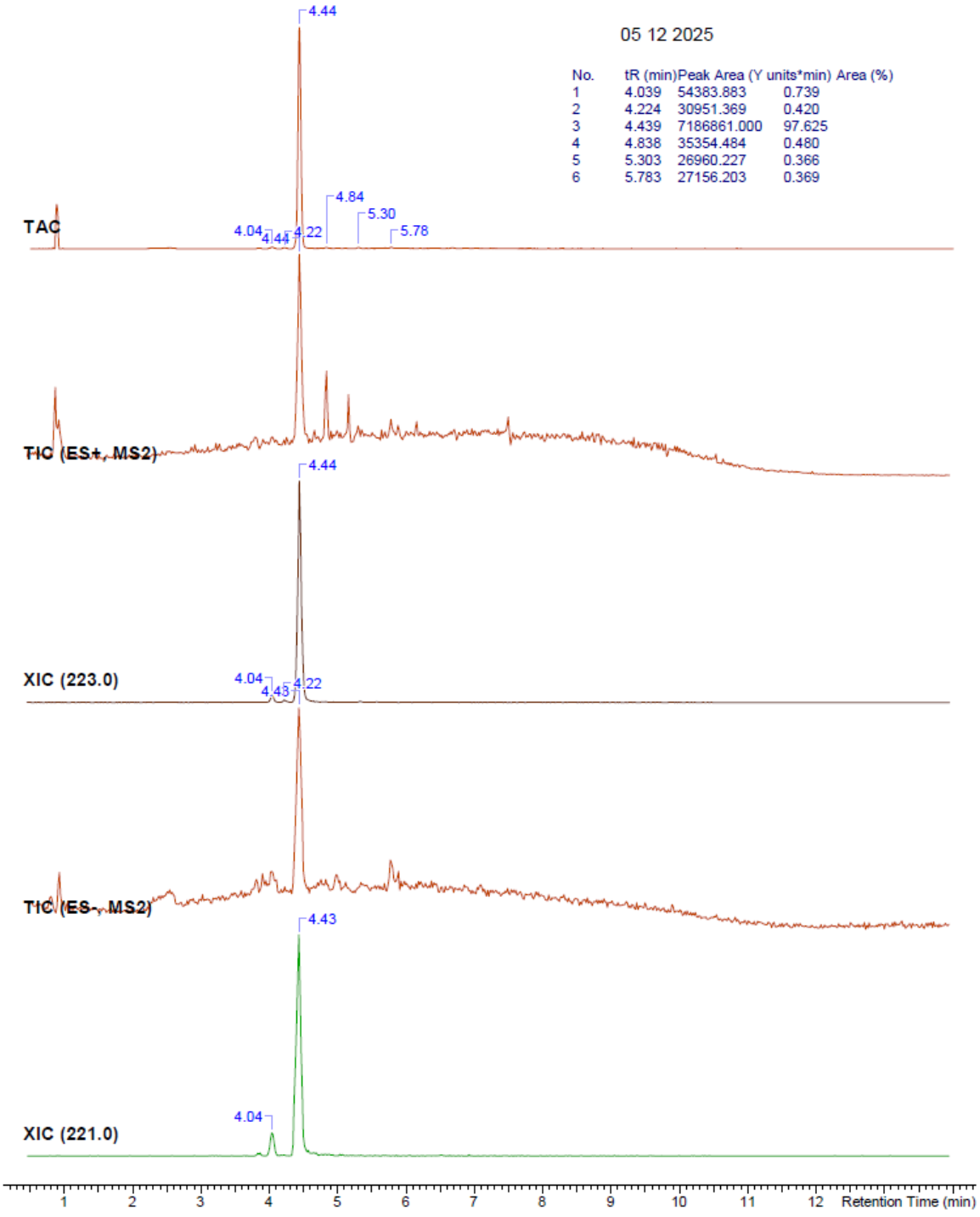
2.15.1. ^{1}H NMR

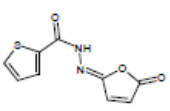
05.12.2025 01:36:44

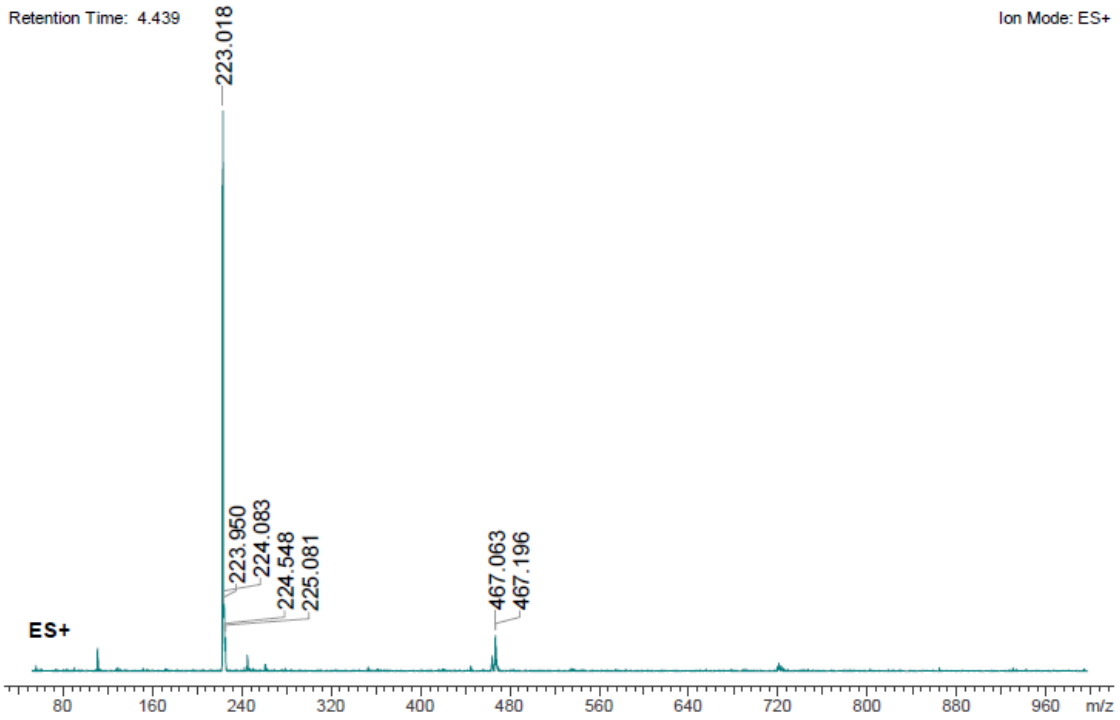
Acquisition Time (sec)	2.0479	*Date*	02 Dec 2025 12:02:31			*Date Stamp*	02 Dec 2025 12:01:52
File Name	C:\Users\Admin\OneDrive - Uniwersytet Jagielloński\nmr\2025\izomal-tiof_935_03_PROTON-1-1.jdf					*Frequency (MHz)*	500.16
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	19225
Owner	delta	*Points Count*	131072	*Pulse Sequence*	single_pulse.jxp	*Solvent*	CHLOROFORM-d
Spectrum Offset (Hz)	3251.0396	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	9387.80	*Temperature (degree C)*	20.800

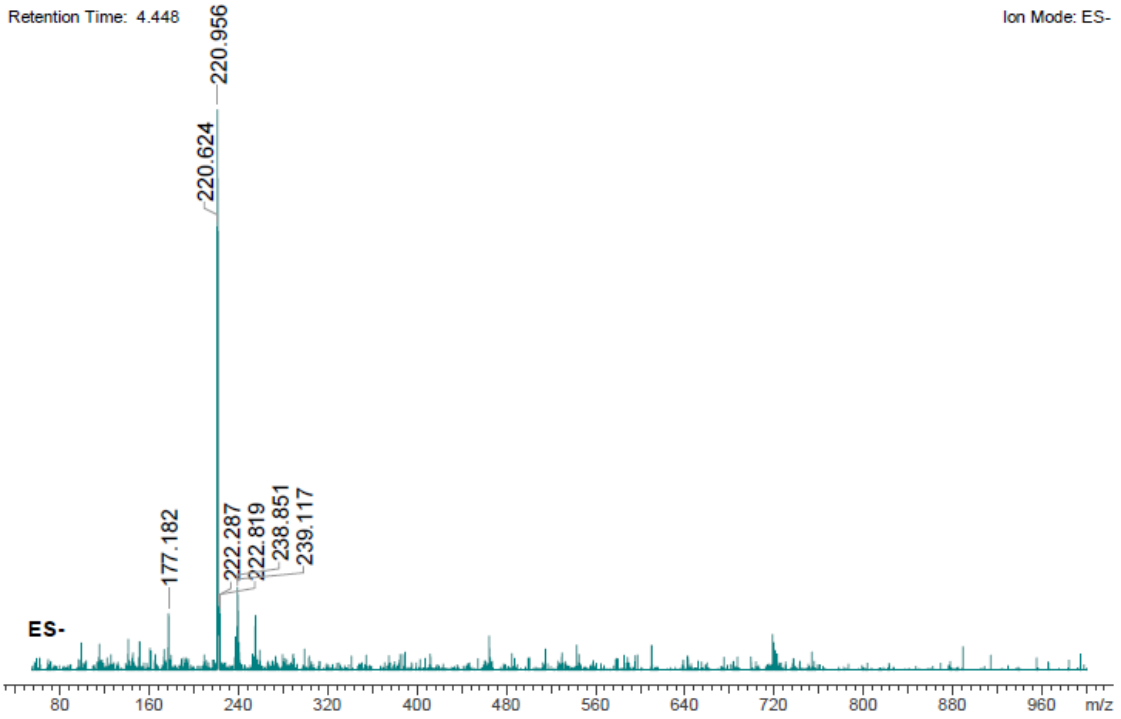


2.15.2. UPLC-MS

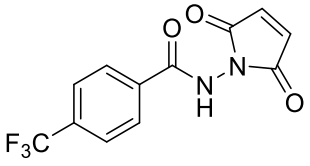


Comp	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	M+·	M-·	MF	Structure	Area (%)
1	4.440	222.010	223.017	221.003	222.009	222.010	$C_5H_6N_2O_3S$		TIC (ES-, MS2) = 100.00 Single XIC = 91.96 TIC (ES+, MS2) = 100.00 Single XIC = 96.78 TAC = 97.63


Retention Time: 4.439
Ion Mode: ES+
223.018
223.950
224.083
224.548
225.081
467.063
467.196
ES+
80
160
240
320
400
480
560
640
720
800
880
960
m/z


Retention Time: 4.448
Ion Mode: ES-
220.956
220.624
177.182
222.287
222.819
238.851
239.117
ES-
80
160
240
320
400
480
560
640
720
800
880
960
m/z

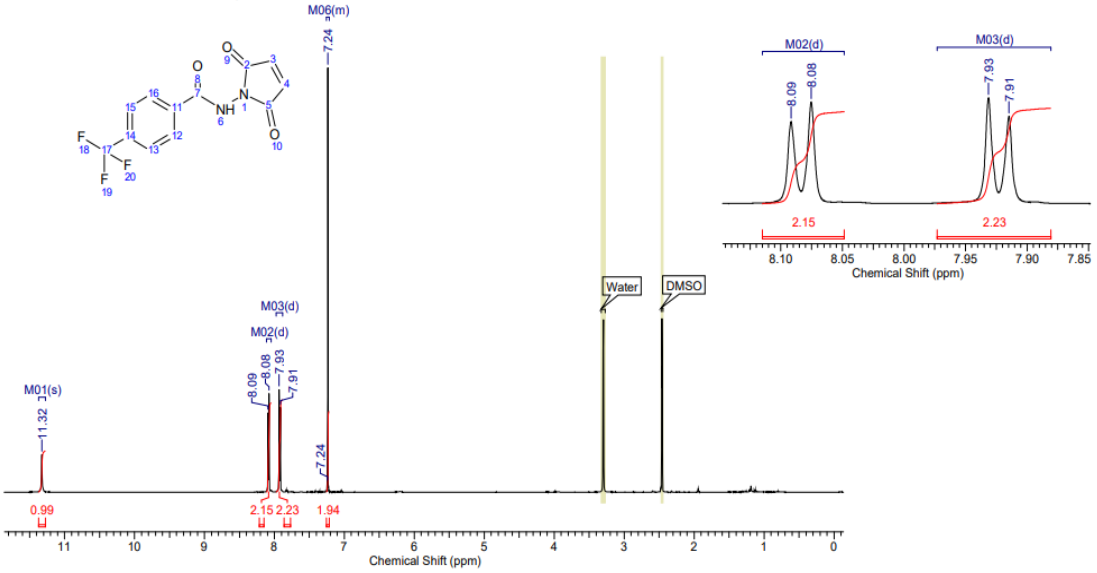
2.16.*N*-(2,5-Dioxo-2,5-dihydro-*1H*-pyrrol-1-yl)-4-(trifluoromethyl)benzamide (3a)



2.16.1. ^{1}H NMR

Acquisition Time (sec)	2.0479	**Date**	12 Sep 2025 07:48:02			**Date Stamp**	12 Sep 2025 07:47:23
File Name	C:\Users\panczykk\Desktop\Widma_KPS_PZ\NMR\2025\KPS25003_935_43_PROTON-1-1.jdf					**Frequency (MHz)**	500.16
Nucleus	1H	**Number of Transients**	8	**Origin**	ECA	**Original Points Count**	19225
Owner	delta	**Points Count**	131072	**Pulse Sequence**	single_pulse.jxp	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	3251.0396	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	9387.80	**Temperature (degree C)**	21.100

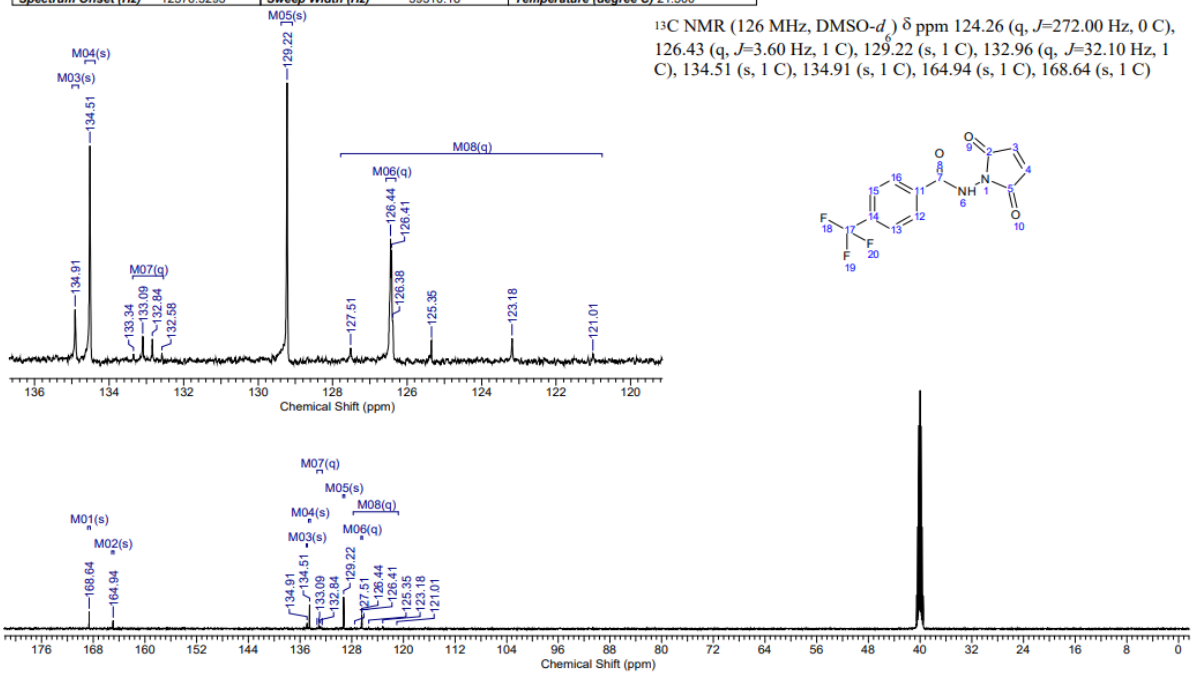
^{1}H NMR (500 MHz, DMSO-d_6) δ ppm 11.32 (s, 1H), 8.08 (d, *J*=8.17 Hz, 2H), 7.92 (d, *J*=8.31 Hz, 2H), 7.22 - 7.26 (m, 2H)



2.16.2. ^{13}C NMR

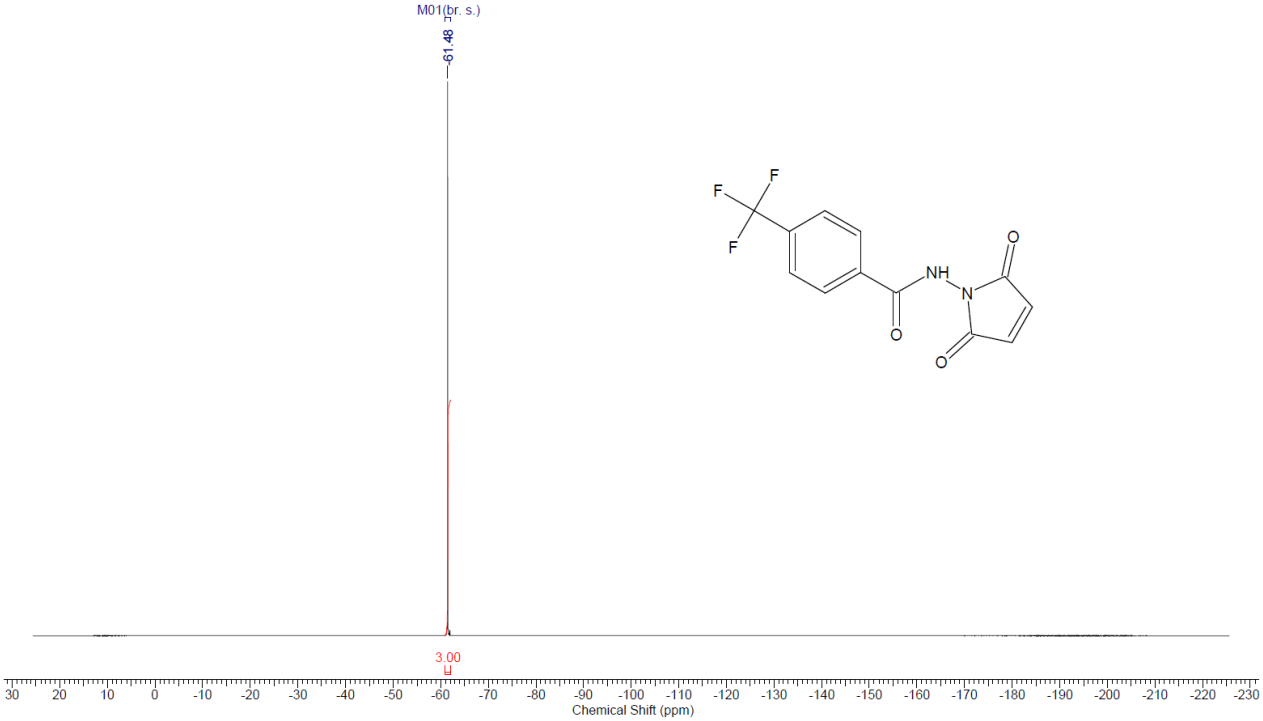
Acquisition Time (sec)	1.9996	**Date**	12 Sep 2025 10:13:01			**Date Stamp**	12 Sep 2025 09:20:58
File Name	C:\Users\panczykk\Desktop\Widma_KPS_PZ\NMR\2025\KPS25003_935_43_CARBON-1-1.jdf					**Frequency (MHz)**	125.77
Nucleus	13C	**Number of Transients**	1024	**Origin**	ECA	**Original Points Count**	78604
Owner	delta	**Points Count**	131072	**Pulse Sequence**	carbon.jxp	**Solvent**	DMSO-d6
Spectrum Offset (Hz)	12576.5293	**Sweep Width (Hz)**	39310.18	**Temperature (degree C)**	21.500		

^{13}C NMR (126 MHz, DMSO-d_6) δ ppm 124.26 (q, *J*=272.00 Hz, 0 C), 126.43 (q, *J*=3.60 Hz, 1 C), 129.22 (s, 1 C), 132.96 (q, *J*=32.10 Hz, 1 C), 134.51 (s, 1 C), 134.91 (s, 1 C), 164.94 (s, 1 C), 168.64 (s, 1 C)

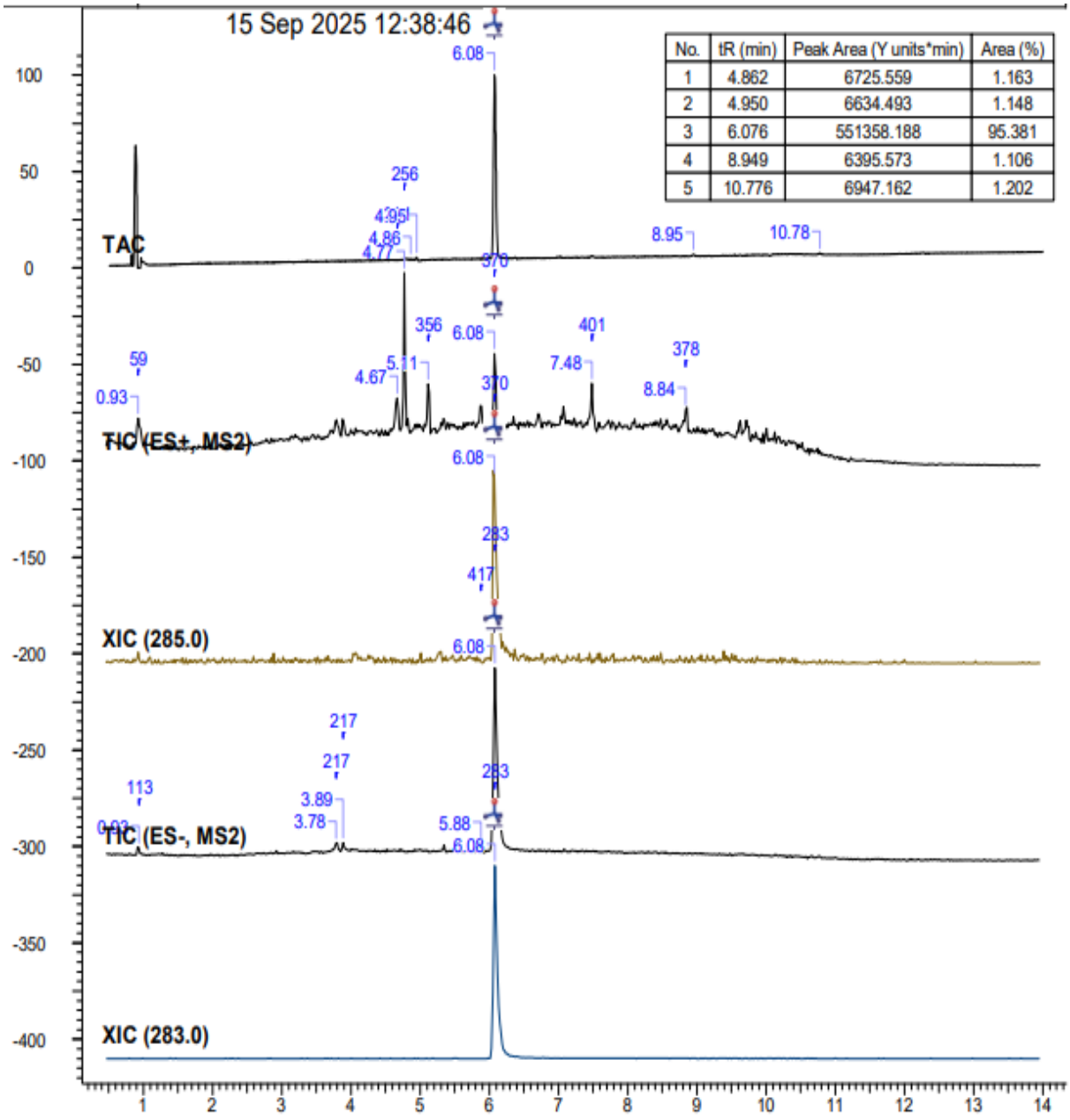


2.16.3. ^{19}F NMR

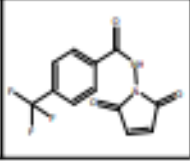
Acquisition Time (sec)	2.9861	***Date***	26 Mar 2024 11:29:23			***Date Stamp***	26 Mar 2024 11:28:36
File Name	C:\Users\Przemek\OneDrive - Uniwersytet Jagielloński\nmr\o2024\CF3-mal_935_03_Fluorine-1-1.jdf					***Frequency (MHz)***	470.62
Nucleus	19F	***Number of Transients***	8	***Origin***	ECA	***Original Points Count***	352967
Owner	delta	***Points Count***	524288	***Pulse Sequence***	single_pulse.jxp	***Solvent***	DMSO-d6
Spectrum Offset (Hz)	-47062.0469	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	118203.65	***Temperature (degree C)***	20.700

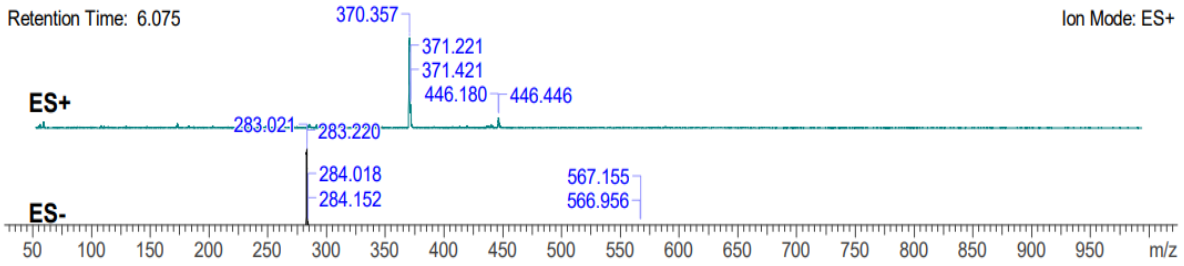


2.16.4. LCMS

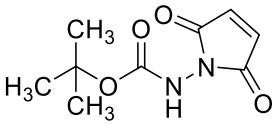


No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	4.862	6725.559	1.163
2	4.950	6634.493	1.148
3	6.076	551358.188	95.381
4	8.949	6395.573	1.106
5	10.776	6947.162	1.202

No.	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	MF	Structure	Name	Area (%)
1	6.08	284.0409	285.0482	283.0336	$C_{12}H_7F_3N_2O_3$			TIC (ES-, MS2) = 89.94 Single XIC = 100.00 TIC (ES+, MS2) = 15.54 Single XIC = 100.00 TAC = 95.38

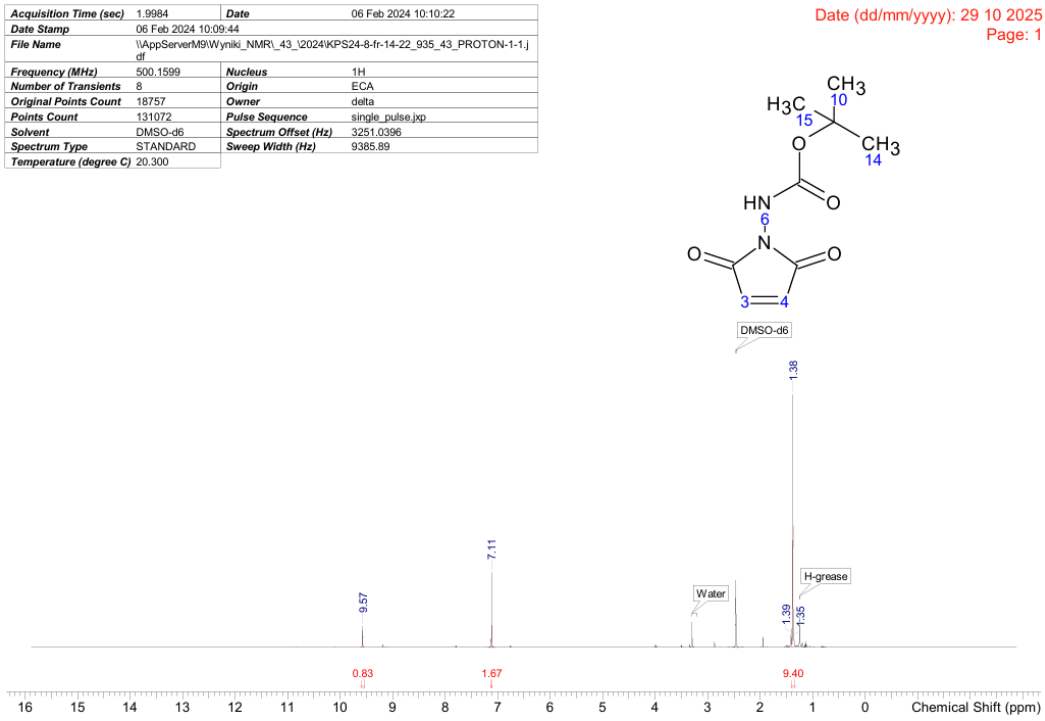

Retention Time: 6.075
Ion Mode: ES+
ES+
ES-
370.357
371.221
371.421
446.180
446.446
283.021
283.220
284.018
284.152
567.155
566.956
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 m/z

2.17. *Tert*-butyl (2,5-dioxo-2,5-dihydro-*1H*-pyrrol-1-yl)carbamate (3b)



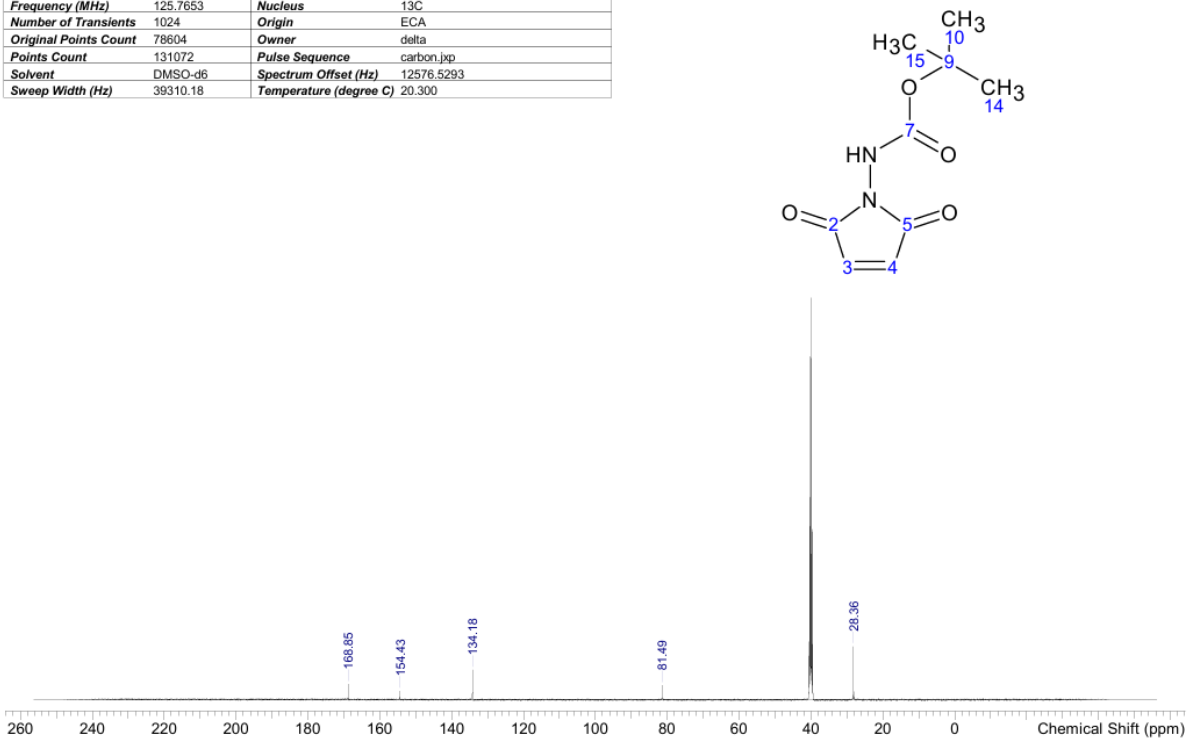
2.17.1. ^{1}H NMR

Acquisition Time (sec)	1.9984	***Date***	06 Feb 2024 10:10:22
Date Stamp	06 Feb 2024 10:09:44		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS24-8-fr-14-22_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	***Nucleus***	1H
Number of Transients	8	***Origin***	ECA
Original Points Count	18757	***Owner***	delta
Points Count	131072	***Pulse Sequence***	single_pulse.jxp
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3251.0396
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9385.89
Temperature (degree C)	20.300		

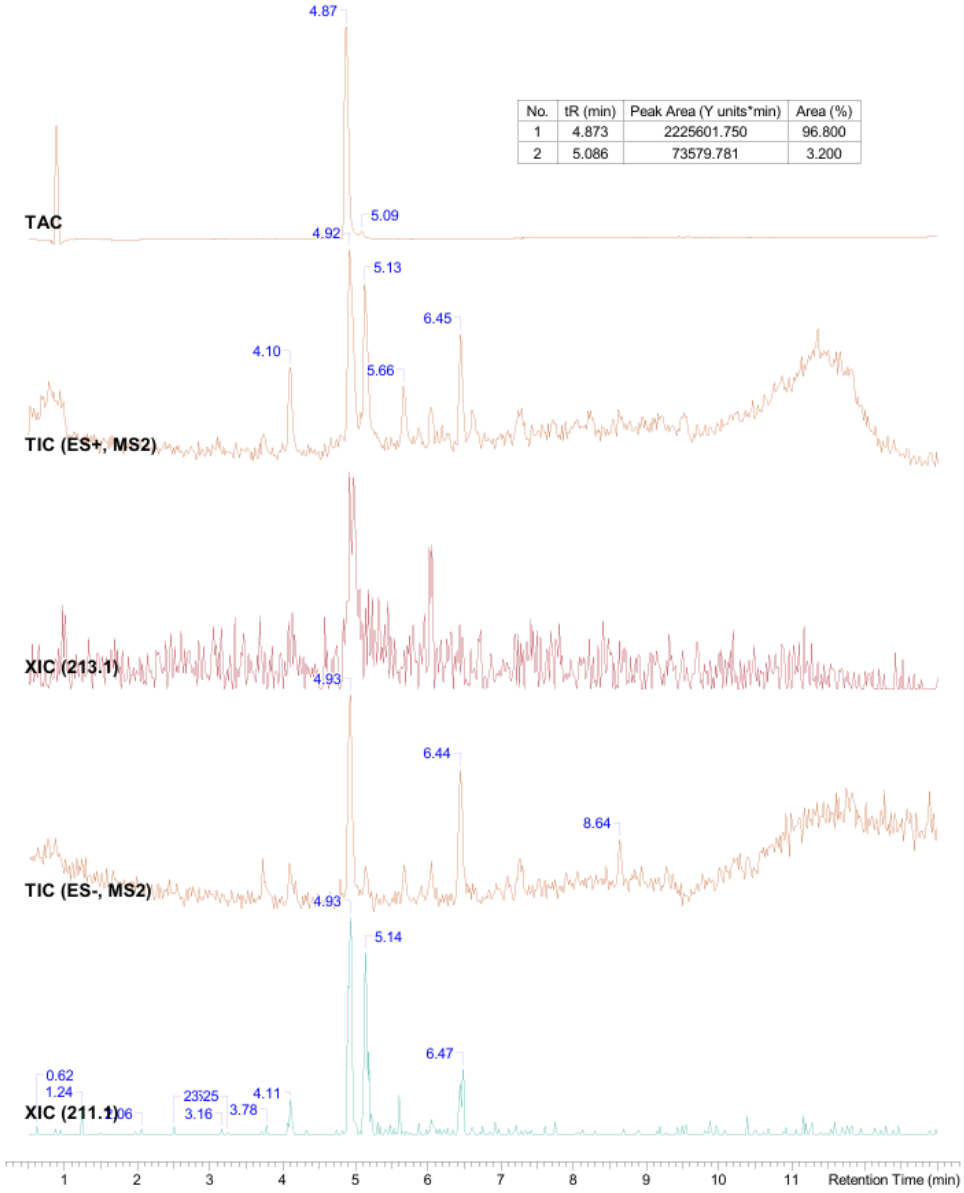


2.17.2. ^{13}C NMR

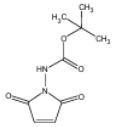
Acquisition Time (sec)	1.9996	***Date***	06 Feb 2024 11:02:55
Date Stamp	06 Feb 2024 10:10:52		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS24-8-fr-14-22_935_43_CARBON-1-1.jdf		
Frequency (MHz)	125.7653	***Nucleus***	13C
Number of Transients	1024	***Origin***	ECA
Original Points Count	78604	***Owner***	delta
Points Count	131072	***Pulse Sequence***	carbon.jxp
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	12576.5293
Sweep Width (Hz)	39310.18	***Temperature (degree C)***	20.300

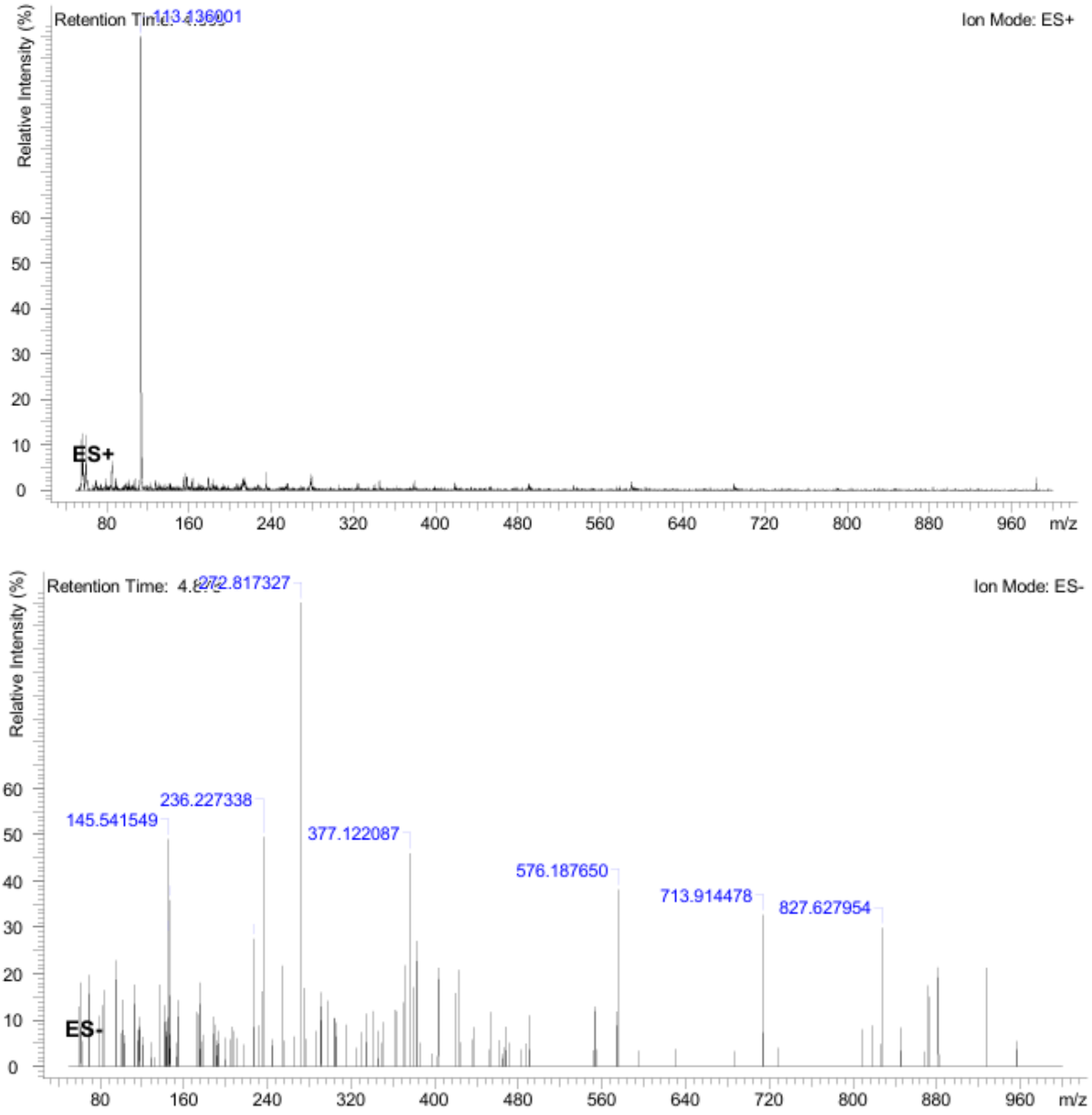


2.17.3. LCMS



No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	4.873	2225601.750	96.800
2	5.086	73579.781	3.200

Compo	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	M+·	M-·	MF	Structure	Area (%)
1	4.873	212.080	213.087	211.072	212.079	212.080	$C_9H_{12}N_2O_4$		TIC (ES-, MS2) = 49.86 Single XIC = 42.95 TIC (ES+, MS2) = 34.81 TAC = 96.80

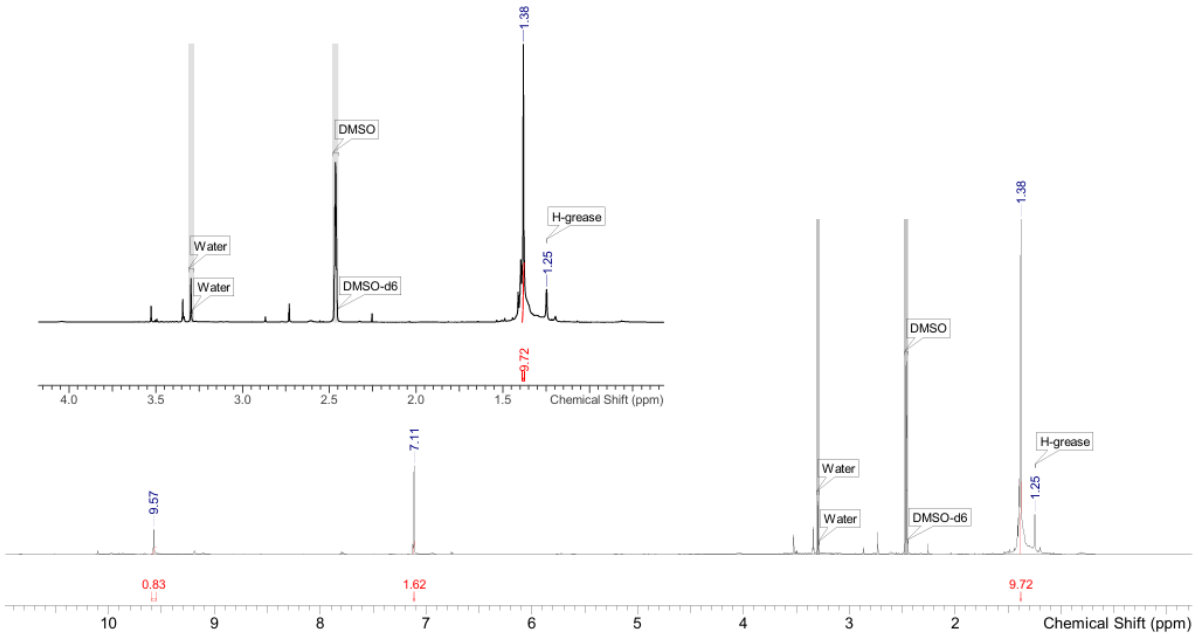


2.17.4. Data before purification by column chromatography

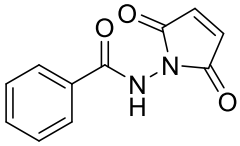
^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm) 1.38 (s, 9H, CH_3) 7.11 (s, 2H, >CH-) 9.57 (s, 1H, NH)

Acquisition Time (sec)	4.3647	***Date***	06 Feb 2024 09:12:17
Date Stamp	06 Feb 2024 09:11:23		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS24-8_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	***Nucleus***	1H
Number of Transients	8	***Origin***	ECA
Original Points Count	40960	***Owner***	delta
Points Count	131072	***Pulse Sequence***	single_pulse.jxp
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3251.0396
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9384.38
Temperature (degree C)	20.100		

Date (dd/mm/yyyy): 28 10 2025
Page: 1



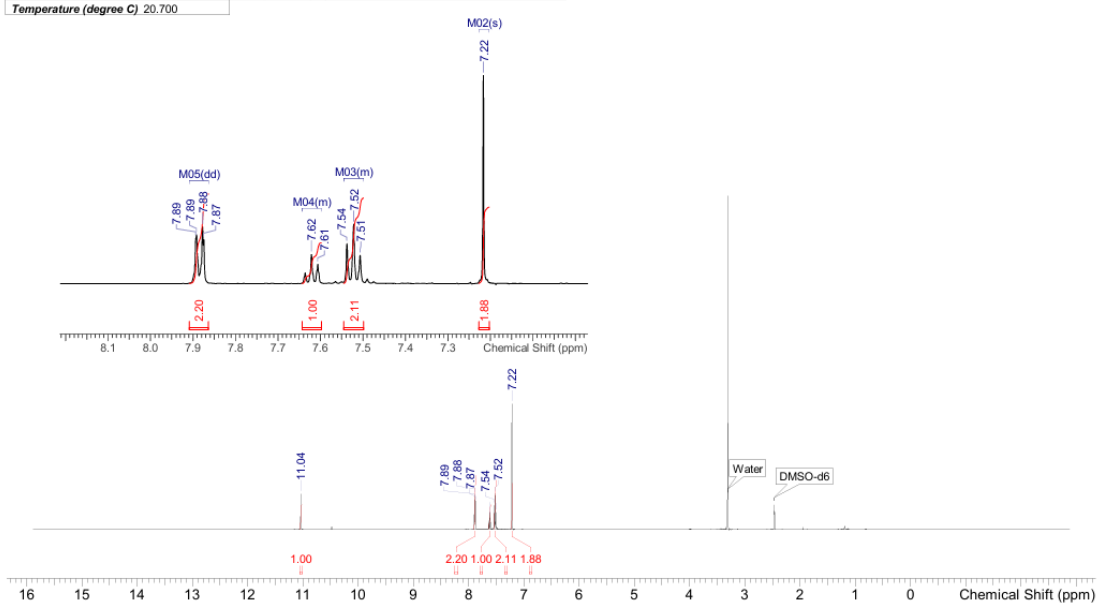
2.18.*N*-(2,5-Dioxo-2,5-dihydro-*1H*-pyrrol-1-yl)benzamide (3c)



2.18.1. ^{1}H NMR

Acquisition Time (sec)	1.9984	***Date***	27 Oct 2023 09:01:31
Date Stamp	27 Oct 2023 09:00:53		
File Name	\\AppServerM9\Wyniki_NMR_43_\2023\KPS23-19_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	***Nucleus***	1H
Number of Transients	8	***Origin***	ECA
Original Points Count	18757	***Owner***	delta
Points Count	131072	***Pulse Sequence***	single_pulse.jxp
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3251.0396
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9385.89
Temperature (degree C)	20.700		

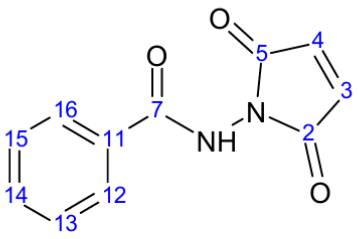
Date (dd/mm/yyyy): 29 10 2025
Page: 1

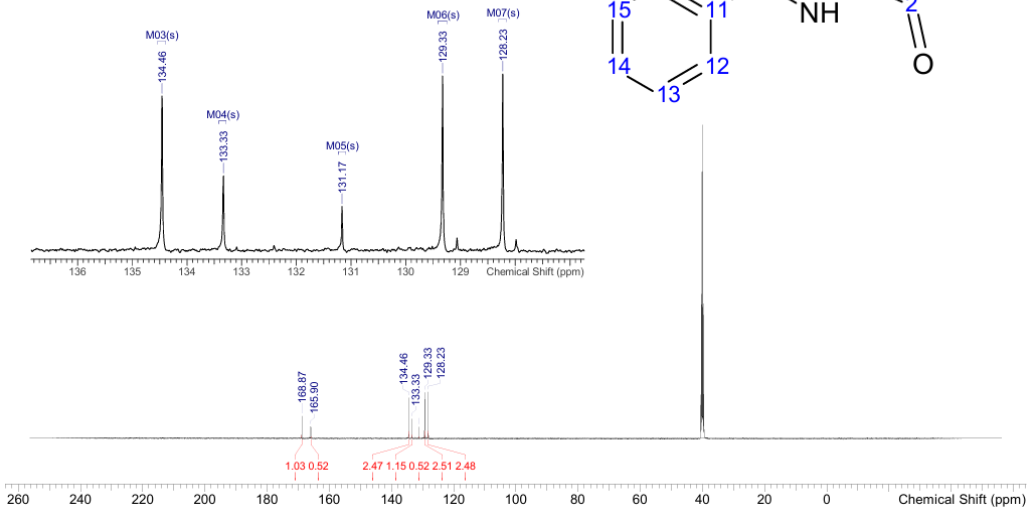


2.18.2. ^{13}C NMR

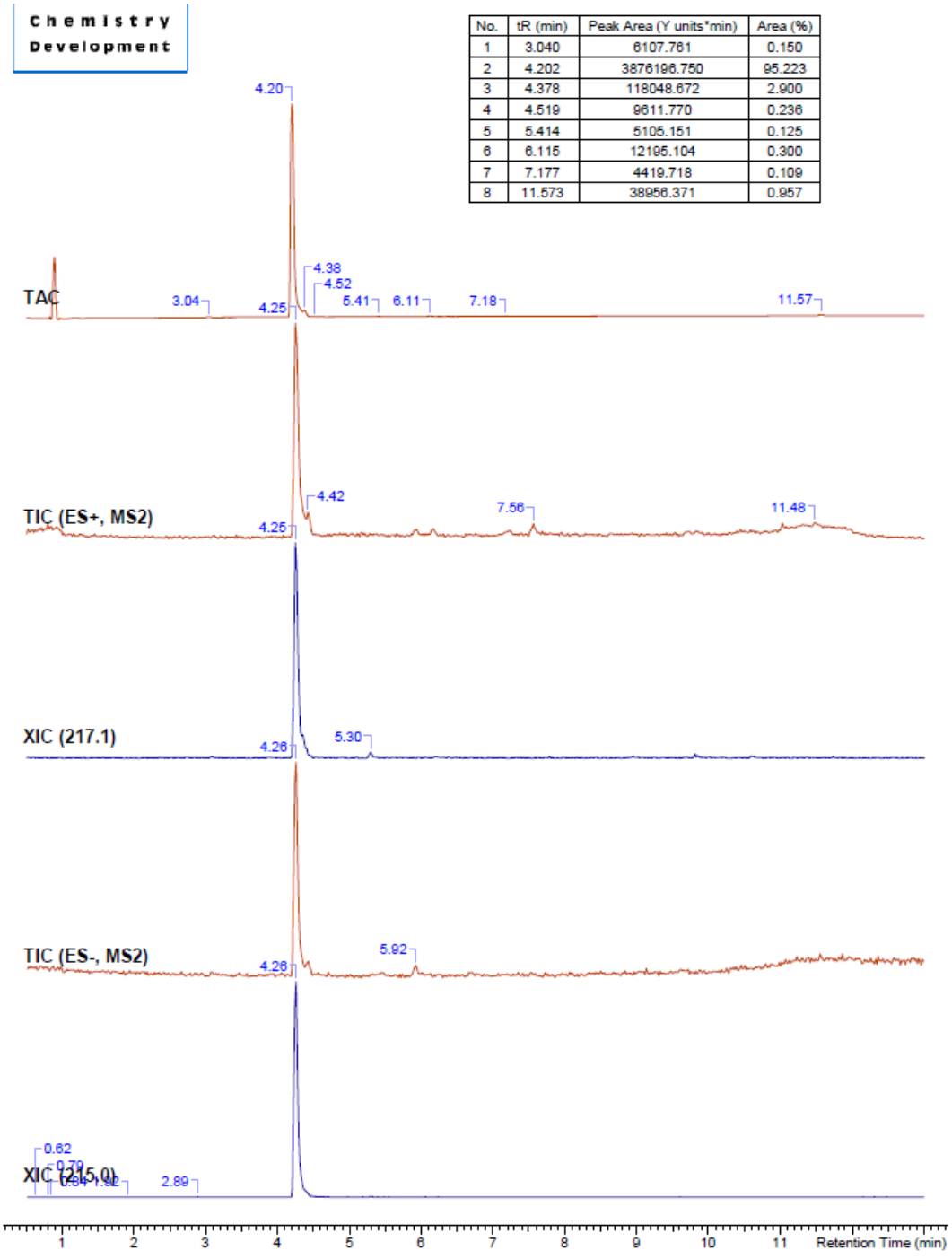
Acquisition Time (sec)	1.9996	***Date***	27 Oct 2023 09:54:04
Date Stamp	27 Oct 2023 09:02:01		
File Name	\\AppServerM9\Wyniki_NMR_43_\2023\KPS23-19_935_43_CARBON-1-1.jdf		
Frequency (MHz)	125.7653	***Nucleus***	13C
Number of Transients	1024	***Origin***	ECA
Original Points Count	78604	***Owner***	delta
Points Count	131072	***Pulse Sequence***	carbon.jxp
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	12576.5293
Sweep Width (Hz)	39310.18	***Temperature (degree C)***	20.900

Date (dd/mm/yyyy): 29 10 2025
Page: 1



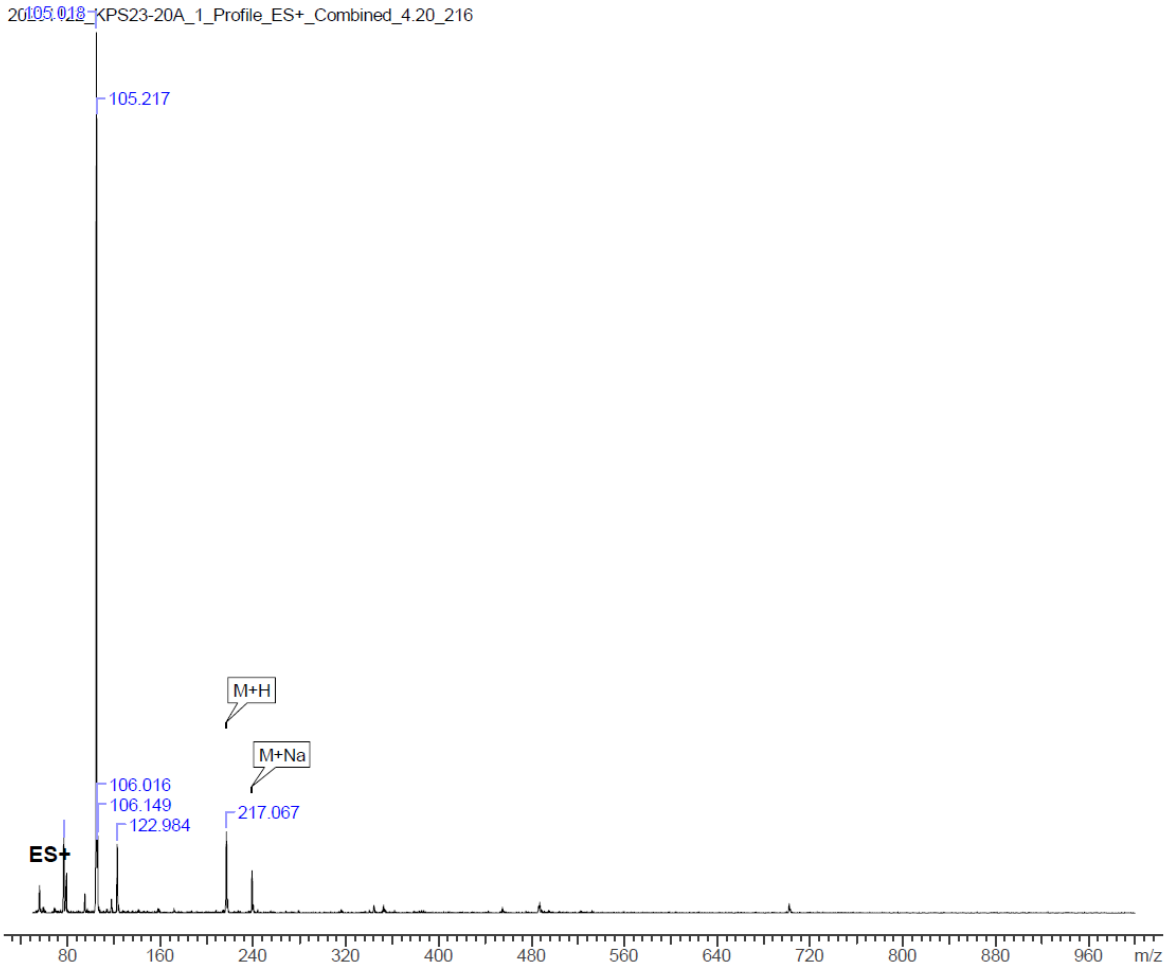


2.18.3. LCMS

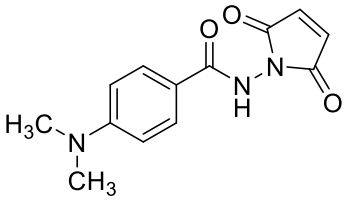


No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	3.040	6107.761	0.150
2	4.202	3876196.750	95.223
3	4.378	118048.672	2.900
4	4.519	9611.770	0.236
5	5.414	5105.151	0.125
6	6.115	12195.104	0.300
7	7.177	4419.718	0.109
8	11.573	38956.371	0.957

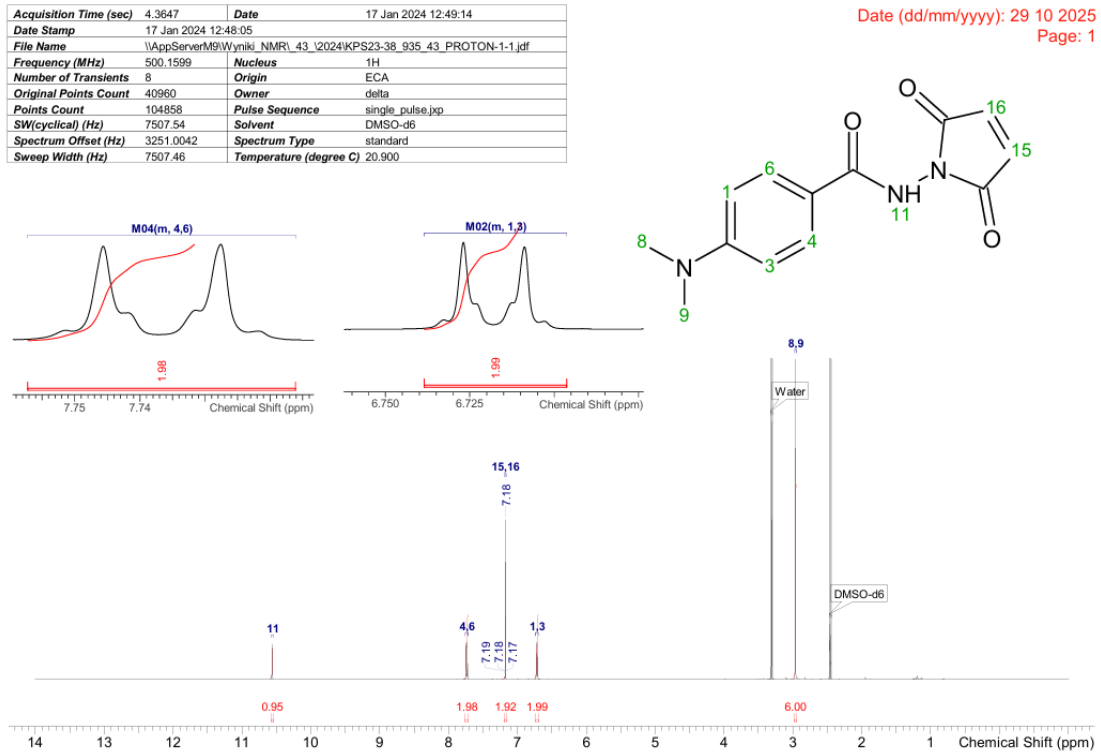
tR (min)	Mass (Ao)	[M+H]+	[M-H]-	Area (%)
4.202	216.053	217.061	215.046	TIC (ES-, MS2) = 93.99 XIC = 89.86 TIC (ES+, MS2) = 81.15 XIC = 59.03 TAC = 95.22


105.018
XPS23-20A_1_Profile_ES+_Combined_4.20_216
105.217
M+H
M+Na
106.016
106.149
122.984
217.067
ES+
80
160
240
320
400
480
560
640
720
800
880
960
m/z

2.19.4-(Dimethylamino)-*N*-(2,5-dioxo-2,5-dihydro-*1H*-pyrrol-1-yl)benzamide (3d)

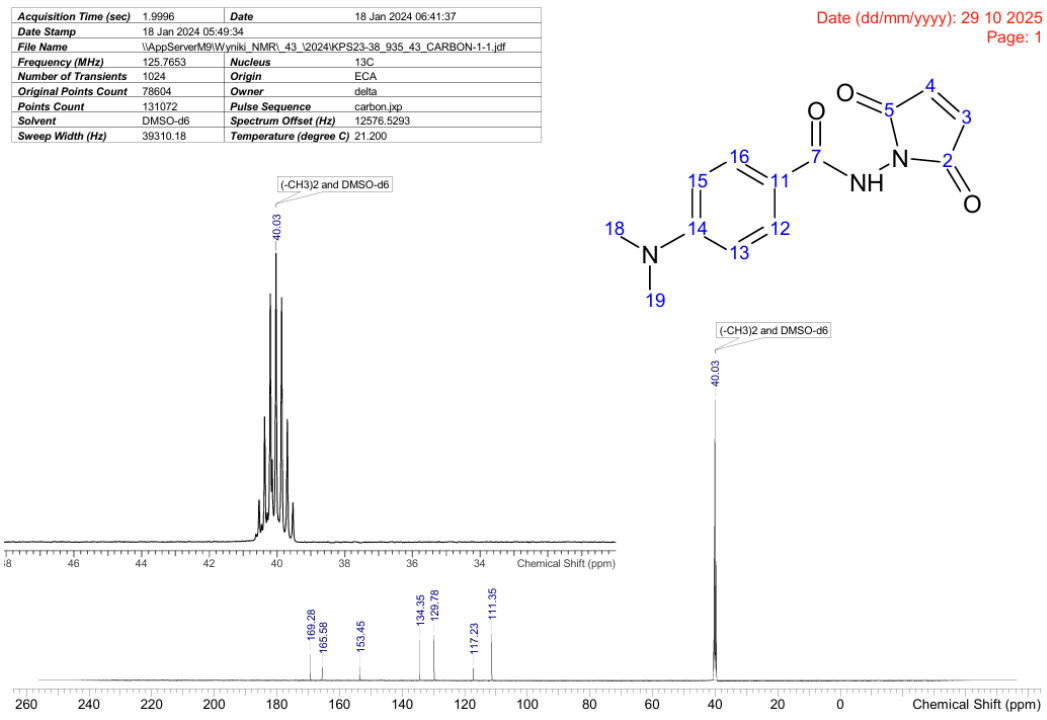


2.19.1. ^{1}H NMR



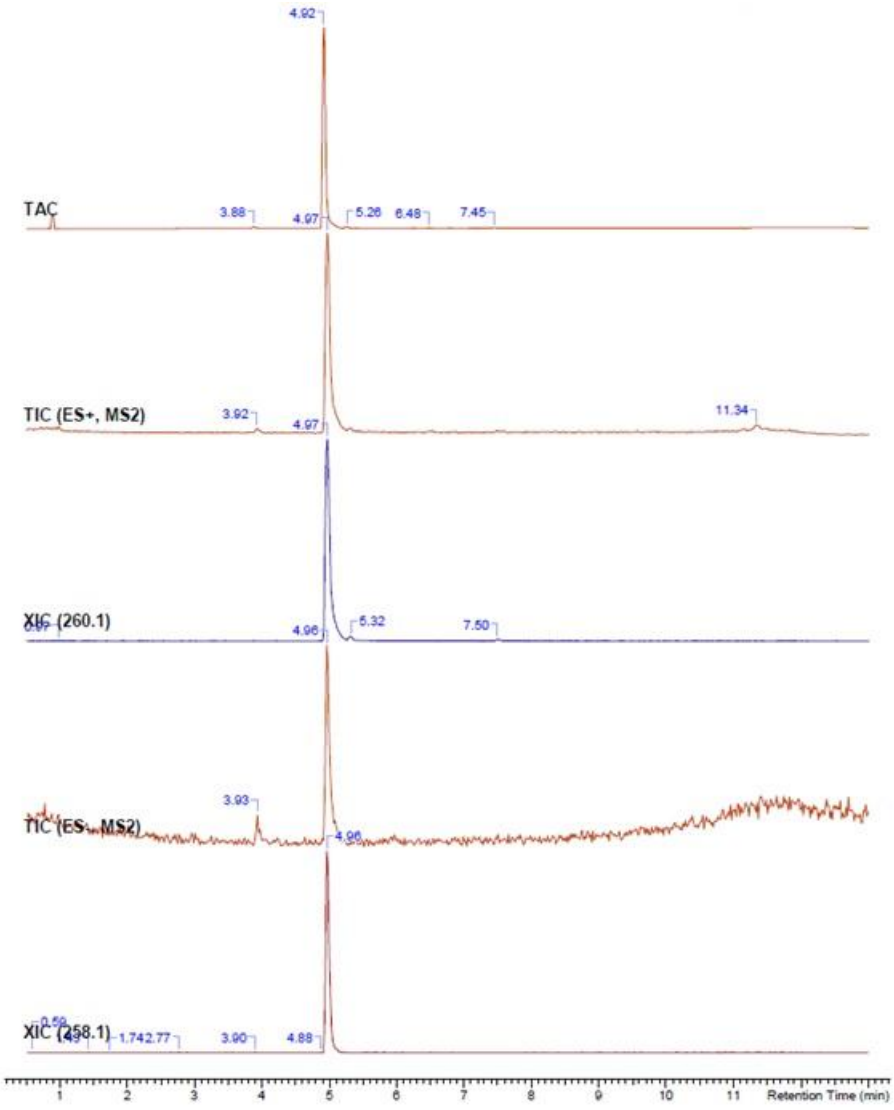
Acquisition Time (sec)	4.3647	Date	17 Jan 2024 12:49:14
Date Stamp	17 Jan 2024 12:48:05		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS23-38_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	Nucleus	1H
Number of Transients	8	Origin	ECA
Original Points Count	40960	Owner	delta
Points Count	104858	Pulse Sequence	single_pulse.jxp
SW(cyclical) (Hz)	7507.54	Solvent	DMSO-d6
Spectrum Offset (Hz)	3251.0042	Spectrum Type	standard
Sweep Width (Hz)	7507.46	Temperature (degree C)	20.900

2.19.2. ^{13}C NMR

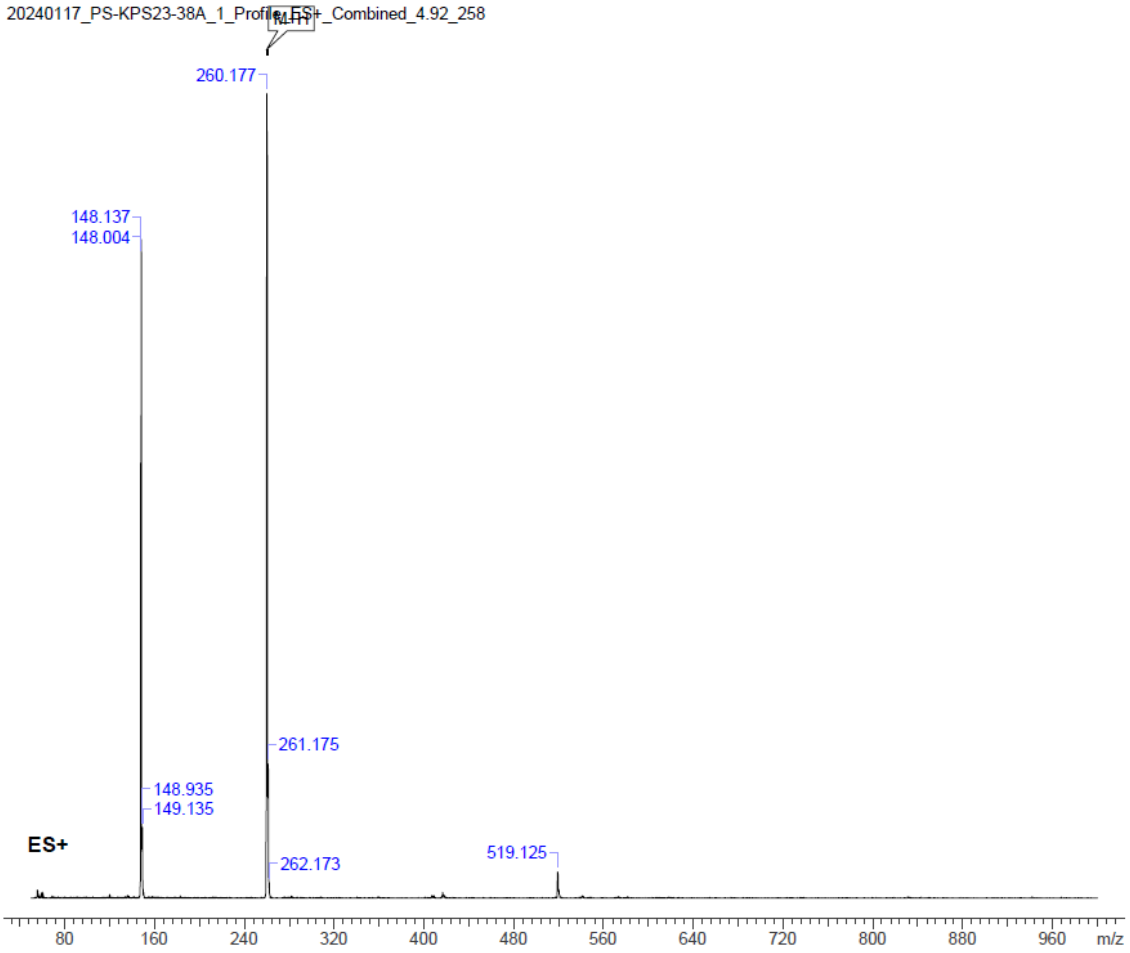


Acquisition Time (sec)	1.9996	Date	18 Jan 2024 06:41:37
Date Stamp	18 Jan 2024 05:49:34		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS23-38_935_43_CARBON-1-1.jdf		
Frequency (MHz)	125.7653	Nucleus	13C
Number of Transients	1024	Origin	ECA
Original Points Count	78604	Owner	delta
Points Count	131072	Pulse Sequence	carbon.jxp
Solvent	DMSO-d6	Spectrum Offset (Hz)	12576.5293
Sweep Width (Hz)	39310.18	Temperature (degree C)	21.200

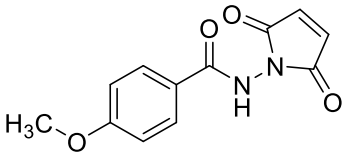
2.19.3. LCMS



tR (min)	Mass (Ao)	[M+H]+	[M-H]-	Area (%)
4.919	259.096	260.103	258.088	TIC (ES-, MS2) = 91.98 XIC = 85.52 TIC (ES+, MS2) = 88.53 XIC = 77.93 TAC = 97.84

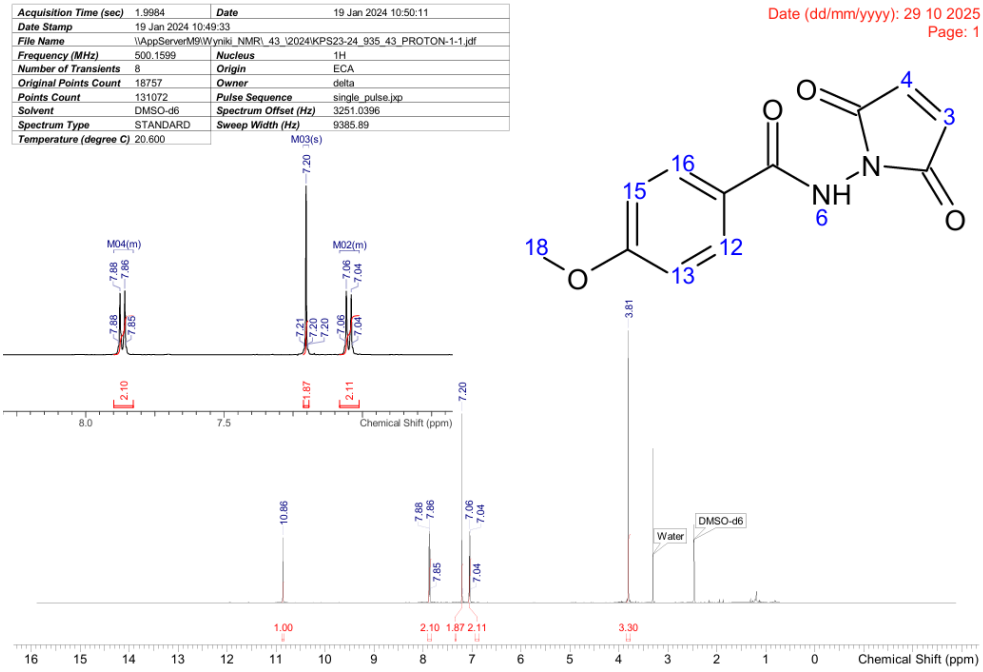

20240117_PS-KPS23-38A_1_Profile_ES+_Combined_4.92_258
M+H+
260.177
148.137
148.004
261.175
148.935
149.135
262.173
519.125
ES+
80
160
240
320
400
480
560
640
720
800
880
960
m/z

2.20.*N*-(2,5-Dioxo-2,5-dihydro-*1H*-pyrrol-1-yl)-4-methoxybenzamide (3e)



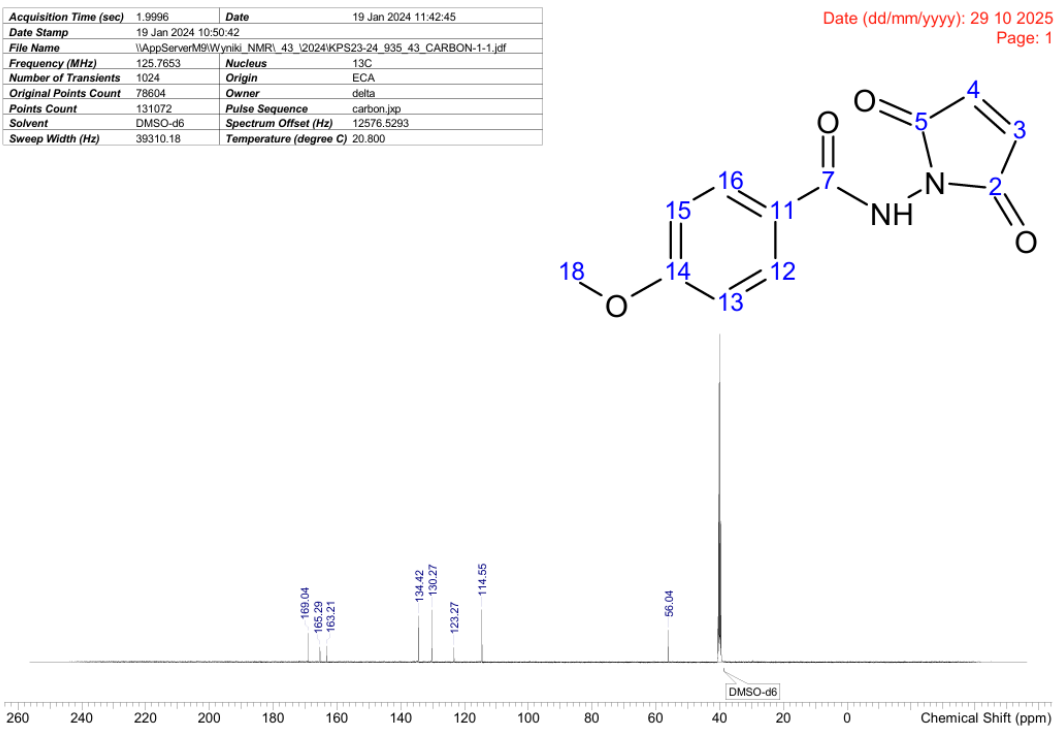
2.20.1. ^{1}H NMR

Acquisition Time (sec)	1.9984	*Date*	19 Jan 2024 10:50:11
Date Stamp	19 Jan 2024 10:49:33		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS23-24_935_43_PROTON-1-1.jdf		
Frequency (MHz)	500.1599	*Nucleus*	1H
Number of Transients	8	*Origin*	ECA
Original Points Count	18757	*Owner*	delta
Points Count	131072	*Pulse Sequence*	single_pulse.jxp
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	3251.0396
Spectrum Type	STANDARD	*Sweep Width (Hz)*	9385.89
Temperature (degree C)	20.600		

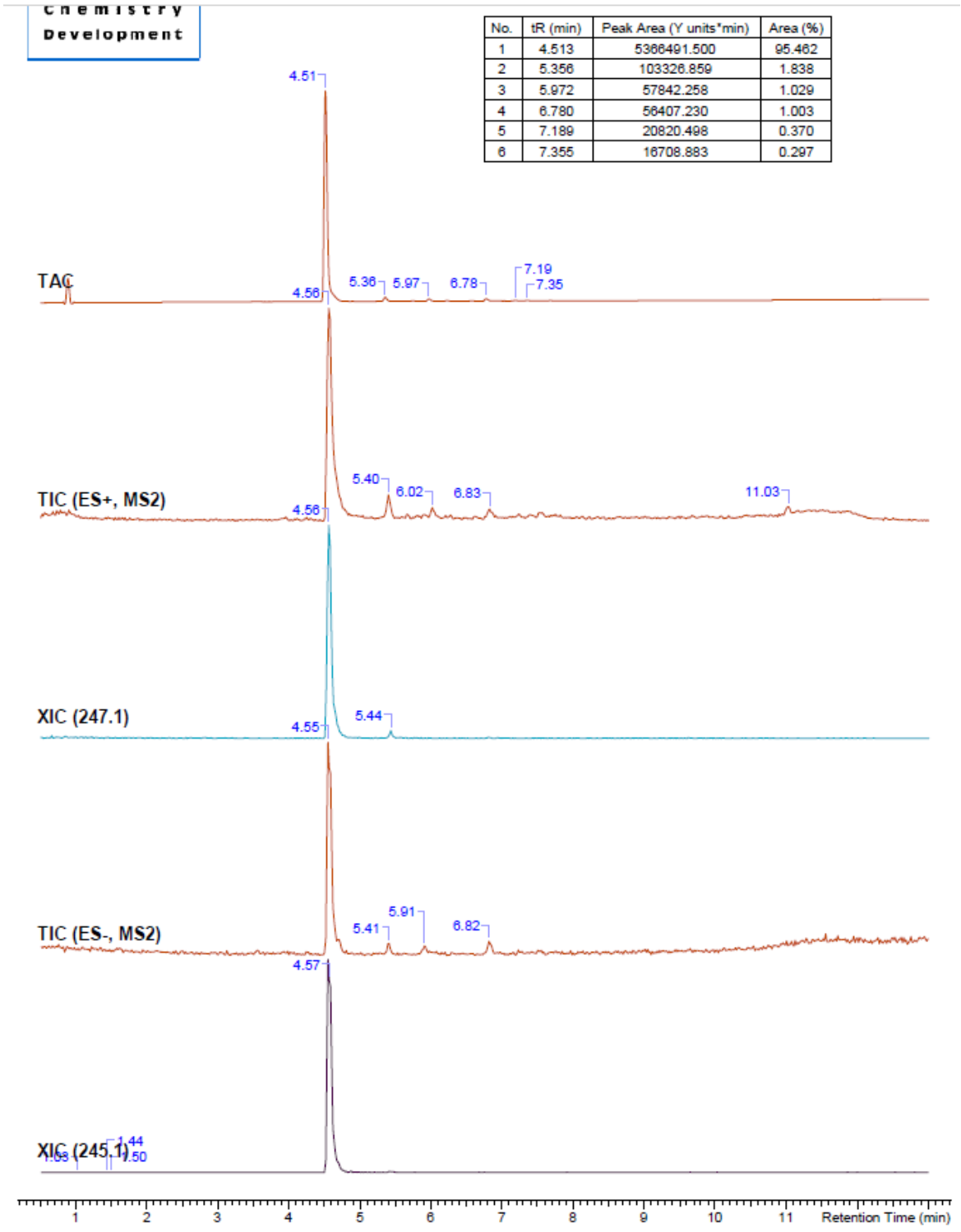


2.20.2. ^{13}C NMR

Acquisition Time (sec)	1.9996	*Date*	19 Jan 2024 11:42:45
Date Stamp	19 Jan 2024 10:50:42		
File Name	\\AppServerM9\Wyniki_NMR_43_\2024\KPS23-24_935_43_CARBON-1-1.jdf		
Frequency (MHz)	125.7653	*Nucleus*	13C
Number of Transients	1024	*Origin*	ECA
Original Points Count	78604	*Owner*	delta
Points Count	131072	*Pulse Sequence*	carbon.jxp
Solvent	DMSO-d6	*Spectrum Offset (Hz)*	12576.5293
Sweep Width (Hz)	39310.18	*Temperature (degree C)*	20.800

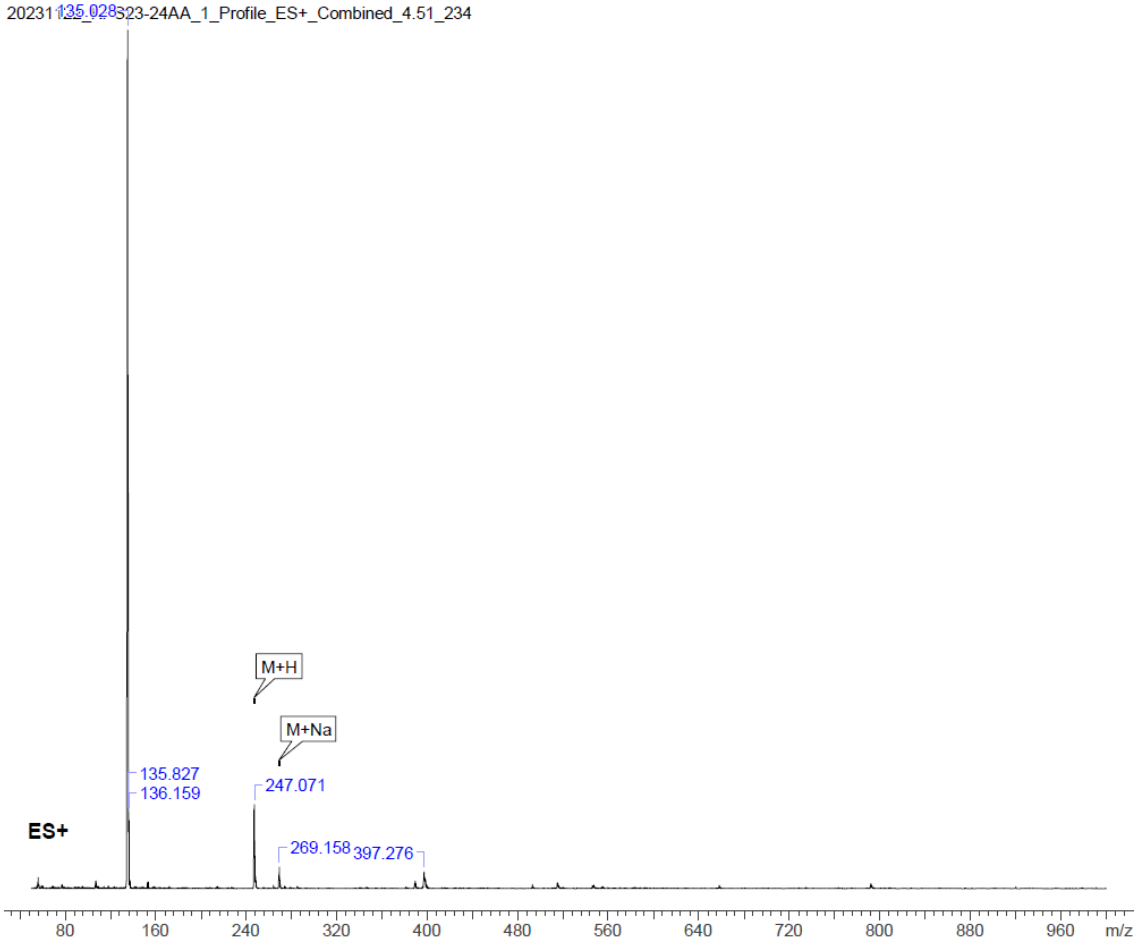


2.20.3. LCMS

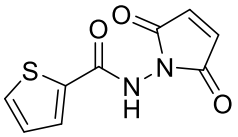


No.	tR (min)	Peak Area (Y units*min)	Area (%)
1	4.513	5366491.500	95.462
2	5.356	103326.859	1.838
3	5.972	57842.258	1.029
4	6.780	56407.230	1.003
5	7.189	20820.498	0.370
6	7.355	16708.883	0.297

tR (min)	Mass (Ao)	[M+H]+	[M-H]-	Area (%)
4.513	246.064	247.071	245.057	TIC (ES-, MS2) = 86.41 XIC = 88.24 TIC (ES+, MS2) = 82.61 XIC = 65.51 TAC = 95.46


20231135_028323-24AA_1_Profile_ES+_Combined_4.51_234
M+H
M+Na
135.827
136.159
247.071
ES+
269.158
397.276
80
160
240
320
400
480
560
640
720
800
880
960
m/z

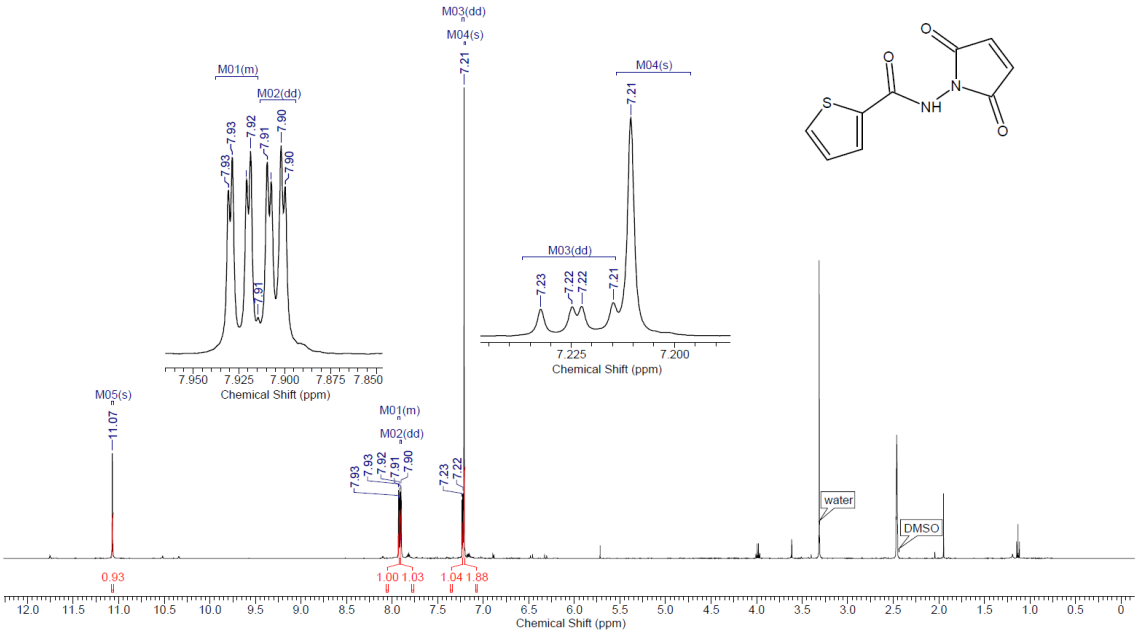
2.21. N-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)thiophene-2-carboxamide 3h



2.21.1. ^{1}H NMR

05.12.2025 02:07:09

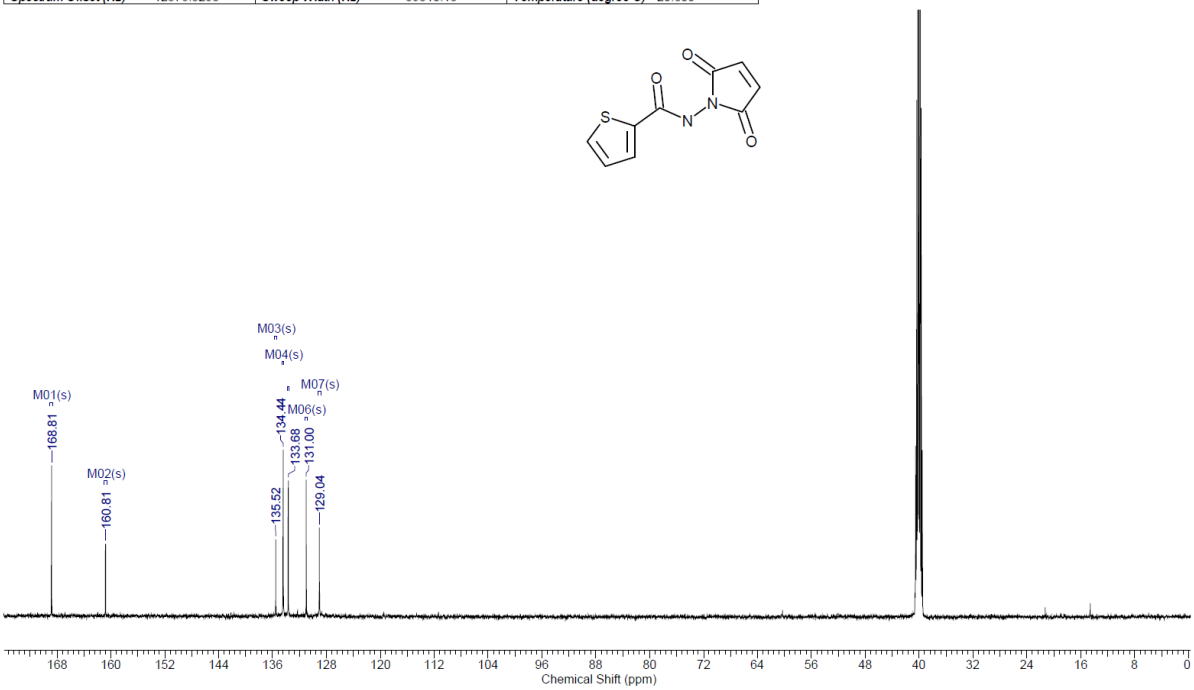
Acquisition Time (sec)	1.9984	*Date*	04 Dec 2025 10:21:44			*Date Stamp*	04 Dec 2025 10:21:06
File Name	C:\Users\Admin\OneDrive - Uniwersytet Jagielloński\nmr\2025\Tiof-mal_935_03_PROTON-1-1.jdf					*Frequency (MHz)*	500.16
Nucleus	1H	*Number of Transients*	8	*Origin*	ECA	*Original Points Count*	18757
Owner	delta	*Points Count*	131072	*Pulse Sequence*	single_pulse.jxp	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	3251.0396	*Spectrum Type*	STANDARD	*Sweep Width (Hz)*	9385.89	*Temperature (degree C)*	20.800



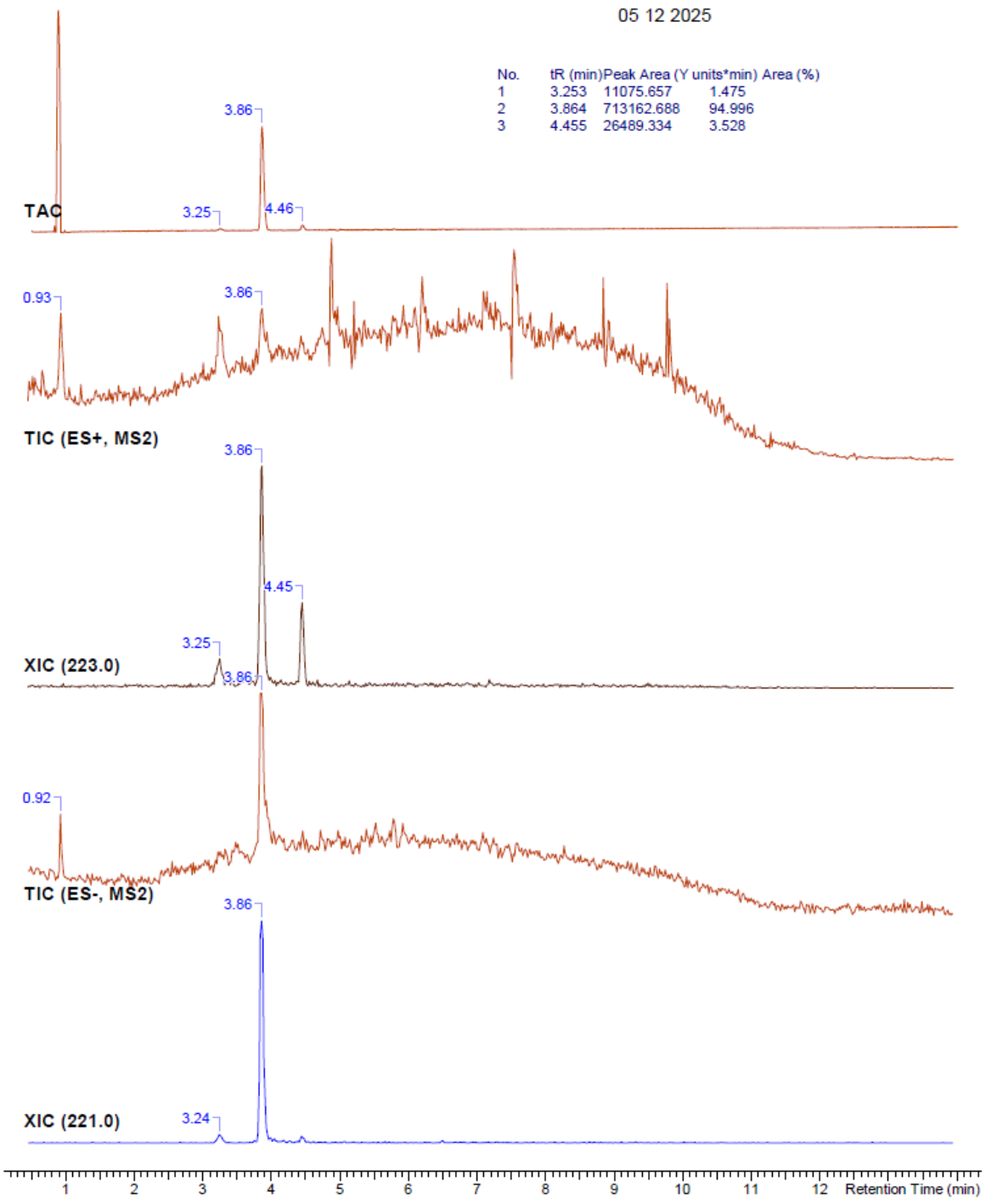
^{13}C NMR

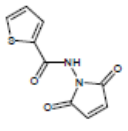
06.12.2025 12:54:56

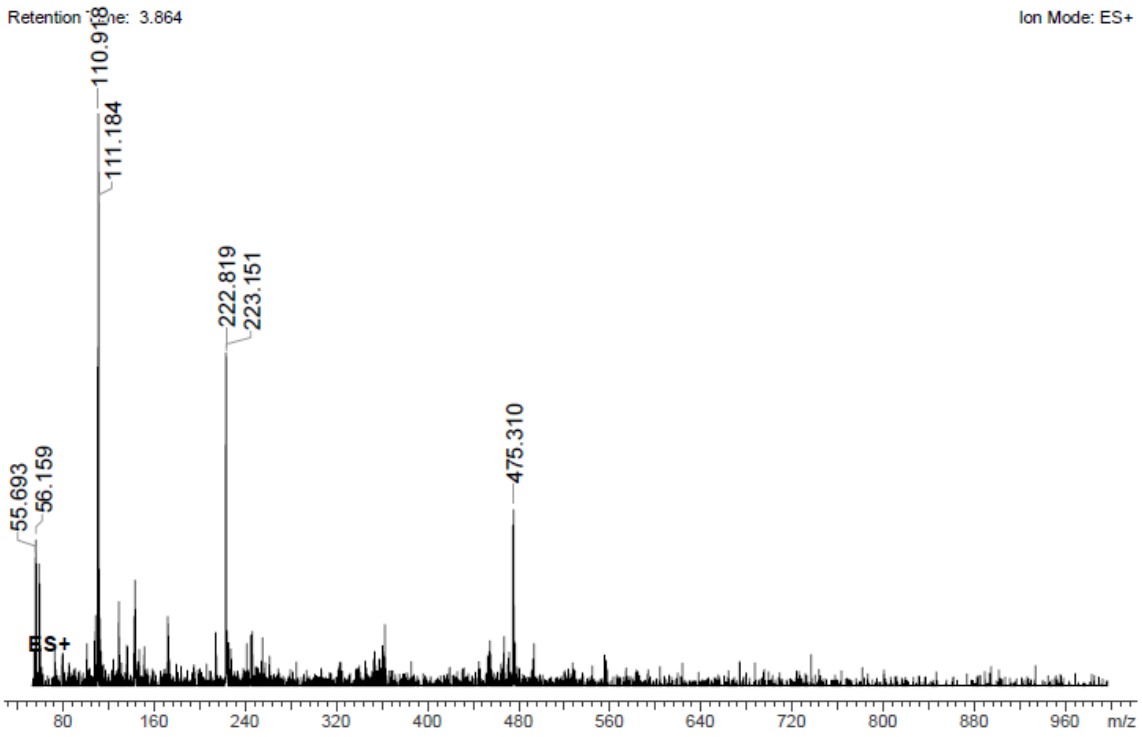
Acquisition Time (sec)	1.9996	*Date*	04 Dec 2025 11:14:18			*Date Stamp*	04 Dec 2025 10:22:15
File Name	C:\Users\Admin\OneDrive - Uniwersytet Jagielloński\nmr\2025\Tiof-mal_935_03_CARBON-2-1.jdf					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	1024	*Origin*	ECA	*Original Points Count*	78604
Owner	delta	*Points Count*	131072	*Pulse Sequence*	carbon.jxp	*Solvent*	DMSO-d6
Spectrum Offset (Hz)	12576.5293	*Sweep Width (Hz)*	39310.18	*Temperature (degree C)*	20.800		

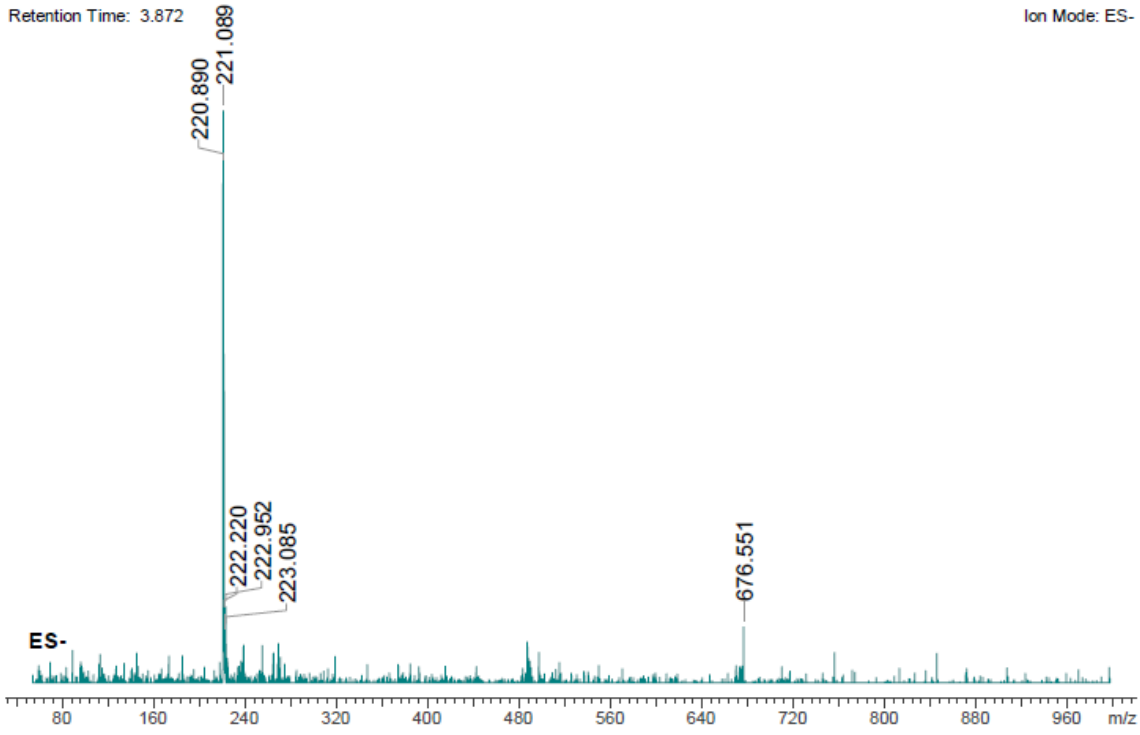


2.21.2. UPLC-MS

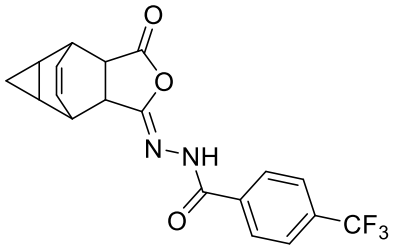


Comp	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	M+·	M-·	MF	Structure	Area (%)
1	3.860	222.010	223.017	221.003	222.009	222.010	$C_9H_6N_2O$		TIC (ES-, MS2) = 87.18 Single XIC = 95.39 TIC (ES+, MS2) = 56.37 Single XIC = 66.15 TAC = 95.00


Retention Time: 3.864
Ion Mode: ES+
110.918
111.184
222.819
223.151
475.310
55.693
56.159
ES+
80
160
240
320
400
480
560
640
720
800
880
960
m/z


Retention Time: 3.872
Ion Mode: ES-
221.089
220.890
222.220
222.952
223.085
676.551
ES-
80
160
240
320
400
480
560
640
720
800
880
960
m/z

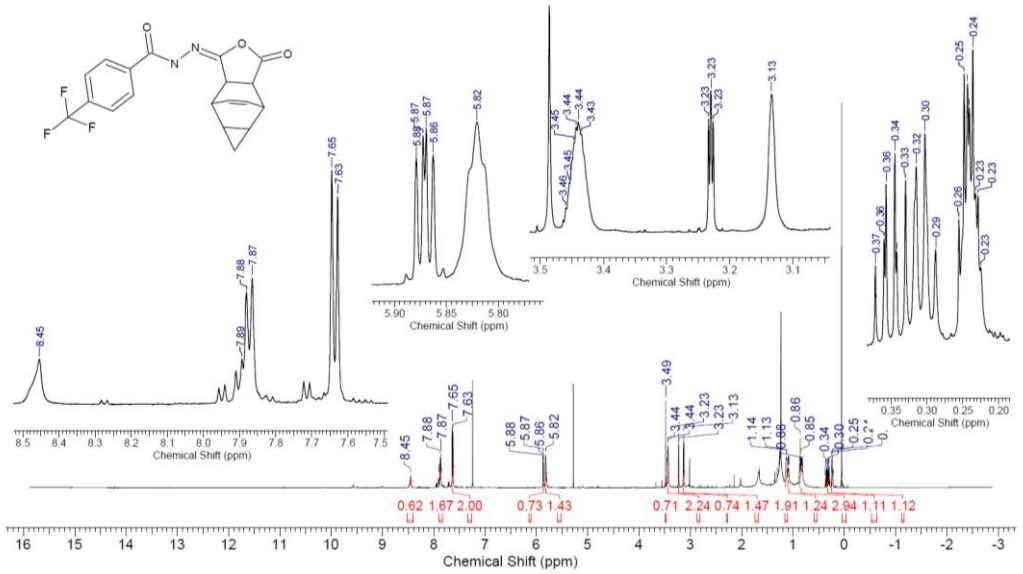
2.22.N'-(3-oxo-3,4,4a,5,5a,6-hexahydro-1H-4,6-ethenocyclopropa[f]isobenzofuran-1-ylidene)-4-(trifluoromethyl)benzohydrazide (4)



2.22.1. ^{1}H NMR

22.11.2025 10:33:15

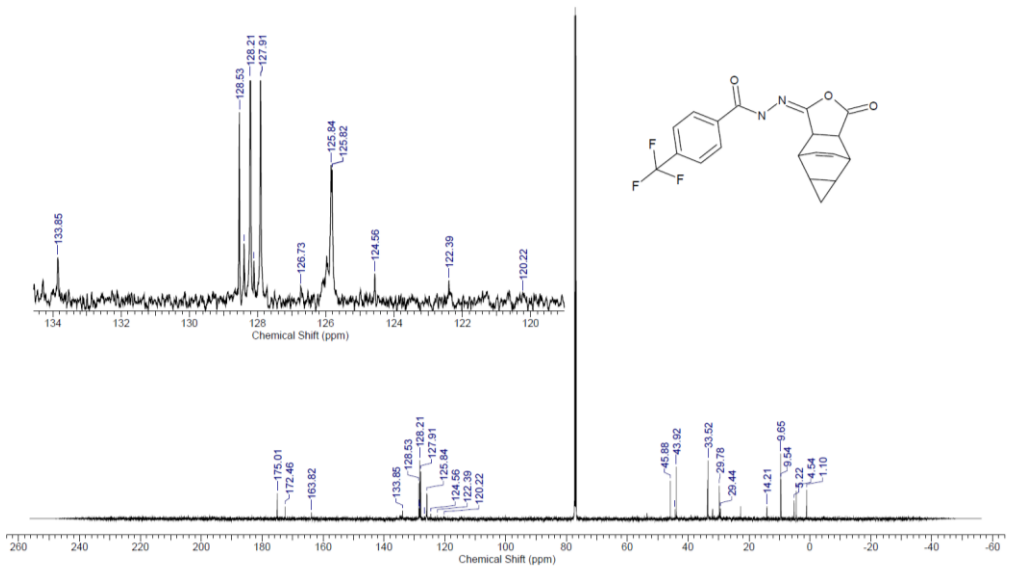
Acquisition Time (sec)	1.9984	Date	29 May 2023 04:06:23			Date Stamp	29 May 2023 04:05:44
File Name	F:\tekowirymat_LCMS\widma_brakujace\izosukc_4AM6I20_935_03_PROTON-1-1.jdf					Frequency (MHz)	500.16
Nucleus	1H	Number of Transients	8	Origin	ECA	Original Points Count	18757
Owner	delta	Points Count	131072	Pulse Sequence	single_pulse.jxp	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3251.0396	Spectrum Type	STANDARD	Sweep Width (Hz)	9385.89	Temperature (degree C)	21.600



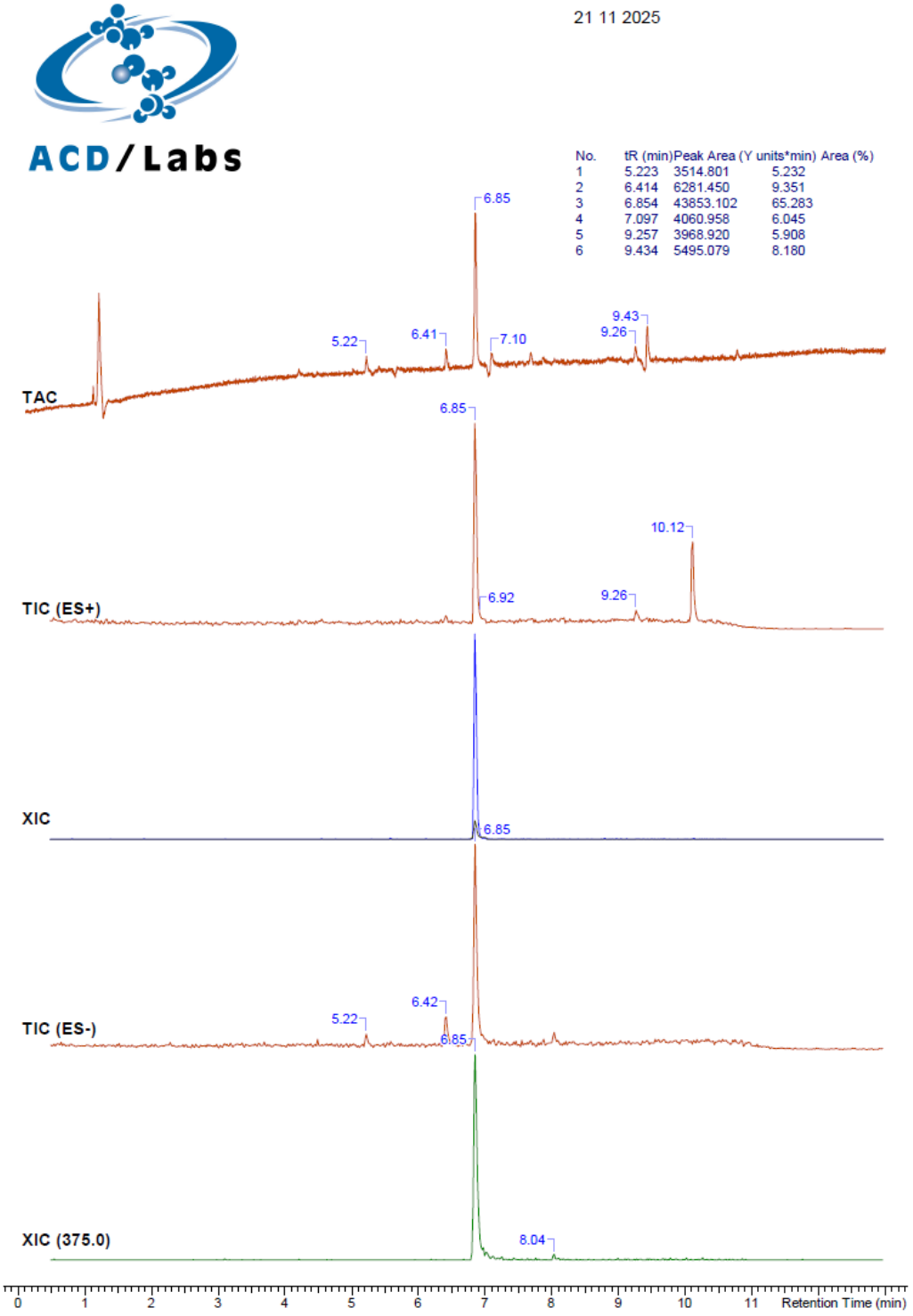
2.22.2. ^{13}C NMR

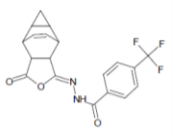
22.11.2025 11:16:03

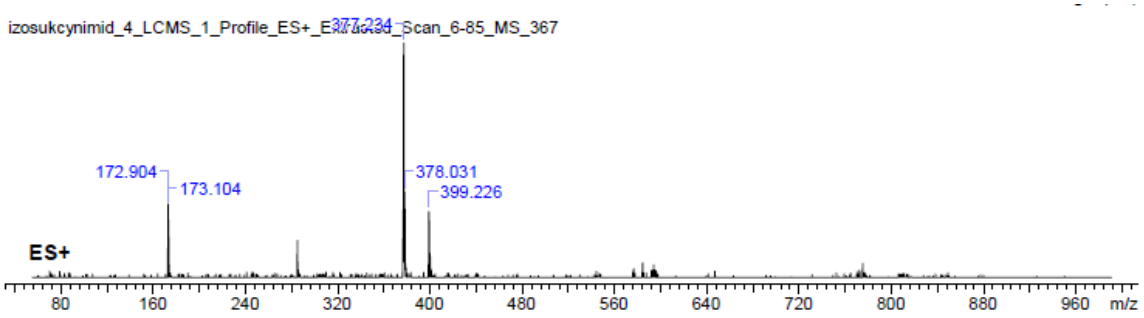
Acquisition Time (sec)	1.9996	Date	29 May 2023 04:58:55			Date Stamp	29 May 2023 04:06:52
File Name	F:\tekowirymat_LCMS\widma_brakujace\izosukcyn4_AM6I20_935_03_CARBON-1-1.jdf					Frequency (MHz)	125.77
Nucleus	13C	Number of Transients	1024	Origin	ECA	Original Points Count	78604
Owner	delta	Points Count	131072	Pulse Sequence	carbon.jxp	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12576.5293	Sweep Width (Hz)	39310.18	Temperature (degree C)	21.400		



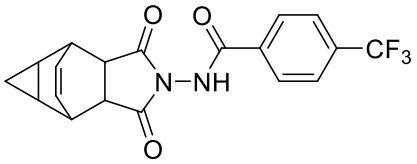
2.22.3. LCMS



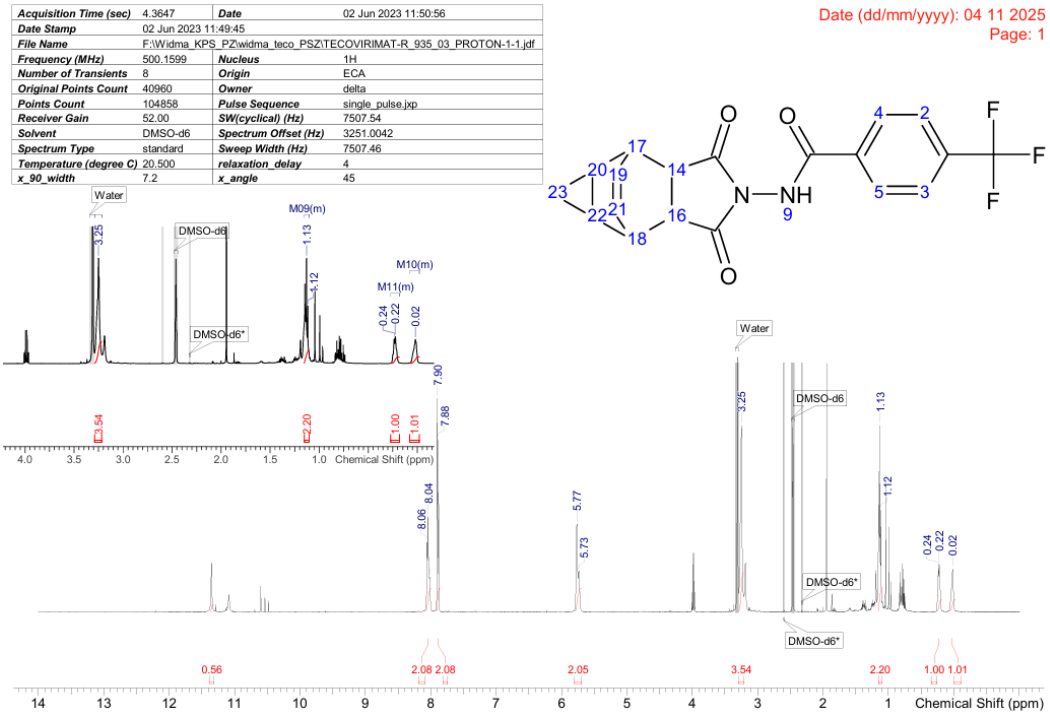
Compor	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	M+·	M-·	MF	Structure	Area (%)
1	6.846	376.103	377.111	375.096	376.103	376.104	$C_{19}H_{15}F_3N_2O_3$		TIC (ES-) = 82.16 Single XIC = 98.69 TIC (ES+) = 41.10 Single XIC = 99.66 TAC = 65.28


izosukcynimid_4_LCMS_1_Profile_ES+_Extracted_Scan_6-85_MS_367
172.904
173.104
378.031
399.226
ES+
80
160
240
320
400
480
560
640
720
800
880
960
m/z

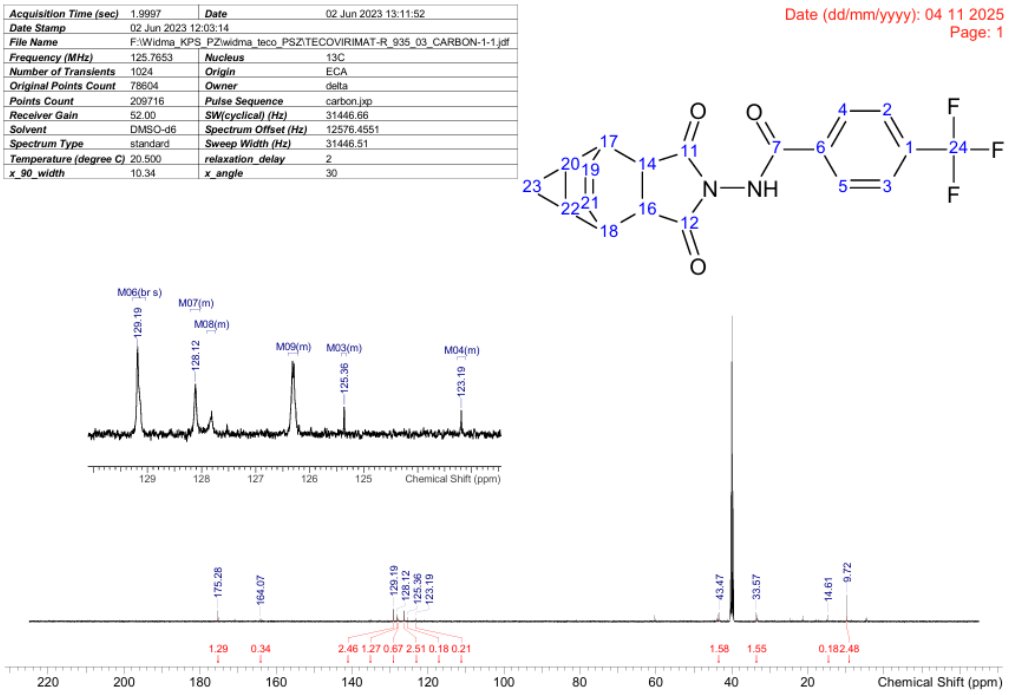
2.23. *N*-(1,3-Dioxo-3,3a,4,4a,5,5a,6,6a-octahydro-4,6-ethenocyclopropa[f]isoindol-2(*1H*)-yl)-4-(trifluoromethyl)benzamide (Tecovirimat, 5)



2.23.1. ^{1}H NMR



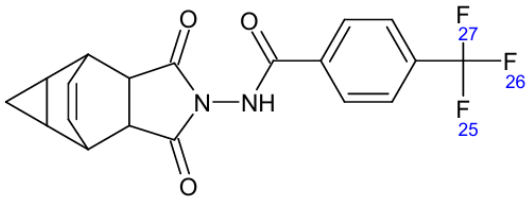
2.23.2. ^{13}C NMR

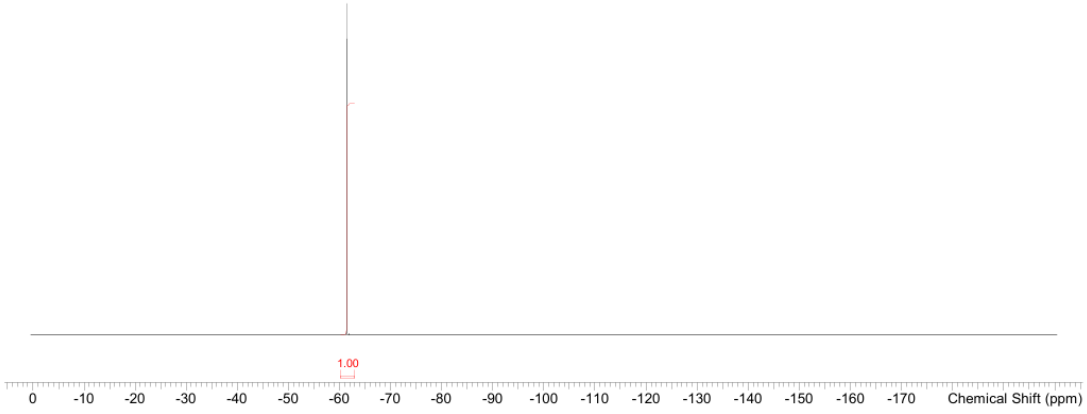


2.23.3. ^{19}F NMR

Acquisition Time (sec)	2.9861	***Date***	02 Jun 2023 11:53:41
Date Stamp	02 Jun 2023 11:52:39		
File Name	F:\Widma_KPS_PZ\widma_teco_PSZ\TECOVIRIMAT-R_935_03_Fluorine-1-1.jdf		
Frequency (MHz)	470.6205	***Nucleus***	19F
Number of Transients	8	***Origin***	ECA
Original Points Count	352967	***Owner***	delta
Points Count	838862	***Pulse Sequence***	single_pulse.jxp
Receiver Gain	62.00	***SW(cyclical) (Hz)***	94562.79
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	-47062.1016
Spectrum Type	standard	***Sweep Width (Hz)***	94562.68
Temperature (degree C)	20.500	***relaxation_delay***	4
x_90_width	7.79	***x_angle***	45

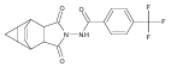
Date (dd/mm/yyyy): 03 11 2025
Page: 1

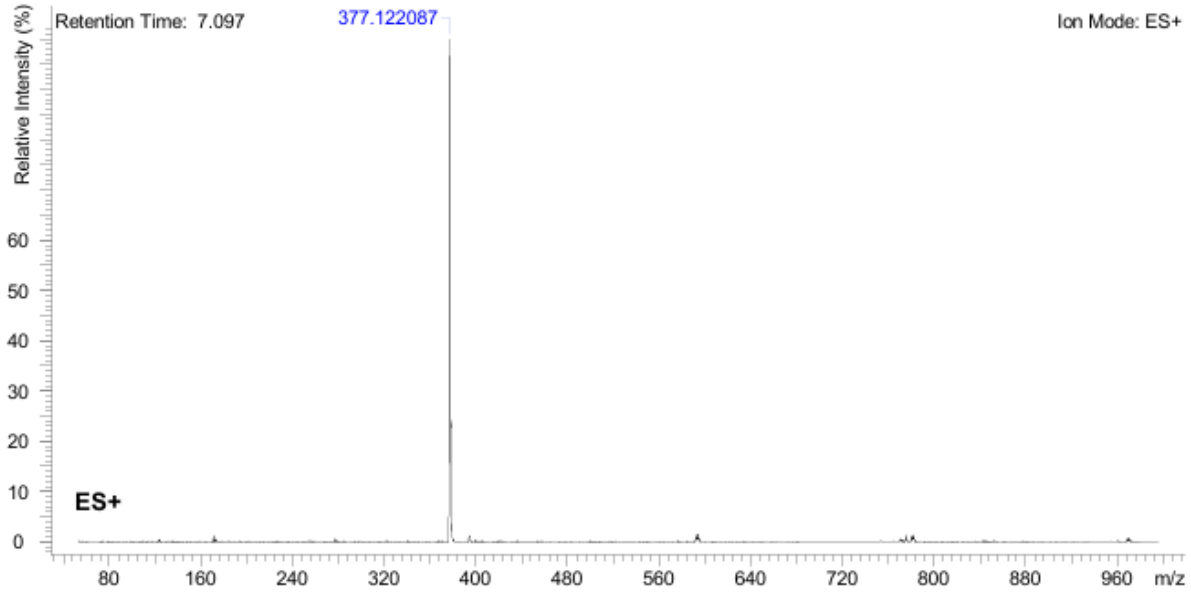




2.23.4. LCMS



Compo	tR(min)	Mass(Ao)	[M+H]+	[M-H]-	M+·	M-·	MF	Structure	Area (%)
1	7.097	376.103	377.111	375.096	376.103	376.104	$C_{19}H_{15}F_3N_2O_3$		TIC (ES-, MS2) = 95.69 Single XIC = 100.00 TIC (ES+, MS2) = 87.09 Single XIC = 99.86 TAC = 95.23


Retention Time: 7.097
377.122087
Ion Mode: ES+
Relative Intensity (%)
60
50
40
30
20
10
0
ES+
80
160
240
320
400
480
560
640
720
800
880
960
m/z

3. Computational results

The computational results for isomaleimides **2a-f, 2h** and isosuccinimide **4** listed below include cartesian coordinates and heat of formation values for the lowest-ΔHf conformations, charge distribution and graphical representations of Molecular Electrostatic Potential (MEP) as well as LUMO and HOMO orbitals with respective energies given in eV.

3.8. *N*'-(5-Oxofuran-2(5H)-ylidene)-4-(trifluoromethyl)benzohydrazide (2a)

Table S1: Heat of formation, atomic coordinates and Net charges for compound **2a**

ΔH_f= 195.81666 kcal/mol					
Atom No.	Element	X	Y	Z	Charge
1	C	-2.794885	3.172267	-0.563112	-0.103436
2	C	-2.385314	3.923163	-1.663580	-0.120605
3	C	-3.129861	3.874683	-2.840226	-0.094041
4	C	-4.268431	3.070335	-2.901056	-0.117186
5	C	-4.686355	2.332116	-1.794332	-0.096921
6	C	-3.943694	2.384254	-0.615951	-0.104778
7	C	-2.036781	3.224658	0.712077	0.571875
8	N	-0.709562	2.821553	0.624449	-0.395417
9	O	-2.517299	3.567497	1.774465	-0.560471
10	F	-5.812211	1.940966	-4.348482	-0.207149
11	N	0.204203	2.904457	1.628264	-0.220851
12	C	-0.078893	2.709416	2.874185	0.296128
13	C	0.667532	2.646329	5.027432	0.615774
14	O	1.054296	2.882417	3.682339	-0.392251
15	C	-1.211862	2.333277	3.754364	-0.073356
16	C	-0.769055	2.295861	5.022102	-0.248698
17	O	1.505079	2.757675	5.869056	-0.435558
18	C	-5.062016	3.029493	-4.174216	0.552244
19	F	-4.332102	3.084940	-5.289749	-0.209010
20	F	-5.923572	4.041821	-4.297248	-0.208564
21	H	-1.493643	4.554952	-1.610519	0.186590
22	H	-2.808946	4.473646	-3.698273	0.187278
23	H	-5.589118	1.714647	-1.824244	0.186669
24	H	-4.264936	1.811428	0.259162	0.185279
25	H	-0.244999	2.640945	-0.280223	0.374824
26	H	-2.203164	2.119376	3.373690	0.213373
27	H	-1.297606	2.056938	5.933788	0.218259

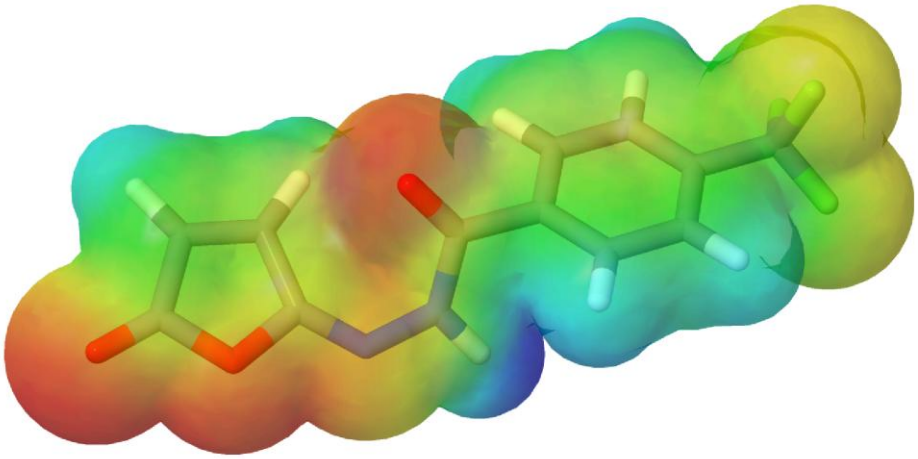


Figure S1: Molecular Electrostatic Potential surface for compound **2a**

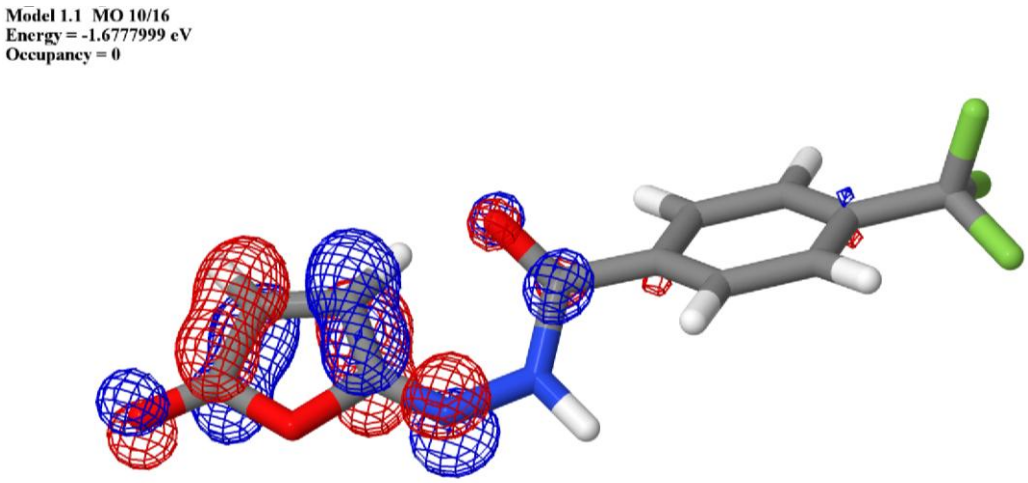


Figure S2: Graphical representation of LUMO orbital for compound **2a**

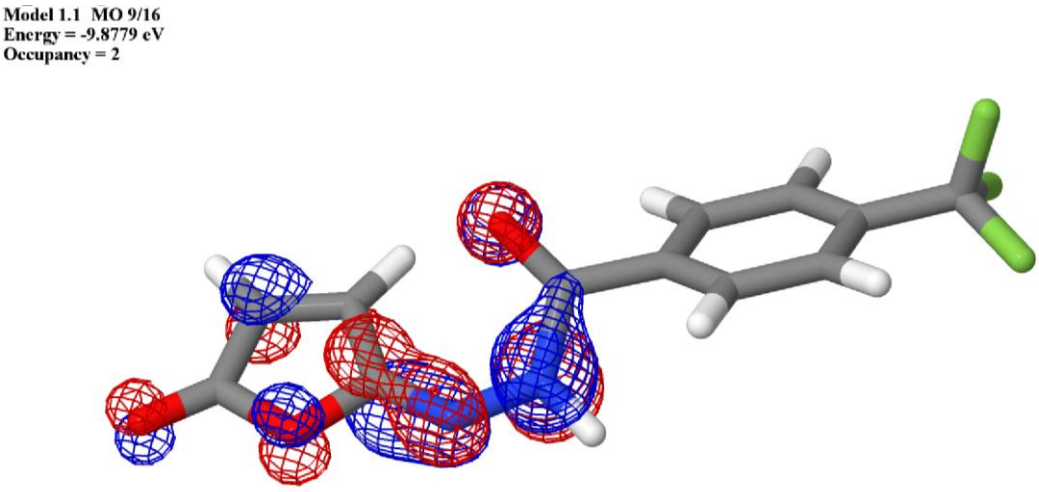


Figure S3: Graphical representation of HOMO orbital for compound **2a**

Tert-butyl 2-(5-oxofuran-2(*5H*)-ylidene)hydrazine-1-carboxylate (2b)

Table S2: Heat of formation, atomic coordinates and Net charges for compound **2b**

ΔH_f= -132.16417 kcal/mol					
Atom No.	Element	X	Y	Z	Net Charge
1	O	2.742612	0.122851	-1.614114	-0.485113
2	C	3.913625	0.899692	-2.041306	0.395310
3	C	2.665697	-1.181438	-1.887277	0.741281
4	N	1.459548	-1.739011	-1.417344	-0.419945
5	O	3.497242	-1.883693	-2.423133	-0.592498
6	N	0.381691	-0.984376	-1.036904	-0.227382
7	C	0.498070	-0.052069	-0.149209	0.303401
8	C	-0.462010	1.598249	1.087817	0.613281
9	O	-0.715893	0.585400	0.123560	-0.381658
10	C	1.546830	0.566779	0.699936	-0.083448
11	C	0.977631	1.540144	1.428633	-0.243231
12	O	-1.382348	2.270581	1.437021	-0.433696
13	C	5.122899	0.396687	-1.273339	-0.518344
14	C	4.060890	0.784931	-3.547710	-0.518497
15	C	3.476158	2.296838	-1.606859	-0.493627
16	H	1.142057	-2.617730	-1.872952	0.373309
17	H	2.572363	0.220244	0.694918	0.208414
18	H	1.412323	2.202747	2.162898	0.216716
19	H	4.944221	0.380343	-0.190661	0.165712
20	H	5.997334	1.037458	-1.450392	0.173016
21	H	5.405294	-0.622951	-1.572627	0.177092
22	H	4.415489	-0.208613	-3.856346	0.177379
23	H	3.108500	0.966482	-4.063539	0.170908
24	H	4.783824	1.517256	-3.932097	0.173321
25	H	4.243458	3.038918	-1.863863	0.174104
26	H	2.544826	2.602774	-2.102367	0.170904
27	H	3.307402	2.359432	-0.524909	0.163291

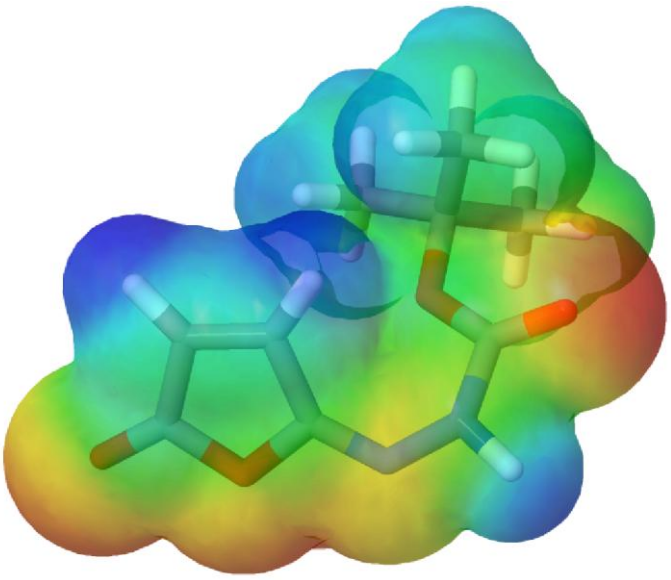


Figure S4: Molecular electrostatic potential surface for compound **2b**

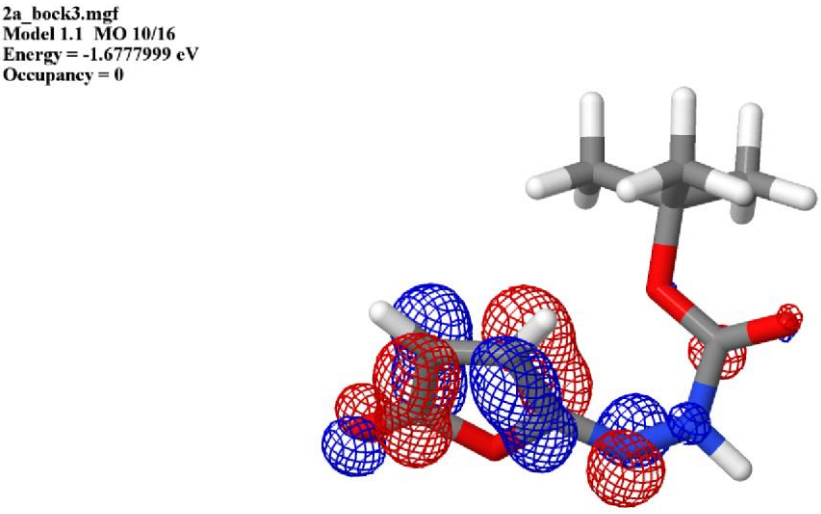


Figure S5: Graphical representation of LUMO orbital for compound **2b**

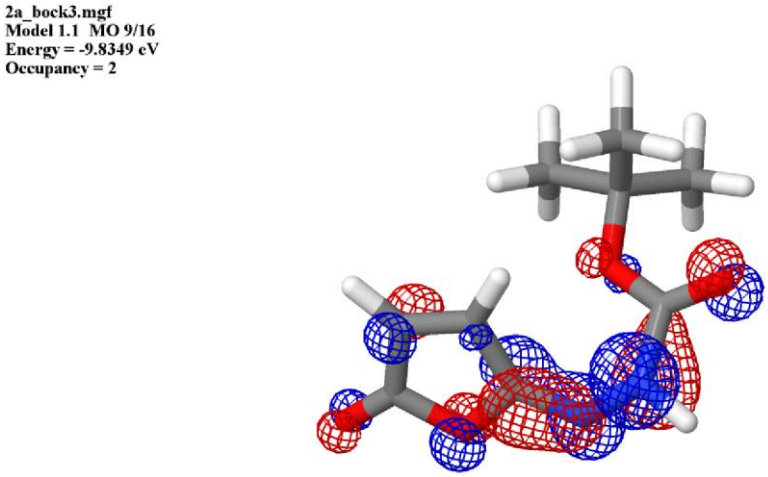


Figure S6: Graphical representation of HOMO orbital for compound **2b**

N'-(5-Oxofuran-2(*5H*)-ylidene)benzohydrazide (2c)

Table S3: Heat of formation, atomic coordinates and Net charges for compound **2c**

ΔH_f= -30.79529 kcal/mol					
Atom No.	Element	X	Y	Z	Charge
1	C	-3.310300169	1.988749772	-1.270934116	-0.158576
2	C	-2.567828802	2.488296597	-2.354330800	-0.072560
3	C	-3.020474927	3.599728154	-3.056250856	-0.191219
4	C	-4.201605065	4.235984237	-2.671855214	-0.092312
5	C	-4.934714881	3.746419904	-1.594370550	-0.186713
6	C	-4.498237304	2.618760939	-0.902543246	-0.073179
7	C	-2.782374657	0.780710958	-0.612377349	0.639709
8	N	-3.391356606	0.067762765	0.434710891	-0.421094
9	O	-1.764717768	0.225908866	-1.007156648	-0.594337
10	N	-4.373273138	0.589883446	1.217055032	-0.184113
11	C	-4.990500624	-0.211693496	2.031364634	0.237159
12	C	-6.380721606	-0.602974586	3.781806320	0.609023
13	O	-5.904585270	0.401344514	2.888991203	-0.364700
14	C	-4.959477727	-1.661356140	2.334554122	-0.102946
15	C	-5.779997279	-1.892241949	3.372389592	-0.229614
16	O	-7.130735286	-0.261193296	4.643455042	-0.440169
17	H	-1.633149164	2.001177273	-2.651139682	0.177157
18	H	-2.458385497	3.976043957	-3.911032826	0.168189
19	H	-4.551456731	5.115957483	-3.214800708	0.161602
20	H	-5.857240426	4.239671336	-1.288990585	0.169723
21	H	-5.104051152	2.238968161	-0.075561302	0.186044
22	H	-2.913079134	-0.795347692	0.740391584	0.341023
23	H	-4.376272106	-2.362438041	1.753920795	0.206228
24	H	-6.024913612	-2.819185241	3.872344935	0.215673

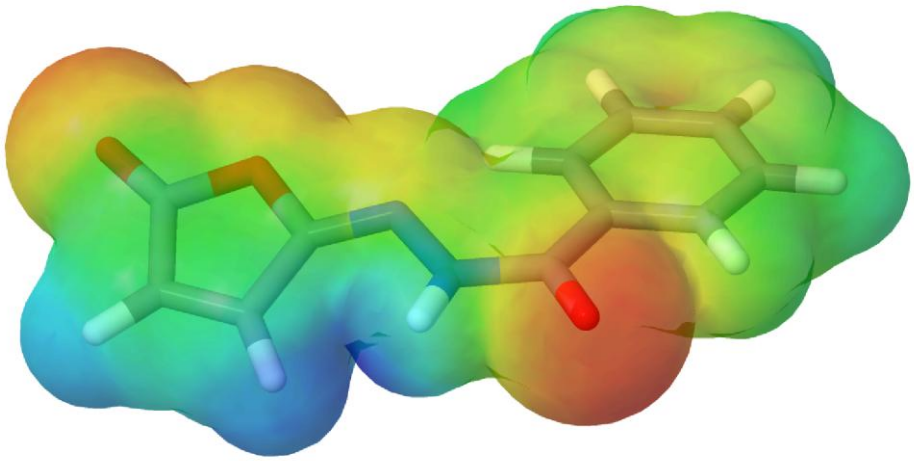


Figure S7: Molecular electrostatic potential surface for compound **2c**

2c_bzk1.mgf
Model 1.1 MO 10/16
Energy = -1.7238 eV
Occupancy = 0

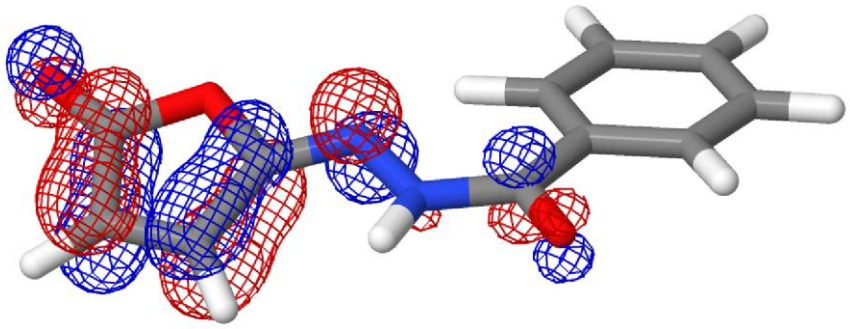


Figure S8: Graphical representation of LUMO orbital for compound **2c**

2c_bzk1.mgf
Model 1.1 MO 9/16
Energy = -9.6381 eV
Occupancy = 2

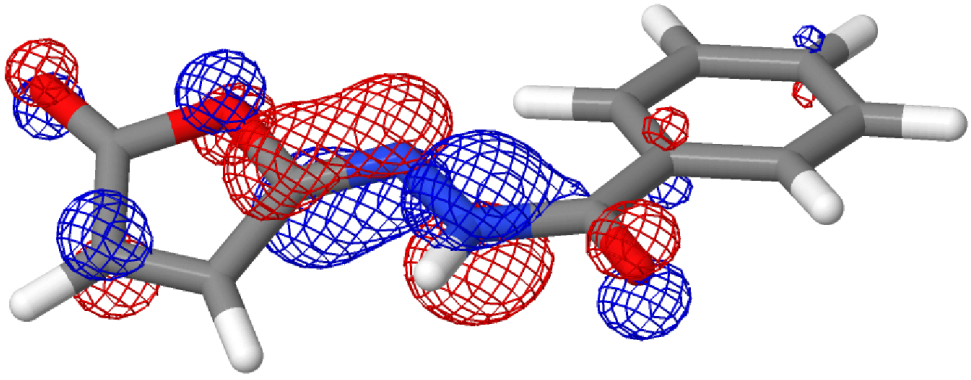


Figure S9: Graphical representation of HOMO orbital for compound **2c**

4-(Dimethylamino)-N'-(5-oxofuran-2(*5H*)-ylidene)benzohydrazide (2d)

Table S4: Heat of formation, atomic coordinates and net charges for compound **2d**

ΔHf = -41.95193 kcal/mol					
Atom No.	Element	X	Y	Z	Charge
1	C	-2.908996771	2.966759508	0.628357206	-0.296697
2	C	-2.394197058	4.163955151	0.111242429	0.012251
3	C	-2.608737519	5.363084042	0.762202807	-0.341241
4	C	-3.349917066	5.402793804	1.971892572	0.291036
5	C	-3.819211445	4.175950726	2.510904344	-0.335304
6	C	-3.608441175	2.986682198	1.840961065	-0.008013
7	C	-2.652362812	1.736682358	-0.122105243	0.618385
8	N	-3.642282456	0.743212255	-0.042464058	-0.410460
9	O	-1.658303782	1.529659317	-0.794627719	-0.592676
10	N	-3.700503321	6.606351290	2.548074245	-0.381793
11	N	-3.662581777	-0.397012431	-0.774762073	-0.211612
12	C	-2.608858731	-1.062100254	-1.114108275	0.274847
13	C	-1.764652380	-2.871100472	-2.215258301	0.620152
14	O	-2.958622887	-2.191804290	-1.878550869	-0.395961
15	C	-1.136481527	-1.064006790	-0.956386209	-0.058659
16	C	-0.640434264	-2.130948398	-1.606665924	-0.267784
17	O	-1.859249434	-3.858746650	-2.880194173	-0.455458
18	C	-2.988976355	7.826286773	2.141940307	-0.260837
19	C	-4.171080868	6.622711848	3.939630309	-0.261345
20	H	-1.814571399	4.143871096	-0.819428358	0.173884
21	H	-2.200226132	6.277505785	0.337702396	0.178438
22	H	-4.351213008	4.161902962	3.459801408	0.177025
23	H	-3.981930959	2.054854547	2.278862879	0.168618
24	H	-4.584615134	0.953461171	0.323374168	0.367555
25	H	-0.608566079	-0.311522123	-0.382055216	0.214778
26	H	0.381070962	-2.463943459	-1.710730789	0.215144
27	H	-1.900854431	7.766338430	2.321117657	0.153258
28	H	-3.373271633	8.703610615	2.692954647	0.165791
29	H	-3.161845031	8.026187101	1.067623794	0.164386
30	H	-3.409427059	6.257756488	4.650376483	0.152250
31	H	-4.453869252	7.647467198	4.242136539	0.167014
32	H	-5.078952254	6.000959857	4.045227047	0.163024

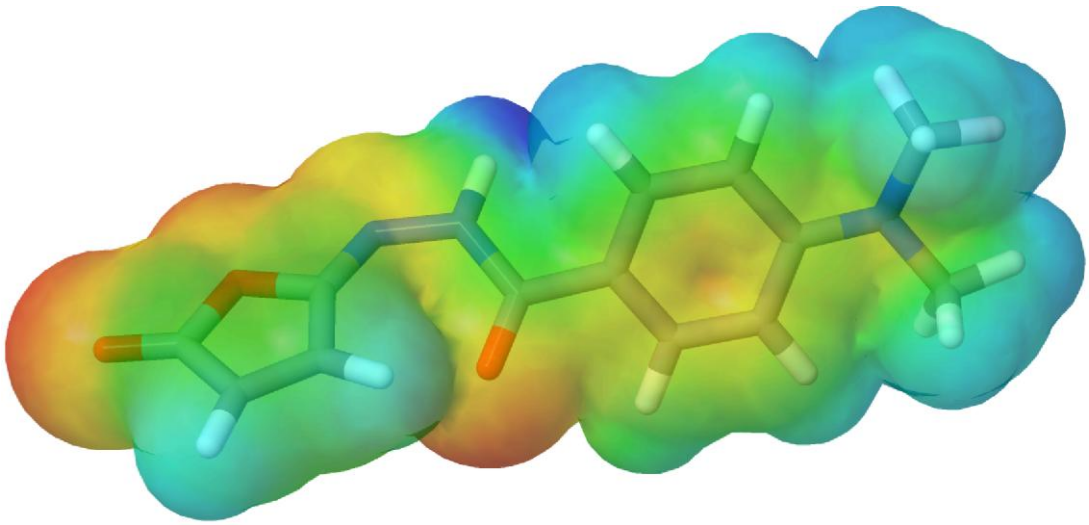


Figure S10: Graphical representation molecular electrostatic potential for compound **2d**

LUMO

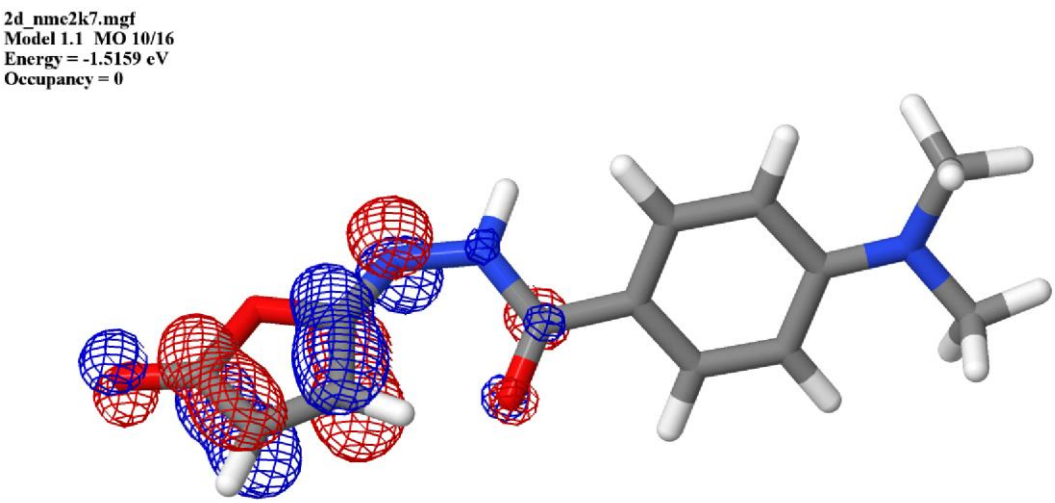


Figure S11: Graphical representation LUMO orbital for compound **2d**

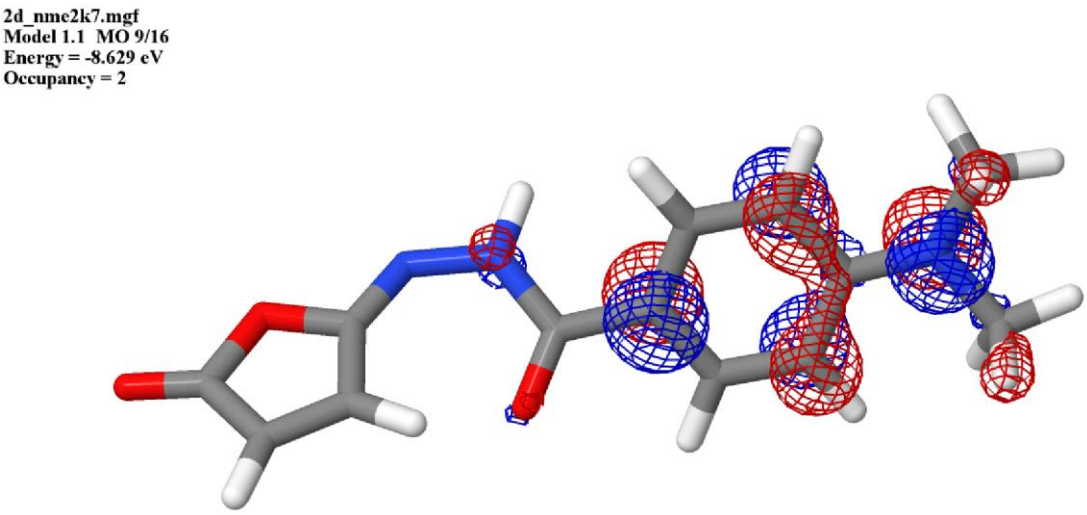


Figure S12: Graphical representation HOMO orbital for compound **2d**

4-Methoxy-*N*'-(5-oxofuran-2(*5H*)-ylidene)benzohydrazide (2e)

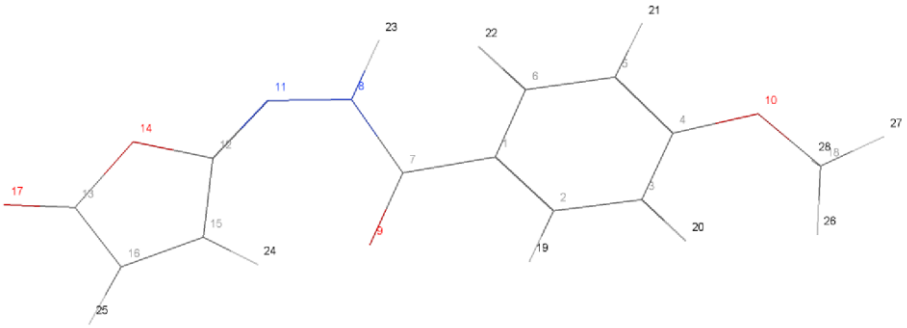


Table S5: Heat of formation, atomic coordinates and Net charges for compound **2e**

ΔHf = -79.61865 kcal/mol					
Atom No.	Element	X	Y	Z	Charge
1	C	-2.506009457	2.619469738	-1.513766588	-0.252353
2	C	-3.657687287	2.115131807	-0.902753804	-0.000541
3	C	-4.771150357	2.928198124	-0.729205868	-0.323797
4	C	-4.715838697	4.247491928	-1.187263260	0.304150
5	C	-3.566664155	4.764359789	-1.815433463	-0.286565
6	C	-2.465308012	3.942096510	-1.974510680	-0.027169
7	C	-1.366310729	1.705592206	-1.689423862	0.605044
8	N	-0.101855128	2.259946786	-1.454758789	-0.404911
9	O	-1.463012113	0.540810144	-2.026754921	-0.579122
10	O	-5.714840538	5.152089890	-1.091109463	-0.345969
11	N	1.061787962	1.561344363	-1.429972887	-0.216686
12	C	1.321052101	0.562591241	-2.206980372	0.282986
13	C	2.812335268	-1.048854674	-2.820509638	0.618537
14	O	2.598908433	0.040128898	-1.940424659	-0.394690
15	C	0.734164846	-0.223512406	-3.317619899	-0.064430
16	C	1.614778212	-1.172833859	-3.677467194	-0.260720
17	O	3.847936425	-1.635894644	-2.731402910	-0.448251
18	C	-6.933386281	4.736811288	-0.480569417	-0.201509
19	H	-3.682325320	1.075376549	-0.557989472	0.177711
20	H	-5.663325392	2.533688472	-0.247010046	0.186831
21	H	-3.559361398	5.795162495	-2.167338903	0.187453
22	H	-1.569125805	4.327915244	-2.471286909	0.176794
23	H	0.005957998	3.159513116	-0.957677481	0.370386
24	H	-0.240889988	-0.005757423	-3.737608080	0.214568
25	H	1.543359478	-1.927239426	-4.446915299	0.216486
26	H	-7.398205504	3.923602866	-1.048062657	0.149910
27	H	-7.546772008	5.647865327	-0.540490497	0.166359
28	H	-6.771330216	4.453801083	0.564954217	0.149500

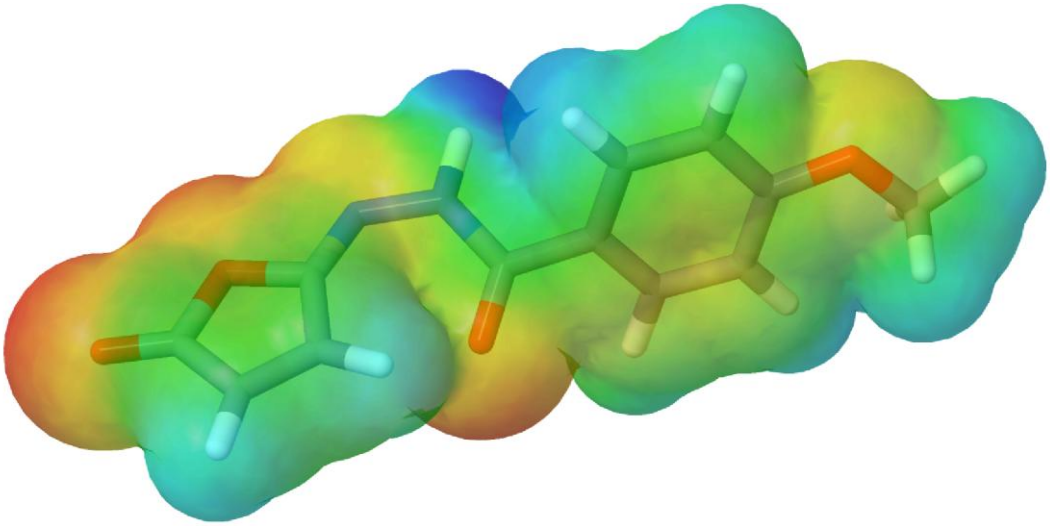


Figure S13: Graphical representation molecular electrostatic potential for compound **2e**

LUMO

2e_omek2.mgf
Model 1.1 MO 10/16
Energy = -1.5738 eV
Occupancy = 0

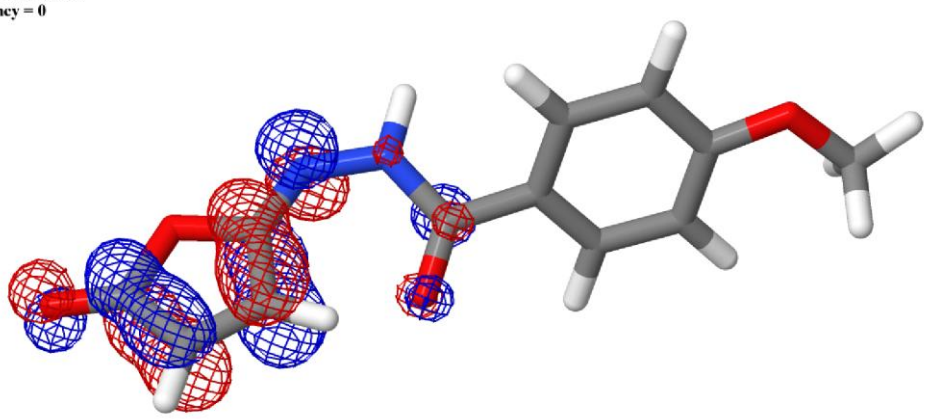


Figure S14: Graphical representation LUMO orbital for compound **2e**

2e_omek2.mgf
Model 1.1 MO 9/16
Energy = -9.5131 eV
Occupancy = 2

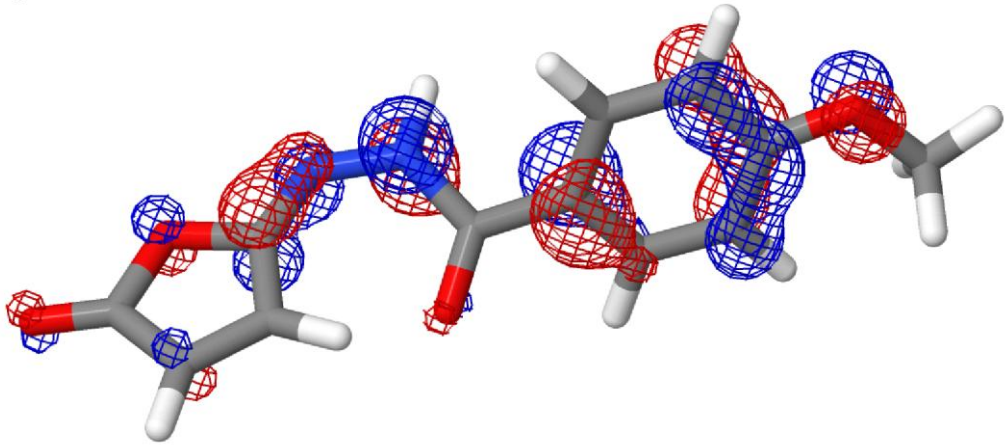


Figure S15: Graphical representation HOMO orbital for compound **2e**

5-(2-Phenylhydrazineylidene)furan-2(5*H*)-one (2f)

Table S6: Heat of formation, atomic coordinates and Net charges for compound **2f**

ΔHf = 10.56278 kcal/mol					
Atom No.	Element	X	Y	Z	Charge
1	N	1.936337379	-0.292358032	0.216521163	-0.354656
2	N	1.134468845	-0.771609912	1.236336034	-0.263508
3	C	1.654659060	-1.193024473	2.343313264	0.295418
4	C	1.467978746	-1.873779574	4.501832827	0.605076
5	O	0.734908449	-1.477800958	3.346403340	-0.373273
6	C	3.020295137	-1.463403442	2.865441272	-0.135747
7	C	2.906599743	-1.884093398	4.133913437	-0.198914
8	O	0.853525284	-2.104766930	5.494957866	-0.418401
9	C	2.142576254	-1.190074144	-0.881385011	0.152482
10	C	1.363144956	-2.330884145	-1.096187704	-0.223075
11	C	1.577046340	-3.092532930	-2.242675839	-0.105316
12	C	2.551336004	-2.722805319	-3.167024381	-0.201708
13	C	3.336062194	-1.592424038	-2.938095678	-0.103153
14	C	3.142668432	-0.824169060	-1.796967853	-0.243846
15	H	2.813538046	0.161142642	0.536780545	0.296340
16	H	3.906202704	-1.347168257	2.257799588	0.204837
17	H	3.664761985	-2.200516263	4.837030627	0.218172
18	H	0.601878258	-2.631640615	-0.376172450	0.181610
19	H	0.983748953	-3.993558271	-2.410853165	0.165265
20	H	2.710376469	-3.320795182	-4.063153311	0.164798
21	H	4.116724080	-1.315749006	-3.649458282	0.163081
22	H	3.767375494	0.050108651	-1.614675656	0.174517

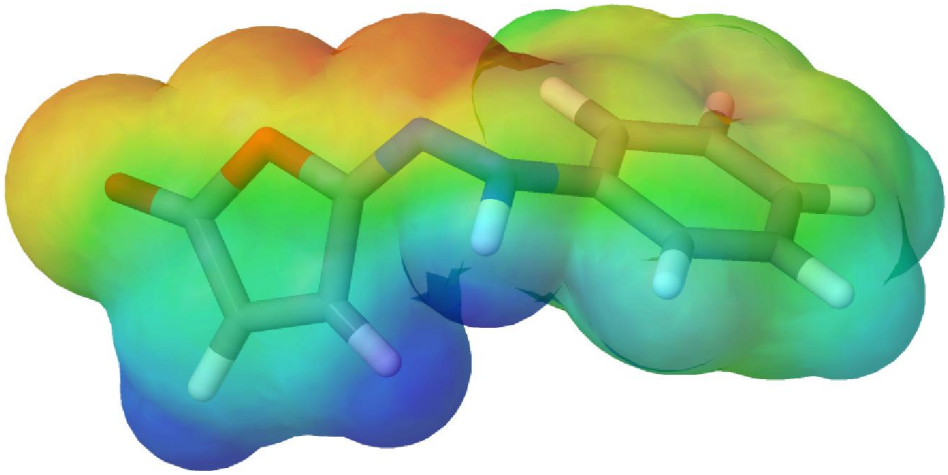


Figure S16: Graphical representation of molecular electrostatic potential for compound **2f**

2f_phhk1.mgf
Model 1.1 MO 10/16
Energy = -1.7045 eV
Occupancy = 0

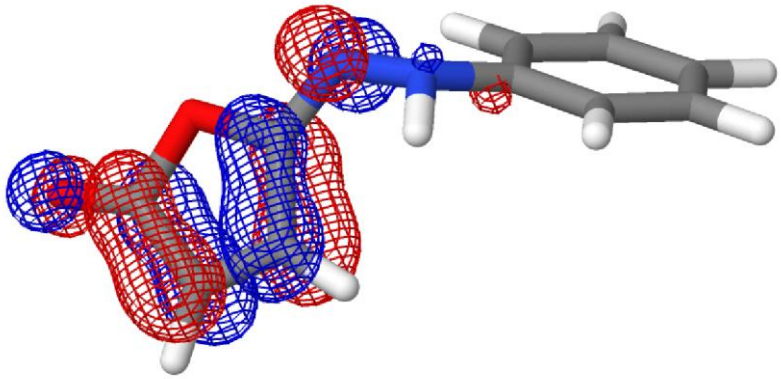


Figure S17: Graphical representation of LUMO orbital for compound **2f**

2f_phhk1.mgf
Model 1.1 MO 9/16
Energy = -9.1692 eV
Occupancy = 2

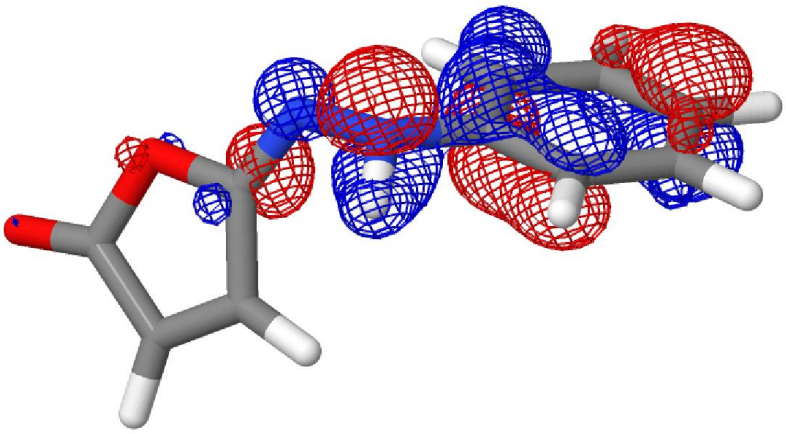


Figure S18: Graphical representation of HOMO orbital for compound **2f**

N'-[5-oxo-2,5-dihydrofuran-2-ylidene]thiophene-2-carbohydrazide (2h)

Table S7: Heat of formation, atomic coordinates and net charges for compound **2h**

ΔH_f= -28.06851 kcal/mol					
Atom No	Element	x	y	z	Charge
1	O	0,50333	-2,9166	-0,78211	-0,37475
2	C	-0,12238	-3,97455	-1,50627	0,602352
3	C	-1,30993	-3,40239	-2,18703	-0,21296
4	C	-1,39186	-2,1007	-1,87407	-0,1184
5	C	-0,26246	-1,76995	-0,96558	0,316244
6	O	0,380073	-5,05164	-1,44911	-0,40975
7	N	0,178959	-0,74362	-0,3114	-0,23698
8	N	-0,49694	0,451409	-0,38245	-0,42544
9	C	-1,78925	0,671153	0,098	0,624138
10	C	-2,62996	-0,43885	0,518493	-0,37197
11	O	-2,15291	1,83807	0,105924	-0,58069
12	S	-4,28771	-0,56677	0,003176	0,313625
13	C	-2,32078	-1,44268	1,402242	-0,07312
14	C	-3,411	-2,33716	1,632285	-0,20791
15	C	-4,53866	-1,99971	0,935138	-0,21495
16	H	-1,94182	-4,008	-2,82177	0,218232
17	H	-2,10002	-1,35617	-2,20938	0,208704
18	H	0,158378	1,248482	-0,4617	0,373274
19	H	-1,36188	-1,56412	1,897383	0,187015
20	H	-3,32519	-3,18896	2,295774	0,186359
21	H	-5,48427	-2,52439	0,9353	0,196959

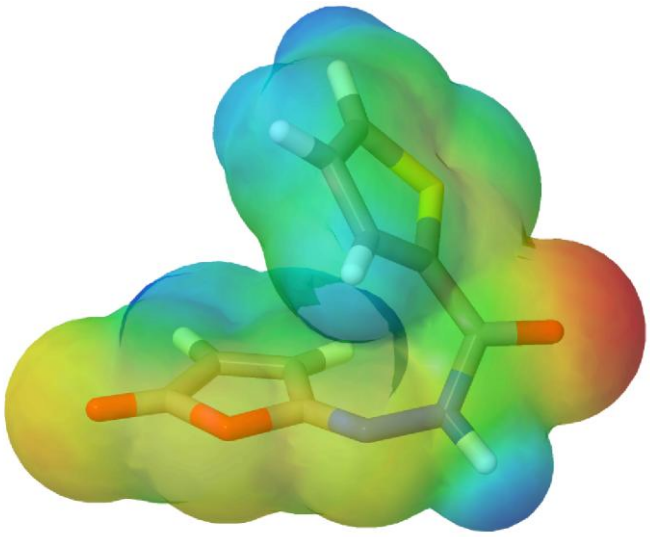


Figure S19: Graphical representation of molecular electrostatic potential for compound **2h**

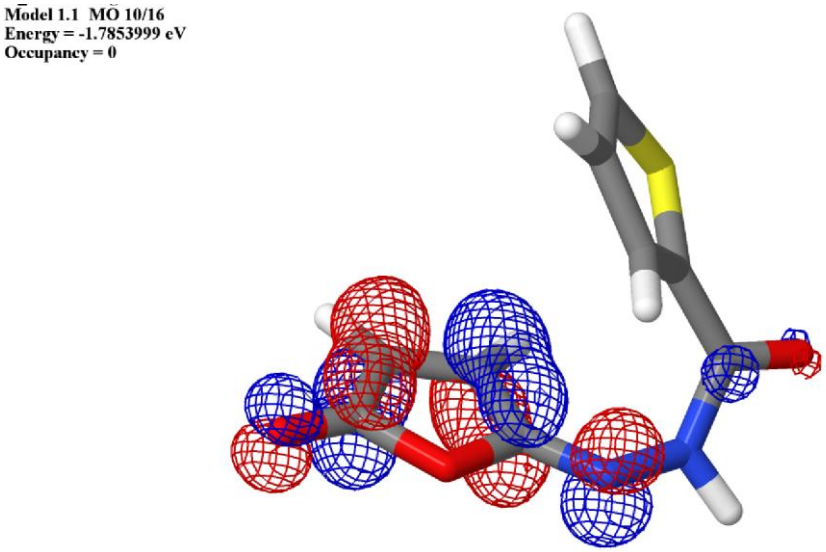


Figure S20: Graphical representation of LUMO orbital for compound **2h**

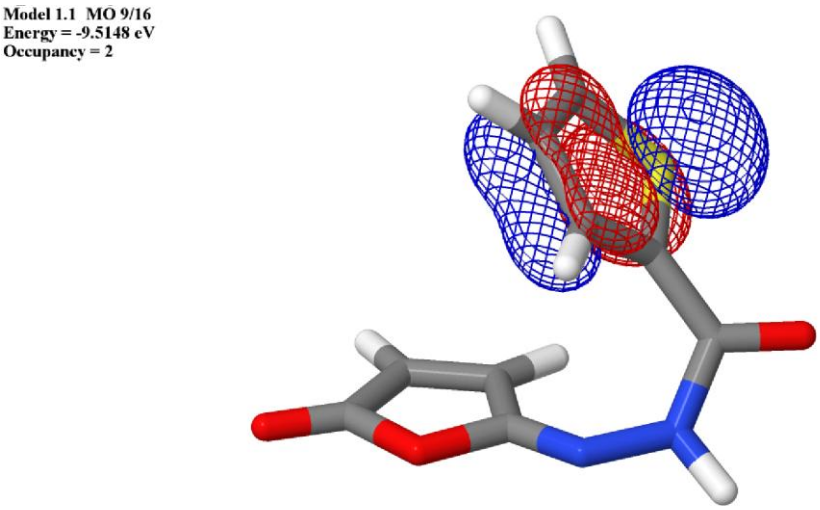


Figure S21: Graphical representation of HOMO orbital for compound **2h**

N'-(3-oxo-3,4,4a,5,5a,6-hexahydro-1H-4,6-ethenocyclopropa[f]isobenzofuran-1-ylidene)-4-(trifluoromethyl)benzohydrazide (4)

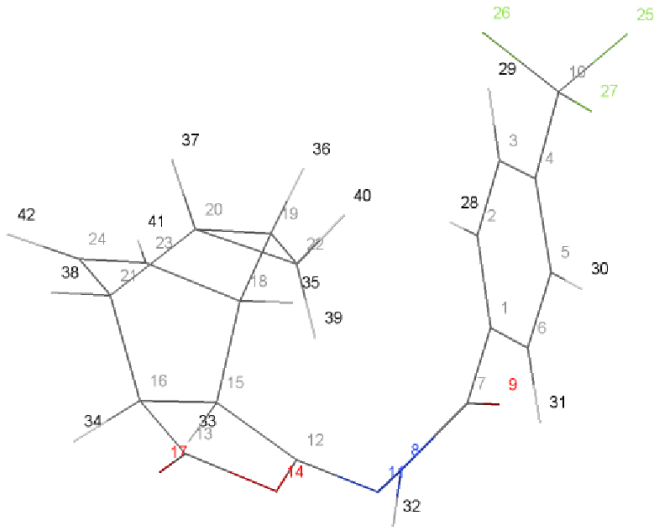


Table S8: Heat of formation, atomic coordinates and net charges for compound **4**

ΔHf = -180.02504 kcal/mol					
Atom No.	Element	X	Y	Z	Charge
1	C	0.736164350	-1.571609311	0.877008494	-0.093137
2	C	-0.142536648	-2.266674886	1.709714742	-0.117370
3	C	-0.242312948	-3.650471087	1.599273770	-0.106344
4	C	0.543095645	-4.322960547	0.660609430	-0.118645
5	C	1.435875874	-3.632420823	-0.155744079	-0.097263
6	C	1.533774489	-2.245358712	-0.044378615	-0.106421
7	C	0.815965565	-0.098655244	1.037655670	0.599307
8	N	0.526064563	0.747345780	-0.022380162	-0.423611
9	O	1.018853705	0.431085415	2.120637990	-0.596176
10	C	0.397274339	-5.812941701	0.563918456	0.556291
11	N	0.627187376	0.295391959	-1.335129721	-0.325546
12	C	-0.479152443	0.044181977	-1.967005534	0.398981
13	C	-1.496312603	-0.589951314	-3.925222598	0.616800
14	O	-0.262844129	-0.320762174	-3.278494843	-0.394075
15	C	-1.948203372	0.117709107	-1.661974452	-0.189014
16	C	-2.630055875	-0.270584065	-3.004036446	-0.225758
17	O	-1.428983799	-0.980685238	-5.048145270	-0.427994
18	C	-2.472115225	-0.797896819	-0.526139990	-0.087123
19	C	-2.331507098	-2.294829078	-0.807829378	-0.175688
20	C	-3.007240079	-2.663313966	-2.131550539	-0.180110
21	C	-3.633878793	-1.427641392	-2.779364514	-0.080387
22	C	-1.526899009	-2.879582265	-1.940178486	-0.332405
23	C	-3.978272275	-0.567839081	-0.549959962	-0.163032
24	C	-4.573991682	-0.889755014	-1.707495739	-0.162922
25	F	0.729755658	-6.459791521	1.683831114	-0.214598
26	F	-0.849758589	-6.218159999	0.311656439	-0.212728
27	F	1.122011603	-6.415116127	-0.378482821	-0.207761
28	H	-0.746920331	-1.730038448	2.446417094	0.183218
29	H	-0.933280929	-4.192193033	2.251858363	0.184839

30	H	2.066434781	-4.147575084	-0.886231238	0.187646
31	H	2.232603683	-1.694500734	-0.683121765	0.190950
32	H	0.713135760	1.758532512	0.064723545	0.361024
33	H	-2.200866587	1.178931886	-1.385384870	0.207056
34	H	-3.195521803	0.606159001	-3.426888678	0.215916
35	H	-2.004336444	-0.523269372	0.440684497	0.160203
36	H	-2.474230904	-2.903152800	0.089151481	0.170167
37	H	-3.644631959	-3.547181669	-2.217138917	0.172156
38	H	-4.151393153	-1.683306033	-3.727702505	0.170221
39	H	-0.762180742	-2.334711876	-2.469059111	0.165474
40	H	-1.176142115	-3.911157109	-1.839039206	0.172863
41	H	-4.455837476	-0.177501698	0.332953754	0.163043
42	H	-5.623626893	-0.806764128	-1.934222699	0.161953

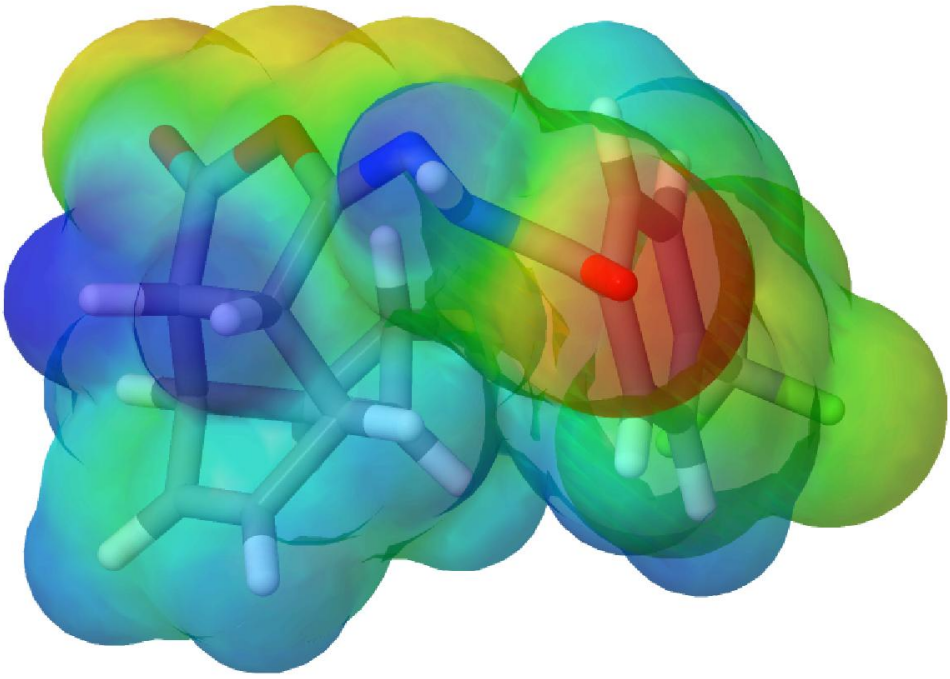


Figure S22: Graphical representation of molecular electrostatic potential for compound **4**

Model 1.1 MO 10/16
Energy = -1.1416 eV
Occupancy = 0

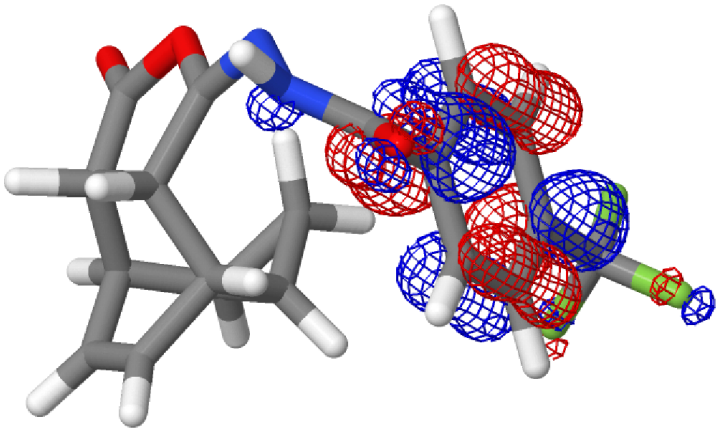


Figure S23: Graphical representation of LUMO orbital for compound **4**

Model 1.1 MO 11/16
Energy = -0.4535 eV
Occupancy = 0

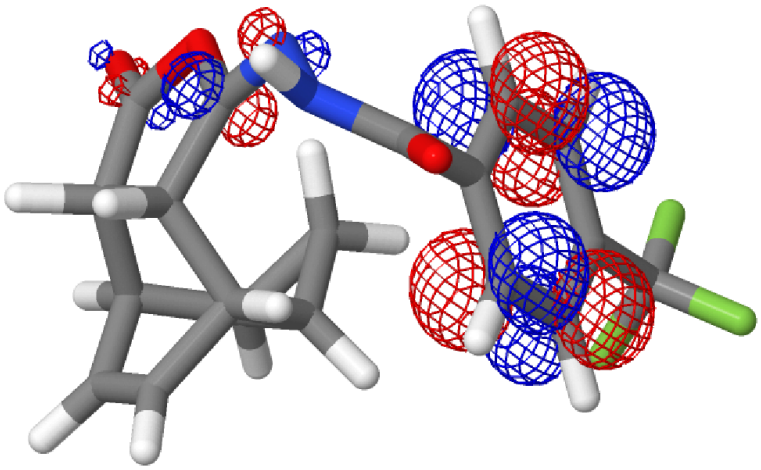


Figure S24: Graphical representation of second unoccupied molecular orbital (LUMO+1) for compound **4**

Model 1.1 MO 12/16
Energy = -0.3538 eV
Occupancy = 0

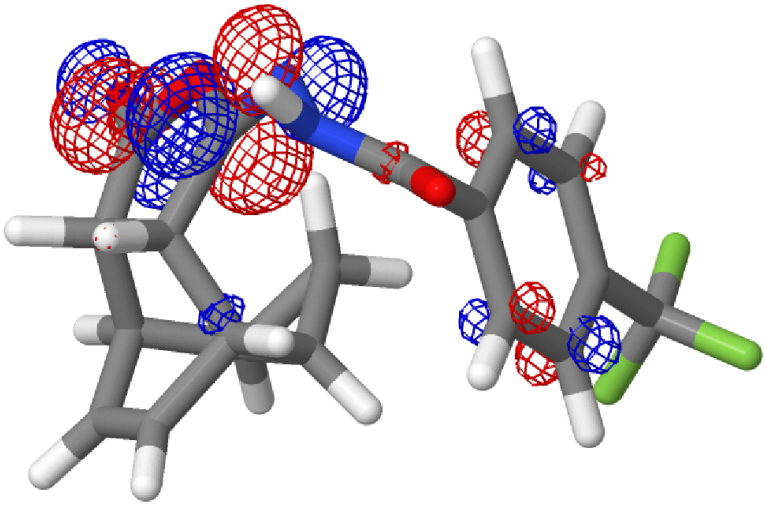


Figure S25: Graphical representation of third unoccupied molecular orbital (LUMO+2) for compound **4**

Model 1.1 MO 9/16
Energy = -10.0138 eV
Occupancy = 2

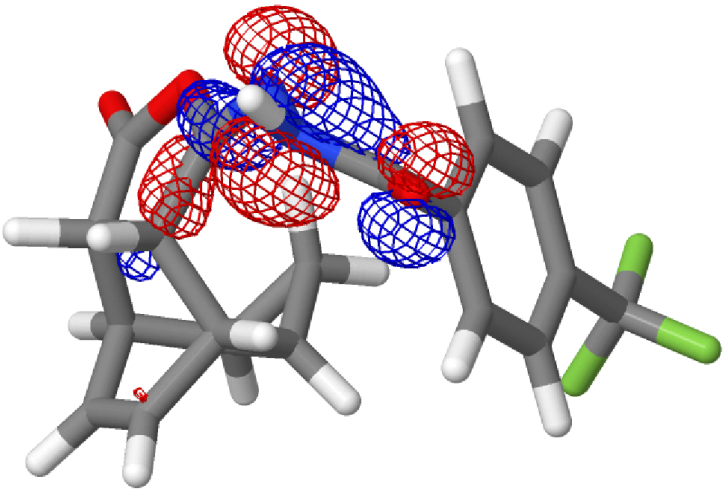


Figure S26: Graphical representation of HOMO orbital for compound **4**