Supplementary material

1. Table S1. Pearson's correlation matrix for descriptors collected in Table 1 and the experimental pIC_{50} = -log (IC_{50}) values.

2. Table S2-S3. Effect of compound **3a** on cell cycle distribution in the RPMI 8226 and A549 cell lines cultures.

3. Table S4-S5. Effects of compound **3a** on apoptosis (early + late apoptosis) induction in the RPMI 8226 and A549 cells.

4. ^{1}H, ^{13}C NMR and LC-ESI-HRMS spectra of compounds **3a**-**3h**.

5. Molecular orbital distribution plots of HOMO-LUMO for compound **3a**-**3h** at B3LYP/ 6-311G** level

6. Geometrical parameters of the investigated compounds **3a**-**3h** at B3LYP/6-311G** level.

7. Scheme S1. Structure of isomers 1 and 2 of investigated compounds.

8. Table S6. Fractional populations [%] of isomers 1 and 2 of investigated compounds.

Table S1. Pearson's correlation matrix for descriptors collected in Table 1 and the experimental $pIC_{50} = -\log (IC_{50})$ values.

	log*P*	HBA	HBD	MW	NRB	TPSA	E_{HOMO}	E_{LUMO}	ΔE	η	S	IP	EA	χ	pIC_{50}
log*P*	1.000														
HBA	-0.450	1.000													
HBD	-0.666	-0.124	1.000												
MW	0.355	0.036	-0.052	1.000											
NRB	-0.615	0.435	0.545	0.133	1.000										
TPSA	-0.864	0.749	0.432	-0.094	0.532	1.000									
E_{HOMO}	-0.128	-0.536	0.571	-0.264	0.078	-0.295	1.000								
E_{LUMO}	0.019	-0.648	0.575	-0.016	0.194	-0.397	0.872	1.000							
ΔE	0.129	-0.623	0.480	0.177	0.249	-0.408	0.626	0.928	1.000						
η	0.128	-0.623	0.481	0.176	0.249	-0.408	0.627	0.928	1.000	1.000					
S	-0.138	0.629	-0.479	-0.156	-0.228	0.412	-0.622	-0.925	-0.999	-0.999	1.000				
IP	0.128	0.536	-0.571	0.264	-0.078	0.295	-1.000	-0.872	-0.626	-0.627	0.622	1.000			
EA	-0.019	0.648	-0.575	0.016	-0.194	0.397	-0.872	-1.000	-0.928	-0.928	0.925	0.872	1.000		
χ	0.030	0.630	-0.591	0.100	-0.161	0.375	-0.940	-0.987	-0.854	-0.855	0.851	0.940	0.987	1.000	
pIC_{50}	-0.472	-0.459	0.694	-0.282	0.260	0.134	0.410	0.384	0.298	0.299	-0.295	-0.410	-0.384	-0.404	1.000

Table S2. Effect of compound **3a** on cell cycle distribution in the RPMI 8226 cell line culture. After the treatment with various concentrations of compound 1 for 24 and 48 h, the cells were stained with propidium iodide and analyzed by flow cytometry. $*p < 0.05$, $**p < 0.01$, and $p < 0.001$*** in comparison to the control; one-way ANOVA test

Concentration (μM)	24 h				48 h			
	Cell cycle distribution [% of cells]							
	Sub-G1	G0/G1	S	G2	Sub-G1	G0/G1	S	G2
0	11.56±5.5	41.93±6.15	26.36±2.04	20.35±3.78	8.6±2.85	40.57±1.8	28.8±1.53	22.71±1.92
2.5	15.53±2.23	41.14±1.03	21.59±1.77	22.35±1.19	21.49±0.94**	35.8±1.49	26.22±0.97	16.99±2
5	21.32±6.2*	38.23±6.83	18.68±2.58	21.31±4.02	25.53±7.59***	40.3±3.15	19.12±2.51	15.23±5.04
10	23.53±7.04**	38.08±9.38	21.4±3.5	17.45±2.75	28.01±5.09***	38.5±2.77	18.61±4.5	18.78±2.32
20	24.09±2.62**	42.63±4.03	19.83±2.92	15.7±5.79	29.68±10.49***	31.66±10.94	20.74±2.14	17.47±1.42

Table S3. Effect of compound **3a** on cell cycle distribution in the A549 cell line culture. After the treatment with various concentrations of compound 1 for 24 and 48 h, the cells were stained with propidium iodide and analyzed by flow cytometry. $*p < 0.05$, and $p < 0.001$*** in comparison to the control; one-way ANOVA test

Concentration (μM)	24 h				48 h			
	Cell cycle distribution [% of cells]							
	sub-G1	G0/G1	S	G2/M	sub-G1	G0/G1	S	G2/M
0	8.29±4.27	64.55±2.73	13.13±2.69	14.49±2.12	13.81±4.87	70.70±6.85	7.22±2.75	8.41±1.53
2.5	8.81±3.73	64.49±1.89	12.39±2.34	14.68±2.11	11.98±3.62	73.22±1.97	6.07±1.54	8.91±2.22
5	8.94±3.39	65.90±2.36	12.18±2.45	13.62±2.25	15.74±6.03	68.55±8.03	6.81±2.66	9.05±1.72
10	13.23±7.01	66.51±4.46	9.82±2.73	11.43±2.88	16.15±6.33	68.54±6.87	7.07±2.63	8.44±1.47
20	22.36±12.24***	66.45±9.20	5.23±2.38*	7.16±2.15	27.32±6.78***	63.07±6.59*	4.61±1.21	5.19±0.93
40	35.46±9.33***	41.03±2.93***	11.34±0.58	12.87±5.29	75.27±4.12***	16.49±3.46***	6.05±0.87	2.19±0.38

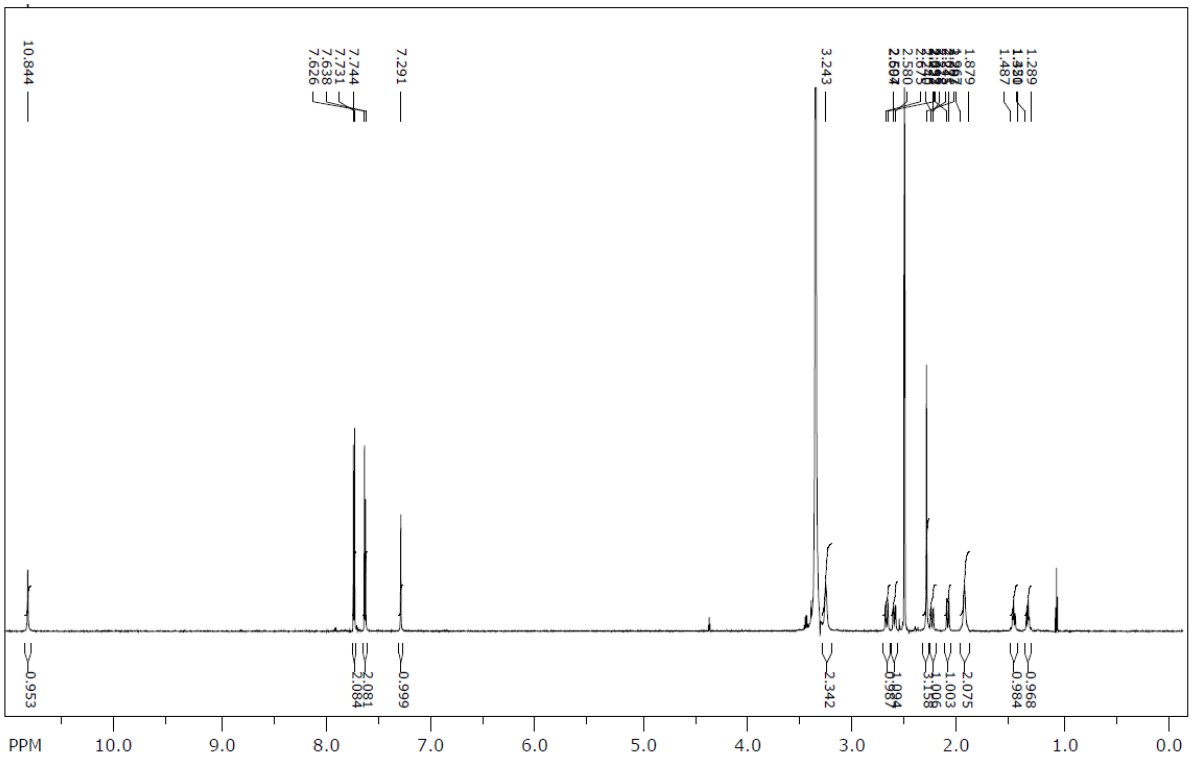
Table S4. Effects of compound **3a** on apoptosis (early + late apoptosis) induction in the RPMI 8226 cells. After the 24-h and 48-h exposure, the cells were stained with AnnexinV-FITC/propidium iodide and examined with flow cytometry. Statistically significant at $p < 0.01$** or at $p < 0.001$*** in comparison to the vehicle control; one-way ANOVA test.

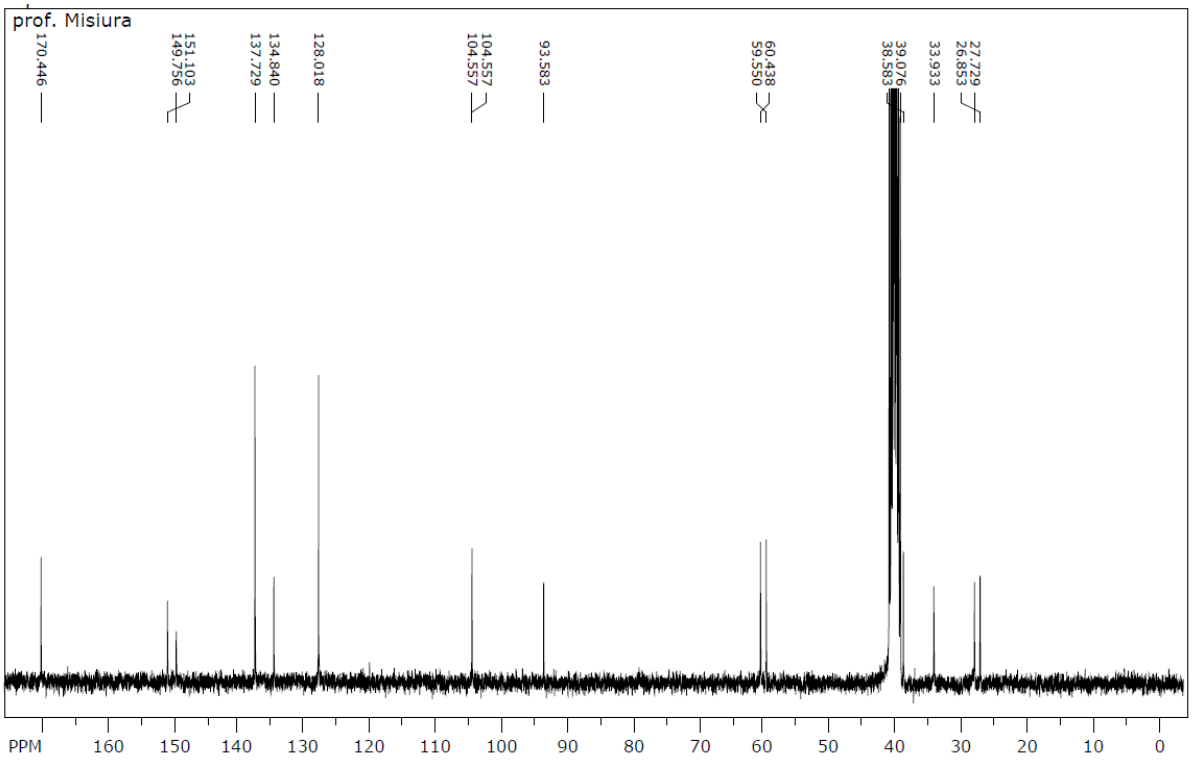
Concentration [μM]	24 hours		48 hours	
	Apoptosis [% of cells ± SD]	Necrosis [% of cells ± SD]	Apoptosis [% of cells ± SD]	Necrosis [% of cells ± SD]
0	14.33 ± 0.87	5.03 ± 0.86	12.99 ± 2.44	5.48 ± 2.25
2.5	19.53 ± 2.64**	3.62 ± 0.87	20.93 ± 1.83***	5.54 ± 0.44
5	22.23 ± 6.01**	6.35 ± 2.57	31.71 ± 11.36***	7.53 ± 2.61
10	39.58 ± 9.33***	9.94 ± 2.73	58.25 ± 21.57***	11.08 ± 5.38
20	60.41 ± 0.99***	18.5 ± 2.38***	76.93 ± 14.34***	20.18 ± 11.99***

Table S5. Effects of compound **3a** on apoptosis (early + late apoptosis) induction in the A549 cells. After the 24-h and 48-h exposure, the cells were stained with AnnexinV-FITC/propidium iodide and examined with flow cytometry. Statistically significant at $p < 0.01$** or at $p < 0.001$*** in comparison to the vehicle control; one-way ANOVA test.

Concentration [μM]	24 hours		48 hours	
	Apoptosis [% of cells ± SD]	Necrosis [% of cells ± SD]	Apoptosis [% of cells ± SD]	Necrosis [% of cells ± SD]
0	14.14±1.77	4.72±1.29	13.65±3.71	5.01±2.20
2.5	14.30±2.21	4.79±1.14	18.41±3.95	4.11±1.44
5	14.82±2.42	4.40±1.66	22.48±8.36	4.93±4.26
10	18.18±2.52	4.87±1.35	27.17±11.71**	4.09±2.58
20	23.43±4.57**	4.56±1.90	40.20±9.87***	4.87±3.04
40	73.96±19.94***	7.89±1.10	89.43±6.65***	8.81±6.51

3a




prof. Misiura
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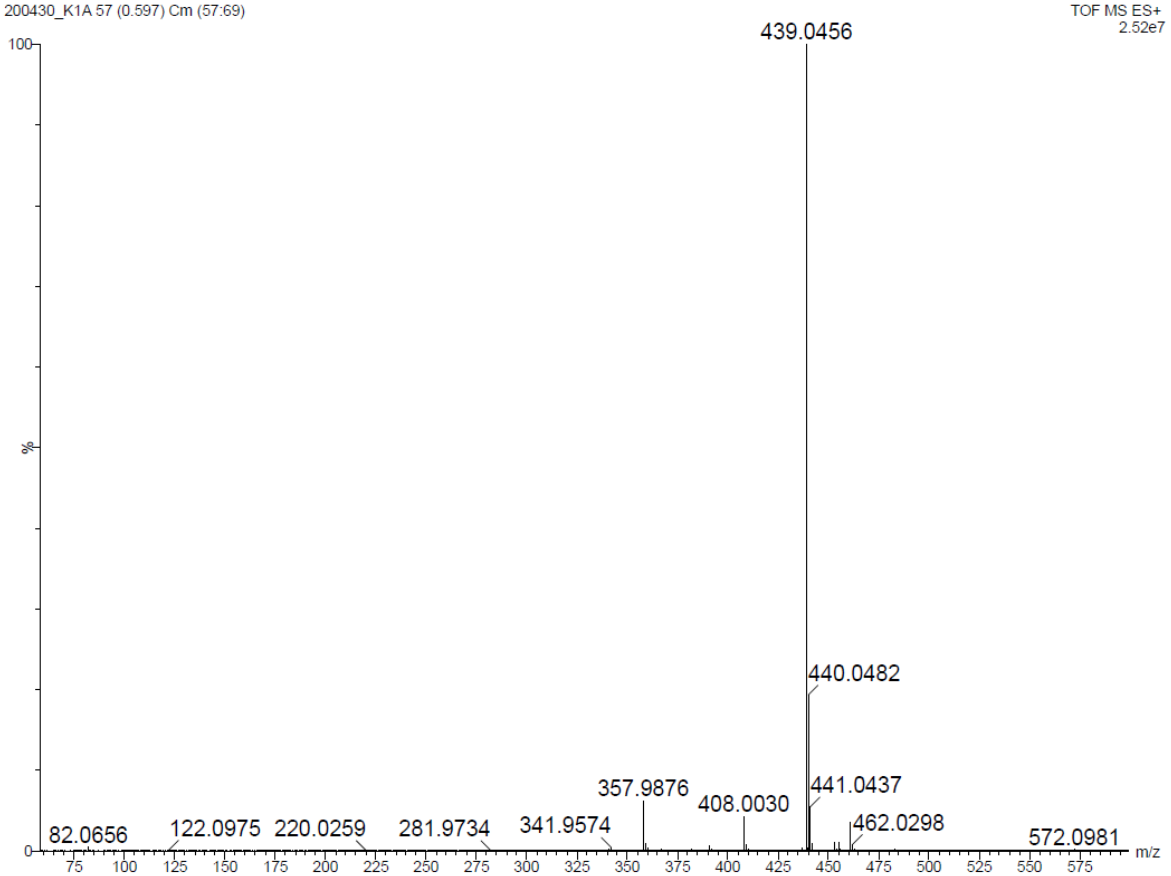
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82.0656
572.0981
m/z
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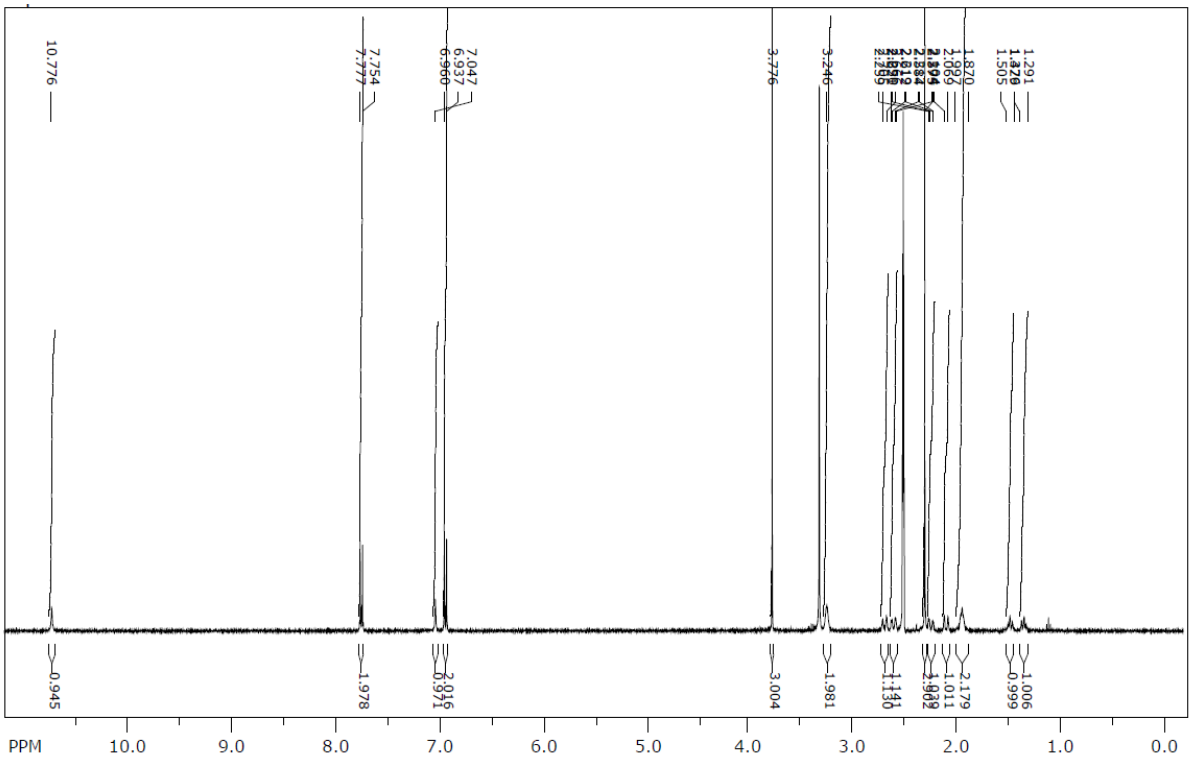
475
500
525
550
575

3b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3.004
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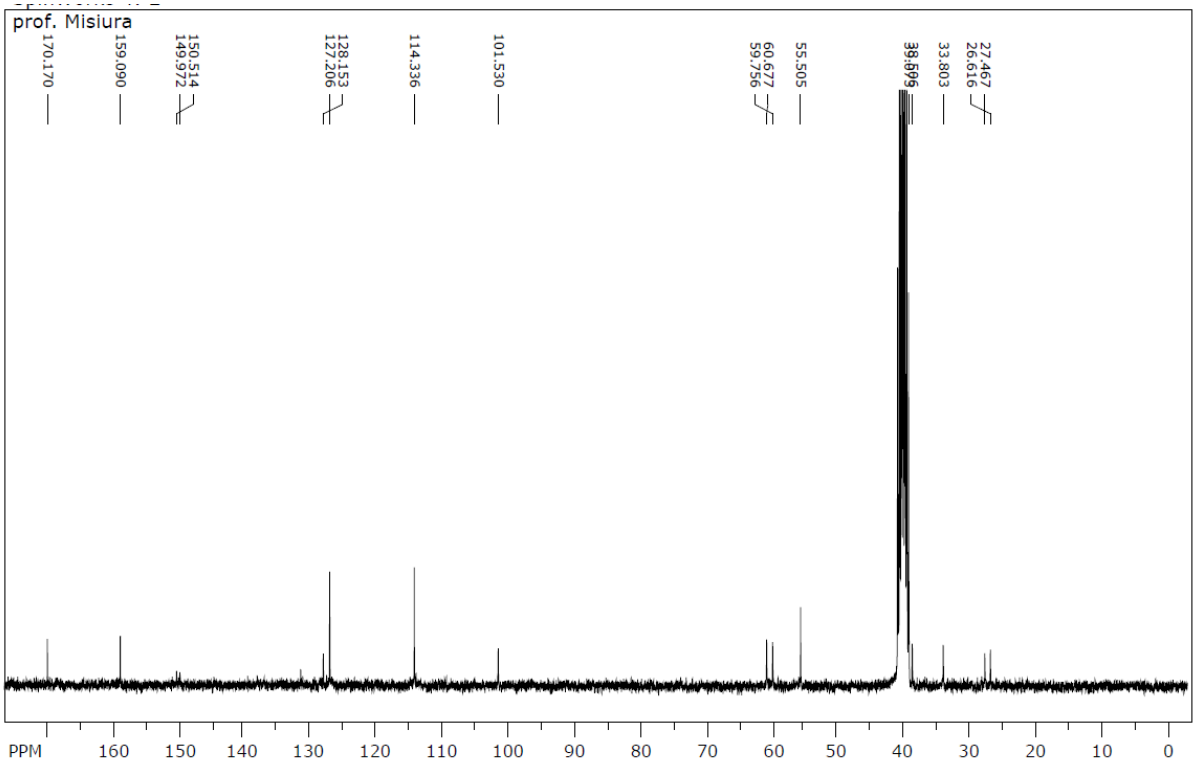
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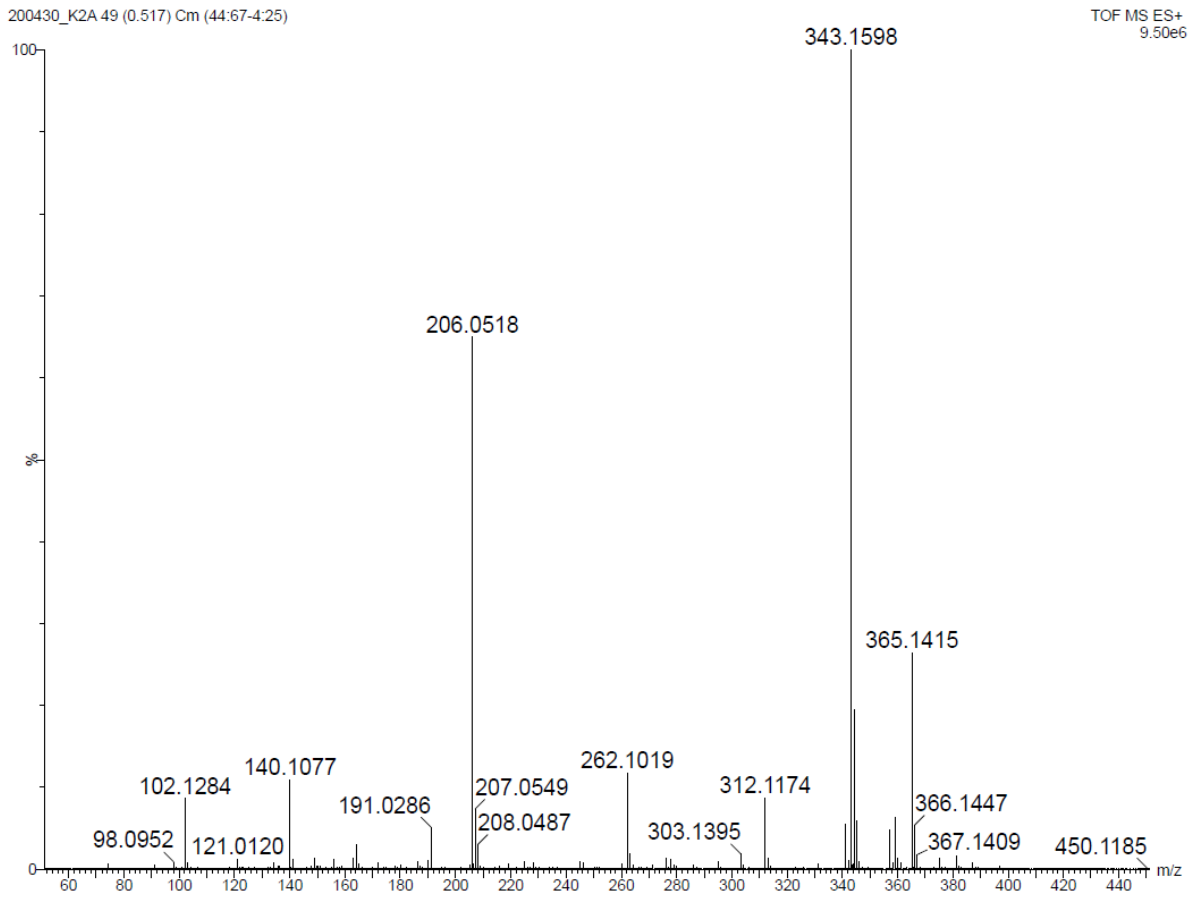
20
10
0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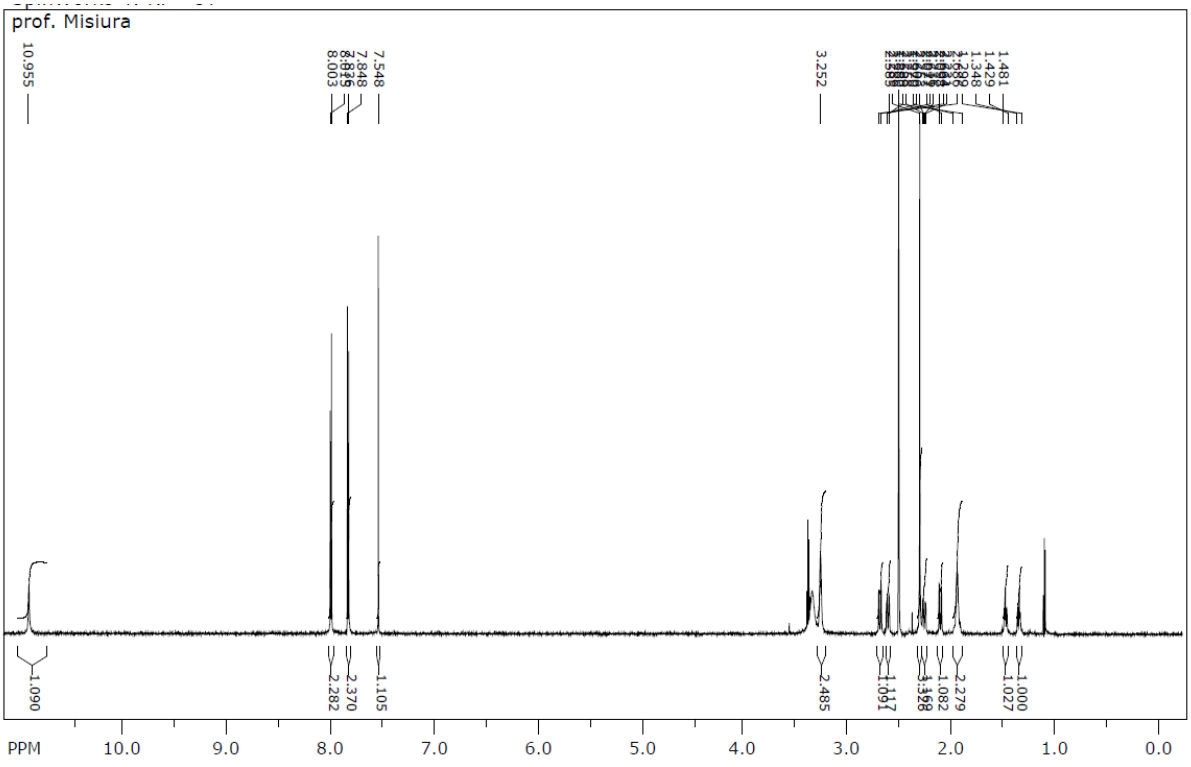
%
m/z

3c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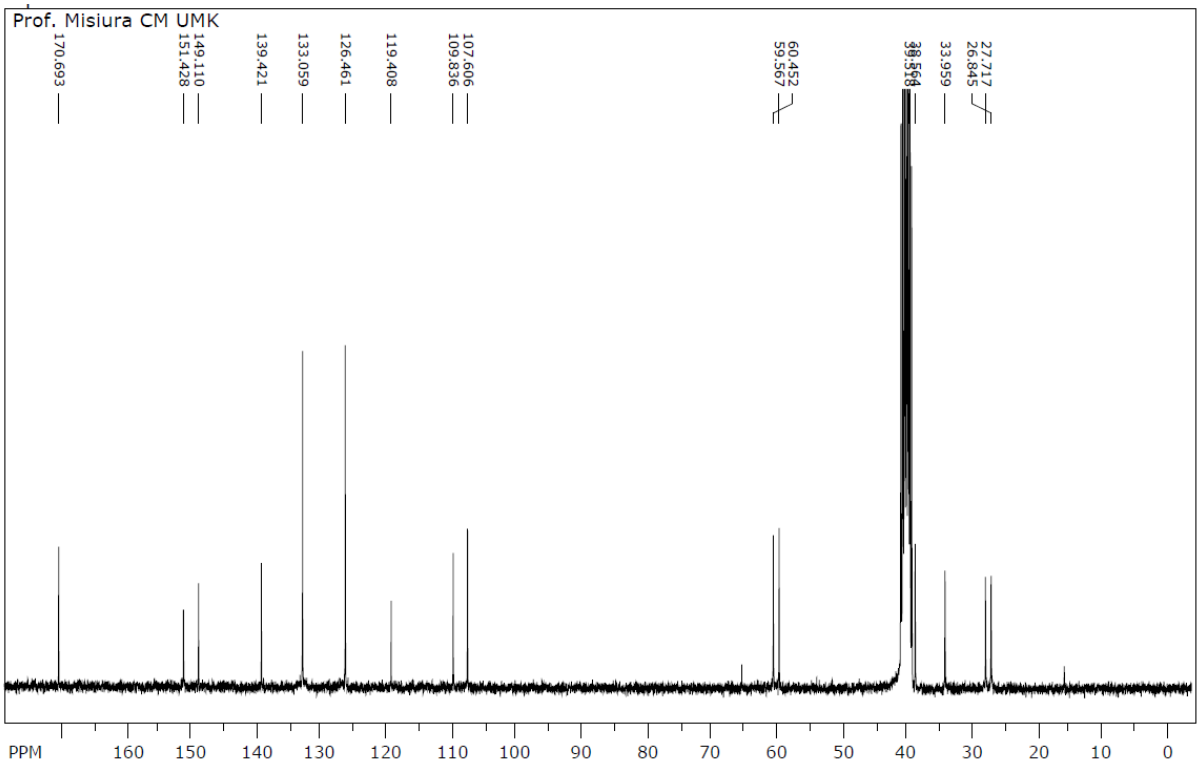
Prof. Misiura CM UMK
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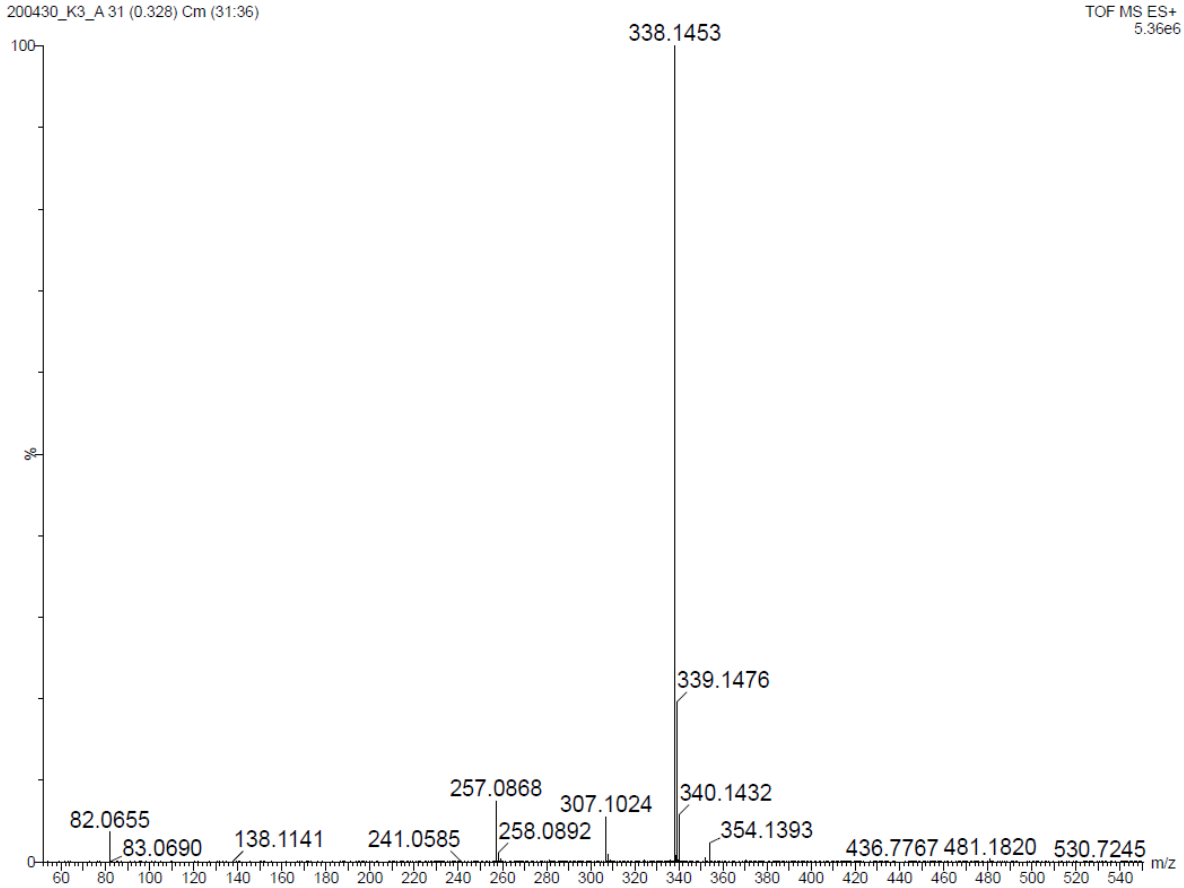
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m/z
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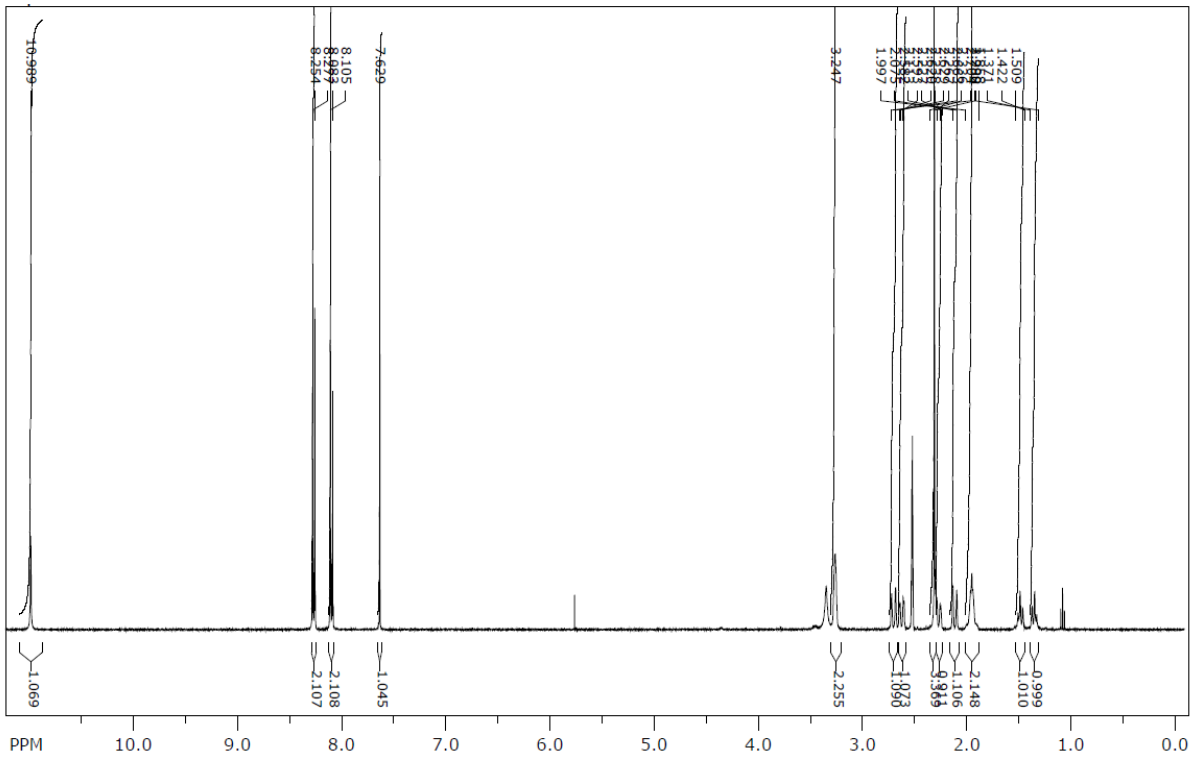
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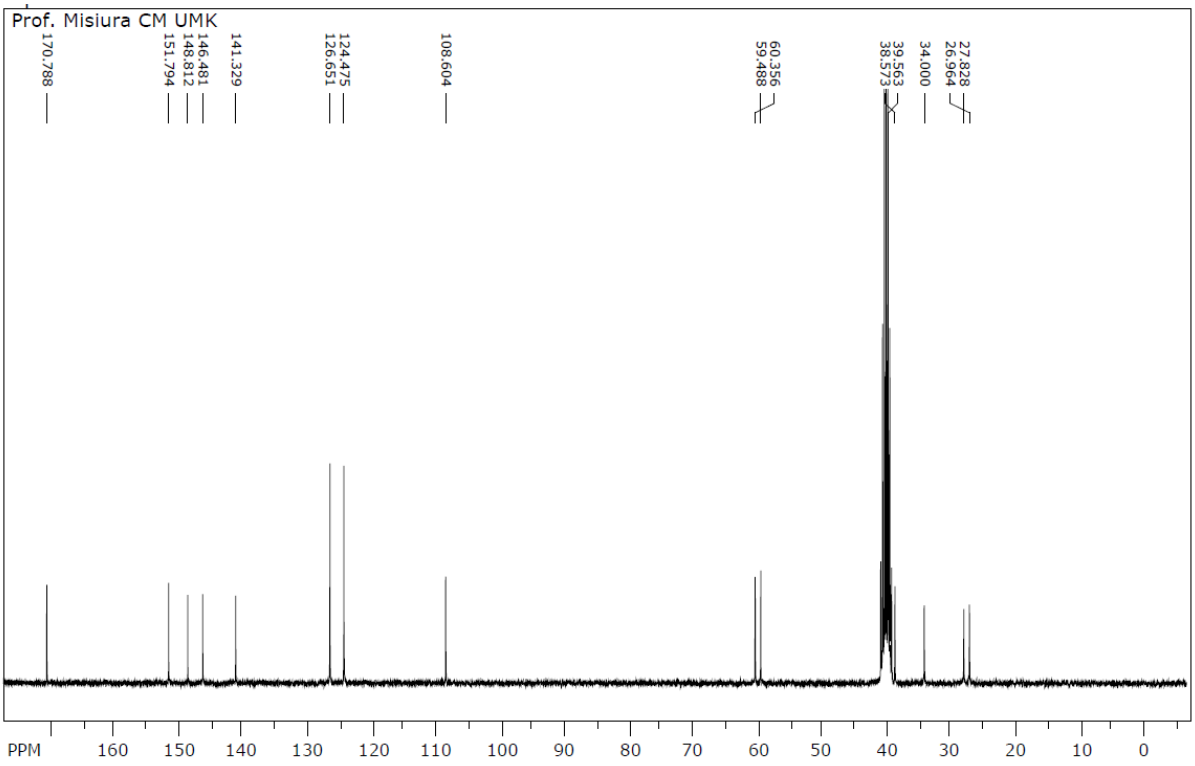
Prof. Misiura CM UMK
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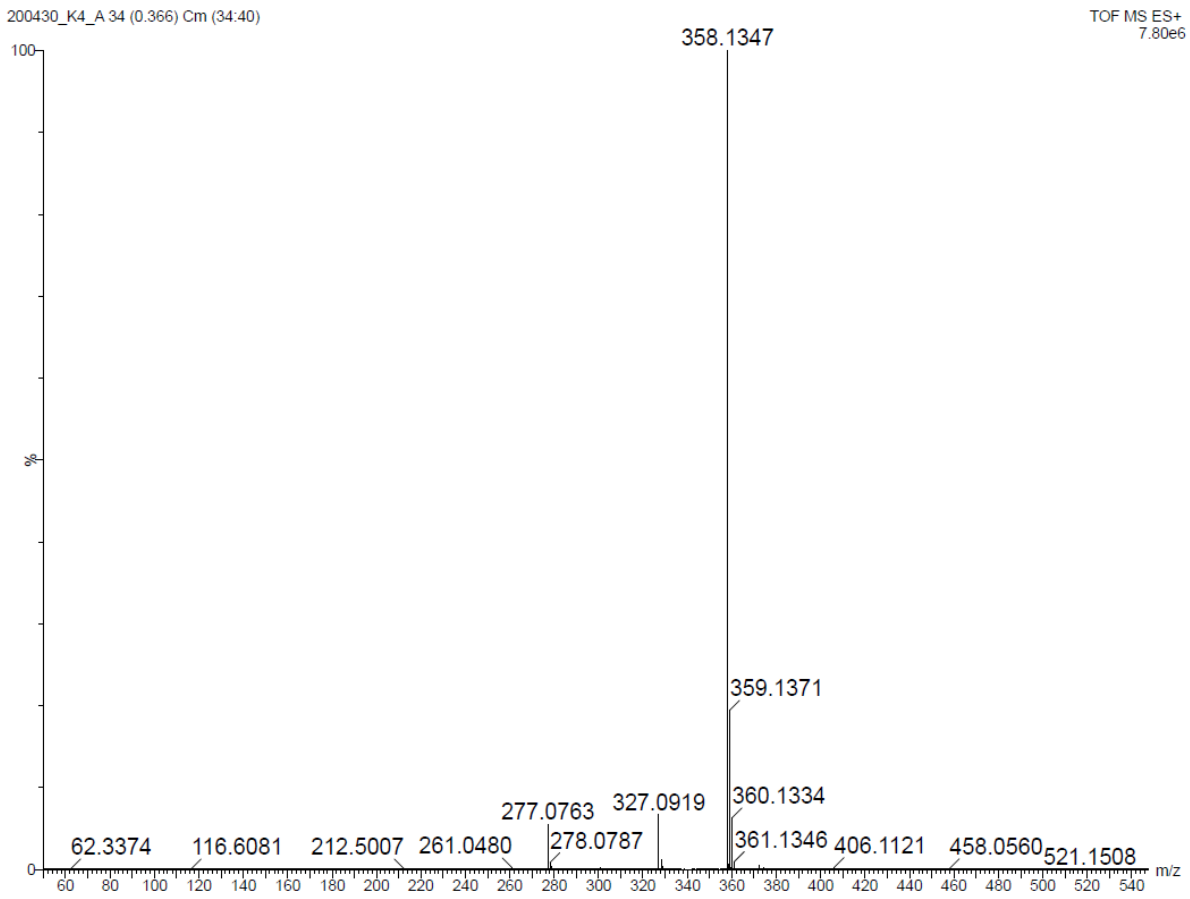
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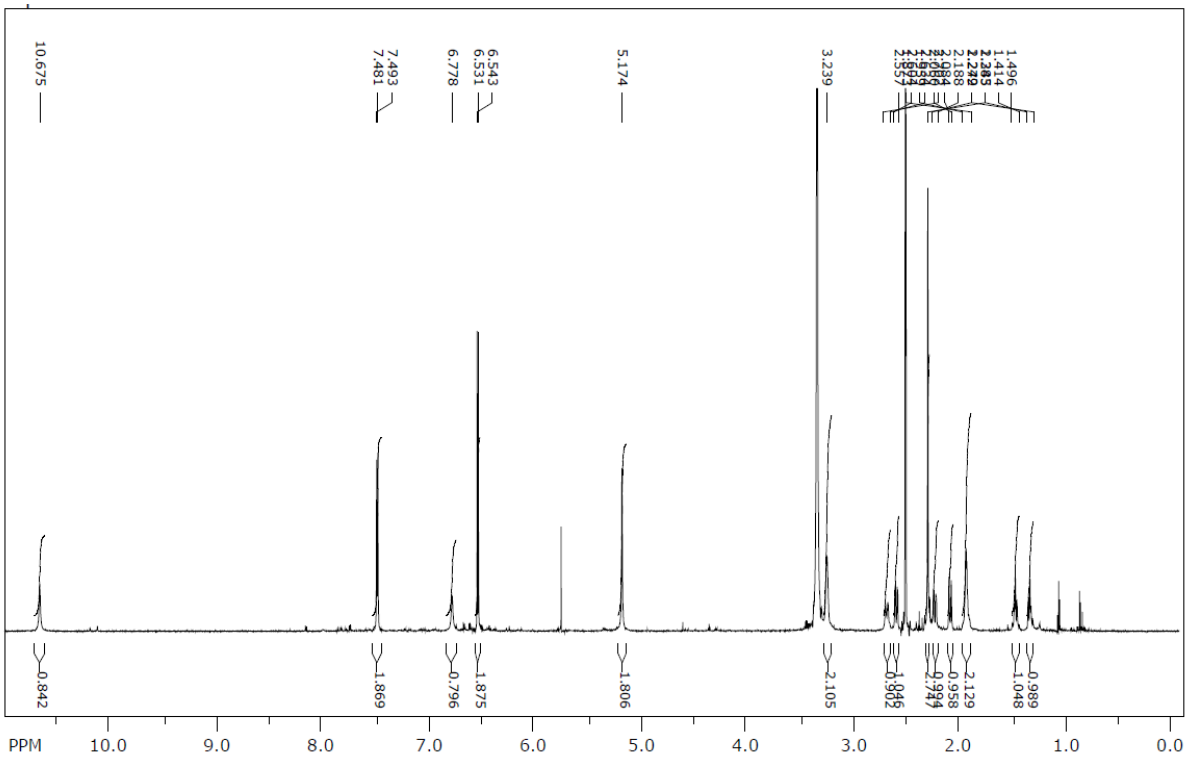
m/z

3e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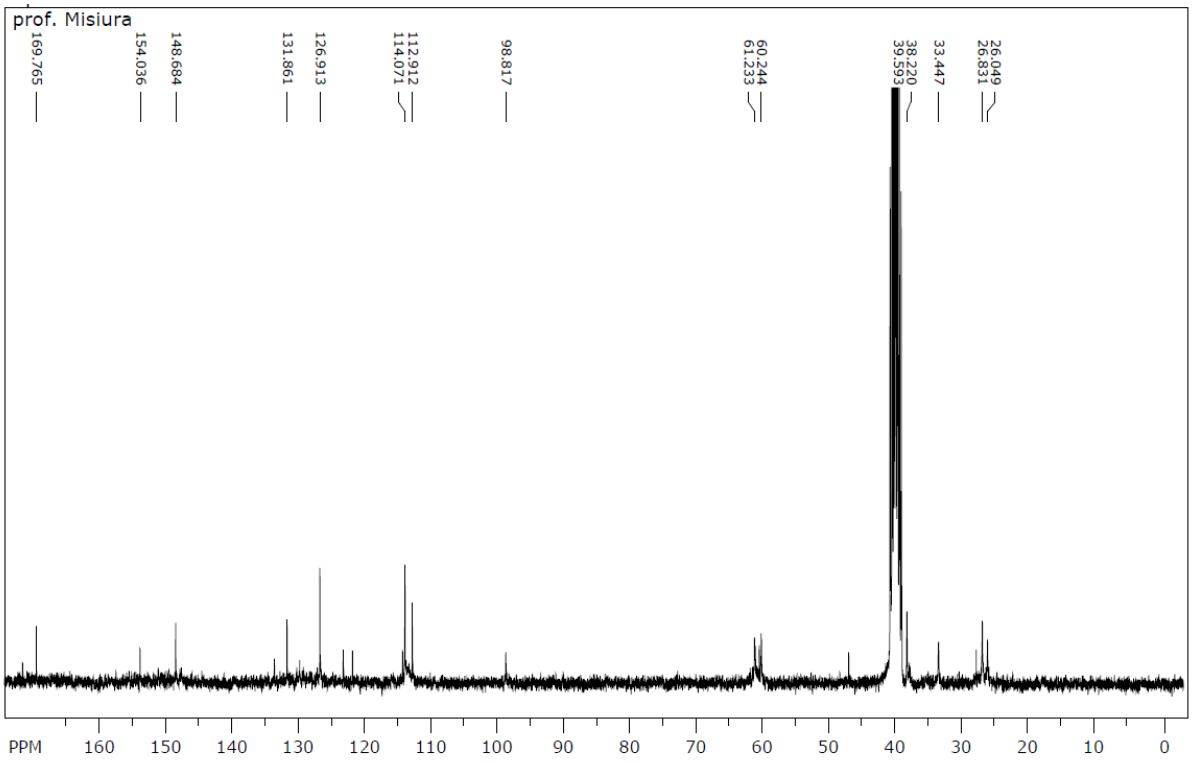
PPM


prof. Misiura
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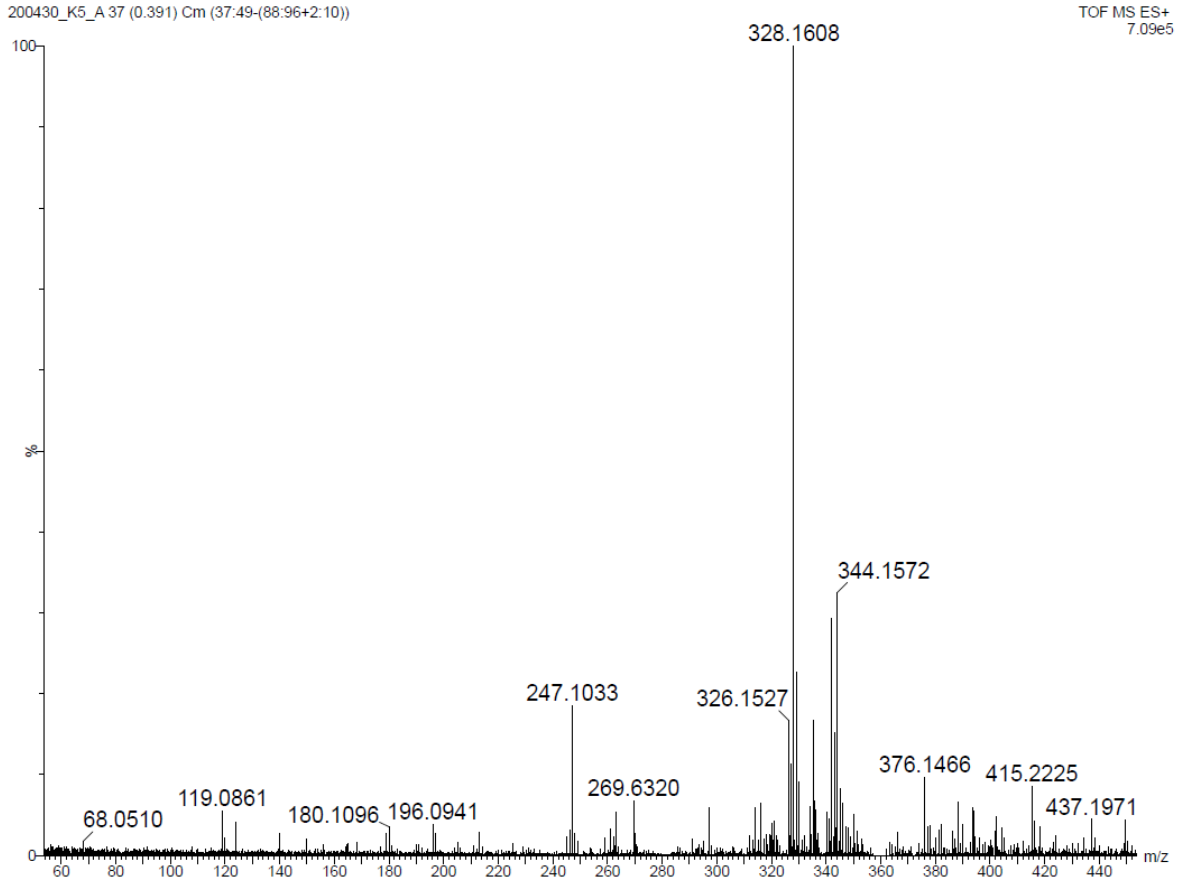
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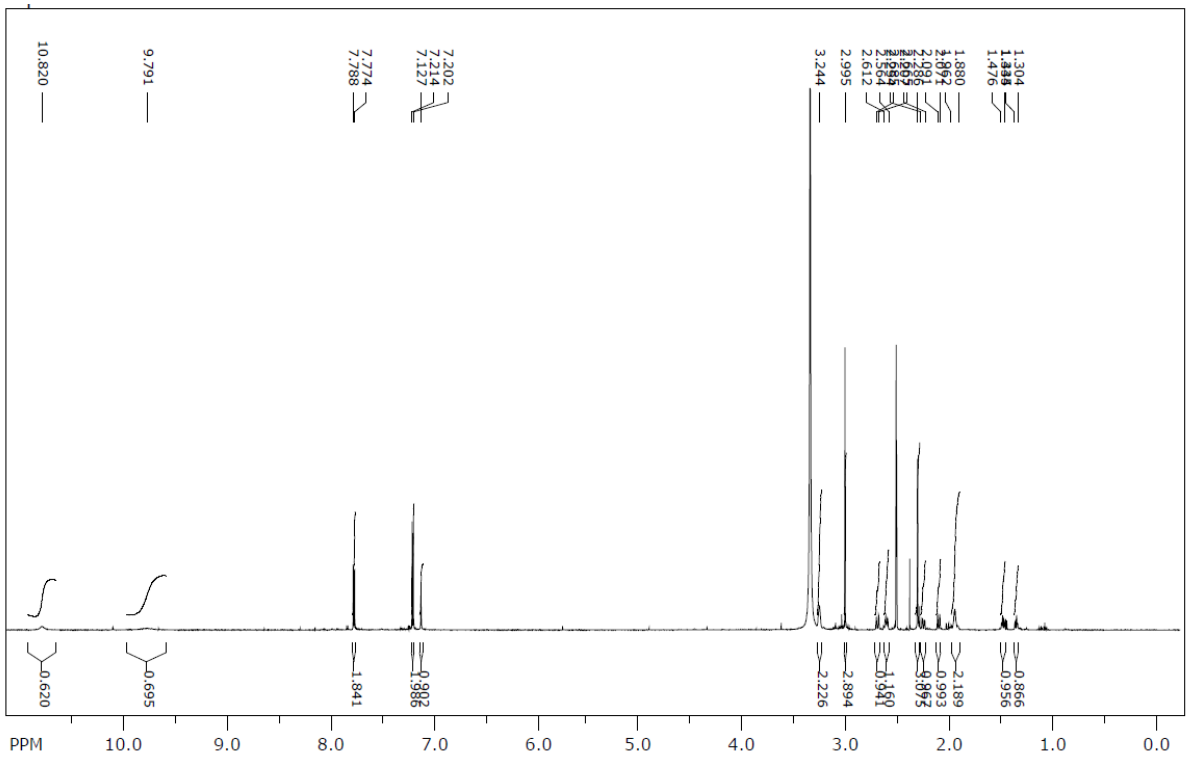
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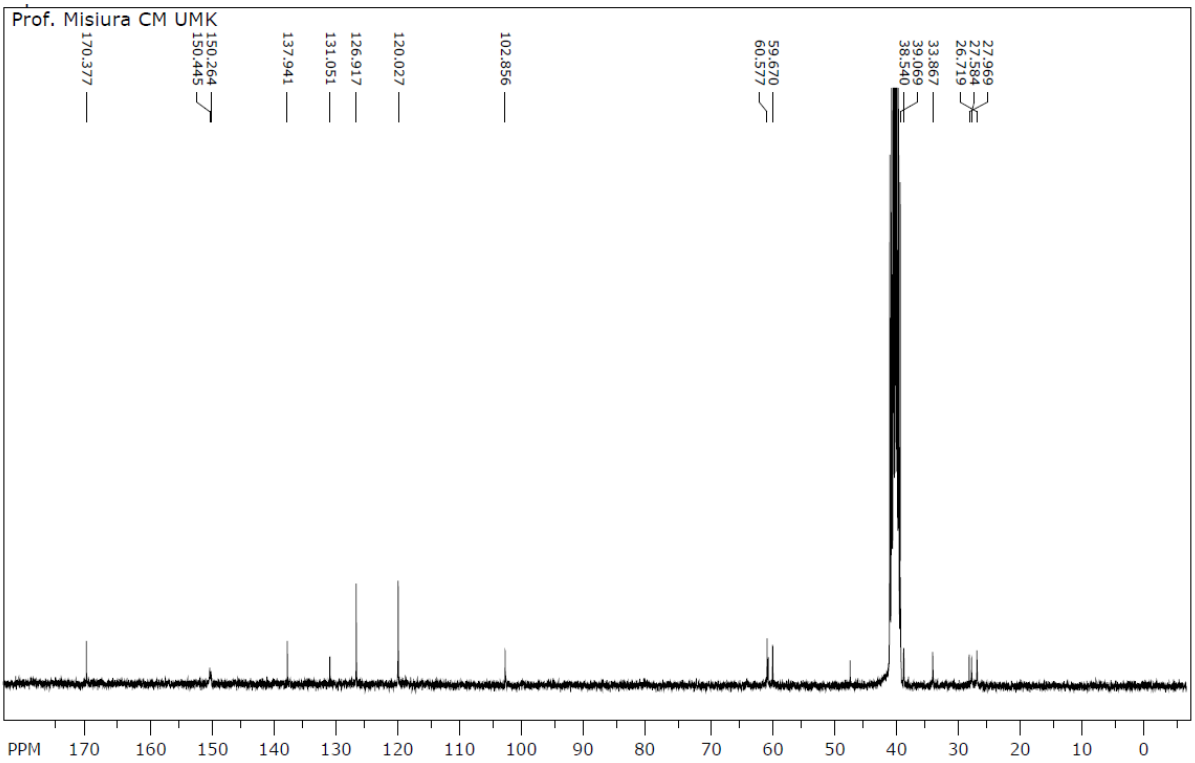
Prof. Misiura CM UMK
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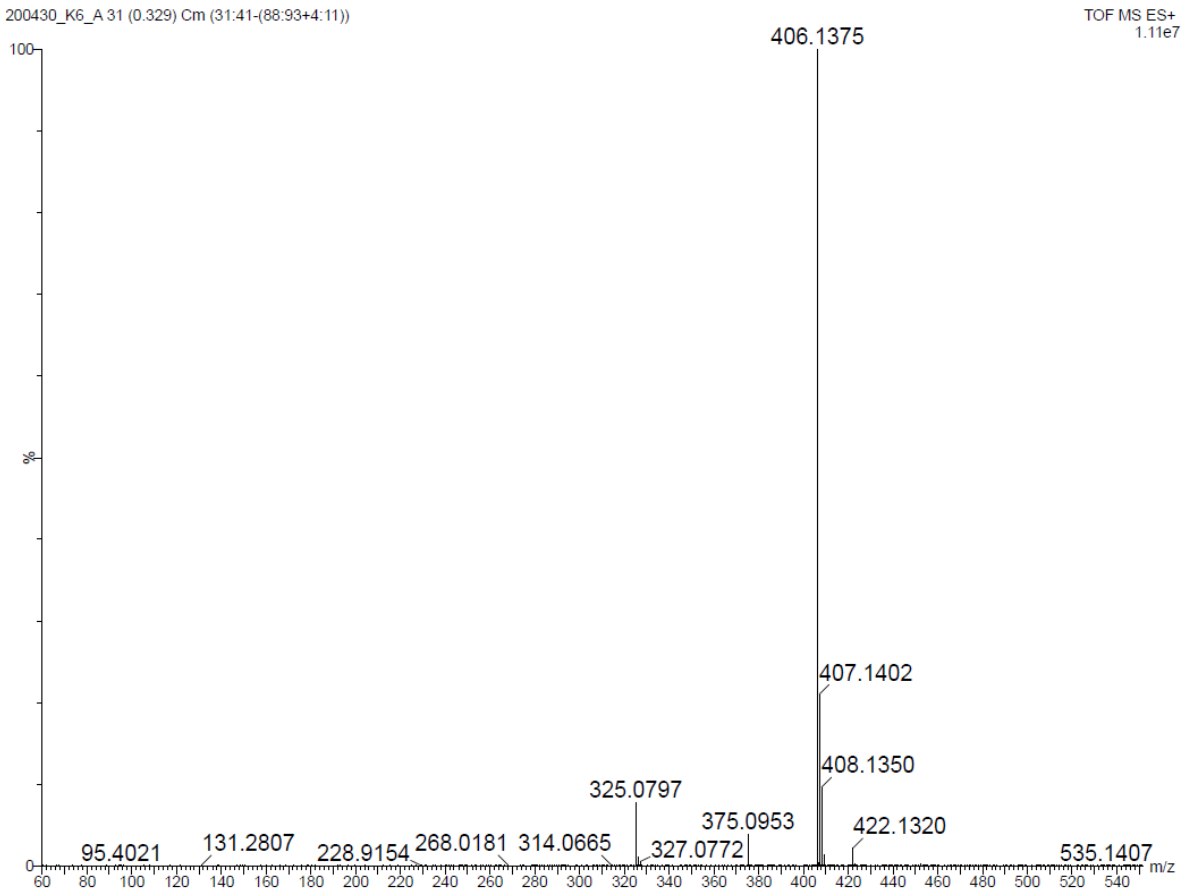
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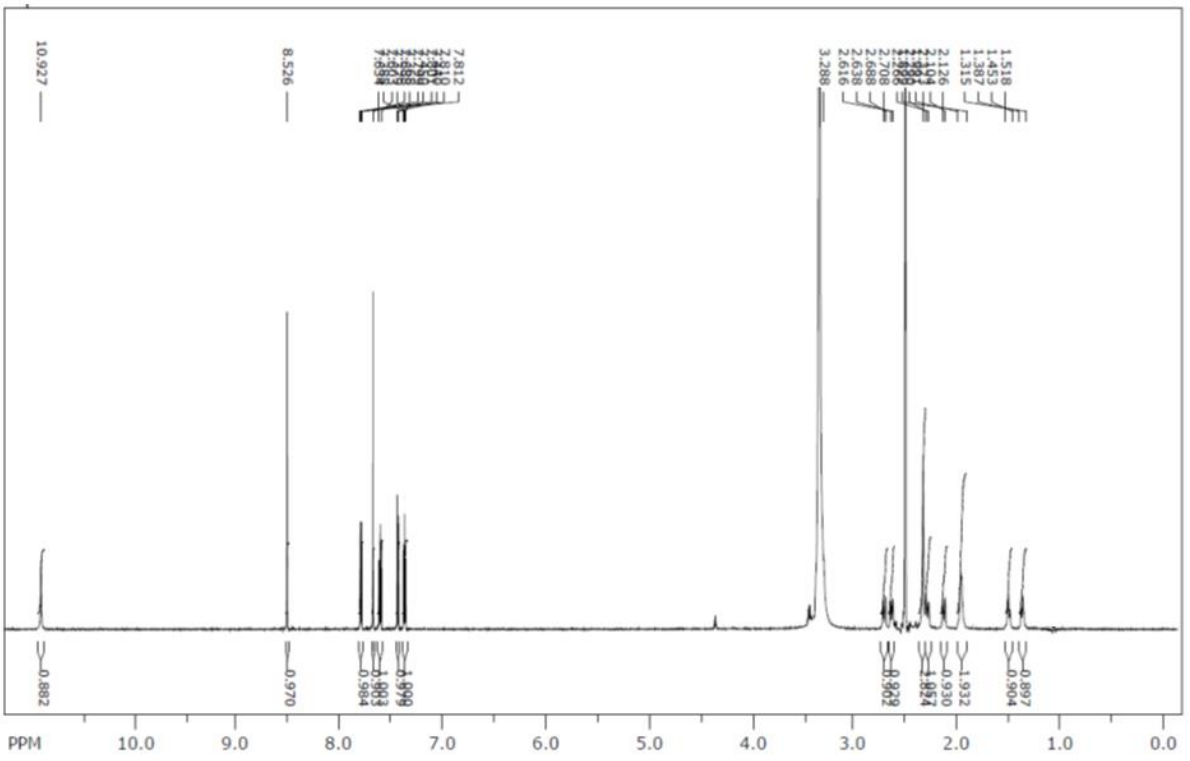
m/z

3g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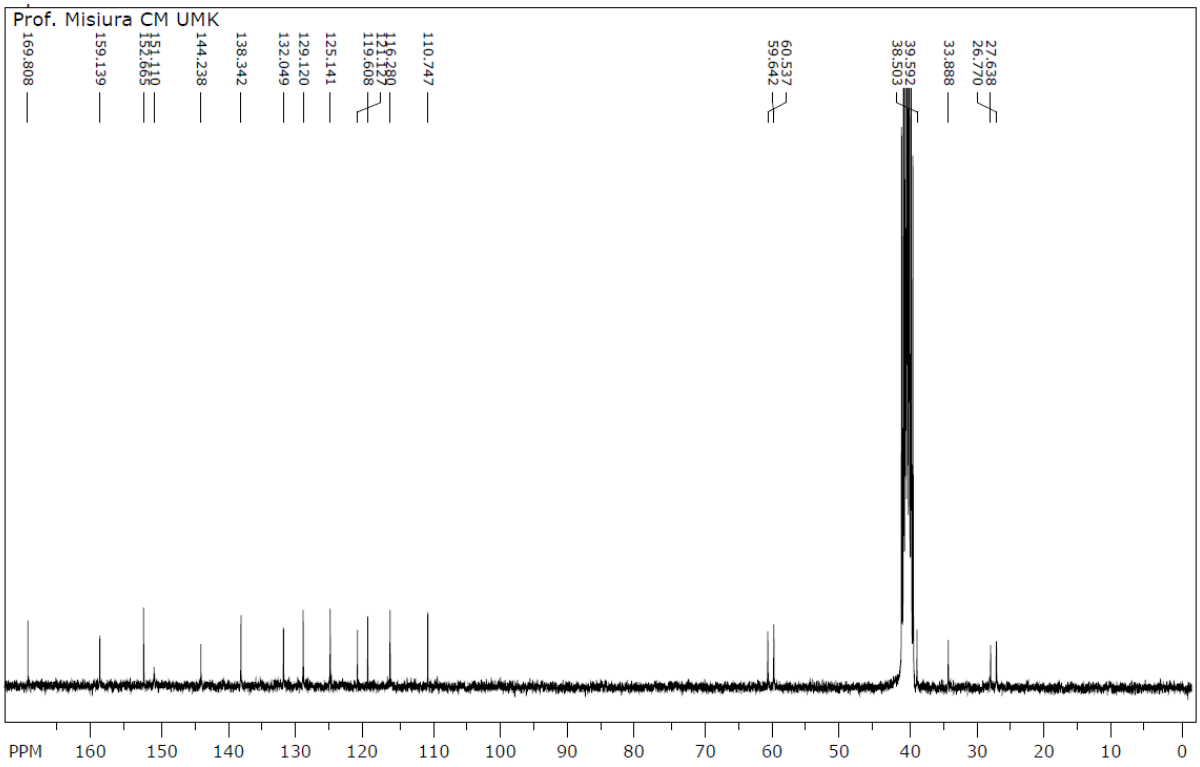
PPM


Prof. Misiura CM UMK
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33.888
27.638
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PPM
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140
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120
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100
90
80
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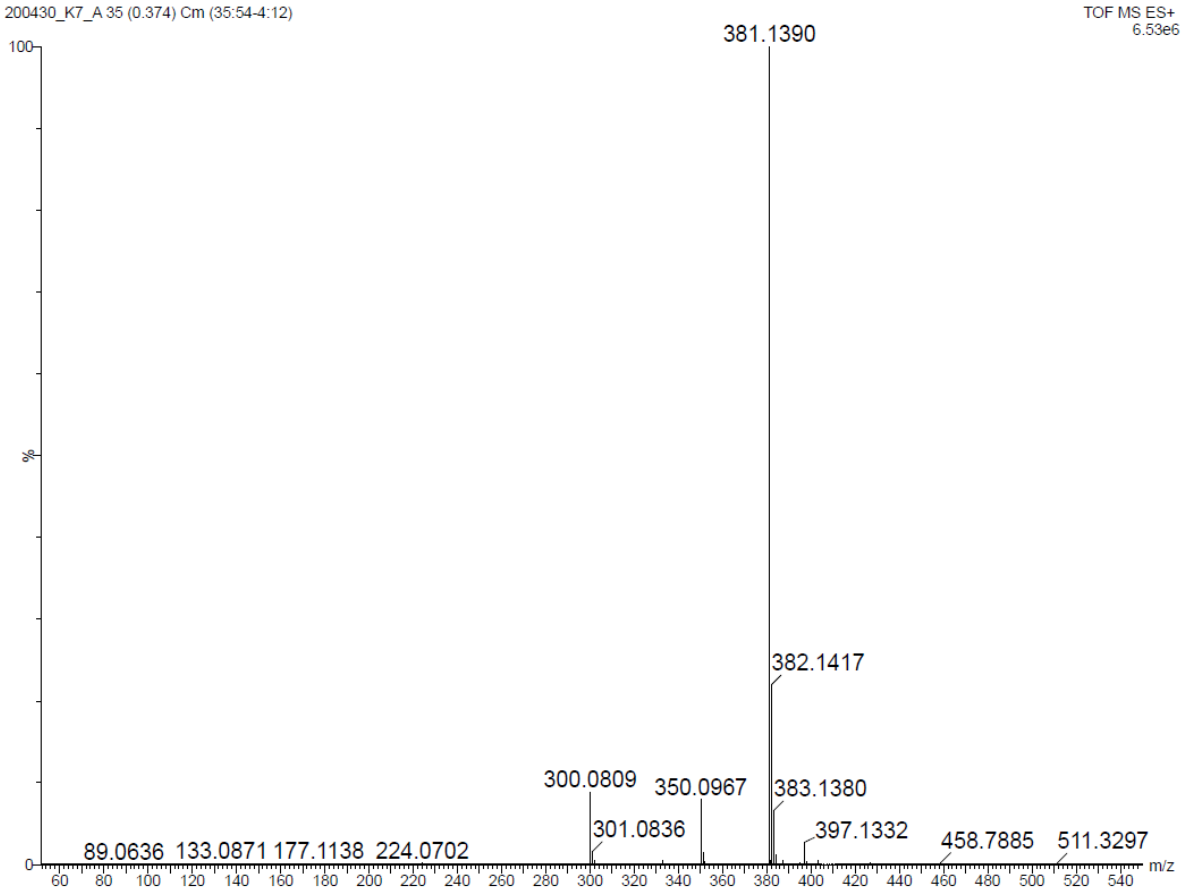
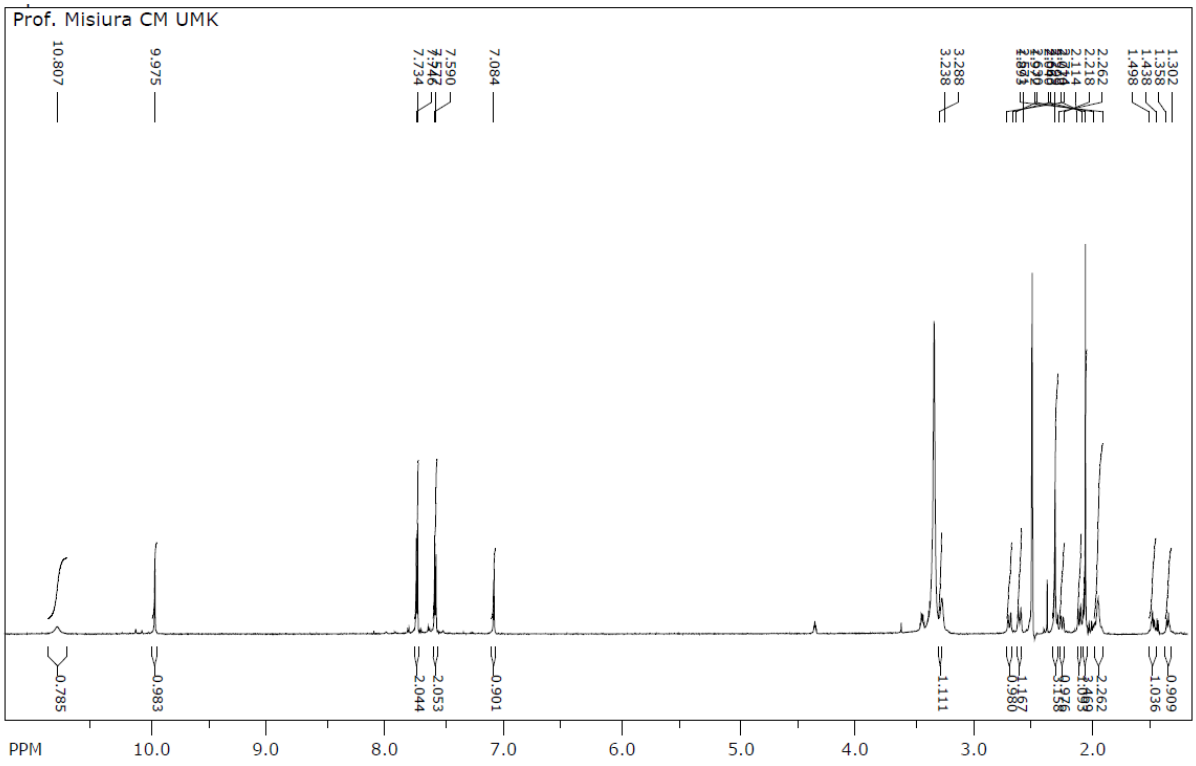
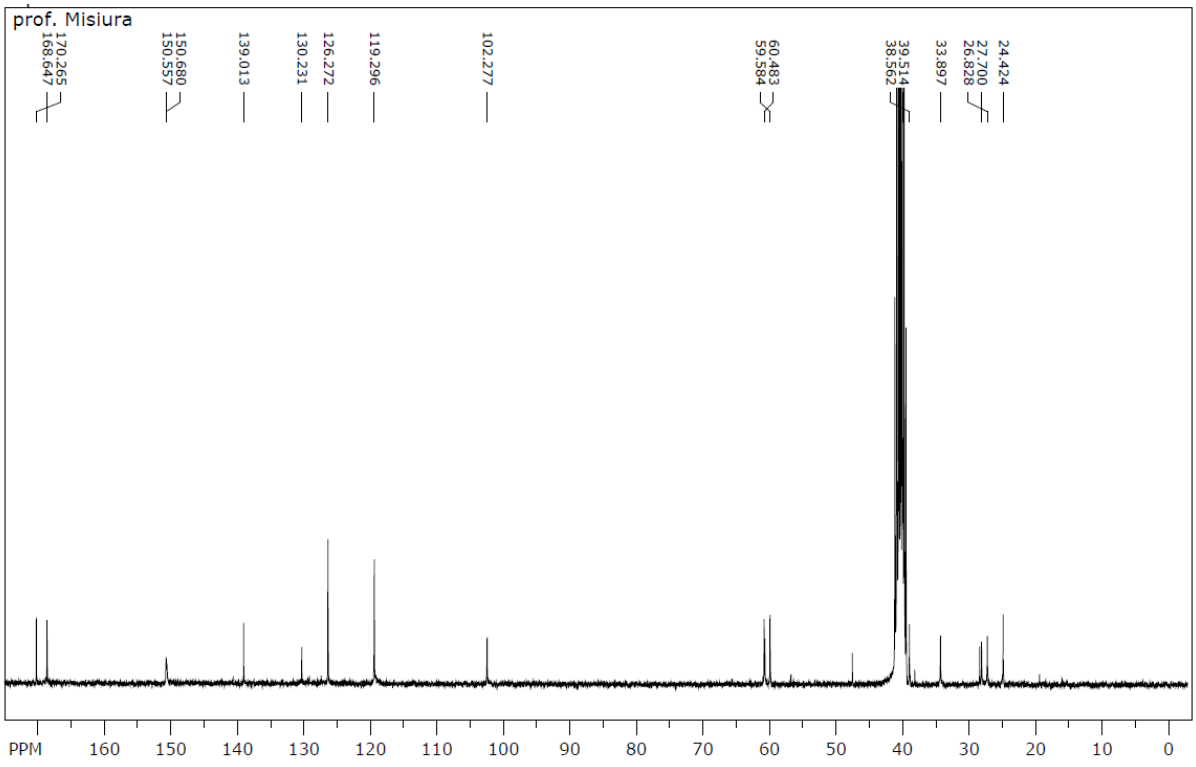
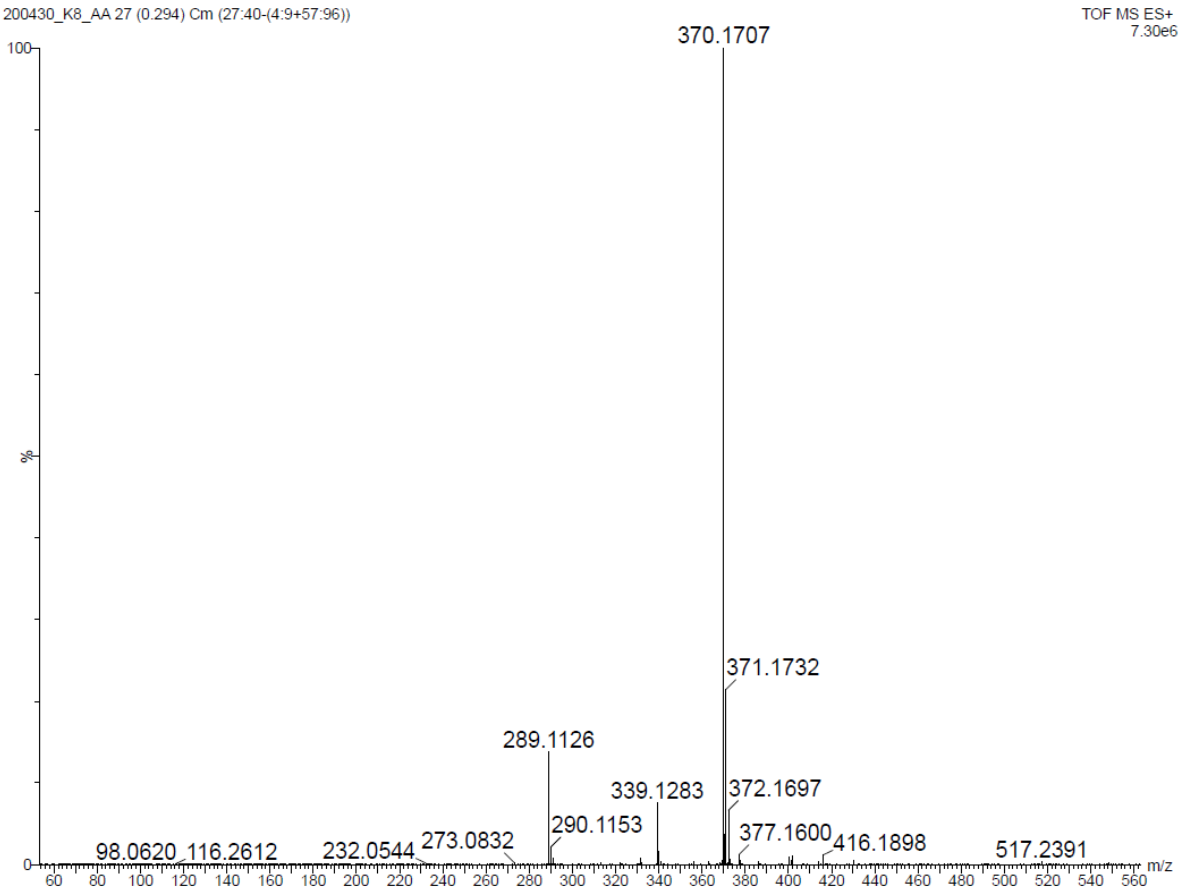
20
10
0


200430_K7_A 35 (0.374) Cm (35:54-4:12)
TOF MS ES+
6.53e6
100
%
0
381.1390
382.1417
300.0809
350.0967
383.1380
301.0836
397.1332
458.7885
511.3297
89.0636
133.0871
177.1138
224.0702
m/z
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540

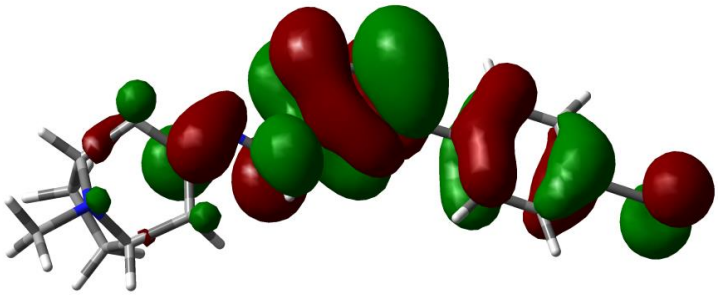
3h


Prof. Misiura CM UMK
10.807
9.975
7.734
7.590
7.547
7.084
3.288
3.238
2.262
2.218
1.498
1.438
1.358
1.302
0.785
0.983
2.044
2.053
0.901
1.111
1.036
0.909
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0

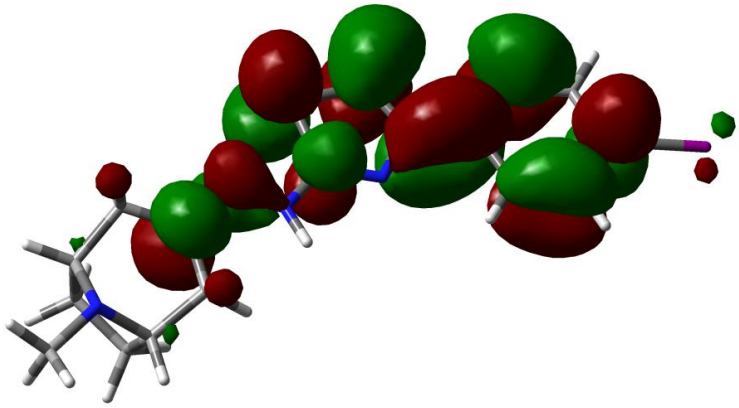

prof. Misiura
170.265
168.647
150.680
150.557
139.013
130.231
126.272
119.296
102.277
60.483
59.584
39.514
38.562
33.897
27.700
26.828
24.424
PPM
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


200430_K8_AA 27 (0.294) Cm (27:40-(4:9+57:96))
TOF MS ES+
7.30e6
100
%
0
370.1707
371.1732
289.1126
339.1283
372.1697
290.1153
377.1600
416.1898
517.2391
98.0620
116.2612
232.0544
273.0832
m/z
60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560

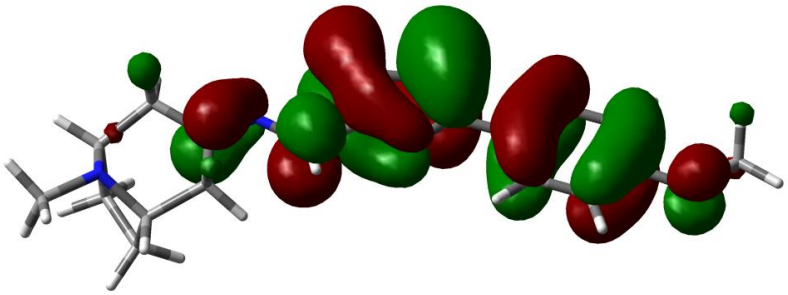
3a-HOMO



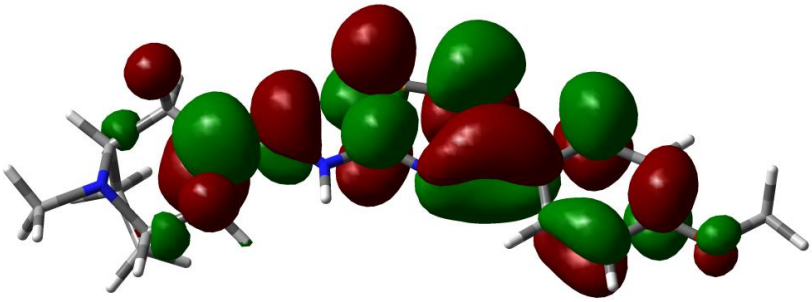
3a-LUMO



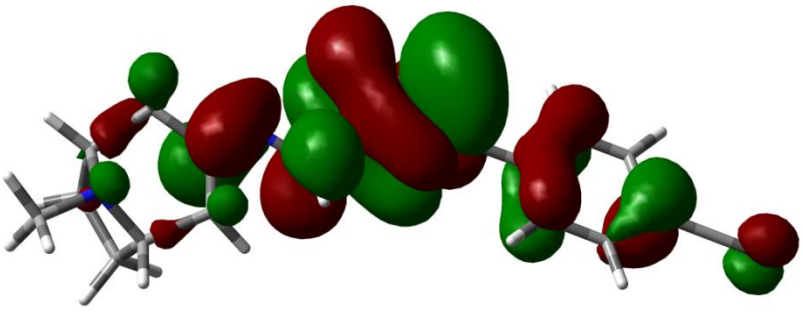
3b-HOMO



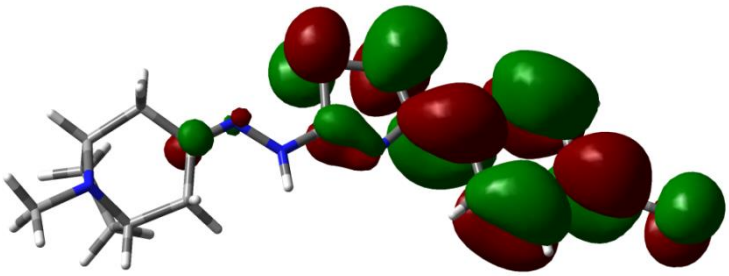
3b-LUMO



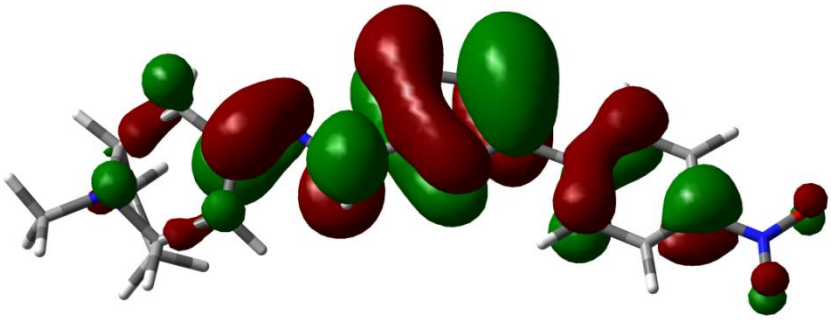
3c-HOMO



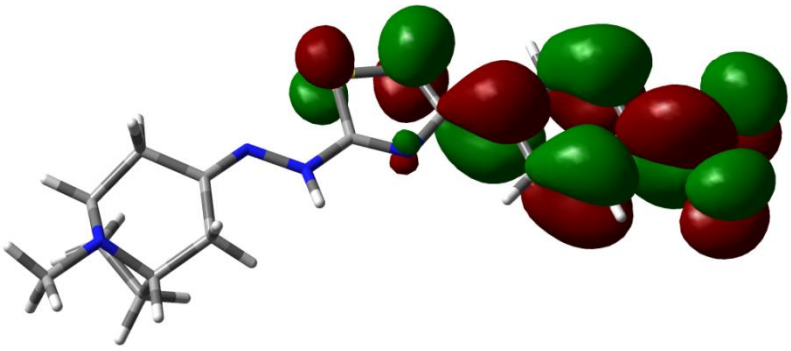
3c-LUMO



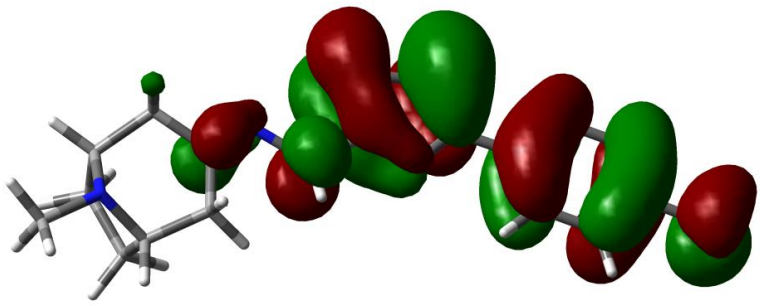
3d-HOMO



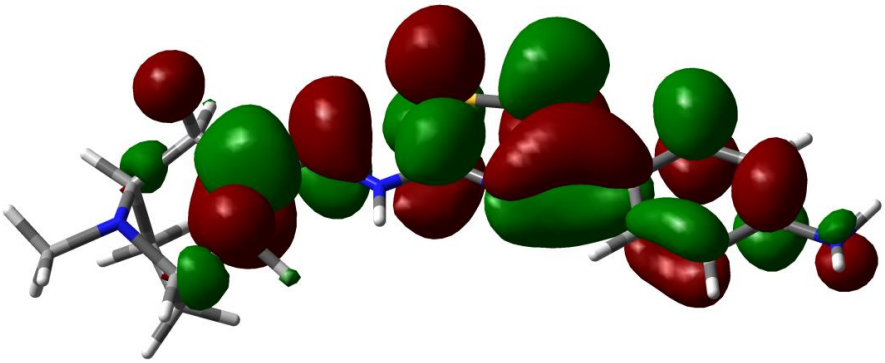
3d-LUMO



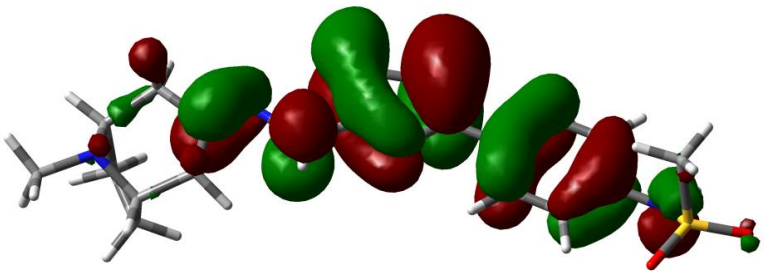
3e-HOMO



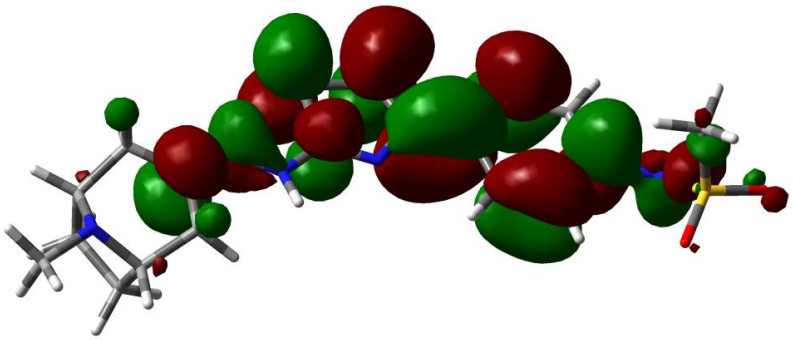
3e-LUMO



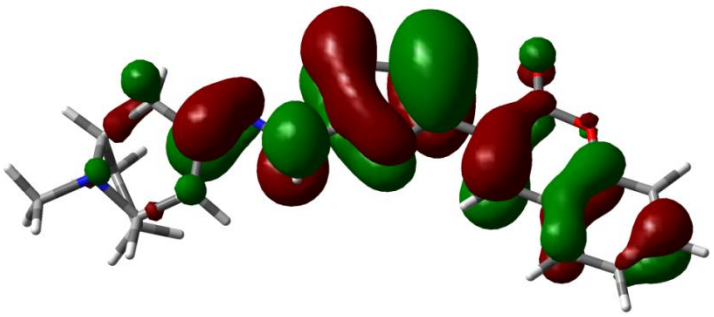
3f-HOMO



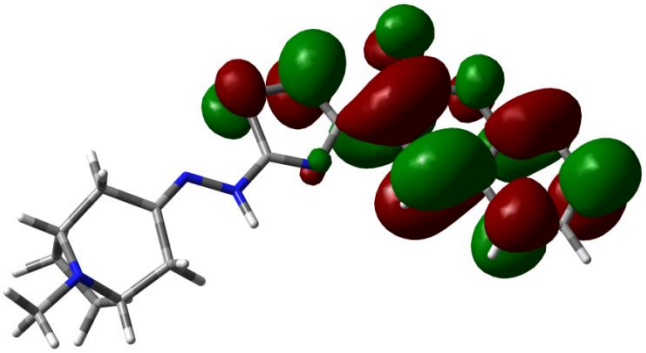
3f-LUMO



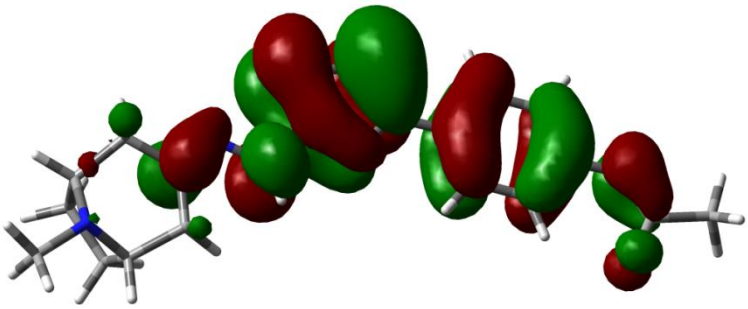
3g-HOMO



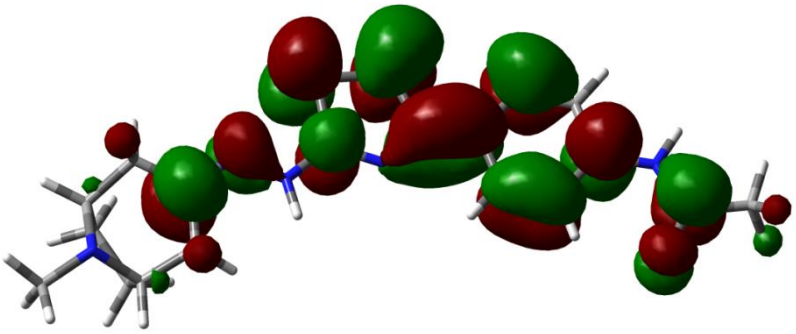
3g-LUMO



3h-HOMO



3h-LUMO



Geometrical parameters of the investigated compounds **3a**-**3h**.

3a

C	6.219519	-1.800700	0.071662
C	6.281359	-1.356748	1.564416
C	6.954401	0.041600	1.504665
C	7.206689	0.264051	-0.015559
N	7.318579	-1.087679	-0.602102
C	6.013896	0.954744	-0.699862
C	4.895781	-1.363732	-0.592391
C	4.747389	0.143257	-0.548161
C	8.626767	-1.708985	-0.408964
N	3.651911	0.793698	-0.399481
N	2.470416	0.125229	-0.312440
C	1.305809	0.832471	-0.175670
S	1.318609	2.576170	0.049455
C	-0.422897	2.500634	0.132989
C	-0.866141	1.216848	-0.013024
N	0.135730	0.274015	-0.187837
C	-2.268831	0.764373	-0.000011
C	-2.565270	-0.596588	-0.153636
C	-3.879369	-1.054913	-0.145404
C	-4.917732	-0.145308	0.018293
C	-4.654770	1.213195	0.172954
C	-3.337830	1.657268	0.162632
I	-6.942665	-0.836968	0.032705
H	6.341169	-2.878785	-0.051467
H	6.881517	-2.058191	2.147476

H	5.290735	-1.325979	2.023239
H	6.325931	0.826668	1.929528
H	7.895876	0.048034	2.057680
H	8.117932	0.832485	-0.212343
H	6.251067	1.046747	-1.766349
H	5.843454	1.958804	-0.305730
H	4.902810	-1.702454	-1.635231
H	4.062227	-1.859996	-0.085118
H	8.622191	-2.705102	-0.858070
H	8.937044	-1.811773	0.644372
H	9.384426	-1.116507	-0.927115
H	2.374656	-0.857629	-0.537940
H	-0.989344	3.405358	0.278662
H	-1.748365	-1.294672	-0.280313
H	-4.084366	-2.110791	-0.265802
H	-5.463604	1.920860	0.299928
H	-3.150942	2.717851	0.283426

3b

C	4.991037	-1.597393	0.058782
C	5.018879	-1.158218	1.554001
C	5.571930	0.291954	1.501210
C	5.801135	0.543627	-0.018144
N	6.025120	-0.790715	-0.612642
C	4.552908	1.135300	-0.696305
C	3.633701	-1.269475	-0.599762
C	3.359217	0.219583	-0.546300

C	7.381037	-1.300949	-0.424712
N	2.213139	0.774373	-0.390638
N	1.093145	0.009590	-0.303496
C	-0.130029	0.614099	-0.164904
S	-0.272727	2.349491	0.067185
C	-2.002642	2.117432	0.147418
C	-2.330283	0.800109	-0.006882
N	-1.244736	-0.046875	-0.182240
C	-3.685094	0.220229	0.002408
C	-3.856836	-1.172228	-0.079335
C	-5.118190	-1.742862	-0.067724
C	-6.258721	-0.937564	0.025422
C	-6.109987	0.450300	0.104273
C	-4.835327	1.010678	0.090837
O	-7.455344	-1.593180	0.029581
C	-8.646369	-0.826472	0.122247
H	5.203000	-2.660733	-0.070673
H	5.676872	-1.810113	2.132255
H	4.029911	-1.212892	2.014090
H	4.880488	1.018850	1.931674
H	6.510883	0.374319	2.052583
H	6.661196	1.187580	-0.213068
H	4.779668	1.253290	-1.762569
H	4.299732	2.119225	-0.295828
H	3.665803	-1.601779	-1.644265
H	2.846123	-1.836181	-0.092830
H	7.459571	-2.291195	-0.880057

H	7.700898	-1.384025	0.627617
H	8.085502	-0.643682	-0.939888
H	1.078963	-0.975080	-0.540721
H	-2.647040	2.966255	0.304937
H	-2.977063	-1.797790	-0.152446
H	-5.249403	-2.816556	-0.129838
H	-6.971372	1.101018	0.172760
H	-4.749696	2.089864	0.145839
H	-8.684484	-0.252015	1.054873
H	-8.753402	-0.143464	-0.728216
H	-9.464641	-1.544817	0.110083

3c

C	4.799742	-1.615901	0.069242
C	4.826016	-1.171228	1.562742
C	5.383521	0.277154	1.505360
C	5.615770	0.522235	-0.014509
N	5.836256	-0.814571	-0.603943
C	4.370584	1.115260	-0.697292
C	3.444524	-1.286896	-0.593727
C	3.174302	0.202981	-0.548391
C	7.191050	-1.328245	-0.414776
N	2.029434	0.762396	-0.401886
N	0.905437	-0.000925	-0.318147
C	-0.310214	0.609762	-0.178520
S	-0.432981	2.352064	0.037354
C	-2.160906	2.142373	0.128516

C	-2.503539	0.826384	-0.008650
N	-1.433752	-0.037837	-0.182523
C	-3.866043	0.269947	0.014301
C	-4.999684	1.084030	0.172649
C	-6.273235	0.540951	0.192676
C	-6.450648	-0.844542	0.053022
C	-5.326671	-1.666823	-0.106483
C	-4.055353	-1.113862	-0.125118
C	-7.763394	-1.408707	0.073328
N	-8.825444	-1.864466	0.090013
H	5.008265	-2.680277	-0.056116
H	5.481200	-1.822797	2.144303
H	3.836386	-1.221784	2.022042
H	4.694368	1.008060	1.932799
H	6.321993	0.358466	2.057454
H	6.477474	1.163342	-0.210744
H	4.599014	1.228181	-1.763613
H	4.118955	2.101329	-0.301263
H	3.478763	-1.621959	-1.637161
H	2.654193	-1.850132	-0.087182
H	7.266482	-2.319959	-0.867197
H	7.510491	-1.408832	0.637686
H	7.897038	-0.674582	-0.932226
H	0.891649	-0.990507	-0.533930
H	-2.795709	3.000782	0.272969
H	-4.889321	2.156003	0.281117
H	-7.138425	1.180638	0.315470

H	-5.458512	-2.736405	-0.214899
H	-3.185053	-1.744012	-0.247981

3d

C	5.181681	-1.660712	0.082789
C	5.212806	-1.208421	1.573915
C	5.803372	0.226583	1.510578
C	6.046035	0.457927	-0.009800
N	6.238265	-0.886739	-0.591133
C	4.816769	1.075062	-0.700043
C	3.836494	-1.304855	-0.586884
C	3.599773	0.190881	-0.550002
C	7.580507	-1.429804	-0.394439
N	2.467573	0.776969	-0.409582
N	1.326094	0.039571	-0.325312
C	0.125288	0.678515	-0.189629
S	0.044070	2.425122	0.016949
C	-1.687481	2.257554	0.108286
C	-2.061821	0.949061	-0.021827
N	-1.013542	0.058222	-0.190716
C	-3.437238	0.427609	0.003204
C	-4.549051	1.272411	0.166080
C	-5.836947	0.763202	0.187617
C	-6.021361	-0.609773	0.044317
C	-4.944571	-1.474443	-0.119057
C	-3.659685	-0.952111	-0.138769
N	-7.388831	-1.156682	0.066604

O	-7.520398	-2.368073	-0.061569
O	-8.315481	-0.367927	0.212174
H	5.366392	-2.730201	-0.036044
H	5.850940	-1.871462	2.161408
H	4.220718	-1.233953	2.029989
H	5.129792	0.975372	1.931857
H	6.741702	0.289497	2.065280
H	6.922537	1.078423	-0.206663
H	5.050924	1.176545	-1.766258
H	4.586249	2.068831	-0.310488
H	3.867172	-1.645550	-1.628577
H	3.031974	-1.847960	-0.080719
H	7.635029	-2.425459	-0.841139
H	7.894416	-1.511676	0.659558
H	8.302789	-0.795132	-0.913016
H	1.290590	-0.951191	-0.533108
H	-2.301867	3.131656	0.246817
H	-4.410387	2.340530	0.277398
H	-6.698664	1.403640	0.312313
H	-5.127297	-2.534394	-0.227326
H	-2.805446	-1.602968	-0.264356

3e

C	4.616223	-1.557718	0.074465
C	4.645583	-1.094018	1.562245
C	5.176511	0.363162	1.483005
C	5.394034	0.593581	-0.041410

N	5.634709	-0.746813	-0.615587
C	4.133619	1.155694	-0.722119
C	3.250684	-1.260612	-0.581612
C	2.954401	0.224967	-0.550990
C	6.998951	-1.233890	-0.426875
N	1.800818	0.764999	-0.398650
N	0.693015	-0.014267	-0.293498
C	-0.539674	0.573596	-0.159751
S	-0.709283	2.308811	0.051229
C	-2.435713	2.049619	0.139729
C	-2.743057	0.725045	0.003663
N	-1.643048	-0.105719	-0.165448
C	-4.086897	0.123729	0.023844
C	-5.252595	0.896311	0.133467
C	-6.510030	0.313501	0.153017
C	-6.657744	-1.079746	0.059724
C	-5.497142	-1.858517	-0.050715
C	-4.242254	-1.266620	-0.068817
N	-7.918479	-1.672558	0.137871
H	4.843481	-2.619767	-0.038945
H	5.316390	-1.726608	2.147225
H	3.660009	-1.155890	2.028626
H	4.476309	1.086464	1.905255
H	6.116922	0.468552	2.027980
H	6.243539	1.246809	-0.251319
H	4.353282	1.260245	-1.791299
H	3.867894	2.141997	-0.335848

H	3.281821	-1.610096	-1.620566
H	2.474272	-1.830052	-0.060665
H	7.089883	-2.229990	-0.866948
H	7.325555	-1.295596	0.624894
H	7.690959	-0.574541	-0.956123
H	0.692207	-1.002327	-0.516569
H	-3.093157	2.890371	0.285919
H	-5.183556	1.976183	0.200514
H	-7.392386	0.939553	0.243264
H	-5.583352	-2.938724	-0.119409
H	-3.354999	-1.879894	-0.157602
H	-7.985494	-2.593836	-0.269263
H	-8.689557	-1.081819	-0.136820

3f

C	6.011390	-1.893713	0.206241
C	6.184845	-1.261651	1.620291
C	6.916139	0.078715	1.336721
C	7.085029	0.085828	-0.211005
N	7.098579	-1.335178	-0.616204
C	5.886006	0.743706	-0.916318
C	4.670975	-1.477543	-0.437191
C	4.594892	0.027722	-0.590515
C	8.386295	-1.995112	-0.413641
N	3.540419	0.749232	-0.476983
N	2.336698	0.161730	-0.240816
C	1.214886	0.940551	-0.141196

S	1.316989	2.695580	-0.164851
C	-0.418966	2.721666	0.019191
C	-0.925488	1.454151	0.076046
N	0.022798	0.446351	-0.014344
C	-2.342130	1.079913	0.229348
C	-3.372602	2.030050	0.194076
C	-4.699889	1.652632	0.335085
C	-5.038305	0.309603	0.539538
C	-4.022029	-0.649068	0.590227
C	-2.698284	-0.262529	0.421383
N	-6.401828	-0.041495	0.730998
S	-7.184060	-1.302350	-0.074804
O	-8.589133	-1.135441	0.270402
O	-6.465576	-2.537526	0.200282
C	-6.977094	-0.949693	-1.834326
H	6.075722	-2.983571	0.222479
H	6.786789	-1.911577	2.258556
H	5.226625	-1.118029	2.124251
H	6.351460	0.945269	1.686103
H	7.889023	0.107320	1.831647
H	8.007795	0.573734	-0.531440
H	6.062666	0.682853	-1.996704
H	5.785688	1.798336	-0.651254
H	4.597772	-1.951849	-1.423109
H	3.848186	-1.856040	0.177801
H	8.308374	-3.039775	-0.724389
H	8.755811	-1.975611	0.625320

H	9.137037	-1.517115	-1.047266
H	2.184428	-0.836569	-0.320008
H	-0.934600	3.665485	0.083068
H	-3.144378	3.077391	0.035453
H	-5.481936	2.403818	0.286076
H	-4.274629	-1.685516	0.768802
H	-1.911612	-1.004471	0.455138
H	-7.040861	0.728297	0.884439
H	-7.420084	-1.786336	-2.373324
H	-5.912874	-0.877410	-2.054249
H	-7.496279	-0.022411	-2.070657

3g

C	-5.341797	1.728893	0.139691
C	-5.400021	1.212283	1.609069
C	-6.035485	-0.198664	1.477898
C	-6.272079	-0.355045	-0.052968
N	-6.417075	1.019801	-0.575235
C	-5.056912	-0.979943	-0.760682
C	-4.002857	1.359967	-0.535124
C	-3.813684	-0.142981	-0.561499
C	-7.742698	1.596022	-0.362379
N	-2.702102	-0.770364	-0.436134
N	-1.539205	-0.076357	-0.308623
C	-0.356604	-0.758489	-0.198011
S	-0.323826	-2.512455	-0.059243
C	1.412449	-2.402581	0.041570

C	1.821175	-1.100599	-0.037018
N	0.797509	-0.170120	-0.173527
C	3.197945	-0.599977	0.007899
C	4.313219	-1.550640	0.150901
O	5.592303	-1.004034	0.186098
C	5.846865	0.331126	0.096994
C	4.795820	1.251324	-0.039481
C	3.461643	0.733743	-0.080624
C	7.176429	0.743573	0.146187
C	7.463073	2.099115	0.057692
C	6.433030	3.039876	-0.079064
C	5.114972	2.619586	-0.127001
O	4.235561	-2.748140	0.240530
H	-5.492142	2.808010	0.067413
H	-6.021483	1.868996	2.221204
H	-4.411301	1.185071	2.072243
H	-5.389435	-0.986412	1.870110
H	-6.980099	-0.255752	2.022613
H	-7.166356	-0.937623	-0.283330
H	-5.285258	-1.027456	-1.831994
H	-4.861537	-1.996680	-0.413493
H	-4.013279	1.747819	-1.560698
H	-3.186092	1.853860	0.001089
H	-8.480962	1.008560	-0.913194
H	-7.762526	2.611995	-0.764172
H	-8.062010	1.640779	0.692349
H	-1.469766	0.918914	-0.483373

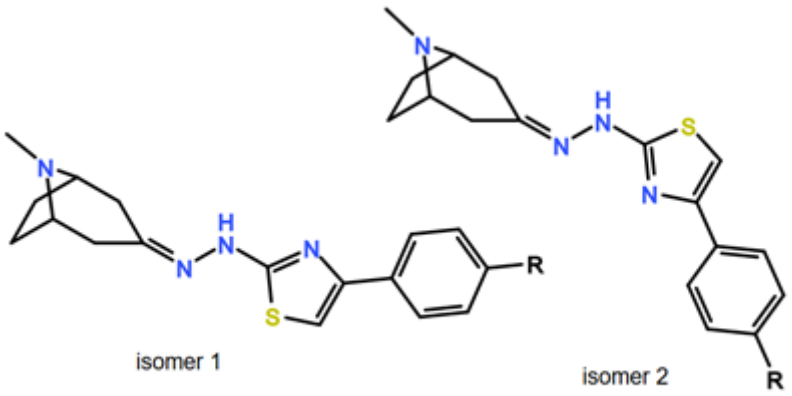
H	2.024084	-3.280864	0.146135
H	2.627006	1.416746	-0.185234
H	7.954281	-0.002021	0.252207
H	8.494665	2.429262	0.095088
H	6.669979	4.094856	-0.147103
H	4.309761	3.338357	-0.232647

3h

C	5.421725	-1.843080	0.085299
C	5.498108	-1.381830	1.572145
C	6.197031	0.002709	1.492318
C	6.448095	0.201151	-0.031501
N	6.532073	-1.159880	-0.601158
C	5.266162	0.905854	-0.720308
C	4.104068	-1.388899	-0.578973
C	3.984778	0.121185	-0.552655
C	7.828584	-1.803598	-0.403752
N	2.902588	0.794272	-0.406610
N	1.709651	0.150728	-0.305164
C	0.556922	0.880157	-0.172493
S	0.596970	2.625724	0.029264
C	-1.146559	2.576327	0.120861
C	-1.610039	1.297233	-0.006637
N	-0.620573	0.338895	-0.172610
C	-3.017676	0.863889	0.018796
C	-4.076697	1.773645	0.155038
C	-5.391636	1.340337	0.178306

C	-5.701517	-0.023304	0.065148
C	-4.656695	-0.944231	-0.073073
C	-3.341470	-0.494256	-0.094547
N	-7.064809	-0.384466	0.097666
C	-7.634754	-1.635287	0.007792
O	-7.004604	-2.667481	-0.119835
C	-9.154851	-1.639054	0.080839
H	5.522350	-2.924784	-0.024655
H	6.087355	-2.087178	2.161675
H	4.510055	-1.326577	2.034124
H	5.584538	0.804682	1.908846
H	7.140354	-0.001356	2.042304
H	7.369551	0.749274	-0.238454
H	5.501246	0.979658	-1.788727
H	5.116859	1.918006	-0.338413
H	4.099848	-1.741156	-1.617367
H	3.263357	-1.862608	-0.062099
H	7.803487	-2.805248	-0.839764
H	8.140328	-1.898752	0.649949
H	8.595936	-1.232591	-0.931758
H	1.593672	-0.832862	-0.517730
H	-1.698551	3.491089	0.259107
H	-3.878452	2.835393	0.242837
H	-6.192072	2.066975	0.284545
H	-4.884208	-1.994891	-0.161486
H	-2.535159	-1.207770	-0.201696
H	-7.704415	0.387650	0.201337

H	-9.457977	-2.270599	0.918236
H	-9.542593	-2.097727	-0.830953
H	-9.604177	-0.650896	0.200126



Scheme S1. Structure of isomers 1 and 2 of investigated compounds.

Table S6. Fractional populations of isomers 1 and 2 of investigated compounds [%].

Molecule	isomer 1 [%]	isomer 2 [%]
3a	100.00	0.00
3b	100.00	0.00
3c	100.00	0.00
3d	100.00	0.00
3e	100.00	0.00
3f	99.99	0.01
3g	99.99	0.01
3h	99.99	0.01