

Supplementary Material

Synthesis of substituted 1,3-oxazino[5,4,3-*ij*]quinolin-1,3-diones by the oxidation of various pyrrolo[3,2,1-*ij*]quinoline-1,2-diones with *m*-chloroperbenzoic acid

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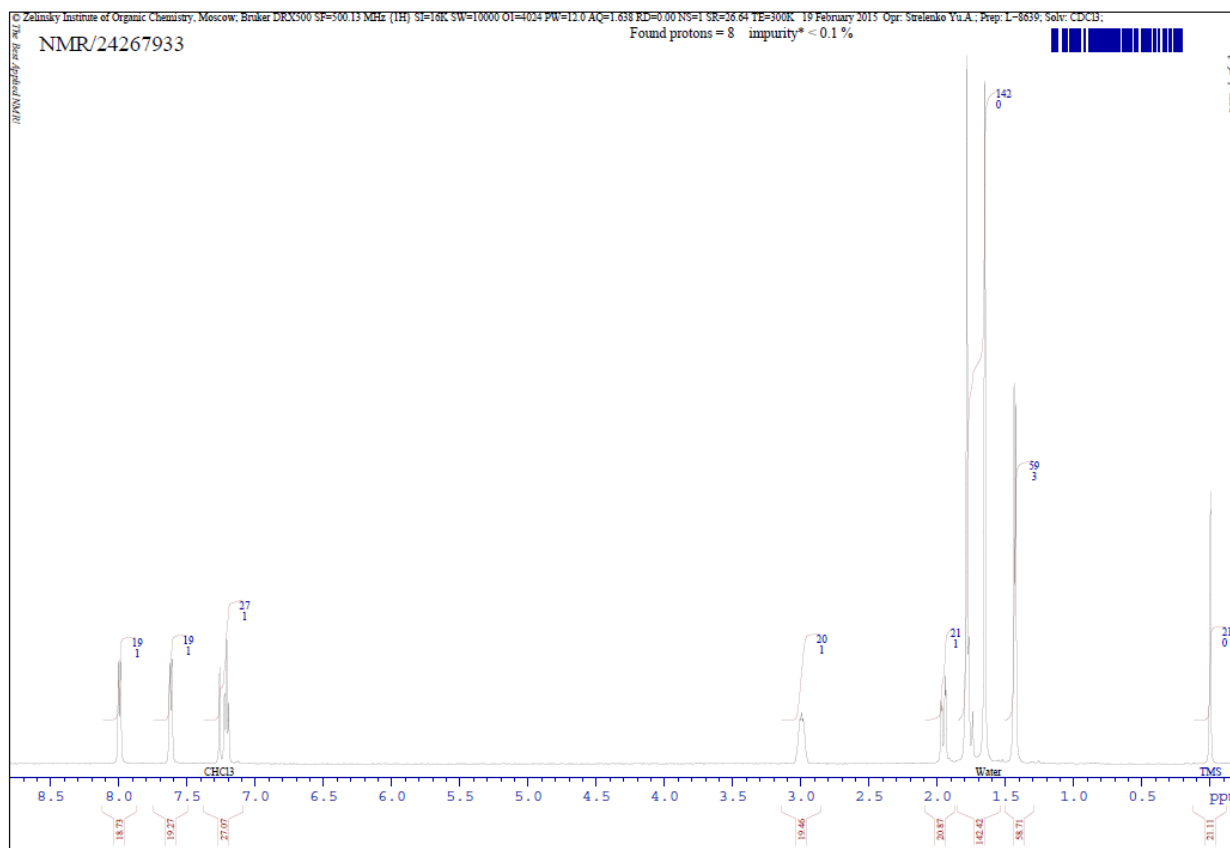
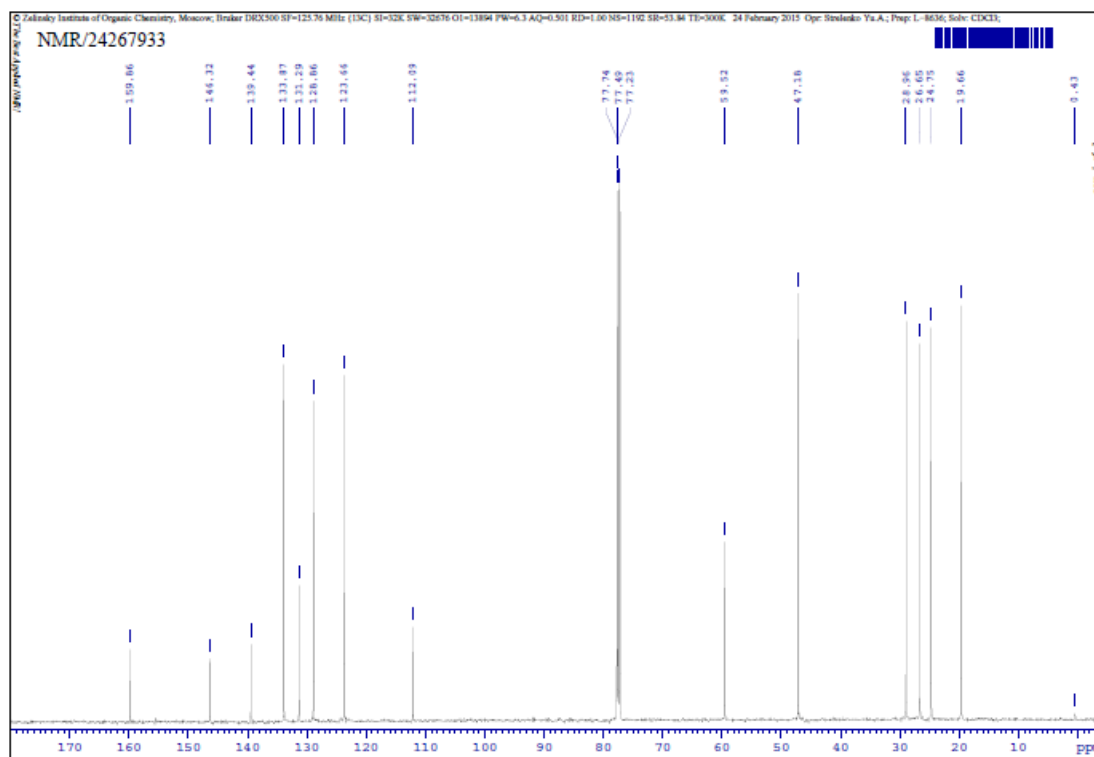
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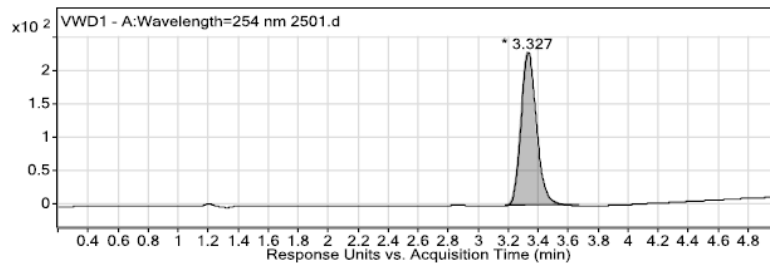
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Figure 1. NMR ^1H spectra of compound 10a.Figure 2. NMR ^{13}C spectra of compound 10a.

Data Filename	2501.d	Sample Name	
Sample Type	Sample	Position	Vial 12
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	2/24/2022 3:14:22 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.18	3.327	3.673	229.41	1657.68	100

User Spectra

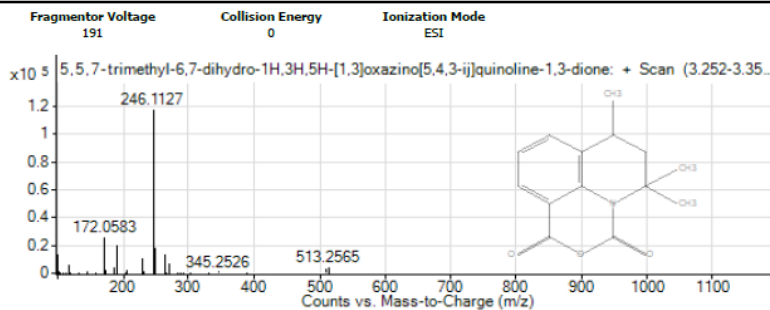
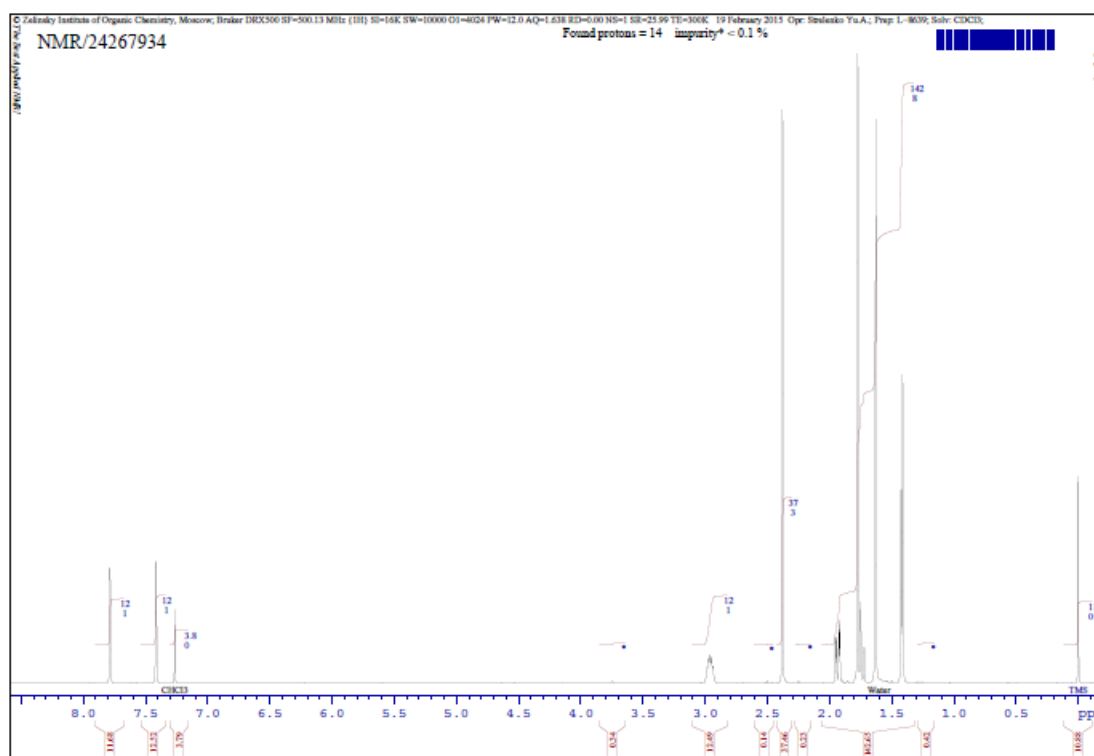
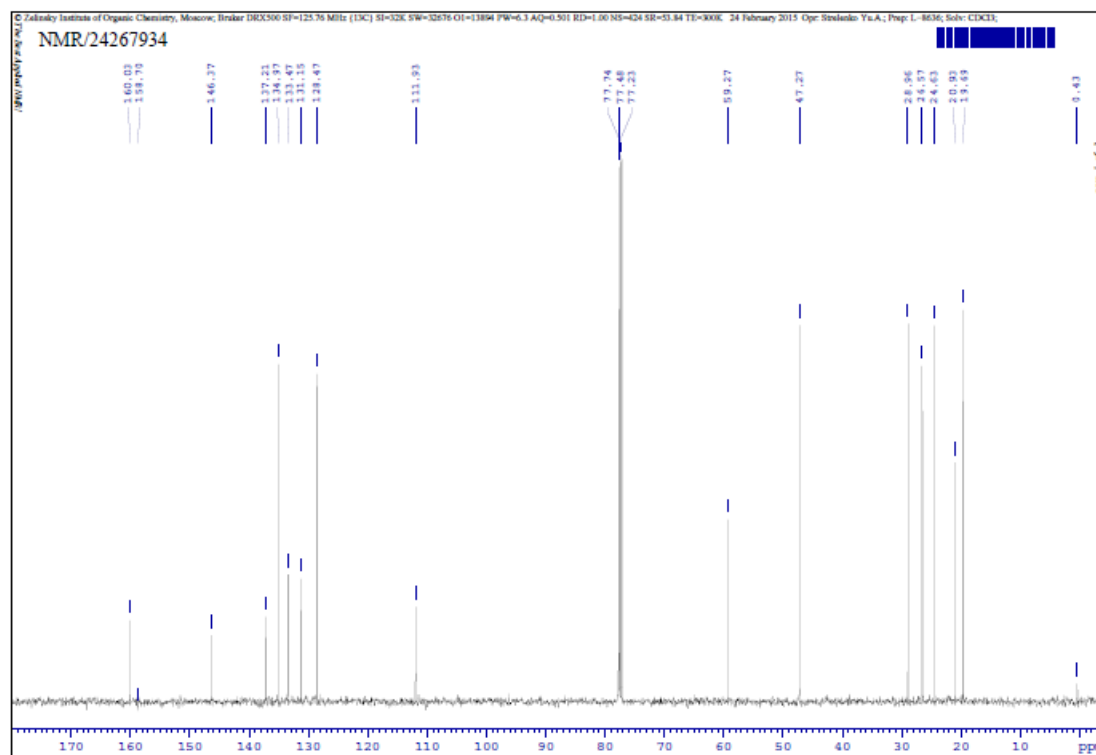


Figure 3. HPLC-HRMS-ESI spectra of compound 10a.

Mass spectrum NMR/24267933: formula C₁₄H₁₅N₃O₃, mol. mass 245.28
 Max intensity: 999 for mass 186
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

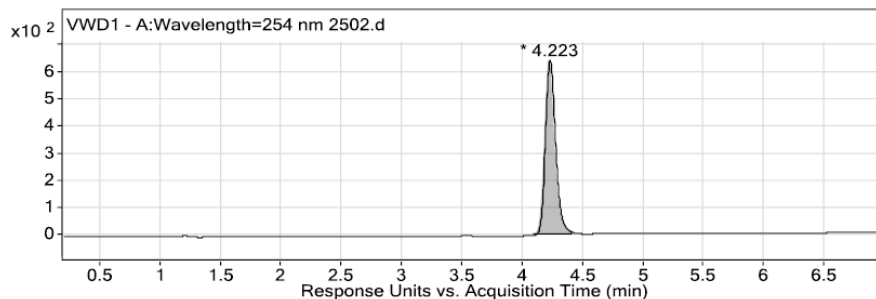
Mass	Intens.	Rel.Int (%)	Mass	*** Graphic ***	Rel.Int (%)
39	75	7.51	39	*	7.51
41	72	7.21	41	*	7.21
91	63	6.31	91	*	6.31
115	58	5.81	115	*	5.81
116	50	5.01	116	*	5.01
117	52	5.21	117	*	5.21
118	117	11.71	118	**	11.71
158	130	13.01	158	**	13.01
172	59	5.91	172	*	5.91
186	999	100.00	186	*****	100.00
187	151	15.12	187	***	15.12
200	15	1.50	200	-->	1.50
201	172	17.22	201	***	17.22
202	45	4.50	202	*	4.50
245	185	18.52	245	mol.mass: ***	18.52
246	29	2.90	246	-->	2.90

Figure 4. Mass-spectra of compound 10a.

Figure 5. NMR ^1H spectra of compound 10b.Figure 6. NMR ^{13}C spectra of compound 10b.

Data Filename	2502.d	Sample Name	
Sample Type	Sample	Position	Vial 13
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	2/24/2022 3:26:13 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.09	4.223	4.41	643.12	3862.22	100

User Spectra

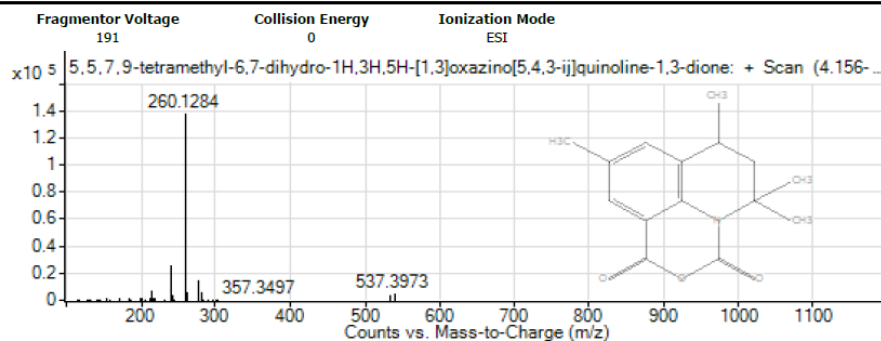
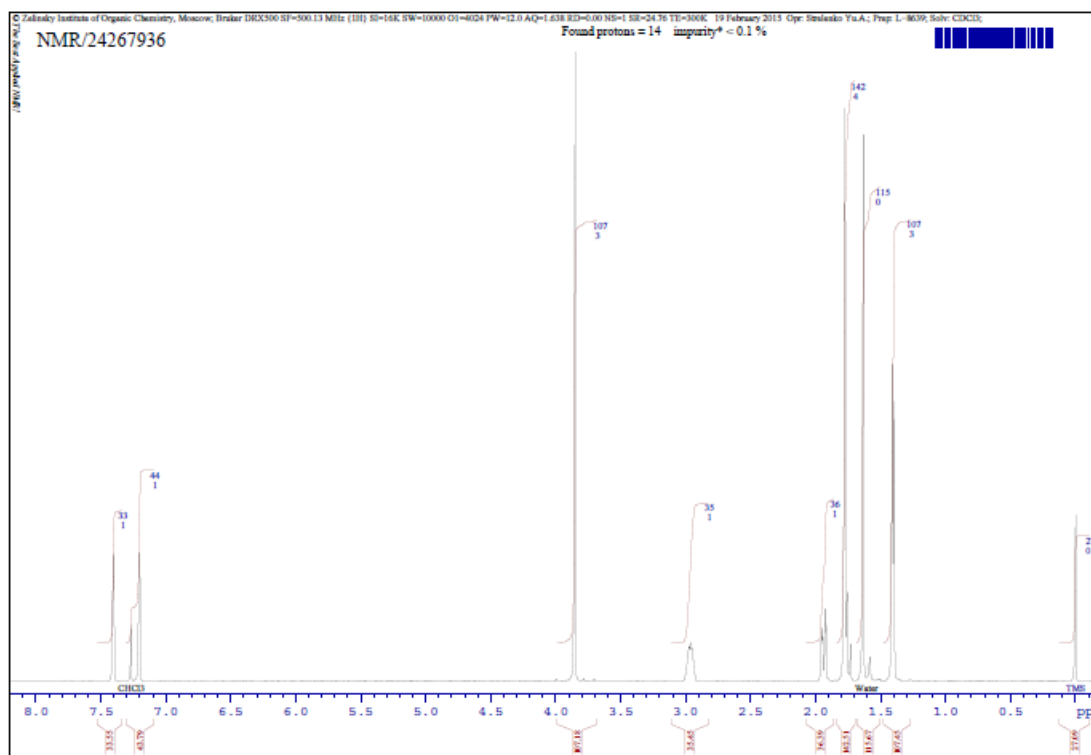
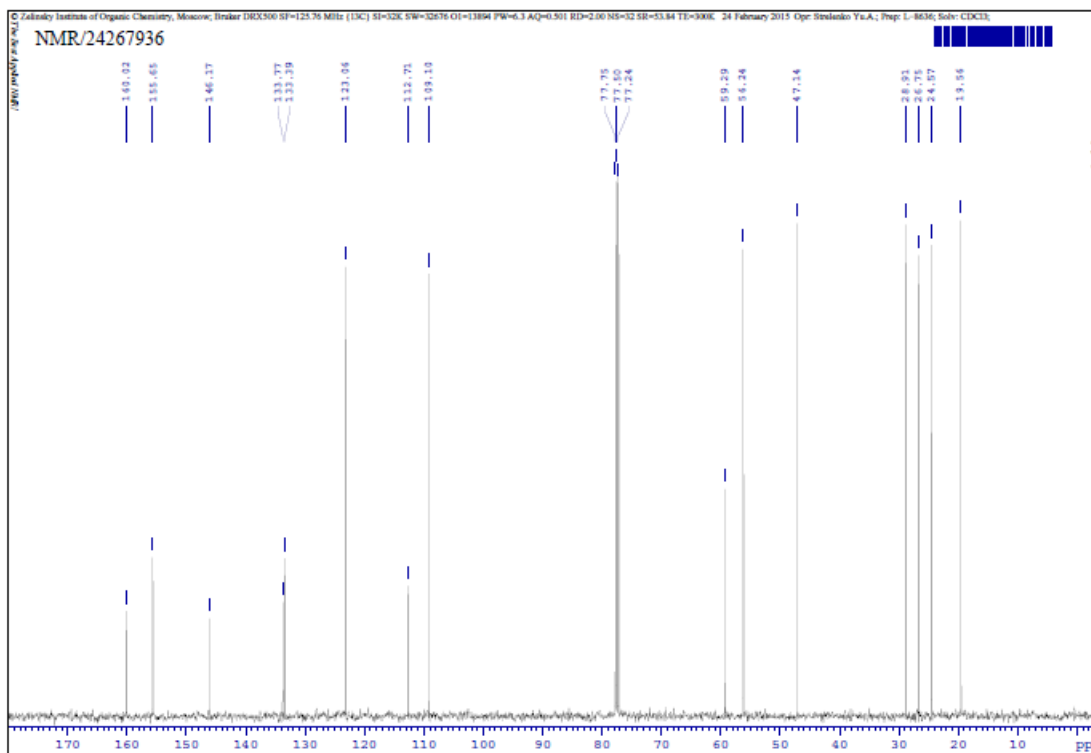


Figure 7. HPLC-HRMS-ESI spectra of compound 10b.

Mass spectrum NMR/24267934: formula C₁₅H₁₇NO₃, mol. mass 259.30
 Max intensity: 999 for mass 200
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

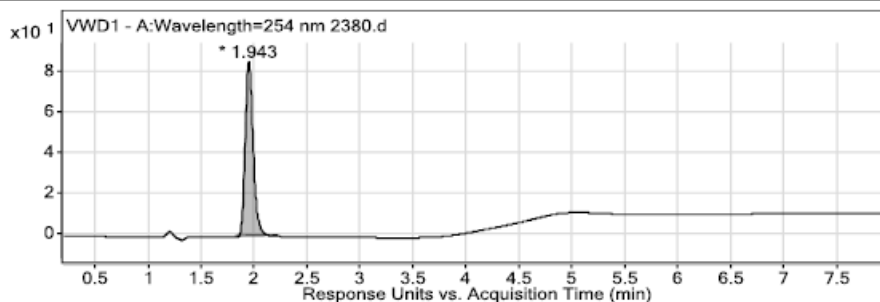
Mass	Intens.	Rel.Int (%)		Mass	*** Graphic ***	
130	63	6.31		130	*	6.31
132	78	7.81		132	*	7.81
172	95	9.51		172	**	9.51
186	54	5.41		186	*	5.41
200	999	100.00		200	*****	100.00
201	146	14.61		201	***	14.61
214	16	1.60	-->	214		1.60
215	177	17.72	-->	215	***	17.72
216	34	3.40	-->	216		3.40
259	188	18.82	mol.mass:	259	***	18.82
260	31	3.10	-->	260		3.10

Figure 8. Mass-spectra of compound 10b.

Figure 9. NMR ¹H spectra of compound 10c.Figure 10. NMR ¹³C spectra of compound 10c.

Data Filename	2380.d	Sample Name	
Sample Type	Sample	Position	Vial 91
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	1/21/2022 11:18:31 AM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1.827	1.943	2.23	86.19	456.59	100

User Spectra

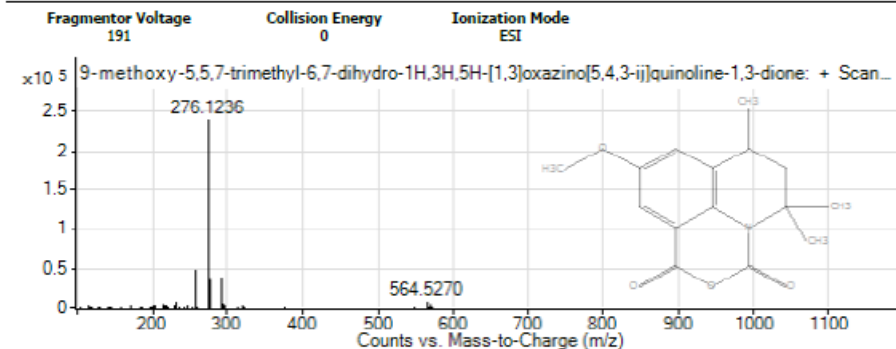
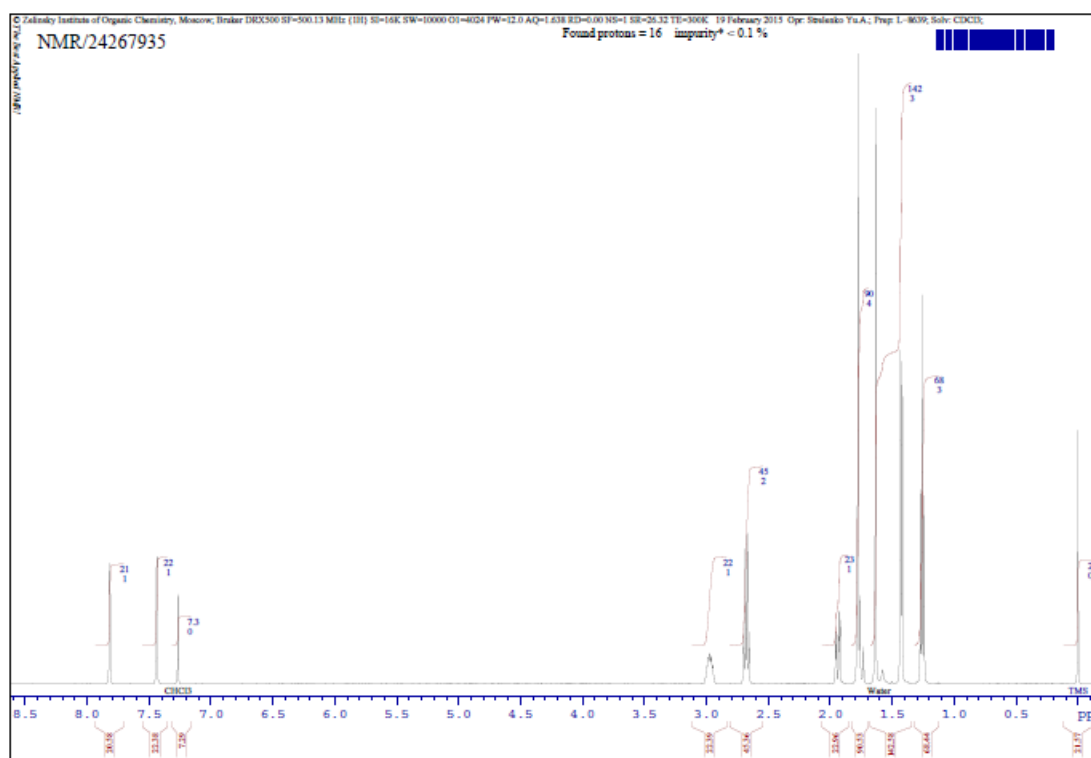
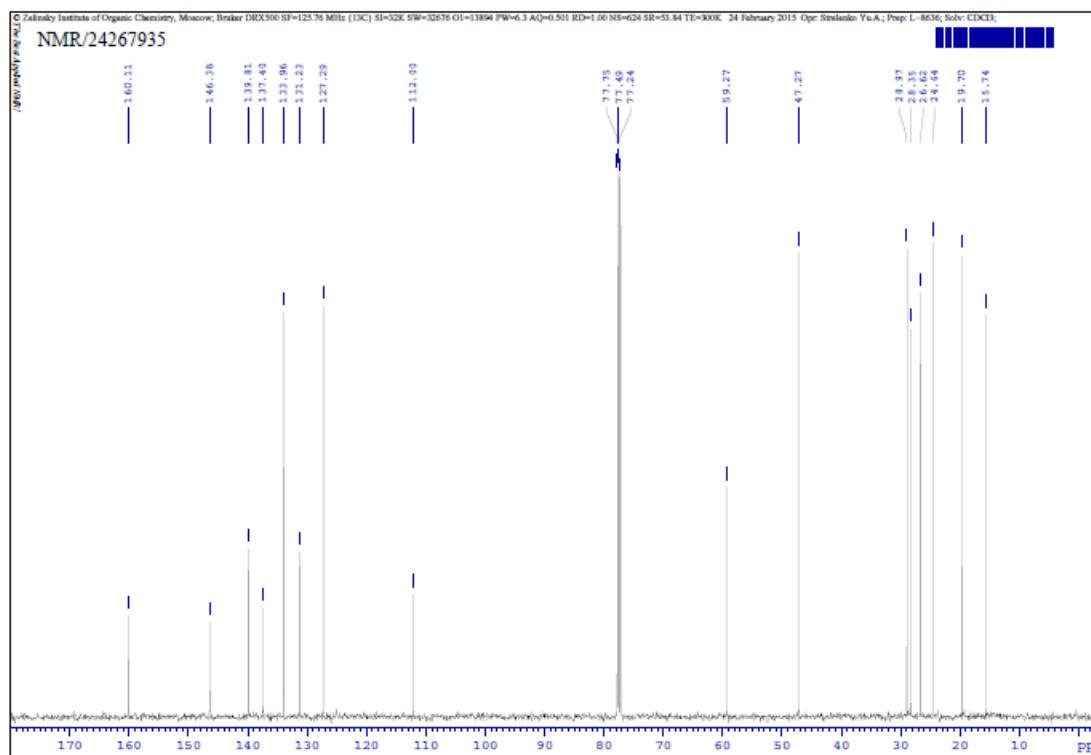


Figure 11. HPLC-HRMS-ESI spectra of compound 10c.

Mass spectrum NMR/24267936: formula C₁₅H₁₇N₂O₄, mol. mass 275.30
 Max intensity: 999 for mass 216
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

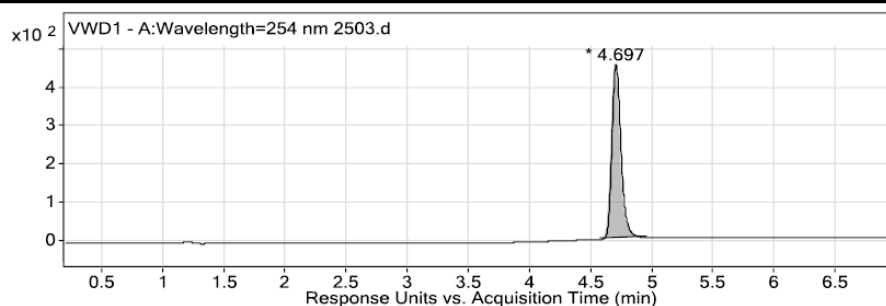
Mass	Intens.	Rel.Int(%)		Mass	*** Graphic ***	
188	84	8.41		188	*	8.41
202	55	5.51		202	*	5.51
216	999	100.00		216	*****	100.00
217	145	14.51		217	***	14.51
230	10	1.00	-->	230		1.00
231	170	17.02	-->	231	***	17.02
232	43	4.30	-->	232		4.30
275	213	21.32	mol.mass:	275	****	21.32
276	37	3.70	-->	276		3.70

Figure 12. Mass-spectra of compound 10c.

Figure 13. NMR ¹H spectra of compound 10d.Figure 14. NMR ¹³C spectra of compound 10d.

Data Filename	2503.d	Sample Name	
Sample Type	Sample	Position	Vial 14
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	2/24/2022 3:38:08 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.573	4.697	4.96	454.21	2334.65	100

User Spectra

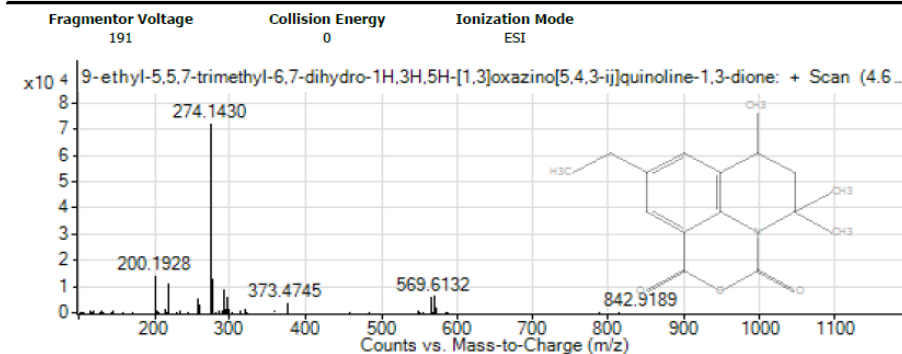
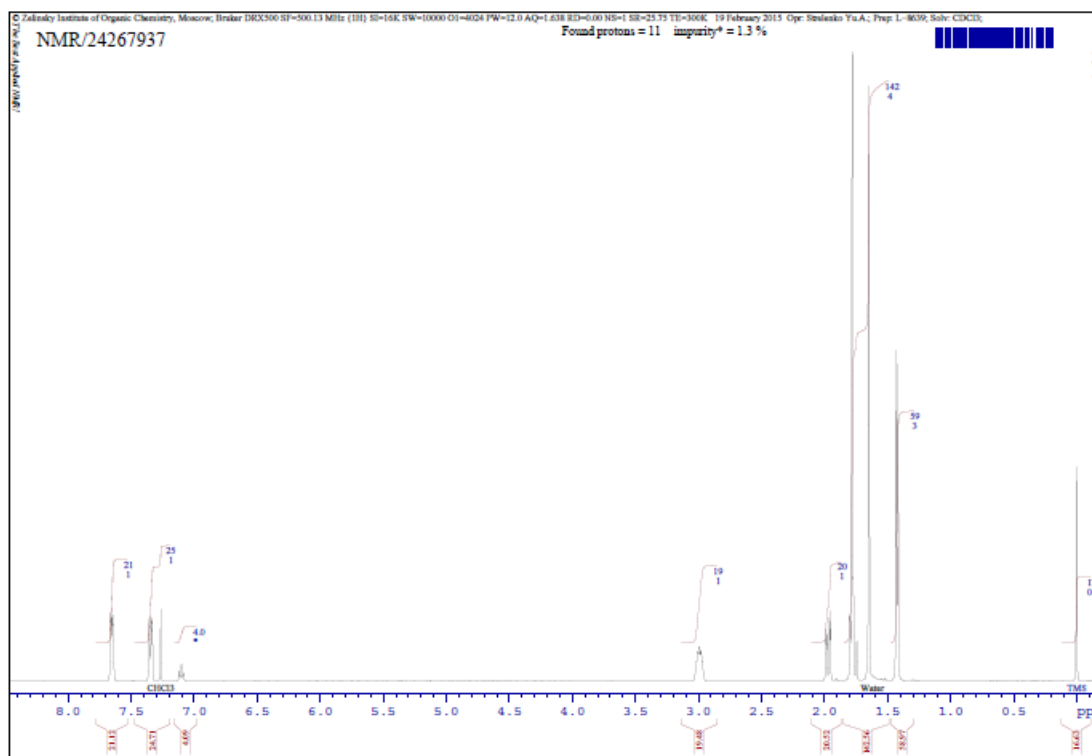
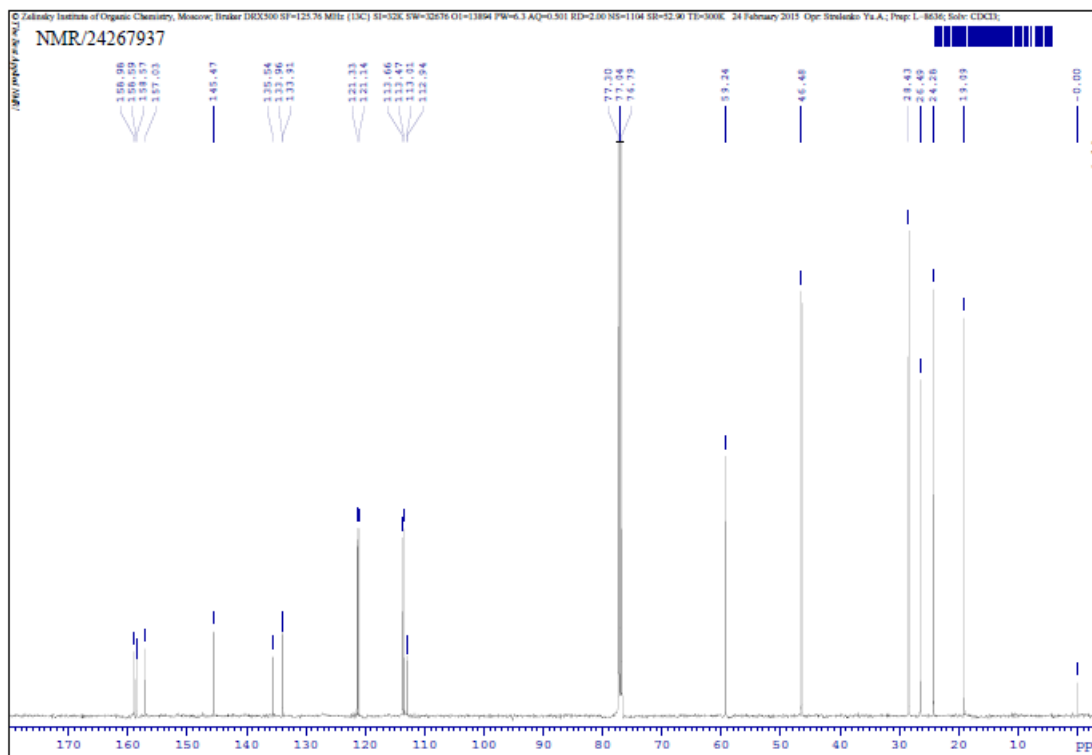


Figure 15. HPLC-HRMS-ESI spectra of compound 10d.

Mass spectrum NMR/24267935: formula C₁₆H₁₉NO₃, mol. mass 273.33
 Max intensity: 999 for mass 214
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

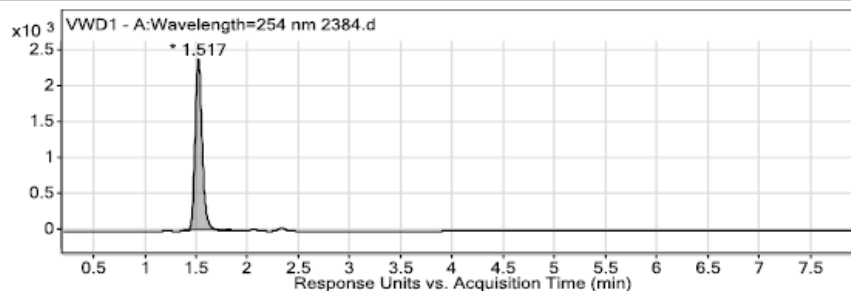
Mass	Intens.	Rel.Int (%)		Mass	*** Graphic ***	
29	65	6.51		29	*	6.51
41	70	7.01		41	*	7.01
130	64	6.41		130	*	6.41
146	76	7.61		146	*	7.61
186	75	7.51		186	*	7.51
214	999	100.00		214	*****	100.00
215	170	17.02		215	***	17.02
229	148	14.81	-->	229	***	14.81
230	33	3.30	-->	230	***	3.30
273	151	15.12	mol.mass:	273	***	15.12
274	27	2.70	-->	274	***	2.70

Figure 16. Mass-spectra of compound 10d.

Figure 17. NMR ¹H spectra of compound 10e.Figure 18. NMR ¹³C spectra of compound 10e.

Data Filename	2384.d	Sample Name	
Sample Type	Sample	Position	Vial 95
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	1/21/2022 12:10:11 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	1.377	1.517	1.843	2378.8	11542.63	100

User Spectra

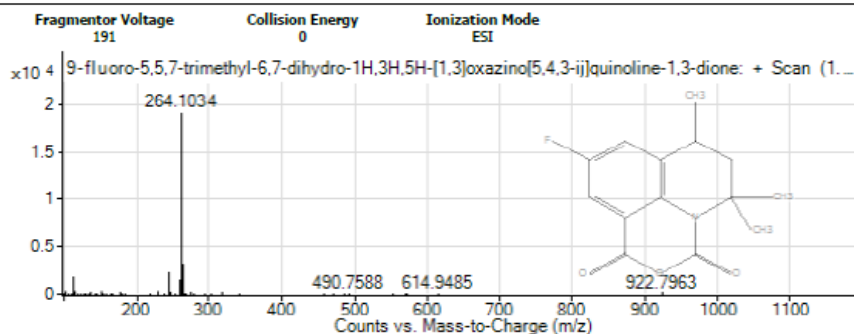
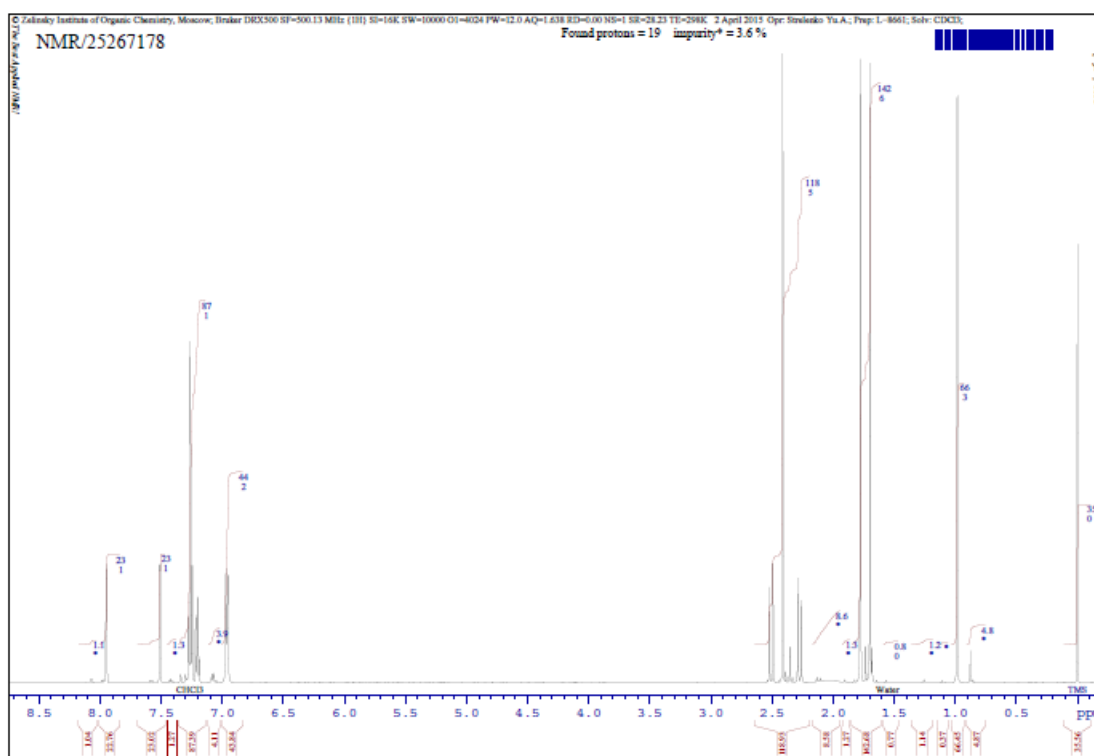
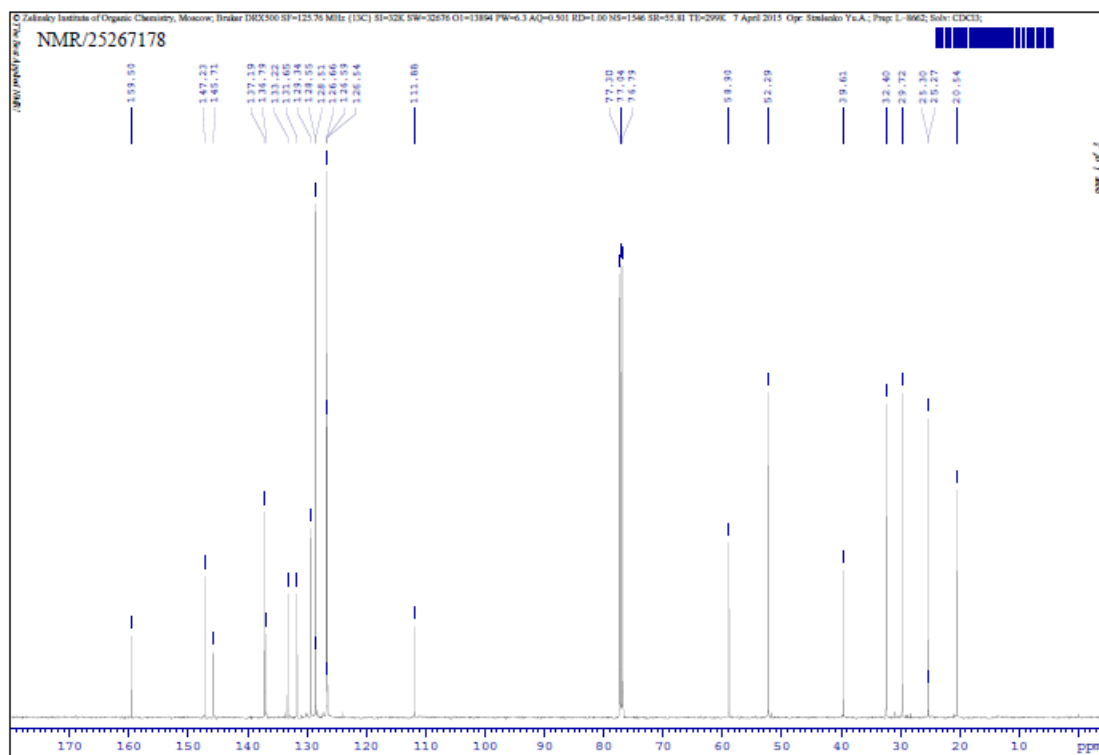


Figure 19. HPLC-HRMS-ESI spectra of compound 10e.

Mass spectrum NMR/24267937: formula C₁₄H₁₄FN₃O₃, mol. mass 263.27
 Max intensity: 999 for mass 204
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

Mass	Intens.	Rel.Int(%)		Mass	*** Graphic ***	
41	63	6.31		41	*	6.31
136	84	8.41		136	*	8.41
176	107	10.71		176	**	10.71
190	72	7.21		190	*	7.21
204	999	100.00		204	*****	100.00
205	140	14.01		205	**	14.01
218	9	0.90	-->	218		0.90
219	157	15.72	-->	219	***	15.72
220	34	3.40	-->	220		3.40
263	155	15.52	mol.mass:	263	***	15.52
264	23	2.30	-->	264		2.30
276	19	1.90	-->	276		1.90

Figure 20. Mass-spectra of compound 10e.

Figure 21. NMR ¹H spectra of compound **10f**.Figure 22. NMR ¹³C spectra of compound **10f**.

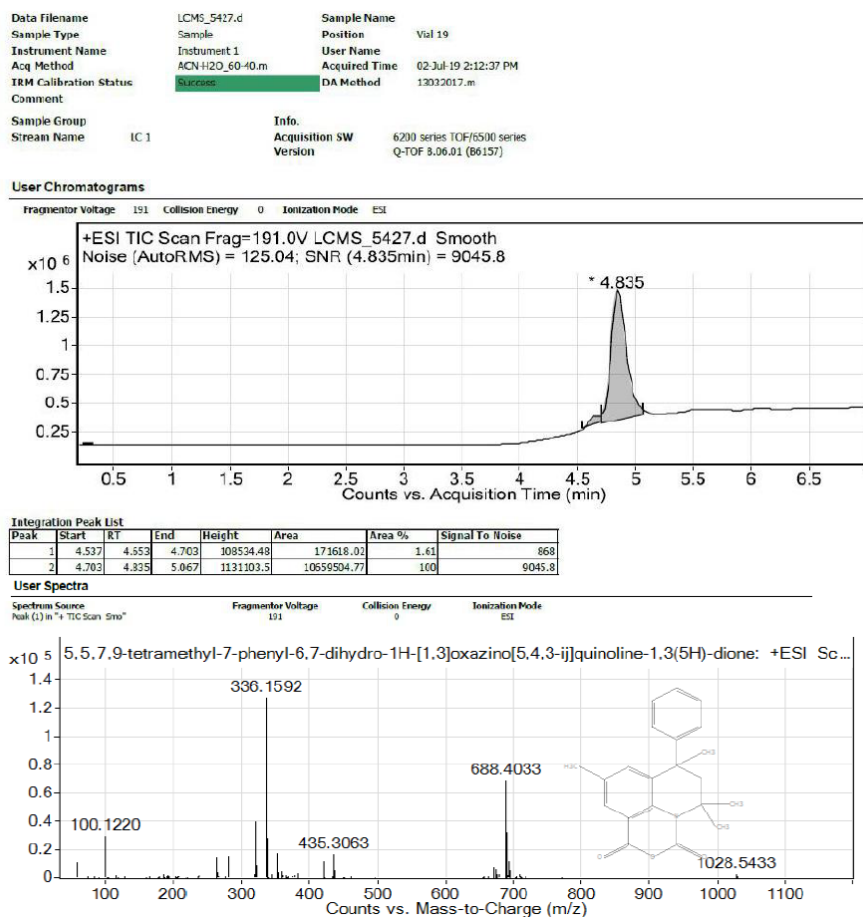


Figure 23. HPLC-HRMS-ESI spectra of compound 10f.

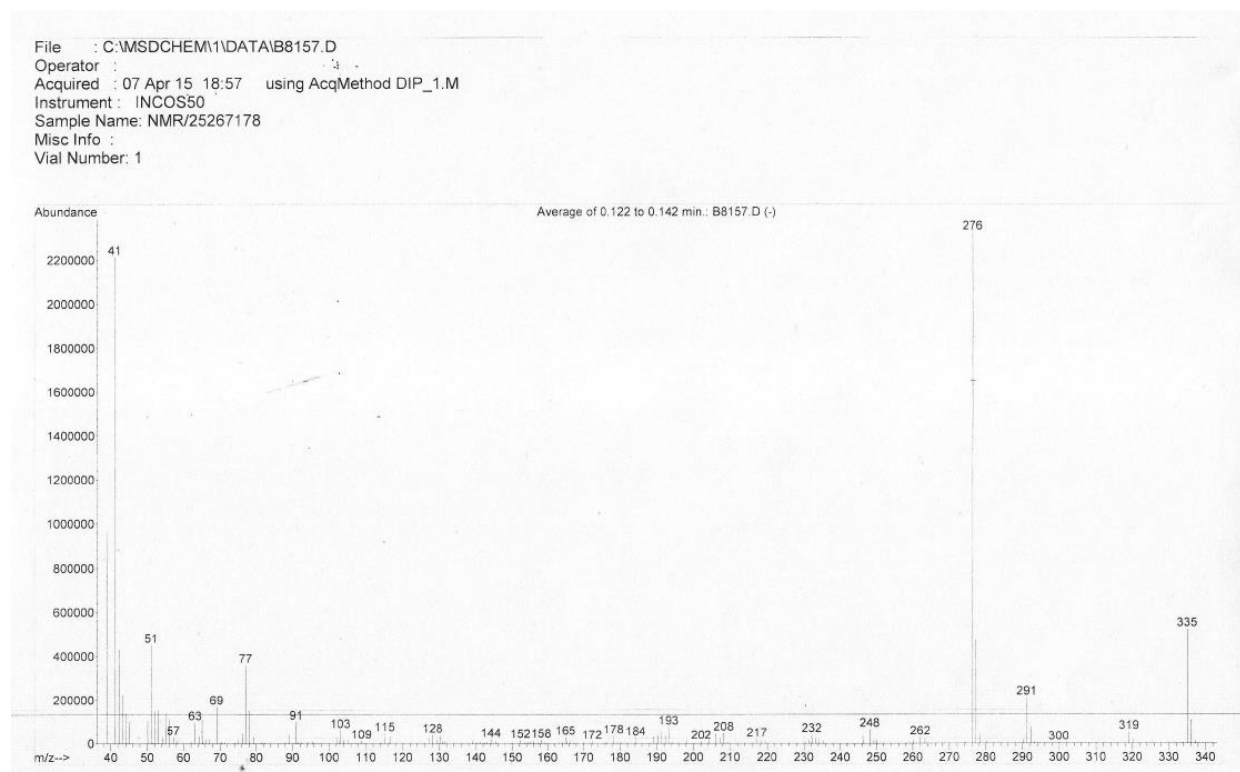
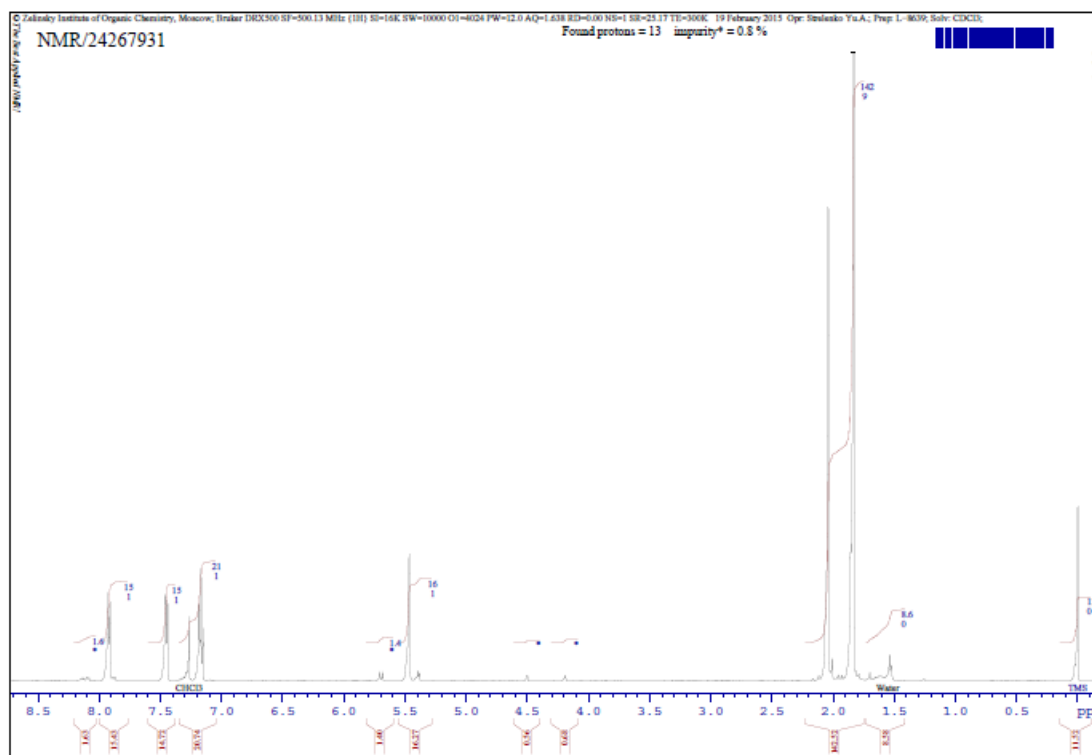
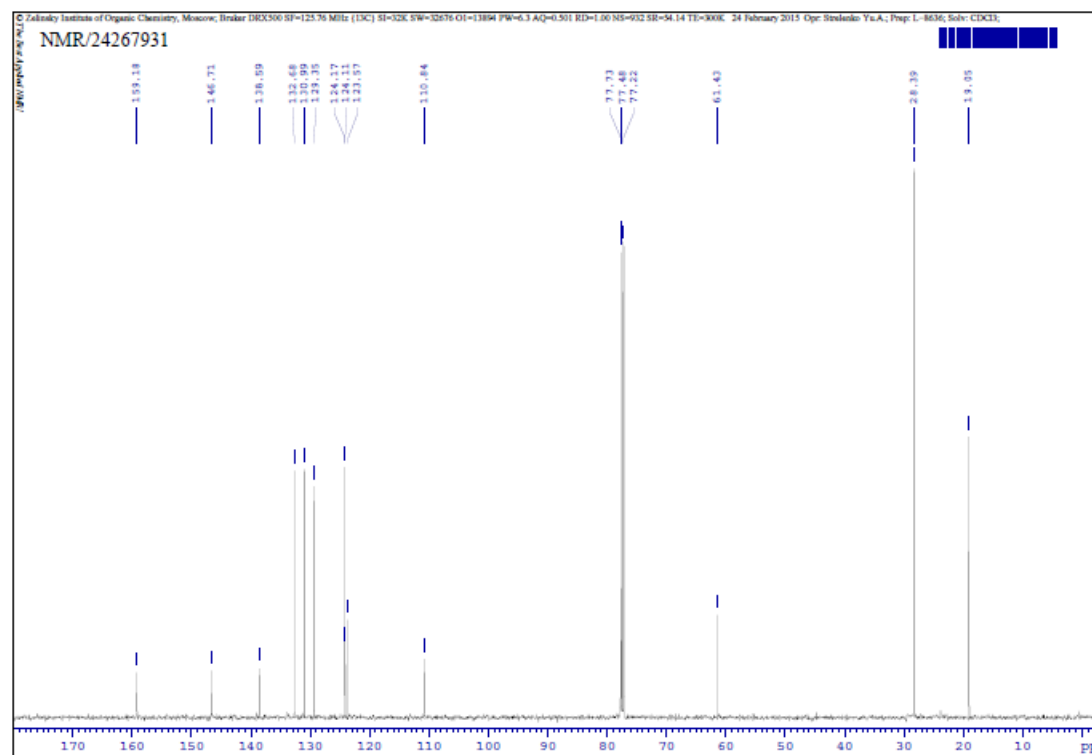
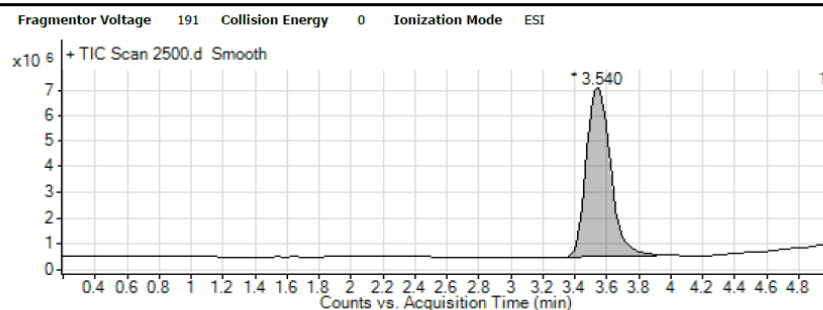


Figure 24. Mass-spectra of compound 10f.

Figure 25. NMR ¹H spectra of compound **12a**.Figure 26. NMR ¹³C spectra of compound **12a**.

Data Filename	2500.d	Sample Name	
Sample Type	Sample	Position	Vial 11
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	2/24/2022 3:04:31 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.325	3.54	3.905	6590441.04	70010421.29	100

User Spectra

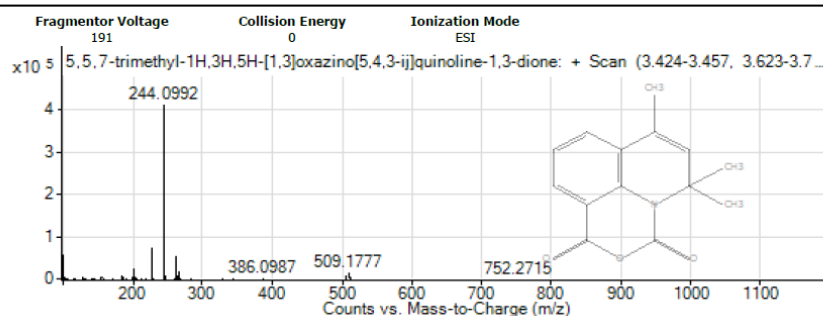
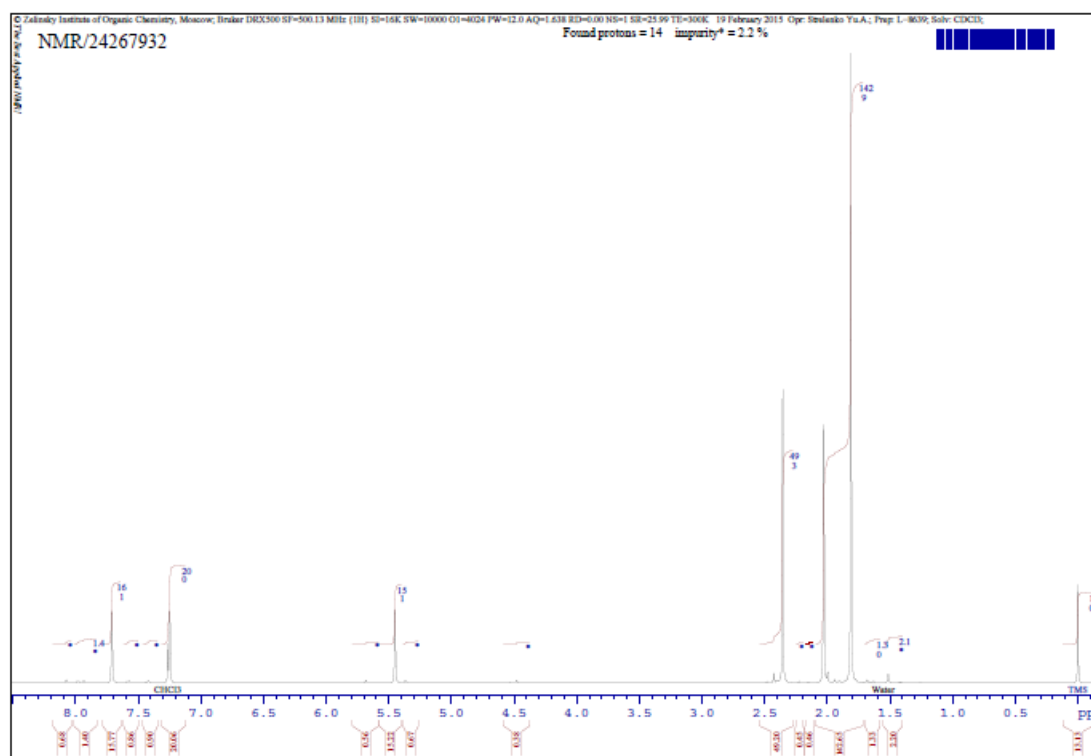
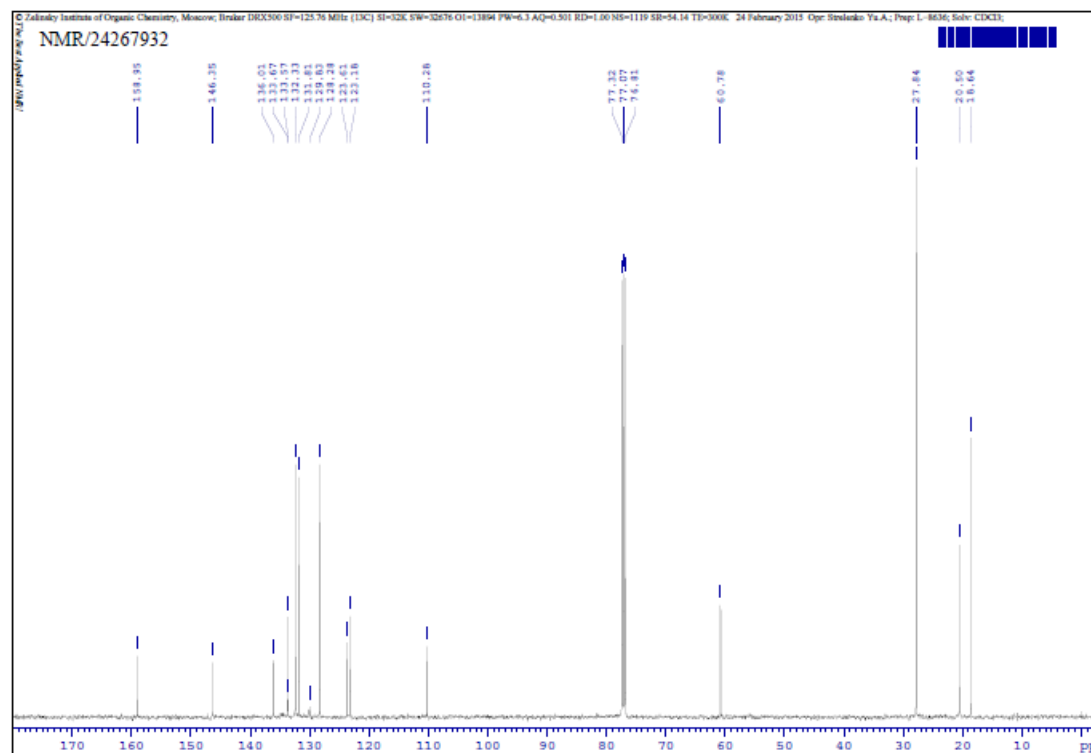


Figure 27. HPLC-HRMS-ESI spectra of compound 12a.

Mass spectrum NMR/24267931: formula C₁₄H₁₃NO₃, mol. mass 243.26
 Max intensity: 999 for mass 184
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

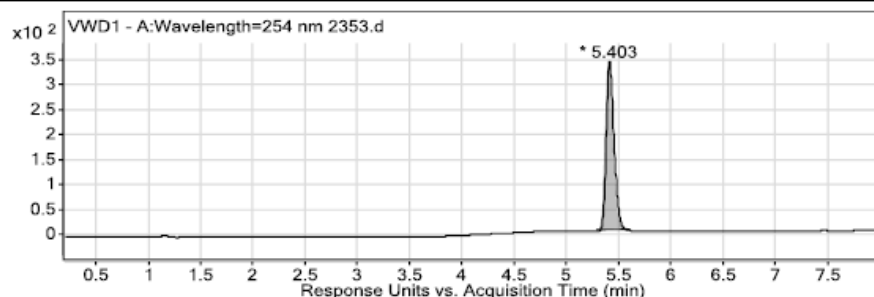
Mass	Intens.	Rel.Int(%)		Mass	*** Graphic ***	
128	68	6.81		128	*	6.81
129	50	5.01		129	*	5.01
156	86	8.61		156	*	8.61
184	999	100.00		184	*****	100.00
185	132	13.21		185	**	13.21
198	9	0.90	-->	198		0.90
200	17	1.70	-->	200		1.70
228	81	8.11	-->	228	*	8.11
229	12	1.20	-->	229		1.20
243	108	10.81	mol.mass:	243	**	10.81
244	15	1.50	-->	244		1.50

Figure 28. Mass-spectra of compound 12a.

Figure 29. NMR ¹H spectra of compound 12b.Figure 30. NMR ¹³C spectra of compound 12b.

Data Filename	2353.d	Sample Name	
Sample Type	Sample	Position	Vial 12
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	1/11/2022 3:23:20 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

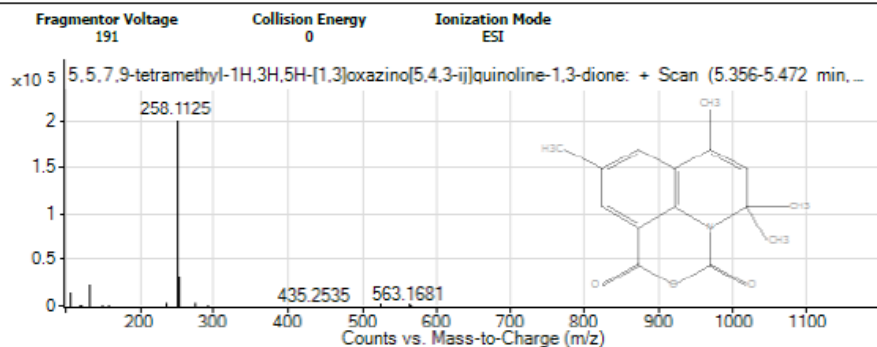
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	5.287	5.403	5.613	337.7	1755.63	100

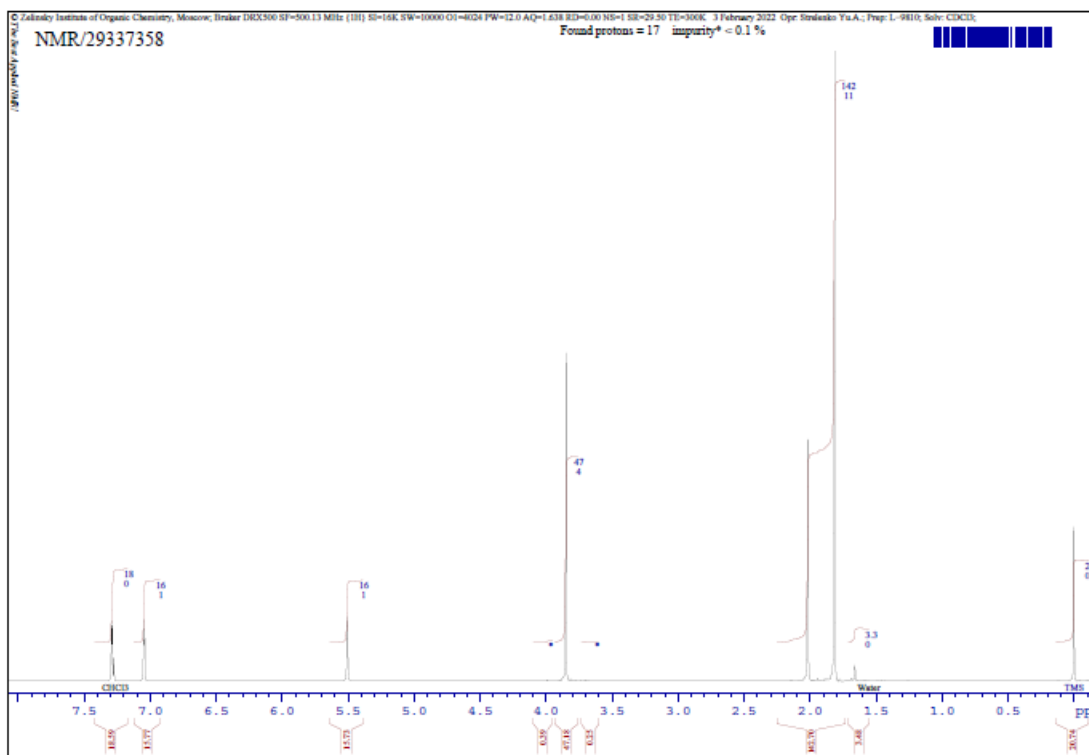
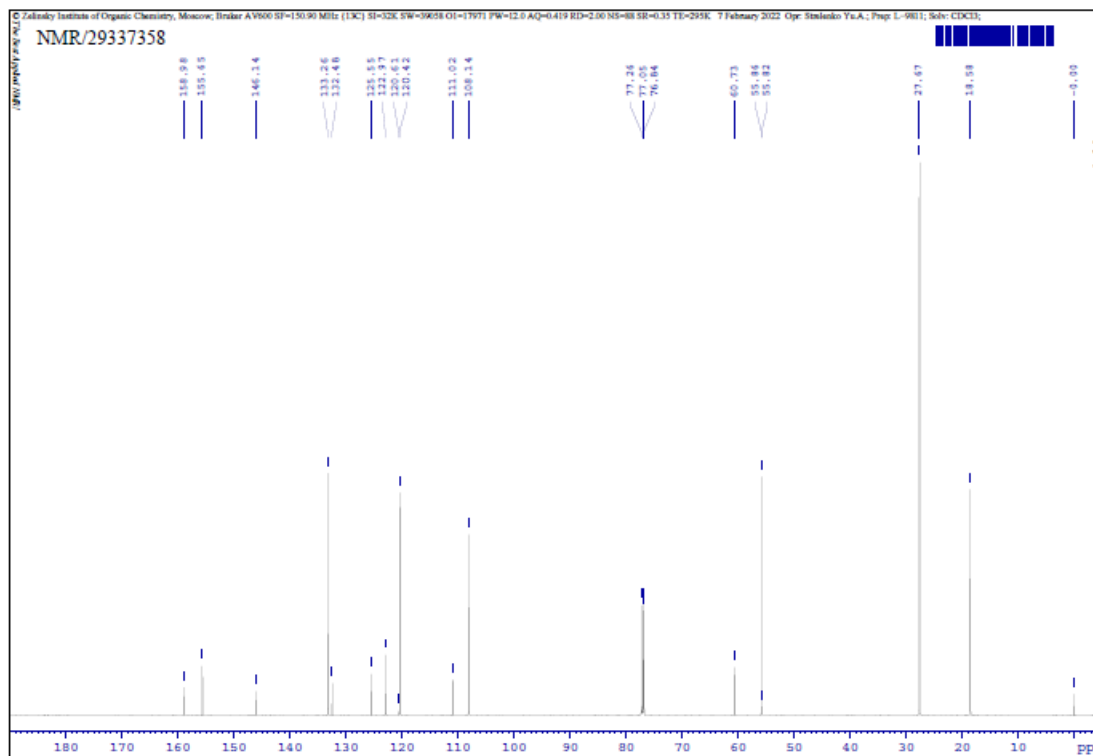
User Spectra

Figure 31. HPLC-HRMS-ESI spectra of compound **12b**.

Mass spectrum NMR/24267932: formula C₁₅H₁₅NO₃, mol. mass 257.29
 Max intensity: 999 for mass 198
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

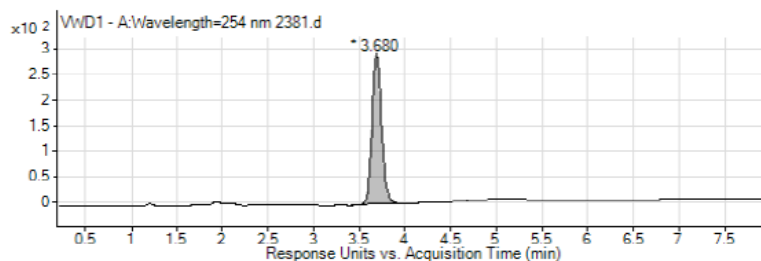
Mass	Intens.	Rel.Int (%)	Mass	*** Graphic ***	Rel.Int (%)
39	65	6.51	39	*	6.51
115	86	8.61	115	*	8.61
127	72	7.21	127	*	7.21
128	121	12.11	128	**	12.11
154	51	5.11	154	*	5.11
198	999	100.00	198	*****	100.00
199	142	14.21	199	**	14.21
212	8	0.80	212		0.80
242	39	3.90	242		3.90
257	65	6.51	257	*	6.51
258	9	0.90	258		0.90

Figure 32. Mass-spectra of compound **12b**.

Figure 33. NMR ^1H spectra of compound 12c.Figure 34. NMR ^{13}C spectra of compound 12c.

Data Filename	2381.d	Sample Name	
Sample Type	Sample	Position	Vial 92
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	1/21/2022 11:31:21 AM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	3.417	3.68	4.023	297.15	2181.31	100

User Spectra

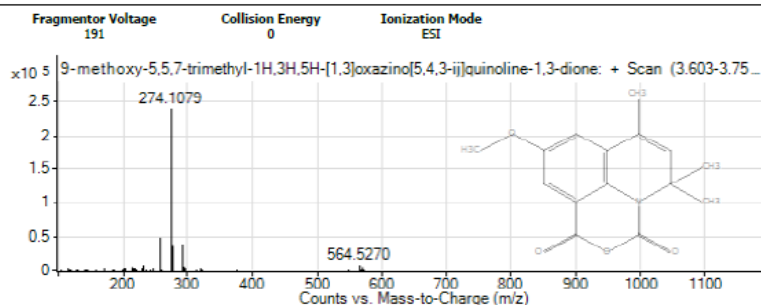
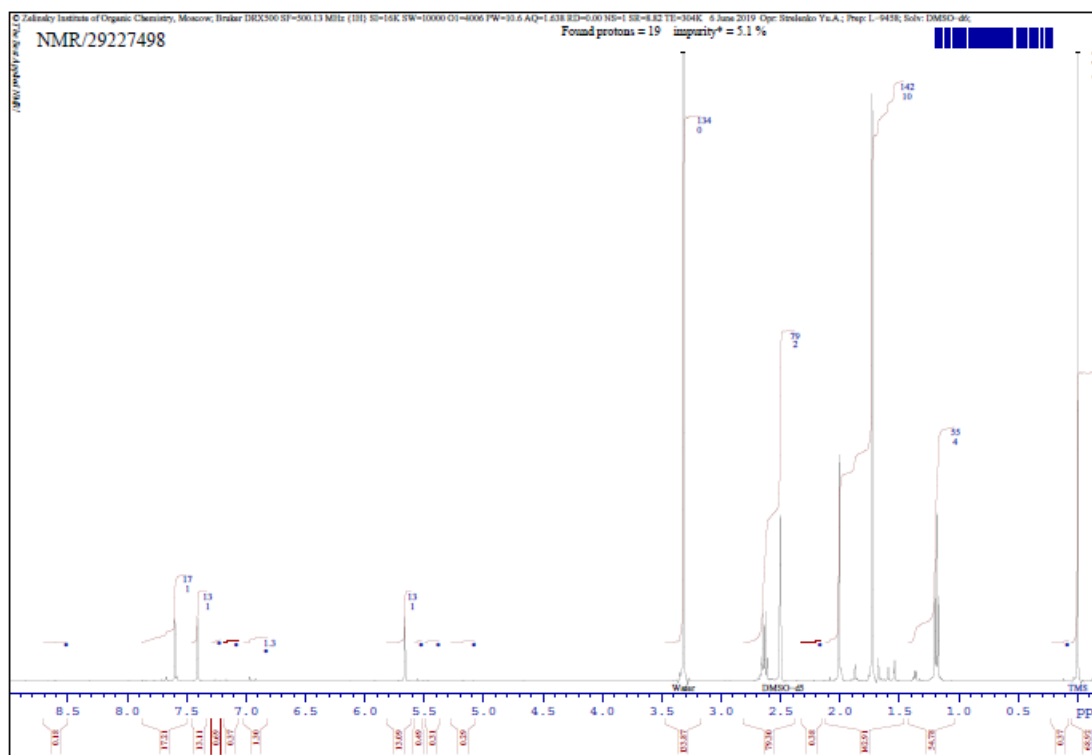
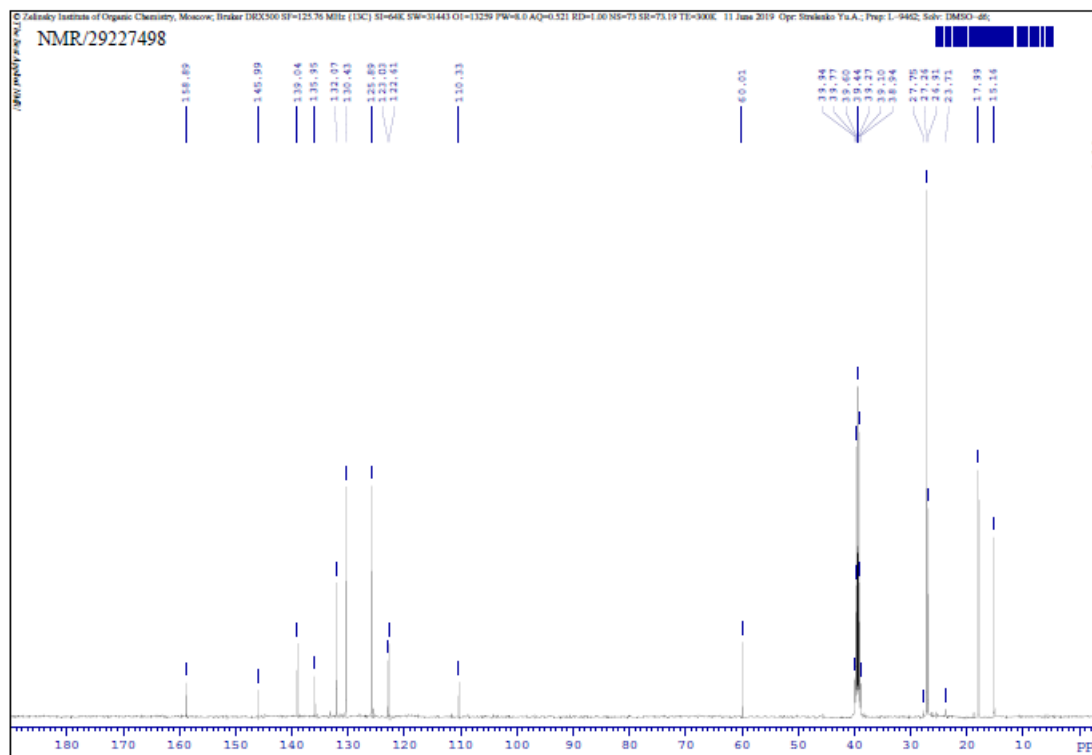


Figure 35. HPLC-HRMS-ESI spectra of compound 12c.

Mass spectrum NMR/24267929: formula C₁₅H₁₅NO₄, mol. mass 273.28
 Max intensity: 999 for mass 214
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

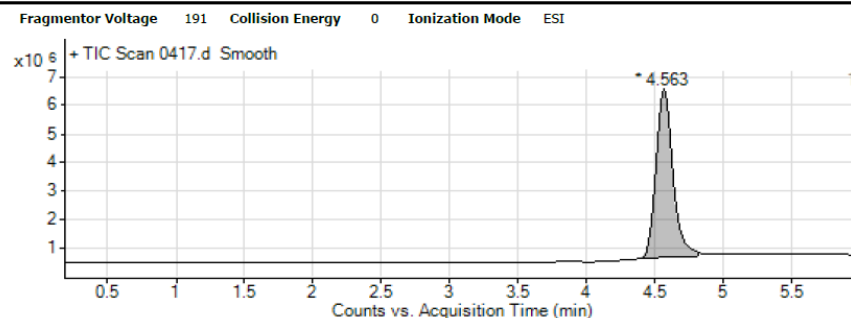
Mass	Intens.	Rel.Int (%)		Mass	*** Graphic ***	
27	126	12.61		27	**	12.61
39	51	5.11		39	*	5.11
144	94	9.41		144	*	9.41
170	53	5.31		170	*	5.31
186	105	10.51		186	**	10.51
187	5	0.50	-->	187		0.50
200	75	7.51	-->	200	*	7.51
214	999	100.00	-->	214	*****	100.00
215	121	12.11	-->	215	**	12.11
228	9	0.90	-->	228		0.90
229	818	81.88	mol.mass:	229	***	14.61
273	113	11.31	-->	273	**	11.31
274	11	1.10	-->	274		1.10

Figure 36. Mass-spectra of compound 12c.

Figure 37. NMR ^1H spectra of compound **12d**.Figure 38. NMR ^{13}C spectra of compound **12d**.

Data Filename	0417.d	Sample Name	
Sample Type	Sample	Position	Vial 14
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	9/29/2020 2:24:01 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

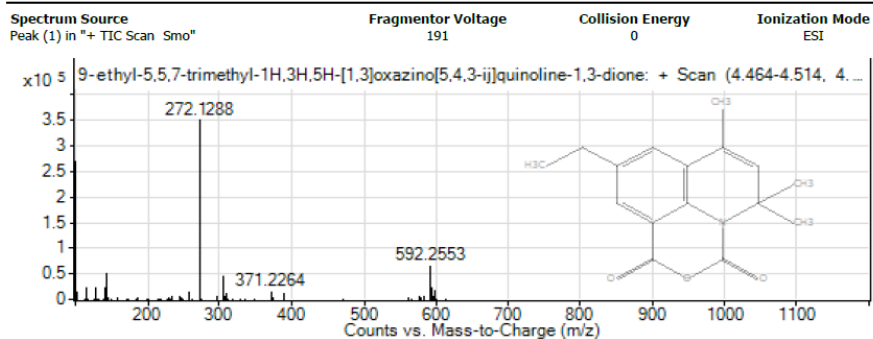
User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.381	4.563	4.812	5932631.91	49620708.99	100

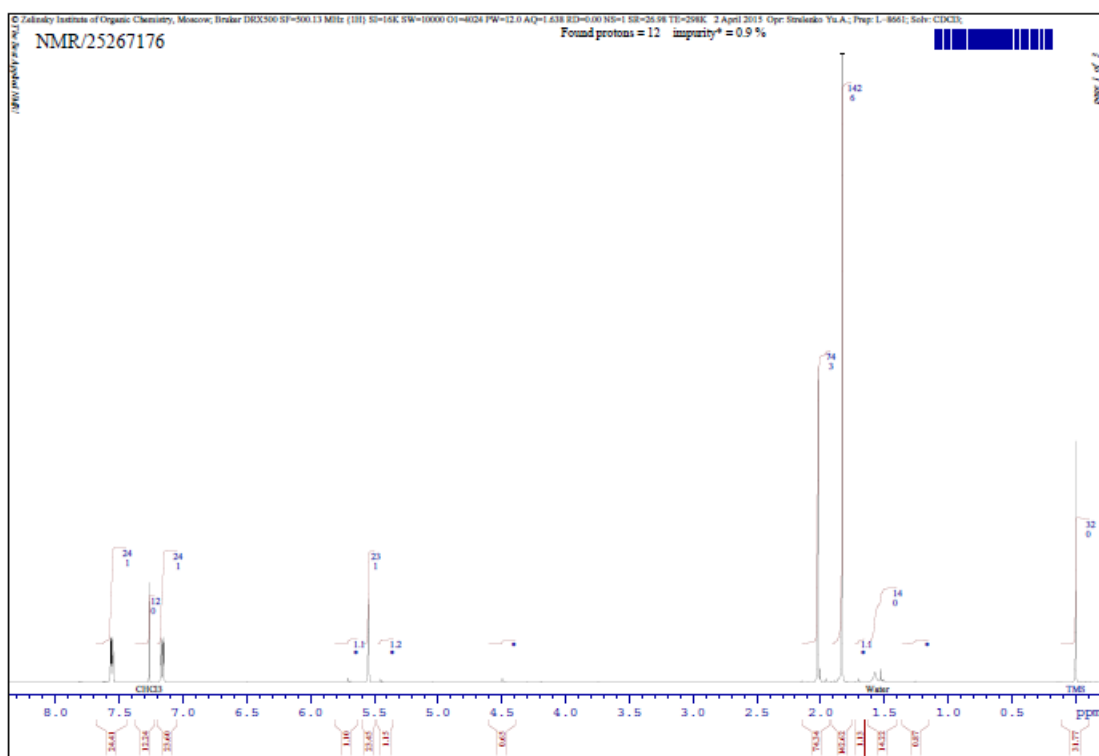
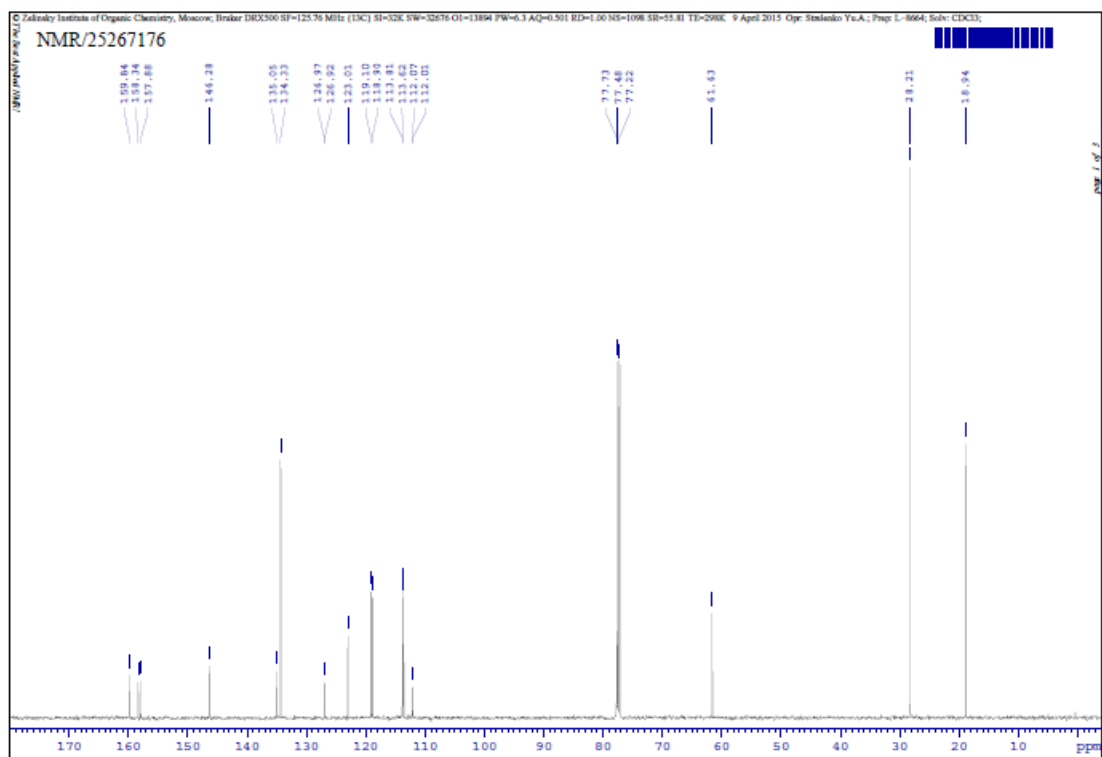
User Spectra

Figure 39. HPLC-HRMS-ESI spectra of compound **12d**.

Mass spectrum NMR/24267930: formula C₁₆H₁₇NO₃, mol. mass 271.31
 Max intensity: 999 for mass 212
 Discrimination level for relative intensity: 5.0%,
 within the interval of (molecular mass+50): 0.5% (marked with -->)
 One symbol '*' on graphic = 5% of maximum relative intensity

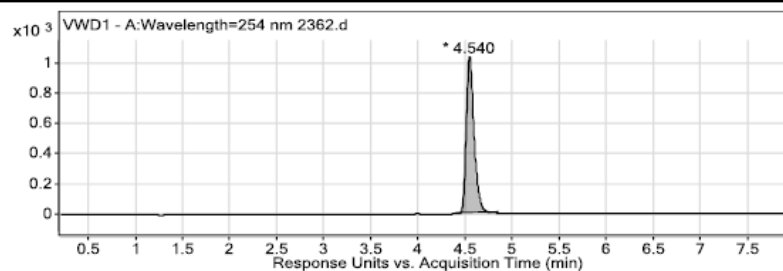
Mass	Intens.	Rel.Int(%)		Mass	*** Graphic ***	
27	76	7.61		27	*	7.61
39	142	14.21		39	**	14.21
128	61	6.11		128	*	6.11
144	55	5.51		144	*	5.51
184	65	6.51		184	*	6.51
212	999	100.00	-->	212	*****	100.00
213	160	16.02	-->	213	***	16.02
214	15	1.50	-->	214		1.50
216	11	1.10	-->	216		1.10
227	341	34.13	-->	227	*****	34.13
228	51	5.11	-->	228	*	5.11
230	15	1.50	-->	230		1.50
271	103	10.31	-->	271	**	10.31
272	12	1.20	-->	272		1.20

Figure 40. Mass-spectra of compound **12d**.

Figure 41. NMR ¹H spectra of compound **12e**.Figure 42. NMR ¹³C spectra of compound **12e**.

Data Filename	2362.d	Sample Name	
Sample Type	Sample	Position	Vial 21
Instrument Name	Instrument 1	User Name	
Acq Method	ACN-H2O_60-40.m	Acquired Time	1/11/2022 5:19:43 PM
IRM Calibration Status	Success	DA Method	111.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Chromatograms



Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	4.403	4.54	4.86	1041.26	5948.94	100

User Spectra

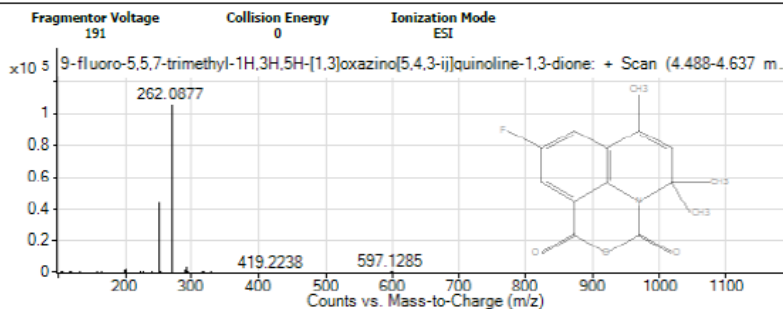


Figure 43. HPLC-HRMS-ESI spectra of compound 12e.

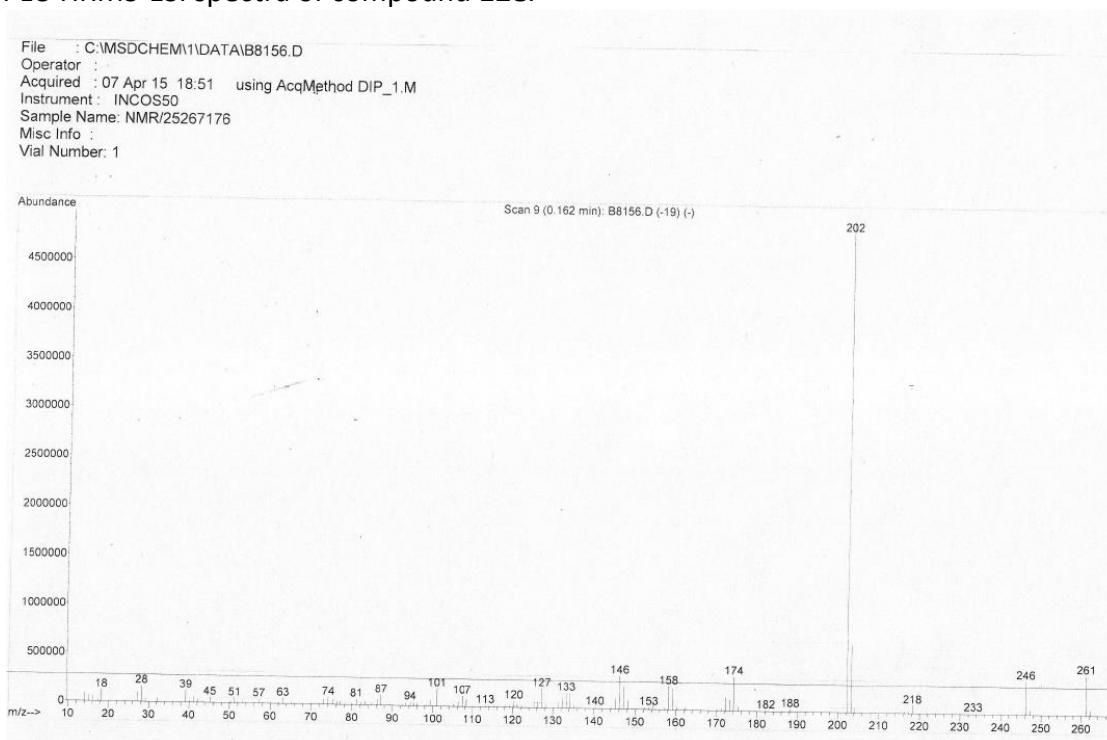


Figure 44. Mass-spectra of compound 12e.

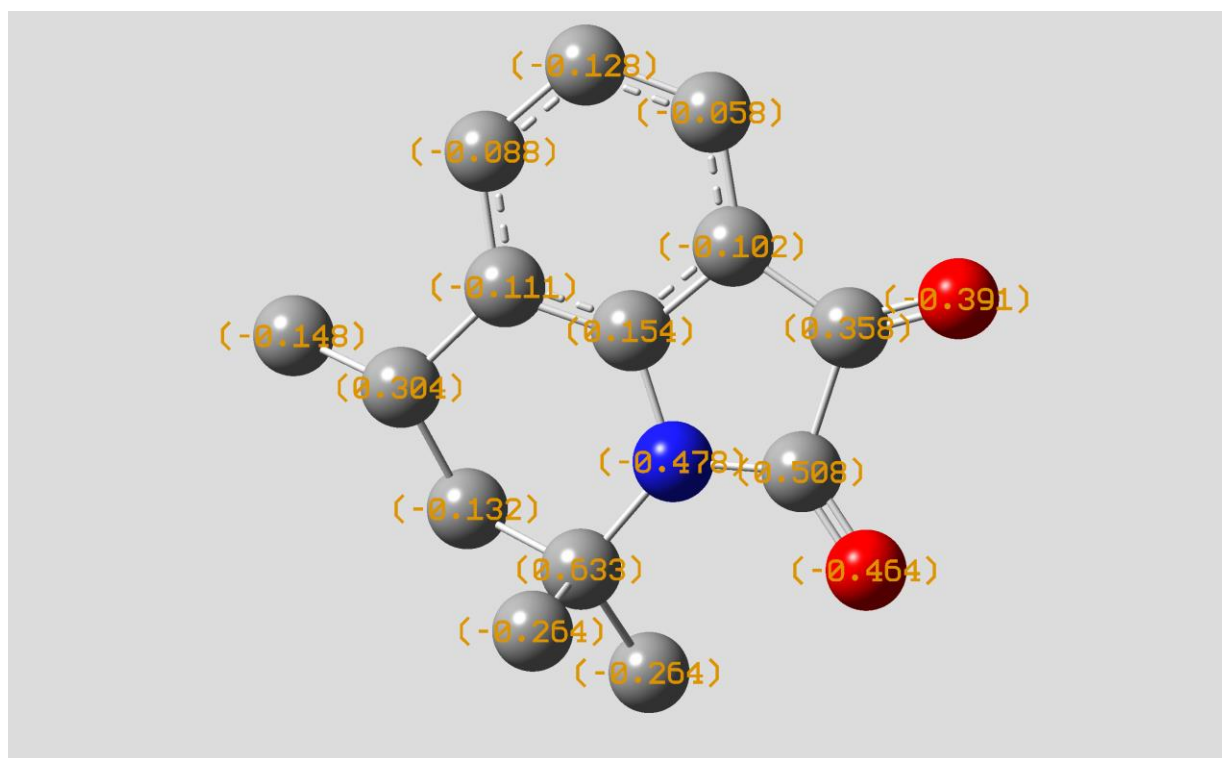


Figure 45. Calculated atomic charges according to CHELPG on the atoms of compound 10a.

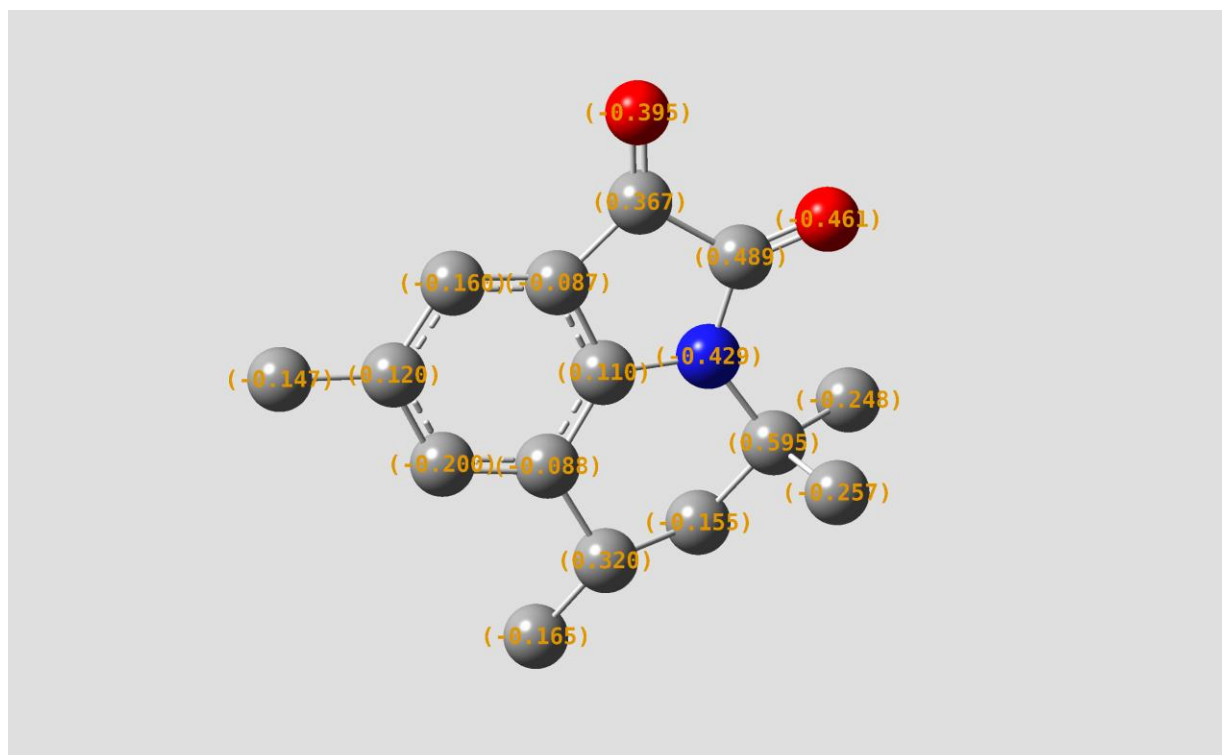


Figure 46. Calculated atomic charges according to CHELPG on the atoms of compound 10b.

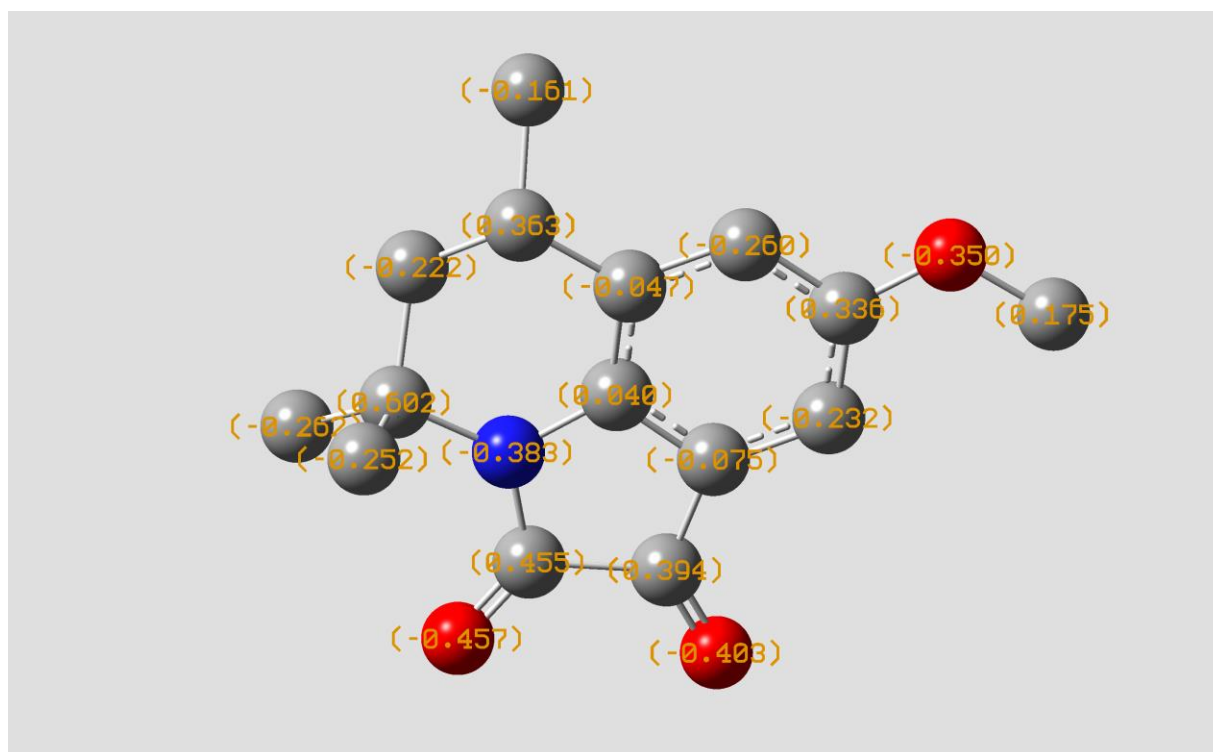


Figure 47. Calculated atomic charges according to CHELPG on the atoms of compound 10c.

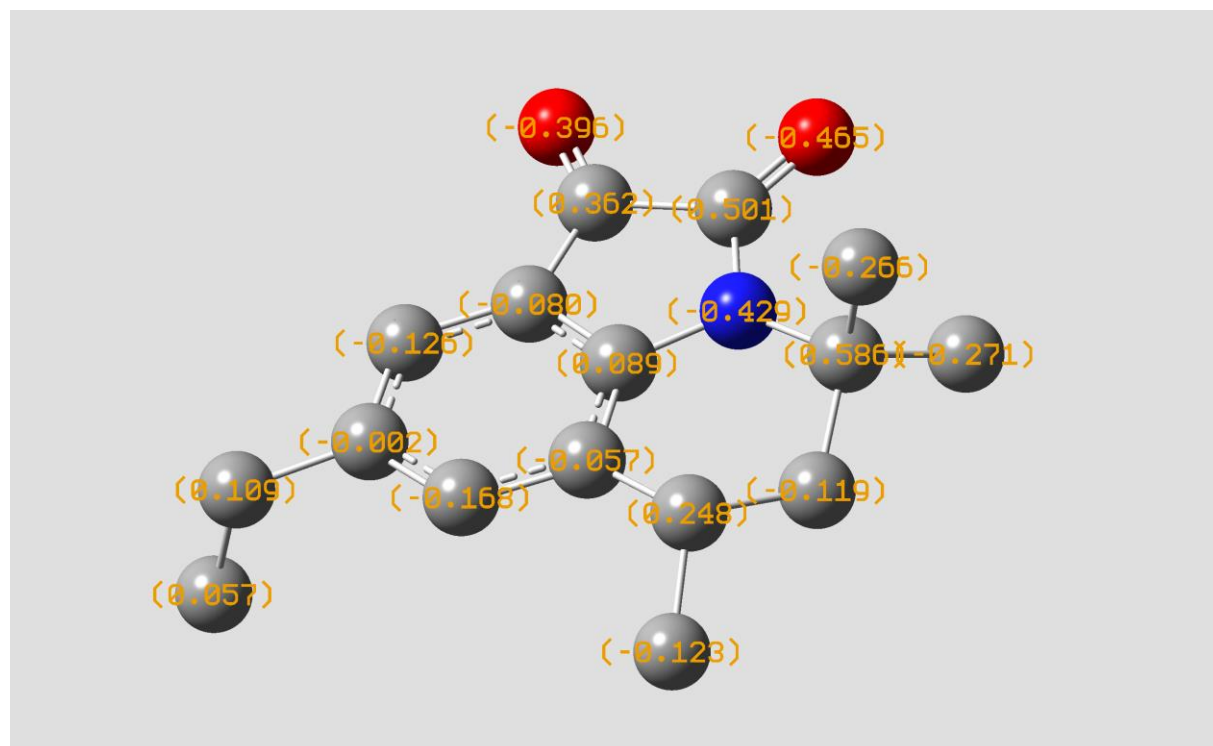


Figure 48. Calculated atomic charges according to CHELPG on the atoms of compound 10d.

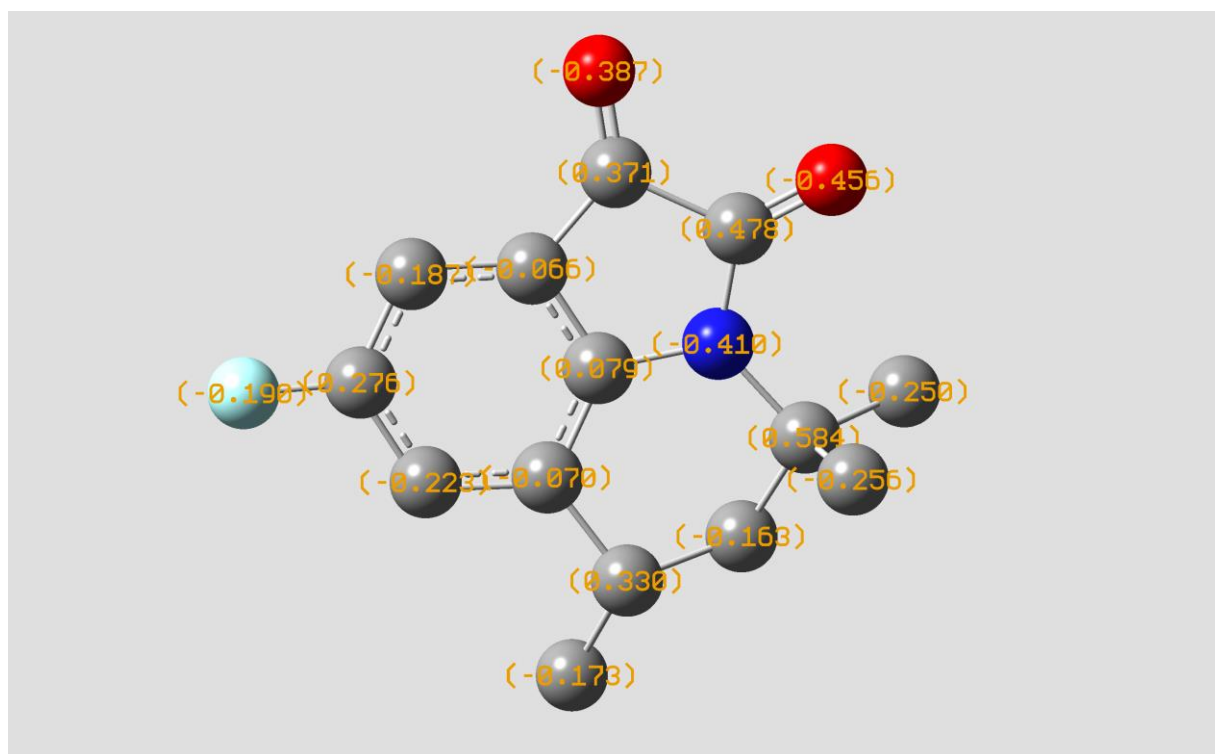


Figure 49. Calculated atomic charges according to CHELPG on the atoms of compound 10e.

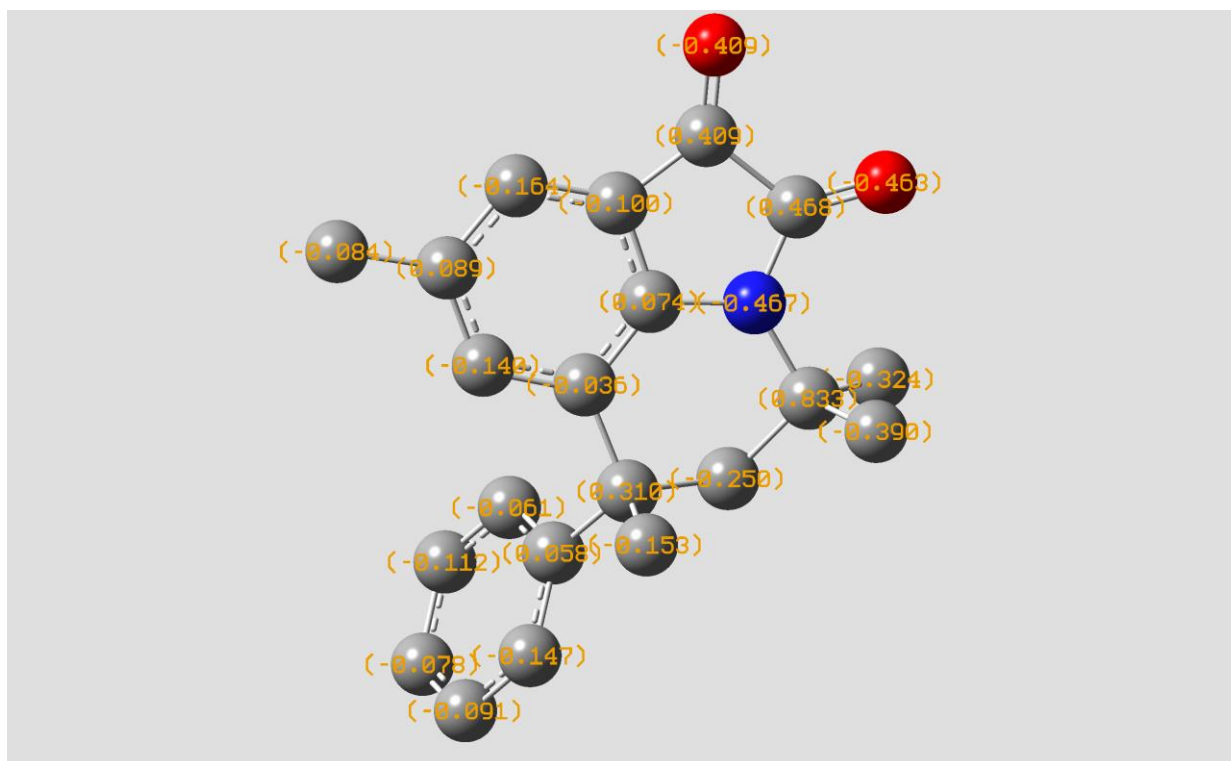


Figure 50. Calculated atomic charges according to CHELPG on the atoms of compound 10f.

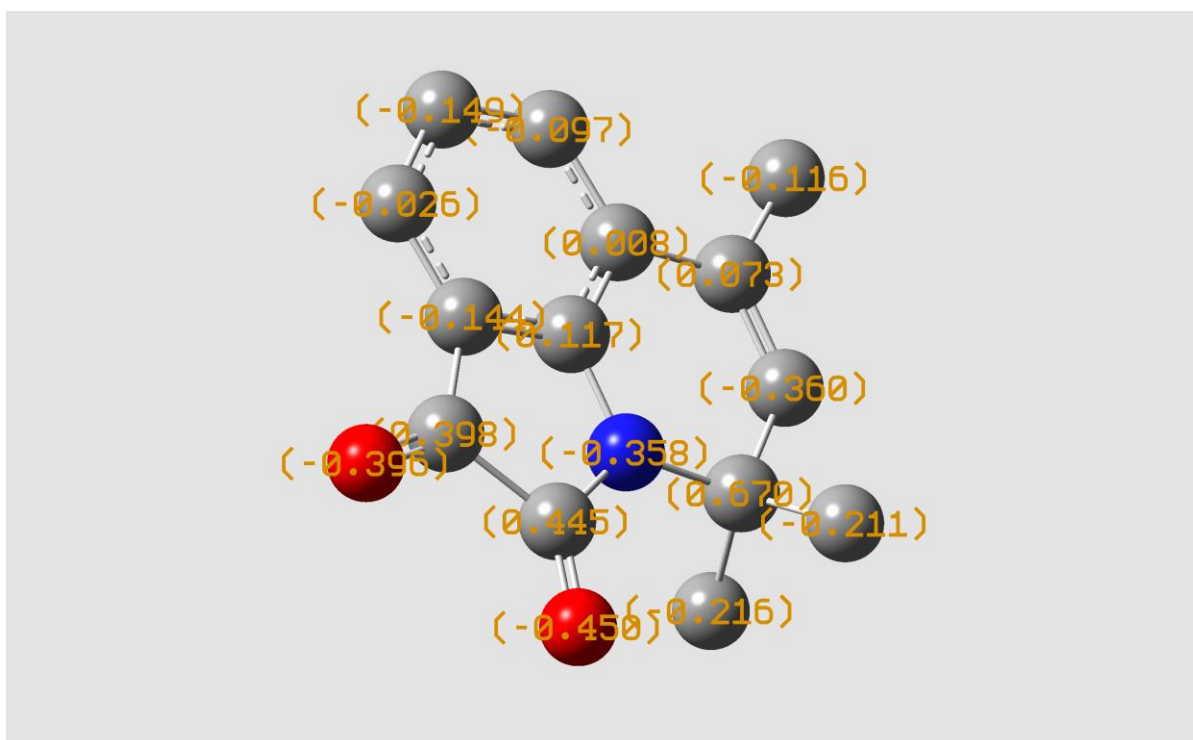


Figure 51. Calculated atomic charges according to CHELPG on the atoms of compound **12a**.

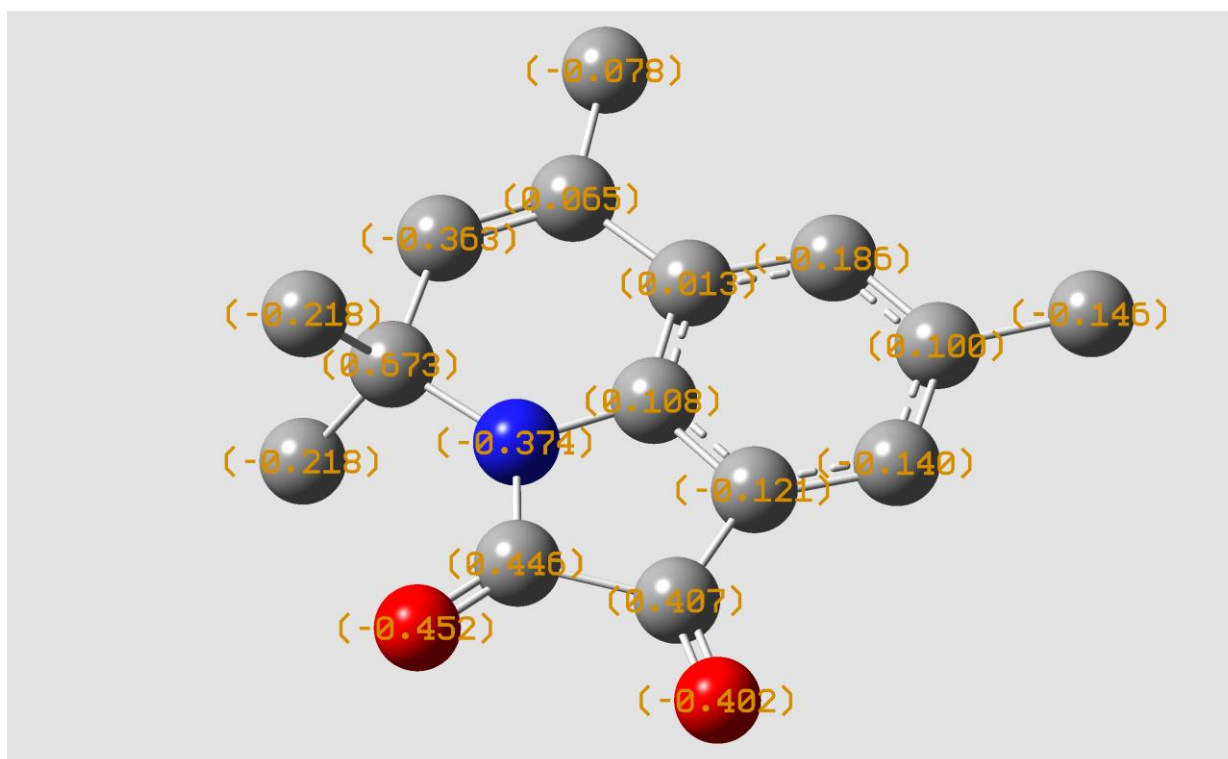


Figure 52. Calculated atomic charges according to CHELPG on the atoms of compound **12b**.

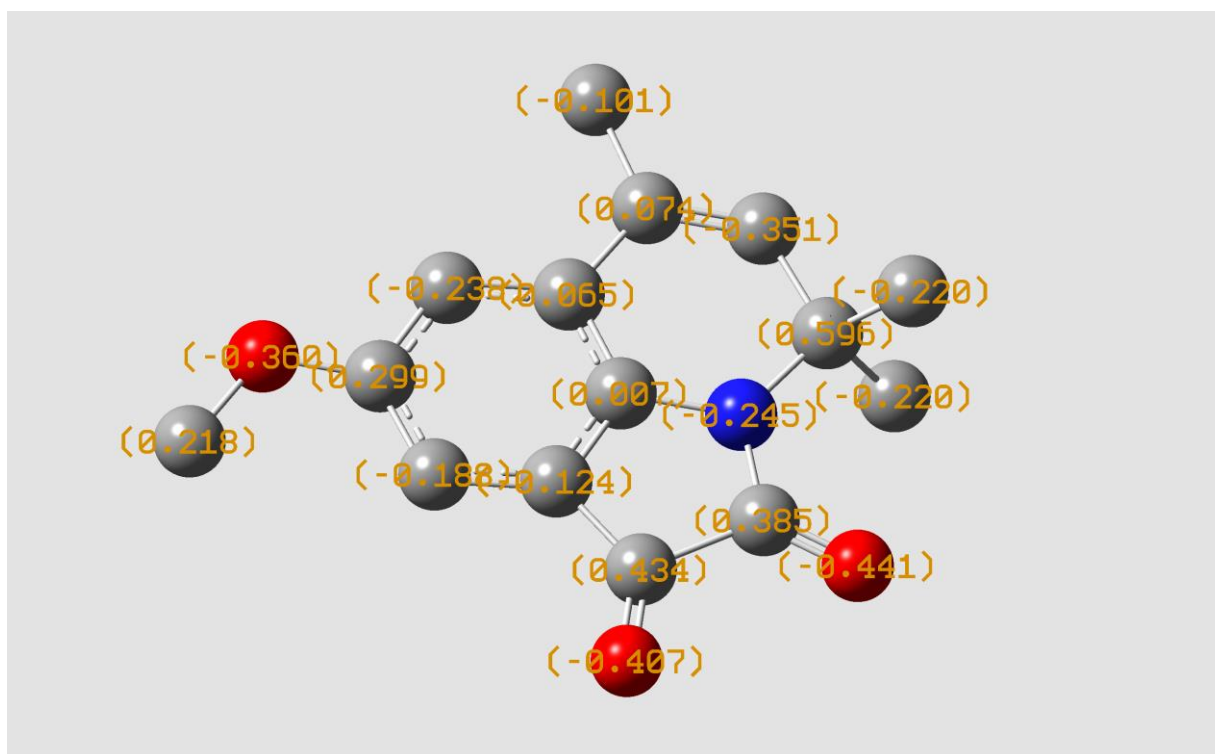


Figure 53. Calculated atomic charges according to CHELPG on the atoms of compound 12c.

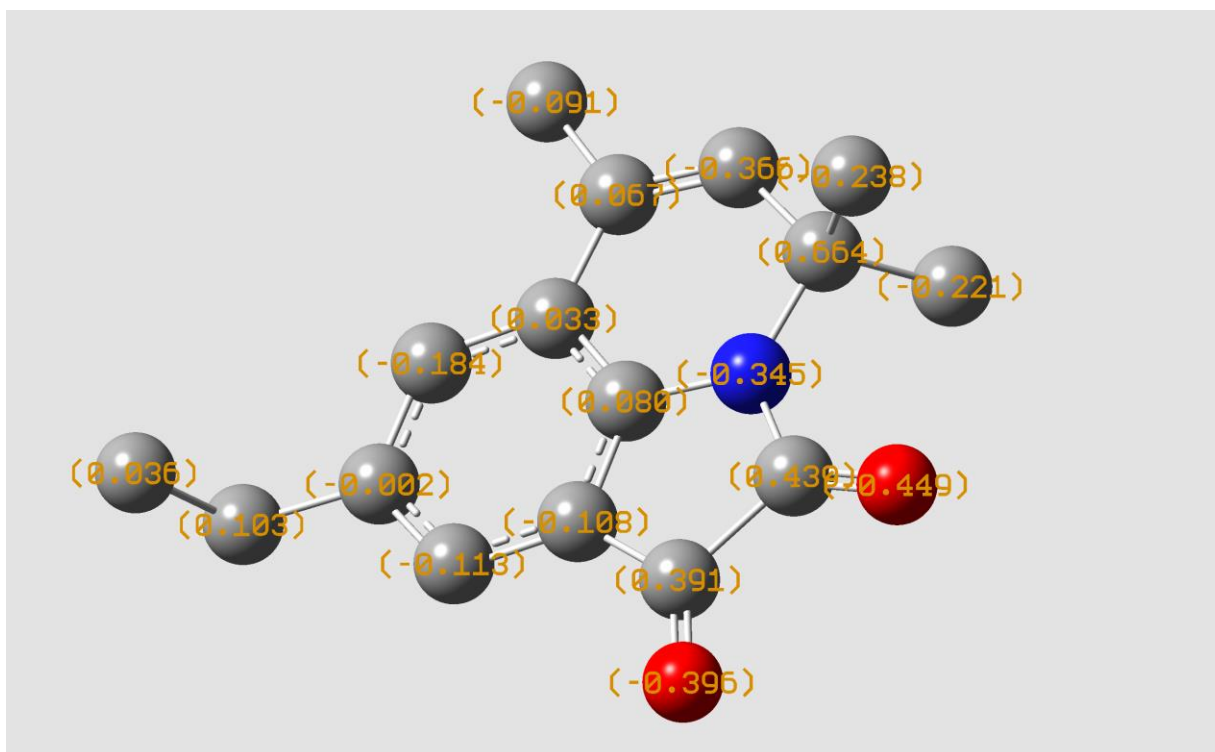


Figure 54. Calculated atomic charges according to CHELPG on the atoms of compound 12d.

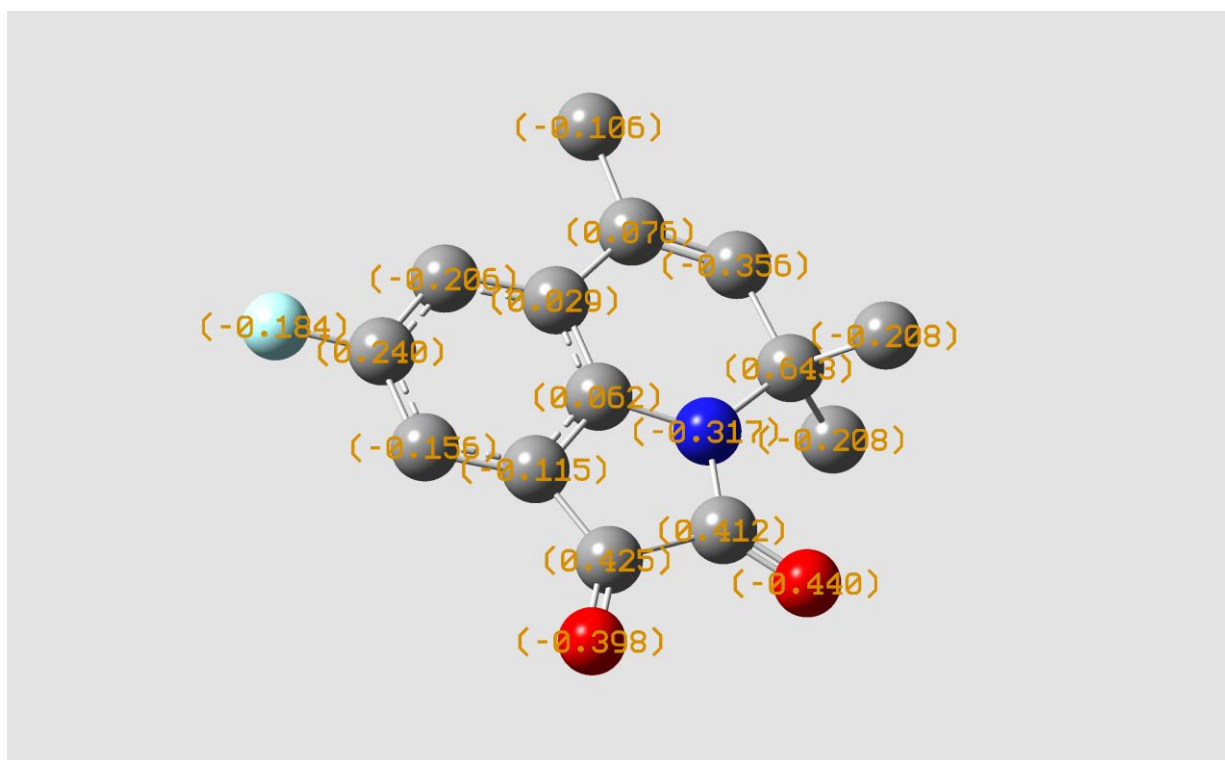


Figure 55. Calculated atomic charges according to CHELPG on the atoms of compound **12e**.