# 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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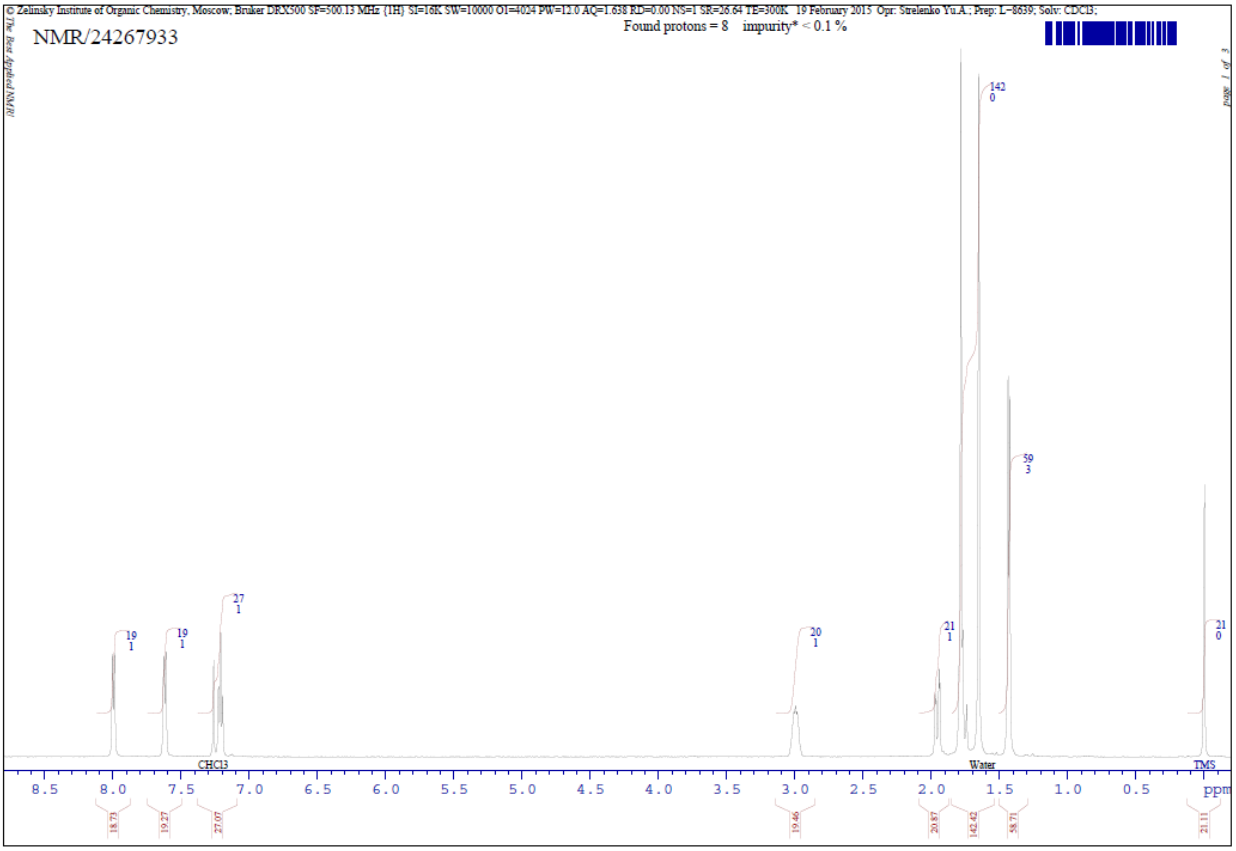



**Figure 1**. NMR $^{1}$H spectra of compound **10a**.

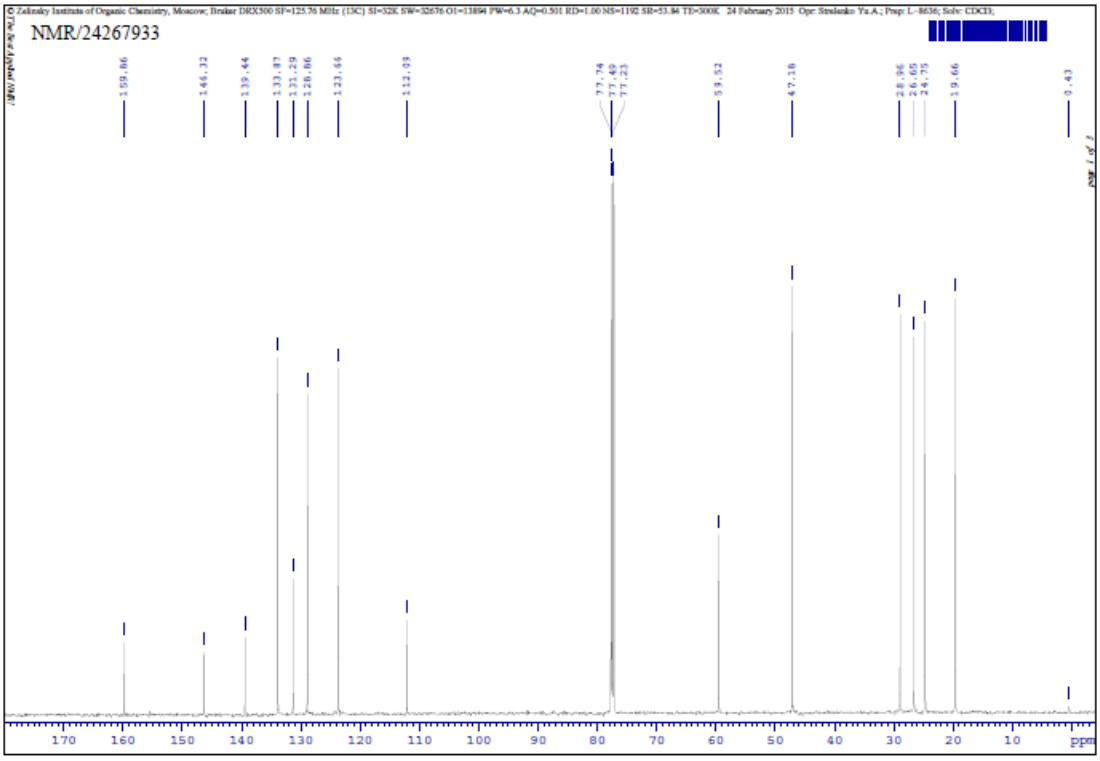



**Figure 2**. NMR $^{13}$C spectra of compound **10a**.

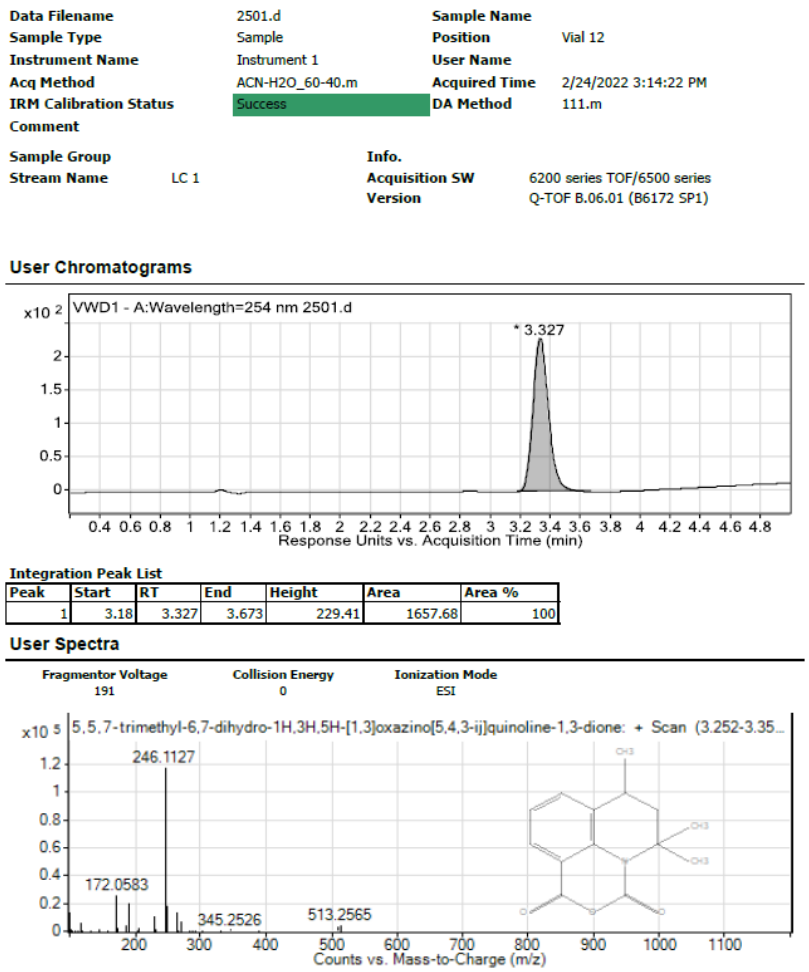



**Figure 3**. HPLC-HRMS-ESI spectra of compound **10a**.

```
    Mass spectrum  NMR/24267933: formula C14H15NO3, mol. mass 245.28
    Max intensity: 999 for mass 186
    Discrimination level for relative intensity: 5.0%,
    whithin 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  mol.mass:   245  ***                     18.52
    246       29      2.90        -->   246                          2.90
```

**Figure 4**. Mass-spectra of compound **10a**.

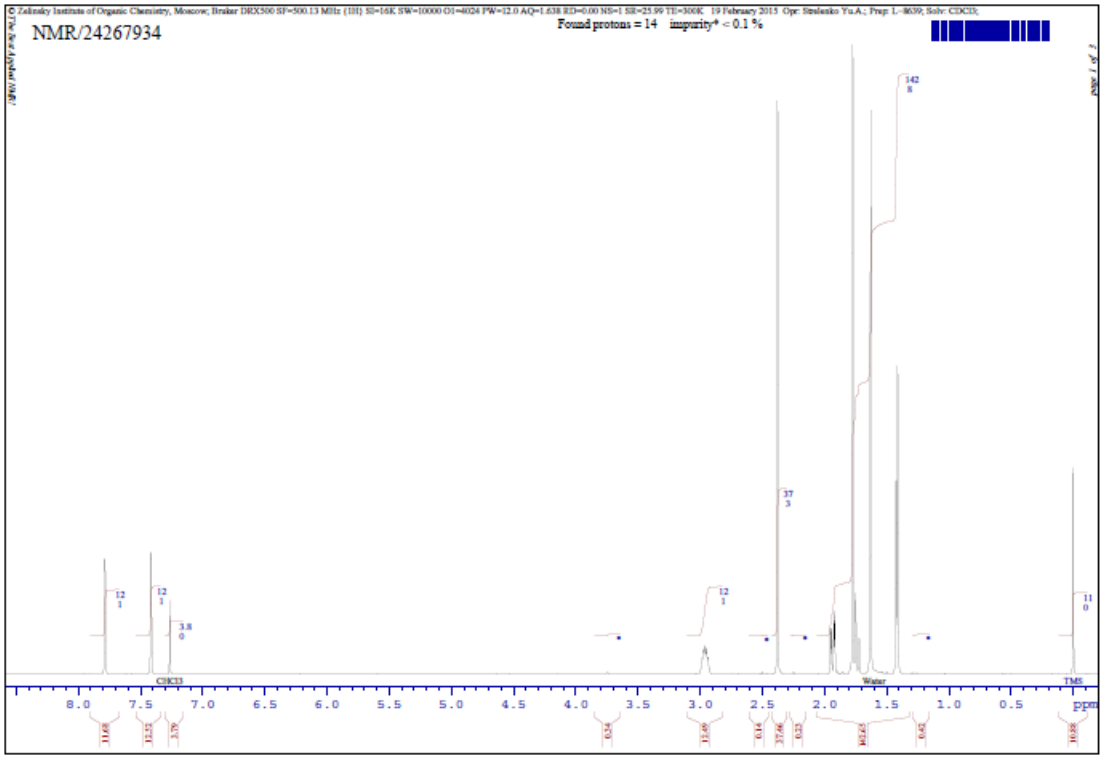



**Figure 5**. NMR $^{1}$H spectra of compound **10b**.

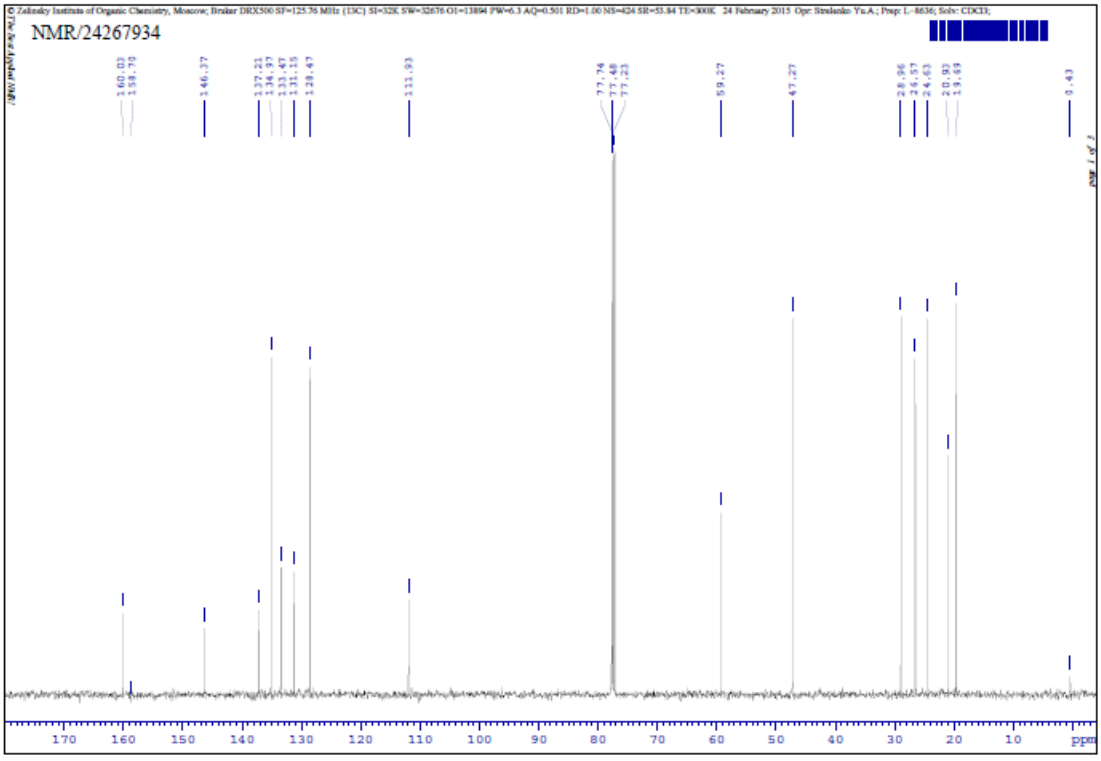
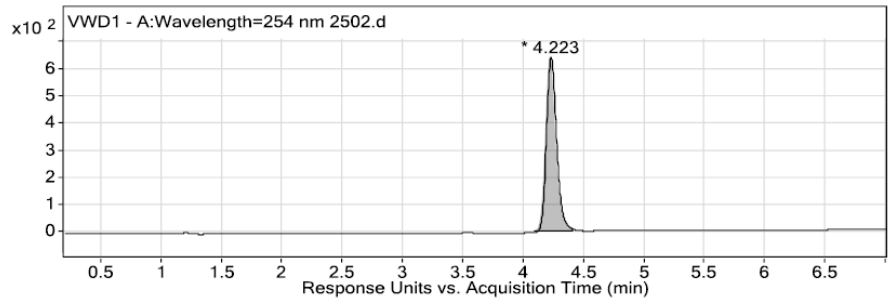



**Figure 6**. NMR $^{13}$C spectra of compound **10b**.

| | | | |
|---|---|---|---|
| **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 Version** | 6200 series TOF/6500 series 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**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 191 | 0 | ESI |

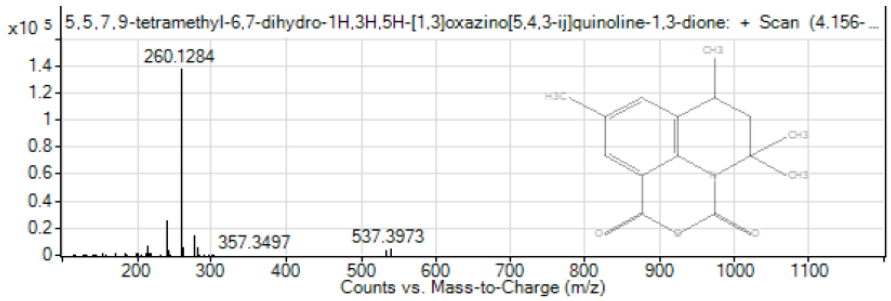



**Figure 7**. HPLC-HRMS-ESI spectra of compound **10b**.

```
Mass spectrum  NMR/24267934: formula C15H17NO3, mol. mass 259.30
Max intensity: 999 for mass 200
Discrimination level for relative intensity: 5.0%,
whithin 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(%)
   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**.

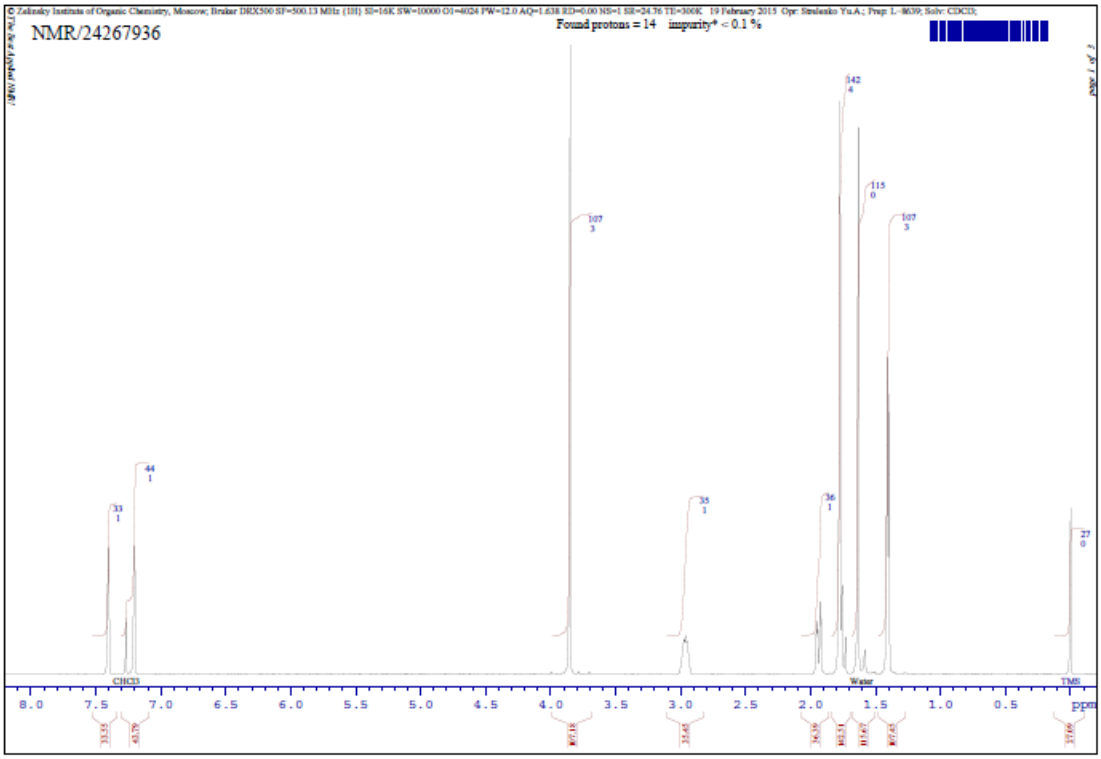



**Figure 9**. NMR $^{1}$H spectra of compound **10c**.

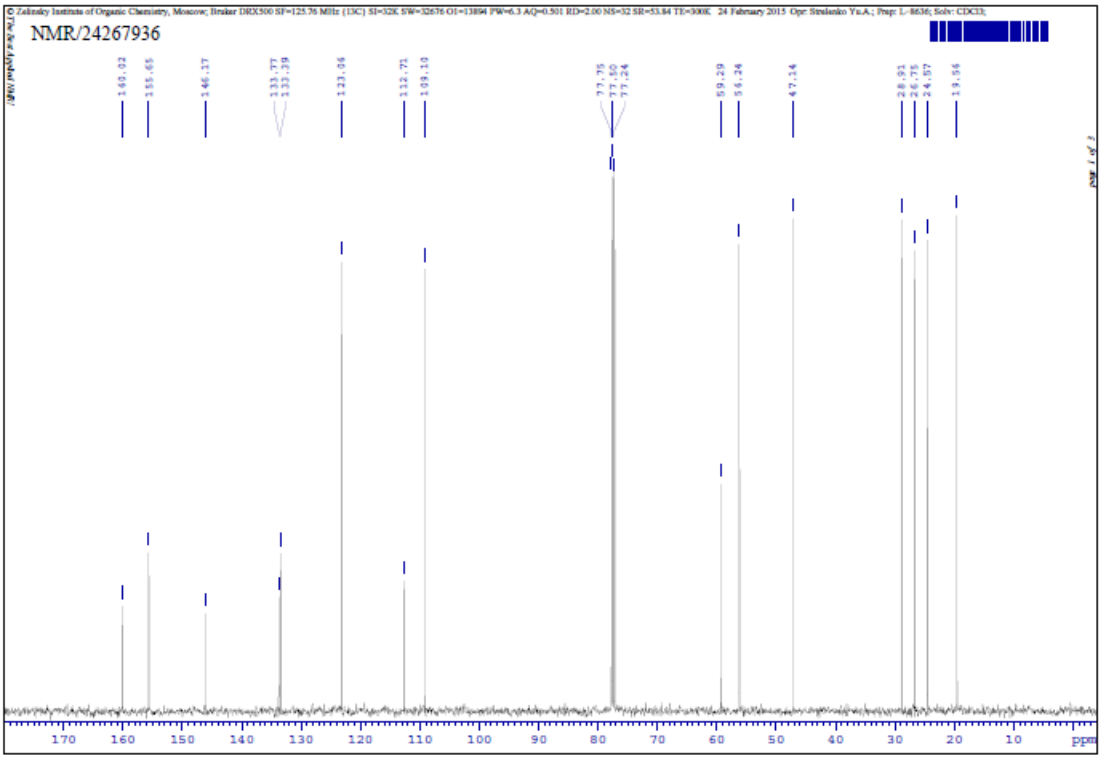
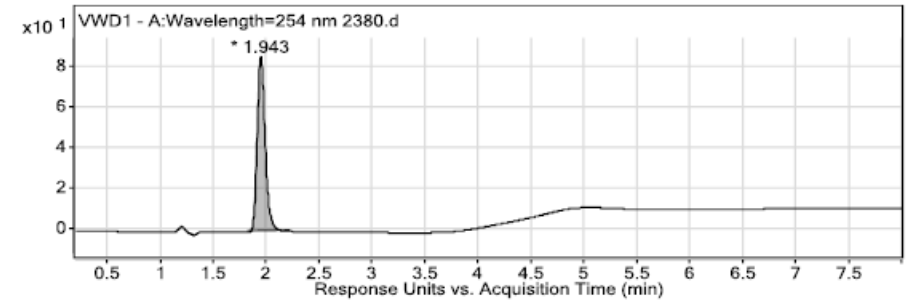



**Figure 10**. NMR $^{13}$C spectra of compound **10c**.

| | | | |
|---|---|---|---|
| **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 Version** | 6200 series TOF/6500 series 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**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 191 | 0 | ESI |

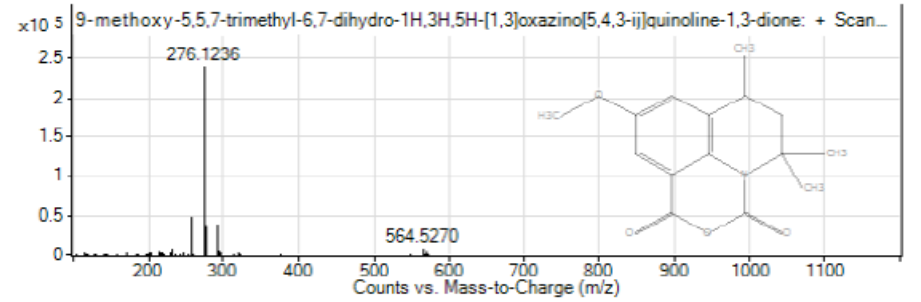



**Figure 11**. HPLC-HRMS-ESI spectra of compound **10c**.

```
Mass spectrum  NMR/24267936: formula C15H17NO4, mol. mass 275.30
Max intensity: 999 for mass 216
Discrimination level for relative intensity: 5.0%,
whithin 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(%)
   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**.

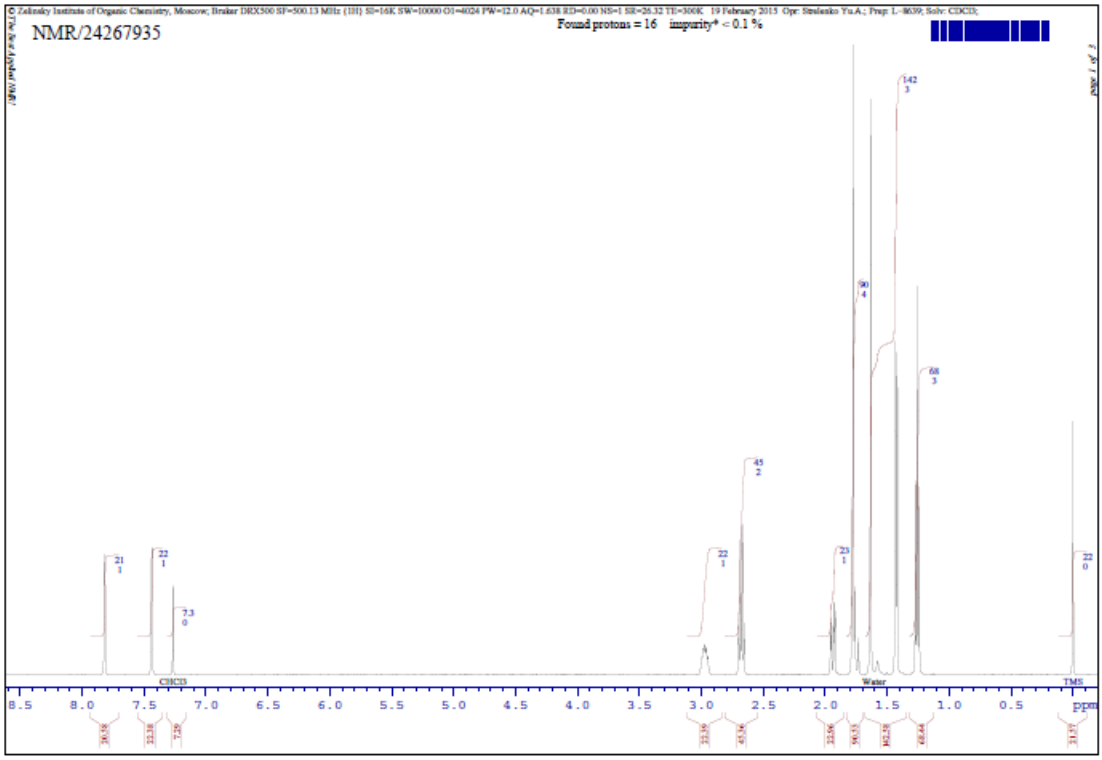



**Figure 13**. NMR $^{1}$H spectra of compound **10d**.

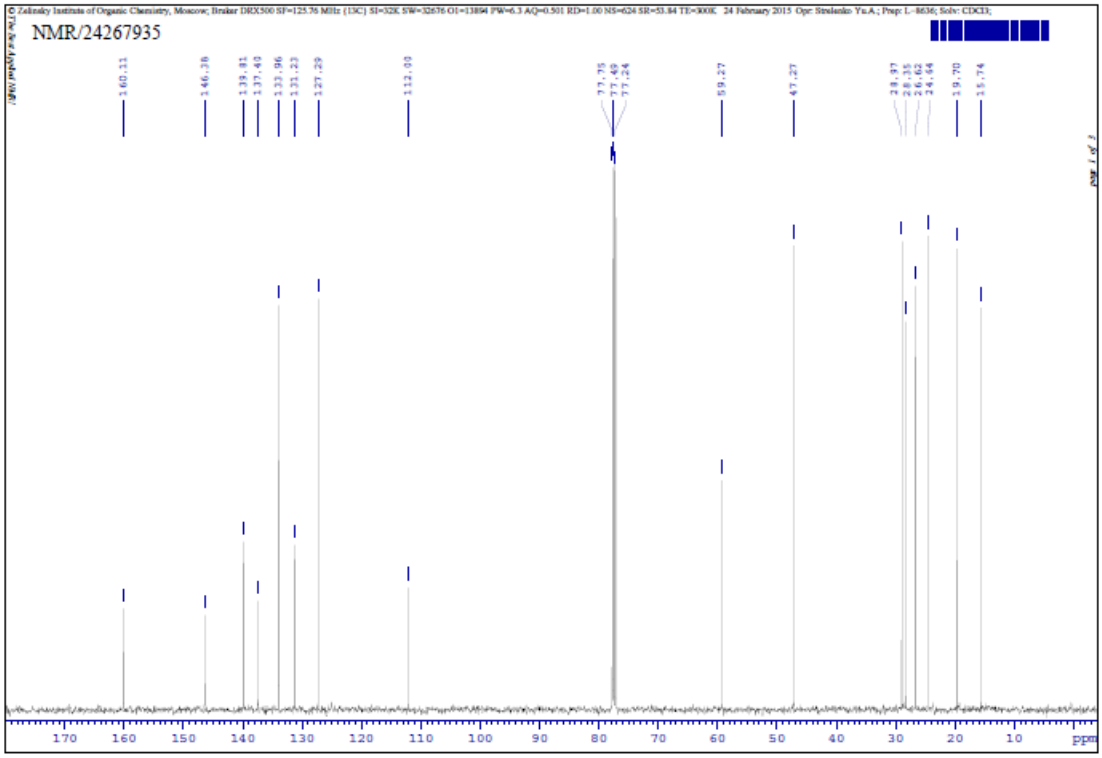
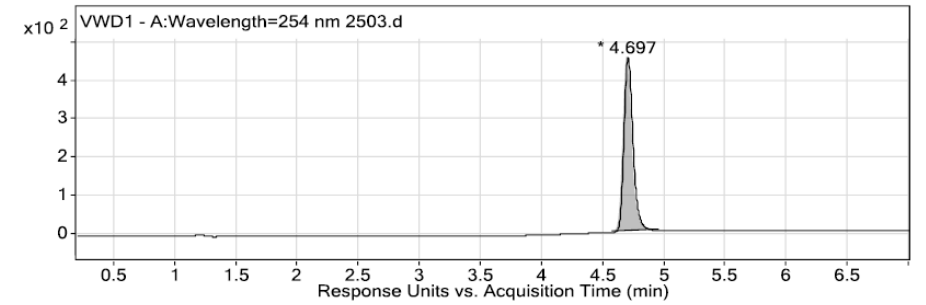



**Figure 14**. NMR $^{13}$C spectra of compound **10d**.

| | | | |
|---|---|---|---|
| **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 Version** | 6200 series TOF/6500 series 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**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 191 | 0 | ESI |

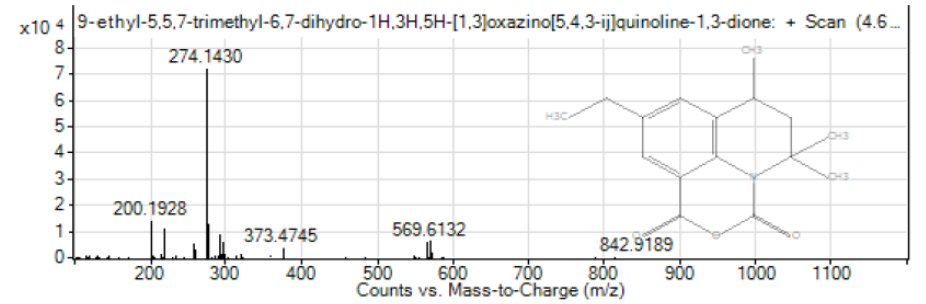



**Figure 15**. HPLC-HRMS-ESI spectra of compound **10d**.

```
Mass spectrum  NMR/24267935: formula C16H19NO3, mol. mass 273.33
Max intensity: 999 for mass 214
Discrimination level for relative intensity: 5.0%,
whithin 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(%)
    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**.

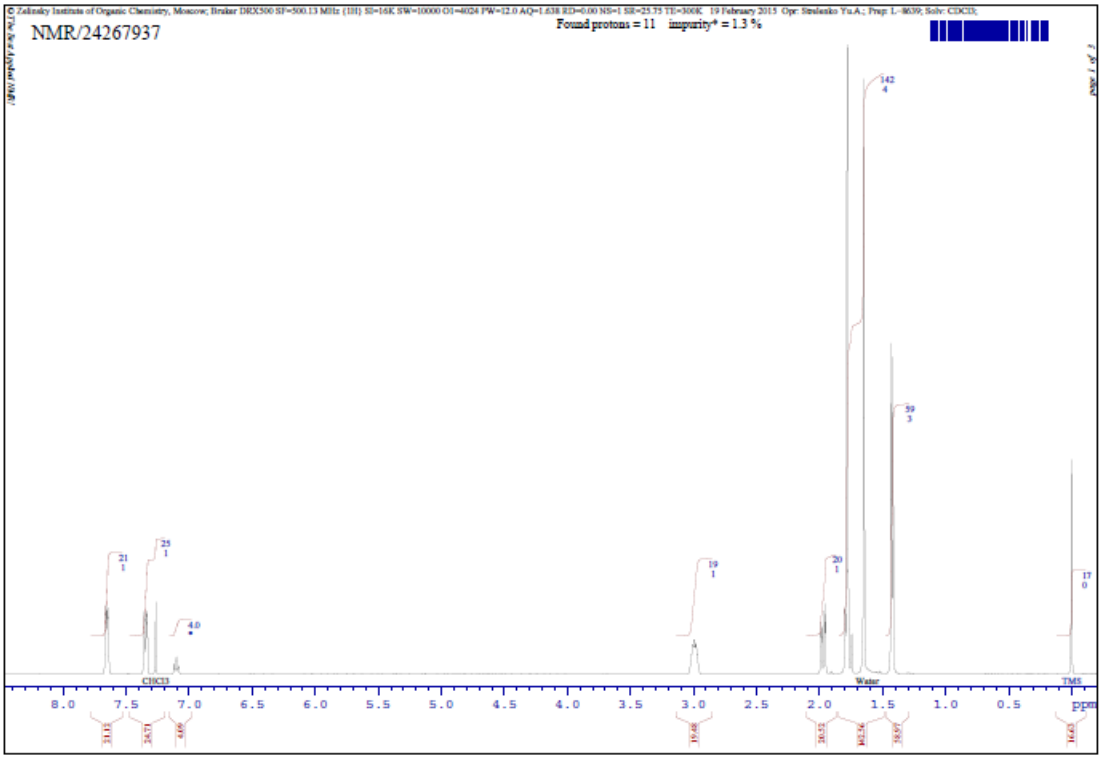



**Figure 17**. NMR $^{1}$H spectra of compound **10e**.

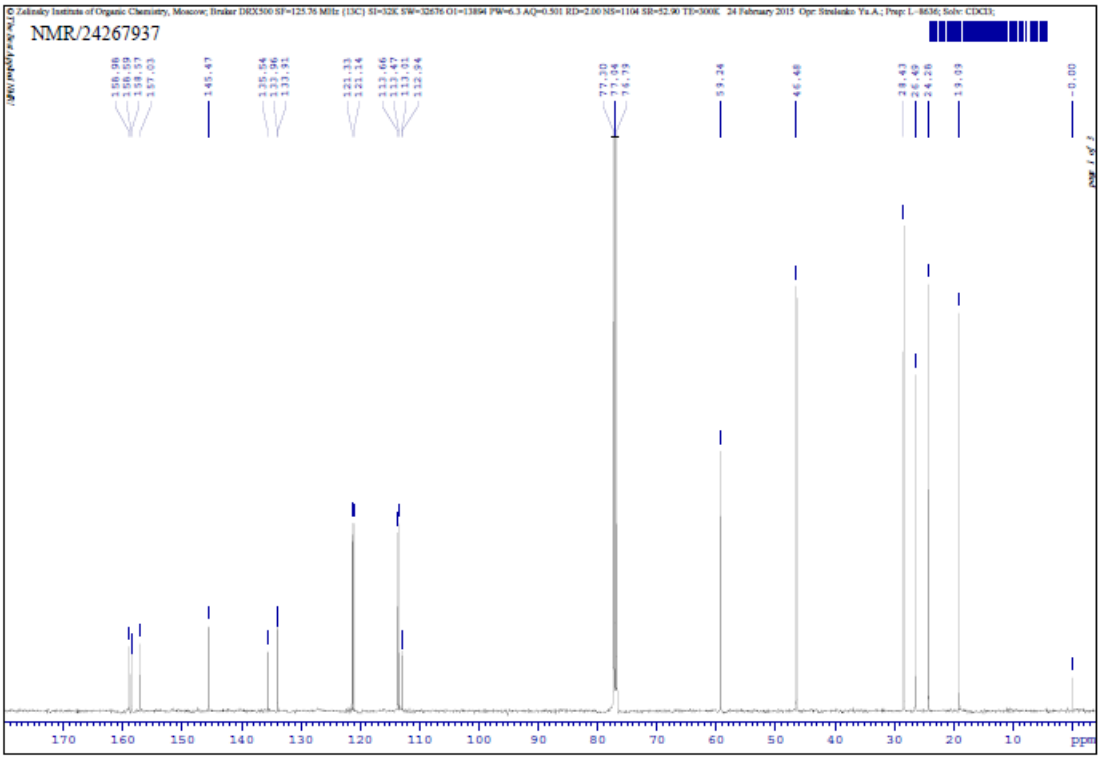
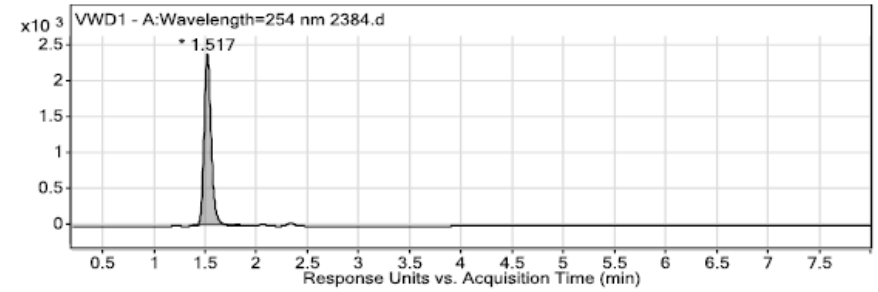



**Figure 18**. NMR $^{13}$C spectra of compound **10e**.

| | | | |
|---|---|---|---|
| **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 Version** | 6200 series TOF/6500 series 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**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 191 | 0 | ESI |

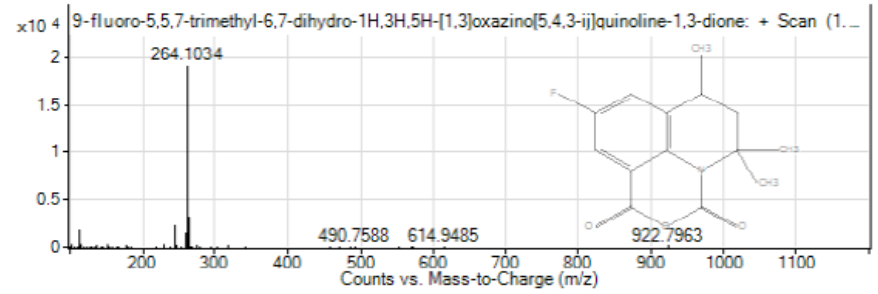



**Figure 19**. HPLC-HRMS-ESI spectra of compound **10e**.

```
Mass spectrum  NMR/24267937: formula C14H14FNO3, mol. mass 263.27
Max intensity: 999 for mass 204
Discrimination level for relative intensity: 5.0%,
whithin 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(%)
    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**.

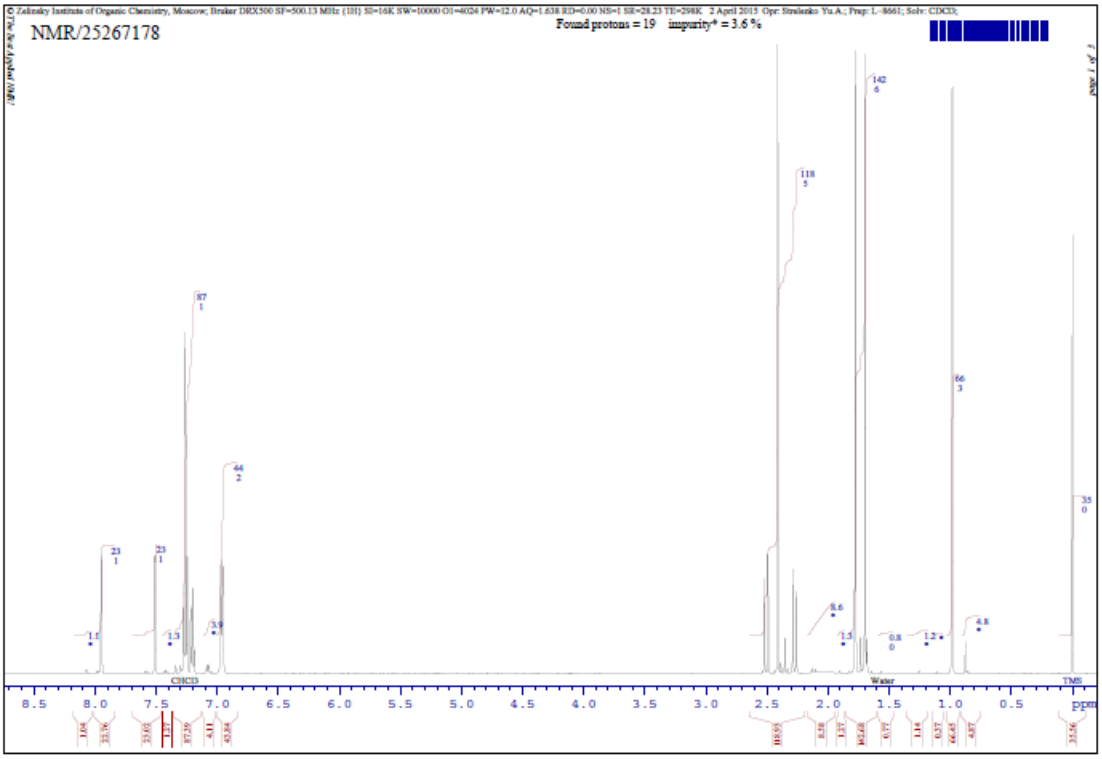



**Figure 21**. NMR $^{1}$H spectra of compound **10f**.

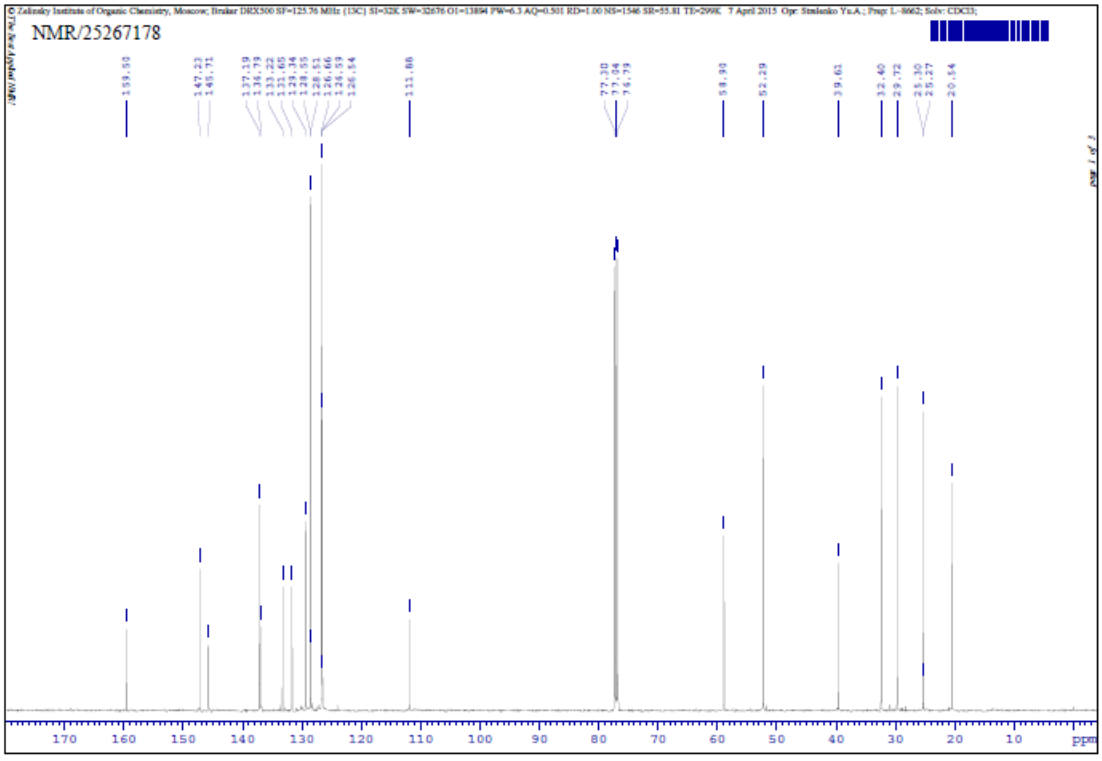



**Figure 22**. NMR $^{13}$C spectra of compound **10f**.

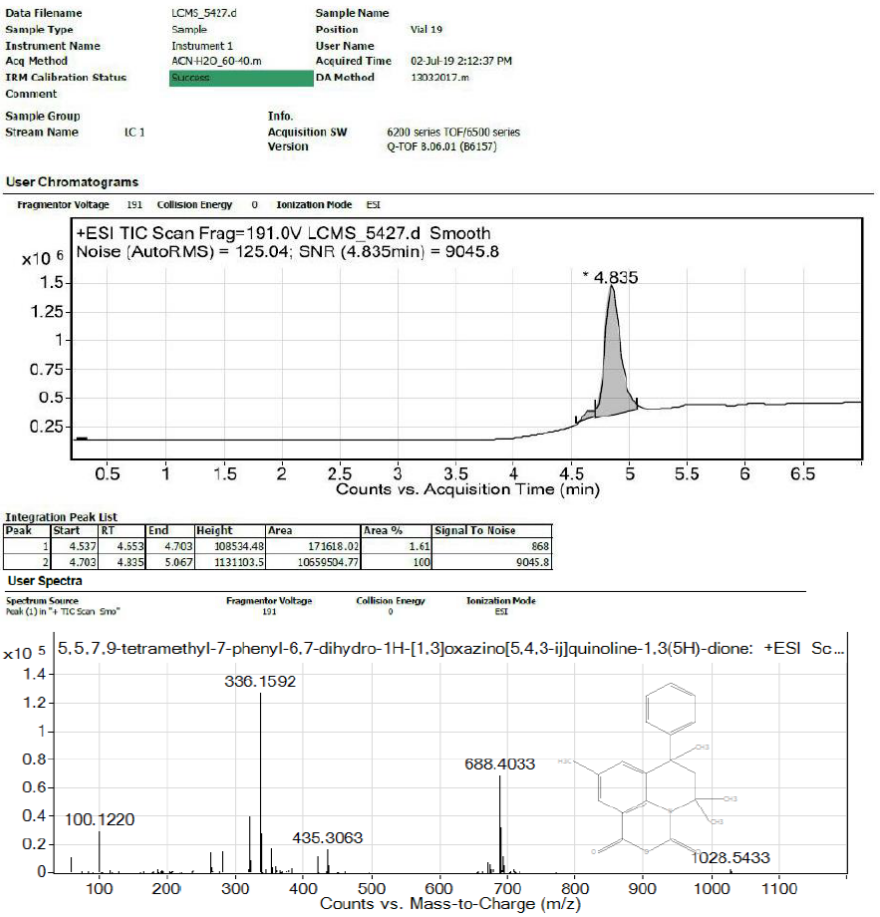



**Figure 23**. HPLC-HRMS-ESI spectra of compound **10f**.

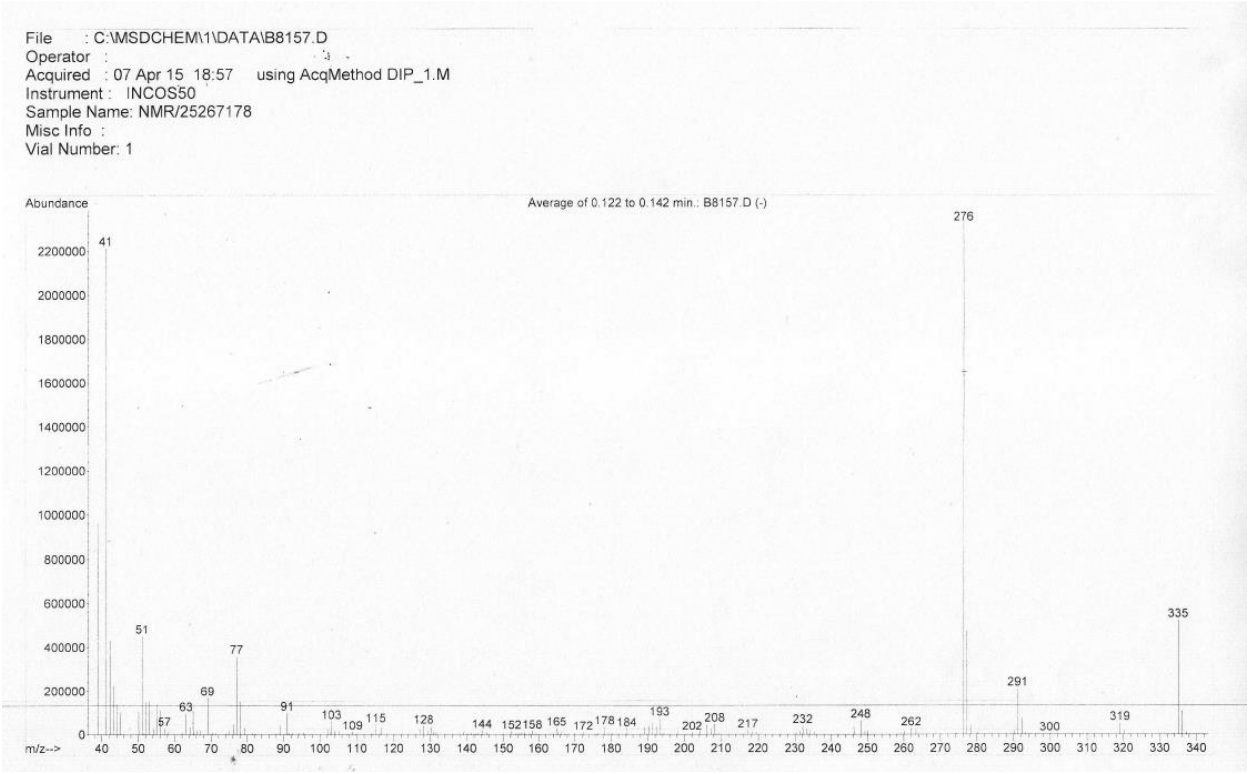



**Figure 24**. Mass-spectra of compound **10f**.

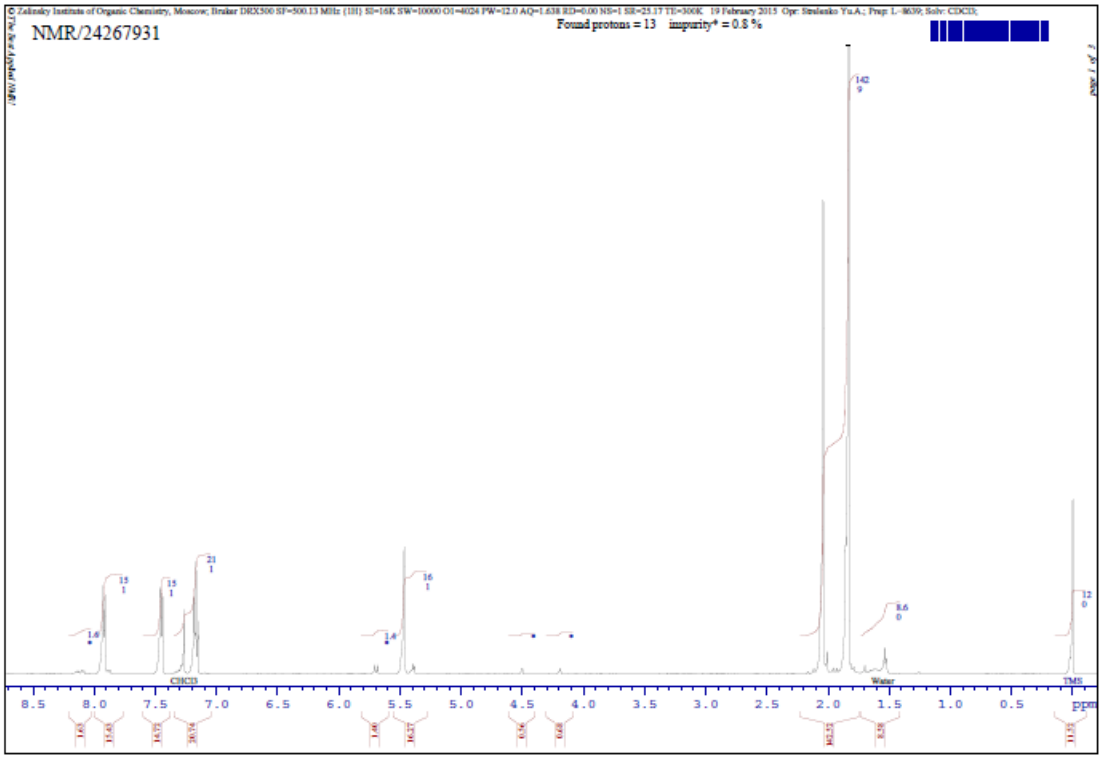



**Figure 25**. NMR $^{1}$H spectra of compound **12a**.

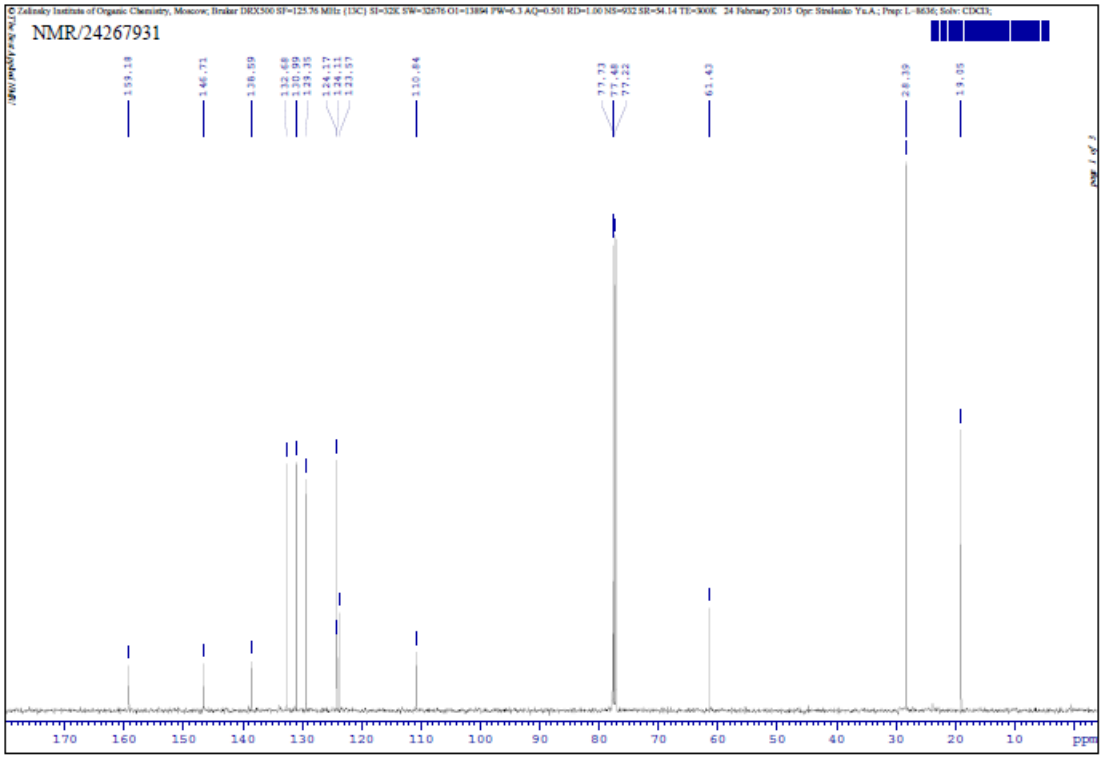
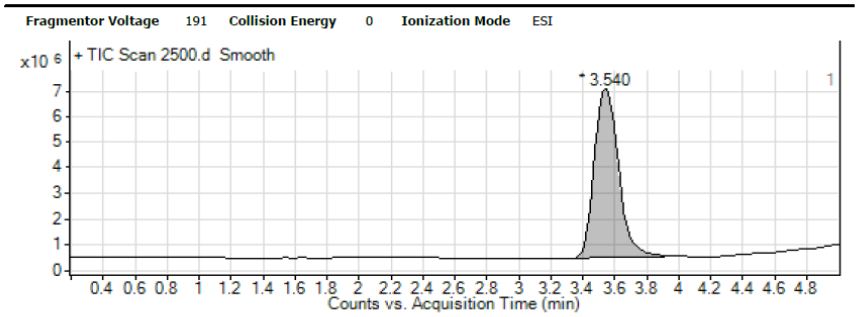



**Figure 26**. NMR $^{13}$C spectra of compound **12a**.

| | | | |
|---|---|---|---|
| **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 Version** | 6200 series TOF/6500 series 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**

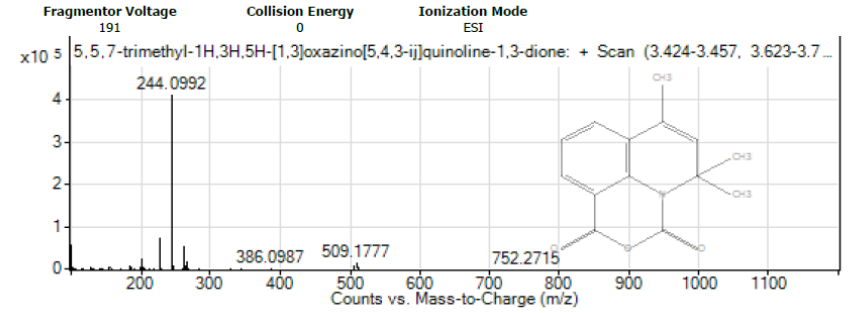



**Figure 27**. HPLC-HRMS-ESI spectra of compound **12a**.

```
    Mass spectrum  NMR/24267931: formula C14H13NO3, mol. mass 243.26
    Max intensity: 999 for mass 184
    Discrimination level for relative intensity: 5.0%,
    whithin 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(%)
    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**.

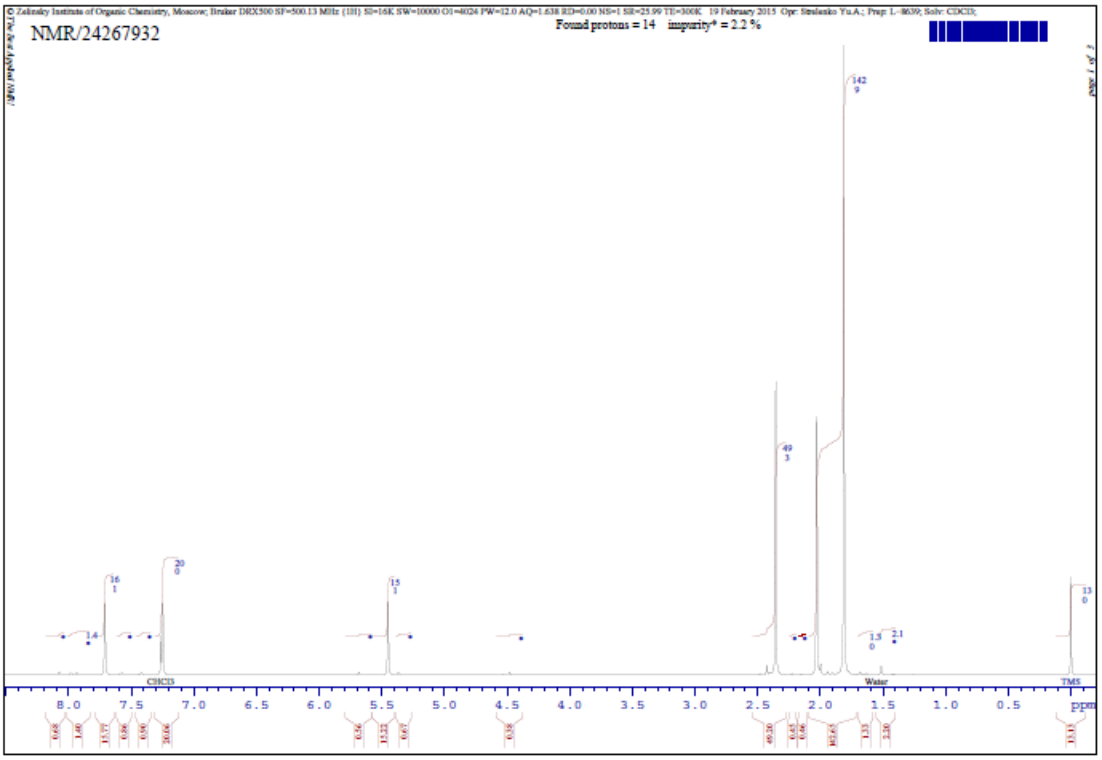



**Figure 29**. NMR $^{1}$H spectra of compound **12b**.

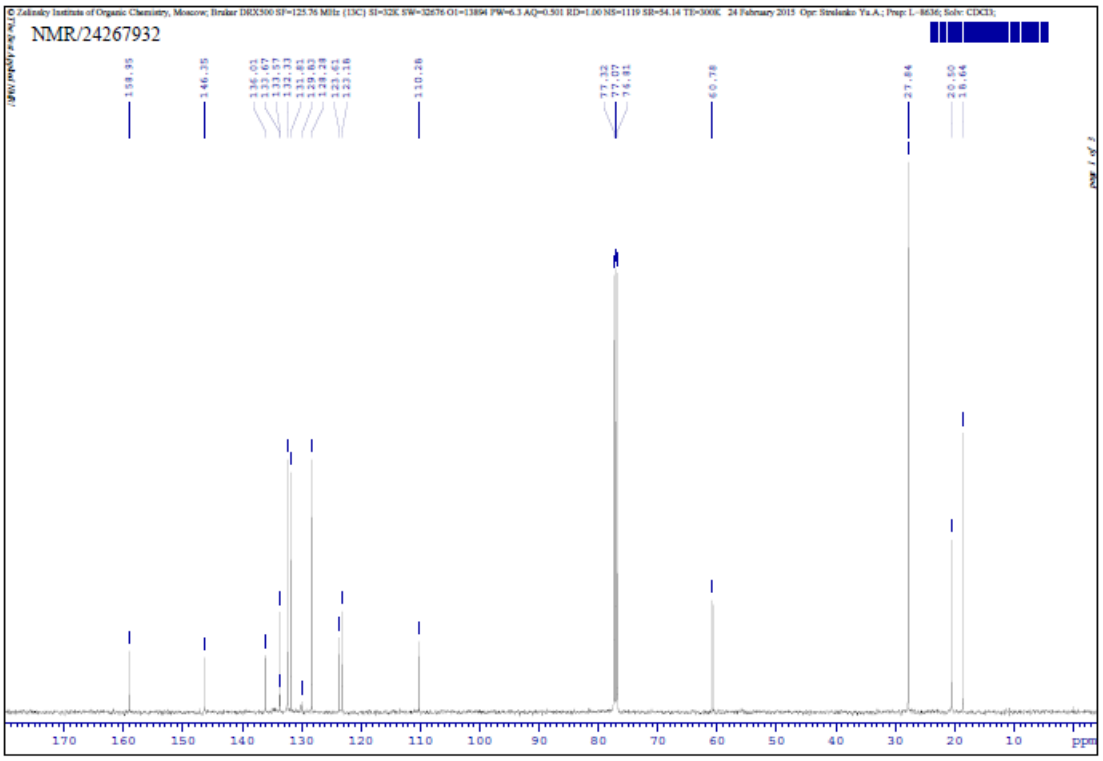
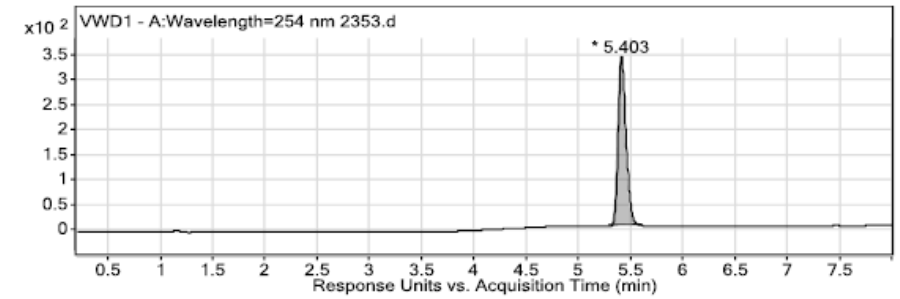



**Figure 30**. NMR $^{13}$C spectra of compound **12b**.

| | | | |
|---|---|---|---|
| **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 Version** | 6200 series TOF/6500 series 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**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 191 | 0 | ESI |

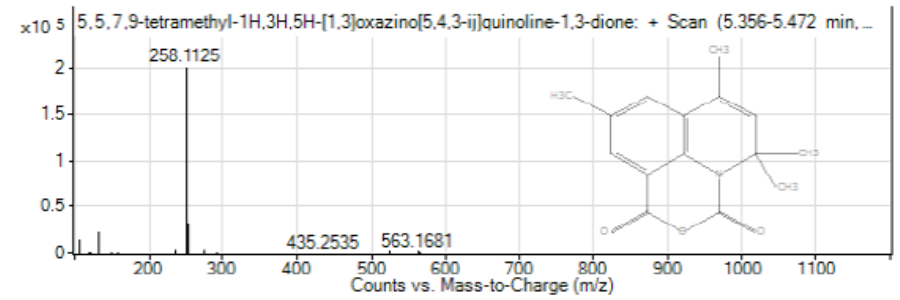



**Figure 31**. HPLC-HRMS-ESI spectra of compound **12b**.

```
Mass spectrum  NMR/24267932: formula C15H15NO3, mol. mass 257.29
Max intensity: 999 for mass 198
Discrimination level for relative intensity: 5.0%,
whithin 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 mol.mass: 257  *                        6.51
    258        9        0.90    -->|    258                           0.90
```

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

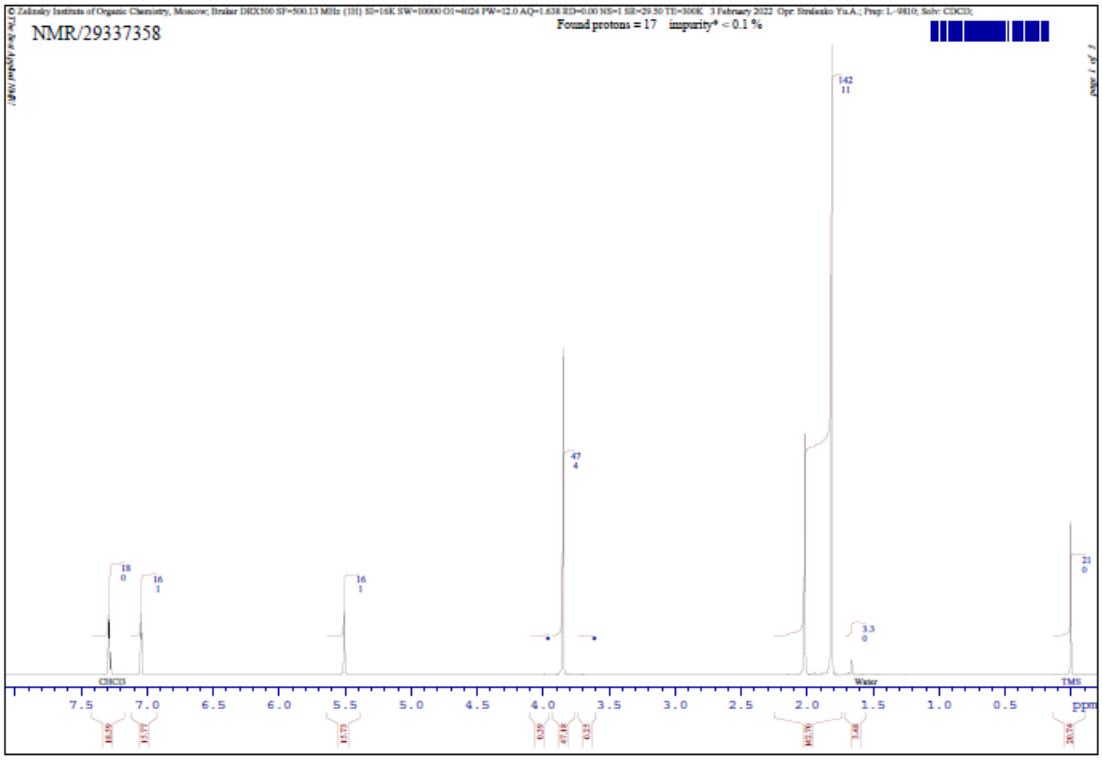



**Figure 33.** NMR $^{1}$H spectra of compound **12c**.

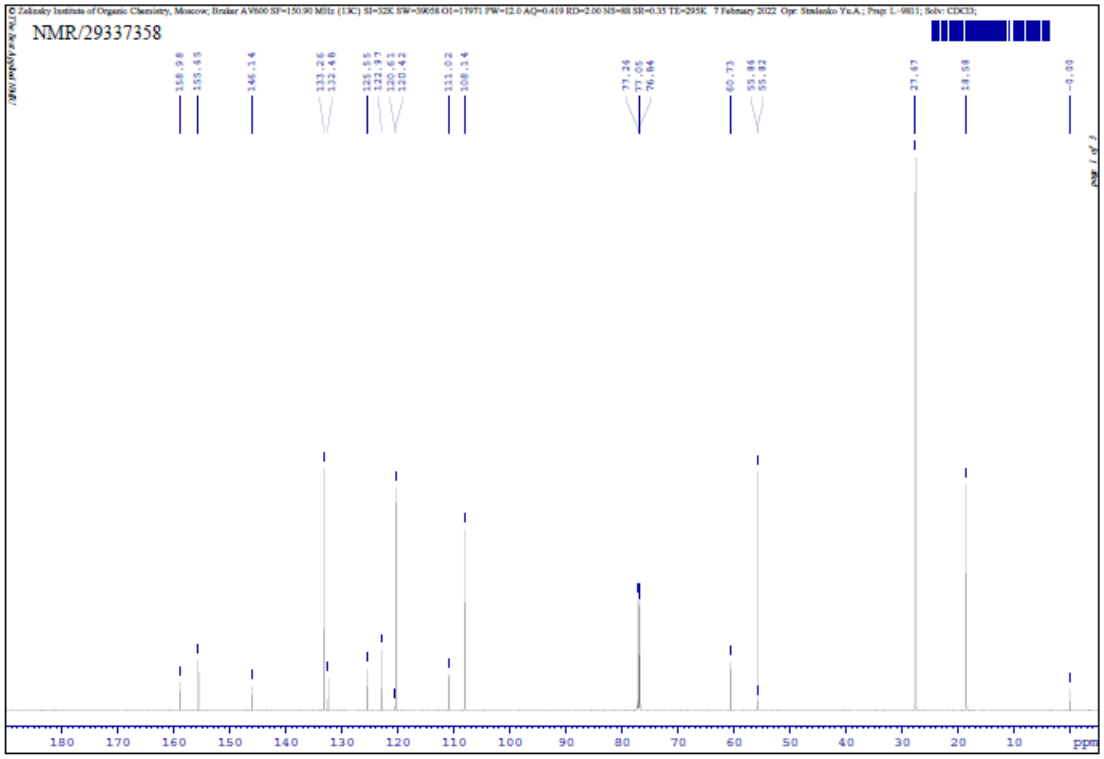



**Figure 34**. NMR $^{13}$C spectra of compound **12c**.

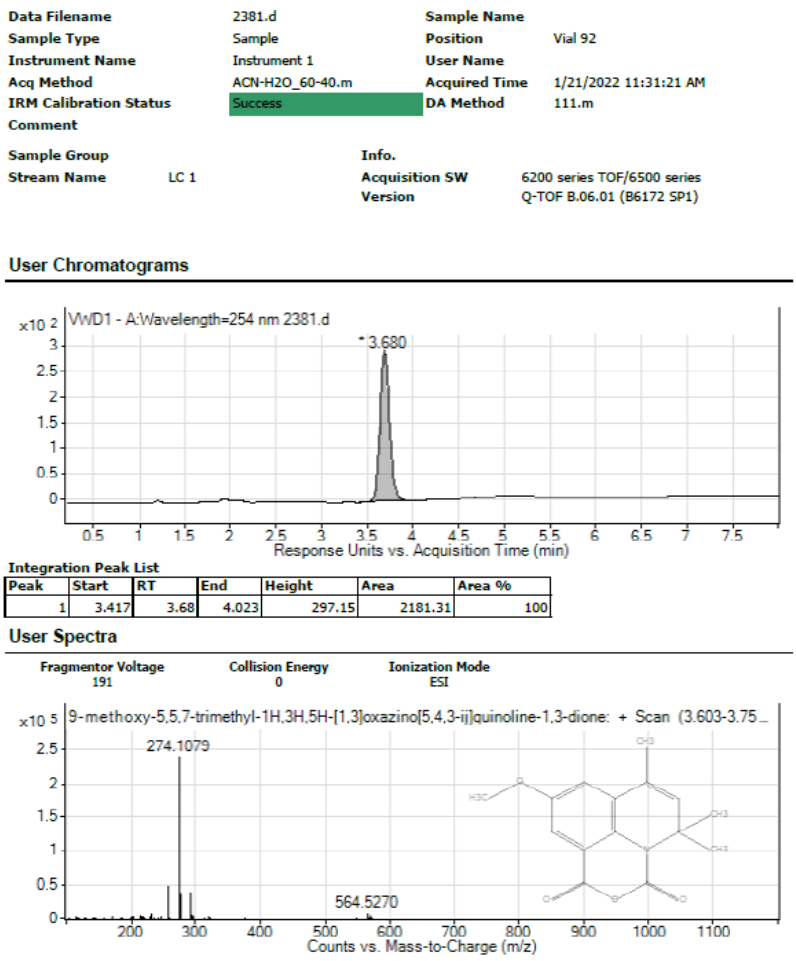



**Figure 35**. HPLC-HRMS-ESI spectra of compound **12c**.

```
Mass spectrum  NMR/24267929: formula C15H15NO4, mol. mass 273.28
Max intensity: 999 for mass 214
Discrimination level for relative intensity: 5.0%,
whithin 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(%)
    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**.

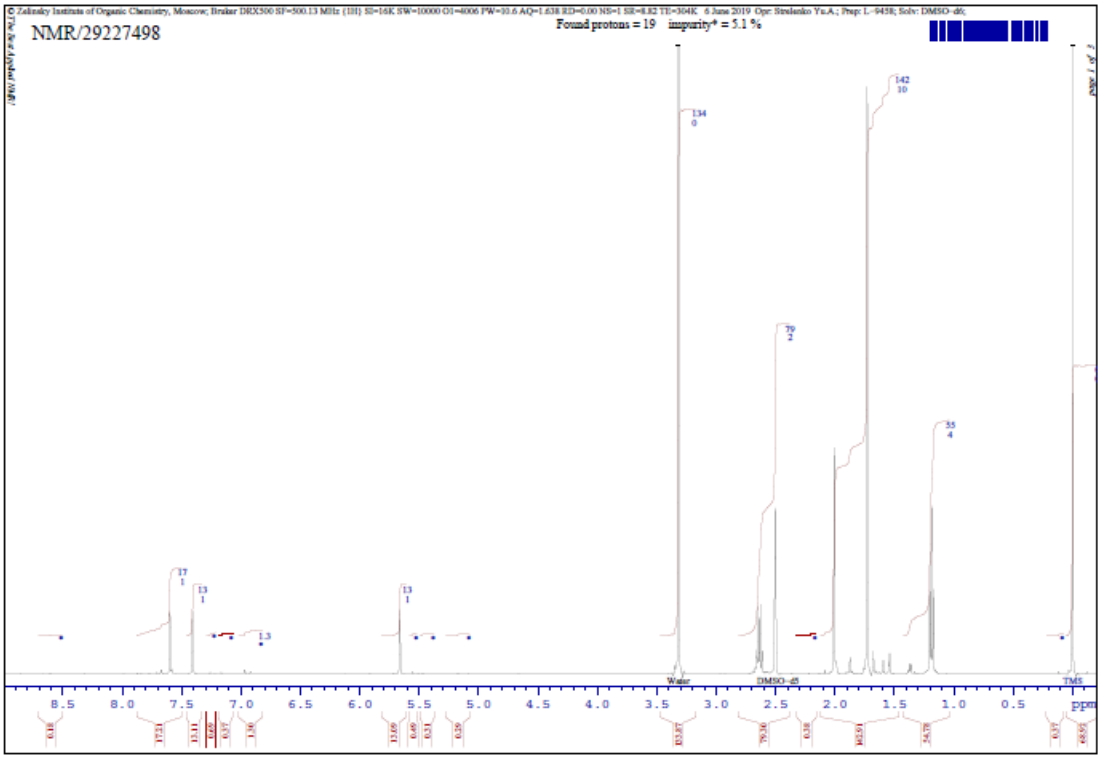



**Figure 37**. NMR $^{1}$H spectra of compound **12d**.

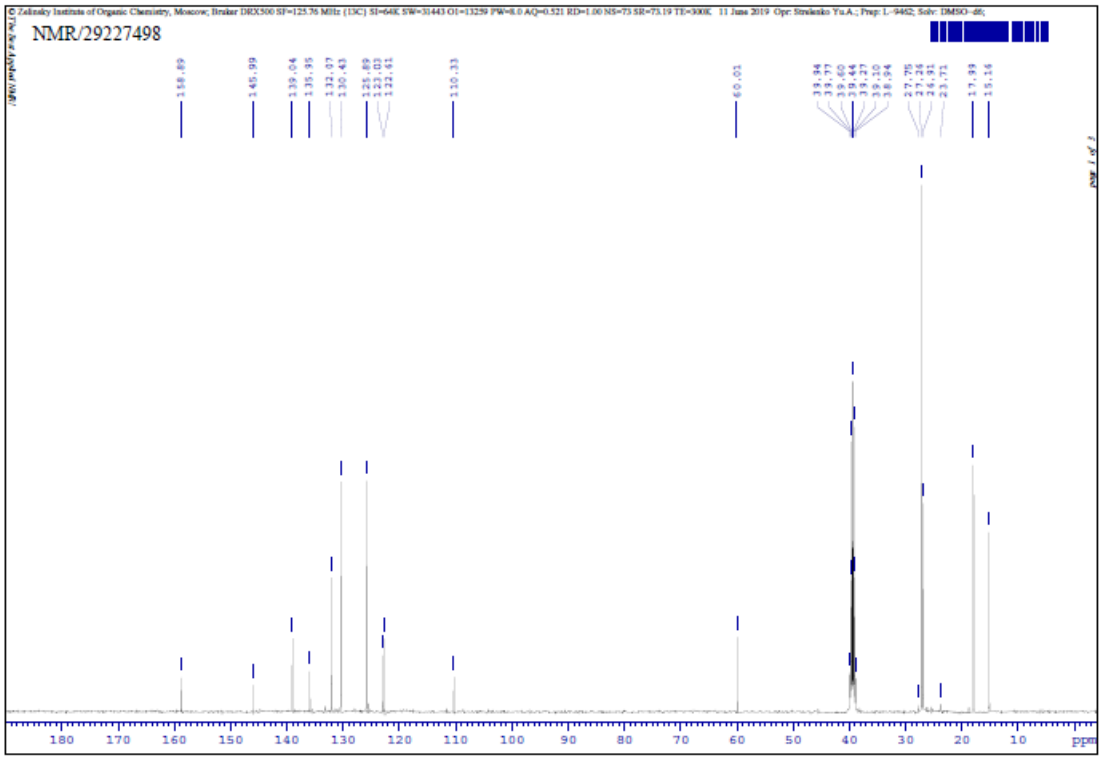


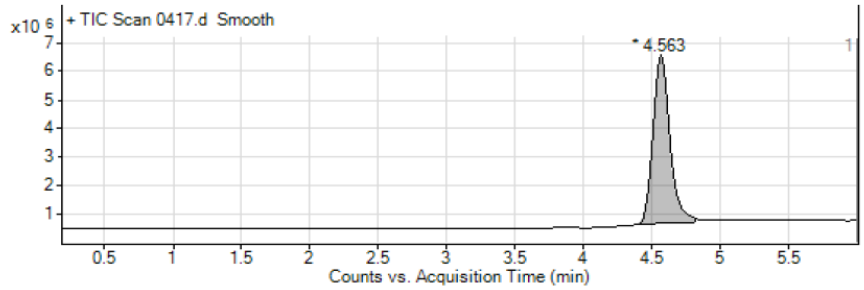

**Figure 38**. NMR $^{13}$C spectra of compound **12d**.

| | | | |
|---|---|---|---|
| **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 Version** | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

**User Chromatograms**

**Fragmentor Voltage** 191 **Collision Energy** 0 **Ionization Mode** ESI




**Integration Peak List**

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

**User Spectra**

| Spectrum Source | Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|---|
| Peak (1) in "+ TIC Scan Smo" | 191 | 0 | ESI |

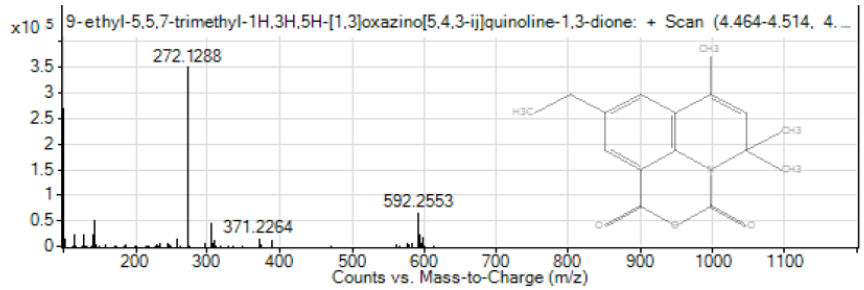



**Figure 39**. HPLC-HRMS-ESI spectra of compound **12d**.

Mass spectrum NMR/24267930: formula C16H17NO3, mol. mass 271.31
Max intensity: 999 for mass 212
Discrimination level for relative intensity: 5.0%,
whithin 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(%) |
|---|---|---|---|---|---|---|
| 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**.

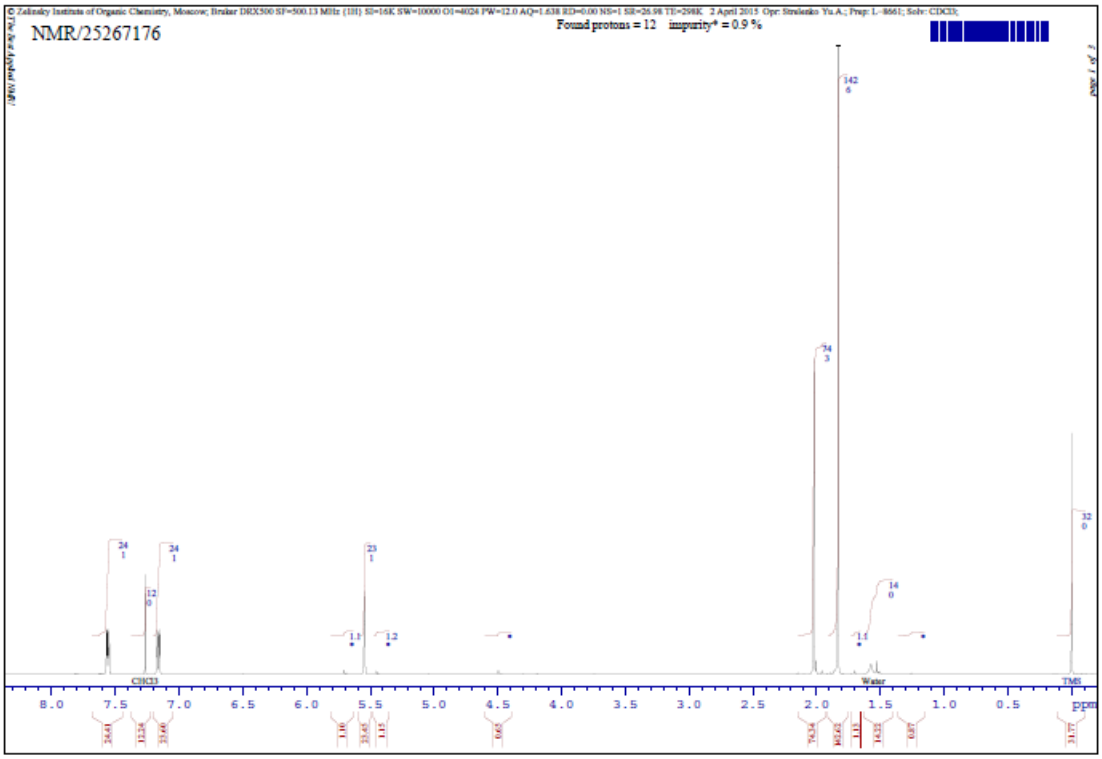



**Figure 41**. NMR $^{1}$H spectra of compound **12e**.

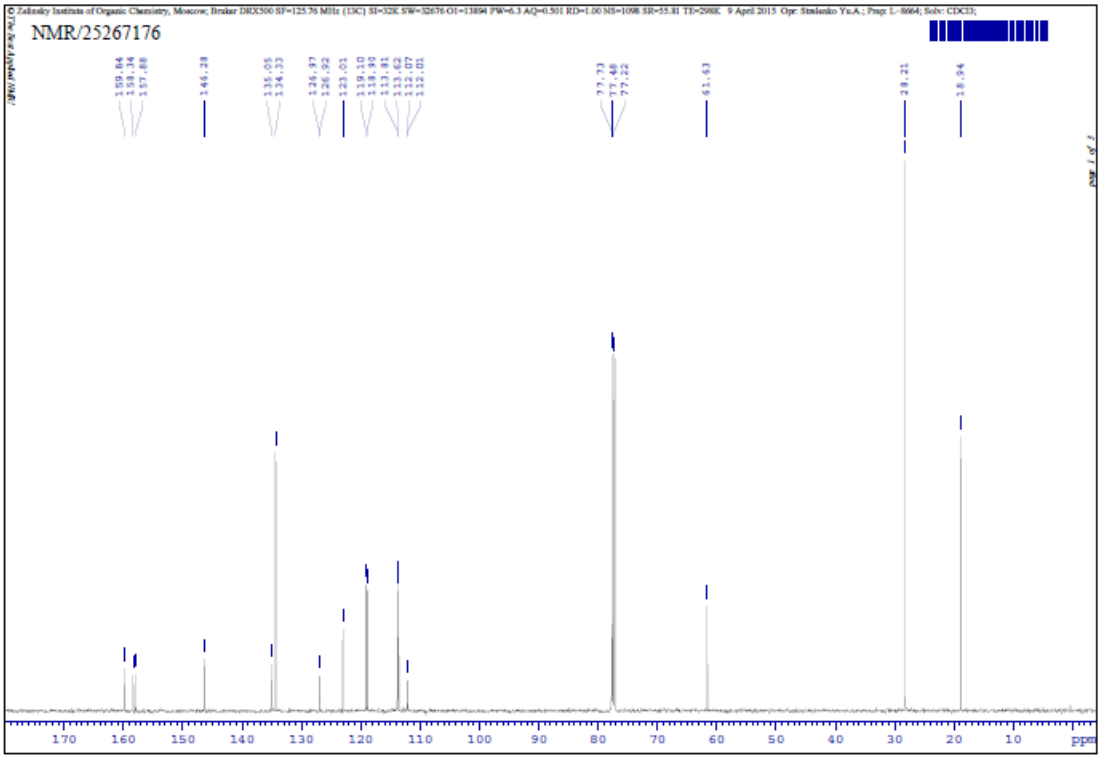



**Figure 42**. NMR $^{13}$C spectra of compound **12e**.

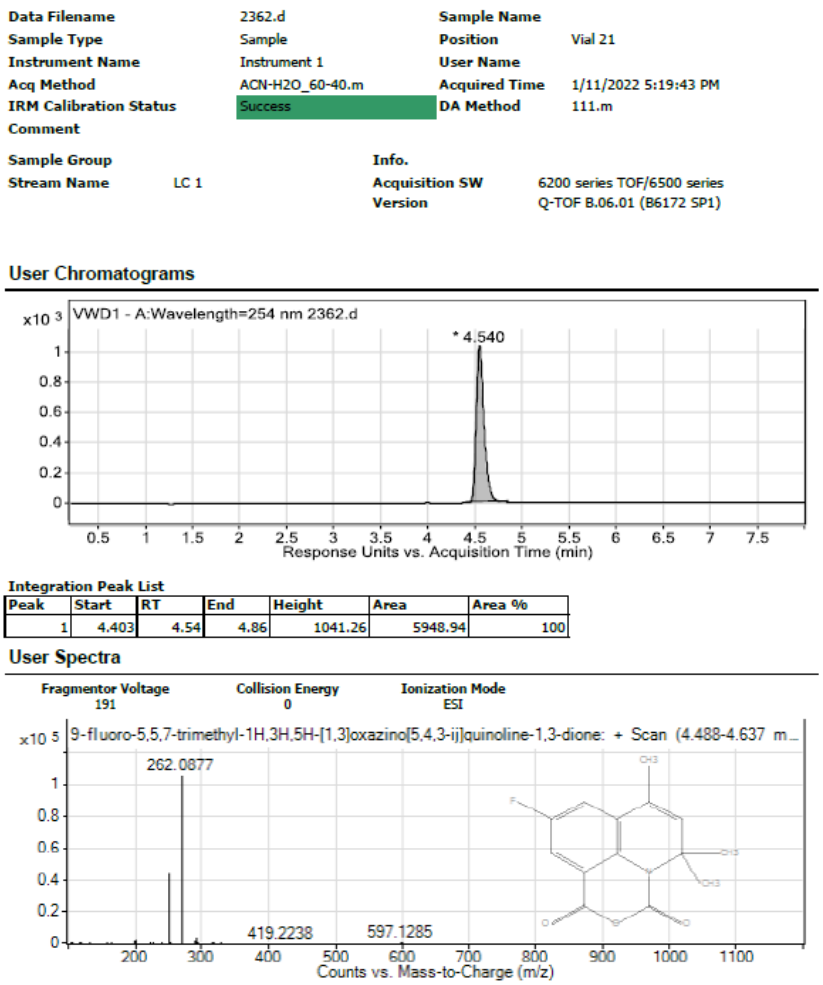



**Figure 43**. HPLC-HRMS-ESI spectra of compound **12e**.

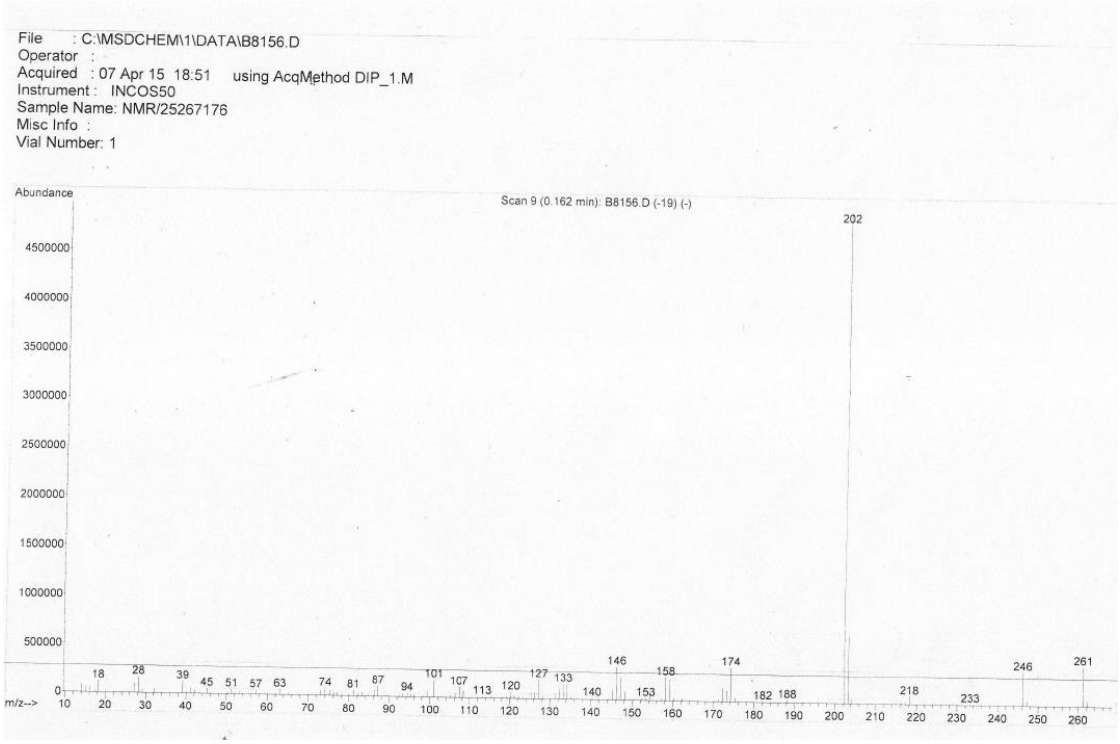



**Figure 44**. Mass-spectra of compound **12e**.

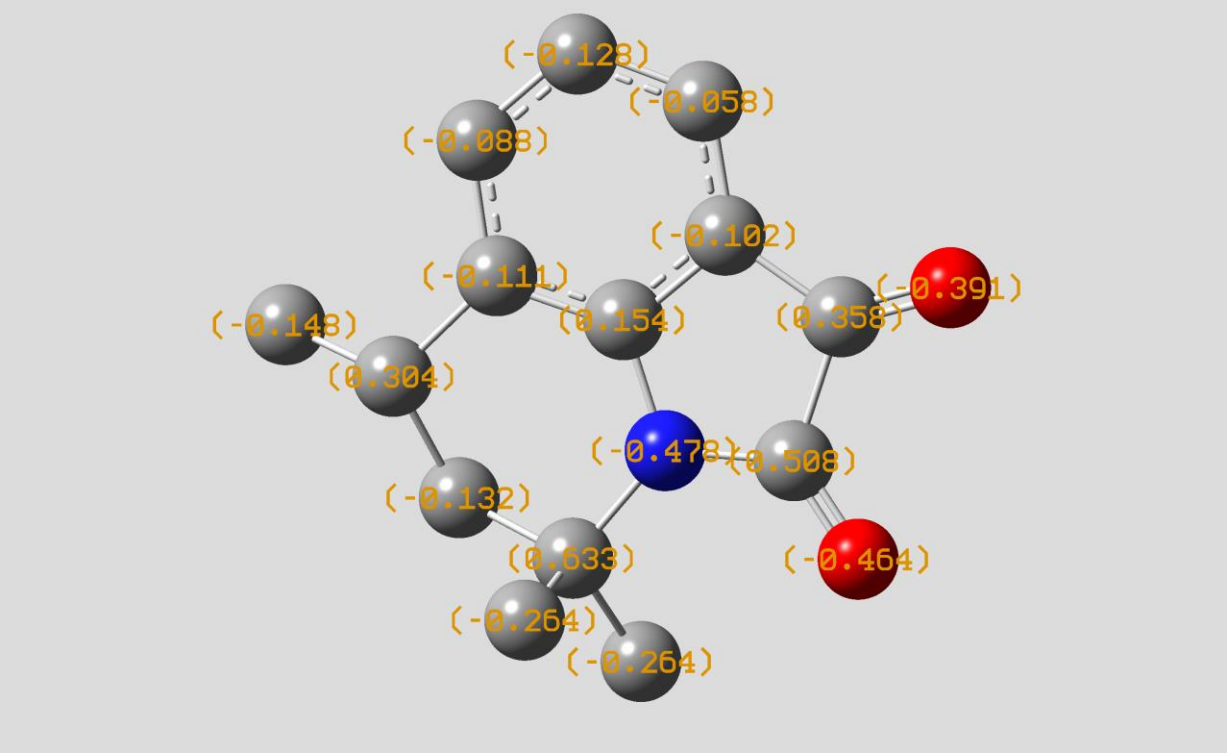



**Figure 45**. Calculated atomic charges according to CHELPG on the atoms of compound **10a.**

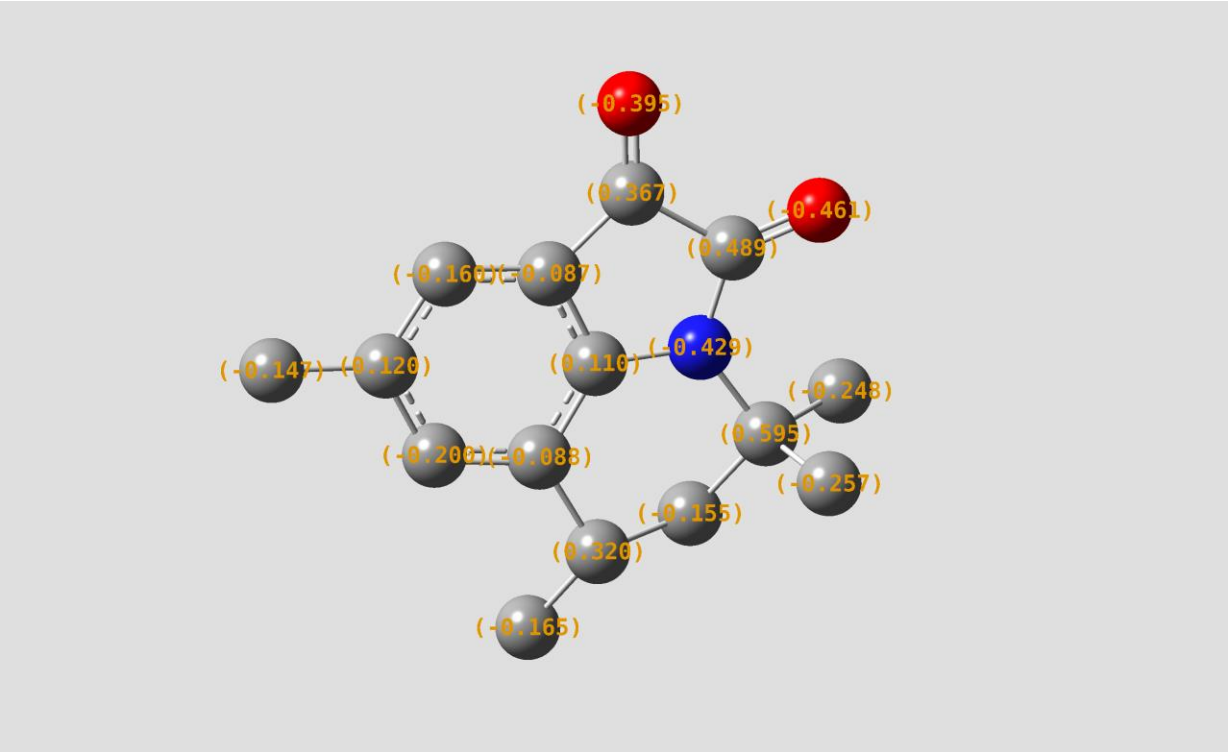



**Figure 46**. Calculated atomic charges according to CHELPG on the atoms of compound **10b.**

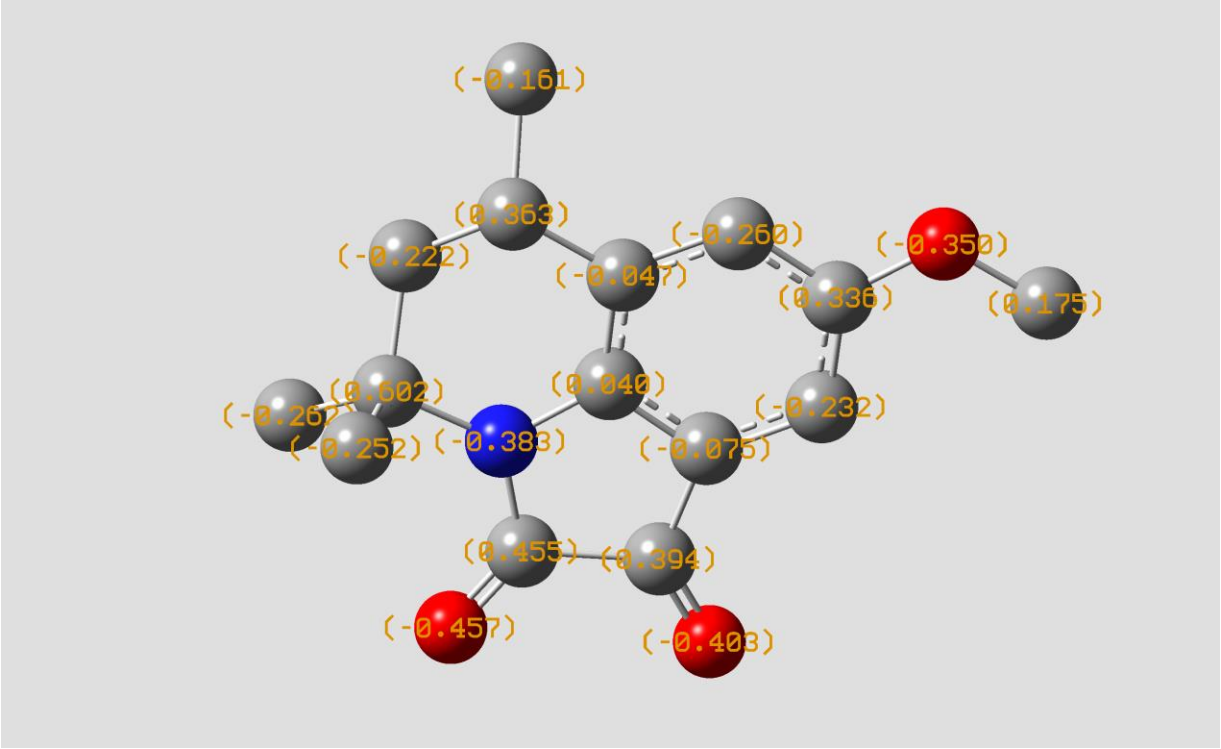



**Figure 47**. Calculated atomic charges according to CHELPG on the atoms of compound **10c.**

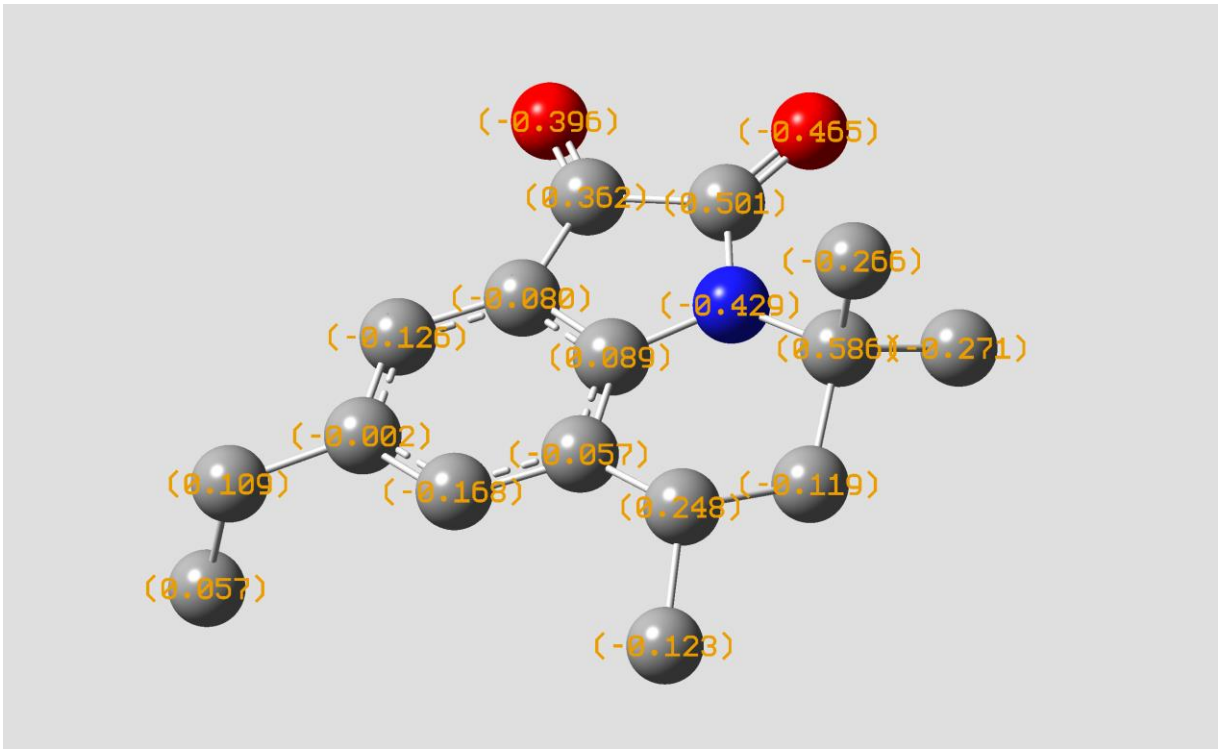



**Figure 48**. Calculated atomic charges according to CHELPG on the atoms of compound **10d.**

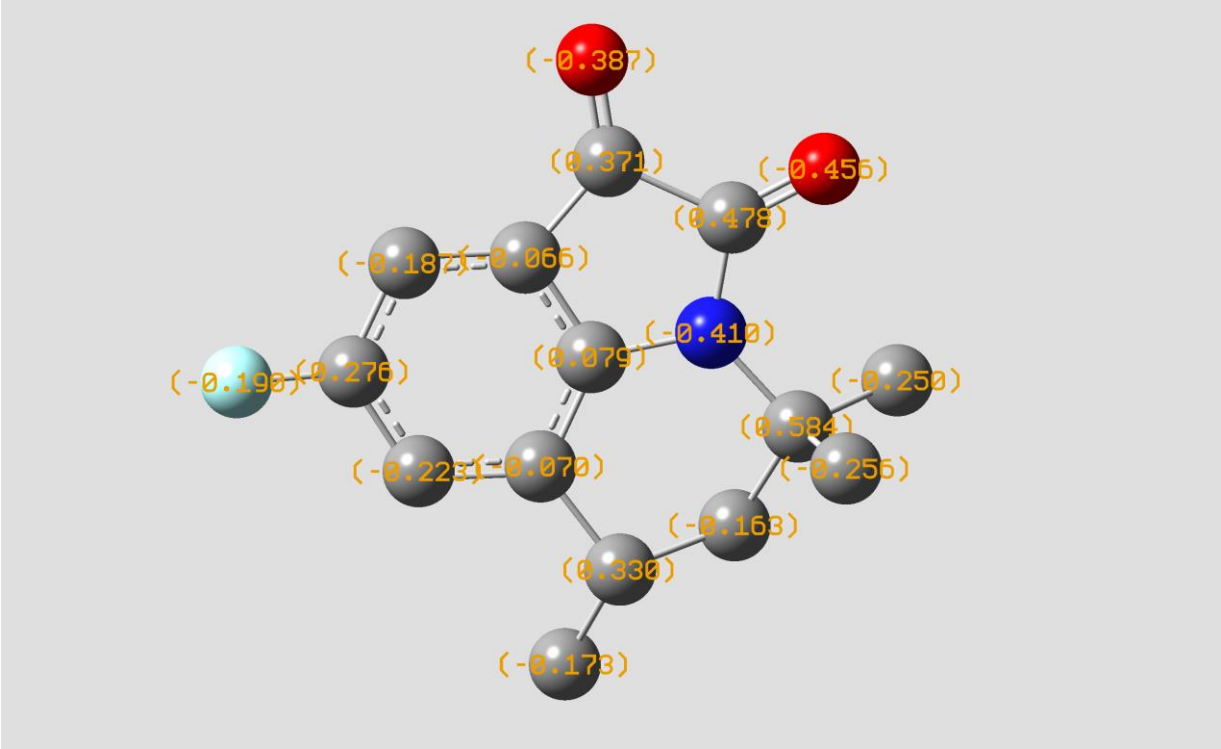



**Figure 49**. Calculated atomic charges according to CHELPG on the atoms of compound **10e.**

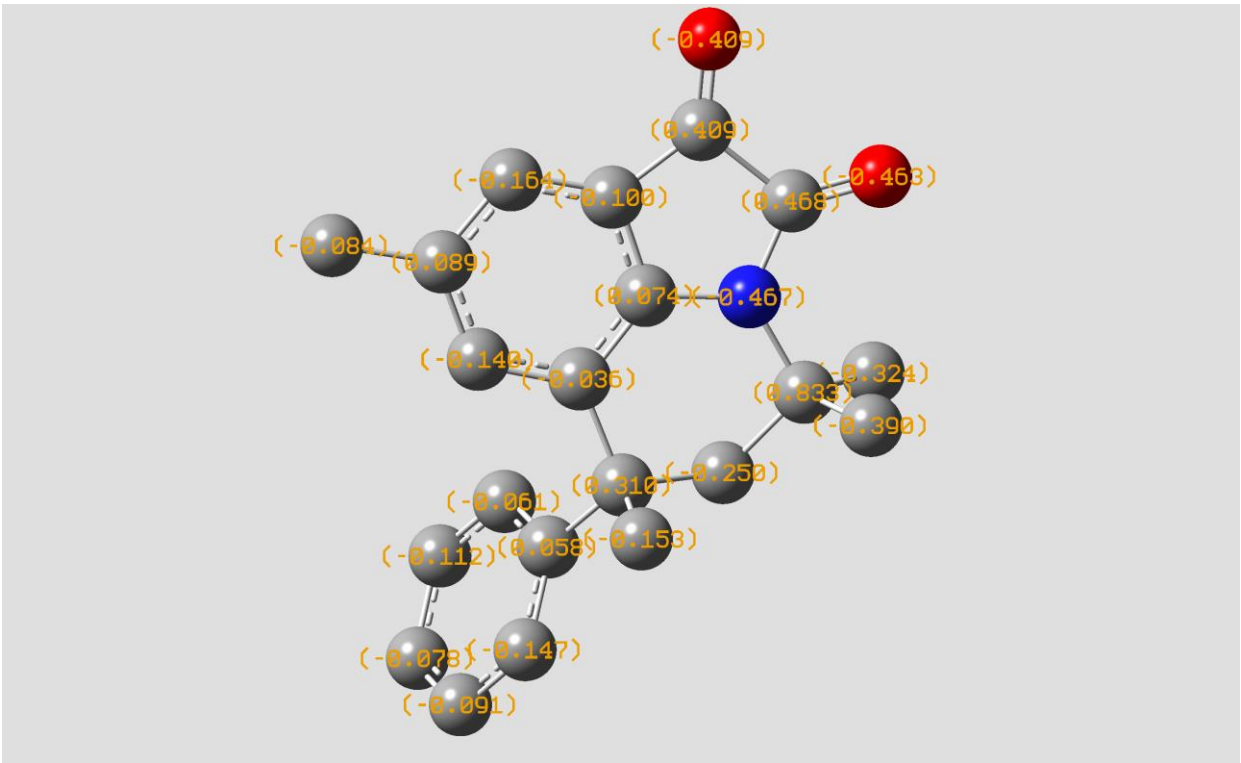



**Figure 50**. Calculated atomic charges according to CHELPG on the atoms of compound **10f.**

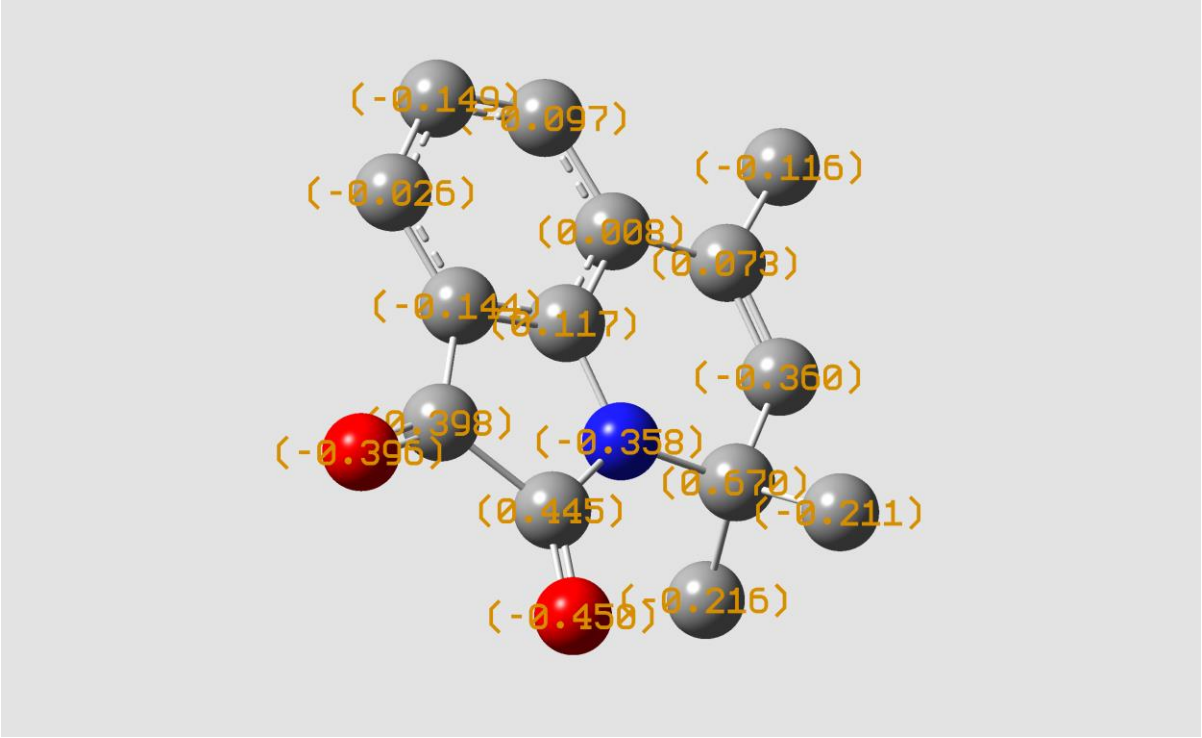



**Figure 51**. Calculated atomic charges according to CHELPG on the atoms of compound **12a.**

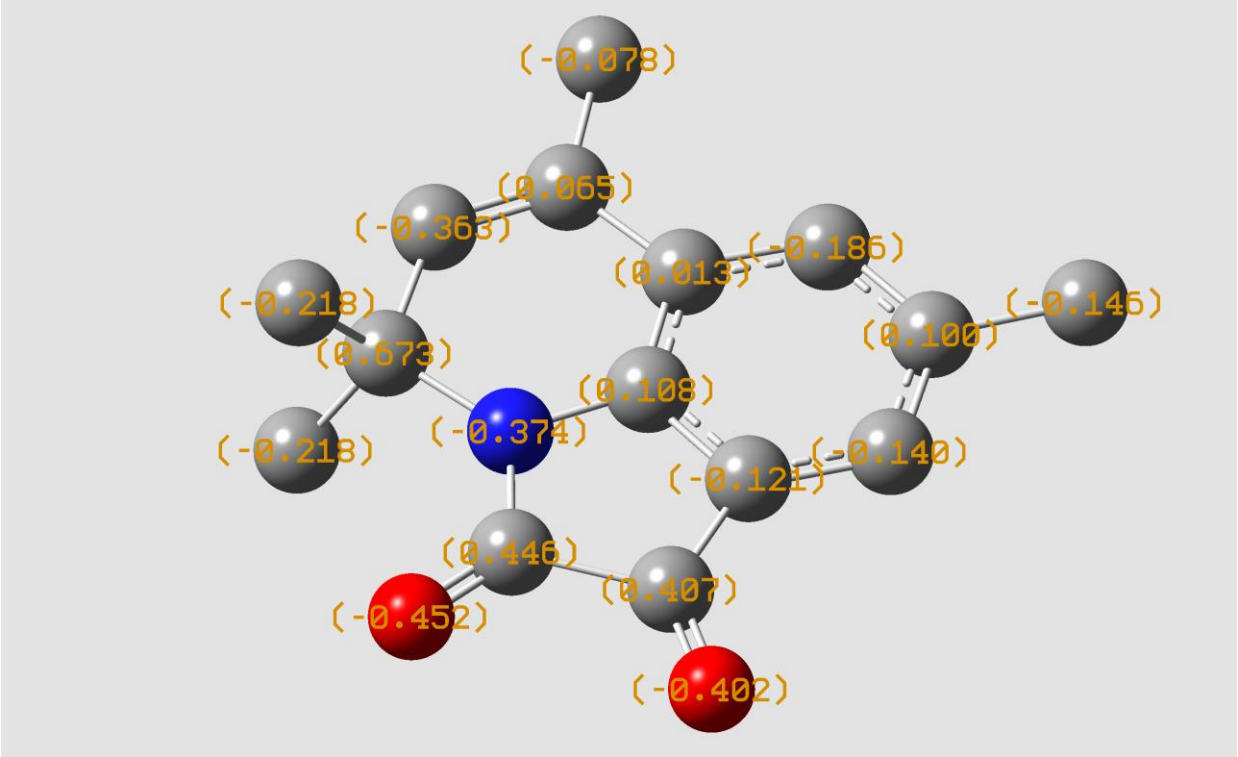



**Figure 52**. Calculated atomic charges according to CHELPG on the atoms of compound **12b.**

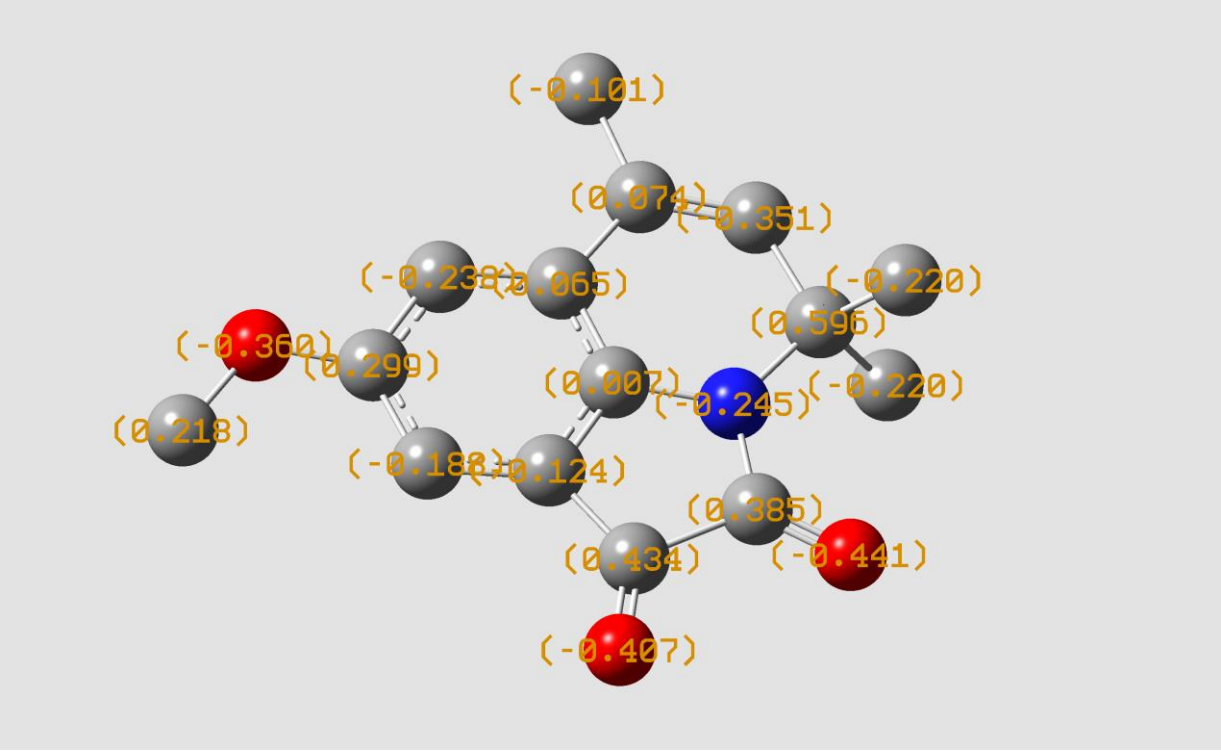



**Figure 53**. Calculated atomic charges according to CHELPG on the atoms of compound **12c.**

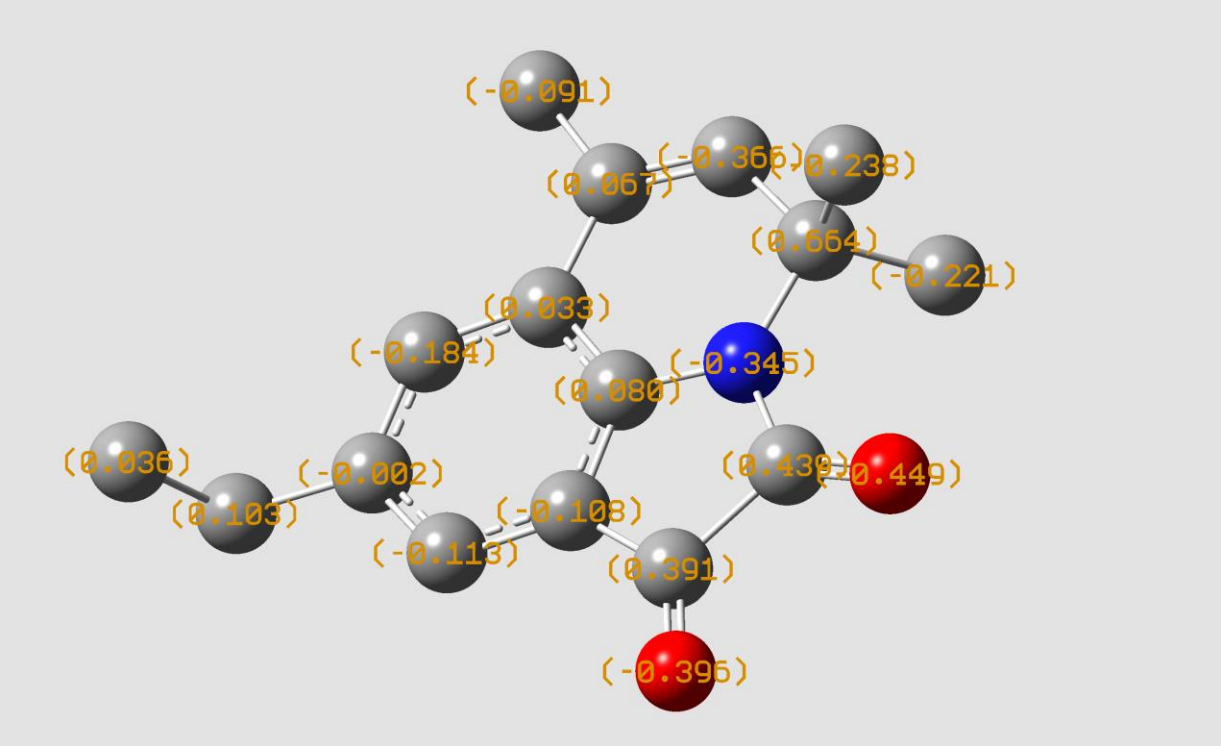



**Figure 54**. Calculated atomic charges according to CHELPG on the atoms of compound **12d.**

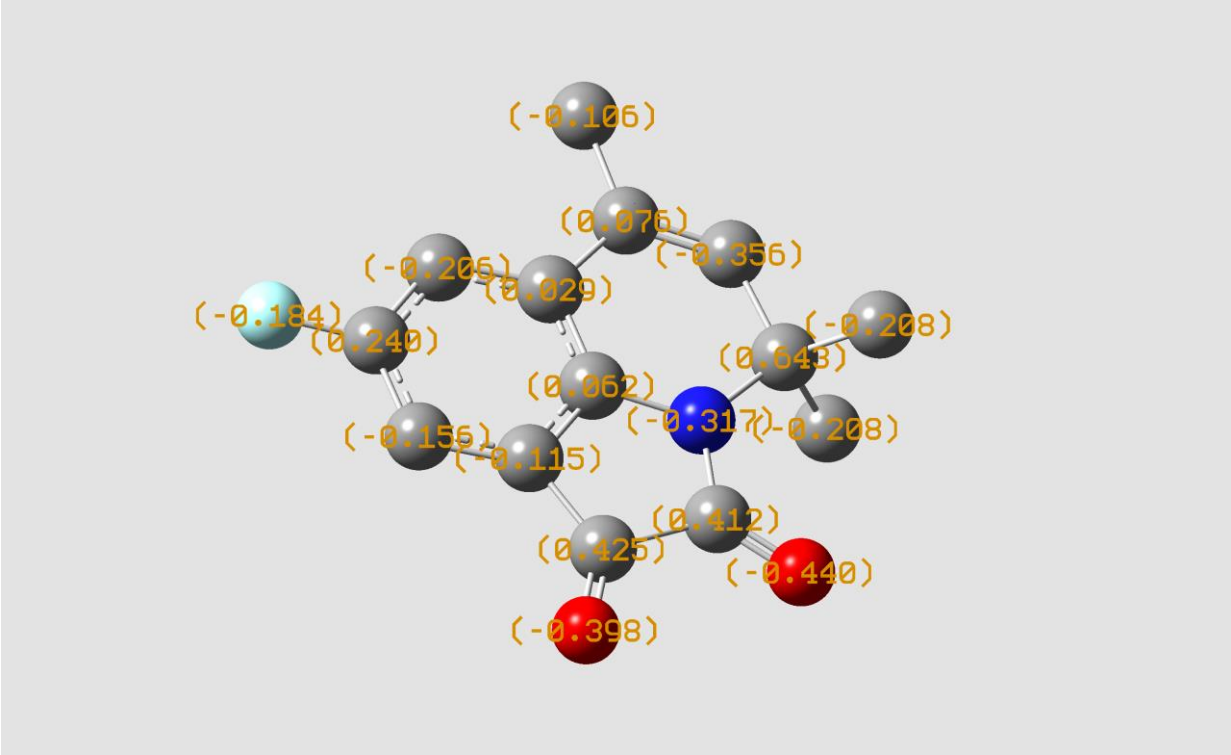



**Figure 55**. Calculated atomic charges according to CHELPG on the atoms of compound **12e.**