

Supplementary Material

Synthesis and some reactions of 5-carbomethoxymethylidene-4-oxo-1,3-thiazol-2-ylguanidine

Nadezhda V. Stolpovskaya,^a Do Van Quy,^a Alexey A. Kruzhilin,^a Evgeniya S. Shvetsova,^a Khidmet S. Shikhaliev,^{*a} and Fedor I. Zubkov^b

^a Department of Organic Chemistry, Voronezh State University, Universitetskaya pl. 1, Voronezh, 394006, Russia

^b Department of Organic Chemistry, Peoples' Friendship University of Russia, 6 Miklukho-Maklaya St., Moscow, 117198, Russian Federation

Email: chocd261@chem.vsu.ru

Table of Contents

| | |
|---|-----|
| 1. X-ray structural analysis data methyl (2Z)-[2[(diaminomethylene)amino]-4-oxothiazol-5(4H)-ylidene]acetate 9 | S2 |
| 2. IR, ¹ H and ¹³ C NMR spectra and data LCMS for compounds 9, 17 a-f | S11 |

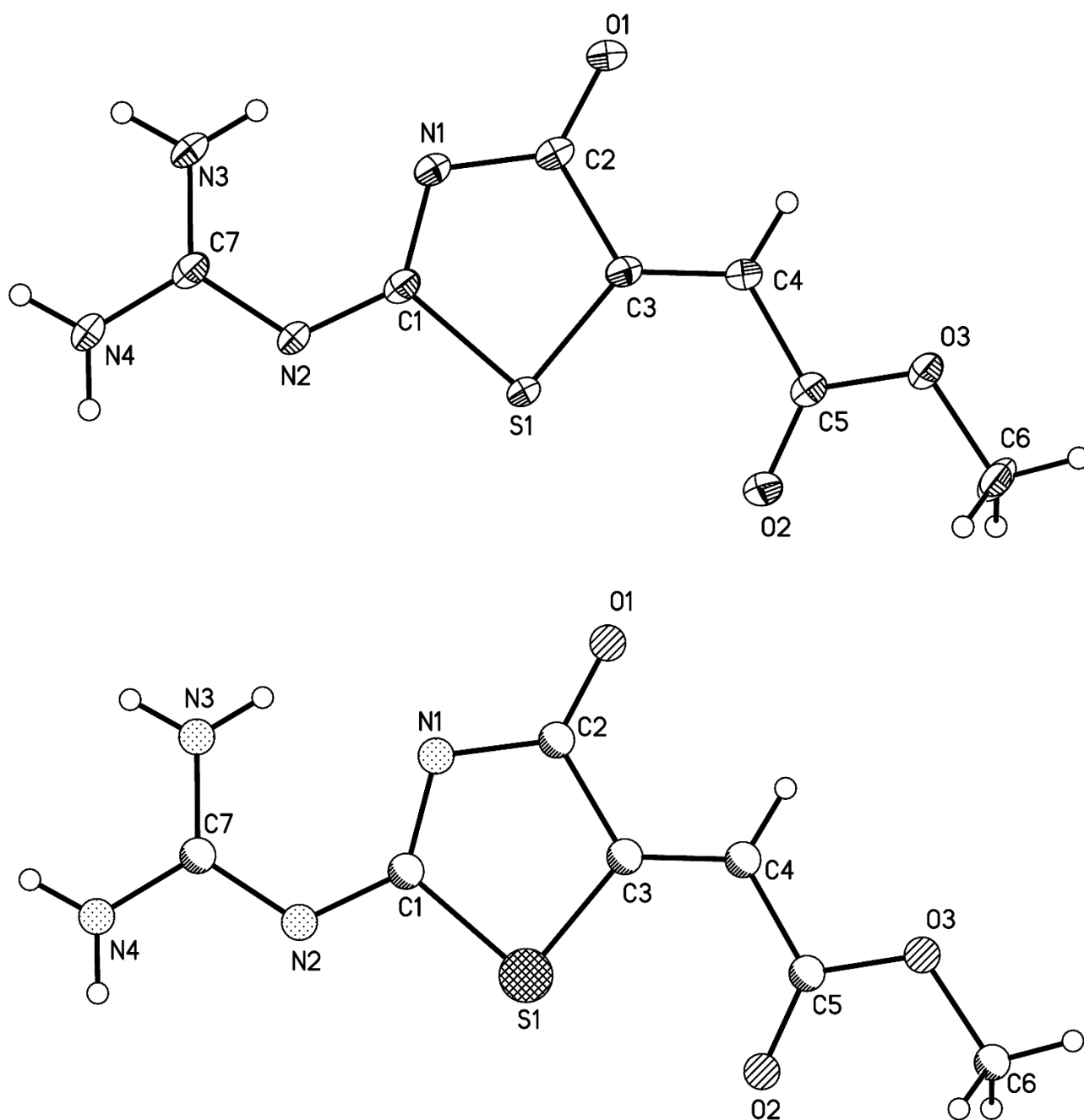


Figure S1. General view of the structure without the DMF solvate molecule (two versions of the image, ellipsoids of atomic displacements are given with a probability of 50%). There are two crystallographically independent molecules of the same structure in the structure; the second molecule is numbered atoms with the index A (not shown in the figure). Structural data deposited as CDCC: 2131042.

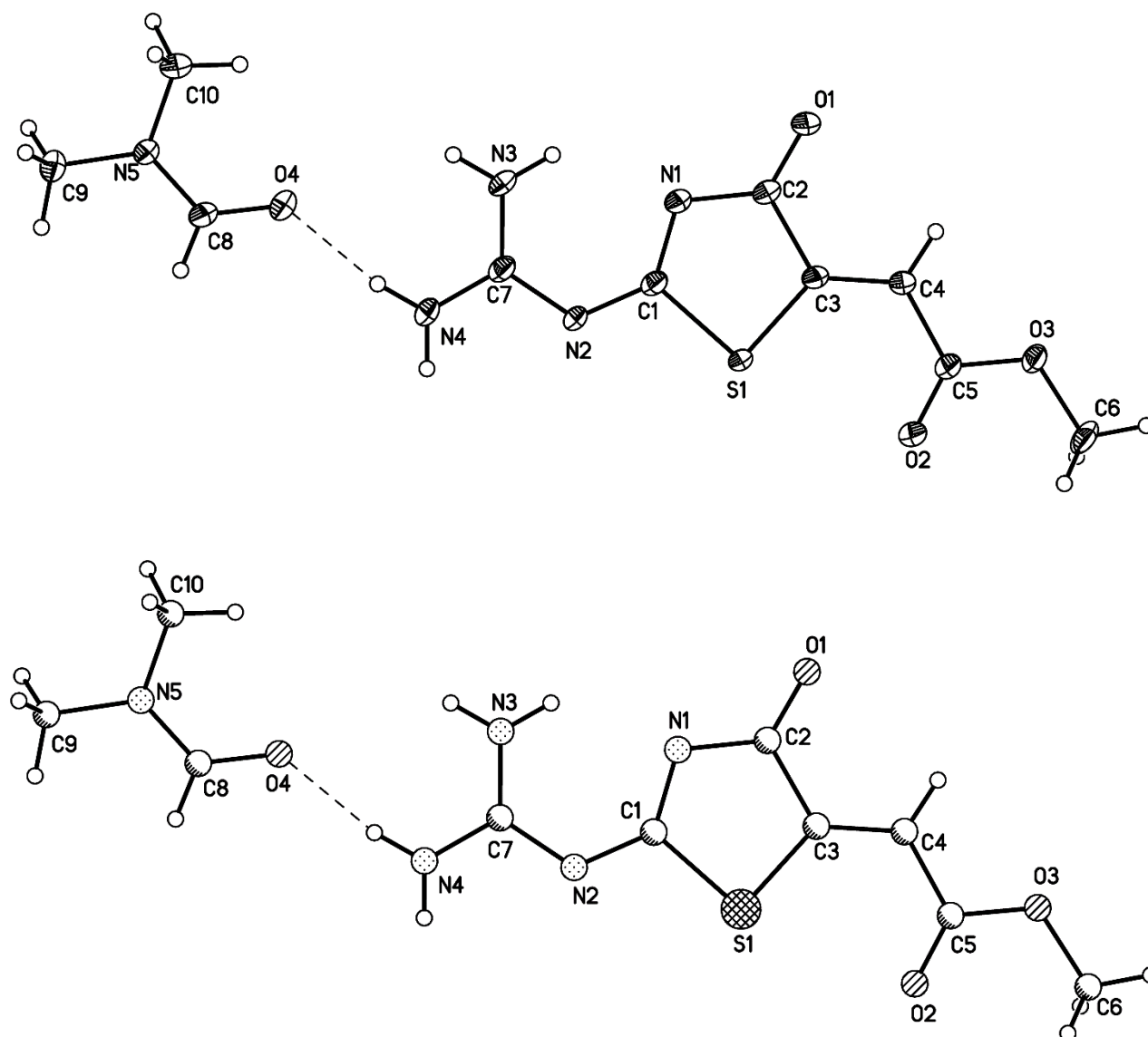


Figure S2. General view of structure 1 with a solvate DMF molecule (two versions of the image, ellipsoids of atomic displacements are given with a probability of 50%). Structural data deposited as CDCC: 2131042.

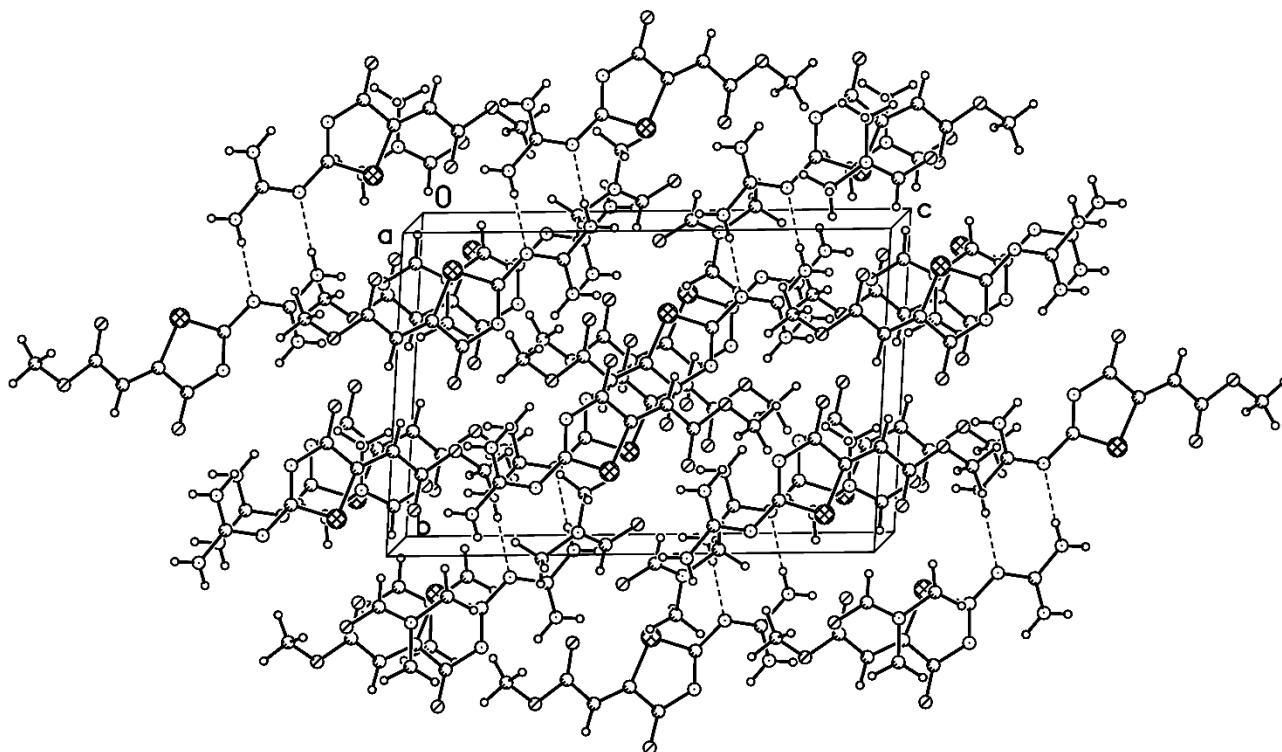


Figure S3. General view of the crystal packing **9**.

Table S1. Crystal data and structure refinement for **9**

| | |
|----------------------------------|-----------------------|
| Identification code | 1 |
| Empirical formula | $C_{10}H_{15}N_5O_4S$ |
| Formula weight | 301.33 |
| Temperature/K | 120 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 8.5470(8) |
| b/Å | 11.0867(10) |
| c/Å | 15.3765(14) |
| $\alpha/^\circ$ | 91.309(2) |
| $\beta/^\circ$ | 98.926(2) |
| $\gamma/^\circ$ | 108.968(2) |
| Volume/Å ³ | 1357.0(2) |
| Z | 4 |
| $\rho_{\text{calc}}/\text{cm}^3$ | 1.475 |
| μ/mm^{-1} | 0.261 |
| F(000) | 632.0 |
| Crystal size/mm ³ | 0.28 × 0.24 × 0.17 |

| | |
|---|--|
| Radiation | MoK α ($\lambda = 0.71073$) |
| 2 θ range for data collection/° | 3.896 to 61.006 |
| Index ranges | -12 \leq h \leq 12, -15 \leq k \leq 15, -21 \leq l \leq 21 |
| Reflections collected | 18774 |
| Independent reflections | 8275 [$R_{\text{int}} = 0.0320$, $R_{\text{sigma}} = 0.0459$] |
| Data/restraints/parameters | 8275/0/367 |
| Goodness-of-fit on F^2 | 1.009 |
| Final R indexes [$I \geq 2\sigma(I)$] | $R_1 = 0.0424$, $wR_2 = 0.1086$ |
| Final R indexes [all data] | $R_1 = 0.0655$, $wR_2 = 0.1227$ |
| Largest diff. peak/hole / e \AA^{-3} | 0.61/-0.35 |

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor

| Atom | x | y | z | U(eq) |
|------|------------|------------|------------|----------|
| S1 | 6926.4(5) | 2750.9(3) | 5396.1(2) | 17.60(9) |
| O1 | 6840.9(14) | 6184.4(10) | 5482.6(7) | 23.9(2) |
| O2 | 8471.2(14) | 2819(1) | 3851.4(7) | 23.9(2) |
| O3 | 9521.7(14) | 4636.9(9) | 3189.5(7) | 22.7(2) |
| N1 | 6059.4(16) | 4438.3(11) | 6304.1(8) | 17.9(2) |
| N2 | 5610.3(15) | 2345.8(11) | 6838.6(8) | 17.5(2) |
| N3 | 4690.2(17) | 3654.2(12) | 7754.9(8) | 24.3(3) |
| N4 | 4567.0(17) | 1607.9(12) | 8075.2(8) | 23.2(3) |
| C1 | 6088.7(17) | 3243.4(13) | 6286.2(9) | 16.4(3) |
| C2 | 6706.7(18) | 5071.7(13) | 5617.3(9) | 18.0(3) |
| C3 | 7320.4(17) | 4266.8(13) | 5024.1(9) | 16.4(3) |
| C4 | 8064.4(18) | 4733.3(13) | 4338.4(9) | 18.8(3) |
| C5 | 8682.1(18) | 3947.1(13) | 3782.7(9) | 18.0(3) |
| C6 | 10134(2) | 3926.7(15) | 2600.7(10) | 25.1(3) |
| C7 | 4953.2(18) | 2566.0(13) | 7560.3(9) | 18.1(3) |
| S1A | 6418.5(5) | 1393.9(3) | 919.9(2) | 17.77(9) |
| O1A | 6501.8(16) | 4870.5(10) | 1076.5(8) | 29.0(3) |
| O2A | 8114.7(14) | 1538.3(10) | -598.0(7) | 23.6(2) |
| O3A | 8815.7(14) | 3311.8(10) | -1352.1(7) | 24.1(2) |
| N1A | 5671.0(16) | 3104.0(11) | 1879.1(8) | 19.2(2) |
| N2A | 5127.7(15) | 977.9(11) | 2370.3(8) | 17.4(2) |
| N3A | 4264.5(16) | 2283.0(12) | 3322.6(8) | 20.4(3) |

| | | | | |
|------|------------|------------|-------------|---------|
| N4A | 4108.8(16) | 215.6(12) | 3609.9(8) | 22.1(3) |
| C1A | 5636.2(17) | 1891.5(13) | 1837.2(9) | 16.6(3) |
| C2A | 6318.9(19) | 3745.7(14) | 1193.5(9) | 20.0(3) |
| C3A | 6852.3(18) | 2923.5(13) | 568.8(9) | 17.6(3) |
| C4A | 7571.7(19) | 3397.9(14) | -121.9(9) | 20.3(3) |
| C5A | 8170.5(19) | 2634.7(14) | -703.9(9) | 19.1(3) |
| C6A | 9512(2) | 2658.1(16) | -1940(1) | 27.7(3) |
| C7A | 4510.3(17) | 1194.8(13) | 3110.0(9) | 17.2(3) |
| O4 | 7136.3(16) | 8002.6(11) | 10629.1(8) | 31.1(3) |
| N5 | 8180.9(16) | 8054.6(12) | 9352.2(8) | 19.5(2) |
| C8 | 7708.2(19) | 8583.4(14) | 10010.2(10) | 21.3(3) |
| C9 | 8917(2) | 8807.2(15) | 8664.9(10) | 23.3(3) |
| C10 | 8009(2) | 6703.2(14) | 9309.0(11) | 25.8(3) |
| O4A | 2692.7(15) | 757(1) | 4982.5(7) | 26.4(2) |
| N5A | 1291.8(16) | 606.2(11) | 6143.2(8) | 19.7(2) |
| C8A | 2098.9(19) | 172.4(14) | 5597.9(9) | 20.9(3) |
| C9A | 576(2) | -154.1(16) | 6833.4(11) | 27.3(3) |
| C10A | 1045(2) | 1829.1(15) | 6039.1(11) | 28.2(3) |

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+...]$

| Atom | U_{11} | U_{22} | U_{33} | U_{23} | U_{13} | U_{12} |
|------|-----------|-----------|-----------|----------|----------|-----------|
| S1 | 25.91(19) | 15.42(16) | 16.42(16) | 1.59(12) | 9.54(13) | 10.82(14) |
| O1 | 37.7(6) | 17.0(5) | 23.9(5) | 2.5(4) | 12.7(5) | 14.8(5) |
| O2 | 33.3(6) | 18.3(5) | 26.5(5) | 3.4(4) | 15.0(5) | 12.6(4) |
| O3 | 31.8(6) | 18.5(5) | 20.8(5) | 0.7(4) | 14.7(4) | 8.0(4) |
| N1 | 23.3(6) | 17.5(6) | 16.2(5) | -0.1(4) | 6.0(5) | 10.0(5) |
| N2 | 23.7(6) | 17.4(5) | 15.0(5) | 0.7(4) | 8.8(5) | 9.4(5) |
| N3 | 36.3(7) | 23.8(6) | 20.6(6) | 0.8(5) | 14.7(5) | 16.4(6) |
| N4 | 34.6(7) | 22.4(6) | 18.2(6) | 2.1(5) | 14.1(5) | 12.8(5) |
| C1 | 17.5(6) | 18.9(6) | 14.6(6) | -1.2(5) | 3.6(5) | 8.4(5) |
| C2 | 21.2(7) | 17.5(6) | 17.7(6) | -1.6(5) | 5.5(5) | 8.7(5) |
| C3 | 20.0(7) | 15.1(6) | 16.1(6) | -0.6(5) | 4.3(5) | 8.3(5) |
| C4 | 26.3(7) | 14.3(6) | 18.9(6) | 1.0(5) | 8.1(6) | 8.9(5) |
| C5 | 21.4(7) | 17.4(6) | 17.1(6) | -0.2(5) | 6.4(5) | 7.7(5) |
| C6 | 29.0(8) | 28.1(8) | 20.0(7) | -3.9(6) | 13.0(6) | 8.3(7) |
| C7 | 20.4(7) | 21.0(7) | 15.2(6) | -1.6(5) | 5.0(5) | 9.1(6) |

| | | | | | | |
|------|-----------|-----------|-----------|----------|----------|-----------|
| S1A | 26.01(19) | 15.84(16) | 15.98(16) | 0.92(12) | 8.69(13) | 10.75(14) |
| O1A | 47.1(7) | 18.3(5) | 31.0(6) | 4.4(4) | 19.7(5) | 17.6(5) |
| O2A | 35.8(6) | 20.0(5) | 22.1(5) | 3.3(4) | 12.0(5) | 15.4(5) |
| O3A | 37.6(6) | 23.3(5) | 21.1(5) | 7.0(4) | 16.8(5) | 17.7(5) |
| N1A | 24.9(6) | 17.7(6) | 18.6(6) | -0.1(4) | 8.2(5) | 10.2(5) |
| N2A | 21.6(6) | 19.0(6) | 14.8(5) | 0.0(4) | 7.0(5) | 9.2(5) |
| N3A | 26.9(6) | 21.3(6) | 17.2(5) | -1.8(4) | 8.1(5) | 11.8(5) |
| N4A | 31.6(7) | 22.3(6) | 18.6(6) | 2.3(5) | 13.4(5) | 12.9(5) |
| C1A | 17.9(6) | 19.2(6) | 14.8(6) | -1.2(5) | 4.9(5) | 8.2(5) |
| C2A | 26.0(7) | 18.9(7) | 19.6(7) | 0.5(5) | 8.0(6) | 11.7(6) |
| C3A | 23.5(7) | 16.1(6) | 16.8(6) | 0.8(5) | 5.5(5) | 10.8(5) |
| C4A | 28.7(8) | 17.0(6) | 20.3(7) | 2.2(5) | 9.1(6) | 12.2(6) |
| C5A | 24.6(7) | 19.8(7) | 16.6(6) | 2.0(5) | 6.7(5) | 10.9(6) |
| C6A | 40.1(9) | 33.9(8) | 21.3(7) | 6.2(6) | 18.5(7) | 22.5(7) |
| C7A | 18.8(7) | 19.3(7) | 14.9(6) | -1.8(5) | 4.5(5) | 8.0(5) |
| O4 | 46.1(7) | 33.8(6) | 26.6(6) | 9.7(5) | 22.2(5) | 23.6(6) |
| N5 | 26.6(6) | 19.7(6) | 16.9(6) | 2.6(4) | 8.6(5) | 11.8(5) |
| C8 | 27.5(8) | 21.9(7) | 20.2(7) | 1.4(5) | 8.2(6) | 13.9(6) |
| C9 | 28.1(8) | 27.2(8) | 18.0(7) | 4.6(6) | 8.7(6) | 11.4(6) |
| C10 | 36.0(9) | 20.3(7) | 27.3(8) | 1.3(6) | 11.3(7) | 15.0(7) |
| O4A | 36.6(6) | 26.5(6) | 22.4(5) | 2.9(4) | 16.4(5) | 14.0(5) |
| N5A | 25.9(6) | 18.8(6) | 20.3(6) | 4.4(4) | 11.9(5) | 11.4(5) |
| C8A | 25.4(7) | 19.2(7) | 21.3(7) | 0.2(5) | 8.5(6) | 9.7(6) |
| C9A | 32.3(9) | 28.9(8) | 25.7(8) | 9.2(6) | 16.0(7) | 11.5(7) |
| C10A | 41.5(10) | 22.6(7) | 28.7(8) | 2.8(6) | 13.5(7) | 18.5(7) |

Table S4. Bond Lengths for **9**

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|------|------|------------|------|------|------------|
| S1 | C1 | 1.7912(14) | O3A | C5A | 1.3403(17) |
| S1 | C3 | 1.7324(14) | O3A | C6A | 1.4540(17) |
| O1 | C2 | 1.2268(17) | N1A | C1A | 1.3347(17) |
| O2 | C5 | 1.2139(17) | N1A | C2A | 1.3724(18) |
| O3 | C5 | 1.3454(16) | N2A | C1A | 1.3225(17) |
| O3 | C6 | 1.4475(17) | N2A | C7A | 1.3735(17) |
| N1 | C1 | 1.3328(17) | N3A | C7A | 1.3321(17) |
| N1 | C2 | 1.3700(17) | N4A | C7A | 1.3286(18) |
| N2 | C1 | 1.3271(18) | C2A | C3A | 1.5255(18) |

| | | | | | |
|-----|-----|------------|-----|------|------------|
| N2 | C7 | 1.3698(17) | C3A | C4A | 1.3419(19) |
| N3 | C7 | 1.3329(18) | C4A | C5A | 1.4724(19) |
| N4 | C7 | 1.3250(18) | O4 | C8 | 1.2357(17) |
| C2 | C3 | 1.5228(18) | N5 | C8 | 1.3359(17) |
| C3 | C4 | 1.3426(19) | N5 | C9 | 1.4542(18) |
| C4 | C5 | 1.4743(18) | N5 | C10 | 1.4559(18) |
| S1A | C1A | 1.7995(13) | O4A | C8A | 1.2394(17) |
| S1A | C3A | 1.7320(14) | N5A | C8A | 1.3367(17) |
| O1A | C2A | 1.2264(17) | N5A | C9A | 1.4555(18) |
| O2A | C5A | 1.2167(17) | N5A | C10A | 1.4469(19) |

Table S5. Bond Angles for **9**

| Atom | Atom | Atom | Angle/° | Atom | Atom | Atom | Angle/° |
|------|------|------|------------|------|------|------|------------|
| C3 | S1 | C1 | 89.18(6) | N1A | C1A | S1A | 116.07(10) |
| C5 | O3 | C6 | 115.13(11) | N2A | C1A | S1A | 113.48(10) |
| C1 | N1 | C2 | 111.86(11) | N2A | C1A | N1A | 130.45(12) |
| C1 | N2 | C7 | 121.32(12) | O1A | C2A | N1A | 125.47(13) |
| N1 | C1 | S1 | 116.32(10) | O1A | C2A | C3A | 121.29(13) |
| N2 | C1 | S1 | 113.68(10) | N1A | C2A | C3A | 113.23(12) |
| N2 | C1 | N1 | 130.00(12) | C2A | C3A | S1A | 109.46(10) |
| O1 | C2 | N1 | 125.25(12) | C4A | C3A | S1A | 128.64(11) |
| O1 | C2 | C3 | 121.43(12) | C4A | C3A | C2A | 121.88(12) |
| N1 | C2 | C3 | 113.30(11) | C3A | C4A | C5A | 122.51(13) |
| C2 | C3 | S1 | 109.31(9) | O2A | C5A | O3A | 124.49(13) |
| C4 | C3 | S1 | 128.29(11) | O2A | C5A | C4A | 124.17(13) |
| C4 | C3 | C2 | 122.39(12) | O3A | C5A | C4A | 111.33(12) |
| C3 | C4 | C5 | 121.59(13) | N3A | C7A | N2A | 124.14(13) |
| O2 | C5 | O3 | 123.90(12) | N4A | C7A | N2A | 115.39(12) |
| O2 | C5 | C4 | 124.50(13) | N4A | C7A | N3A | 120.44(12) |
| O3 | C5 | C4 | 111.61(12) | C8 | N5 | C9 | 121.50(12) |
| N3 | C7 | N2 | 124.10(13) | C8 | N5 | C10 | 120.95(12) |
| N4 | C7 | N2 | 115.64(12) | C9 | N5 | C10 | 117.54(12) |
| N4 | C7 | N3 | 120.27(13) | O4 | C8 | N5 | 124.29(14) |
| C3A | S1A | C1A | 89.20(6) | C8A | N5A | C9A | 121.30(12) |
| C5A | O3A | C6A | 115.47(11) | C8A | N5A | C10A | 120.66(12) |
| C1A | N1A | C2A | 112.02(11) | C10A | N5A | C9A | 117.99(12) |
| C1A | N2A | C7A | 121.31(12) | O4A | C8A | N5A | 124.36(14) |

Table S6. Hydrogen Bonds for **9**

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|-----|------|------------------|----------|----------|------------|---------|
| N3 | H3A | O1A ¹ | 0.88 | 2.18 | 2.9085(16) | 140.3 |
| N3 | H3B | N1 | 0.88 | 2.06 | 2.7091(17) | 129.9 |
| N4 | H4A | O4 ² | 0.88 | 1.88 | 2.7467(16) | 166.4 |
| N3A | H3AA | O1 ¹ | 0.88 | 2.21 | 2.9317(15) | 138.6 |
| N3A | H3AB | N1A | 0.88 | 2.07 | 2.7220(17) | 129.7 |
| N4A | H4AA | O4A | 0.88 | 1.87 | 2.7362(16) | 167.0 |

¹1-X,1-Y,1-Z; ²1-X,1-Y,2-Z**Table S7.** Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for **9**

| Atom | x | y | z | U(eq) |
|------|-------|------|-------|-------|
| H3A | 4258 | 3739 | 8227 | 29 |
| H3B | 4948 | 4288 | 7411 | 29 |
| H4A | 4135 | 1689 | 8548 | 28 |
| H4B | 4742 | 891 | 7945 | 28 |
| H4 | 8196 | 5591 | 4208 | 23 |
| H6A | 10717 | 4501 | 2191 | 38 |
| H6B | 9185 | 3233 | 2267 | 38 |
| H6C | 10914 | 3566 | 2947 | 38 |
| H3AA | 3834 | 2357 | 3797 | 25 |
| H3AB | 4533 | 2928 | 2989 | 25 |
| H4AA | 3677 | 283 | 4085 | 27 |
| H4AB | 4274 | -501 | 3466 | 27 |
| H4AC | 7699 | 4259 | -240 | 24 |
| H6AA | 10458 | 2460 | -1603 | 42 |
| H6AB | 9903 | 3211 | -2405 | 42 |
| H6AC | 8645 | 1863 | -2208 | 42 |
| H8 | 7819 | 9464 | 10002 | 26 |
| H9A | 10085 | 8837 | 8703 | 35 |
| H9B | 8886 | 9678 | 8744 | 35 |
| H9C | 8278 | 8413 | 8085 | 35 |
| H10A | 7255 | 6272 | 8764 | 39 |
| H10B | 7541 | 6316 | 9819 | 39 |
| H10C | 9113 | 6613 | 9315 | 39 |
| H8A | 2226 | -638 | 5688 | 25 |

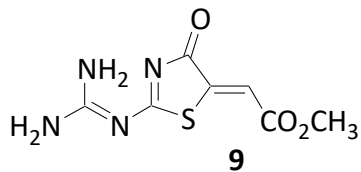
| | | | | |
|------|------|------|------|----|
| H9AA | 855 | -944 | 6839 | 41 |
| H9AB | -647 | -366 | 6719 | 41 |
| H9AC | 1039 | 336 | 7407 | 41 |
| H10D | -160 | 1702 | 5920 | 42 |
| H10E | 1563 | 2227 | 5545 | 42 |
| H10F | 1566 | 2387 | 6582 | 42 |

Experimental

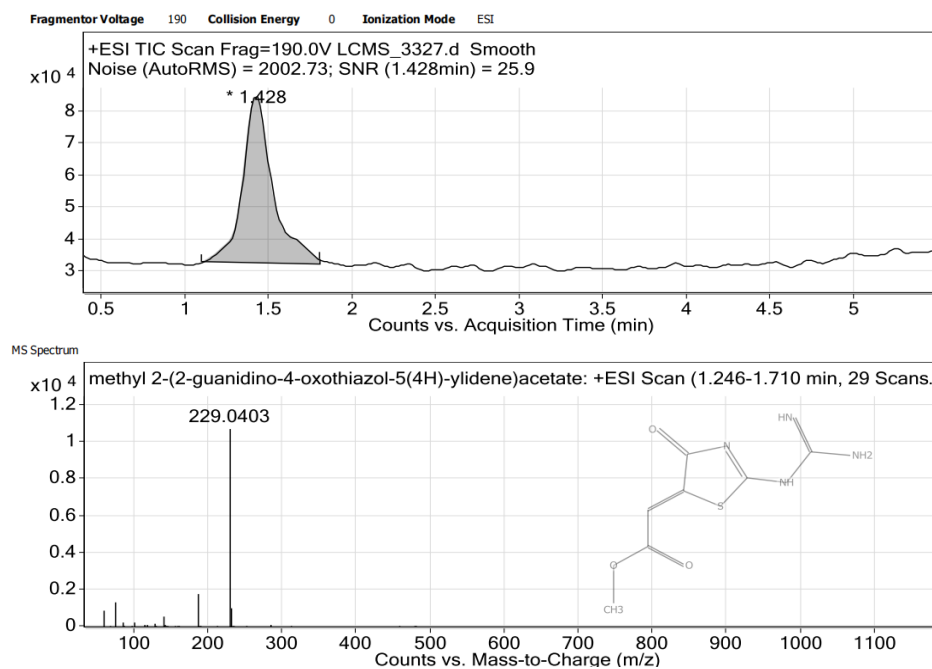
Single crystals of $C_{10}H_{15}N_5O_4S$ were prism. A suitable crystal was selected, and X-ray dataset was collected on a 'Bruker APEX-II CCD' diffractometer. The crystal was kept at 120 K during data collection. Using Olex2 [Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), *J. Appl. Cryst.* 42, 339-341], the structure was solved with the ShelXT [Sheldrick, G.M. (2015). *Acta Cryst.* A71, 3-8] structure solution program using Intrinsic Phasing and refined with the ShelXL [Sheldrick, G.M. (2015). *Acta Cryst.* C71, 3-8] refinement package using Least Squares minimisation.

Crystal structure determination of [Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), *J. Appl. Cryst.* 42, 339-341]

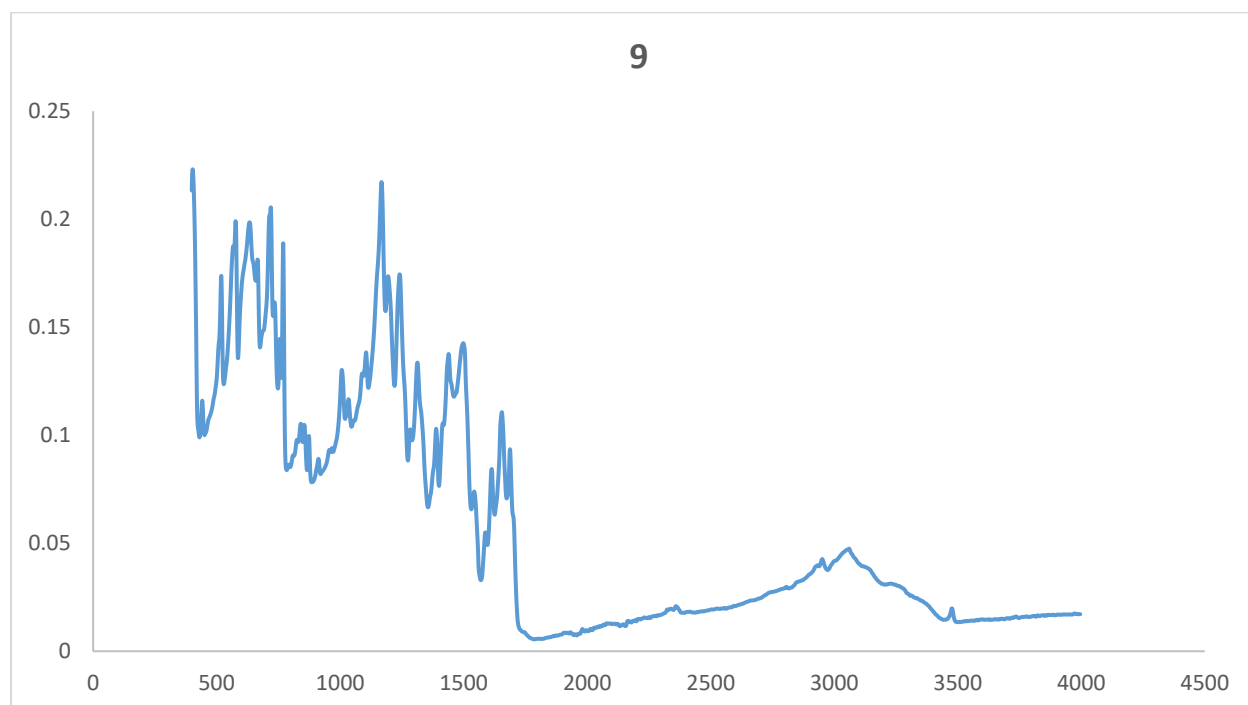
Crystal Data for $C_{10}H_{15}N_5O_4S$ ($M = 301.33$ g/mol): triclinic, space group P-1 (no. 2), $a = 8.5470(8)$ Å, $b = 11.0867(10)$ Å, $c = 15.3765(14)$ Å, $\alpha = 91.309(2)^\circ$, $\beta = 98.926(2)^\circ$, $\gamma = 108.968(2)^\circ$, $V = 1357.0(2)$ Å³, $Z = 4$, $T = 120$ K, $\mu(\text{MoK}\alpha) = 0.261$ mm⁻¹, $D_{\text{calc}} = 1.475$ g/cm³, 18774 reflections measured ($3.896^\circ \leq 2\theta \leq 61.006^\circ$), 8275 unique ($R_{\text{int}} = 0.0320$, $R_{\text{sigma}} = 0.0459$) which were used in all calculations. The final R_1 was 0.0424 ($I > 2\sigma(I)$) and wR_2 was 0.1227 (all data). Structural data deposited as CDCC: 2131042.

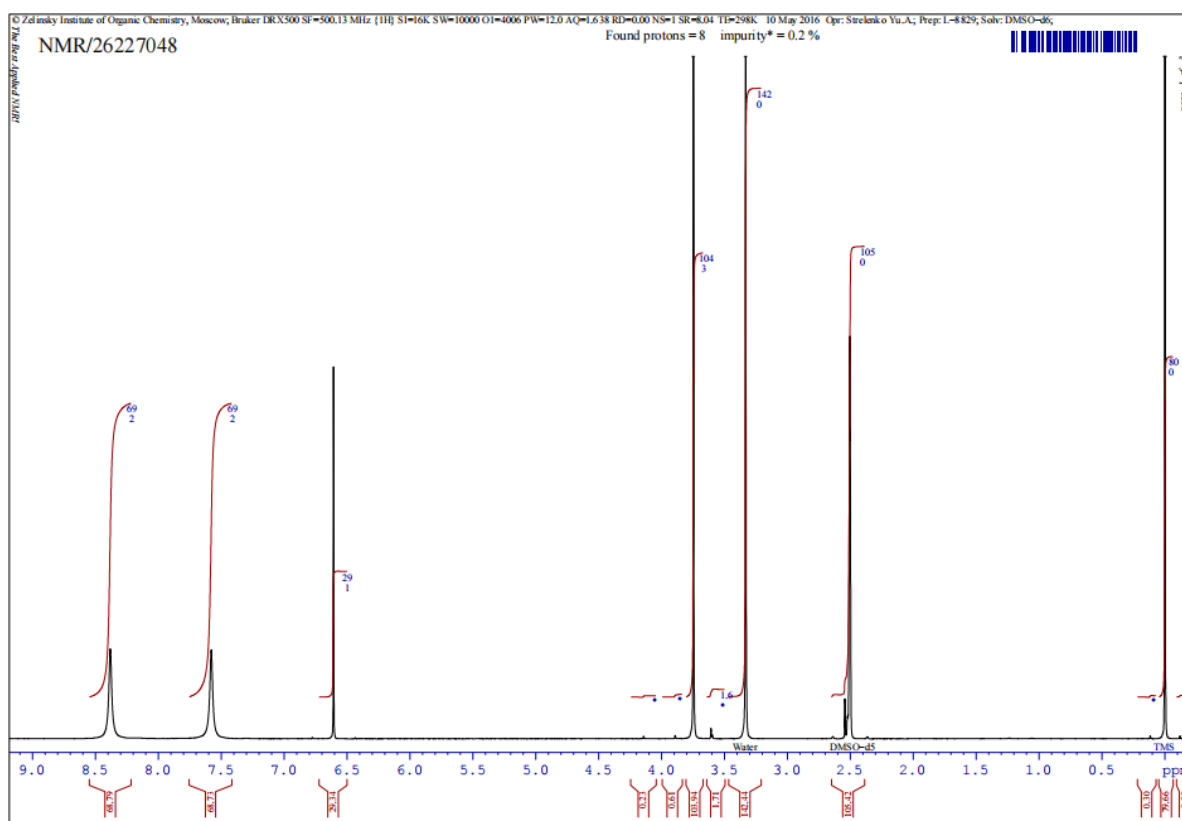
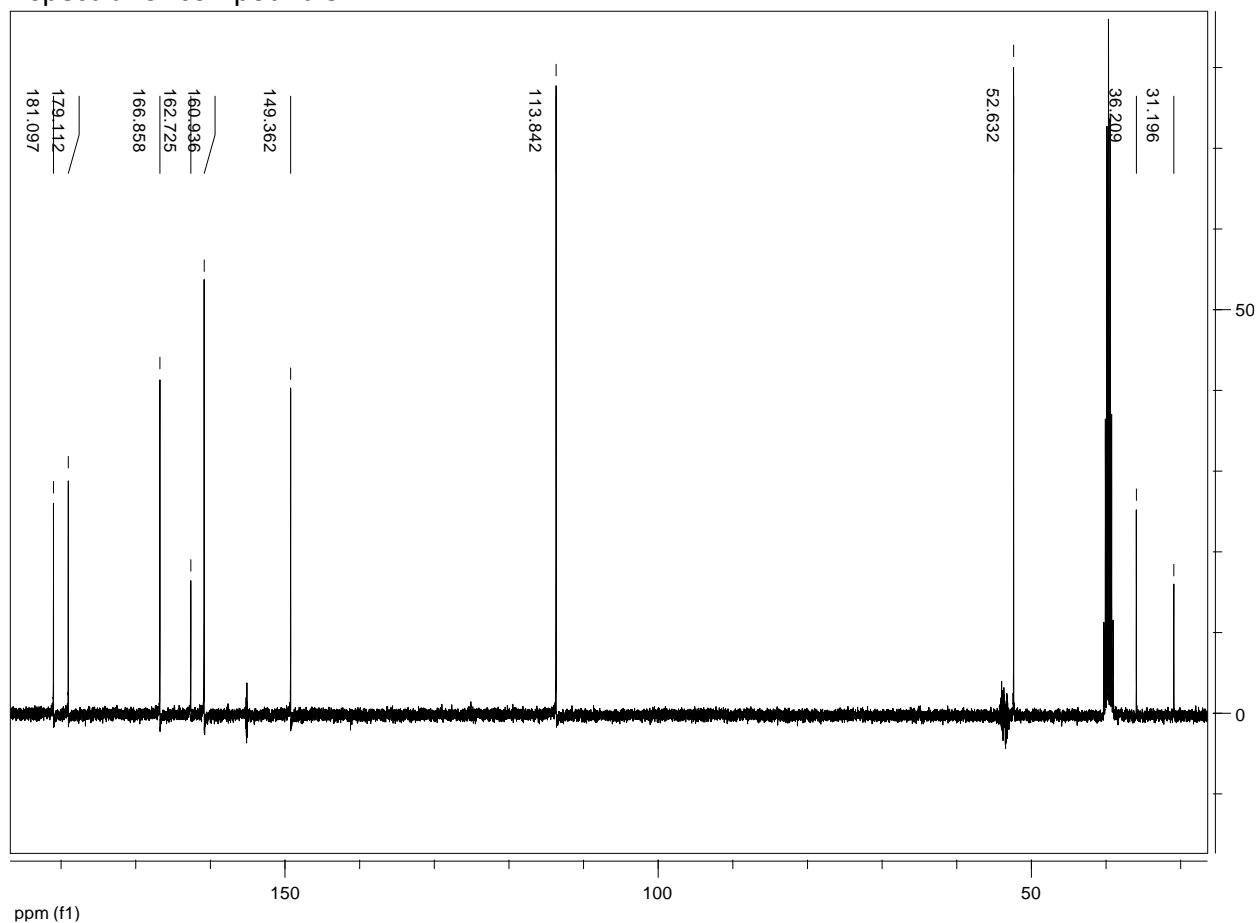
IR, ^1H and ^{13}C NMR spectra and data LCMS for compounds 9, 17 a-f

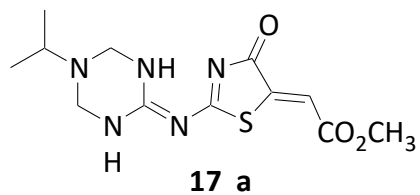
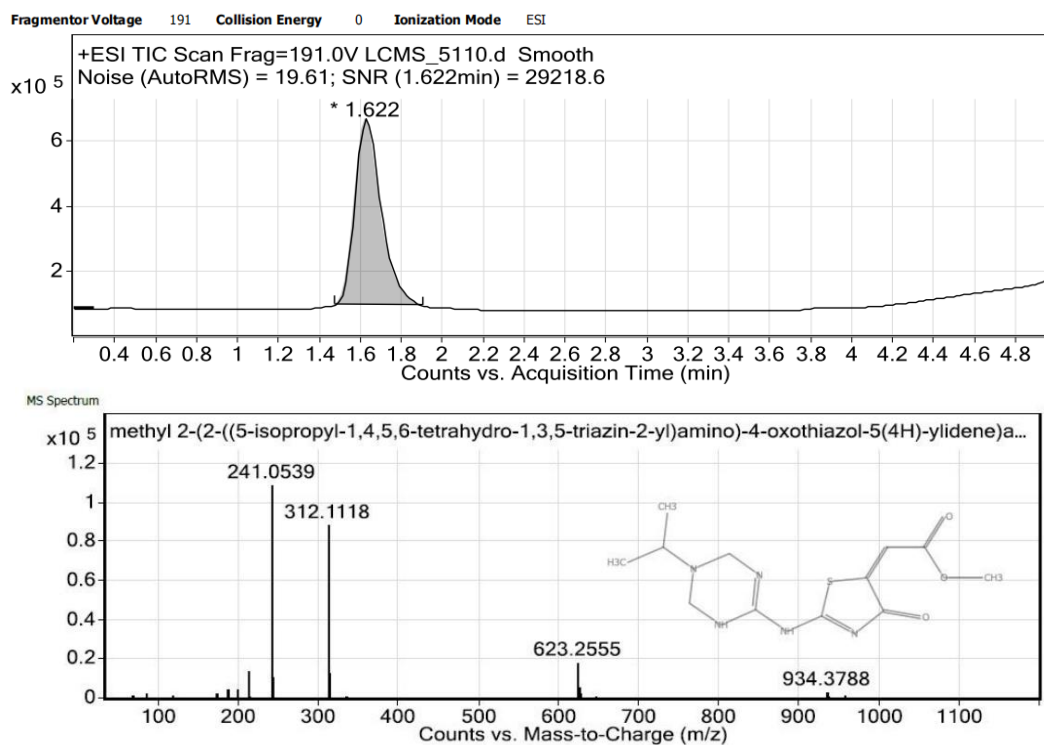
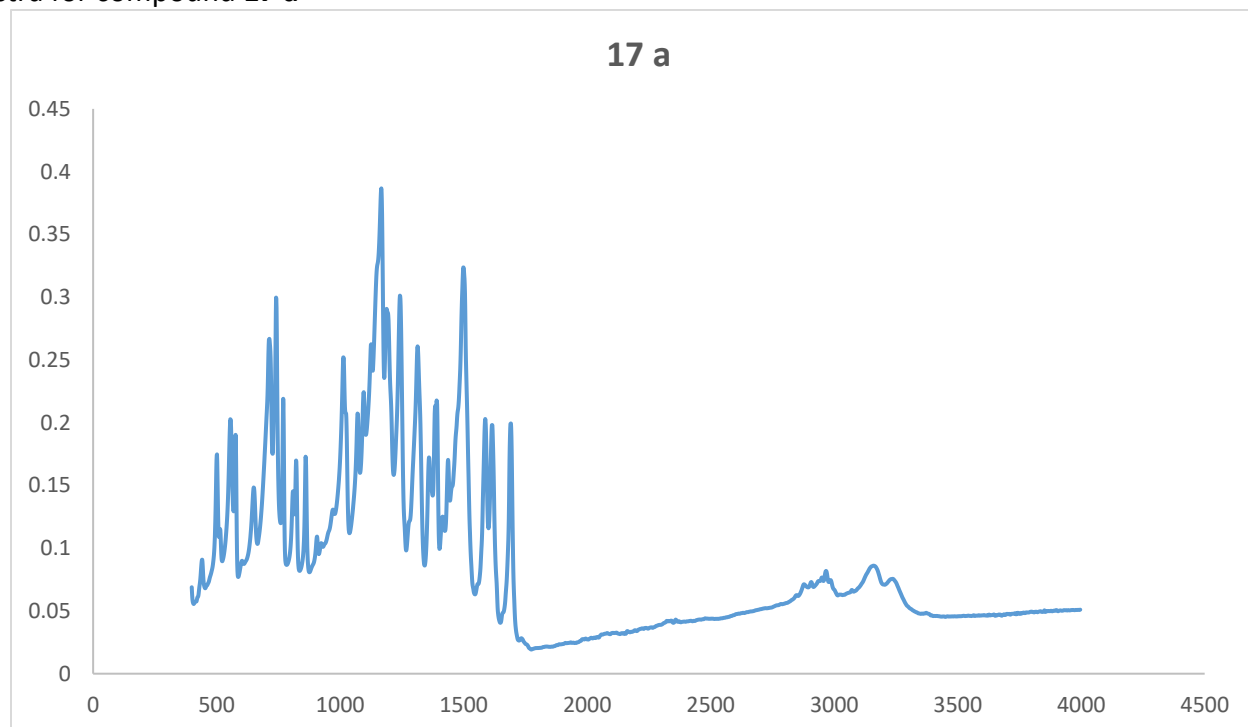
Data LCMS for compound 9

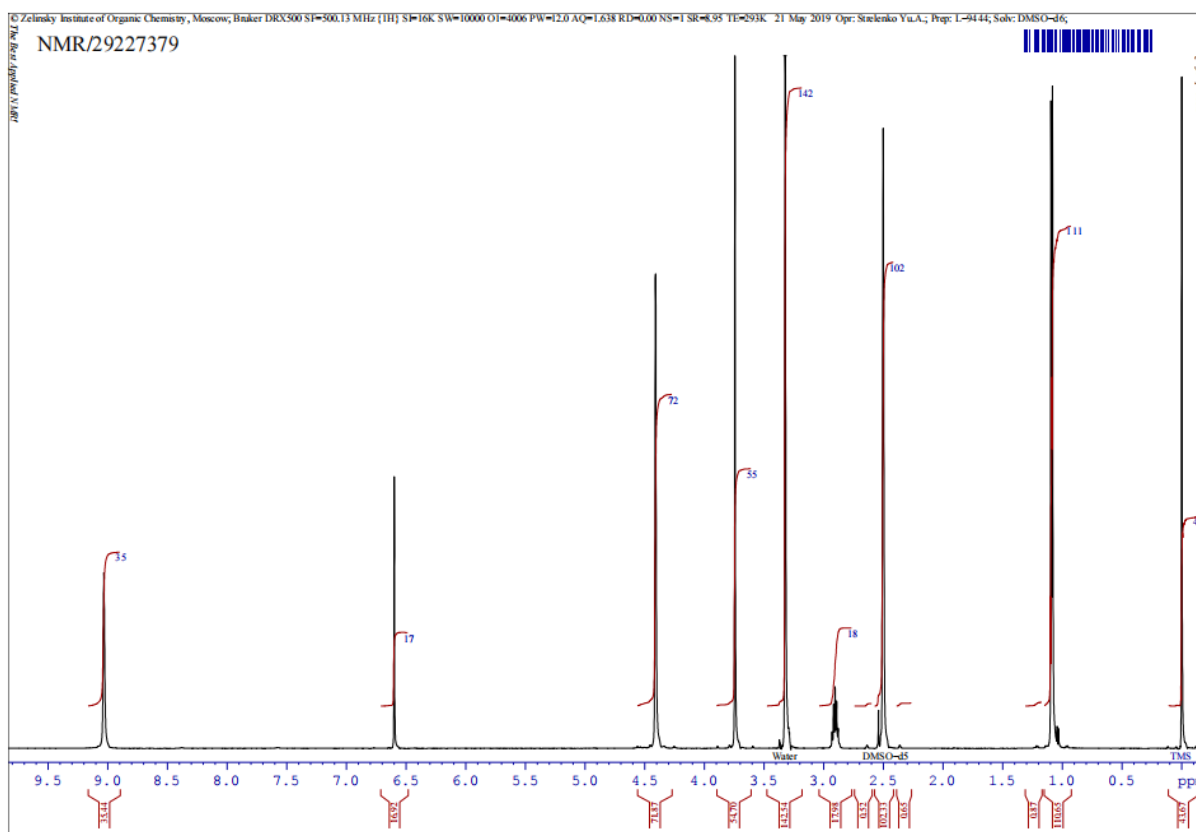
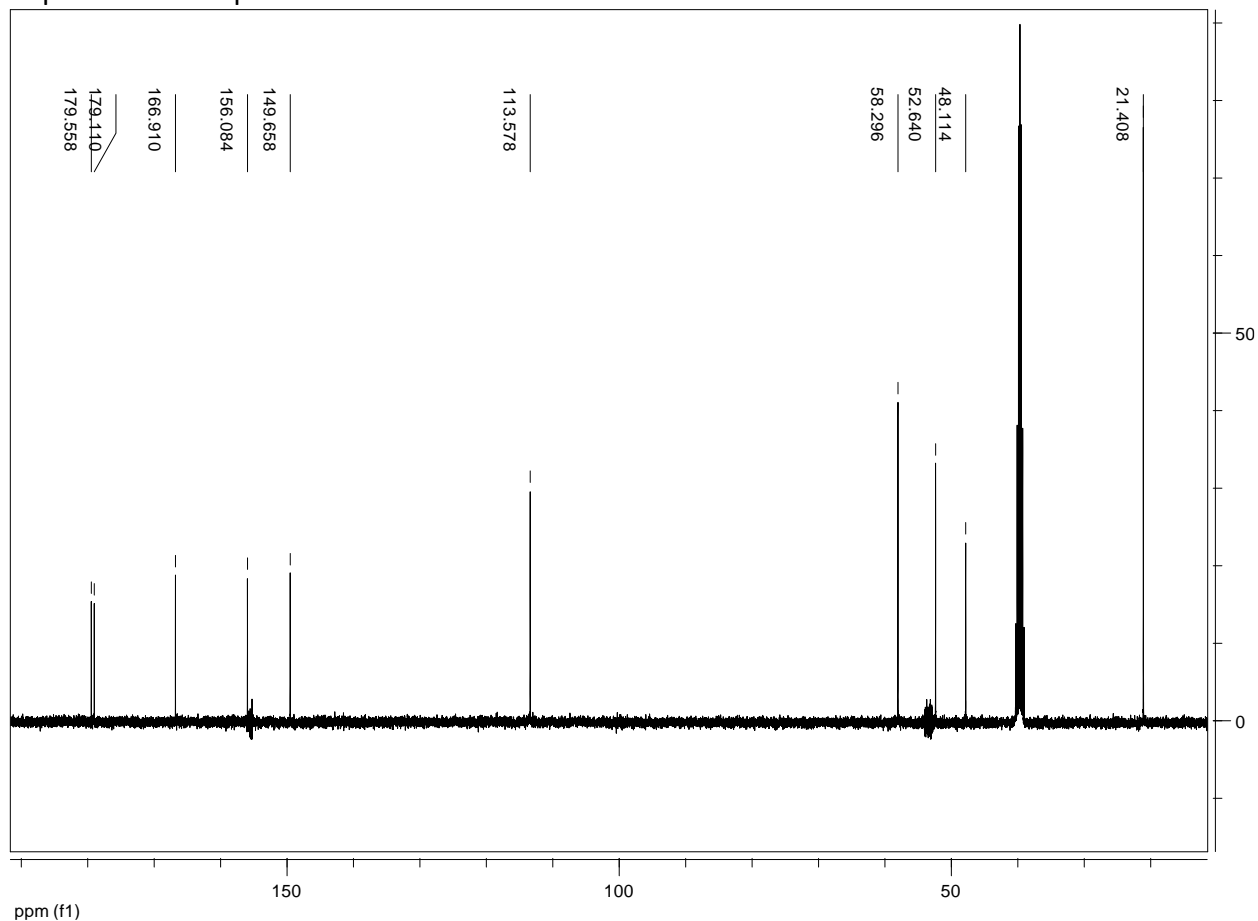


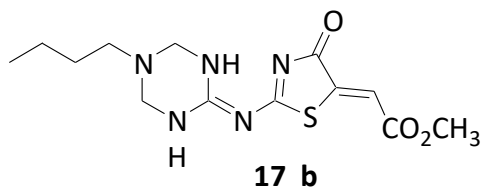
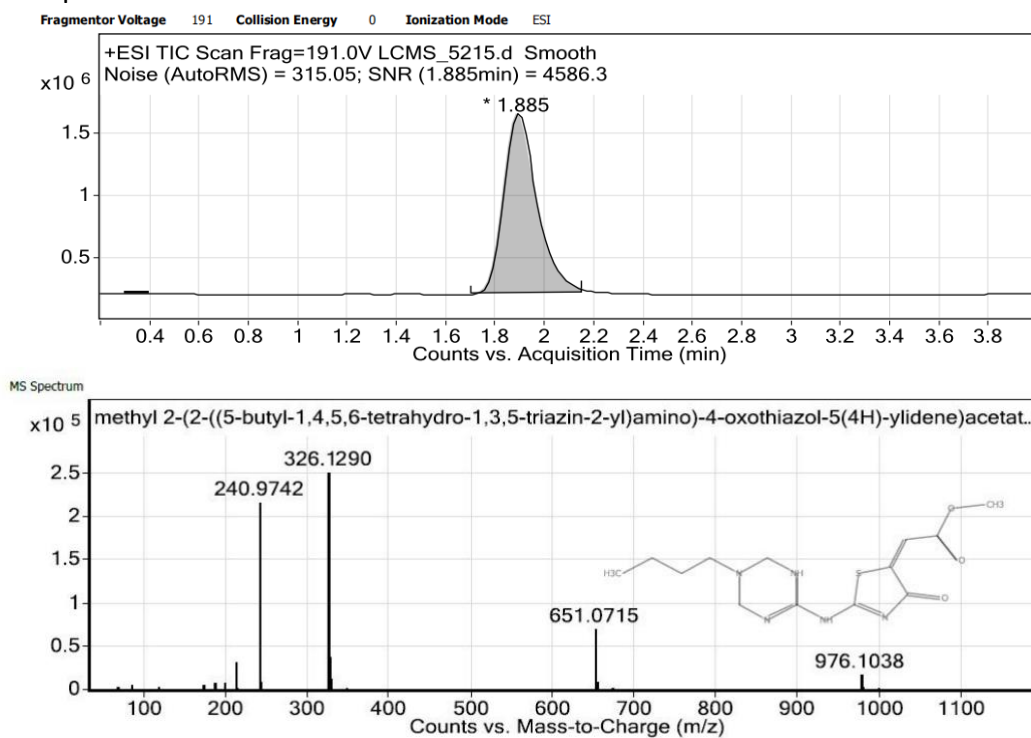
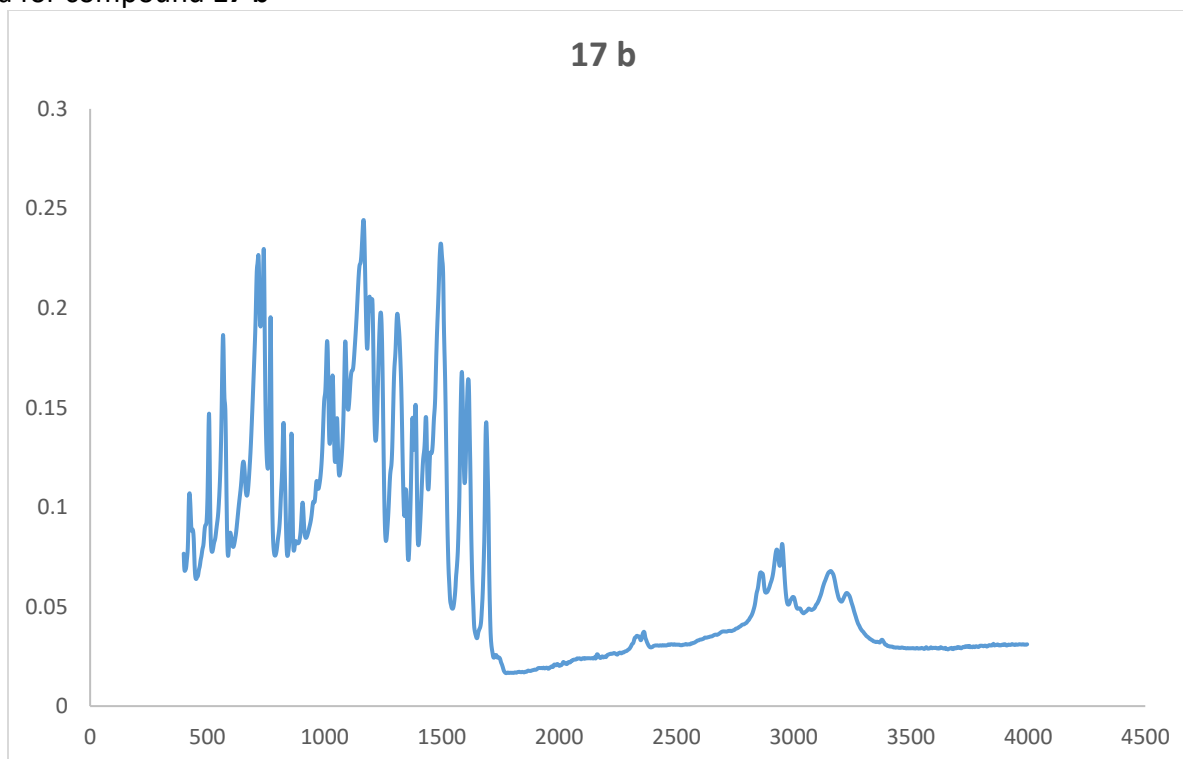
IR spectra for compound 9

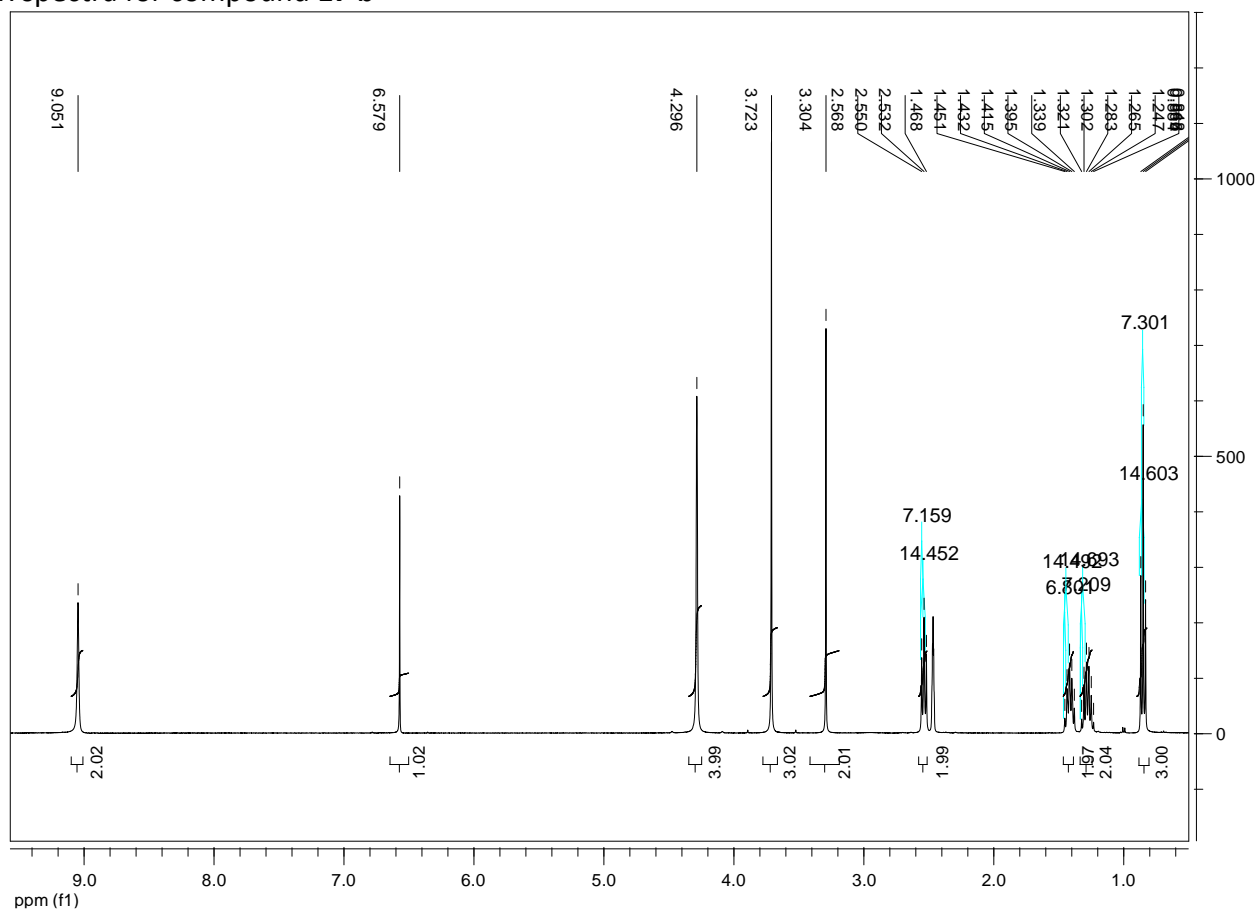
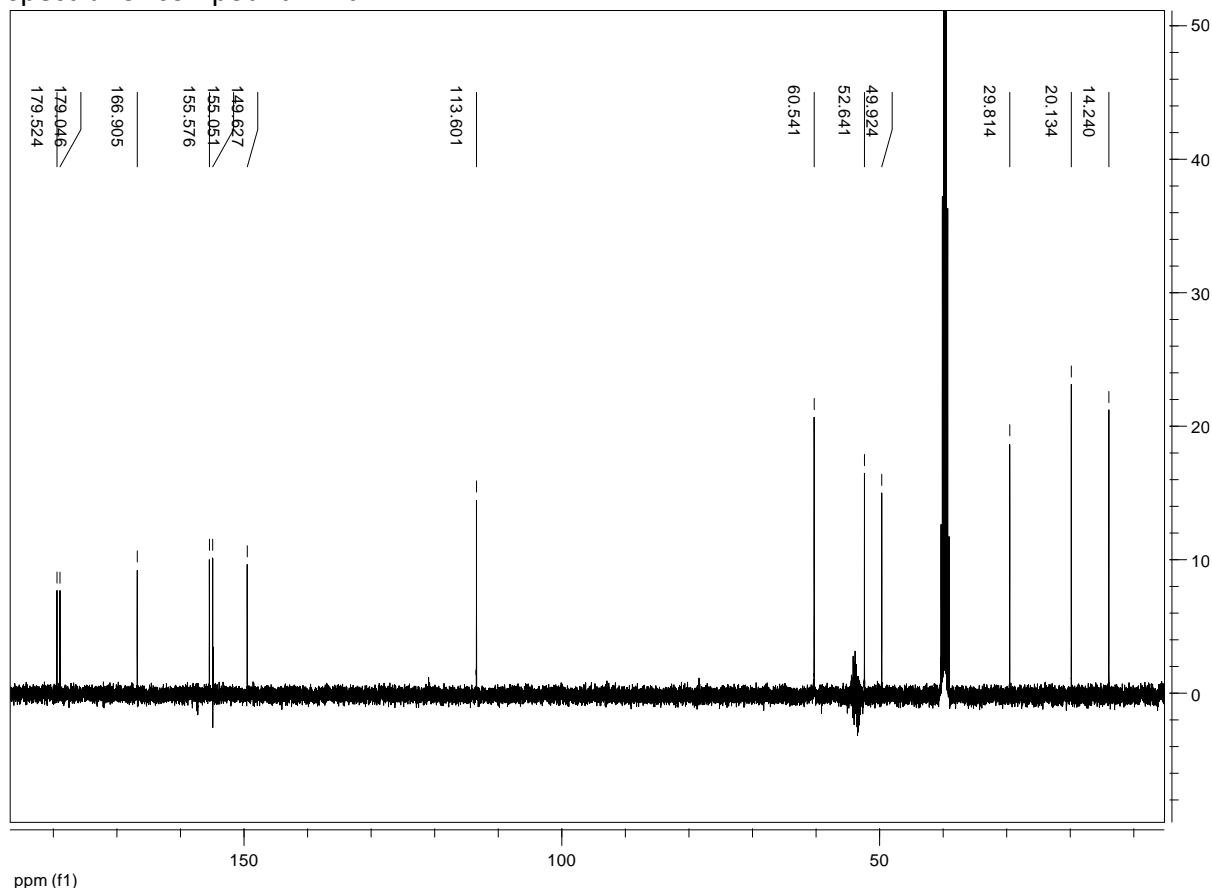


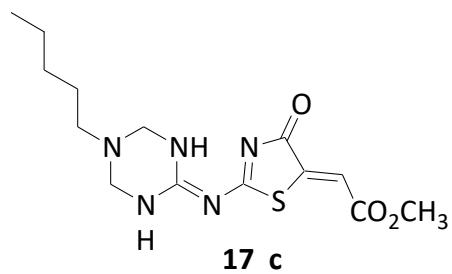
^1H NMR spectra for compound **9** ^{13}C NMR spectra for compound **9**

Data LCMS for compound **17 a**IR spectra for compound **17 a**

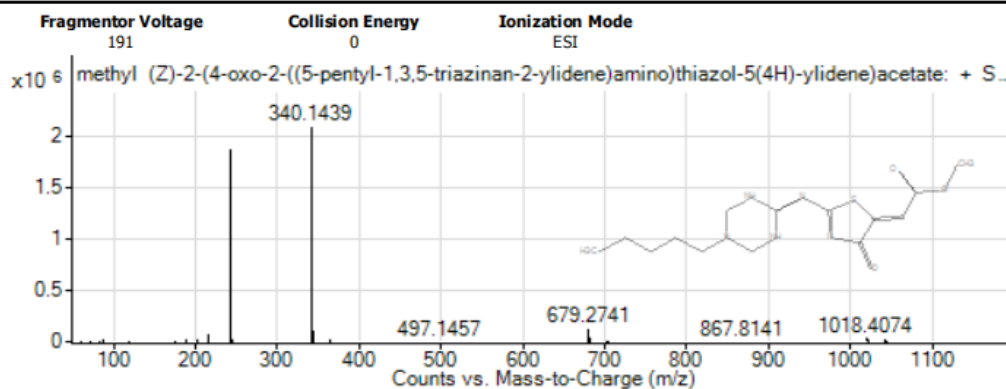
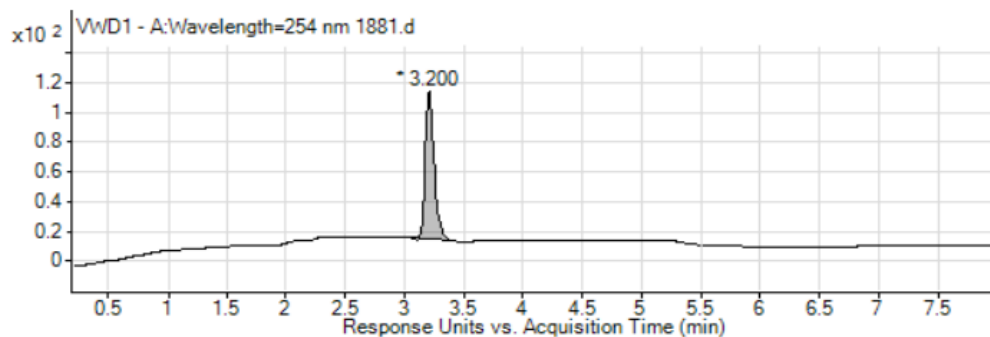
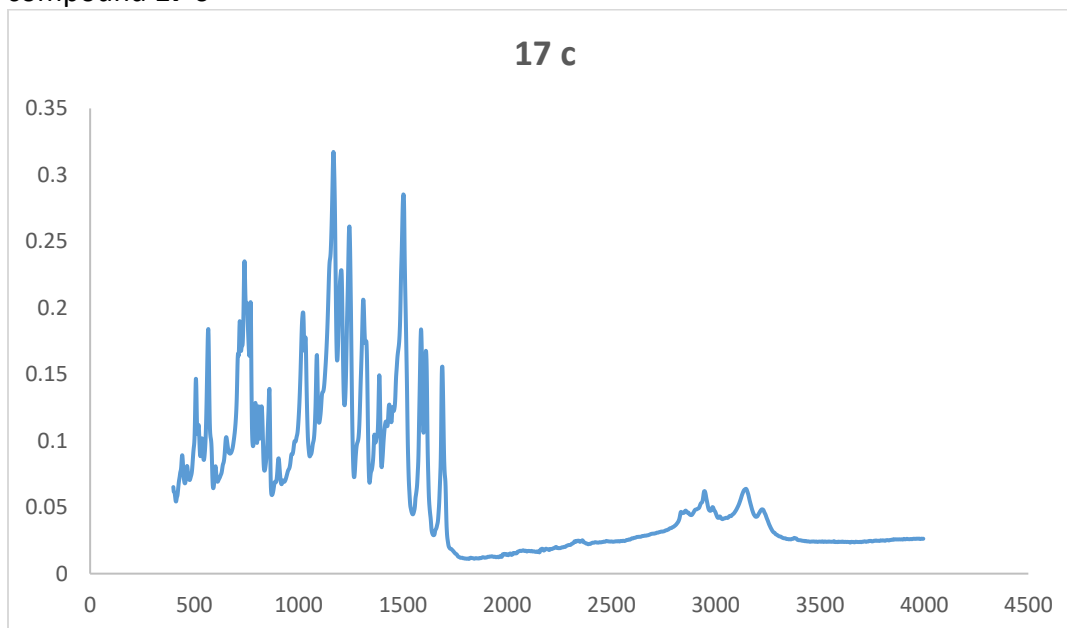
^1H NMR spectra for compound **17 a** ^{13}C NMR spectra for compound **17 a**

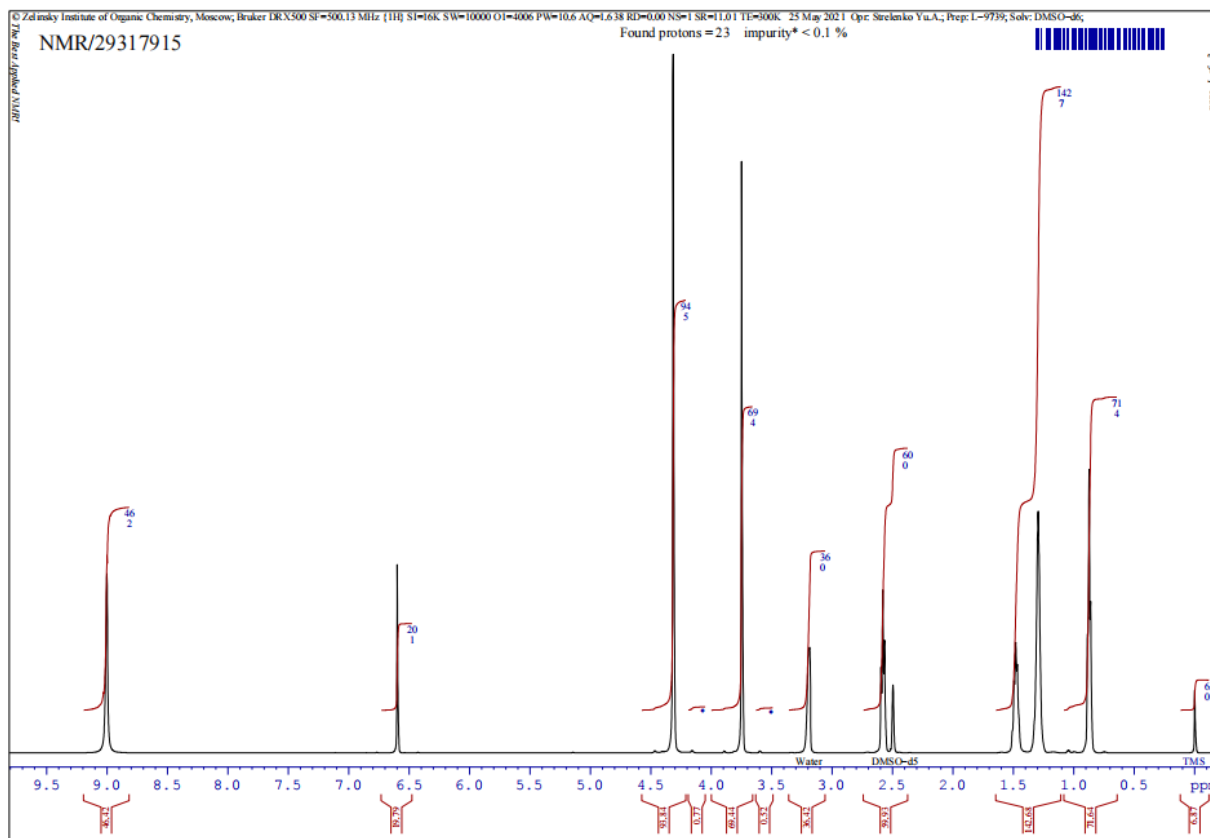
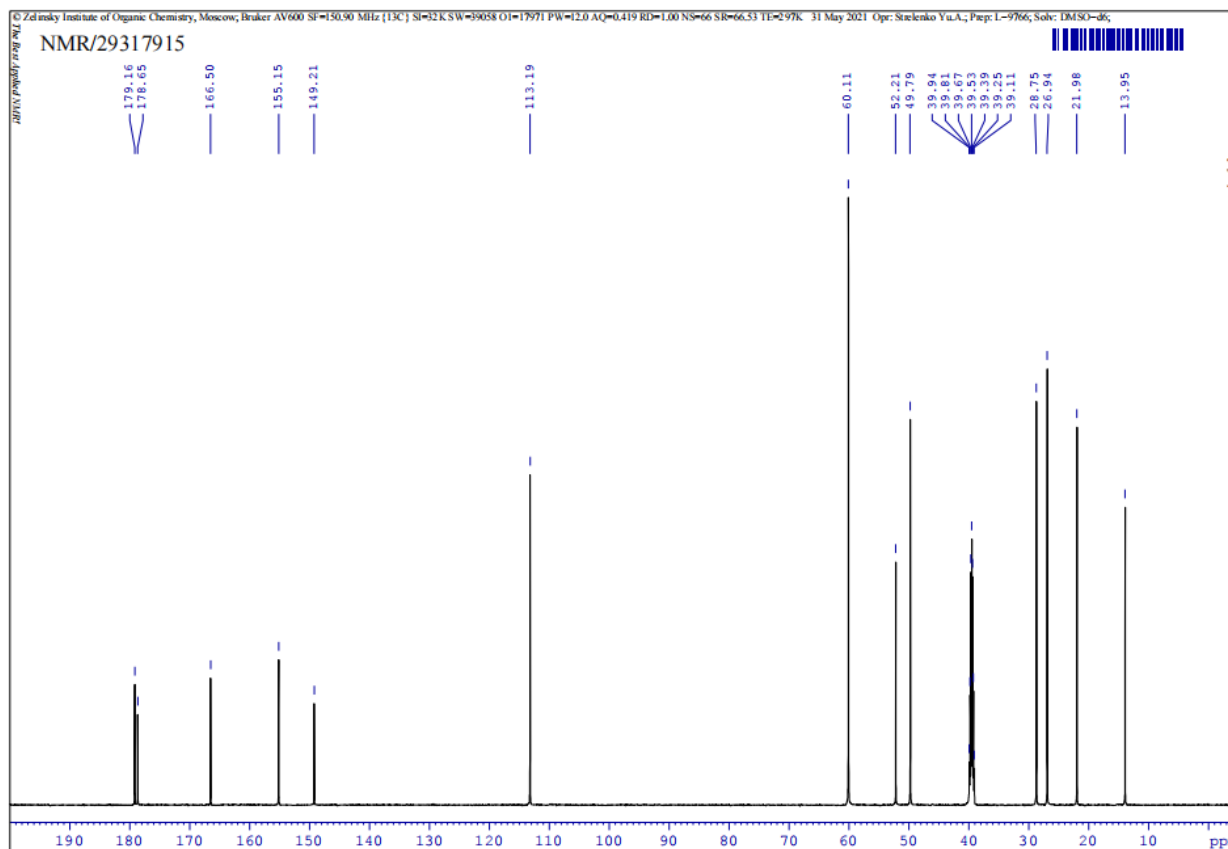
Data LCMS for compound **17 b**IR spectra for compound **17 b**

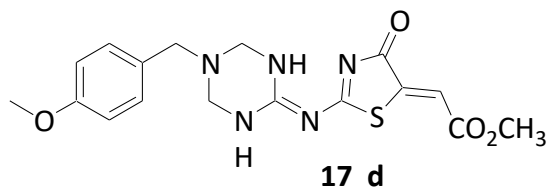
¹H NMR spectra for compound **17 b**¹³C NMR spectra for compound **17 b**

Data LCMS for compound **17 c**

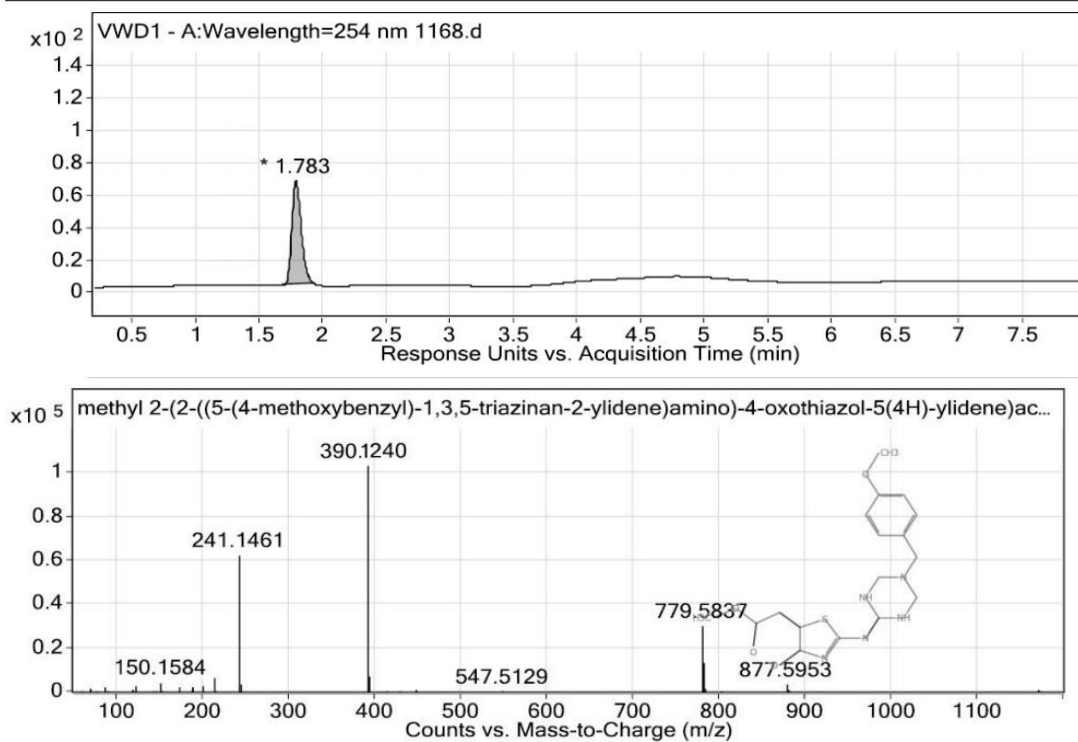
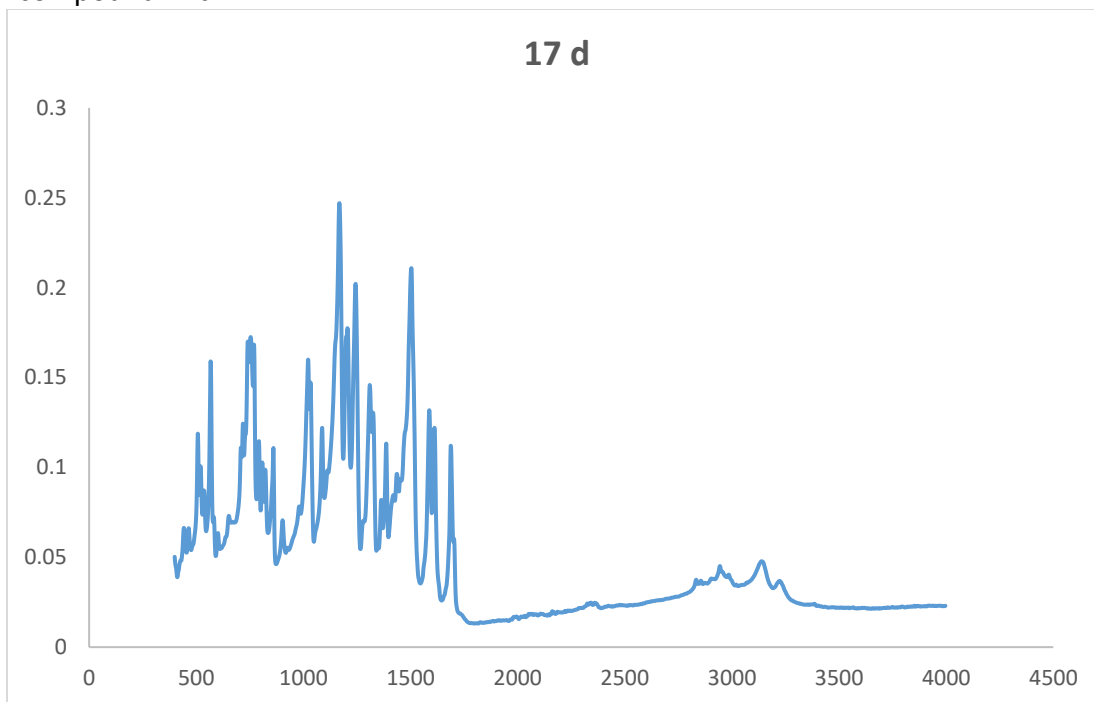
User Chromatograms

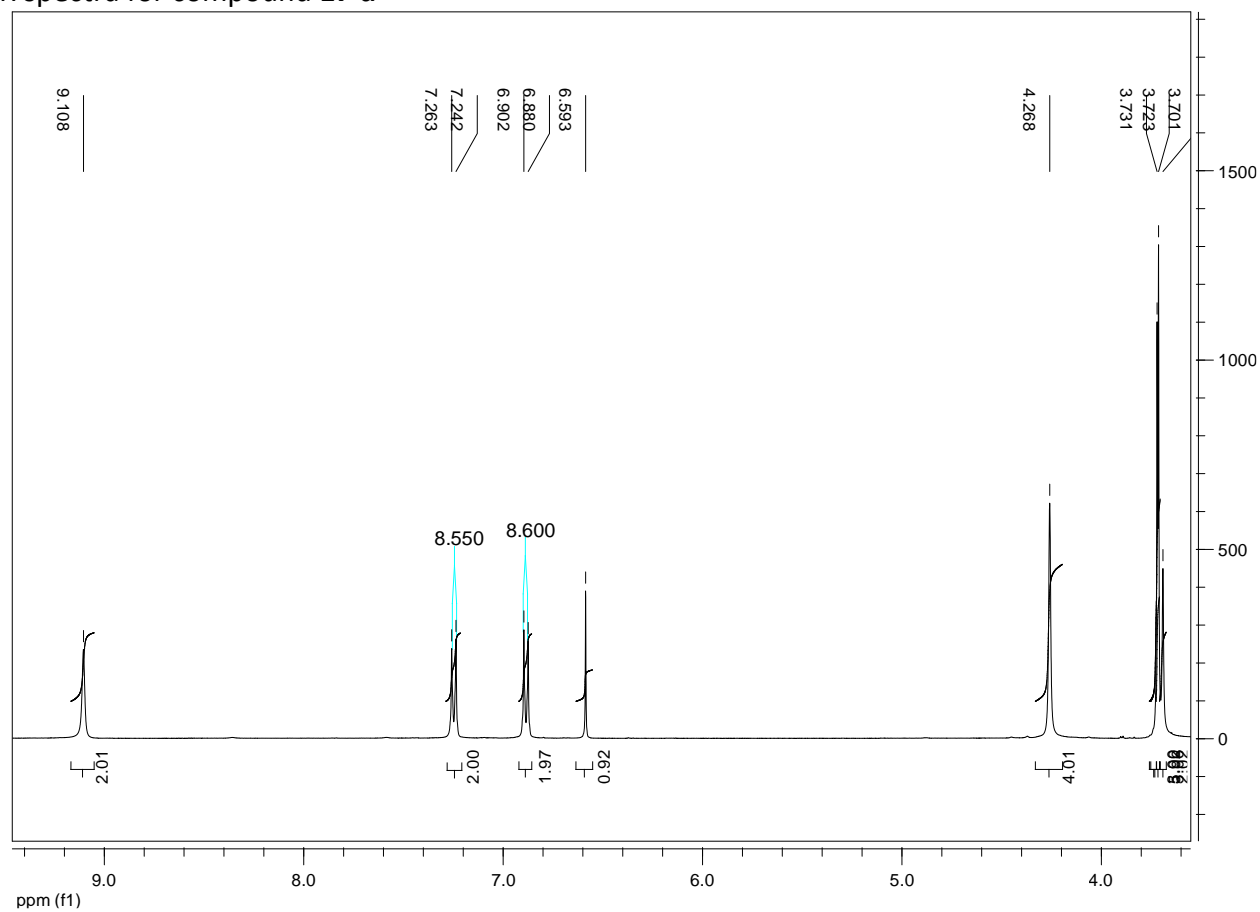
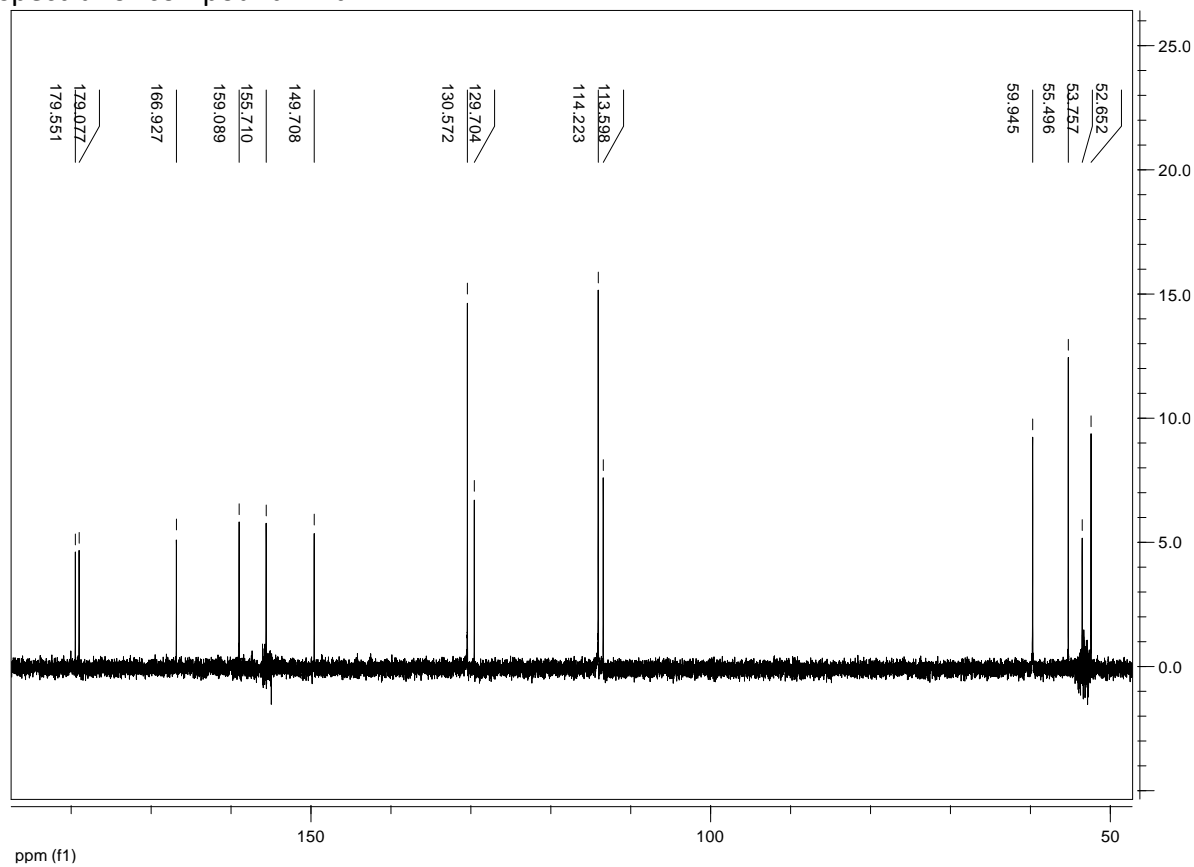
IR spectra for compound **17 c**

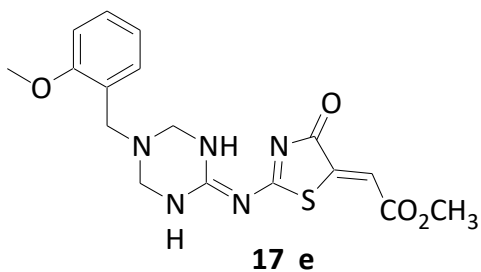
¹H NMR spectra for compound **17 c**¹³C NMR spectra for compound **17 c**

Data LCMS for compound **17 d**

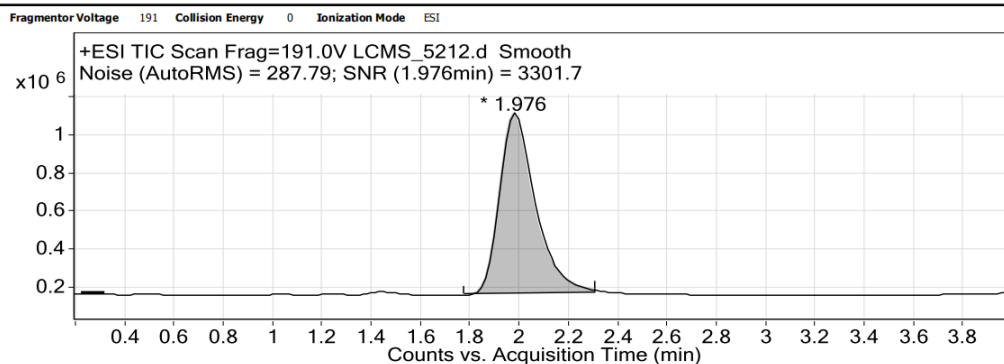
User Chromatograms

IR spectra for compound **17d**

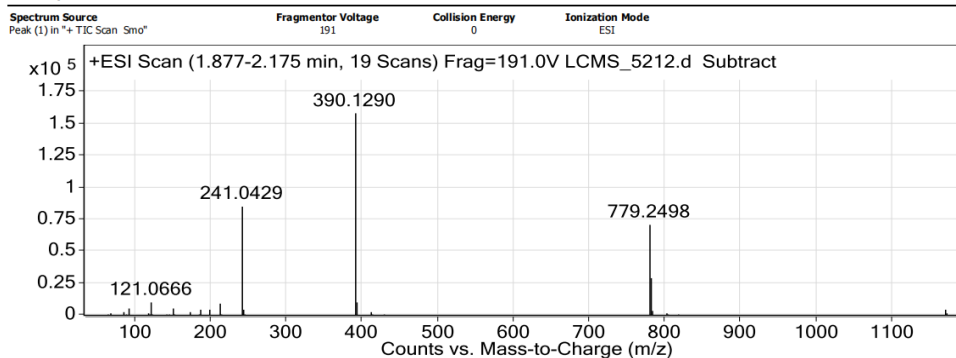
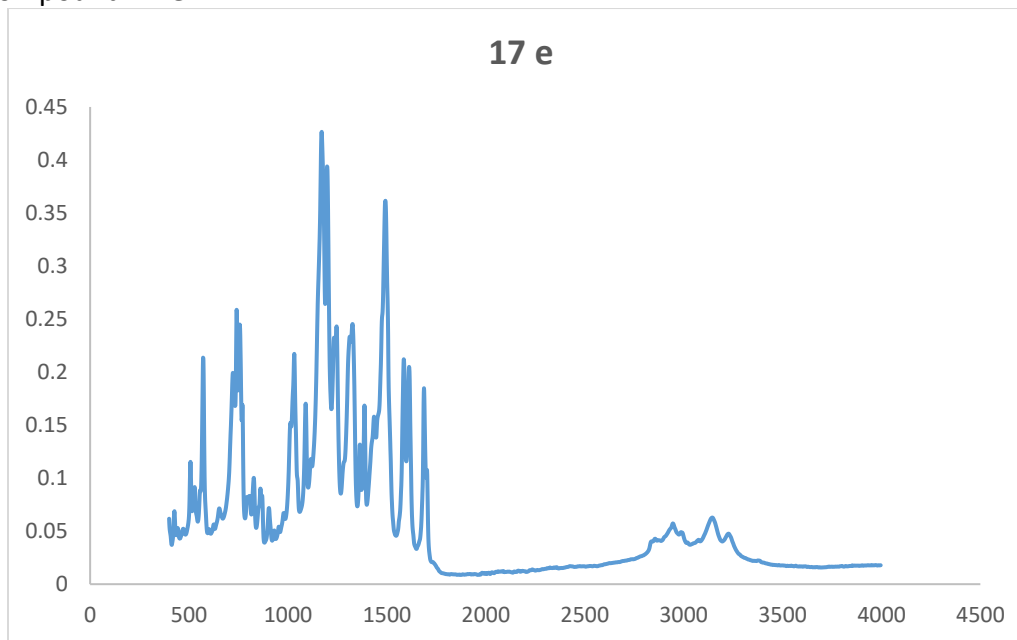
¹H NMR spectra for compound **17 d**¹³C NMR spectra for compound **17 d**

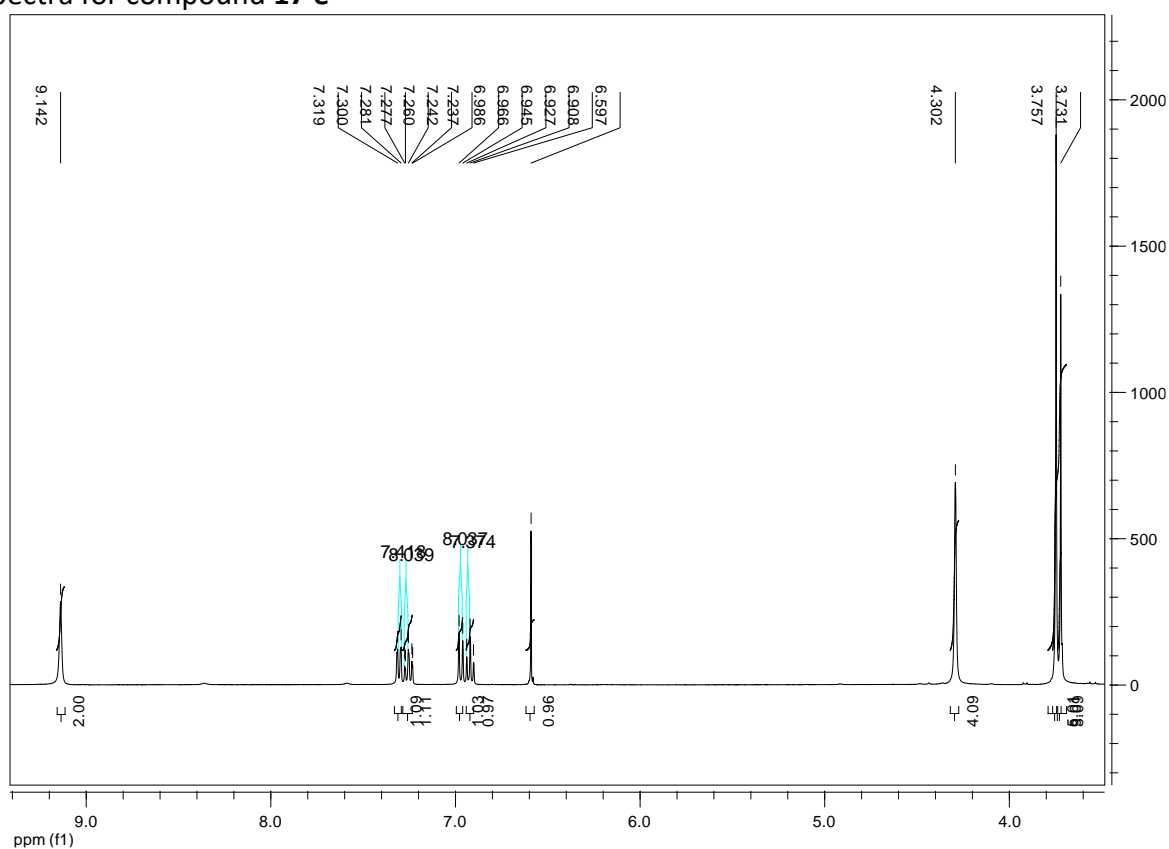
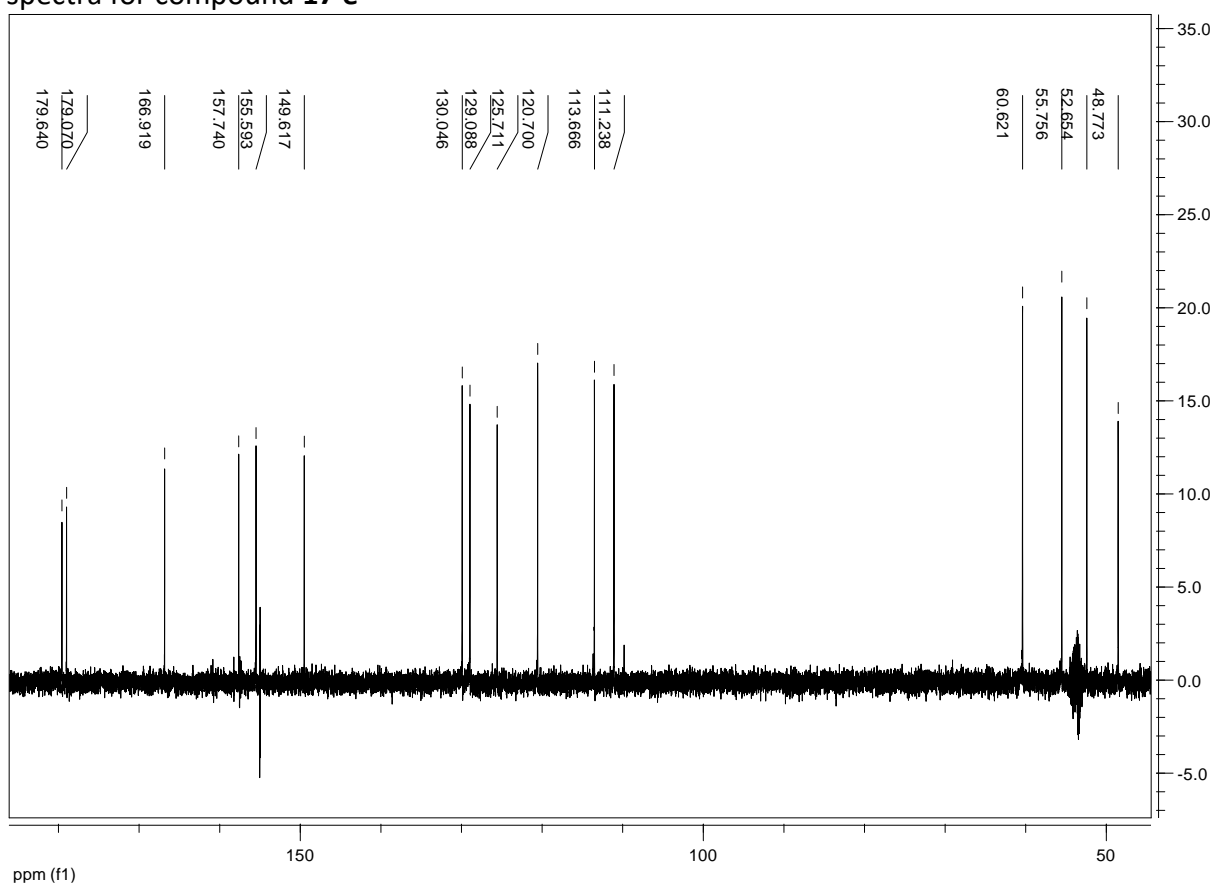
Data LCMS for compound **17 e**

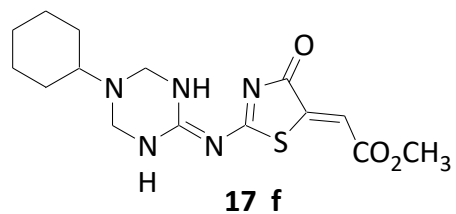
User Chromatograms



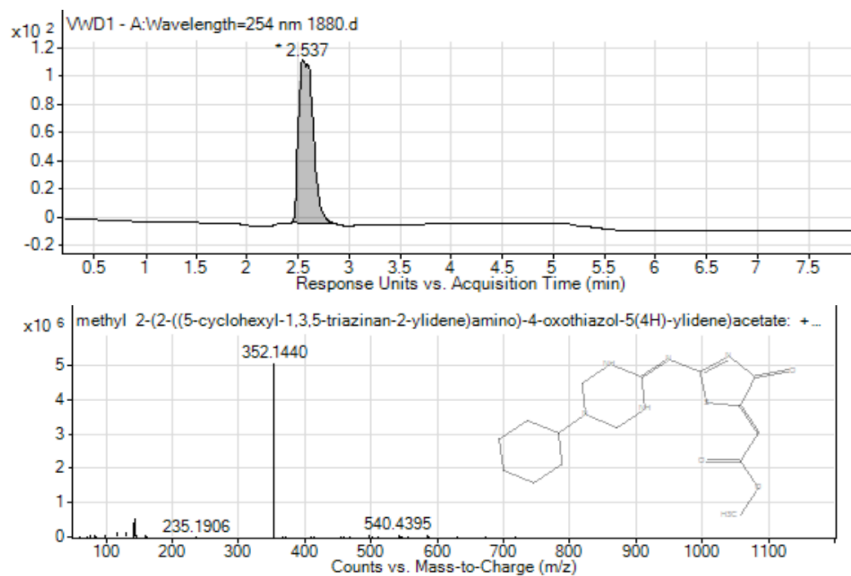
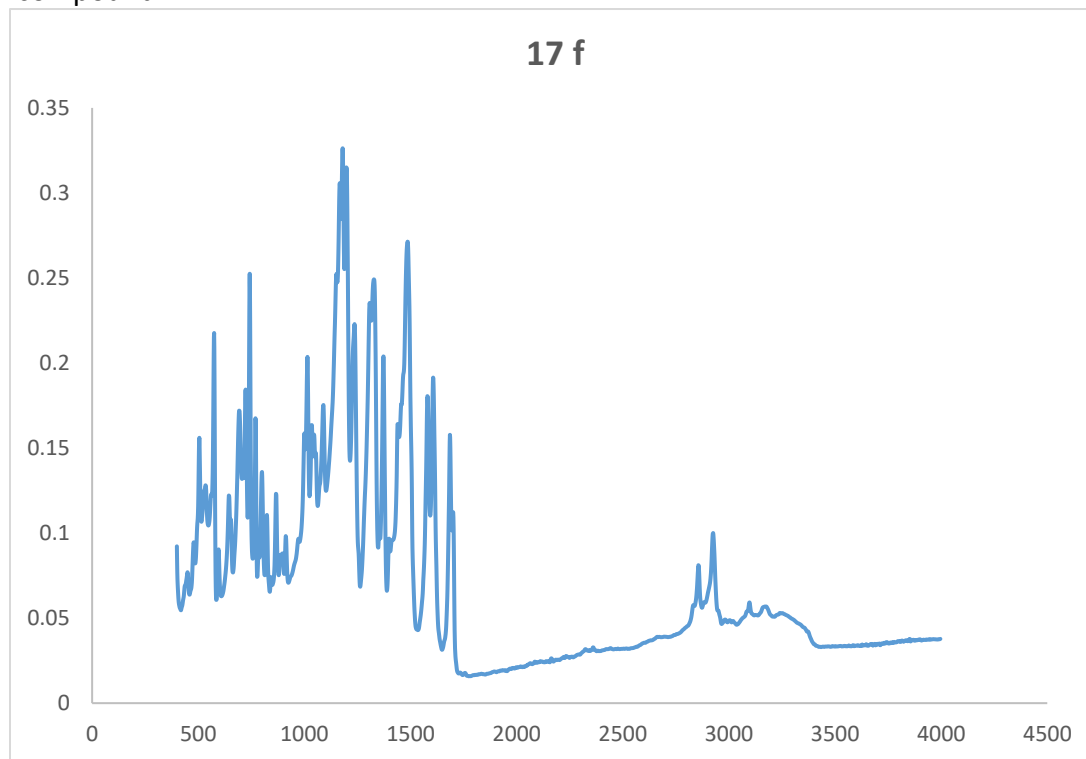
User Spectra

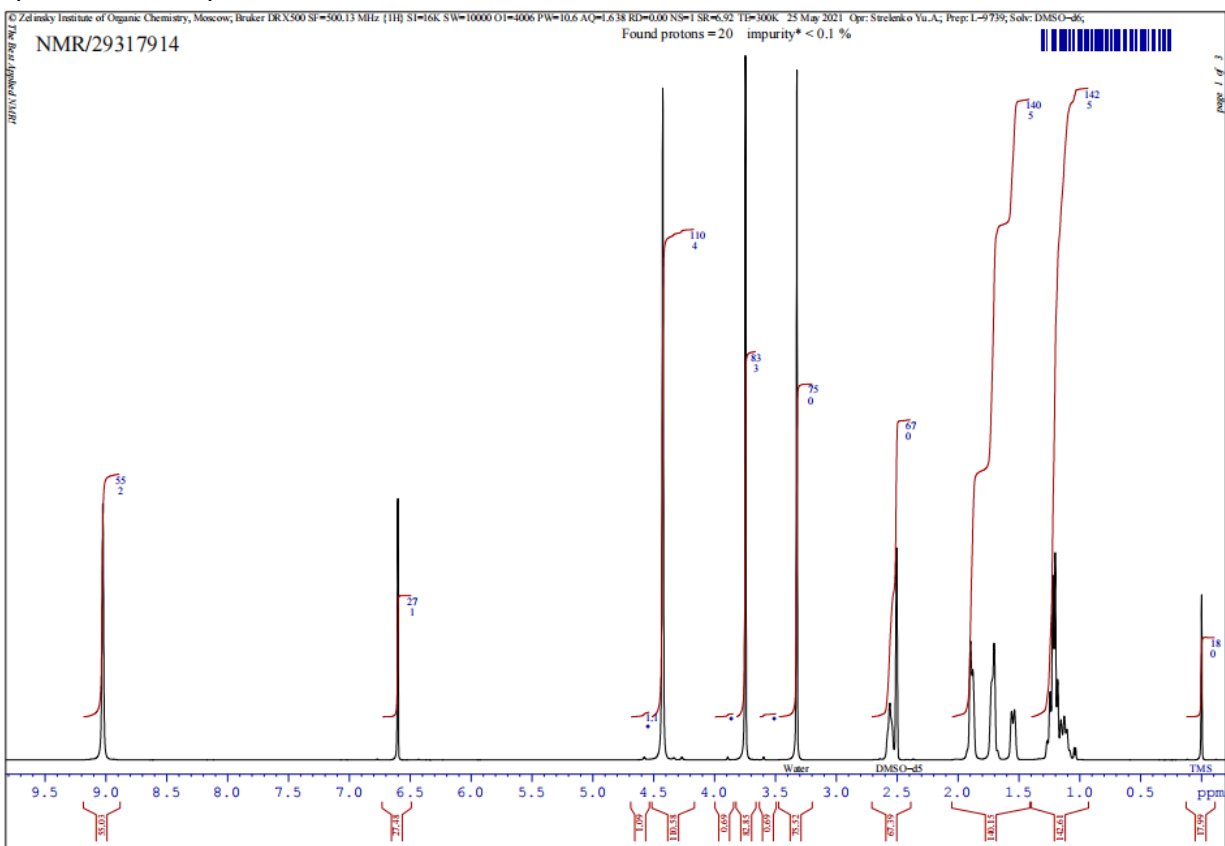
IR spectra for compound **17 e**

^1H NMR spectra for compound **17 e** ^{13}C NMR spectra for compound **17 e**

Data LCMS for compound **17 f**

User Chromatograms

IR spectra for compound **17 f**

^1H NMR spectra for compound **17 f** ^{13}C NMR spectra for compound **17 f**