

SUPPLEMENTARY MATERIALS

Inhibition of Cholinesterases by Benzothiazolone Derivatives

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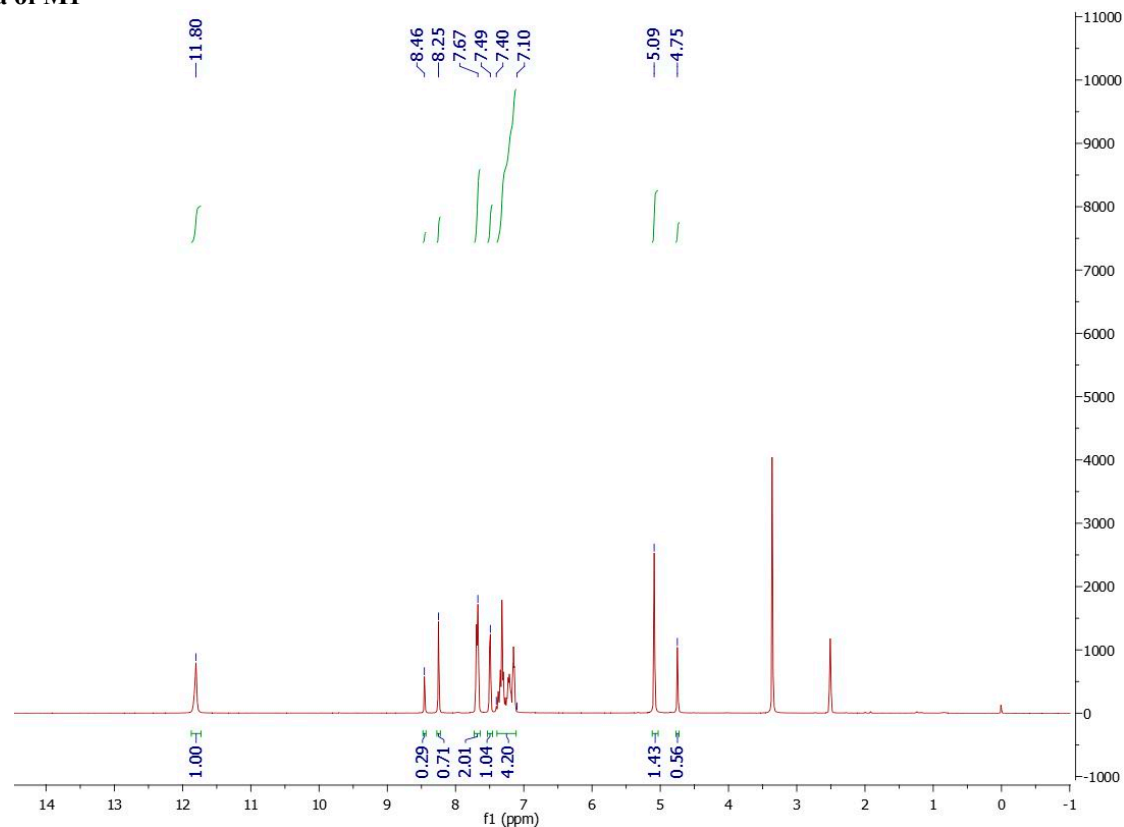
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Table S1. Inhibitions of MAO by **M** series

Figure S. ^1H -NMR, ^{13}C -NMR, and HRMS spectra of the compounds **M1-13**

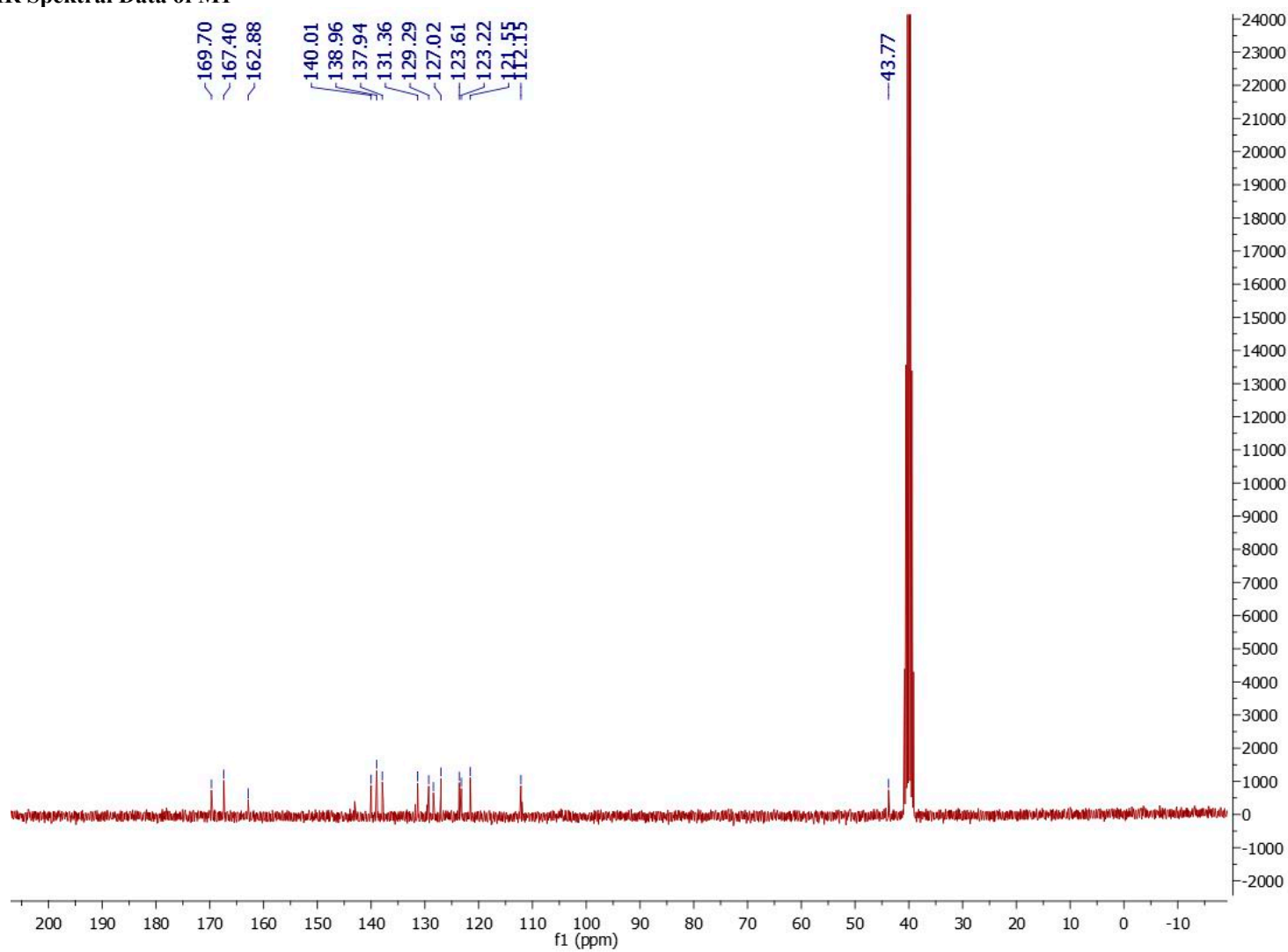
Data 1. ^1H -NMR Spektral Data of **M1**



(*E/Z*;72/28%)-*N'*-(thiophen-2-ylmethylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl)- acetohydrazide (**M1**)

Yield: 91%; mp: 250-2 °C, white powder. ^1H NMR (400 MHz, DMSO-*d*₆): δ 4.75 (s, 2H, -CH₂, %28), 5.09 (s, 2H, -CH₂, %72), 7.13–7.43 (m, 4H, benzothiazolone), 7.49–7.67 (m, 3H, thiophene), 8.14 (s, H, N=CH, %72), 8.35 (s, H, N=CH, %28), 11.80 (s, H, NH). ^{13}C NMR (100 MHz, DMSO-*d*₆) δ 169.70, 167.40, 162.88, 140.01, 138.96, 137.94, 131.36, 129.29, 127.02, 123.61, 123.22, 121.55, 112.15, 43.77. HRMS (ESI): *m/z* calcd for C₁₄H₁₂N₃O₂S₂ [M+H]⁺ 318,0371; found: 318.0366

Data 2. ^{13}C -NMR Spektral Data of M1



Data 3. Mass Spectrum Data of M1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

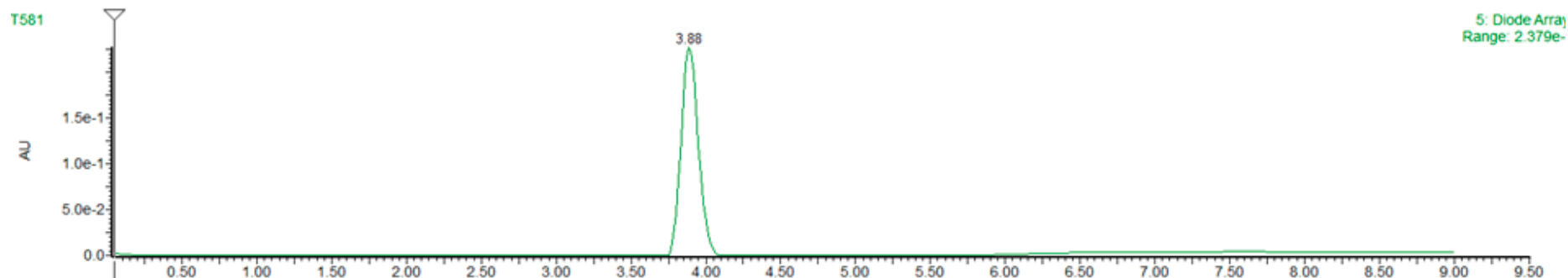
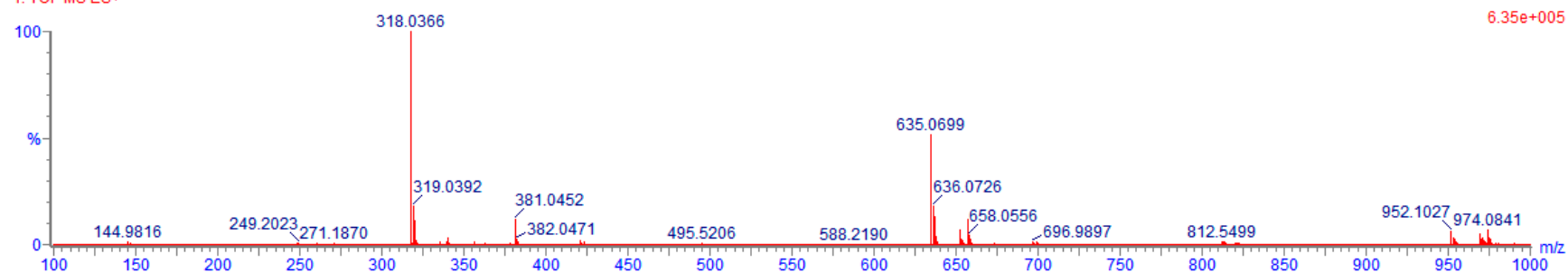
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

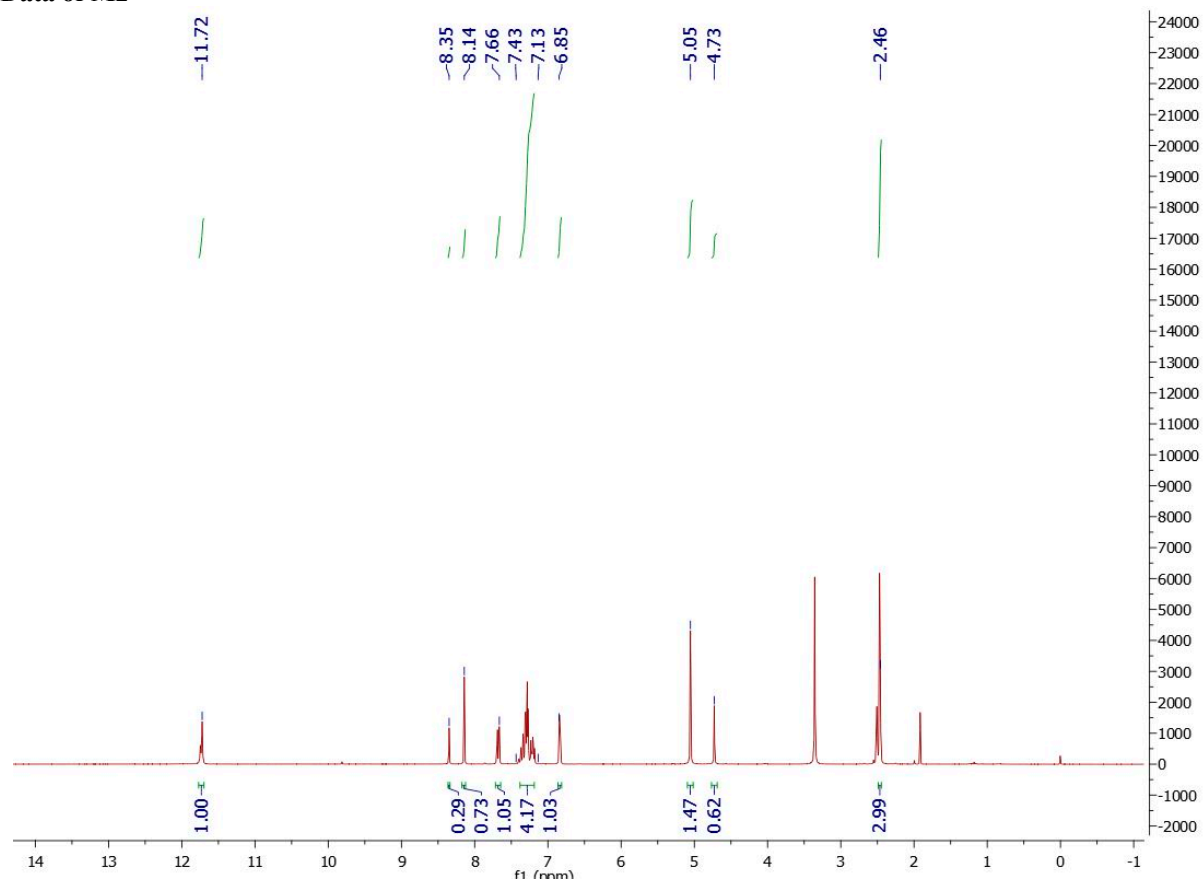
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|------------------|-------|--------------|----|----|---|---|---|
| 318.0366 | 318.0371 | -0.5 | -1.6 | 10.5 | C14 H12 N3 O2 S2 | 527.2 | 0.0 | 14 | 12 | 3 | 2 | 2 |

T581 100 (3.900) Cm (97:105)

1: TOF MS ES+



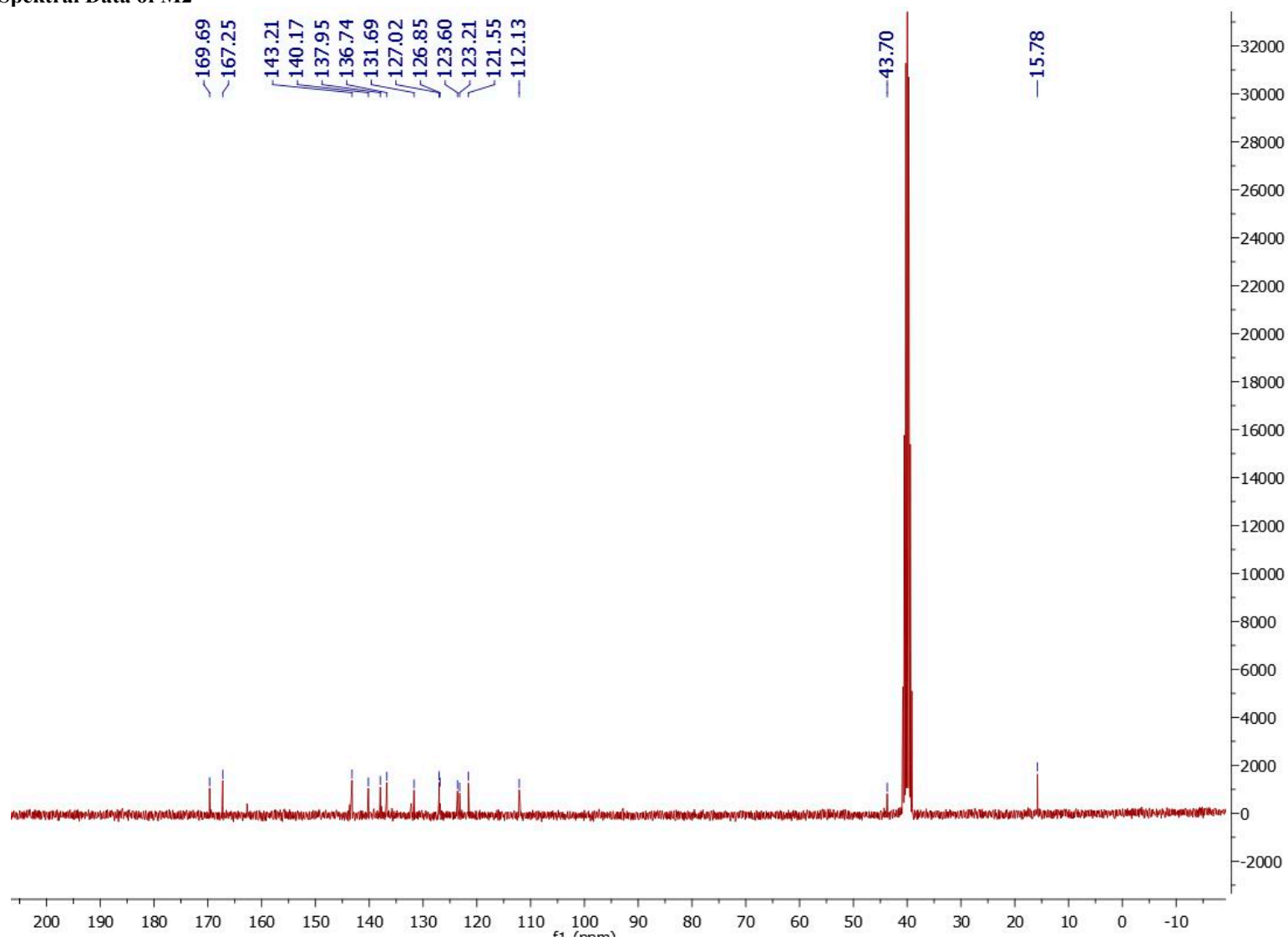
Data 4. ^1H -NMR Spektral Data of M2



E/Z; 72/28%) -N'-((5-methylthiophen-2-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M2**)

Yield: 93%; mp: 284-6 °C, white powder. ^1H NMR (400 MHz, DMSO- d_6): δ 2.46 (s, 3H, CH₃), 4.73 (s, 2H, -CH₂, %28), 5.05 (s, 2H, -CH₂, %72), 6.85 (m, H, thiophene) 7.10–7.40 (m, 4H, benzothiazolone), 7.66 (m, H, thiophene), 8.25 (s, H, N=CH, %72), 8.46 (s, H, N=CH, %28), 11.72 (s, H, NH). ^{13}C NMR (100 MHz, DMSO- d_6) δ 169.69, 167.25, 143.21, 140.17, 137.95, 136.74, 131.69, 127.02, 126.85, 123.60, 123.21, 121.55, 112.13, 43.70, 15.78. HRMS (ESI): m/z calcd for C₁₅H₁₄N₃O₂S₂ [M+H]⁺ 332.0527; found: 332.0525.

Data 5. ^{13}C -NMR Spektral Data of M2



Data 6. Mass Spectrum Data of M2

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

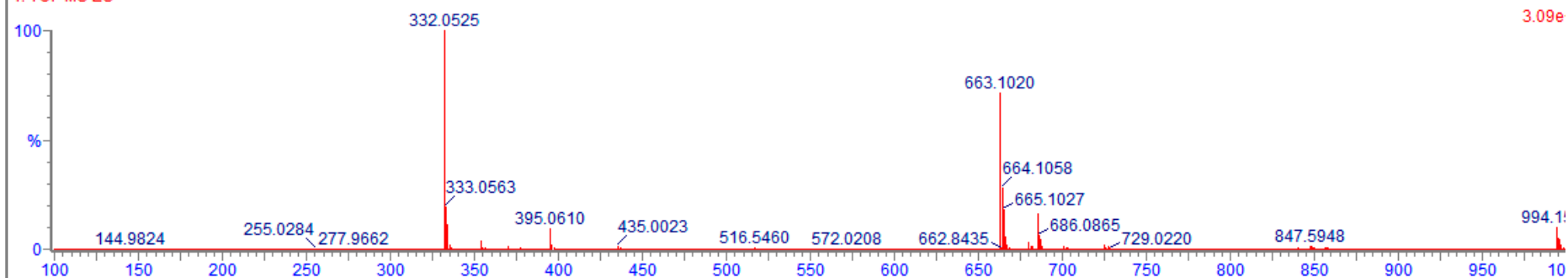
32 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

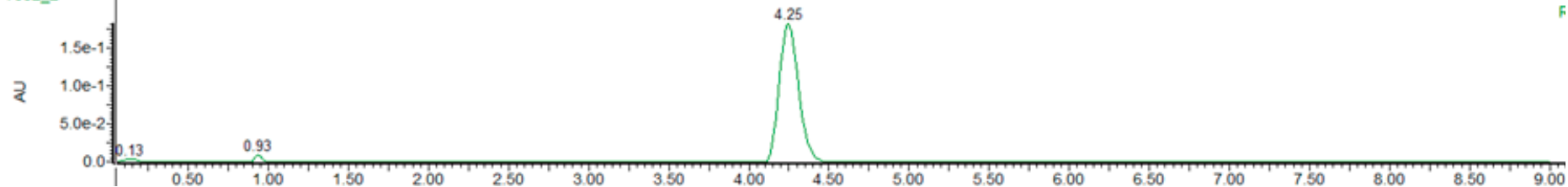
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|------------------|-------|--------------|----|----|---|---|---|
| 332.0525 | 332.0527 | -0.2 | -0.6 | 10.5 | C15 H14 N3 O2 S2 | 457.1 | 0.0 | 15 | 14 | 3 | 2 | 2 |

T582_2 108 (4.212) Cm (106:108)

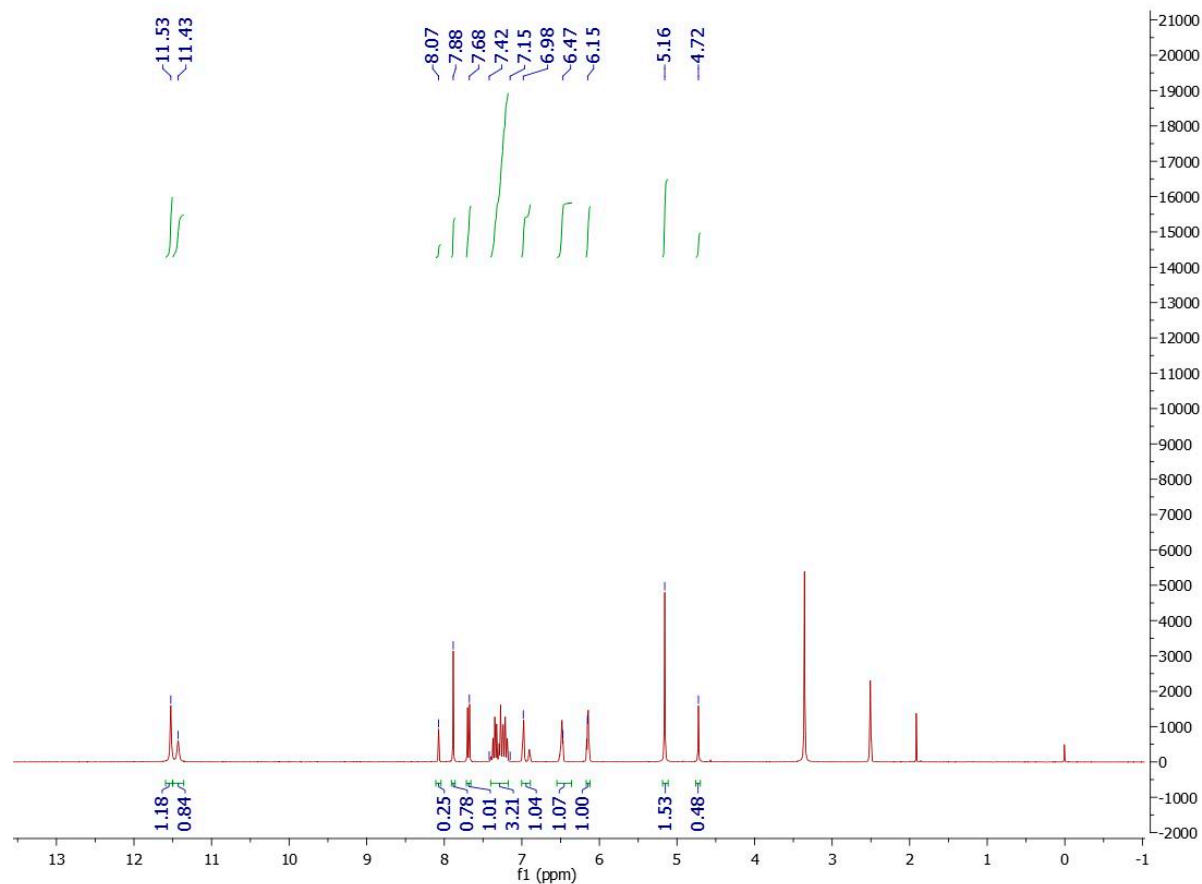
1: TOF MS ES+



T582_2



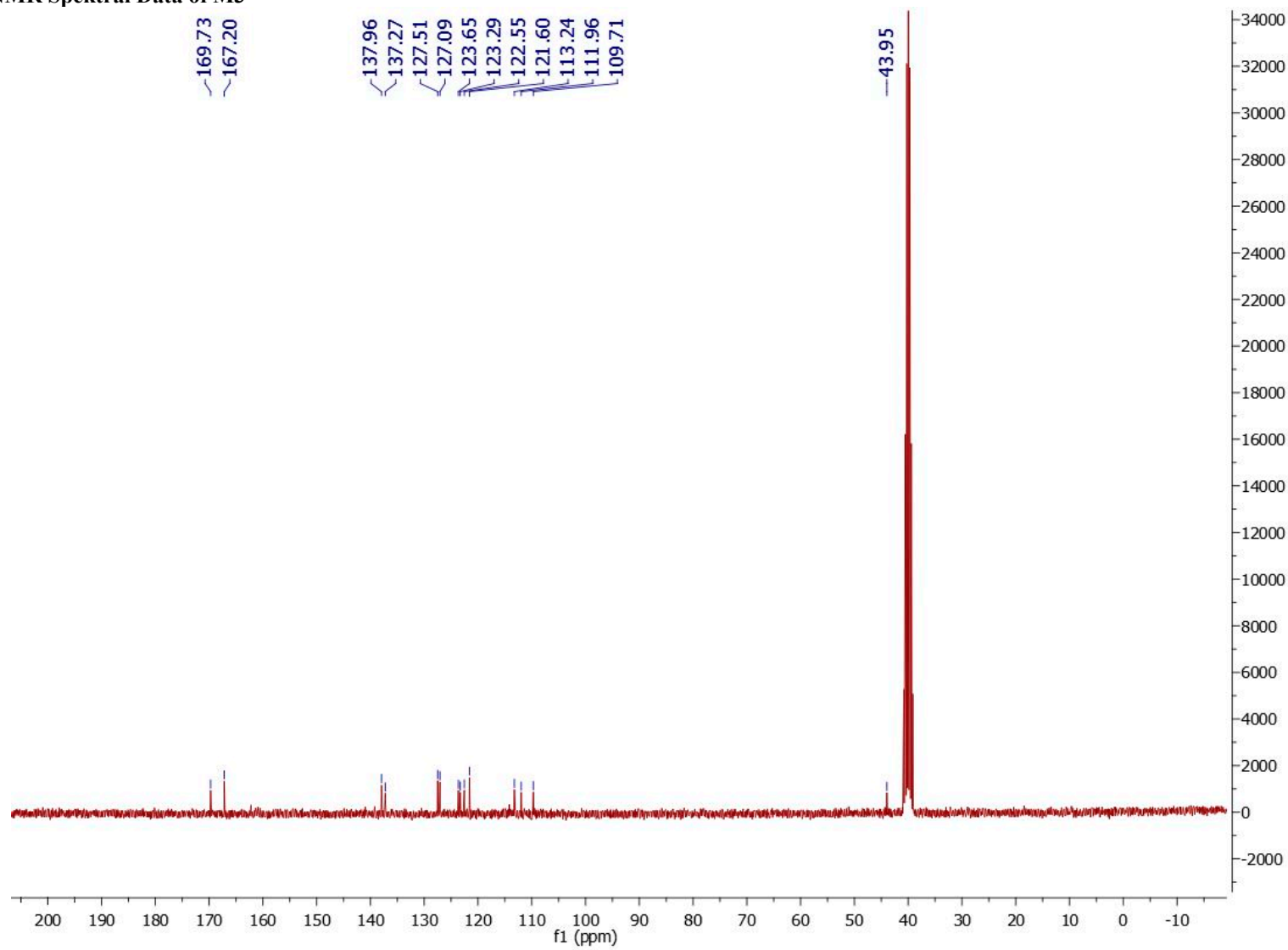
Data 7. ^1H -NMR Spektral Data of M3



E/Z; 76/24%) -N'-((1H-pyrrol-2-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M3**)

Yield: 70%; mp: 238-40 °C, white powder. ^1H NMR (400 MHz, DMSO- d_6): δ 4.72 (s, 2H, -CH₂, %24), 5.16 (s, 2H, -CH₂, %76), 6.15 (m, H, pyrrol), 6.47 (m, H, pyrrol), 6.98 (m, H, pyrrol), 7.15–7.68 (m, 4H, benzothiazolone), 7.88 (s, H, N=CH, %76), 8.07 (s, H, N=CH, %24), 11.43 (s, H, NH, pyrrol), 11.53 (s, H, NH). ^{13}C NMR (100 MHz, DMSO- d_6) δ 169.73, 167.20, 137.96, 137.27, 127.51, 127.09, 123.65, 123.29, 122.55, 121.60, 113.24, 111.96, 109.71, 43.95. HRMS (ESI): m/z calcd for C₁₄H₁₃N₄O₂S [M+H]⁺ 301.0759; found: 301.0747.

Data 8. ^{13}C -NMR Spektral Data of M3



Data 9. Mass Spectrum Data of M3

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

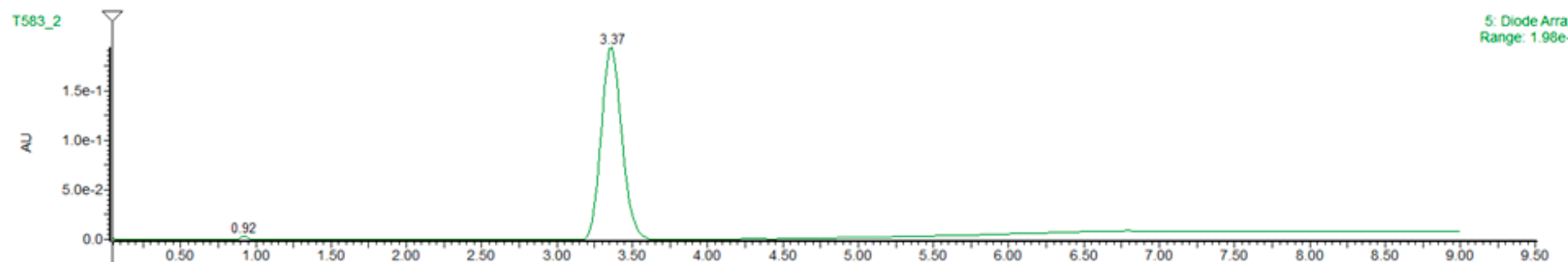
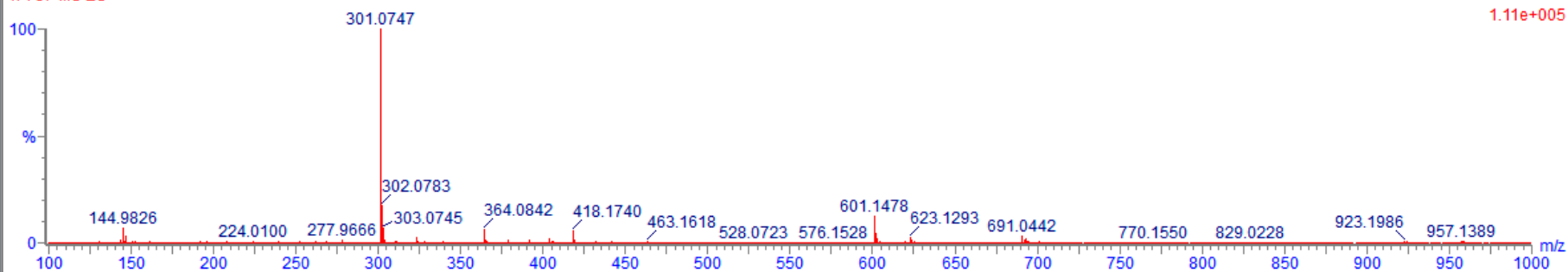
26 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

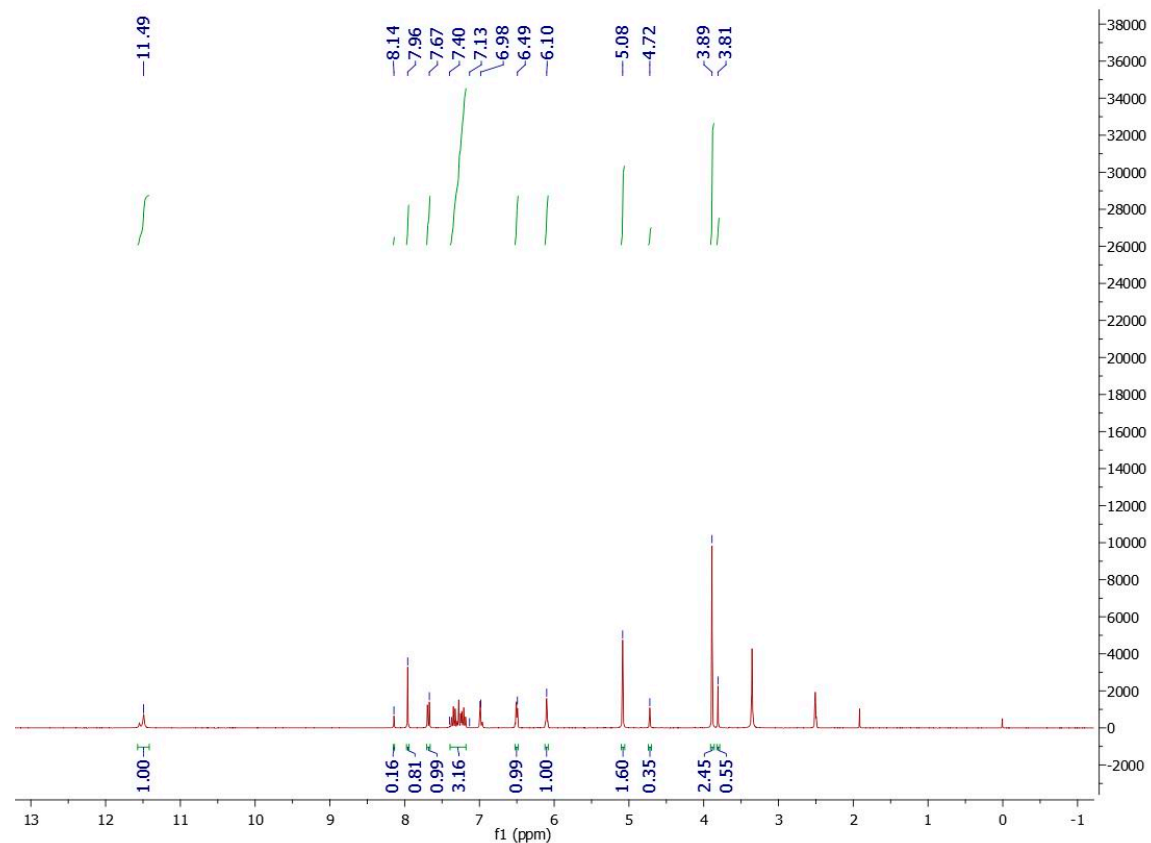
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|-----------------|-------|--------------|----|----|---|---|---|
| 301.0747 | 301.0759 | -1.2 | -4.0 | 10.5 | C14 H13 N4 O2 S | 241.6 | 0.0 | 14 | 13 | 4 | 2 | 1 |

T583_2 90 (3.526) Cm (90:92)

1: TOF MS ES+



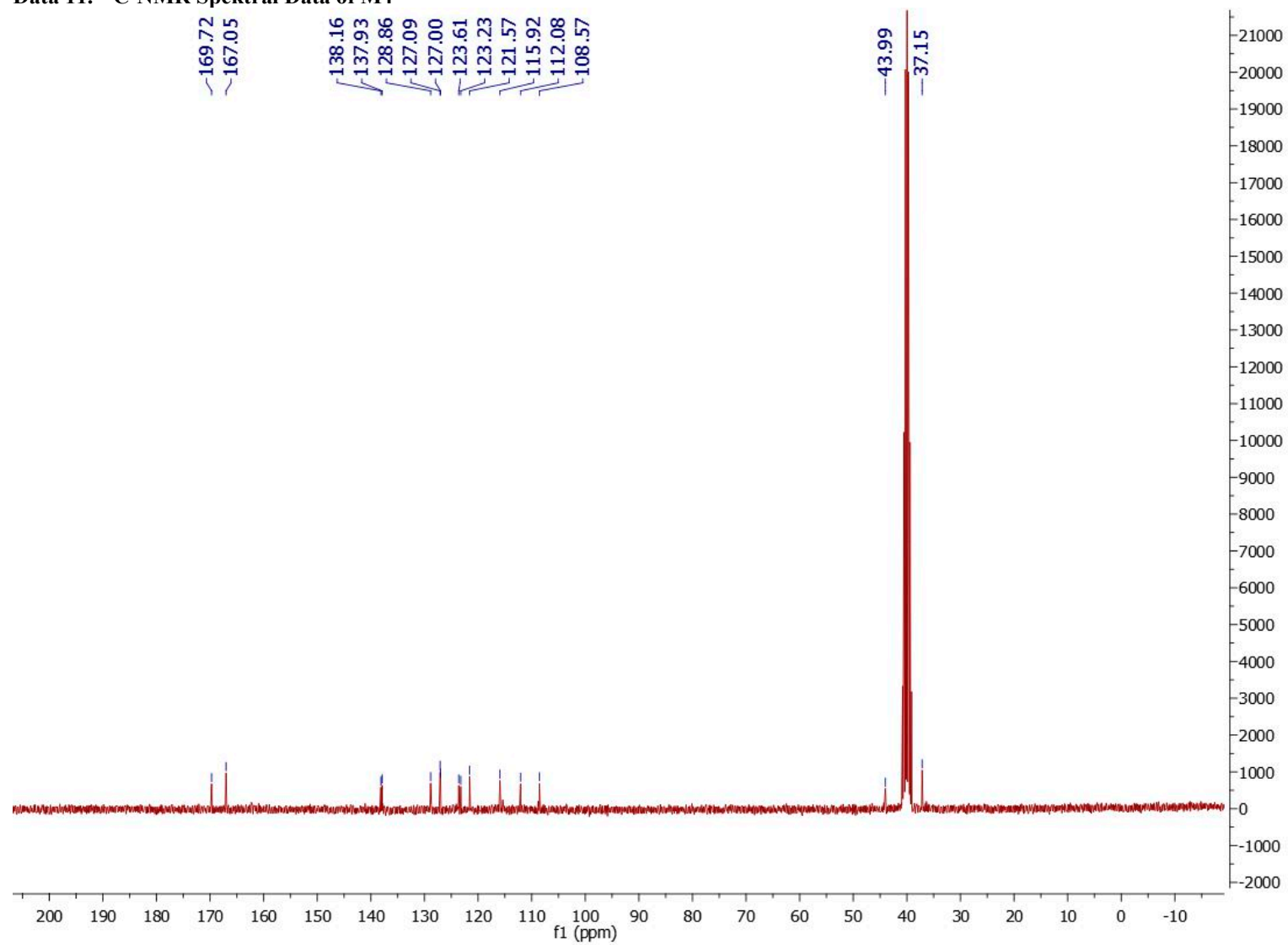
Data 10. ^1H -NMR Spektral Data of M4



(*E/Z*;82/18%)-*N'*-((1-methyl-1H-pyrrol-2-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl)acetohydrazide (**M4**)

Yield: 91%; mp: 264-6 °C, white powder. ^1H NMR (400 MHz, DMSO-*d*₆): δ 3.81 (s, 3H, CH₃, 18%), 3.89 (s, 3H, CH₃, %82), 5.72 (s, 2H, -CH₂, %18), 5.08 (s, 2H, -CH₂, %82), 6.10 (m, H, pyrrol), 6.49 (m, H, pyrrol), 7.05 (m, H, pyrrol), 7.13–7.67 (m, 4H, benzothiazolone), 7.96 (s, H, N=CH, %82), 8.14 (s, H, N=CH, %18). 11.49 (s, H, NH). ^{13}C NMR (100 MHz, DMSO-*d*₆) δ 169.72, 167.05, 138.16, 137.93, 128.86, 127.09, 127.00, 123.61, 123.23, 121.57, 115.92, 112.08, 108.57, 43.99, 37.15. HRMS (ESI): *m/z* calcd for C₁₅H₁₅N₄O₂S [M+H]⁺ 315.0916; found: 315.0905.

Data 11. ^{13}C -NMR Spektral Data of M4



Data 12. Mass Spectrum Data of M4

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

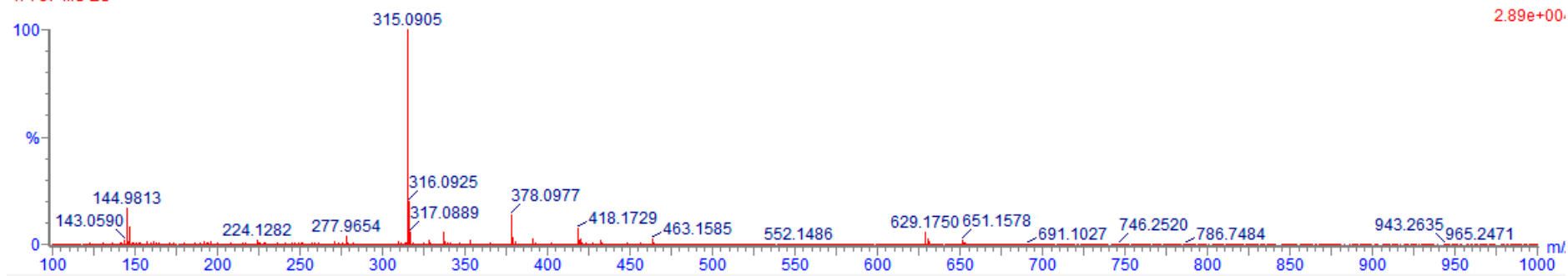
26 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

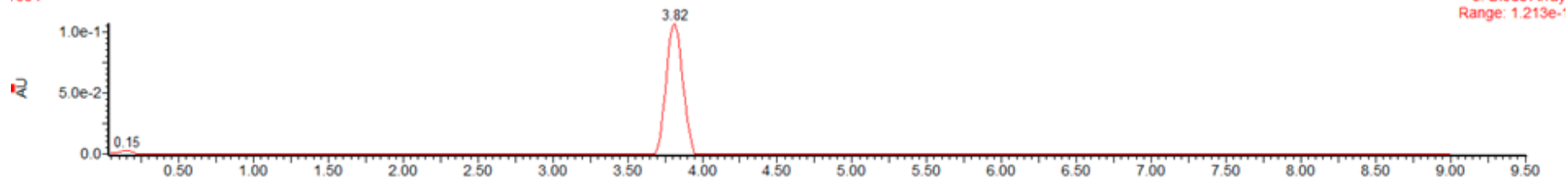
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|-----------------|-------|--------------|----|----|---|---|---|
| 315.0905 | 315.0916 | -1.1 | -3.5 | 10.5 | C15 H15 N4 O2 S | 98.0 | 0.0 | 15 | 15 | 4 | 2 | 1 |

T584 94 (3.682) Cm (93:94)

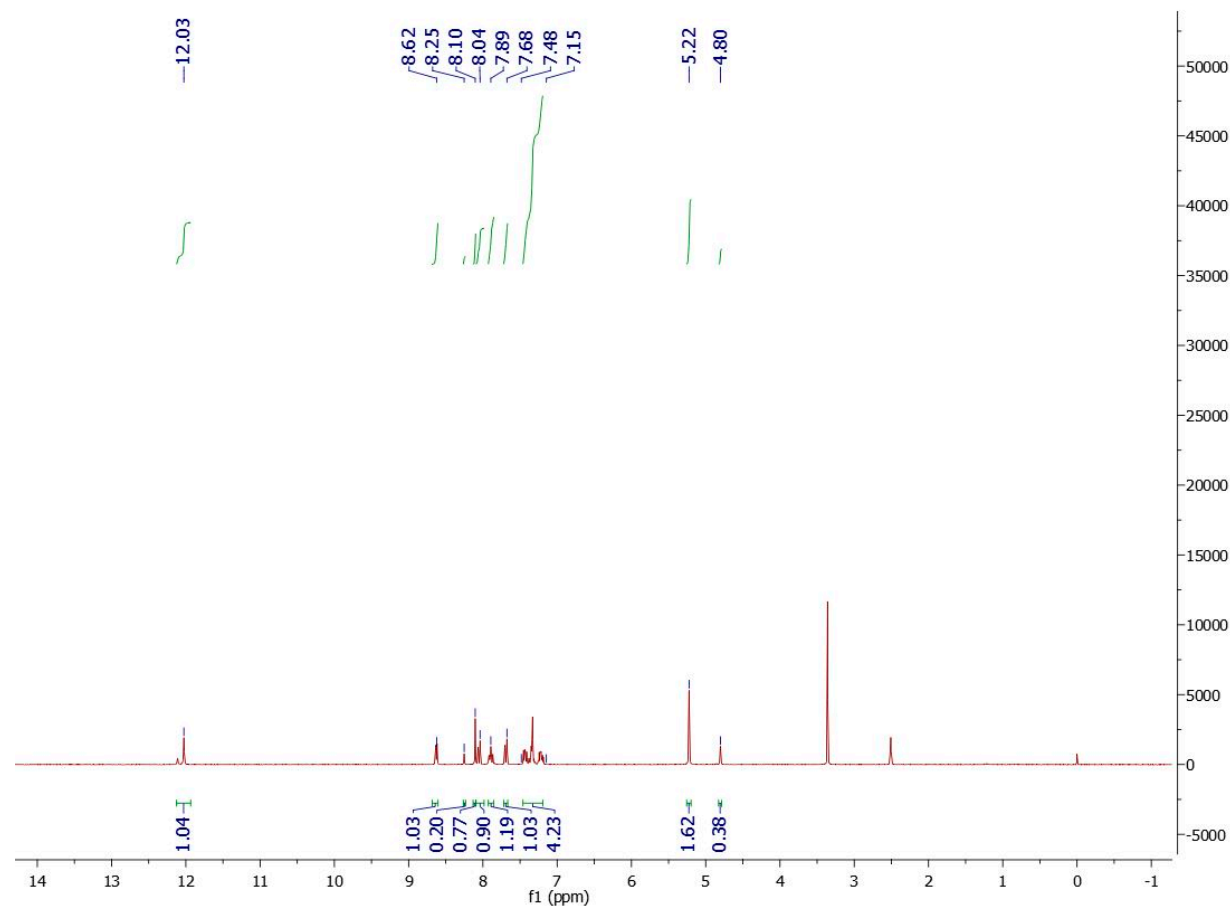
1: TOF MS ES+



T584



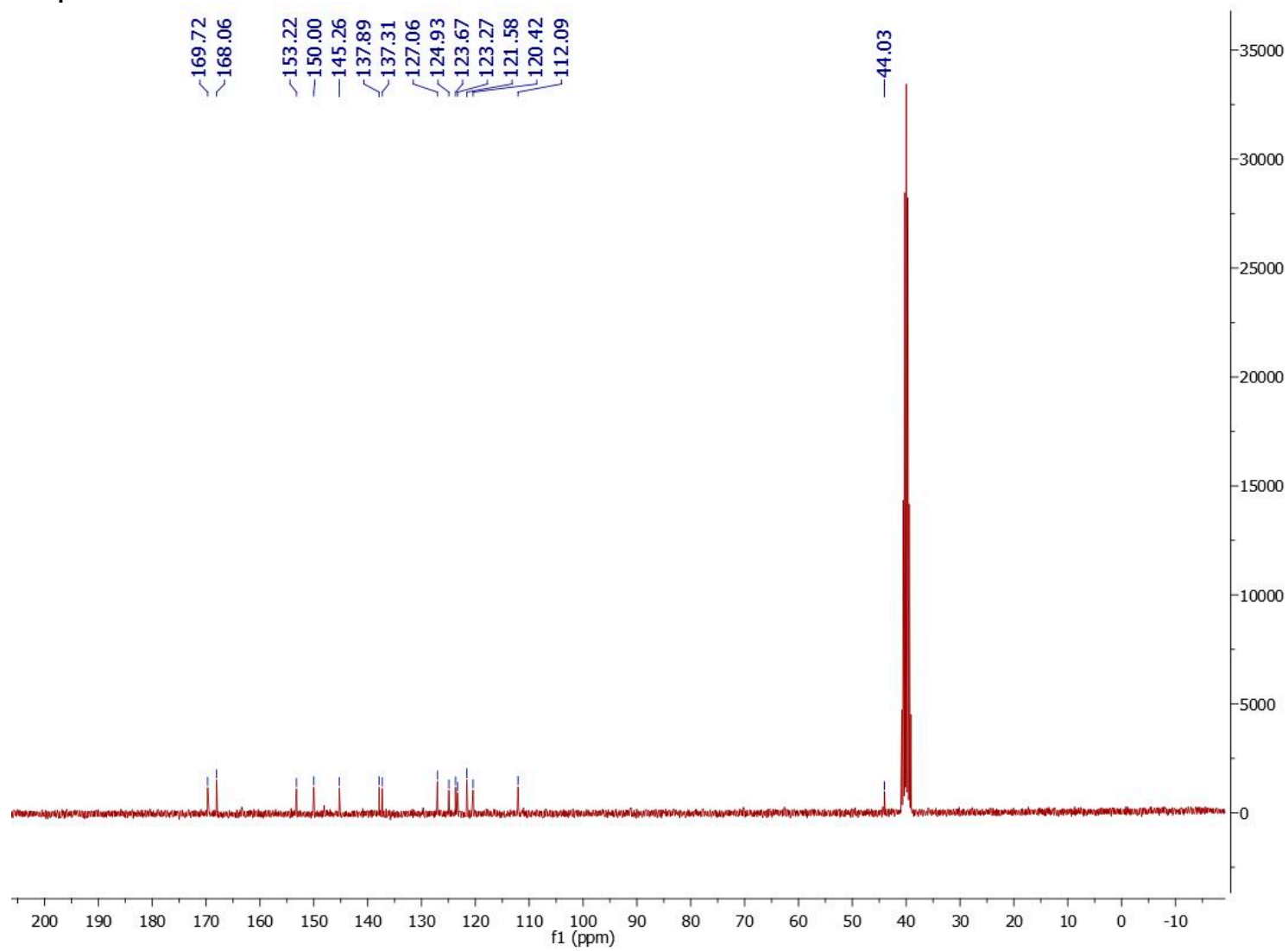
Data 13. ¹H-NMR Spektral Data of M5



E/Z;81/19%)-N'-(pyridin-2-ylmethylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl)- acetohydrazide (**M5**)

Yield: 68%; mp: 228-30 °C, white powder. ¹H NMR (400 MHz, DMSO-d): δ 4.80 (s, 2H, -CH₂, %19), 5.08 (s, 2H, -CH₂, %81), 7.15–7.48 (m, 4H, benzothiazolone), 8.10 (s, H, N=CH, %81), 8.22 (s, H, N=CH, %19), 7.68-8.22 (m, 4H, pyridin), 12.03 (s, H, NH). ¹³C NMR (100 MHz, DMSO-d) δ 169.72, 168.06, 153.22, 150.00, 145.26, 137.89, 137.31, 127.06, 124.93, 123.67, 123.27, 121.58, 120.42, 112.09, 44.03. HRMS (ESI): *m/z* calcd for C₁₅H₁₃N₄O₂S [M+H]⁺ 313.0759; found: 313.0746.

Data 14. ^{13}C -NMR Spektral Data of M5



Data 15. Mass Spectrum Data of M5

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

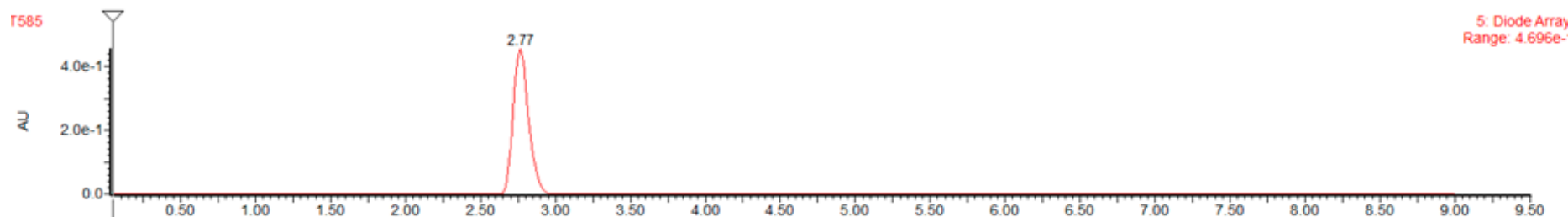
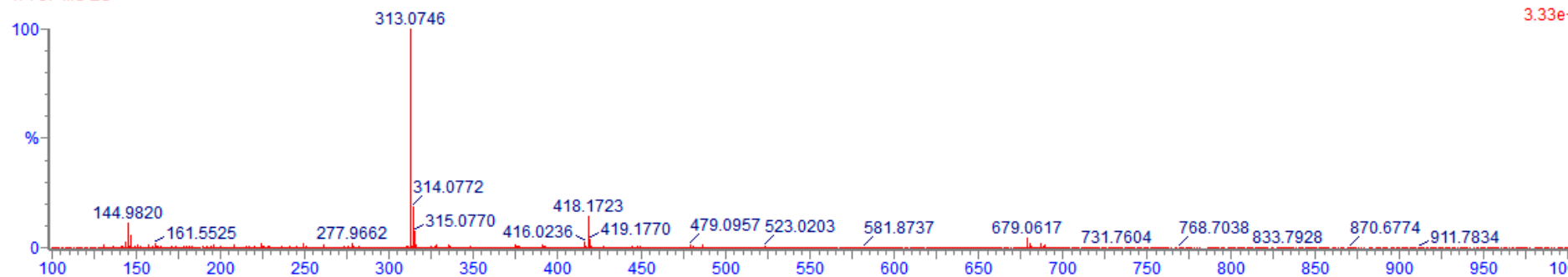
24 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

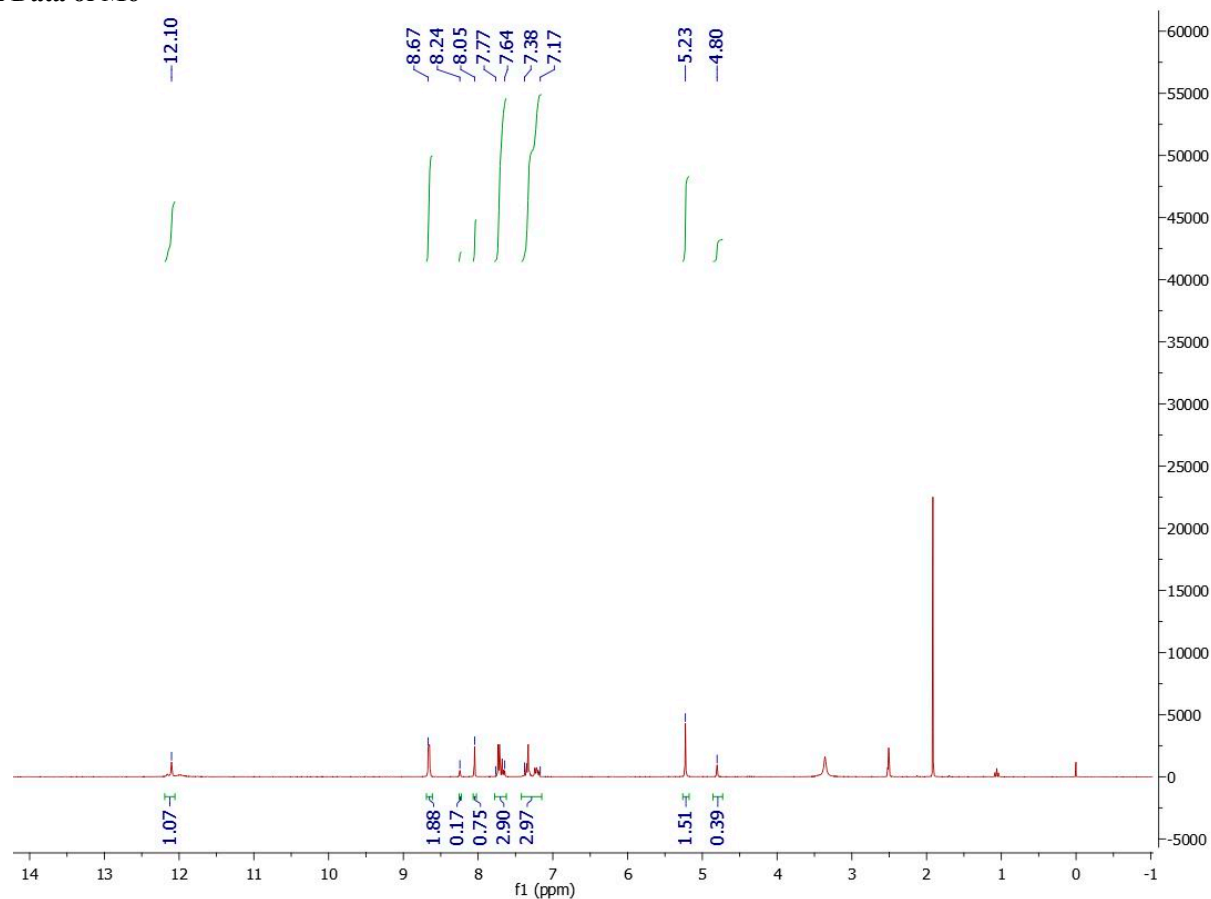
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|-----------------|-------|--------------|----|----|---|---|---|
| 313.0746 | 313.0759 | -1.3 | -4.2 | 11.5 | C15 H13 N4 O2 S | 147.2 | 0.0 | 15 | 13 | 4 | 2 | 1 |

T585 77 (3.024) Cm (77:78)

1: TOF MS ES+



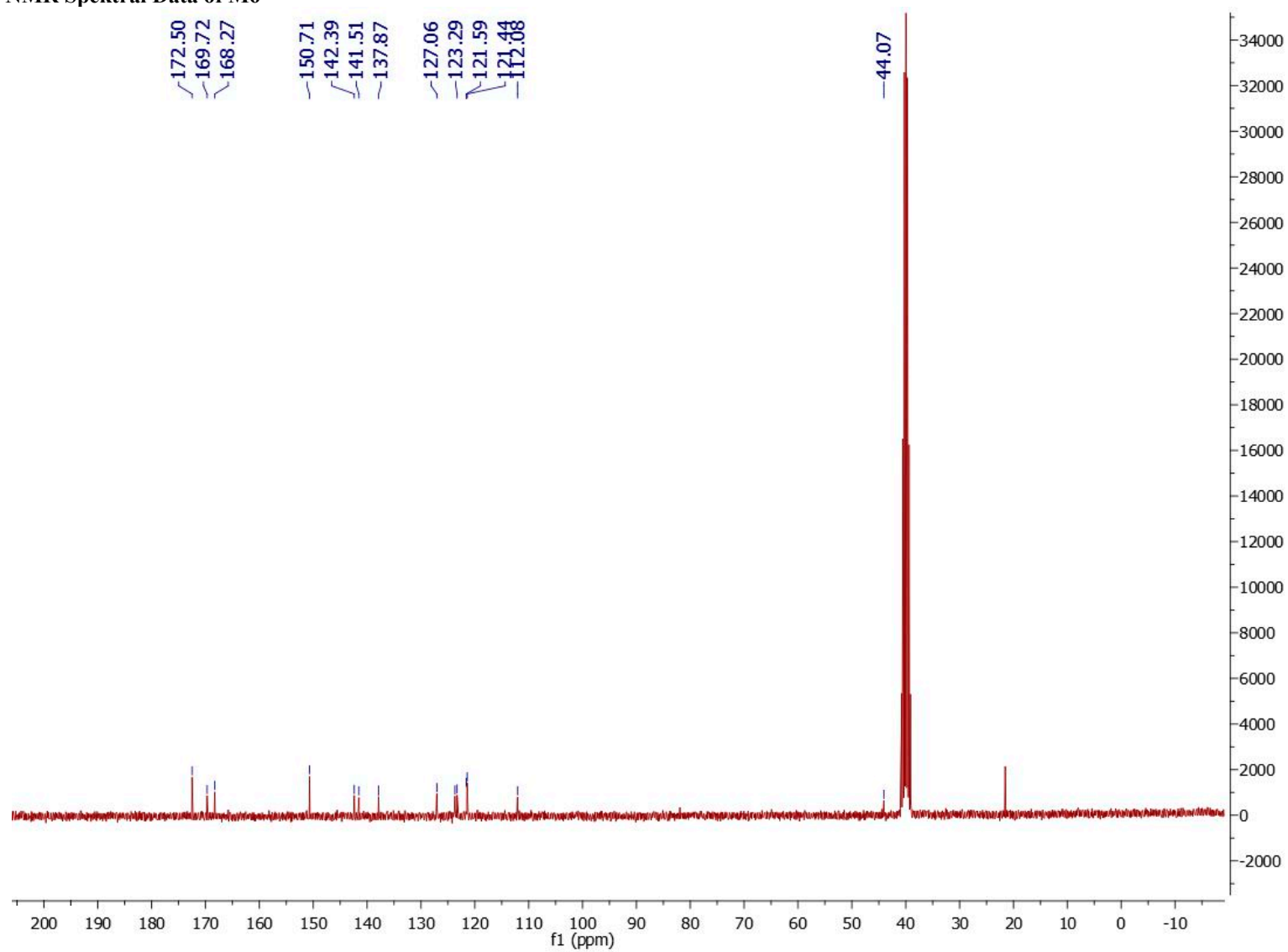
Data 16. ^1H -NMR Spektral Data of M6



(*E/Z*;81/19%)-*N'*-(pyridin-4-ylmethylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M6**)

Yield: 71%; mp:162-4°C, white powder. ^1H NMR (400 MHz, DMSO-*d*): δ 4.80 (s, 2H, -CH₂, %19), 5.23 (s, 2H, -CH₂, %81), 7.17–7.38 (m, 3H), 7.64–7.77 (m, 3H), 8.05 (s, H, N=CH, %81), 8.24 (s, H, N=CH, %19), 8.67 (m, 2H), 12.10 (s, H, NH). ^{13}C NMR (100 MHz, DMSO-*d*) δ 172.50, 169.72, 168.27, 150.71, 142.39, 141.51, 137.87, 127.06, 123.29, 121.59, 121.44, 112.08, 44.07. HRMS (ESI): *m/z* calcd for C₁₅H₁₃N₄O₂S [M+H]⁺ 313.0759; found: 313.0752.

Data 17. ^{13}C -NMR Spektral Data of M6



Data 18. Mass Spectrum Data of M6

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

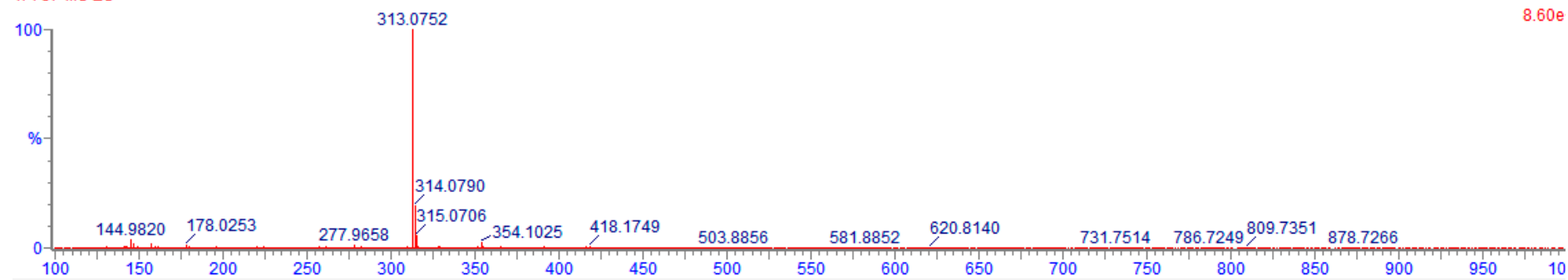
24 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

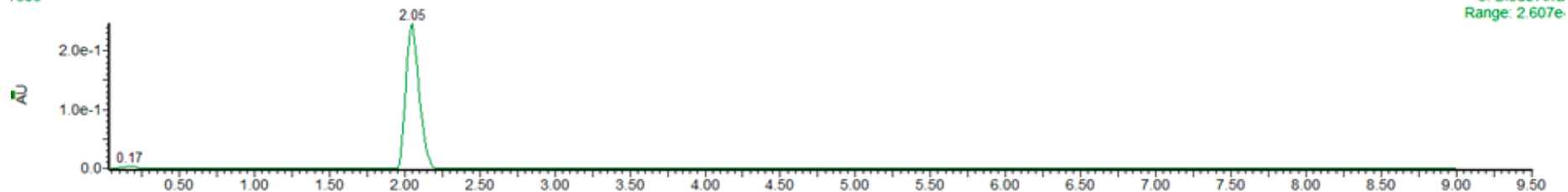
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|-----------------|-------|--------------|----|----|---|---|---|
| 313.0752 | 313.0759 | -0.7 | -2.2 | 11.5 | C15 H13 N4 O2 S | 237.8 | 0.0 | 15 | 13 | 4 | 2 | 1 |

T586 57 (2.241) Cm (57:58)

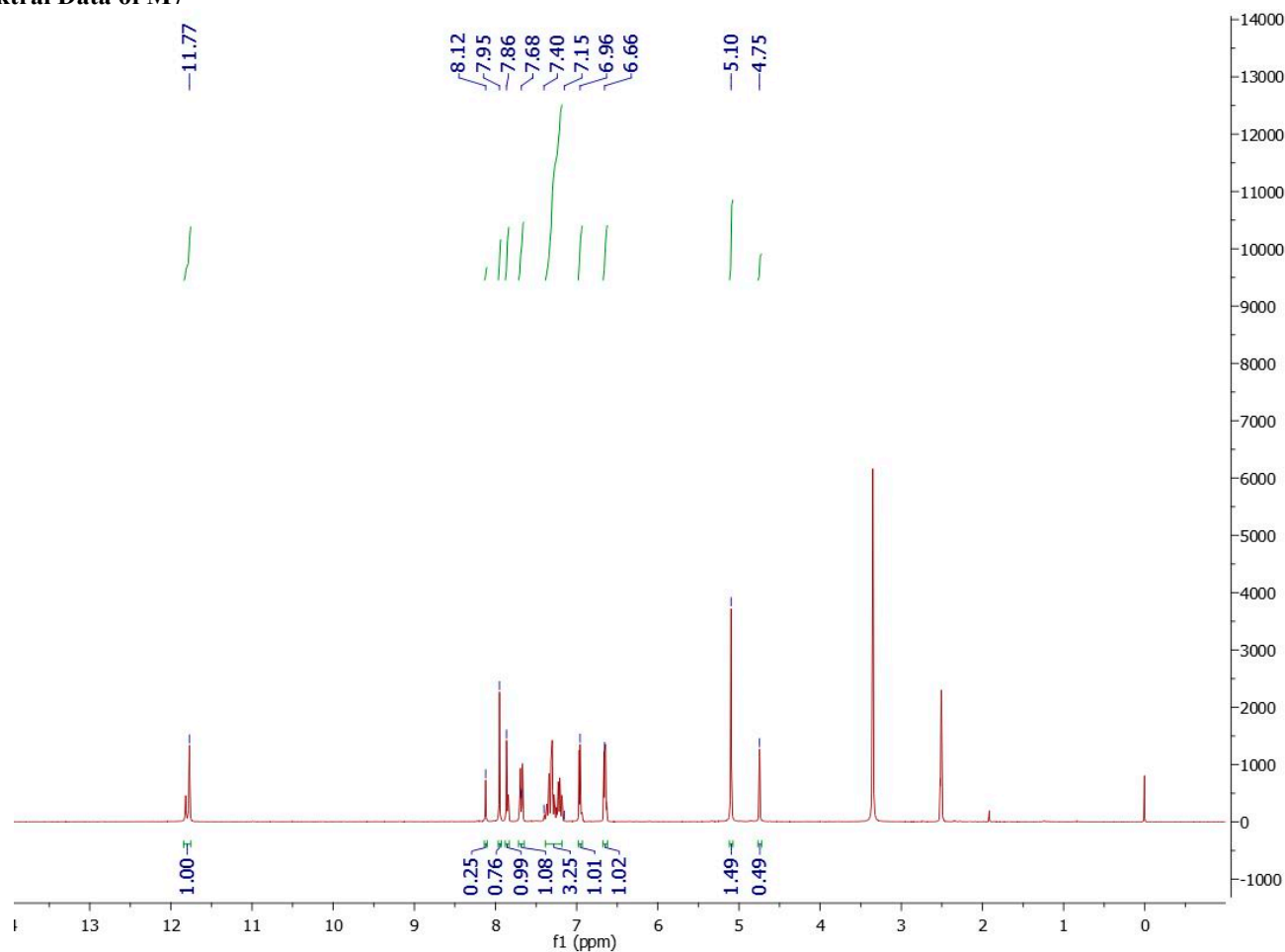
1: TOF MS ES+



T586



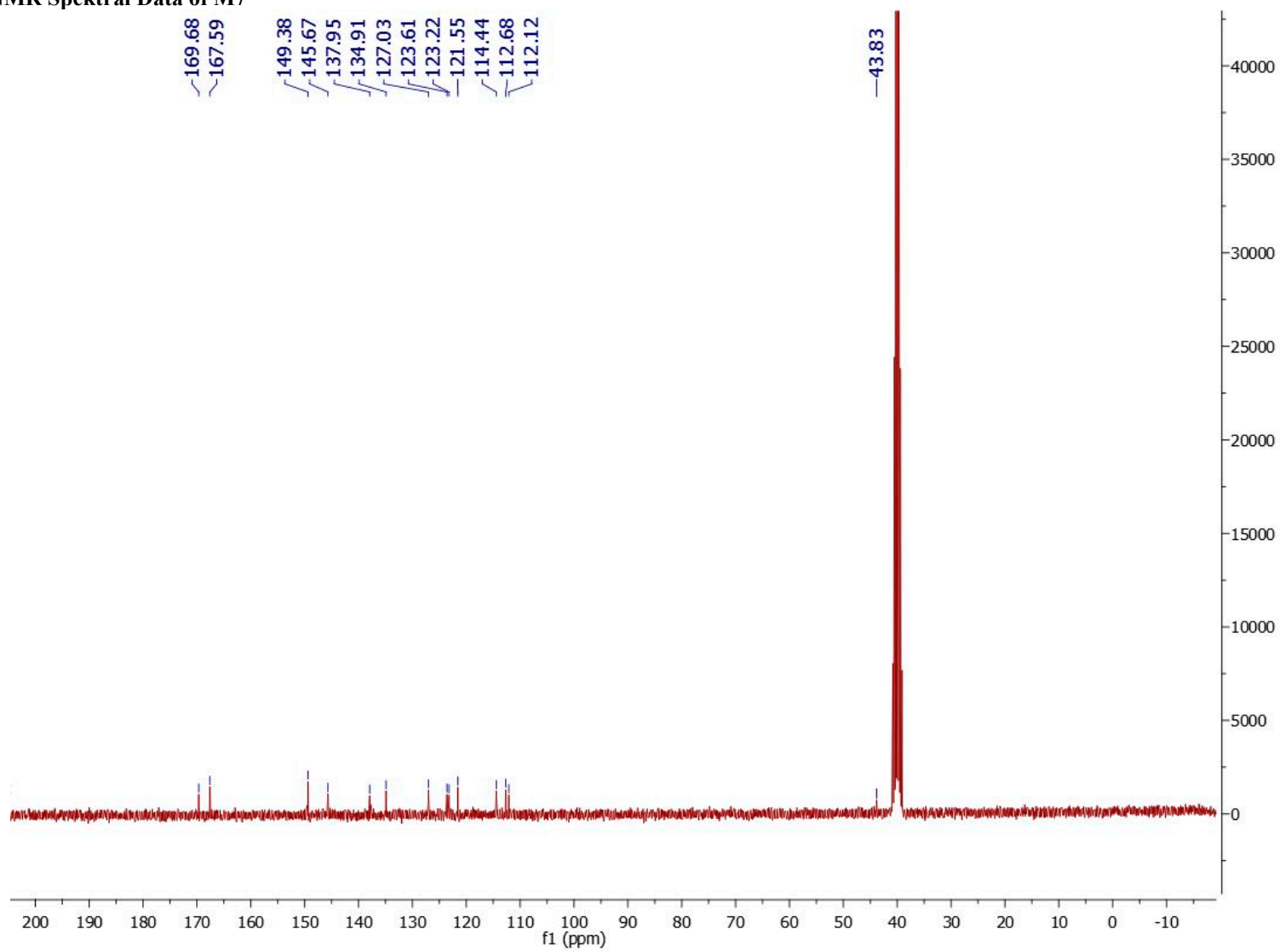
Data 19. ¹H-NMR Spektral Data of M7



(*E/Z*;75/25%)-N'-(furan-2-ylmethylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M7**)

Yield: 71%; mp: 216-7 °C, white powder. ¹H NMR (400 MHz, DMSO-d₆): δ 4.75 (s, 2H, -CH₂, %25), 5.08 (s, 2H, -CH₂, %75), 6.66 (m, H, furan), 6.96 (m, H, furan), 7.15–7.40 (m, 3H, benzothiazolone), 7.68 (m, H), 7.86 (m, H), 7.95 (s, H, N=CH, %75), 8.12 (s, H, N=CH, %25), 11.77 (s, H, NH). ¹³C NMR (100 MHz, DMSO-d₆) δ 169.68, 167.59, 149.38, 145.67, 137.95, 134.91, 127.03, 123.61, 123.22, 121.55, 114.44, 112.68, 112.12, 43.83. HRMS (ESI): *m/z* calcd for C₁₄H₁₂N₃O₃S [M+H]⁺ 302.0599; found: 302.0586.

Data 20. ^{13}C -NMR Spektral Data of M7



Data 21. Mass Spectrum Data of M7

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

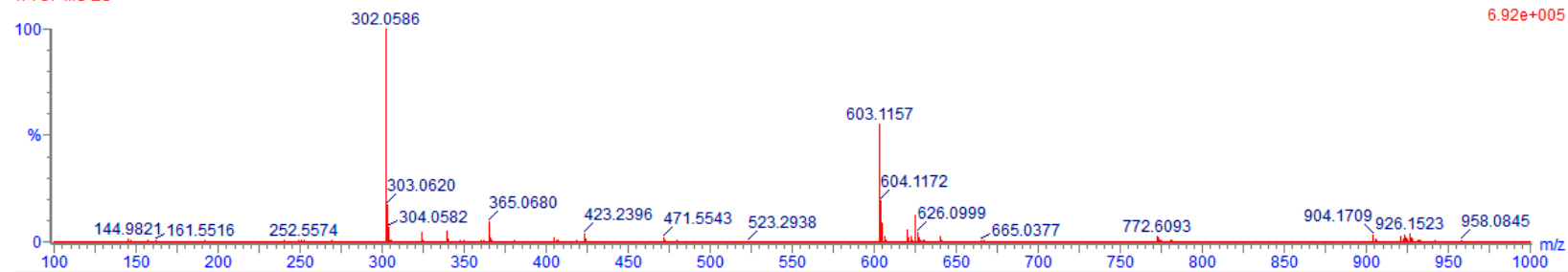
28 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

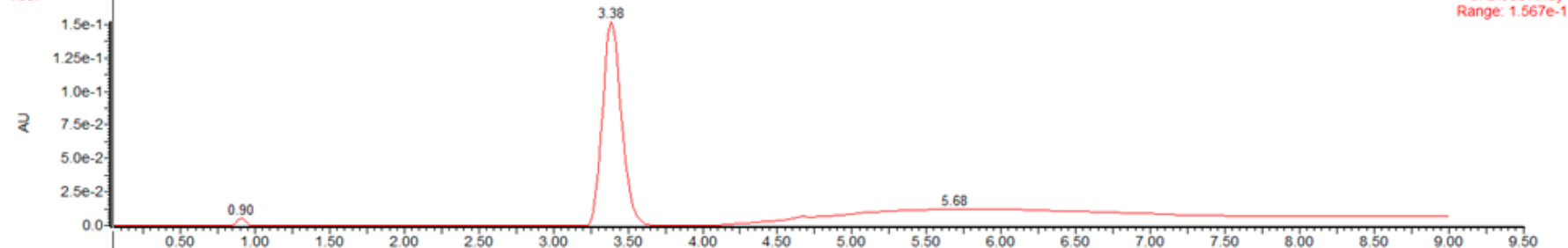
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|-----------------|-------|--------------|----|----|---|---|---|
| 302.0586 | 302.0599 | -1.3 | -4.3 | 10.5 | C14 H12 N3 O3 S | 576.6 | 0.0 | 14 | 12 | 3 | 3 | 1 |

T587 86 (3.369) Cm (83:90)

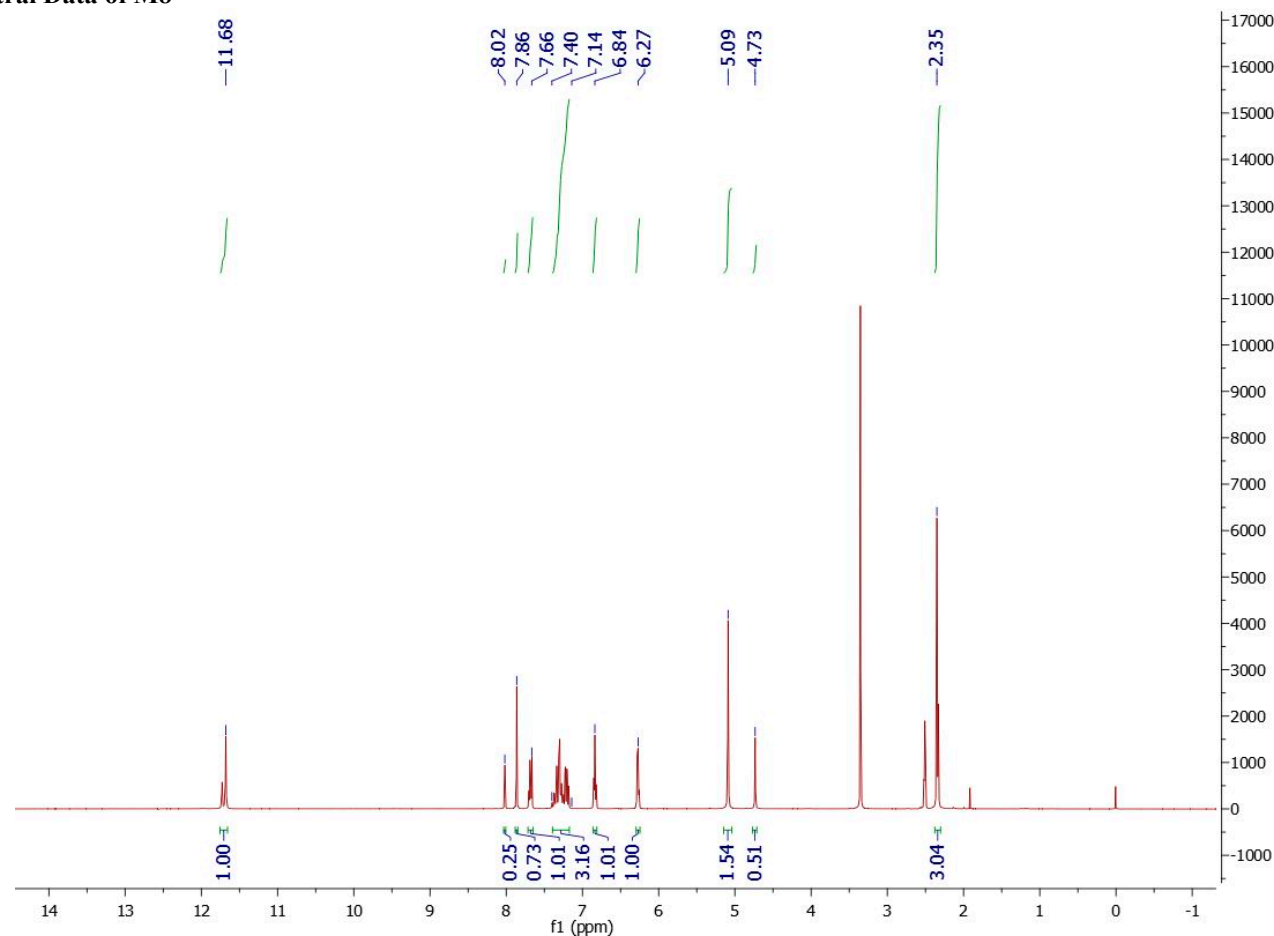
1: TOF MS ES+



T587



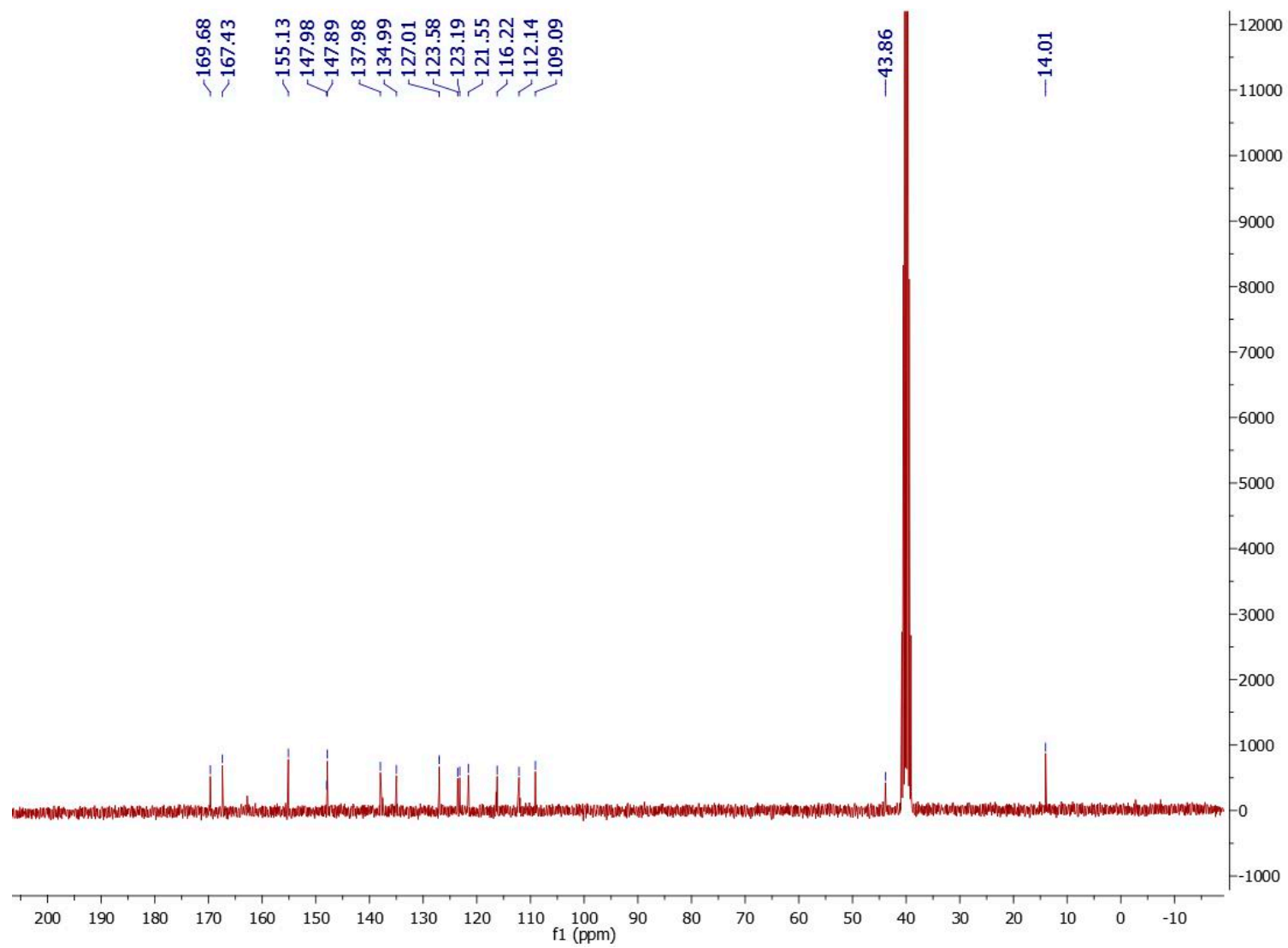
Data 22. ^1H -NMR Spektral Data of M8



(*E/Z*; 75/25%)-*N'*-((5-methylfuran-2-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M8**)

Yield: 80%; mp: 238-40 °C, white powder. ^1H NMR (400 MHz, DMSO- d_6): δ 2.35 (s, 3H, CH_3), 4.73 (s, 2H, $-\text{CH}_2$, %25), 5.09 (s, 2H, $-\text{CH}_2$, %75), 6.27 (m, H, furan), 6.84 (m, H, furan), 7.14–7.40 (m, 3H, benzothiazolone), 7.66 (m, H, benzothiazolone), 7.86 (s, H, $\text{N}=\text{CH}$, %75), 8.02 (s, H, $\text{N}=\text{CH}$, %25), 11.77 (s, H, NH). ^{13}C NMR (100 MHz, DMSO- d_6) δ 169.68, 167.43, 155.13, 147.98, 147.89, 137.98, 134.99, 127.01, 123.58, 123.19, 121.55, 116.22, 112.14, 109.09, 43.86, 14.01. HRMS (ESI): m/z calcd for $\text{C}_{15}\text{H}_{14}\text{N}_3\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$ 316.0756; found: 316.0742.

Data 23. ^{13}C -NMR Spektral Data of M8



Data 24. Mass Spectrum Data of M8

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

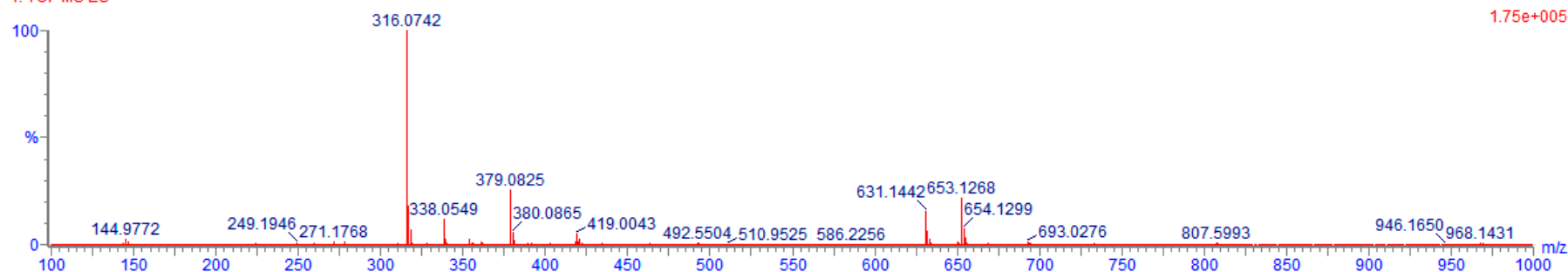
28 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

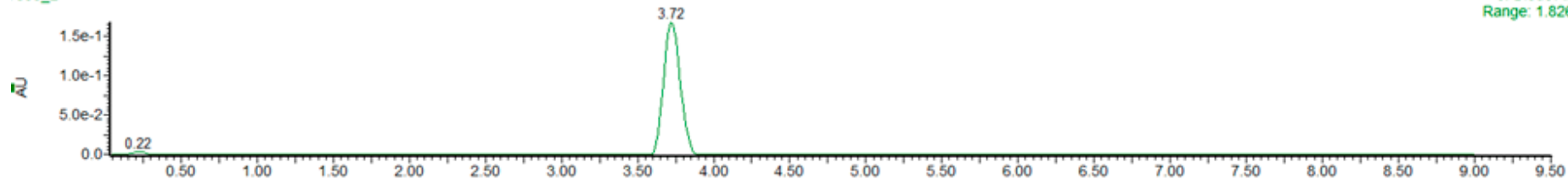
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|-----------------|-------|--------------|----|----|---|---|---|
| 316.0742 | 316.0756 | -1.4 | -4.4 | 10.5 | C15 H14 N3 O3 S | 331.4 | 0.0 | 15 | 14 | 3 | 3 | 1 |

T588_2 99 (3.873) Cm (99:101)

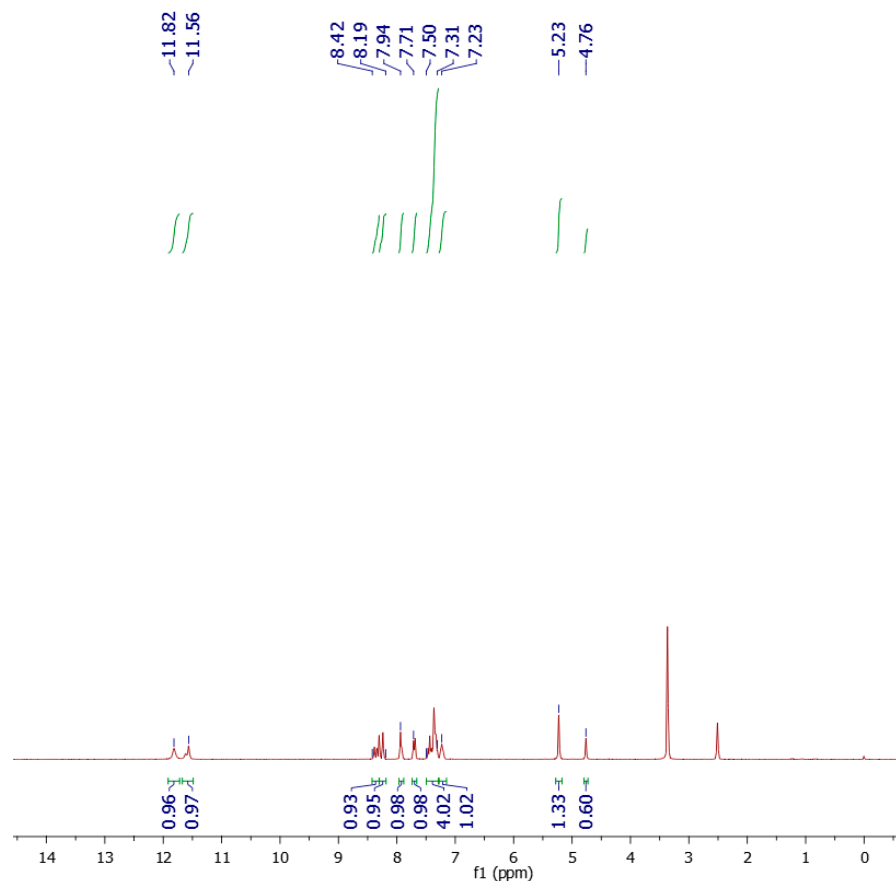
1: TOF MS ES+



T588_2



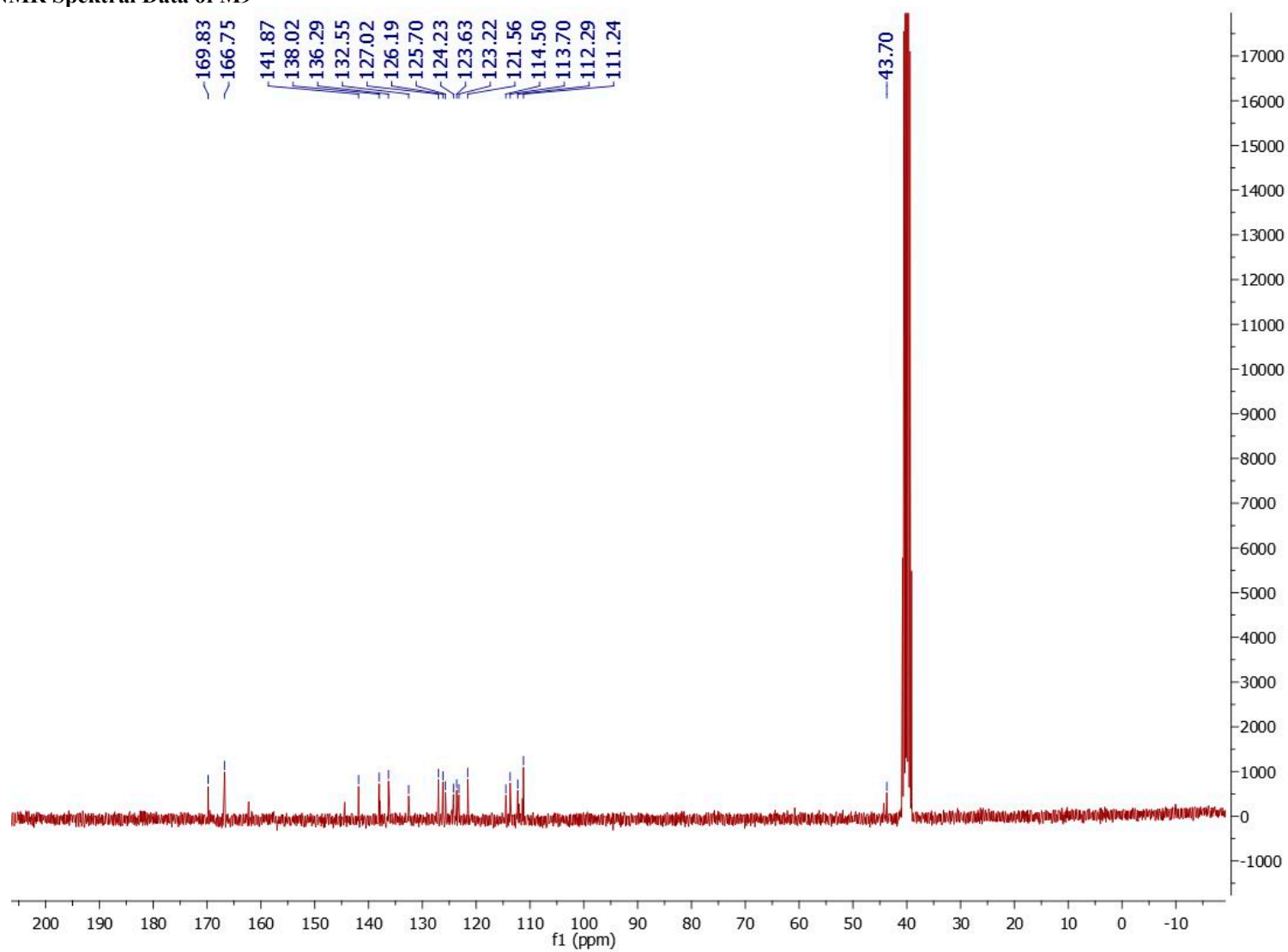
Data 25. ¹H-NMR Spektral Data of M9



(*E/Z*;69/31%)-N'-((5-bromo-1H-indol-3-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M9**)

Yield: 67%; mp: 268-9 °C, white powder. ¹H NMR (400 MHz, DMSO-d): δ 4.76 (s, 2H, -CH₂, %31), 5.23 (s, 2H, -CH₂, %69), 7.23-7.50 (m, 5H), 7.71 (m, H), 7.94 (m, H), 8.19 (m, H), 8.42 (m, H), 11.56 (s, H, NH), 11.82 (s, H, NH). ¹³C NMR (100 MHz, DMSO-d) δ 169.83, 166.85, 14.87, 138.02, 132.55, 127.02, 126.19, 125.70, 124.23, 123.63, 123.22, 121.56, 114.50, 113.70, 112.29, 111.24, 43.70. HRMS (ESI): *m/z* calcd for C₁₈H₁₄N₄O₂SBr [M+H]⁺ 429.0021; found: 429.0011.

Data 26. ^{13}C -NMR Spektral Data of M9



Data 27. Mass Spectrum Data of M9

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

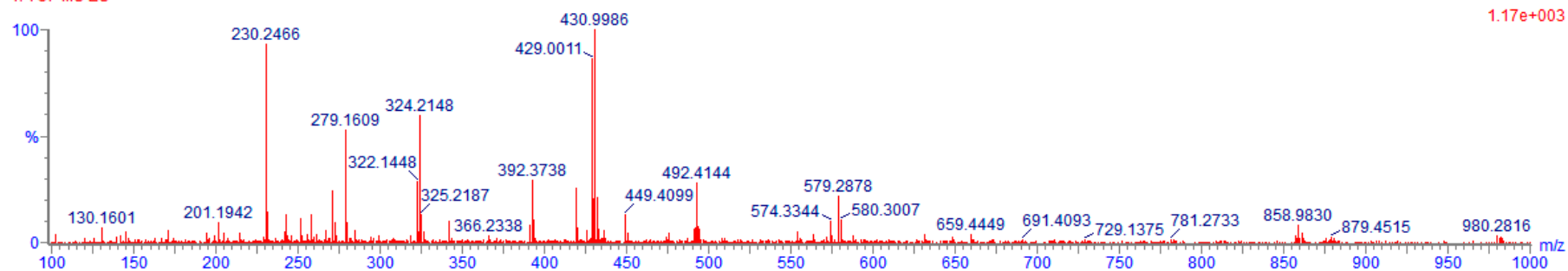
191 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

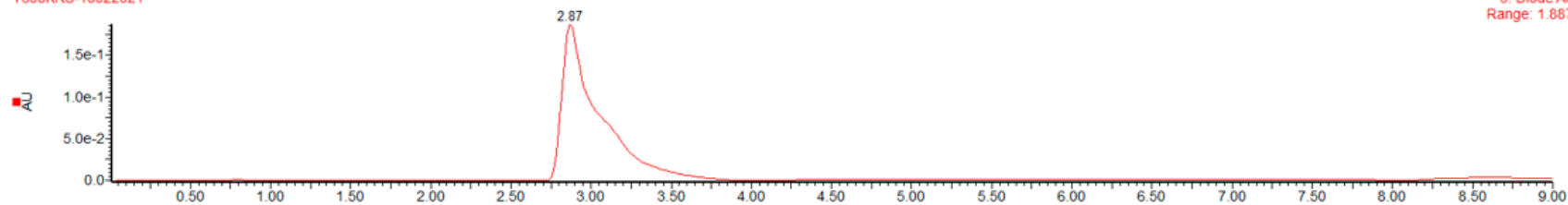
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S | Br |
|----------|------------|------|------|------|--------------------|-------|--------------|----|----|---|---|---|----|
| 429.0011 | 429.0021 | -1.0 | -2.3 | 13.5 | C18 H14 N4 O2 S Br | 55.1 | 0.0 | 18 | 14 | 4 | 2 | 1 | 1 |

T608KRS-18022021 276 (3.949)

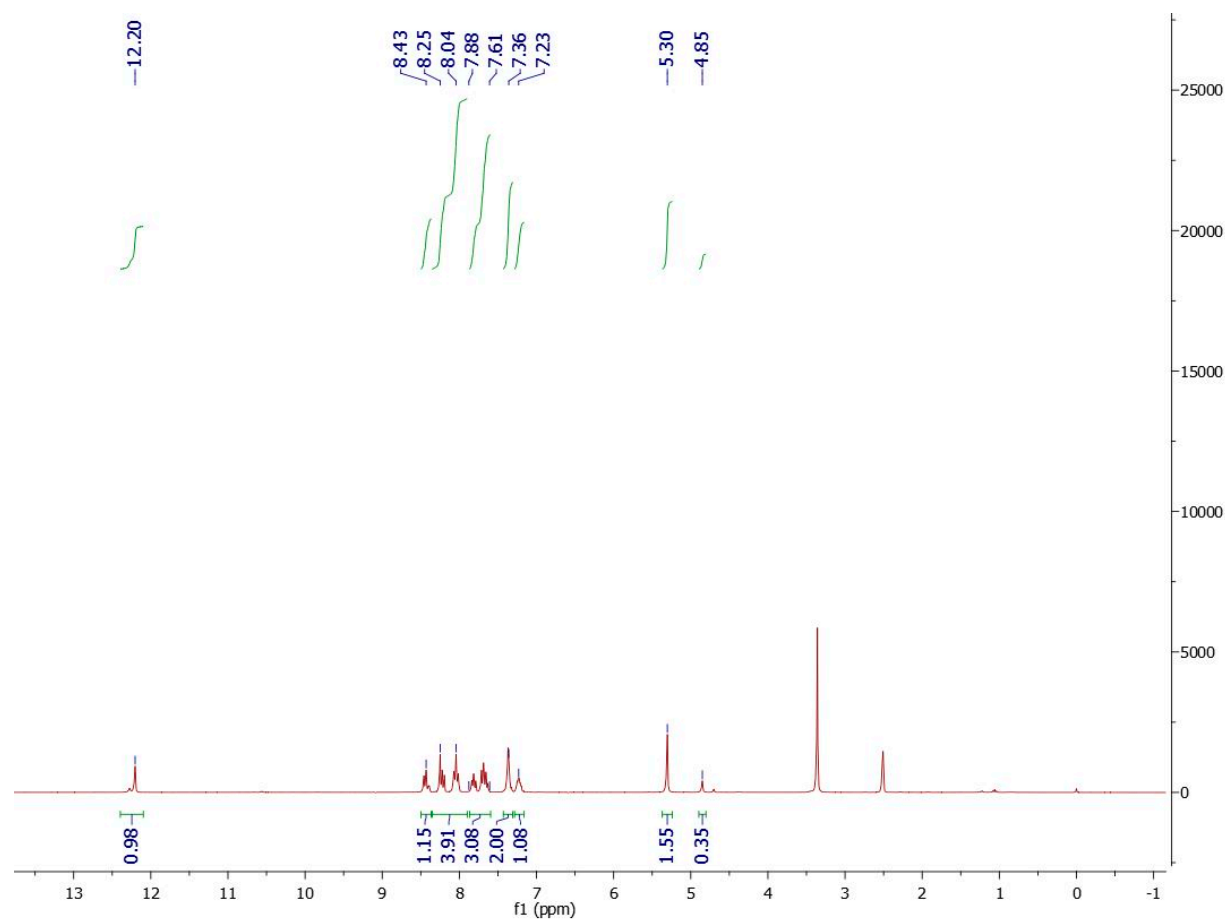
1: TOF MS ES+



T608KRS-18022021



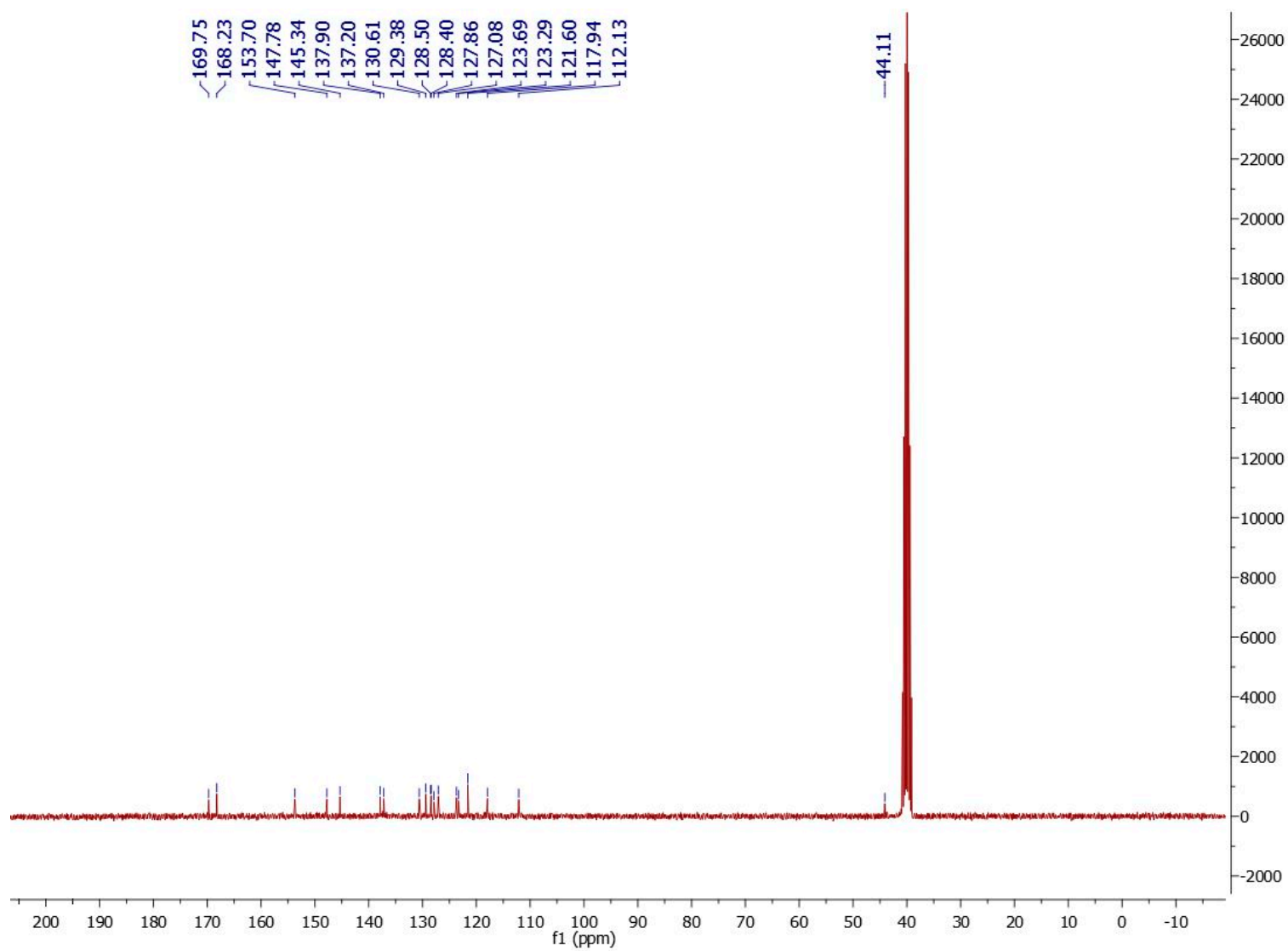
Data 28. ^1H -NMR Spektral Data of M10



(E/Z;82/18)-N'-(quinolin-2-ylmethylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl)- acetohydrazide (**M10**)

Yield: 59%; mp: 271-2 °C, white powder. ^1H NMR (400 MHz, DMSO- d_6): δ 4.85 (s, 2H, $-\text{CH}_2$, %18), 5.30 (s, 2H, $-\text{CH}_2$, %82), 7.23-7.36 (m, 3H), 7.61-7.88 (m, 3H), 8.04-8.25 (m, 4H), 8.43 (m, H, $\text{N}=\text{CH}$), 12.20 (s, H, NH). ^{13}C NMR (100 MHz, DMSO- d_6) δ 169.75, 168.23, 153.70, 147.78, 145.34, 137.90, 137.20, 130.61, 129.38, 128.50, 127.86, 127.08, 123.69, 123.29, 121.60, 117.94, 112.13, 44.11. HRMS (ESI): m/z calcd for $\text{C}_{19}\text{H}_{15}\text{N}_4\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 363.0916; found: 363.0905.

Data 29. ^{13}C -NMR Spektral Data of M10



Data 30. Mass Spectrum Data of M10

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

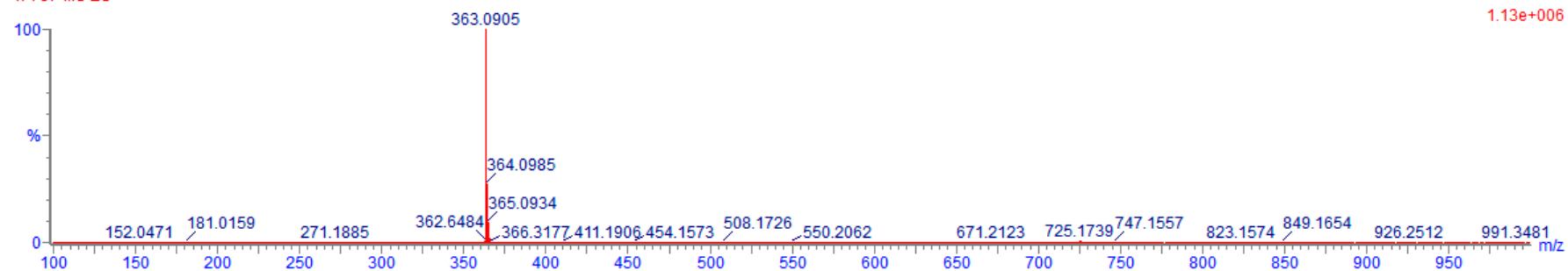
57 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|-----------------|-------|--------------|----|----|---|---|---|
| 363.0905 | 363.0916 | -1.1 | -3.0 | 14.5 | C19 H15 N4 O2 S | 596.1 | 0.0 | 19 | 15 | 4 | 2 | 1 |

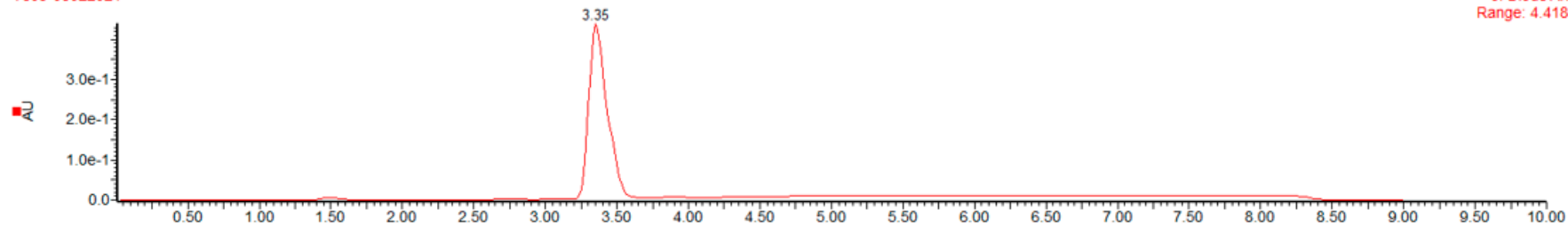
T609-08022021 243 (3.478) Cm (243:248)

1: TOF MS ES+

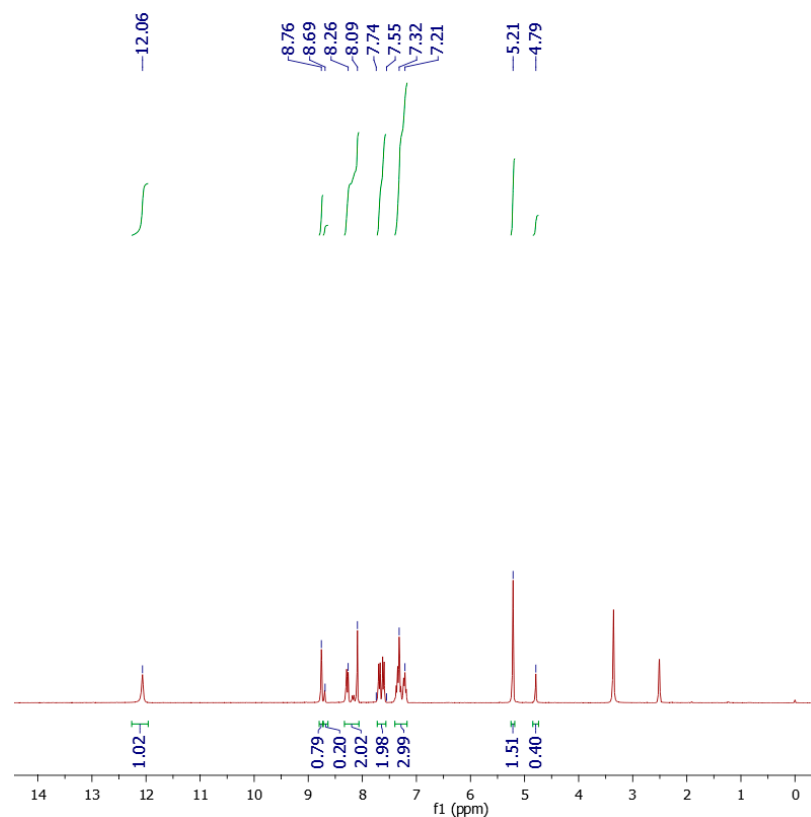


T609-08022021

3: Diode Array
Range: 4.418e-1



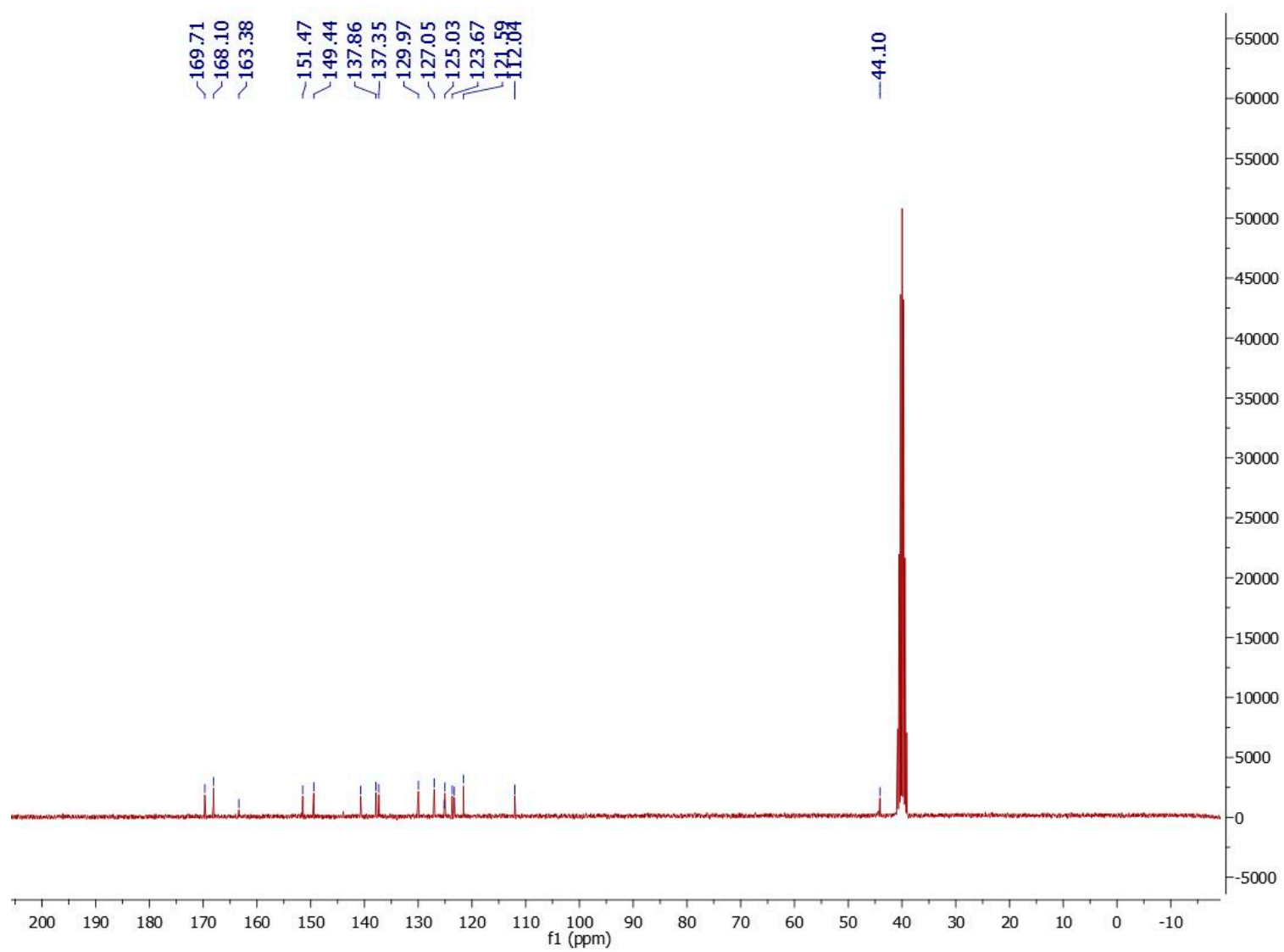
Data 31. ¹H-NMR Spektral Data of M11



(E/Z;79/21)-N'-((6-chloropyridin-3-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M11**)

Yield: 75%; mp: 237-8 °C, white powder. ¹H NMR (400 MHz, DMSO-d₆): δ 4.79 (s, 2H, -CH₂, %21), 5.21 (s, 2H, -CH₂, %79), 7.21-7.32 (m, 3H), 7.55-7.74 (m, 2H), 8.09-8.26 (m, 2H), 8.69 (m, H, N=CH, %21), 8.76 (m, H, N=CH, %79), 12.06 (s, H, NH). ¹³C NMR (100 MHz, DMSO-d₆) δ 169.71, 168.10, 163.38, 151.47, 149.44, 137.86, 137.35, 129.97, 127.05, 125.03, 123.67, 121.59, 112.04, 44.10. HRMS (ESI): *m/z* calcd for C₁₅H₁₂N₄O₂SCl [M+H]⁺ 347.0370; found: 347.0368.

Data 32. ^{13}C -NMR Spektral Data of M11



Data 33. Mass Spectrum Data of M11

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

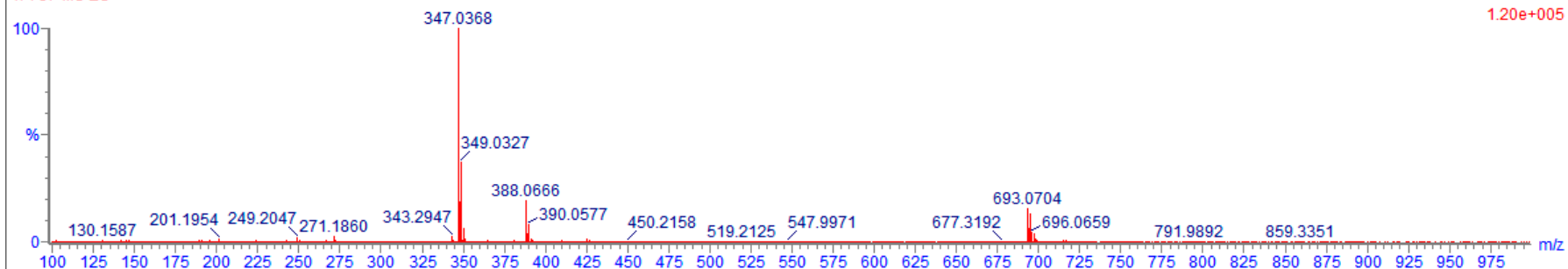
109 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

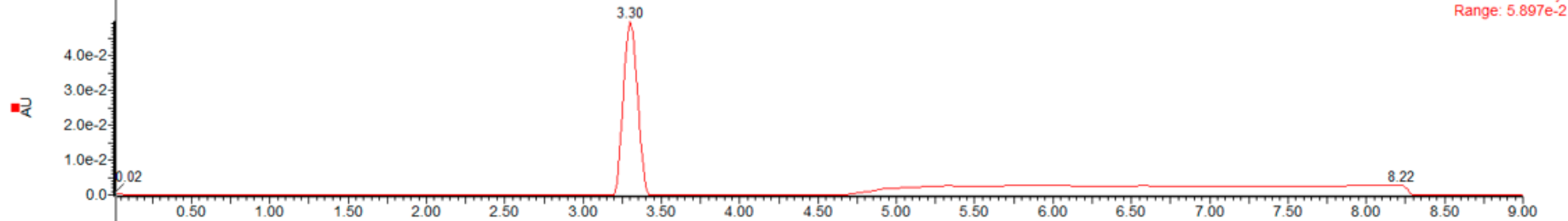
| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S | Cl |
|----------|------------|------|------|------|--------------------|-------|--------------|----|----|---|---|---|----|
| 347.0368 | 347.0370 | -0.2 | -0.6 | 11.5 | C15 H12 N4 O2 S Cl | 292.9 | 0.0 | 15 | 12 | 4 | 2 | 1 | 1 |

T610K-12022021 228 (3.260) Cm (225:228)

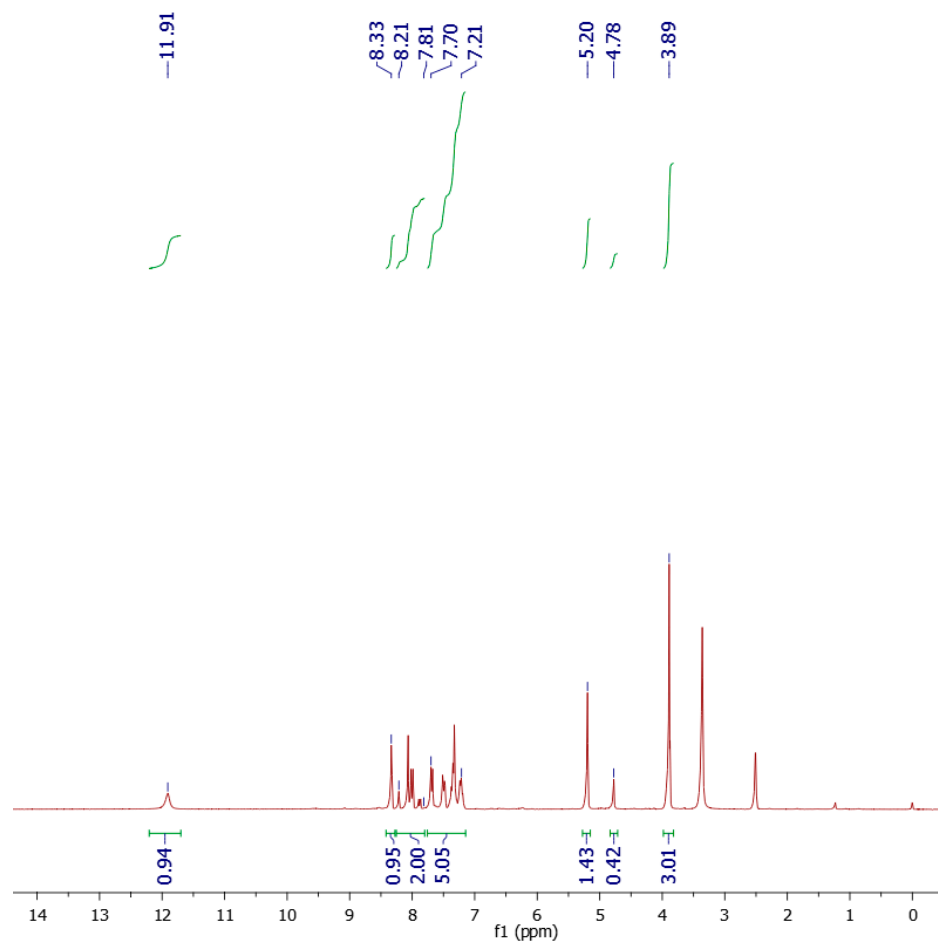
1: TOF MS ES+



T610K-12022021



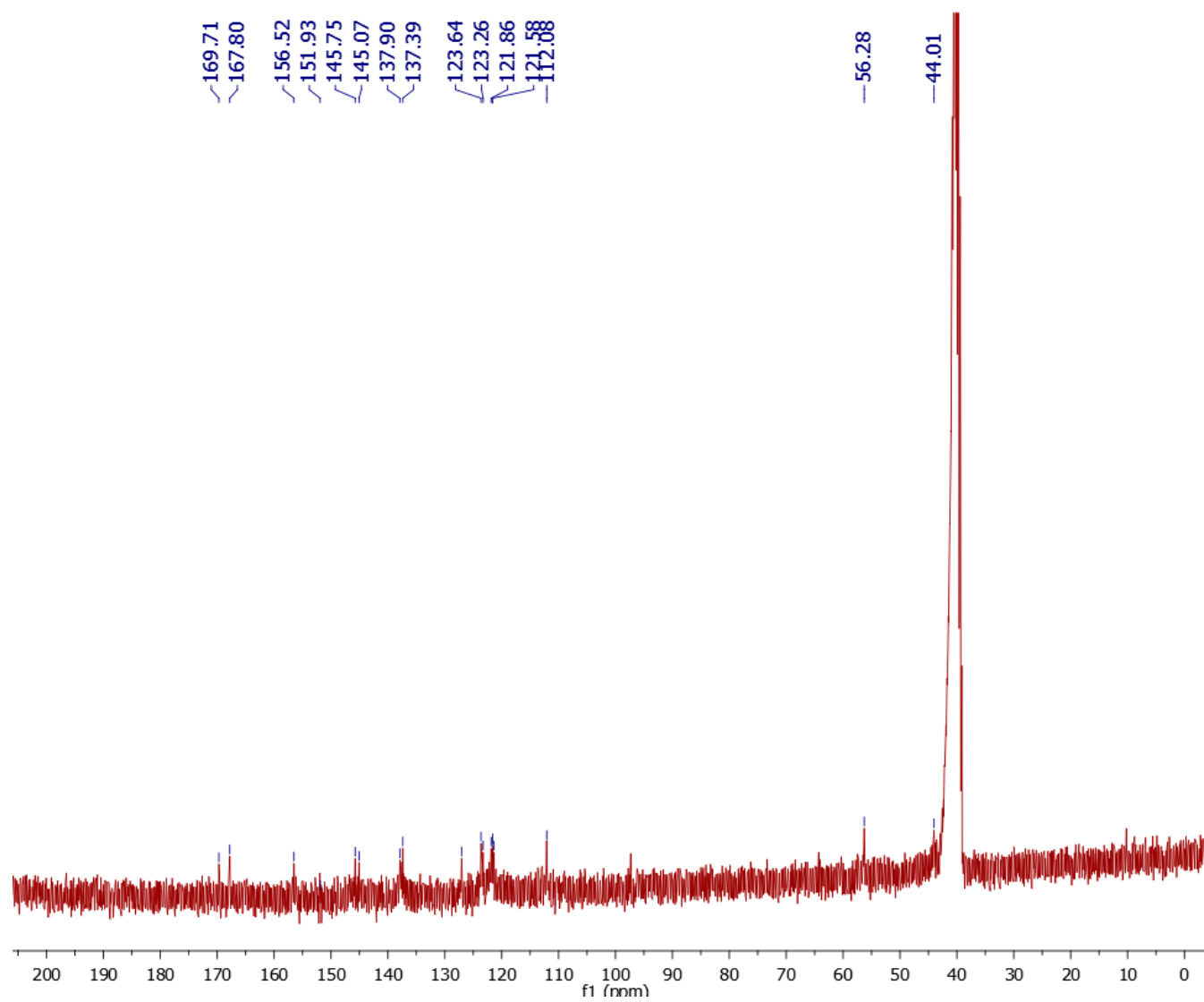
Data 34. ^1H -NMR Spektral Data of M12



(E/Z;78/22)-N'-((6-methoxypyridin-3-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl) acetohydrazide (**M12**)

Yield: 55%; mp: 226-7 °C, white powder. ^1H NMR (400 MHz, DMSO- d_6): δ 3.89 (s, 3H, CH_3) 4.78 (s, 2H, $-\text{CH}_2$, %22), 5.20 (s, 2H, $-\text{CH}_2$, %78), 7.21-7.70 (m, 5H), 7.81-8.21 (m, 2H), 8.33 (m, H, $\text{N}=\text{CH}$), 11.91 (s, H, NH). ^{13}C NMR (100 MHz, DMSO- d_6) δ 169.71, 167.80, 156.52, 151.93, 145.75, 145.07, 137.90, 137.39, 123.64, 123.26, 121.86, 121.58, 112.08, 56.28, 44.01. HRMS (ESI): m/z calcd for $\text{C}_{16}\text{H}_{15}\text{N}_4\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$ 343.0865; found: 343.0868.

Data 35. ^{13}C -NMR Spektral Data of M12



Data 36. Mass Spectrum Data of M12

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

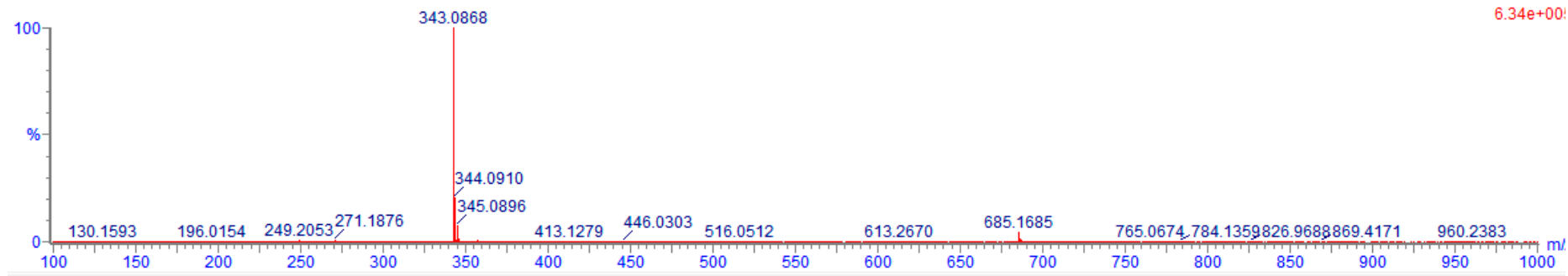
66 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|-----|-----|------|-----------------|-------|--------------|----|----|---|---|---|
| 343.0868 | 343.0865 | 0.3 | 0.9 | 11.5 | C16 H15 N4 O3 S | 463.9 | 0.0 | 16 | 15 | 4 | 3 | 1 |

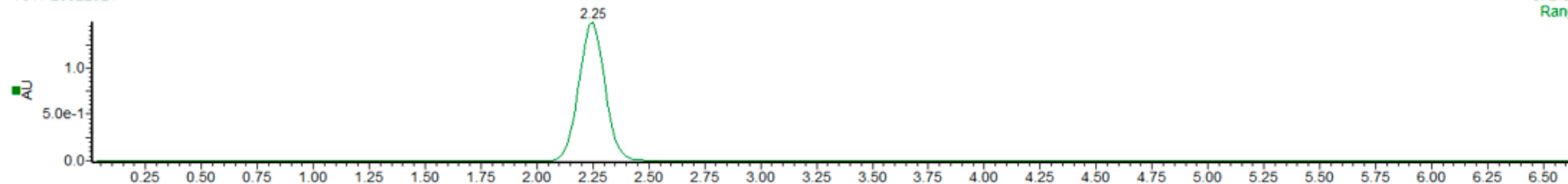
T611-25022021 170 (2.437) Cm (170:172)

1: TOF MS ES+

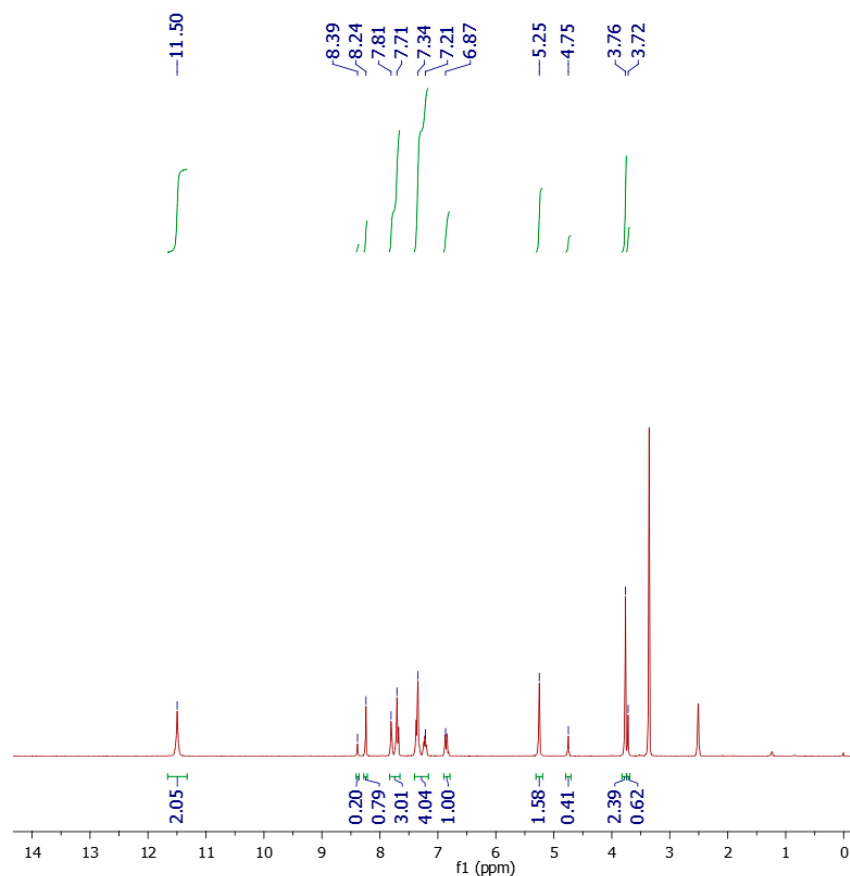


T611-25022021

3: Diode Array
Range: 1.504



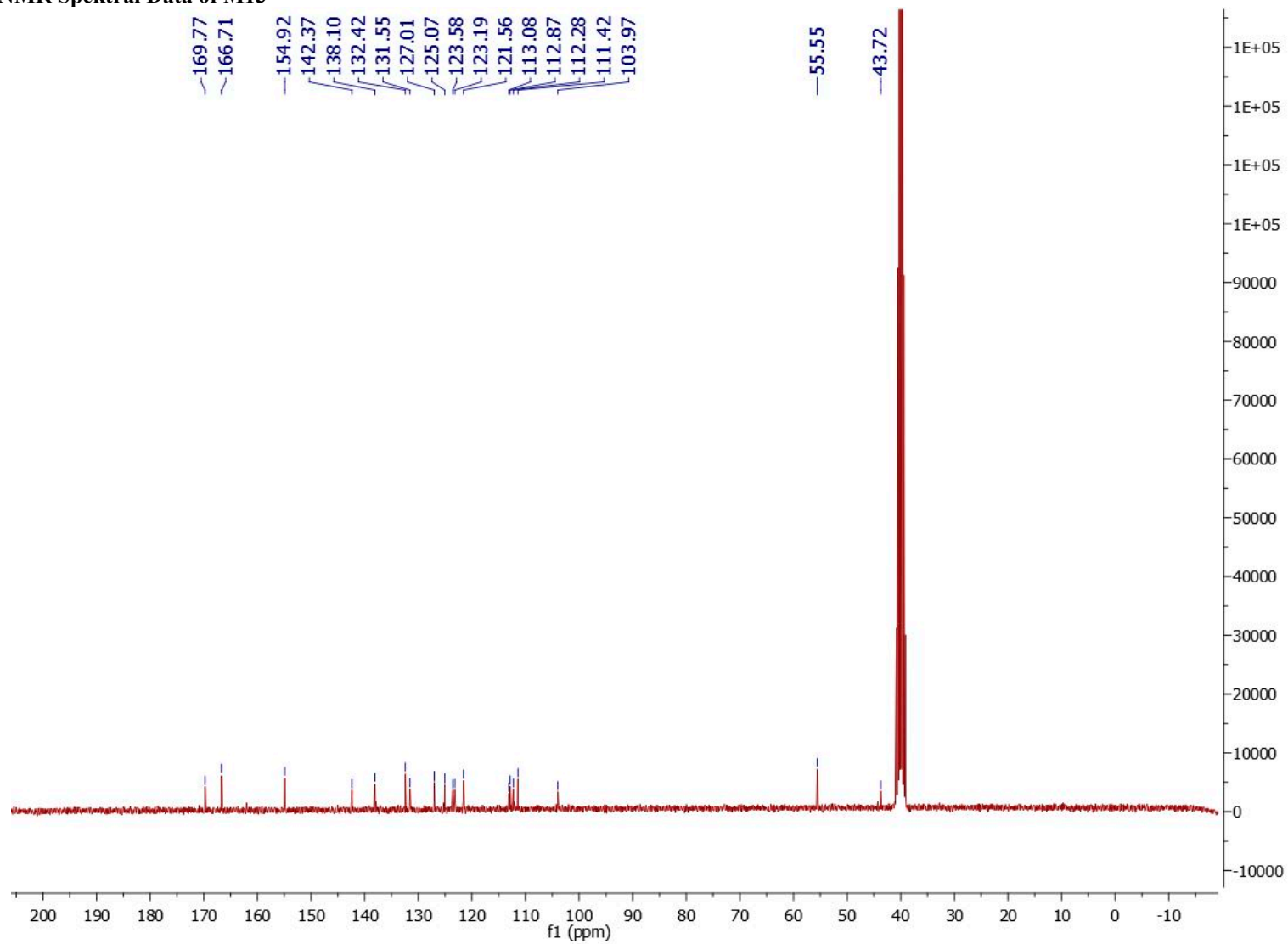
Data 37. ¹H-NMR Spektral Data of M13



(E/Z;79/21)-N'-((6-methoxy-1H-indol-3-yl)methylene)-2-(2-oxobenzo[d]thiazol-3(2H)-yl)acetohydrazide (**M13**)

Yield: 62%; mp: 262-3 °C, white powder. ¹H NMR (400 MHz, DMSO-d): δ 3.72 (s, 3H, CH₃, 21%), 3.76 (s, 3H, CH₃, 79%), 4.75 (s, 2H, -CH₂, %22), 5.25 (s, 2H, -CH₂, %78), 6.87 (m, H), 7.21-7.34 (m, 4H), 7.71-7.81 (m, 3H), 8.24 (s, H, N=CH, 79%), 8.39 (s, H, N=CH, 21%), 11.50 (s, 2H, NH). ¹³C NMR (100 MHz, DMSO-d) δ 169.77, 166.71, 154.92, 142.37, 138.10, 132.42, 131.55, 127.01, 125.07, 123.58, 123.19, 121.56, 113.08, 112.87, 112.28, 111.42, 103.97, 55.55, 43.72. HRMS (ESI): *m/z* calcd for C₁₉H₁₇N₄O₃S [M+H]⁺ 381.1021; found: 381.101

Data 38. ^{13}C -NMR Spektral Data of M13



Data 39. Mass Spectrum Data of M13

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

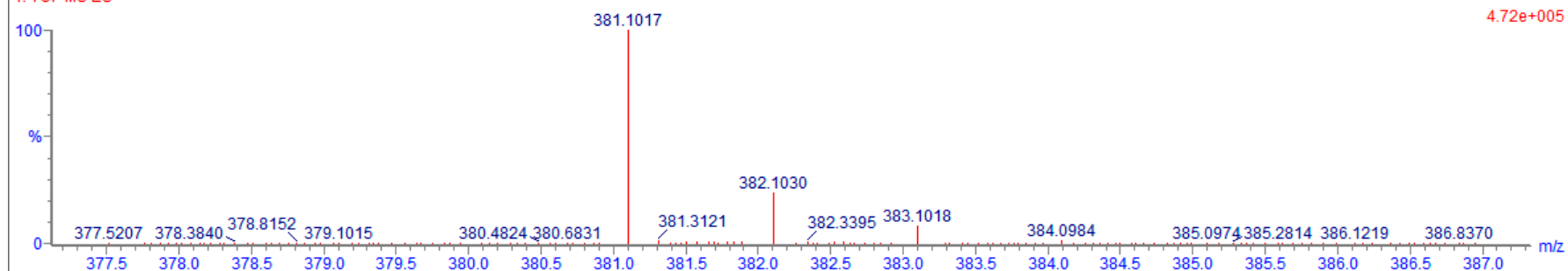
34 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

| Mass | Calc. Mass | mDa | PPM | DBE | Formula | i-FIT | i-FIT (Norm) | C | H | N | O | S |
|----------|------------|------|------|------|---|-------|--------------|----|----|---|---|---|
| 381.1017 | 381.1021 | -0.4 | -1.0 | 13.5 | C ₁₉ H ₁₇ N ₄ O ₃ S | 451.3 | 0.0 | 19 | 17 | 4 | 3 | 1 |

T612KRS-18022021 172 (2.456) Cm (172:175)

1: TOF MS ES+



T612-25022021

3: Diode Array
Range: 1.125

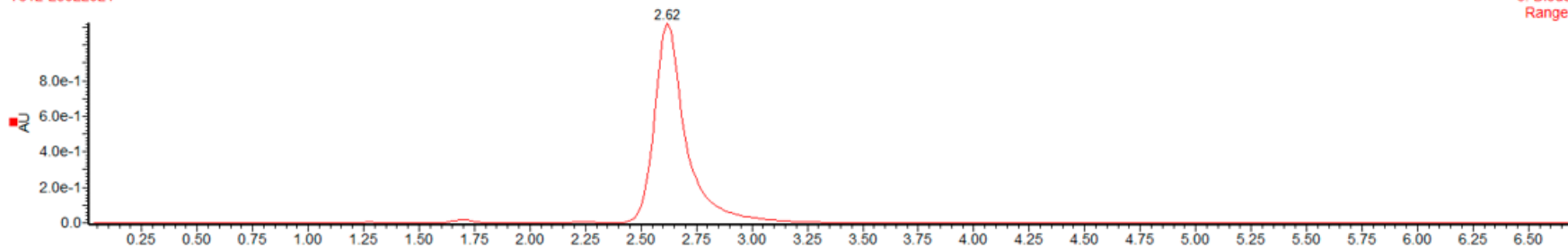


Table S1. Inhibitions of MAO by **M** series^a

| Compound | Residual activity at 10 μ M (%) | |
|-------------------------|-------------------------------------|--|
| | MAO-A | MAO-B |
| M1 | 97.50 \pm 0.36 | 83.52 \pm 0.12 |
| M2 | 88.40 \pm 1.81 | 80.88 \pm 0.01 |
| M3 | 88.31 \pm 2.73 | 73.37 \pm 2.53 |
| M4 | 95.33 \pm 5.03 | 83.25 \pm 0.27 |
| M5 | 85.14 \pm 2.06 | 77.43 \pm 4.11 |
| M6 | 94.20 \pm 3.64 | 83.25 \pm 0.27 |
| M7 | 81.34 \pm 2.71 | 78.89 \pm 5.26 |
| M8 | 102.40 \pm 1.68 | 82.42 \pm 3.79 |
| M9 | 84.39 \pm 2.15 | 76.99 \pm 4.43 |
| M10 | 93.58 \pm 4.30 | 39.17 \pm 0.06^b |
| M11 | 92.97 \pm 2.72 | 89.46 \pm 1.73 |
| M12 | 86.65 \pm 2.30 | 85.90 \pm 5.01 |
| M13 | 98.02 \pm 4.51 | 76.74 \pm 4.42 |
| Toloxatone ^c | 1.080 \pm 0.025 | - |
| Lazabemide ^c | - | 0.110 \pm 0.016 |
| Clorgyline ^c | 0.007 \pm 0.001 | - |
| Pargyline ^c | - | 0.140 \pm 0.006 |

^a Results are the means \pm standard errors of duplicate or triplicate experiments.^b IC₅₀ value of MAO-B was 2.75 \pm 0.44 μ M.^c IC₅₀ value of MAO-A and MAO-B, respectively