



MB03\_crd\_2

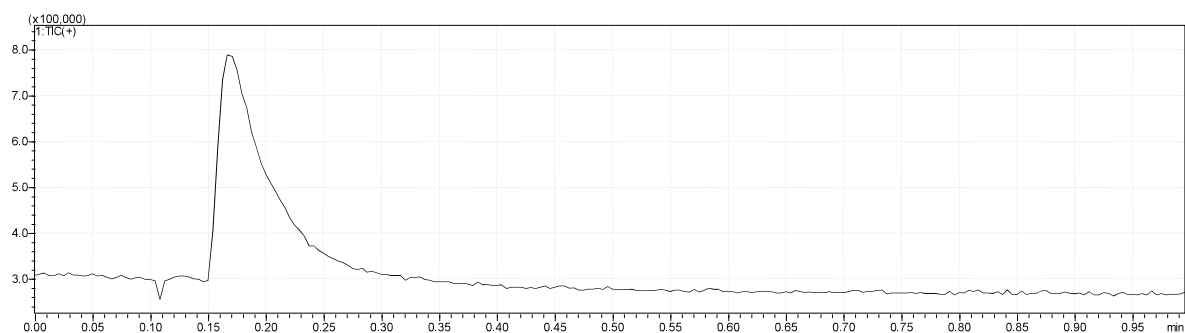
C15H10O3S

$[M+H]^+_{\text{theo}} = 271.0423 \text{ m/z}$

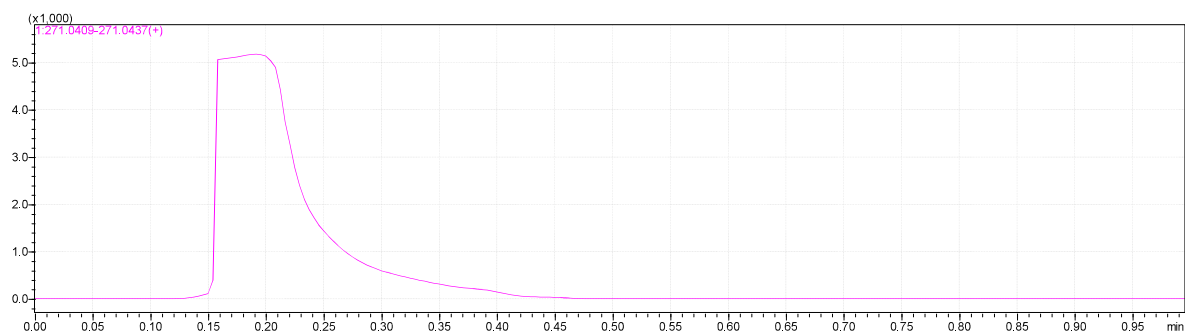
C16H12O3S

$[M+H]^+_{\text{theo}} = 285.0580 \text{ m/z}$

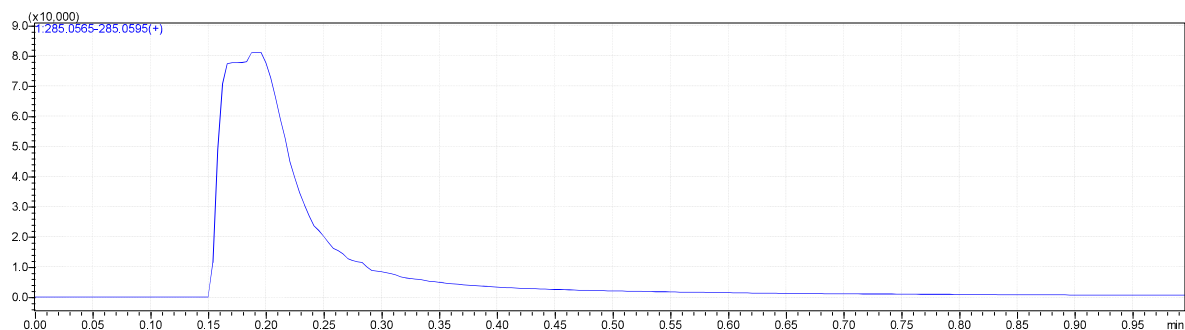
TIC (+)



XIC 271.0423  $m/z \pm 5$  ppm

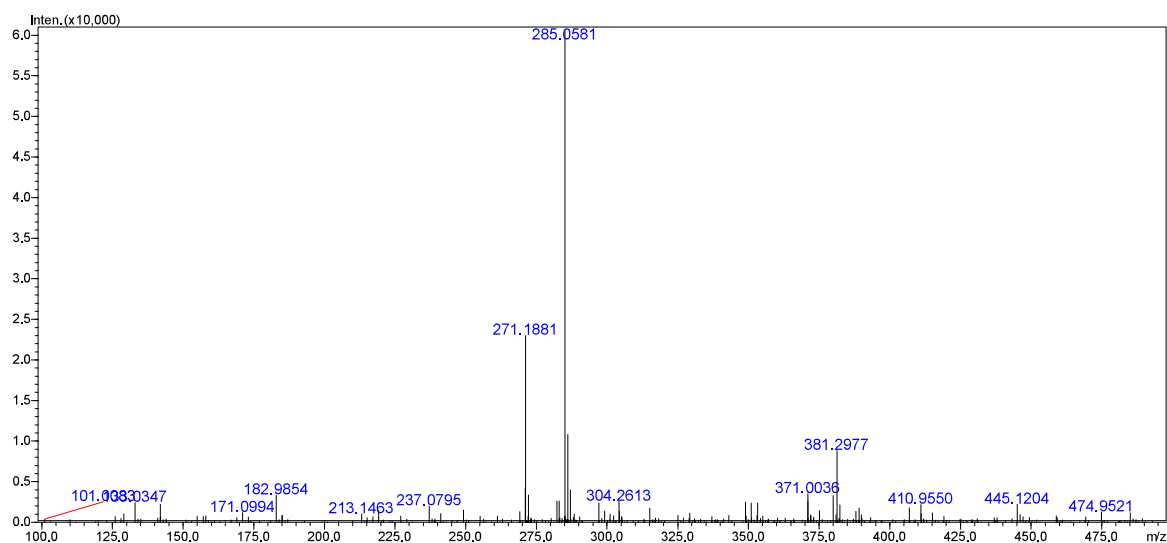
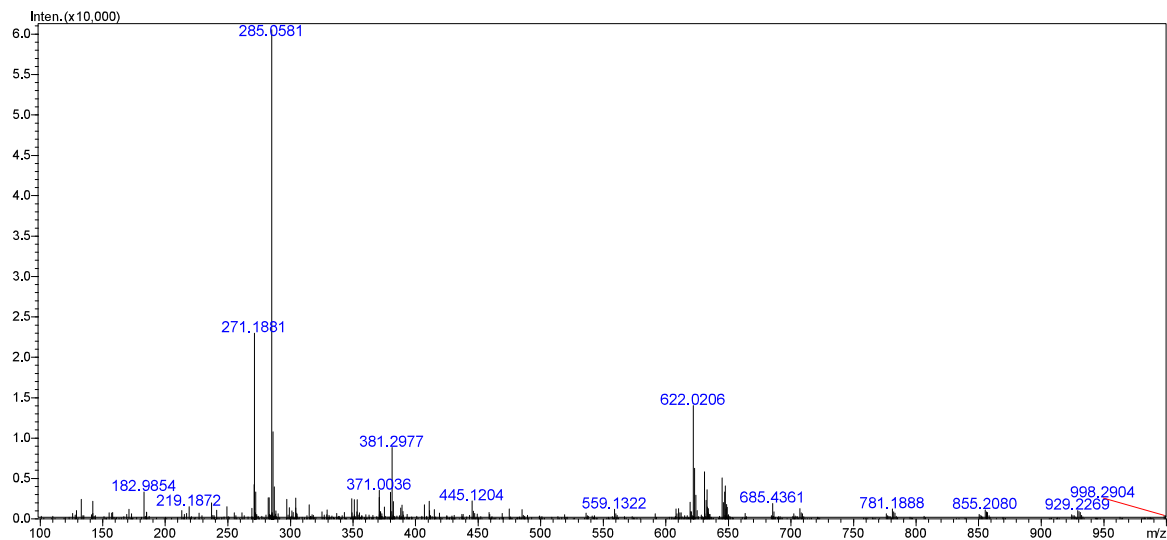


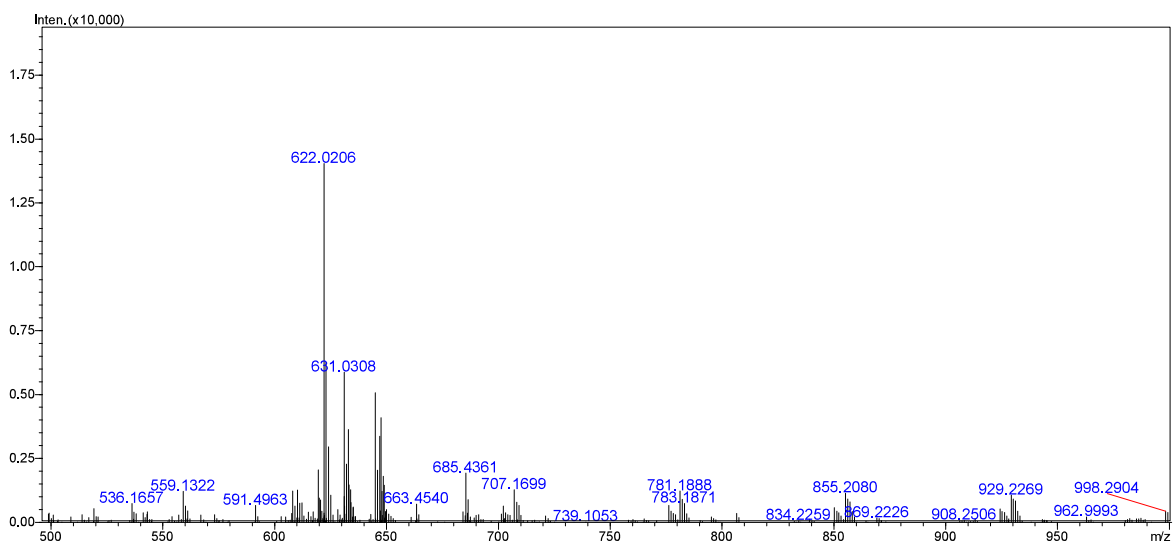
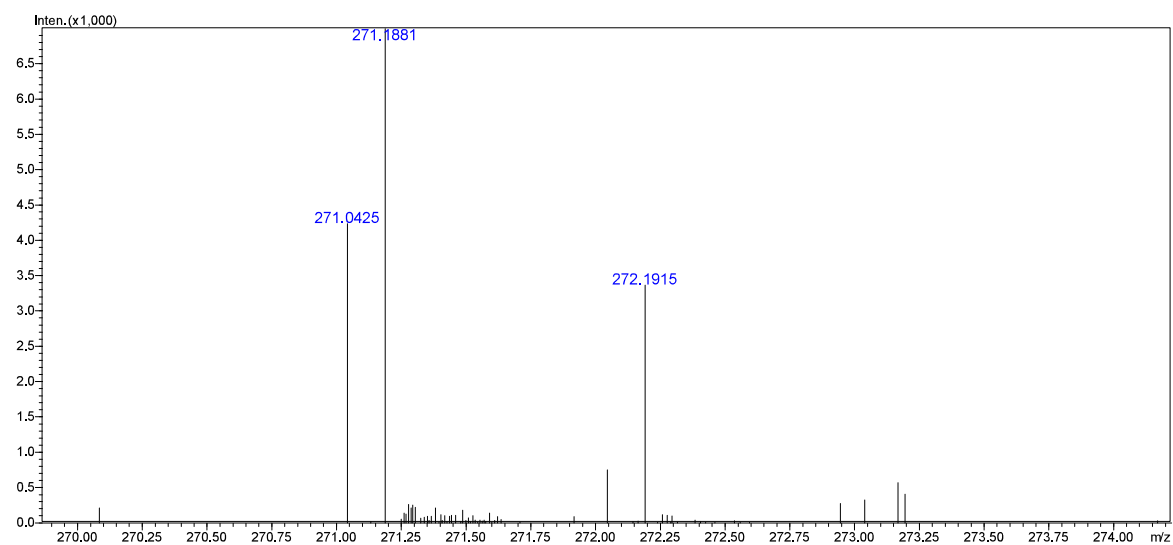
XIC 285.0580  $m/z \pm 5$  ppm





MS (+)



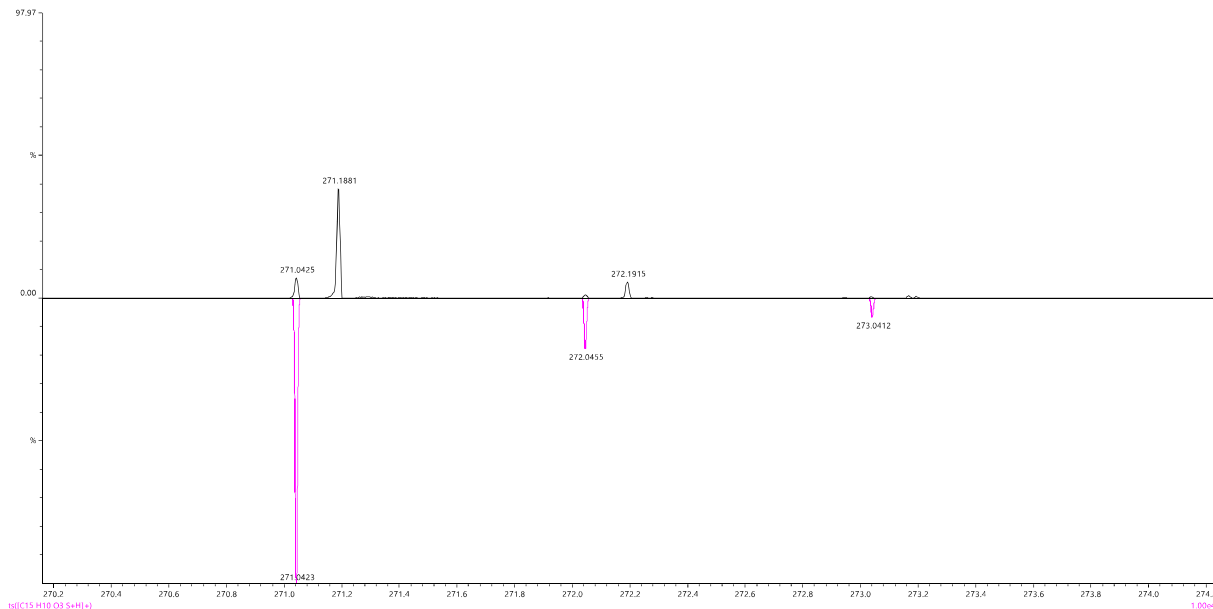




## Isotopic distribution 271.0423 m/z

Event#: 1 MS(E-) Ret. Time: [0.146--0.217]-[0.017--0.125] Scan#: [36--53]-[5--31]

1.53e4

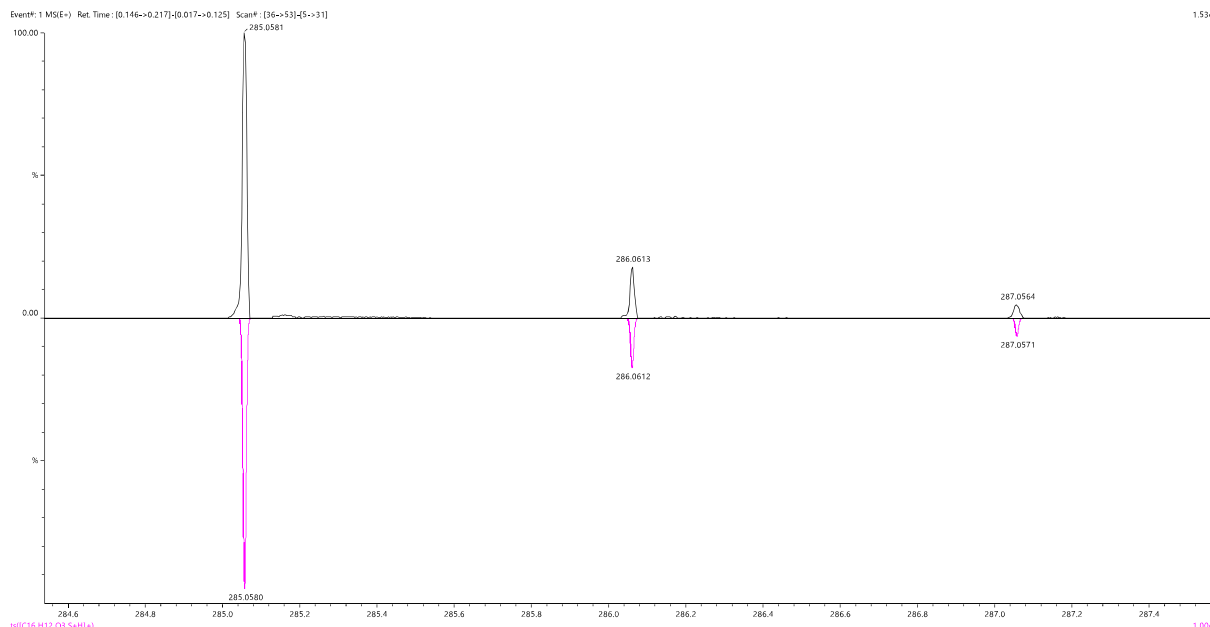


## Formula predictor

| #  | Score | Pred. (M) | Pred. m/z | Meas. m/z | Diff. (mDa) | Formula (M)    | Ion                 | Diff. (ppm) | Iso Score | DBE  |
|----|-------|-----------|-----------|-----------|-------------|----------------|---------------------|-------------|-----------|------|
| 1  | 75.62 | 270.03575 | 271.04303 | 271.04249 | -0.54       | C8 H10 N6 O S2 | [M+H] <sup>+</sup>  | -1.984      | 72.91     | 7.0  |
| 2  | 75.49 | 248.05322 | 271.04244 | 271.04249 | 0.05        | C9 H12 O8      | [M+Na] <sup>+</sup> | 0.192       | 72.77     | 4.0  |
| 3  | 74.37 | 270.03507 | 271.04234 | 271.04249 | 0.15        | C15 H10 O3 S   | [M+H] <sup>+</sup>  | 0.547       | 71.53     | 11.0 |
| 4  | 72.98 | 270.03510 | 271.04238 | 271.04249 | 0.11        | H14 N8 O3 S3   | [M+H] <sup>+</sup>  | 0.419       | 69.97     | -2.0 |
| 5  | 68.69 | 248.05409 | 271.04331 | 271.04249 | -0.82       | C10 H16 O3 S2  | [M+Na] <sup>+</sup> | -3.016      | 65.21     | 3.0  |
| 6  | 68.17 | 232.07675 | 271.03990 | 271.04249 | 2.59        | C2 H12 N6 O7   | [M+K] <sup>+</sup>  | 9.539       | 64.63     | 0.0  |
| 7  | 65.88 | 270.03622 | 271.04350 | 271.04249 | -1.01       | C8 H2 N10 O2   | [M+H] <sup>+</sup>  | -3.711      | 62.09     | 13.0 |
| 8  | 62.52 | 248.05072 | 271.03994 | 271.04249 | 2.55        | C13 H12 O3 S   | [M+Na] <sup>+</sup> | 9.423       | 58.36     | 8.0  |
| 9  | 53.33 | 248.05455 | 271.04378 | 271.04249 | -1.29       | C10 H8 N4 O4   | [M+Na] <sup>+</sup> | -4.743      | 48.15     | 9.0  |
| 10 | 53.27 | 232.07827 | 271.04143 | 271.04249 | 1.06        | C11 H12 N4 S   | [M+K] <sup>+</sup>  | 3.927       | 48.08     | 8.0  |



## Isotopic distribution 285.0580 m/z



## Formula predictor

| #  | Score | Pred. (M) | Pred. m/z | Meas. m/z | Diff. (mDa) | Formula (M)    | Ion                 | Diff. (ppm) | Iso Score | DBE  |
|----|-------|-----------|-----------|-----------|-------------|----------------|---------------------|-------------|-----------|------|
| 1  | 97.84 | 284.05072 | 285.05799 | 285.05814 | 0.15        | C16 H12 O3 S   | [M+H] <sup>+</sup>  | 0.520       | 97.60     | 11.0 |
| 2  | 77.13 | 262.06887 | 285.05809 | 285.05814 | 0.05        | C10 H14 O8     | [M+Na] <sup>+</sup> | 0.182       | 74.59     | 4.0  |
| 3  | 74.87 | 262.06974 | 285.05896 | 285.05814 | -0.82       | C11 H18 O3 S2  | [M+Na] <sup>+</sup> | -2.868      | 72.07     | 3.0  |
| 4  | 74.35 | 284.04988 | 285.05716 | 285.05814 | 0.98        | H12 N8 O8 S    | [M+H] <sup>+</sup>  | 3.448       | 71.50     | -1.0 |
| 5  | 69.88 | 284.05140 | 285.05868 | 285.05814 | -0.54       | C9 H12 N6 O S2 | [M+H] <sup>+</sup>  | -1.887      | 66.53     | 7.0  |
| 6  | 69.37 | 284.05187 | 285.05915 | 285.05814 | -1.01       | C9 H4 N10 O2   | [M+H] <sup>+</sup>  | -3.529      | 65.97     | 13.0 |
| 7  | 63.47 | 262.07154 | 285.06076 | 285.05814 | -2.62       | C12 H6 N8      | [M+Na] <sup>+</sup> | -9.201      | 59.41     | 14.0 |
| 8  | 62.89 | 246.09595 | 285.05911 | 285.05814 | -0.97       | C8 H22 O4 S2   | [M+K] <sup>+</sup>  | -3.401      | 58.76     | -2.0 |
| 9  | 61.69 | 262.06637 | 285.05559 | 285.05814 | 2.55        | C14 H14 O3 S   | [M+Na] <sup>+</sup> | 8.959       | 57.43     | 8.0  |
| 10 | 58.50 | 246.09508 | 285.05824 | 285.05814 | -0.10       | C7 H18 O9      | [M+K] <sup>+</sup>  | -0.351      | 53.89     | -1.0 |



MB03\_crd\_2

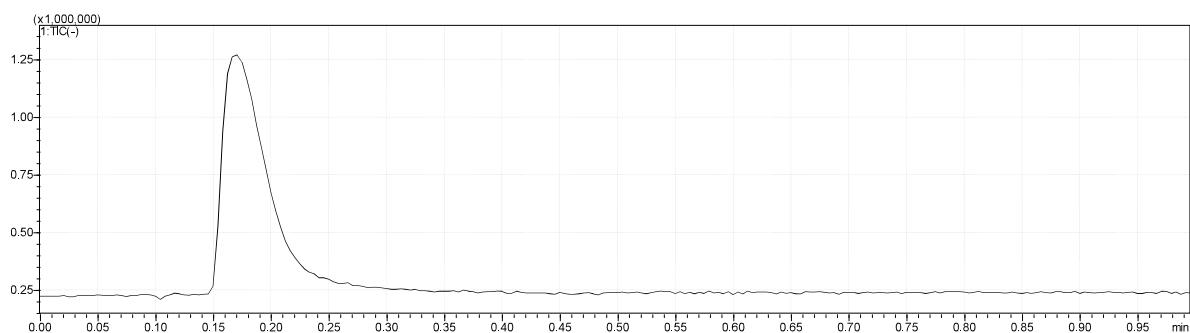
C15H10O3S

$[M-H]^-_{\text{theo}} = 269.0278 \text{ m/z}$

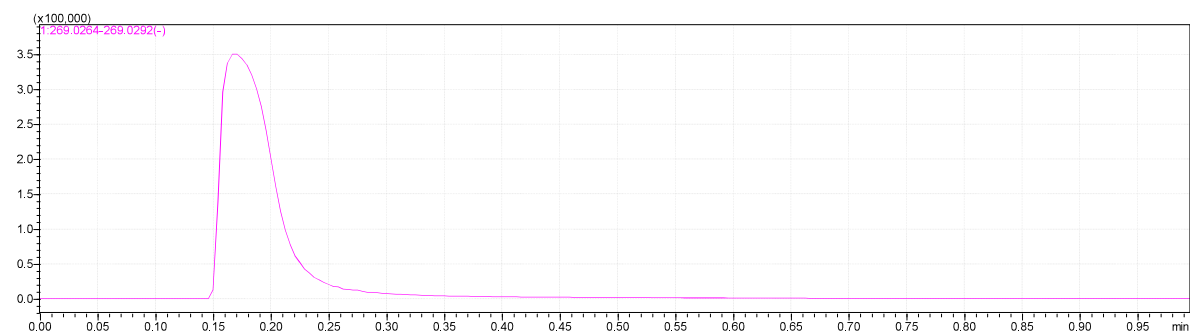
C16H12O3S

$[M-H]^-_{\text{theo}} = 283.0434 \text{ m/z}$

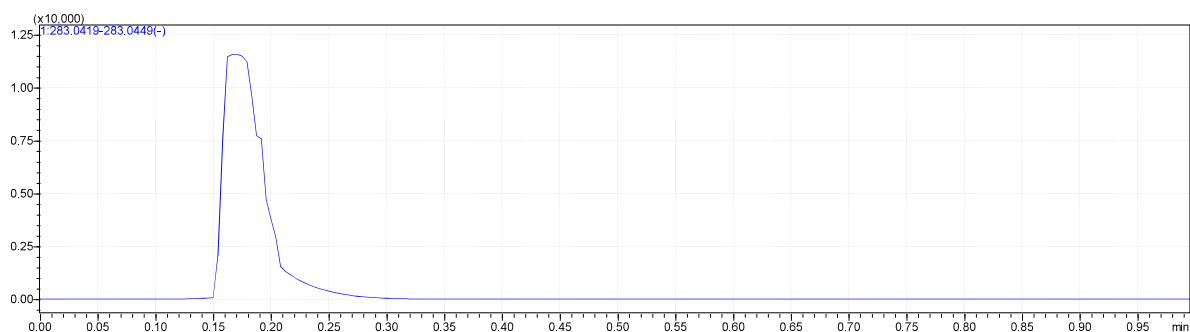
TIC (-)



XIC 269.0278  $m/z \pm 5 \text{ ppm}$



XIC 283.0434  $m/z \pm 5 \text{ ppm}$



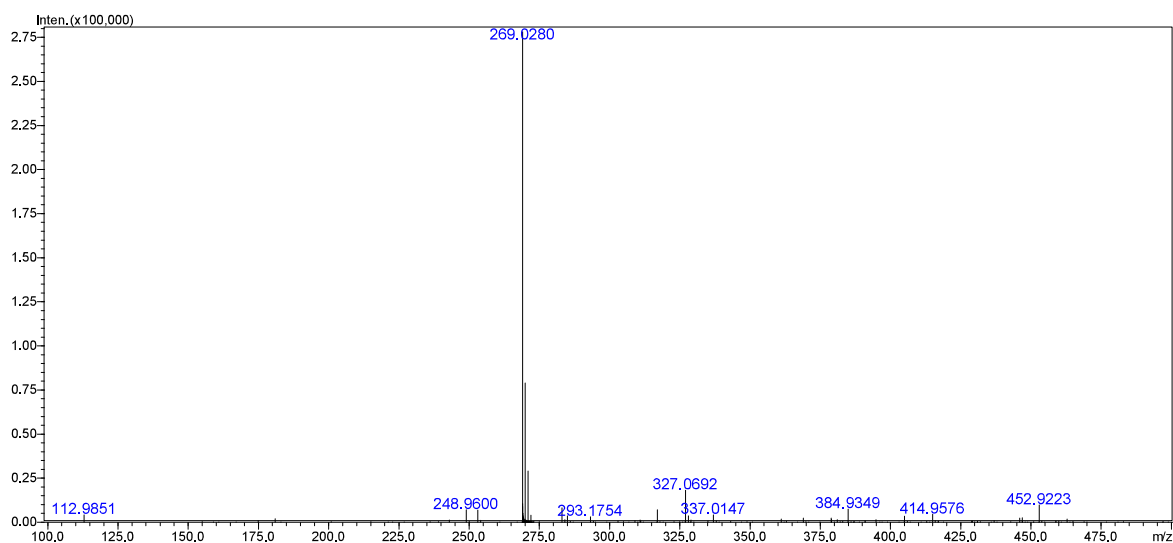
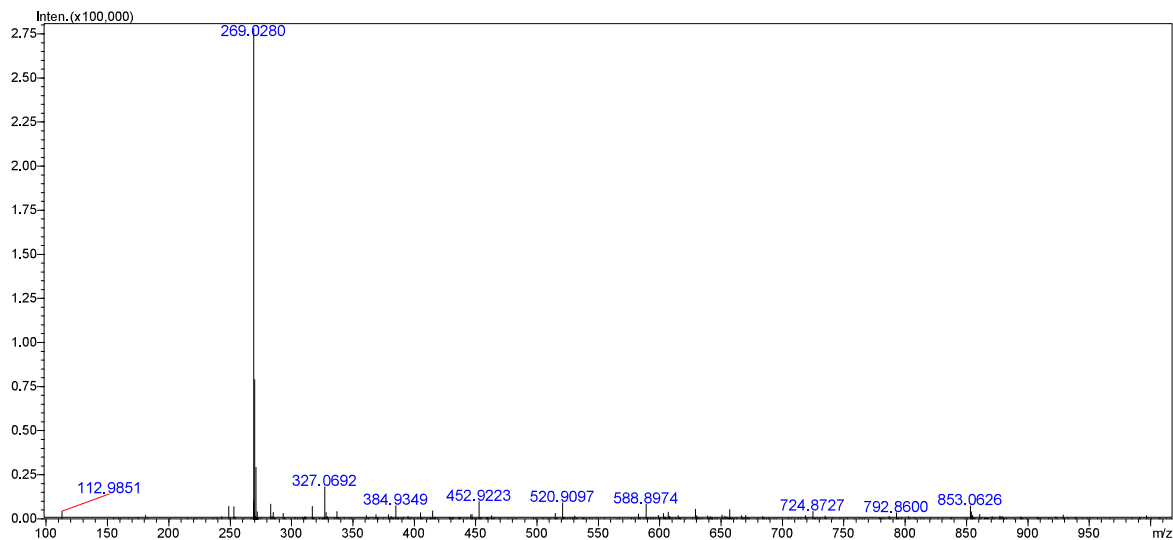


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POMIAROWE - SEKCJA MS

## MS (-)

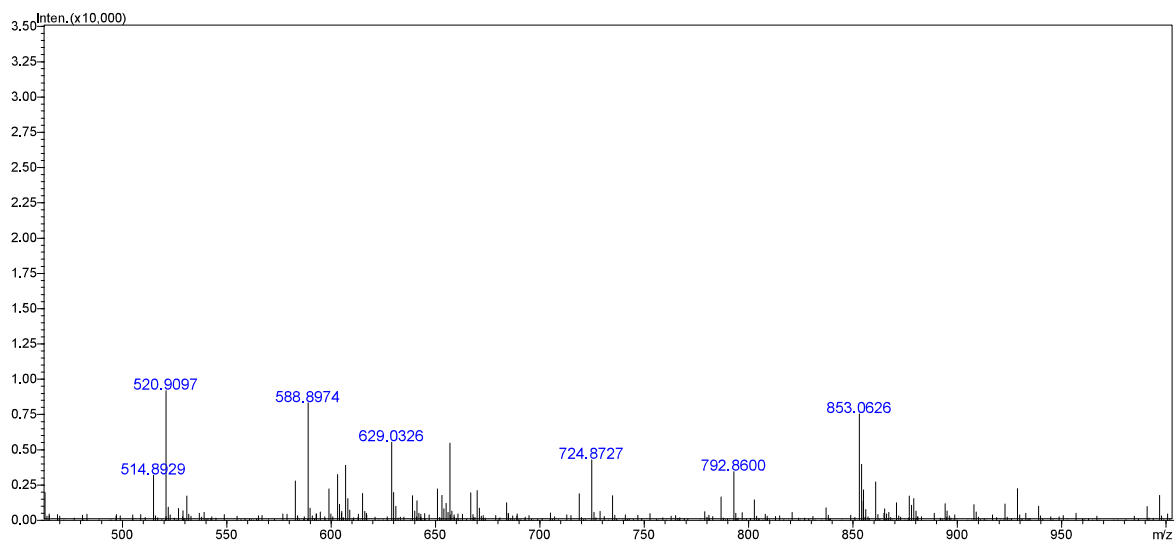
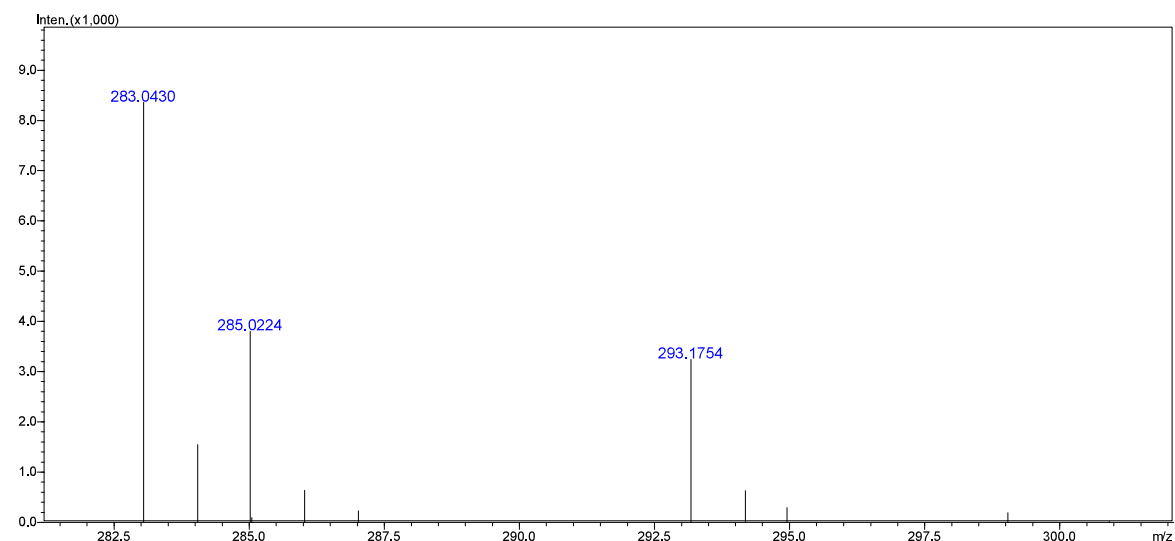
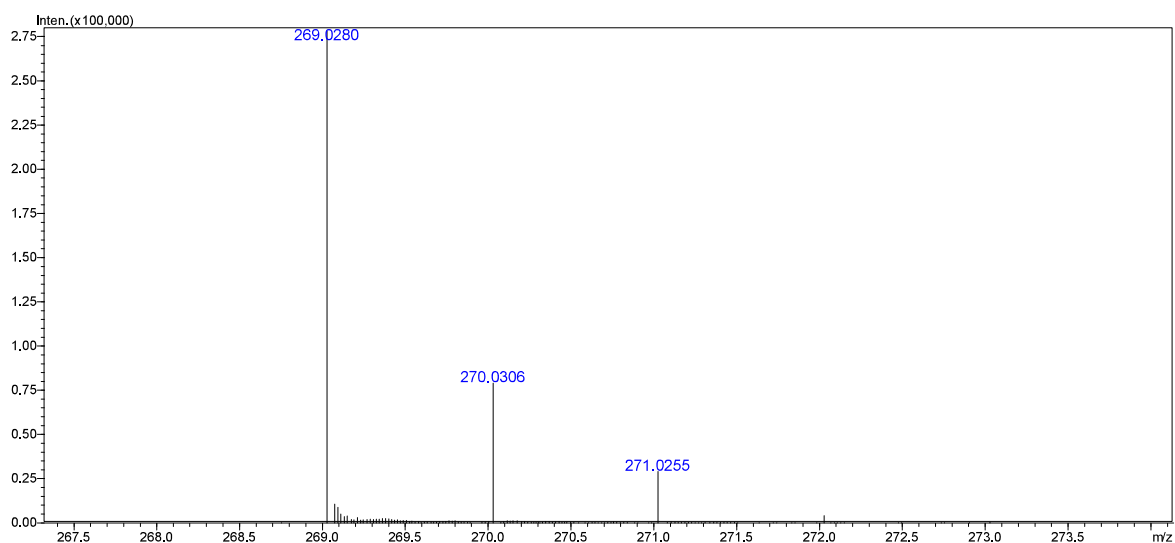




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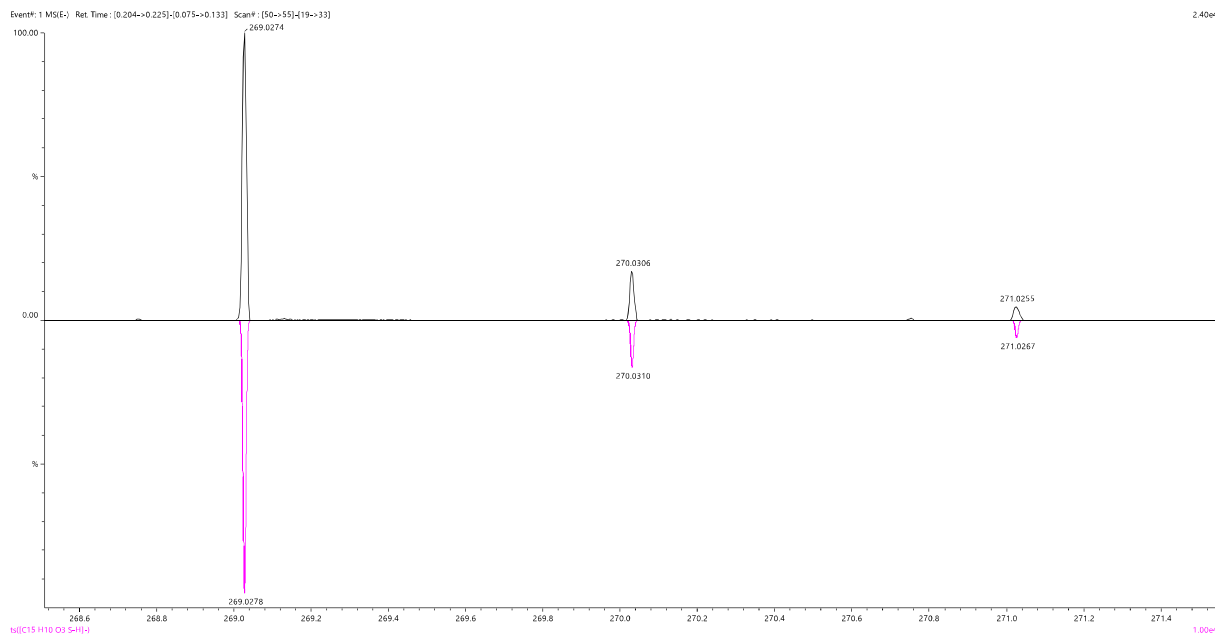


WYDZIAŁOWE LABORATORIUM  
POMIAROWE - SEKCJA MS





### Isotopic distribution 269.0278 m/z

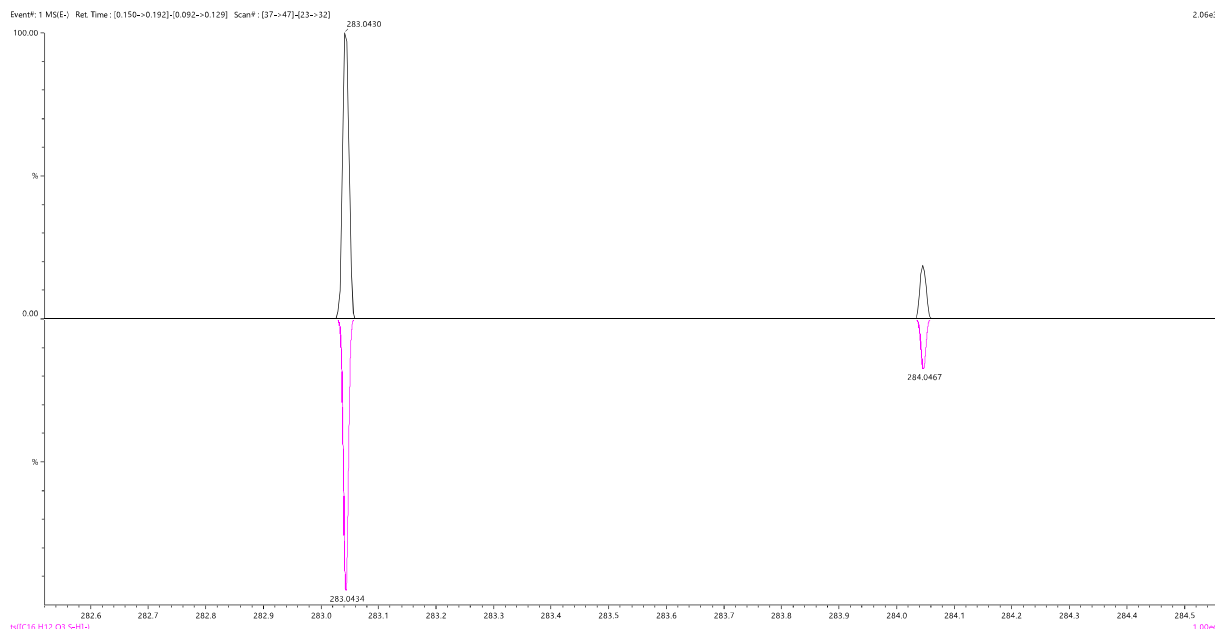


### Formula predictor

| #  | Score | Pred. (M) | Pred. m/z | Meas. m/z | Diff. (mDa) | Formula (M)    | Ion                     | Diff. (ppm) | Iso Score | DBE  |
|----|-------|-----------|-----------|-----------|-------------|----------------|-------------------------|-------------|-----------|------|
| 1  | 90.81 | 270.03507 | 269.02779 | 269.02742 | -0.37       | C15 H10 O3 S   | [M-H] <sup>-</sup>      | -1.371      | 89.79     | 11.0 |
| 2  | 90.81 | 224.02959 | 269.02779 | 269.02742 | -0.37       | C14 H8 O S     | [M+HCOO] <sup>-</sup>   | -1.371      | 89.79     | 11.0 |
| 3  | 90.81 | 210.01394 | 269.02779 | 269.02742 | -0.37       | C13 H6 O S     | [M+CH3COO] <sup>-</sup> | -1.371      | 89.79     | 11.0 |
| 4  | 72.90 | 270.03575 | 269.02847 | 269.02742 | -1.05       | C8 H10 N6 O S2 | [M-H] <sup>-</sup>      | -3.921      | 69.89     | 7.0  |
| 5  | 69.06 | 224.02940 | 269.02761 | 269.02742 | -0.19       | C6 H4 N6 O4    | [M+HCOO] <sup>-</sup>   | -0.689      | 65.62     | 8.0  |
| 6  | 69.06 | 270.03488 | 269.02761 | 269.02742 | -0.19       | C7 H6 N6 O6    | [M-H] <sup>-</sup>      | -0.689      | 65.62     | 8.0  |
| 7  | 69.06 | 210.01375 | 269.02761 | 269.02742 | -0.19       | C5 H2 N6 O4    | [M+CH3COO] <sup>-</sup> | -0.689      | 65.62     | 8.0  |
| 8  | 55.30 | 270.03238 | 269.02510 | 269.02742 | 2.32        | C11 H6 N6 O S  | [M-H] <sup>-</sup>      | 8.610       | 50.33     | 12.0 |
| 9  | 53.71 | 270.03622 | 269.02894 | 269.02742 | -1.52       | C8 H2 N10 O2   | [M-H] <sup>-</sup>      | -5.661      | 48.57     | 13.0 |
| 10 | 53.71 | 224.03074 | 269.02894 | 269.02742 | -1.52       | C7 N10         | [M+HCOO] <sup>-</sup>   | -5.661      | 48.57     | 13.0 |



### Isotopic distribution 283.0434 m/z



### Formula predictor

| #  | Score | Pred. (M) | Pred. m/z | Meas. m/z | Diff. (mDa) | Formula (M)  | Ion         | Diff. (ppm) | Iso Score | DBE  |
|----|-------|-----------|-----------|-----------|-------------|--------------|-------------|-------------|-----------|------|
| 1  | 54.77 | 238.04186 | 283.04007 | 283.04297 | 2.90        | C18 H6 O     | [M+HCOO]-   | 10.254      | 49.74     | 16.0 |
| 2  | 54.77 | 224.02621 | 283.04007 | 283.04297 | 2.90        | C17 H4 O     | [M+CH3COO]- | 10.254      | 49.74     | 16.0 |
| 3  | 54.77 | 284.04734 | 283.04007 | 283.04297 | 2.90        | C19 H8 O3    | [M-H]-      | 10.254      | 49.74     | 16.0 |
| 4  | 39.98 | 284.05072 | 283.04344 | 283.04297 | -0.47       | C16 H12 O3 S | [M-H]-      | -1.657      | 33.32     | 11.0 |
| 5  | 39.98 | 238.04524 | 283.04344 | 283.04297 | -0.47       | C15 H10 O S  | [M+HCOO]-   | -1.657      | 33.32     | 11.0 |
| 6  | 39.98 | 224.02959 | 283.04344 | 283.04297 | -0.47       | C14 H8 O S   | [M+CH3COO]- | -1.657      | 33.32     | 11.0 |
| 7  | 19.95 | 284.05322 | 283.04594 | 283.04297 | -2.97       | C12 H12 O8   | [M-H]-      | -10.496     | 22.17     | 7.0  |
| 8  | 19.95 | 238.04774 | 283.04594 | 283.04297 | -2.97       | C11 H10 O6   | [M+HCOO]-   | -10.496     | 22.17     | 7.0  |
| 9  | 19.95 | 224.03209 | 283.04594 | 283.04297 | -2.97       | C10 H8 O6    | [M+CH3COO]- | -10.496     | 22.17     | 7.0  |
| 10 | 18.71 | 284.05659 | 283.04931 | 283.04297 | -6.34       | C9 H16 O8 S  | [M-H]-      | -22.407     | 20.79     | 2.0  |

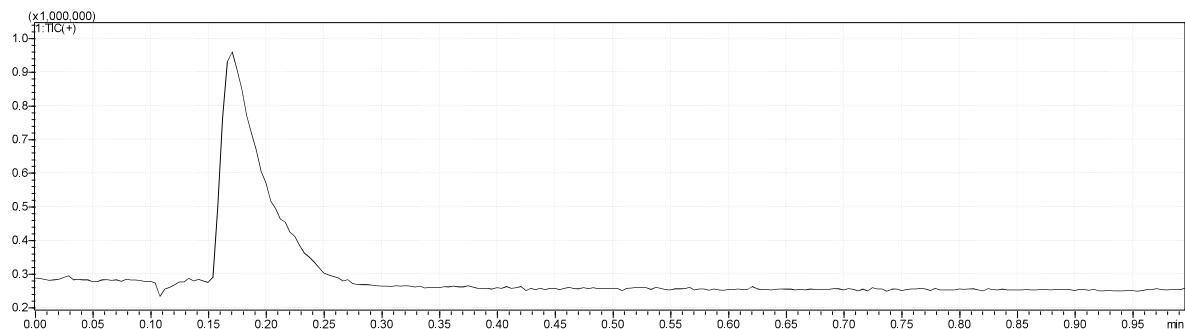


PL1

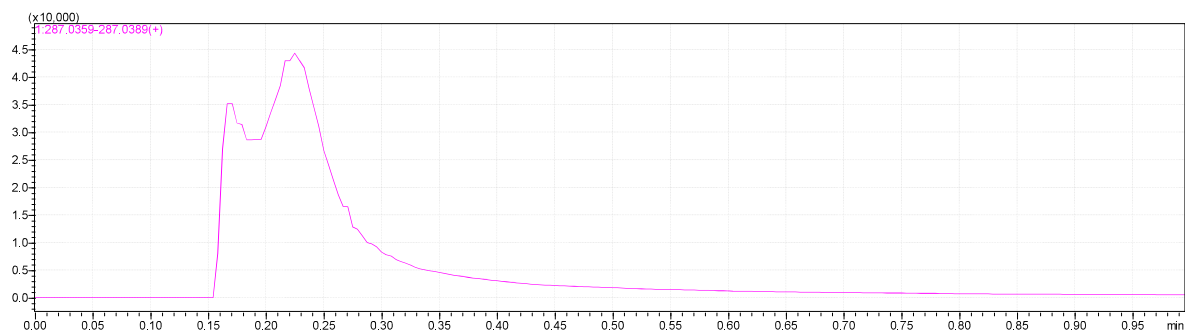
C15H10O4S

$[M+H]^+_{\text{theo}} = 287.0373 \text{ m/z}$

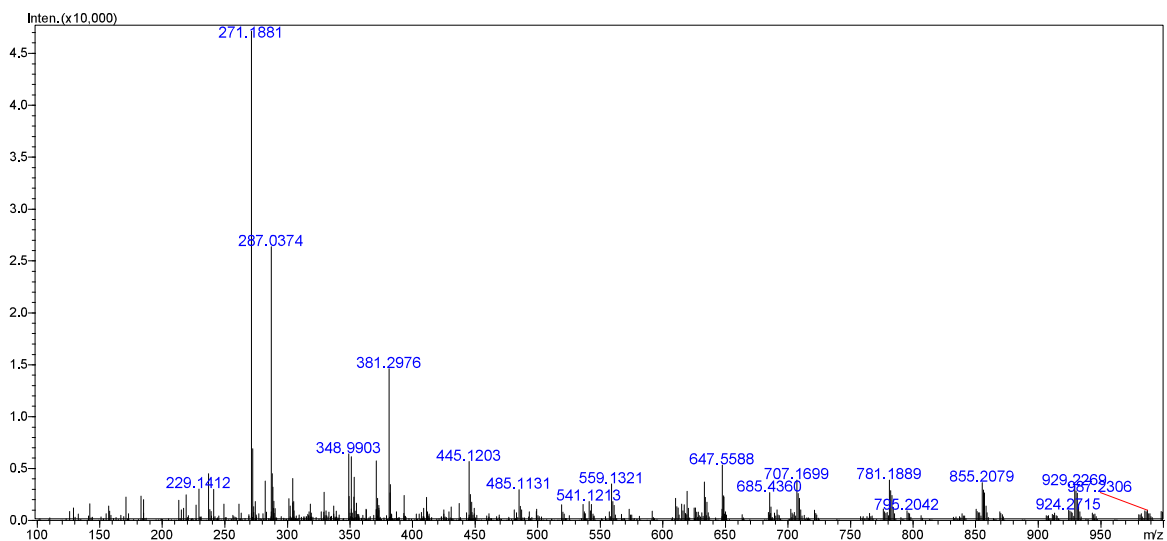
TIC (+)



XIC 287.0373 m/z  $\pm 5$  ppm



MS

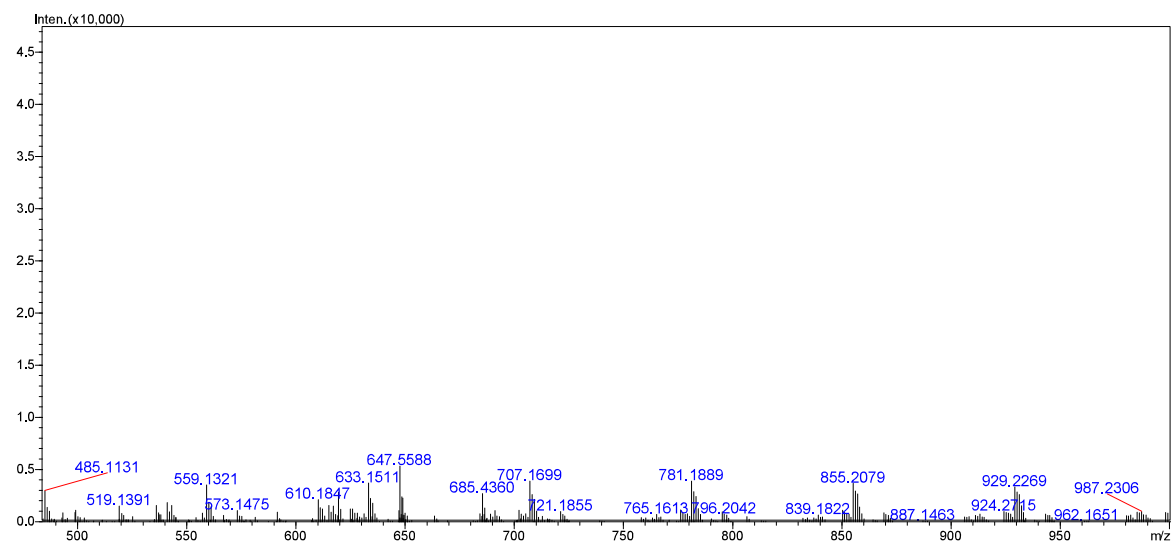
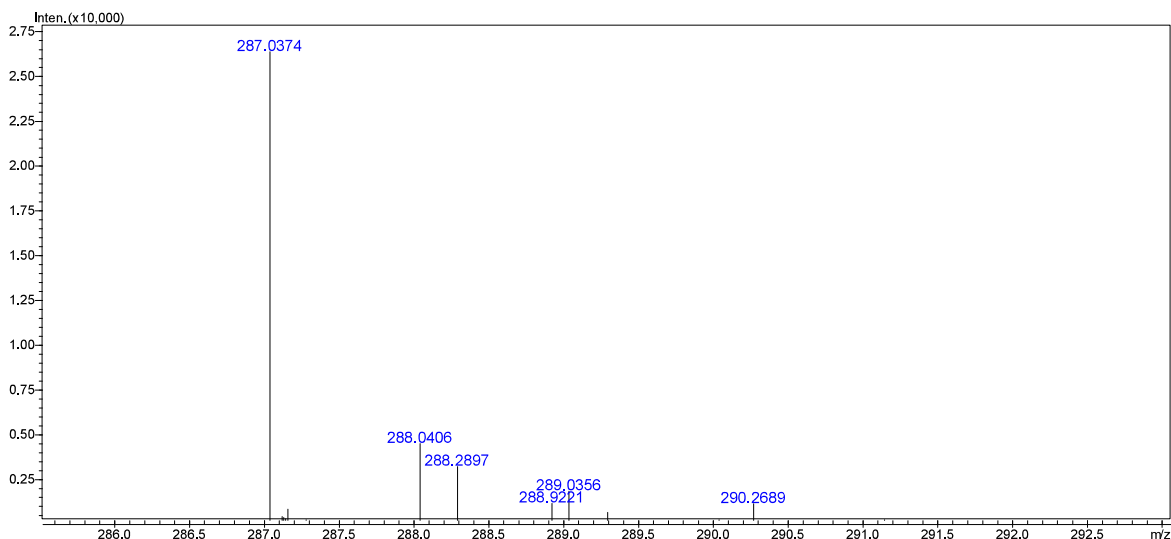
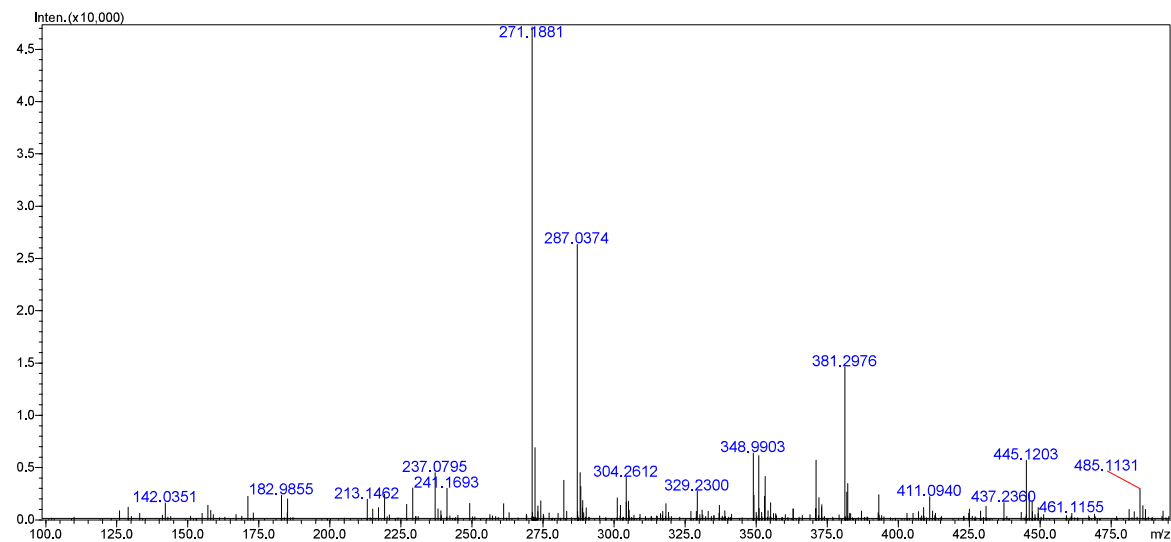




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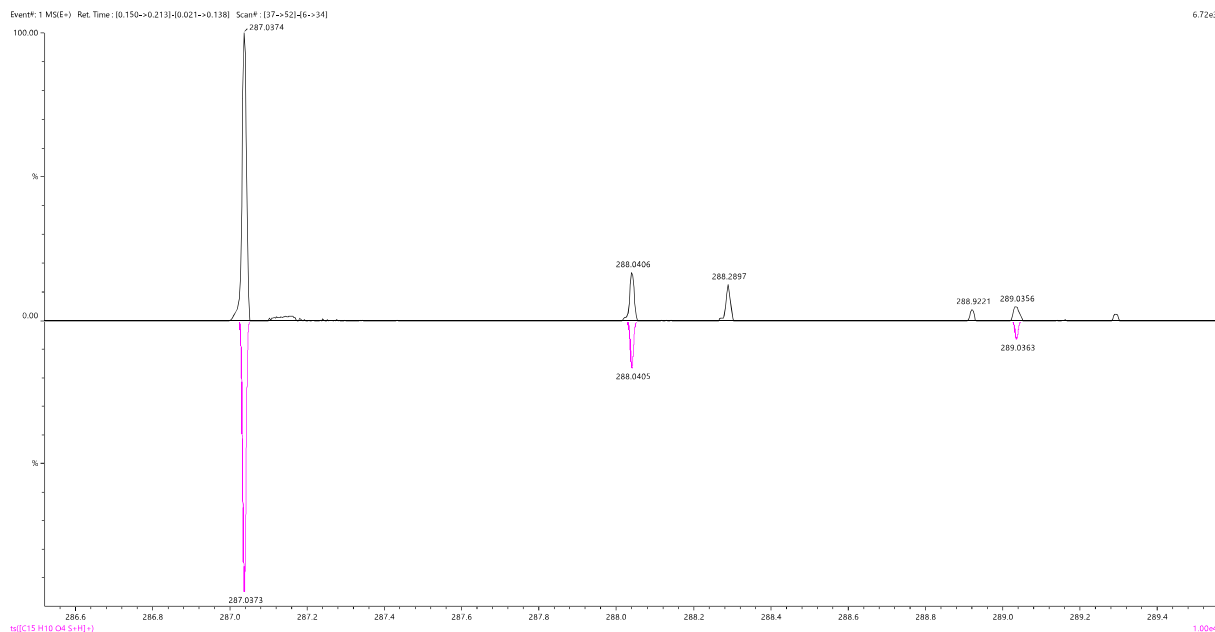


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POMIAROWE - SEKCJA MS





## Isotopic distribution



## Formula Predictor

| #  | Score | Pred. (M) | Pred. m/z | Meas. m/z | Diff. (mDa) | Formula (M)   | Ion                 | Diff. (ppm) | Iso Score | DBE  |
|----|-------|-----------|-----------|-----------|-------------|---------------|---------------------|-------------|-----------|------|
| 1  | 97.73 | 286.02998 | 287.03726 | 287.03740 | 0.14        | C15 H10 O4 S  | [M+H] <sup>+</sup>  | 0.500       | 97.47     | 11.0 |
| 2  | 76.56 | 264.04813 | 287.03735 | 287.03740 | 0.05        | C9 H12 O9     | [M+Na] <sup>+</sup> | 0.165       | 73.95     | 4.0  |
| 3  | 75.25 | 264.04900 | 287.03822 | 287.03740 | -0.82       | C10 H16 O4 S2 | [M+Na] <sup>+</sup> | -2.864      | 72.51     | 3.0  |
| 4  | 63.14 | 248.07522 | 287.03837 | 287.03740 | -0.97       | C7 H20 O5 S2  | [M+K] <sup>+</sup>  | -3.393      | 59.04     | -2.0 |
| 5  | 51.34 | 264.04563 | 287.03485 | 287.03740 | 2.55        | C13 H12 O4 S  | [M+Na] <sup>+</sup> | 8.881       | 57.04     | 8.0  |
| 6  | 49.27 | 248.07435 | 287.03750 | 287.03740 | -0.10       | C6 H16 O10    | [M+K] <sup>+</sup>  | -0.364      | 43.63     | -1.0 |
| 7  | 46.07 | 286.03335 | 287.04063 | 287.03740 | -3.23       | C12 H14 O4 S2 | [M+H] <sup>+</sup>  | -11.245     | 40.08     | 6.0  |
| 8  | 39.96 | 286.03248 | 287.03976 | 287.03740 | -2.36       | C11 H10 O9    | [M+H] <sup>+</sup>  | -8.216      | 33.29     | 7.0  |
| 9  | 39.05 | 248.07184 | 287.03500 | 287.03740 | 2.40        | C10 H16 O5 S  | [M+K] <sup>+</sup>  | 8.352       | 32.28     | 3.0  |
| 10 | 38.69 | 248.06847 | 287.03163 | 287.03740 | 5.77        | C13 H12 O5    | [M+K] <sup>+</sup>  | 20.097      | 42.99     | 8.0  |