

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112223\  
 Data File : BG059847.D  
 Acq On : 23 Nov 2023 11:17  
 Operator : MA/JU  
 Sample : 05449-07  
 Misc :  
 ALS Vial : 29 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 WC-SED-03

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059847.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 5.362       | 331           | 336         | 343          | rVB2     | 51280          | 84969         | 2.36%           | 0.508%        |
| 2         | 5.826       | 408           | 415         | 421          | rBV      | 1027665        | 1631604       | 45.36%          | 9.763%        |
| 3         | 7.459       | 685           | 693         | 701          | rBV      | 1173860        | 2030964       | 56.47%          | 12.153%       |
| 4         | 8.329       | 831           | 841         | 849          | rVB2     | 168378         | 293901        | 8.17%           | 1.759%        |
| 5         | 9.533       | 1038          | 1046        | 1054         | rVB      | 714036         | 1266540       | 35.21%          | 7.579%        |
| 6         | 11.178      | 1319          | 1326        | 1333         | rVB      | 149055         | 270271        | 7.51%           | 1.617%        |
| 7         | 13.582      | 1727          | 1735        | 1743         | rBV      | 1646341        | 2501125       | 69.54%          | 14.966%       |
| 8         | 13.787      | 1761          | 1770        | 1774         | rBV3     | 35903          | 62245         | 1.73%           | 0.372%        |
| 9         | 14.962      | 1963          | 1970        | 1977         | rBV      | 299355         | 468237        | 13.02%          | 2.802%        |
| 10        | 16.449      | 2216          | 2223        | 2231         | rBV      | 1709780        | 2540641       | 70.64%          | 15.202%       |
| 11        | 17.712      | 2433          | 2438        | 2444         | rBV2     | 366628         | 585034        | 16.27%          | 3.501%        |
| 12        | 18.523      | 2572          | 2576        | 2584         | rBV2     | 97611          | 123634        | 3.44%           | 0.740%        |
| 13        | 19.786      | 2787          | 2791        | 2794         | rBV5     | 44672          | 51501         | 1.43%           | 0.308%        |
| 14        | 20.291      | 2871          | 2877        | 2882         | rBV      | 2835796        | 3596626       | 100.00%         | 21.521%       |
| 15        | 21.566      | 3092          | 3094        | 3100         | rVB7     | 33048          | 46408         | 1.29%           | 0.278%        |
| 16        | 22.042      | 3168          | 3175        | 3183         | rVB2     | 316059         | 548870        | 15.26%          | 3.284%        |
| 17        | 24.451      | 3582          | 3585        | 3587         | rBV4     | 32737          | 39796         | 1.11%           | 0.238%        |
| 18        | 25.626      | 3777          | 3785        | 3795         | rVB3     | 176494         | 527938        | 14.68%          | 3.159%        |
| 19        | 29.234      | 4396          | 4399        | 4402         | rBV5     | 33090          | 41750         | 1.16%           | 0.250%        |

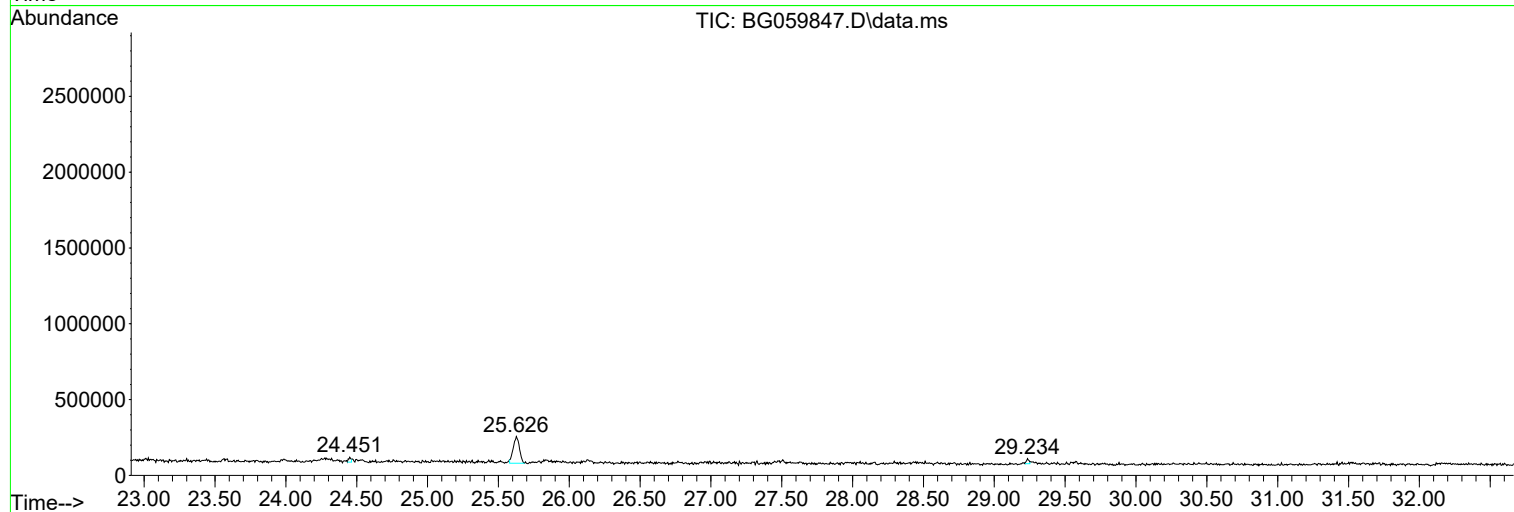
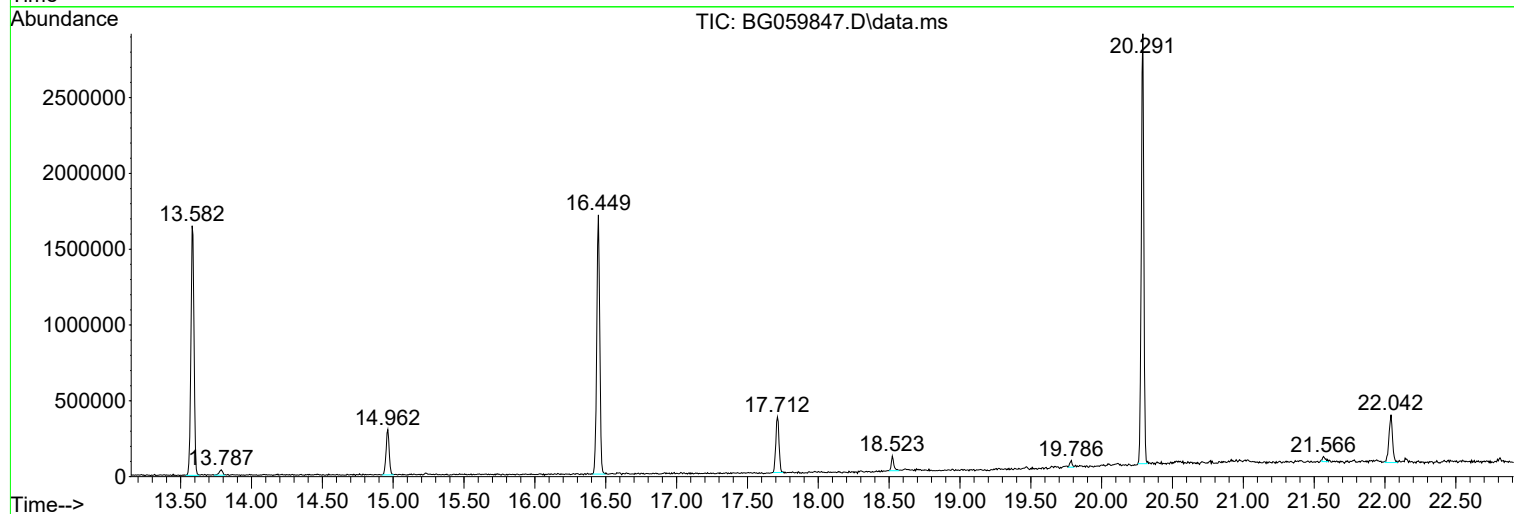
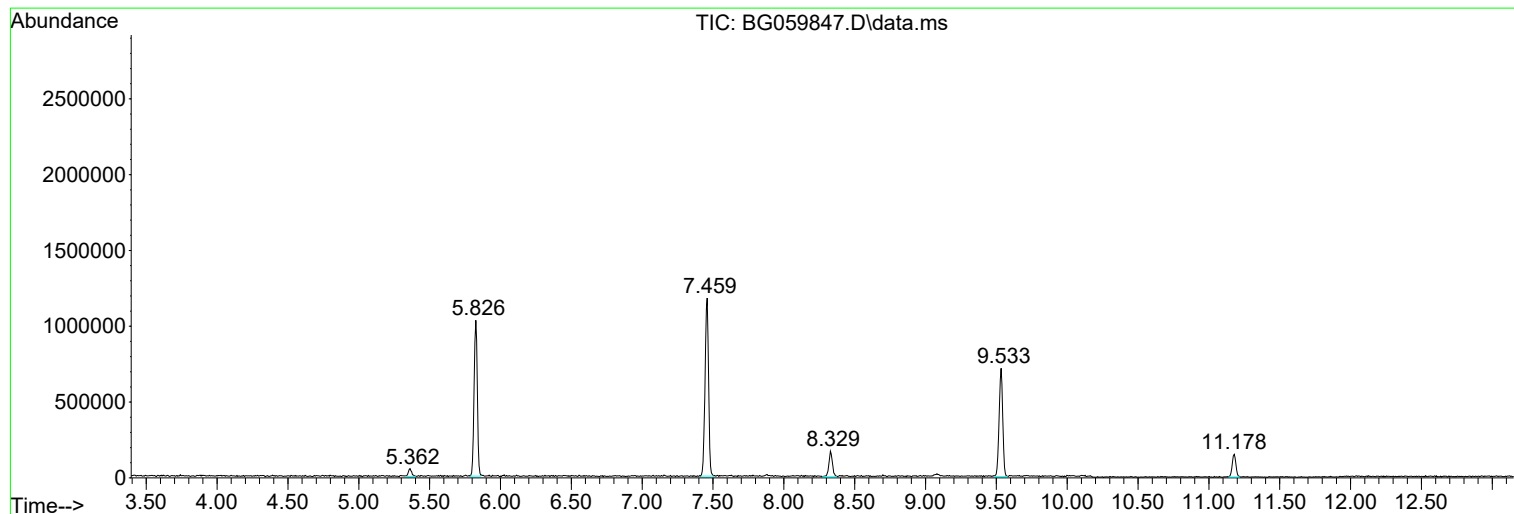
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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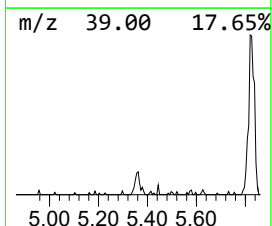
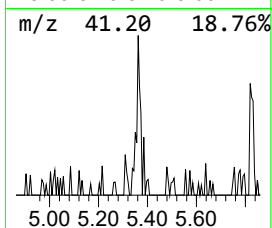
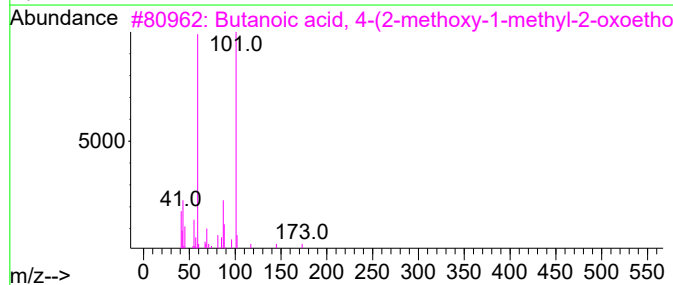
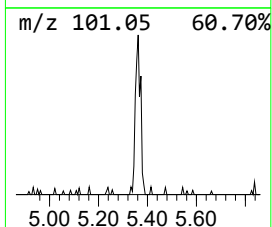
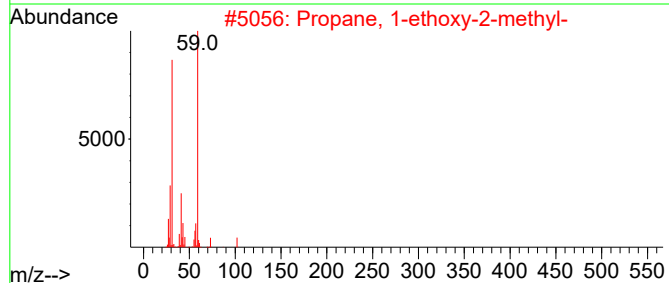
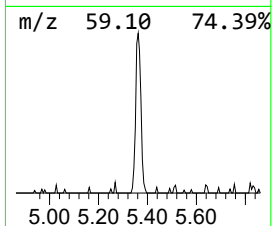
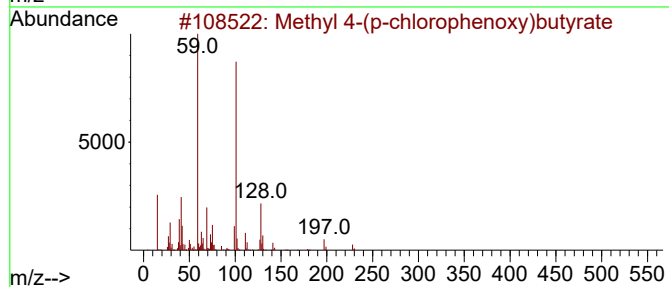
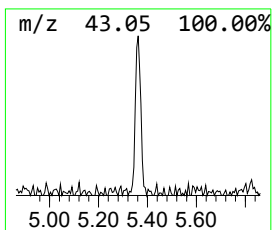
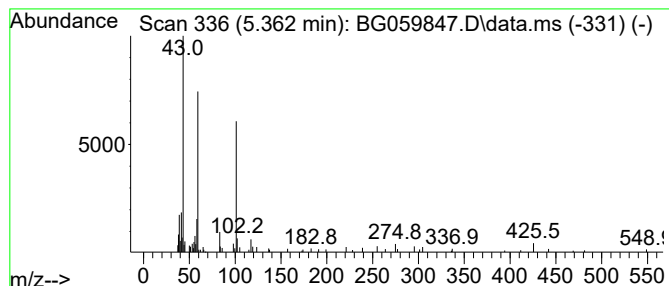
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Methyl 4-(p-chlorophenoxy)b... Concentration Rank 1

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.362 | 5.78 ng | 84969 | 1,4-Dichlorobenzene-d4 | 8.329 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Methyl 4-(p-chlorophenoxy)butyrate  | 228 | C11H13ClO3 | 209052-80-2  | 64   |
| 2    |    |   | Propane, 1-ethoxy-2-methyl-         | 102 | C6H14O     | 000627-02-1  | 43   |
| 3    |    |   | Butanoic acid, 4-(2-methoxy-1-me... | 204 | C9H16O5    | 054966-46-0  | 39   |
| 4    |    |   | Hydrazine, 1-methyl-1-(2-methylp... | 102 | C5H14N2    | 020240-63-5  | 37   |
| 5    |    |   | 5-Fluoroorotyl-N,N-dimethylhydra... | 216 | C7H9FN4O3  | 1000227-24-4 | 25   |



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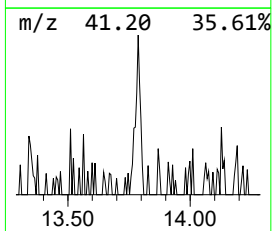
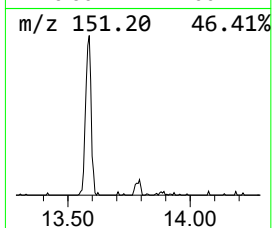
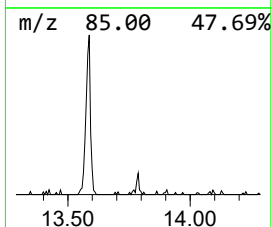
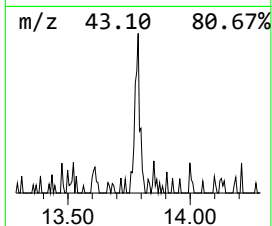
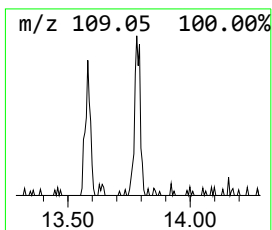
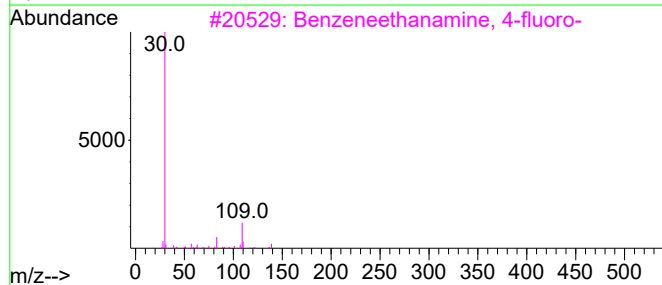
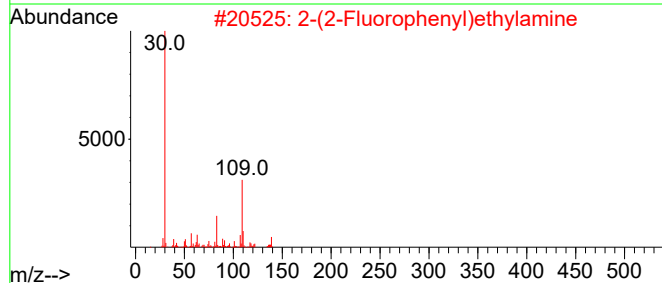
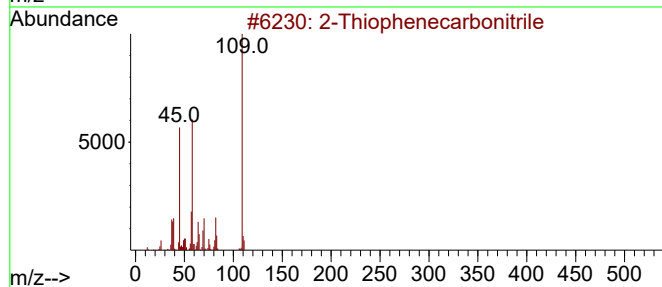
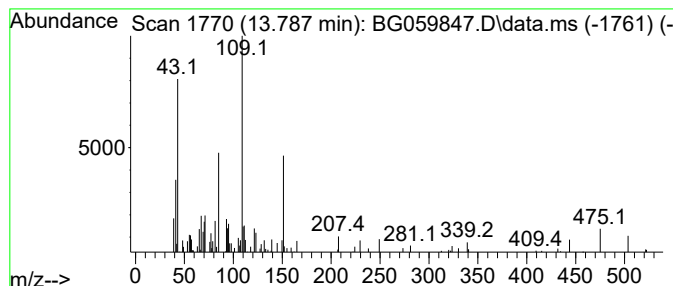
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TIC Library : C:\Database\NIST20.L  
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Peak Number 2 unknown13.787 Concentration Rank 3

| R.T.      | EstConc                         | Area  | Relative to ISTD | R.T.         |      |
|-----------|---------------------------------|-------|------------------|--------------|------|
| 13.787    | 2.66 ng                         | 62245 | Acenaphthene-d10 | 14.962       |      |
| Hit# of 5 | Tentative ID                    | MW    | MolForm          | CAS#         | Qual |
| 1         | 2-Thiophenecarbonitrile         | 109   | C5H3NS           | 001003-31-2  | 12   |
| 2         | 2-(2-Fluorophenyl)ethylamine    | 139   | C8H10FN          | 052721-69-4  | 9    |
| 3         | Benzeneethanamine, 4-fluoro-    | 139   | C8H10FN          | 001583-88-6  | 9    |
| 4         | Butyramide, 4-bromo-N-isobutyl- | 221   | C8H16BrNO        | 1000419-75-7 | 9    |
| 5         | 3-Thiophenecarbonitrile         | 109   | C5H3NS           | 001641-09-4  | 7    |



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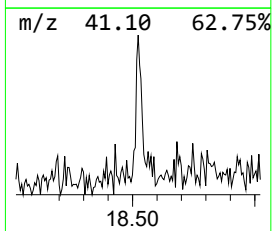
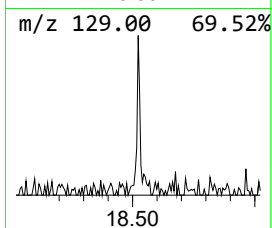
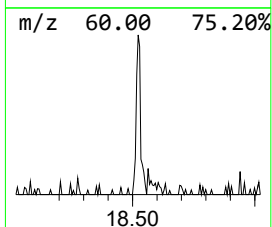
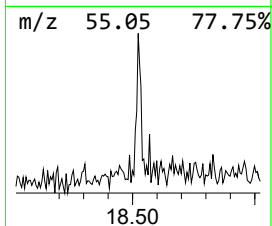
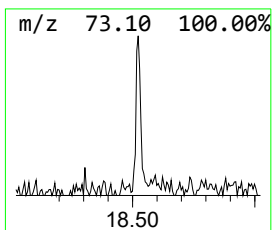
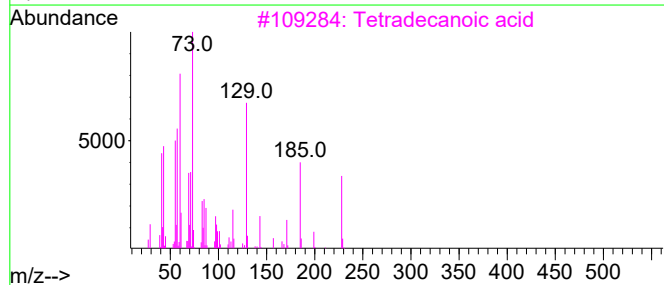
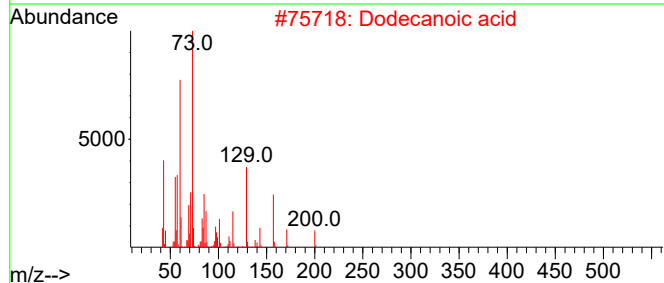
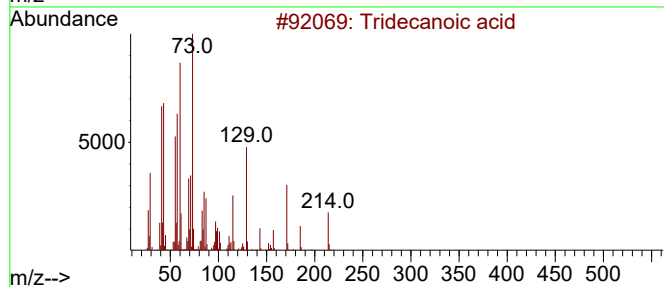
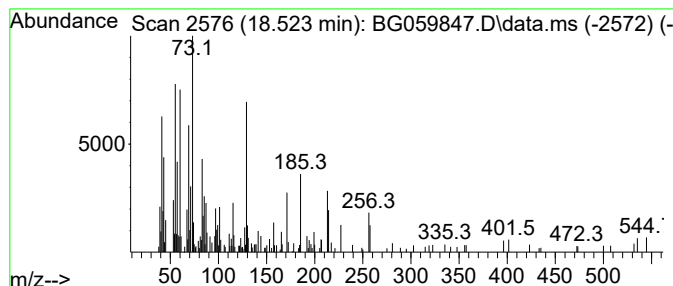
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Peak Number 3 Tridecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.523 | 4.23 ng | 123634 | Phenanthrene-d10 | 17.712 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 93   |
| 2    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 53   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 49   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 49   |
| 5    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 46   |



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TIC Library : C:\Database\NIST20.L  
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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Methyl 4-(p-chl... | 5.362  | 5.8     | ng    | 84969    | 1                     | 8.329  | 293901 | 20.0 |
| unknown13.787      | 13.787 | 2.7     | ng    | 62245    | 3                     | 14.962 | 468237 | 20.0 |
| Tridecanoic acid   | 18.523 | 4.2     | ng    | 123634   | 4                     | 17.712 | 585034 | 20.0 |