

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112423\  
 Data File : BG059865.D  
 Acq On : 24 Nov 2023 19:42  
 Operator : MA/JU  
 Sample : 05449-07  
 Misc :  
 ALS Vial : 4 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: BG059865.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         | 5.809       | 405           | 412         | 420          | rVB      | 376775         | 601895        | 28.97%          | 5.840%        |
| 2         | 7.443       | 683           | 690         | 697          | rVB2     | 374597         | 648714        | 31.22%          | 6.295%        |
| 3         | 8.318       | 831           | 839         | 846          | rBV2     | 100444         | 169376        | 8.15%           | 1.644%        |
| 4         | 9.517       | 1033          | 1043        | 1051         | rBV2     | 248276         | 454617        | 21.88%          | 4.411%        |
| 5         | 11.162      | 1317          | 1323        | 1330         | rVB      | 133697         | 252327        | 12.14%          | 2.448%        |
| 6         | 13.571      | 1726          | 1733        | 1740         | rVB      | 885187         | 1323647       | 63.71%          | 12.844%       |
| 7         | 13.777      | 1759          | 1768        | 1774         | rBV2     | 348035         | 566851        | 27.28%          | 5.500%        |
| 8         | 14.952      | 1961          | 1968        | 1973         | rBV      | 299411         | 487461        | 23.46%          | 4.730%        |
| 9         | 15.222      | 2008          | 2014        | 2020         | rBV3     | 29369          | 42884         | 2.06%           | 0.416%        |
| 10        | 16.432      | 2210          | 2220        | 2228         | rBV      | 974097         | 1497392       | 72.07%          | 14.530%       |
| 11        | 16.908      | 2297          | 2301        | 2308         | rVB4     | 18492          | 27783         | 1.34%           | 0.270%        |
| 12        | 17.701      | 2429          | 2436        | 2442         | rVB      | 425639         | 642570        | 30.93%          | 6.235%        |
| 13        | 18.283      | 2533          | 2535        | 2543         | rVB8     | 19417          | 26789         | 1.29%           | 0.260%        |
| 14        | 18.512      | 2569          | 2574        | 2580         | rBV4     | 104584         | 156638        | 7.54%           | 1.520%        |
| 15        | 19.452      | 2730          | 2734        | 2741         | rBV10    | 30260          | 48894         | 2.35%           | 0.474%        |
| 16        | 19.640      | 2761          | 2766        | 2767         | rBV5     | 15906          | 22276         | 1.07%           | 0.216%        |
| 17        | 19.770      | 2783          | 2788        | 2795         | rBV10    | 54425          | 74990         | 3.61%           | 0.728%        |
| 18        | 20.093      | 2839          | 2843        | 2846         | rBV6     | 15882          | 23955         | 1.15%           | 0.232%        |
| 19        | 20.275      | 2868          | 2874        | 2881         | rBV      | 1674898        | 2077772       | 100.00%         | 20.161%       |
| 20        | 20.439      | 2899          | 2902        | 2904         | rBV4     | 19662          | 24390         | 1.17%           | 0.237%        |
| 21        | 22.020      | 3166          | 3171        | 3179         | rVB      | 304059         | 527823        | 25.40%          | 5.122%        |
| 22        | 22.772      | 3297          | 3299        | 3302         | rBV4     | 17373          | 23057         | 1.11%           | 0.224%        |
| 23        | 23.806      | 3471          | 3475        | 3479         | rBV7     | 20354          | 33639         | 1.62%           | 0.326%        |
| 24        | 25.163      | 3703          | 3706        | 3709         | rBV5     | 18746          | 28045         | 1.35%           | 0.272%        |
| 25        | 25.586      | 3771          | 3778        | 3788         | rVB2     | 161187         | 478227        | 23.02%          | 4.640%        |
| 26        | 29.617      | 4463          | 4464        | 4468         | rBV4     | 16019          | 20798         | 1.00%           | 0.202%        |
| 27        | 32.073      | 4878          | 4882        | 4884         | rBV5     | 15973          | 22976         | 1.11%           | 0.223%        |

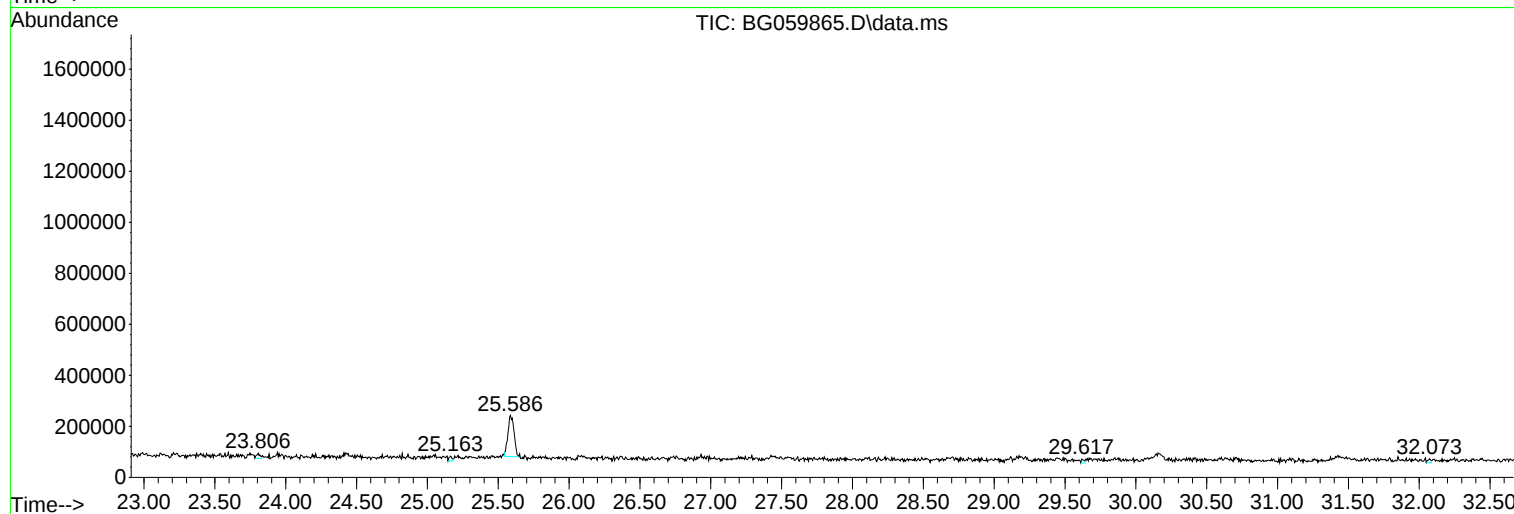
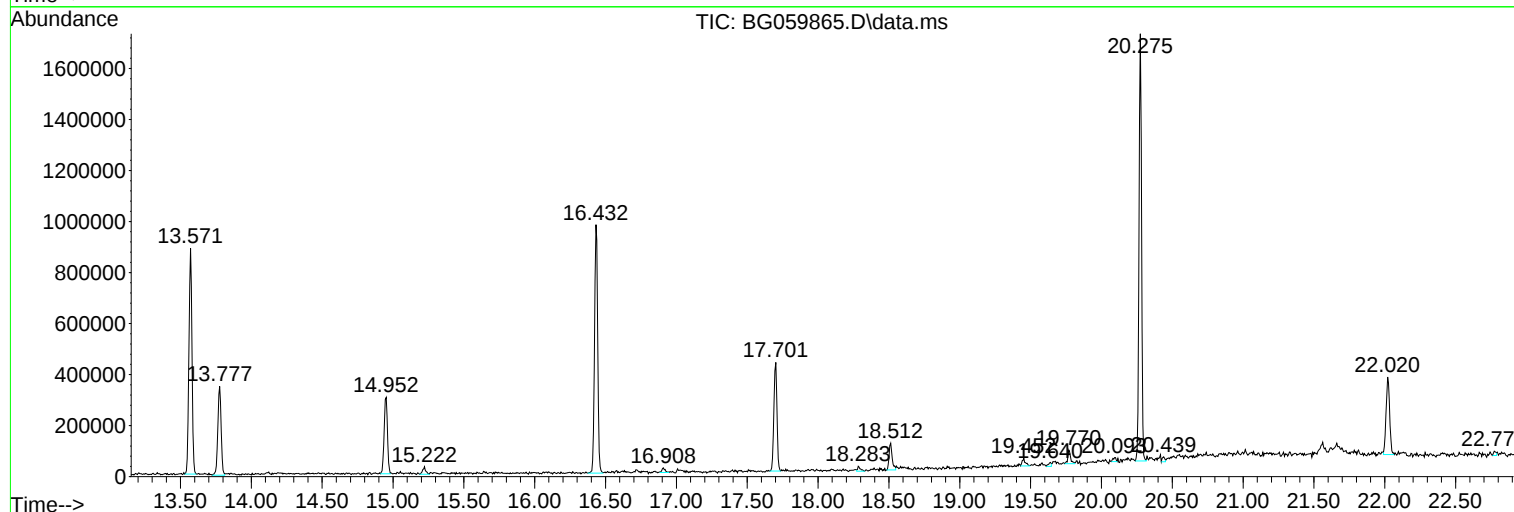
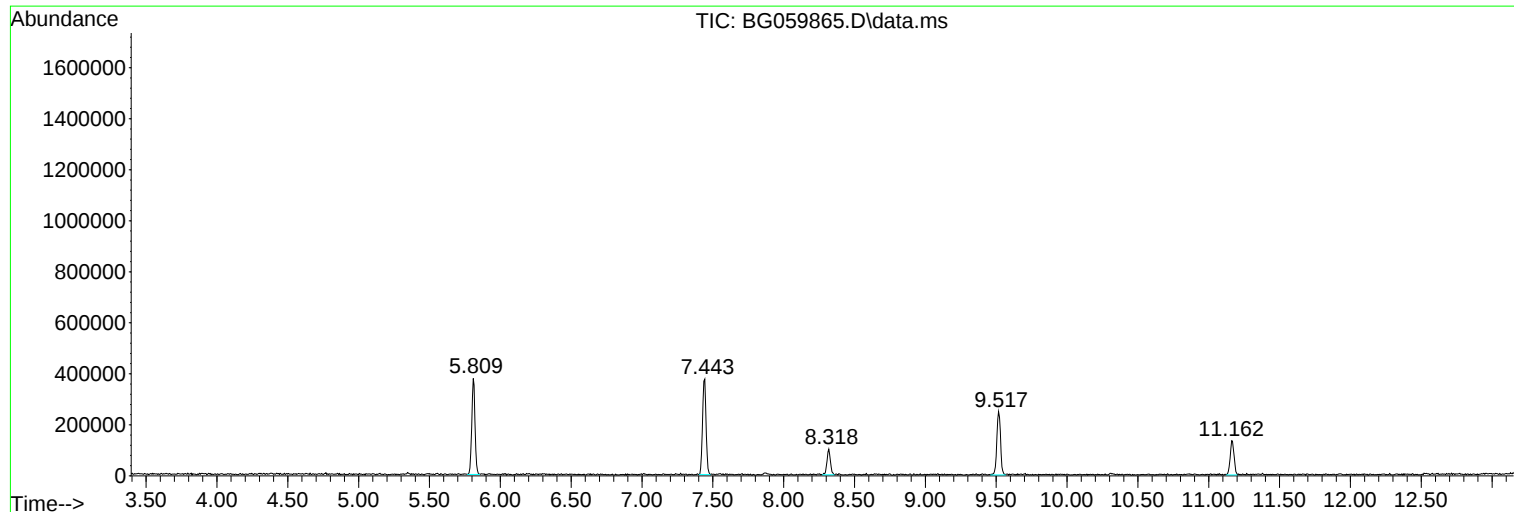
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BNA\_G  
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WC-SED-03

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112423\  
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Instrument :  
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ClientSampleId :  
WC-SED-03

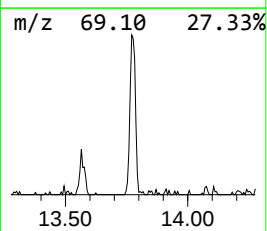
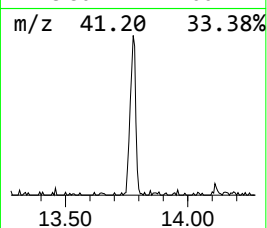
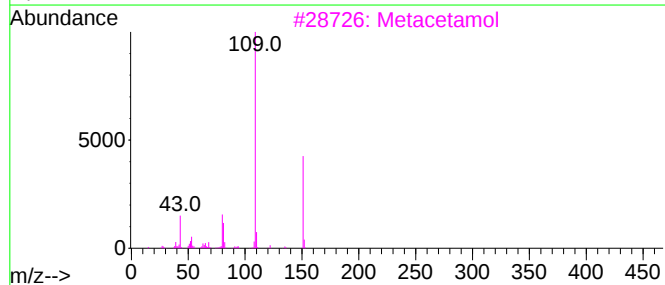
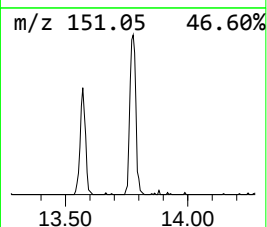
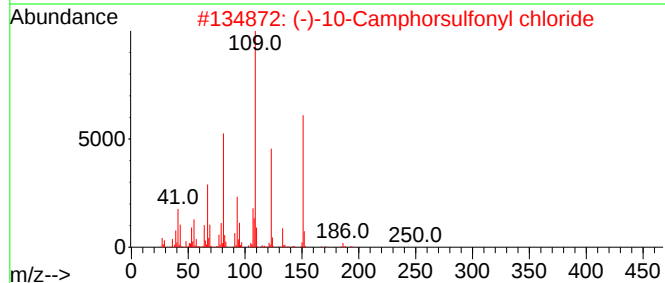
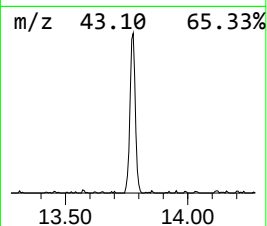
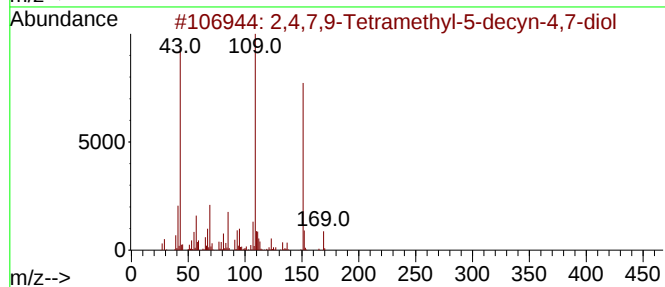
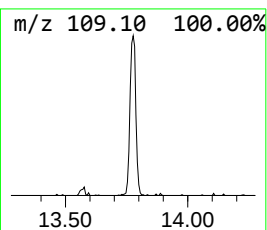
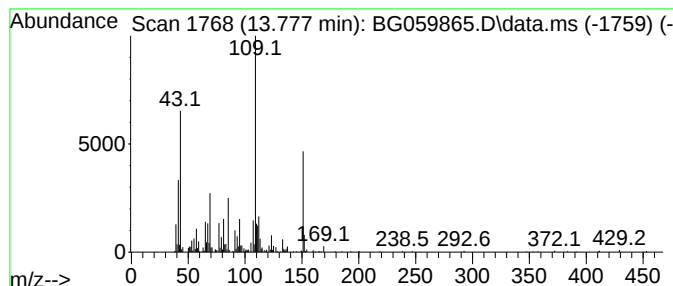
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG11623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

| R.T.      | EstConc                             | Area   | Relative to ISTD |             | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|-------------|-------------|------|
| 13.777    | 23.26 ng                            | 566851 | Acenaphthene-d10 |             | 14.952      |      |
| Hit# of 5 | Tentative ID                        |        | MW               | MolForm     | CAS#        | Qual |
| 1         | 2,4,7,9-Tetramethyl-5-decyn-4,7-... |        | 226              | C14H26O2    | 000126-86-3 | 78   |
| 2         | (-)-10-Camphorsulfonyl chloride     |        | 250              | C10H15ClO3S | 039262-22-1 | 59   |
| 3         | Metacetamol                         |        | 151              | C8H9NO2     | 000621-42-1 | 58   |
| 4         | Acetaminophen                       |        | 151              | C8H9NO2     | 000103-90-2 | 50   |
| 5         | Diacetamate                         |        | 193              | C10H11NO3   | 002623-33-8 | 50   |



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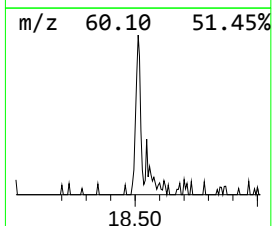
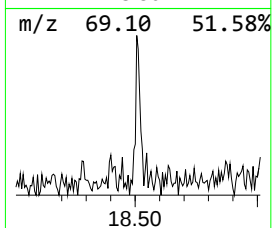
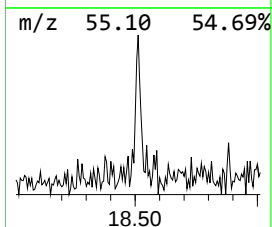
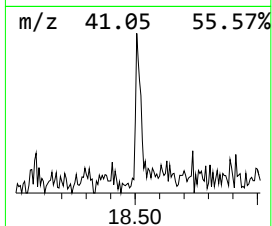
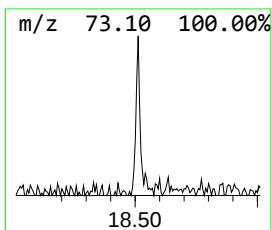
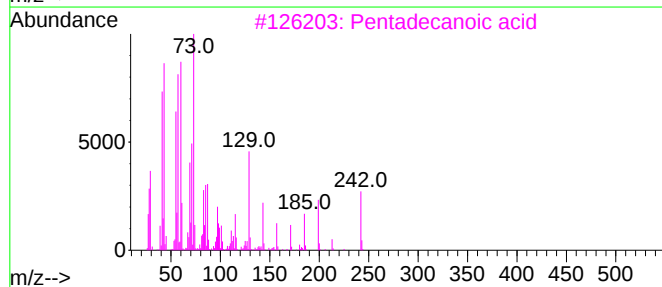
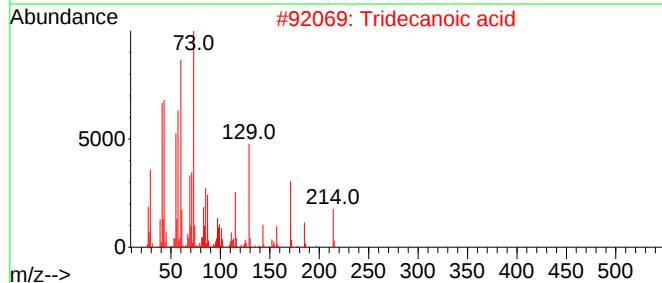
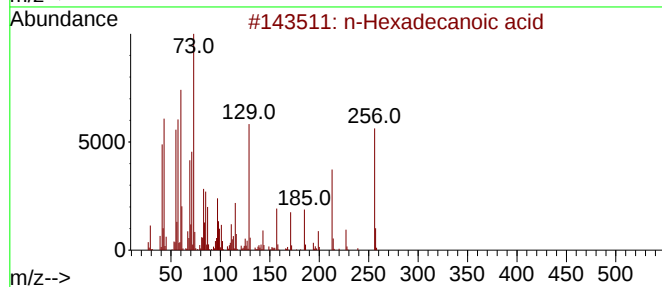
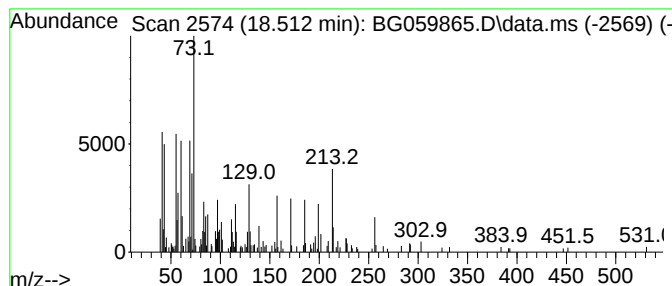
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG11623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown18.512 Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.512 | 4.88 ng | 156638 | Phenanthrene-d10 | 17.701 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 47   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 46   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 35   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 22   |
| 5    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 22   |



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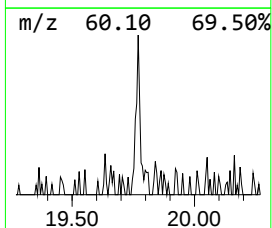
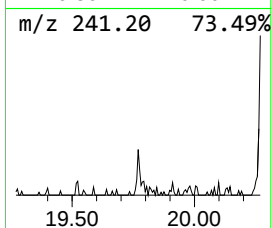
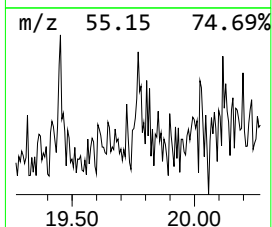
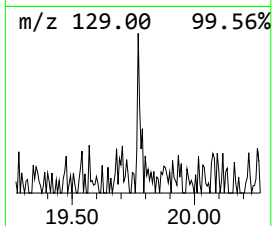
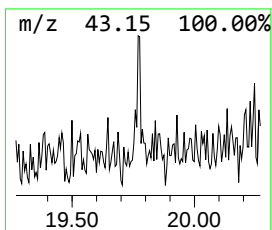
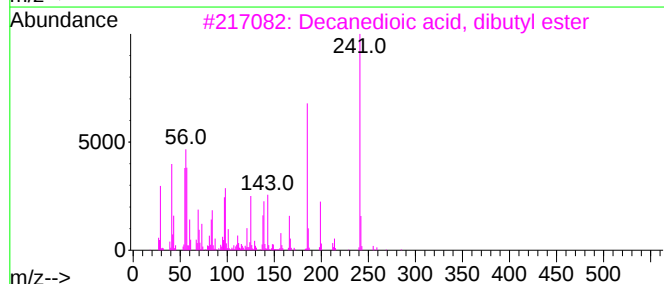
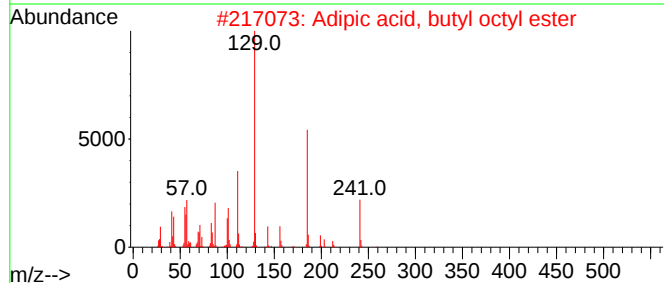
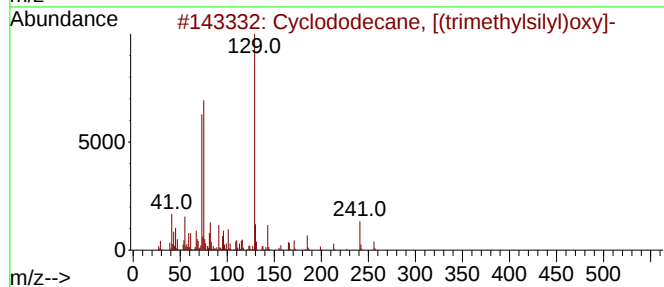
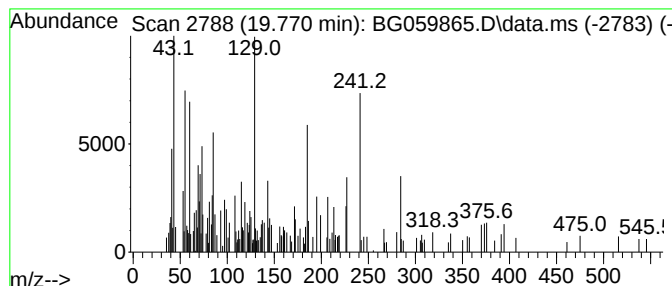
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown19.770 Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 19.770 | 2.33 ng | 74990 | Phenanthrene-d10 | 17.701 |

| Hit# | of | 5 | Tentative ID                               | MW  | MolForm   | CAS#         | Qual |
|------|----|---|--------------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Cyclododecane, [(trimethylsilyl)oxy]-      | 256 | C15H32OSi | 006221-91-6  | 38   |
| 2    |    |   | Adipic acid, butyl octyl ester             | 314 | C18H34O4  | 1000324-46-9 | 27   |
| 3    |    |   | Decanedioic acid, dibutyl ester            | 314 | C18H34O4  | 000109-43-3  | 27   |
| 4    |    |   | Adipic acid, hexyl 3-methylpentyl ester    | 314 | C18H34O4  | 1000353-69-1 | 22   |
| 5    |    |   | Adipic acid, isohexyl 2-methylpentyl ester | 314 | C18H34O4  | 1000353-56-0 | 22   |



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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 |
| 2,4,7,9-Tetrame... | 13.777 | 23.3    | ng    | 566851   | 3                     | 14.952 | 487461 | 20.0 |
| unknown18.512      | 18.512 | 4.9     | ng    | 156638   | 4                     | 17.701 | 642570 | 20.0 |
| unknown19.770      | 19.770 | 2.3     | ng    | 74990    | 4                     | 17.701 | 642570 | 20.0 |