

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120318\  
 Data File : BG038316.D  
 Acq On : 4 Dec 2018 1:36  
 Operator : JU/SJ  
 Sample : J6179-07  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 S7-0-0.5-BGS

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-BG111318.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 5.159       | 313           | 318         | 327          | rVB2     | 10446          | 20227         | 1.21%           | 0.271%        |
| 2         | 5.623       | 390           | 397         | 412          | rVB      | 189882         | 374931        | 22.50%          | 5.026%        |
| 3         | 7.221       | 662           | 669         | 685          | rBV      | 222877         | 457635        | 27.46%          | 6.135%        |
| 4         | 7.603       | 727           | 734         | 745          | rBV      | 212376         | 399968        | 24.00%          | 5.362%        |
| 5         | 8.079       | 808           | 815         | 824          | rBV      | 52721          | 99825         | 5.99%           | 1.338%        |
| 6         | 8.396       | 862           | 869         | 879          | rBV      | 167313         | 313451        | 18.81%          | 4.202%        |
| 7         | 9.254       | 1007          | 1015        | 1026         | rBV      | 140381         | 278323        | 16.70%          | 3.731%        |
| 8         | 10.899      | 1288          | 1295        | 1307         | rBV      | 75403          | 151214        | 9.07%           | 2.027%        |
| 9         | 13.331      | 1701          | 1709        | 1719         | rBV      | 434015         | 699464        | 41.98%          | 9.376%        |
| 10        | 14.154      | 1842          | 1849        | 1857         | rBV      | 46816          | 79244         | 4.76%           | 1.062%        |
| 11        | 14.712      | 1936          | 1944        | 1957         | rVB2     | 153854         | 261081        | 15.67%          | 3.500%        |
| 12        | 16.198      | 2191          | 2197        | 2209         | rBV2     | 569837         | 922750        | 55.38%          | 12.370%       |
| 13        | 17.462      | 2405          | 2412        | 2423         | rBV2     | 260137         | 413322        | 24.81%          | 5.541%        |
| 14        | 18.314      | 2553          | 2557        | 2569         | rBV2     | 39389          | 69325         | 4.16%           | 0.929%        |
| 15        | 19.583      | 2770          | 2773        | 2779         | rBV4     | 16511          | 25826         | 1.55%           | 0.346%        |
| 16        | 20.059      | 2849          | 2854        | 2866         | rVB      | 1211880        | 1666274       | 100.00%         | 22.337%       |
| 17        | 20.587      | 2934          | 2944        | 2951         | rBV10    | 10746          | 39416         | 2.37%           | 0.528%        |
| 18        | 21.340      | 3066          | 3072        | 3079         | rBV3     | 35664          | 69948         | 4.20%           | 0.938%        |
| 19        | 21.745      | 3134          | 3141        | 3149         | rBV      | 317939         | 536293        | 32.19%          | 7.189%        |
| 20        | 23.208      | 3384          | 3390        | 3396         | rBV5     | 8541           | 16973         | 1.02%           | 0.228%        |
| 21        | 24.025      | 3524          | 3529        | 3536         | rVB4     | 9007           | 21782         | 1.31%           | 0.292%        |
| 22        | 25.059      | 3689          | 3705        | 3718         | rBV2     | 171475         | 524188        | 31.46%          | 7.027%        |
| 23        | 26.152      | 3883          | 3891        | 3901         | rBV2     | 6221           | 18383         | 1.10%           | 0.246%        |

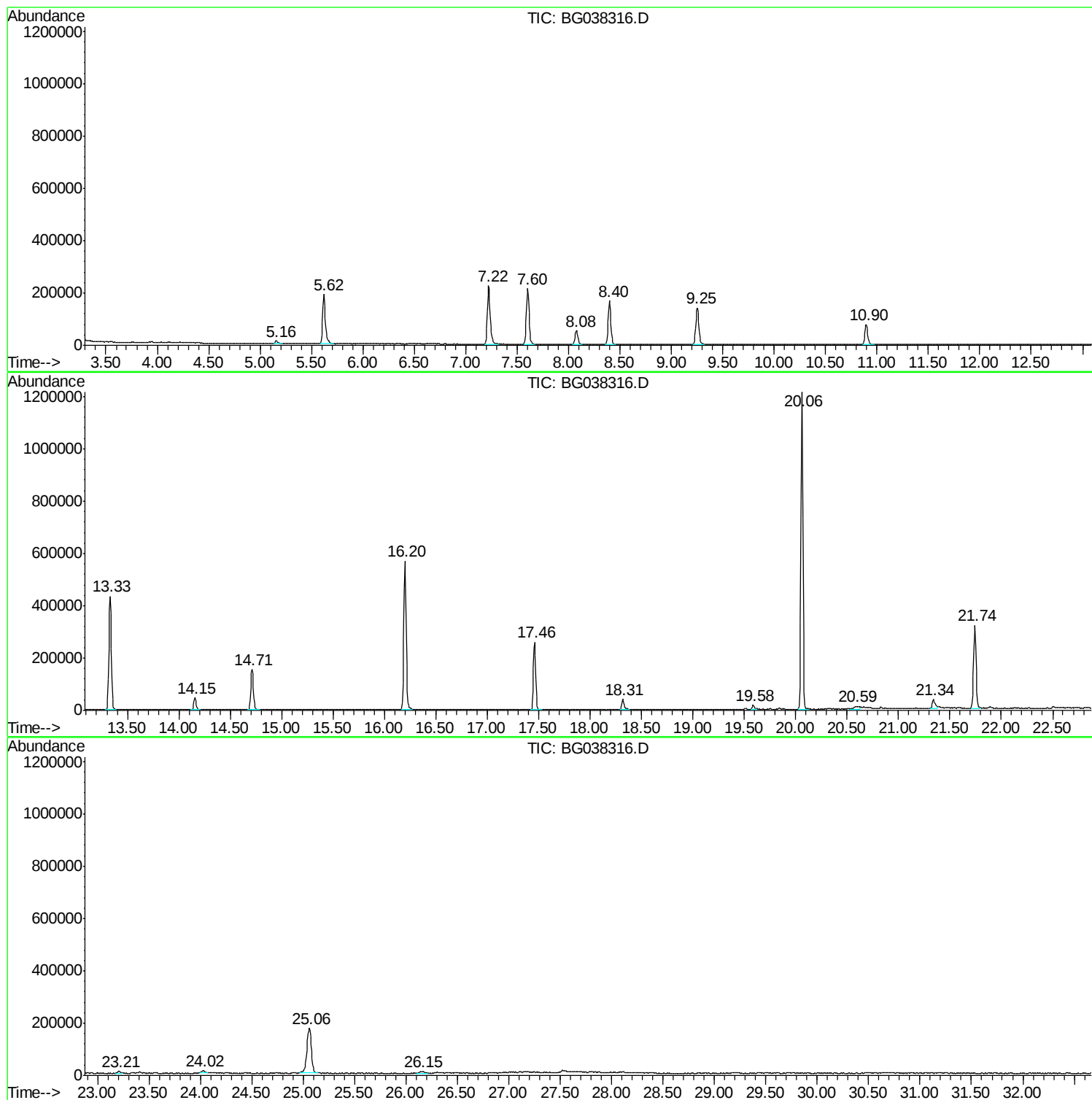
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG111318.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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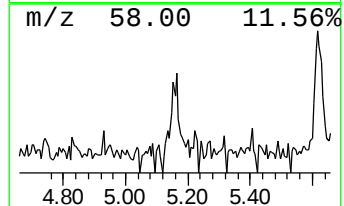
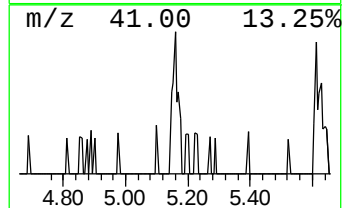
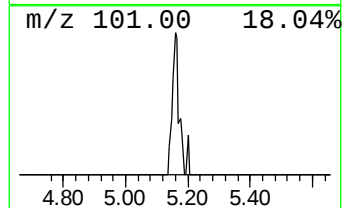
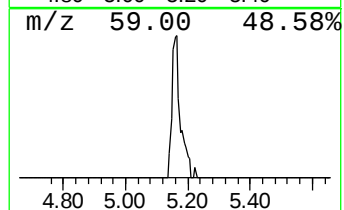
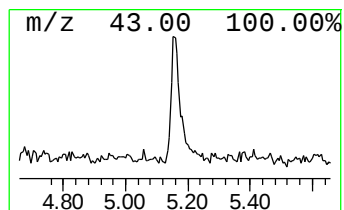
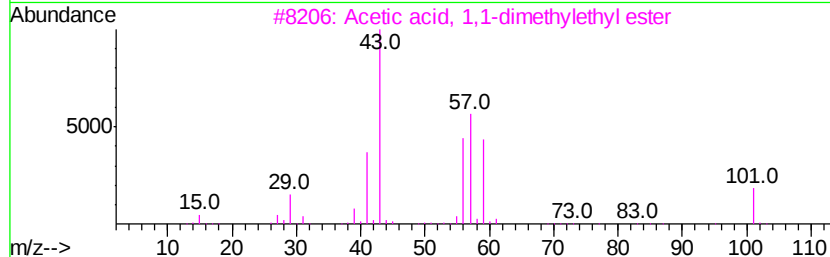
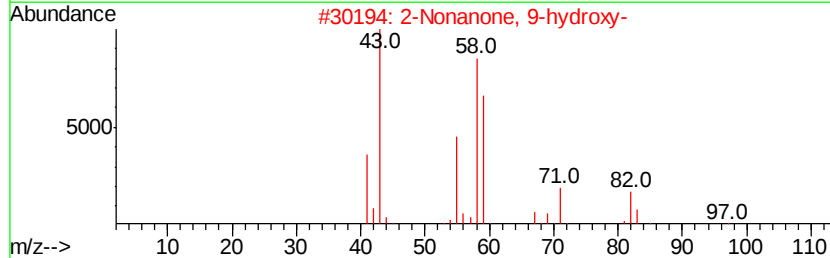
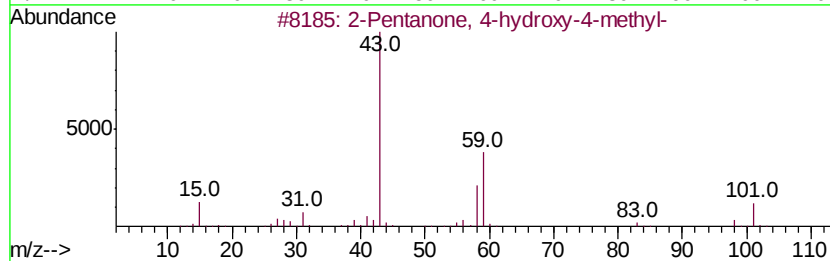
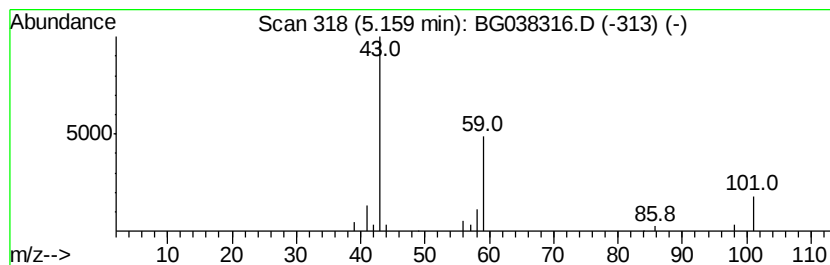
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG111318.M  
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TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 5.16 | 4.05 ng | 20227 | 1,4-Dichlorobenzene-d4 | 8.08 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 50   |
| 2    |    |   | 2-Nonanone, 9-hydroxy-              | 158 | C9H18O2 | 025368-56-3 | 9    |
| 3    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9    |
| 4    |    |   | Diacetamide                         | 101 | C4H7NO2 | 000625-77-4 | 7    |
| 5    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 7    |



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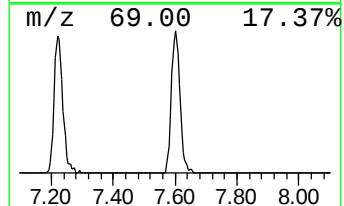
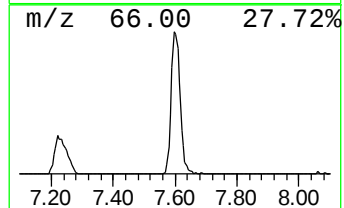
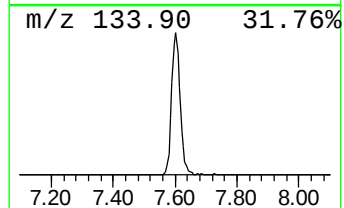
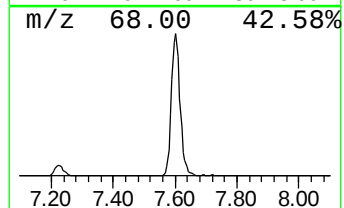
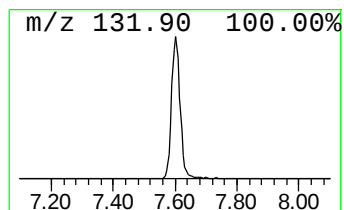
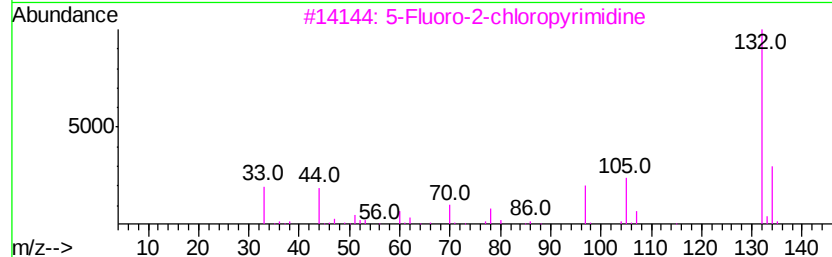
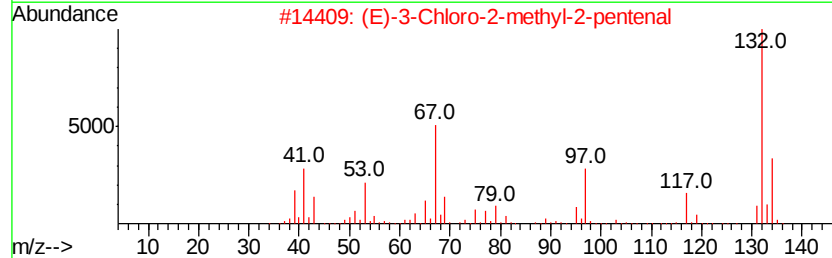
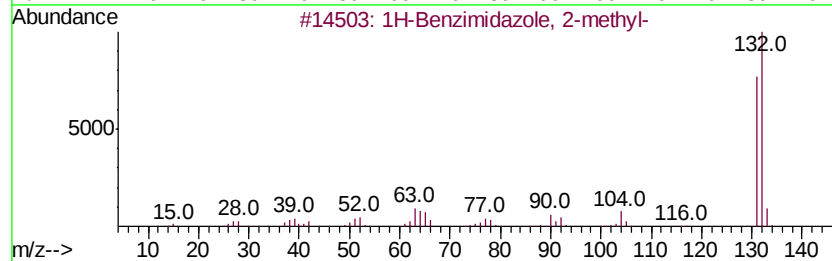
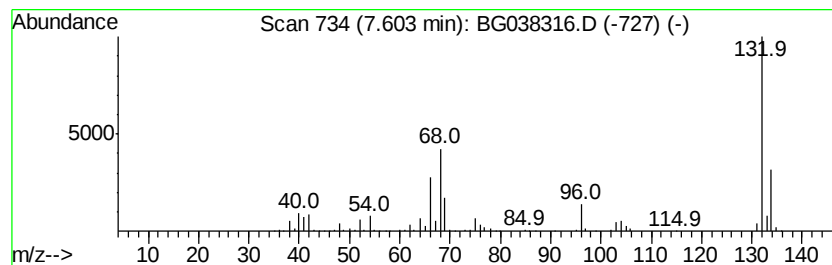
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown7.60 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 7.60 | 80.13 ng | 399968 | 1,4-Dichlorobenzene-d4 | 8.08 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 22   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 16   |
| 3    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 5    |    | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2    | 1000241-93-9 | 10   |



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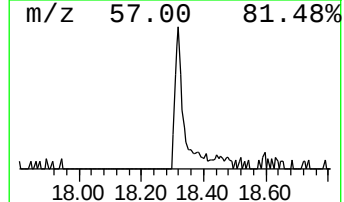
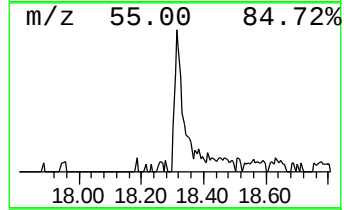
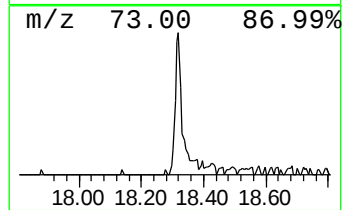
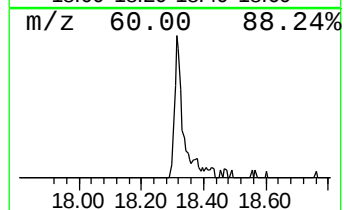
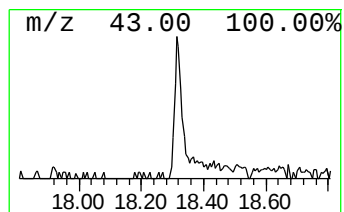
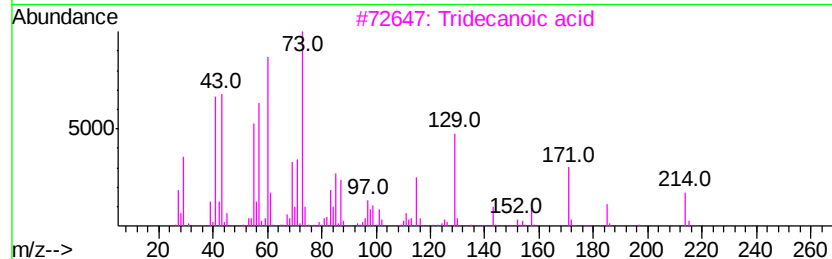
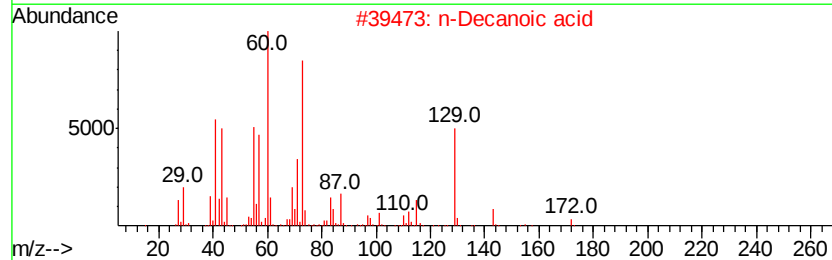
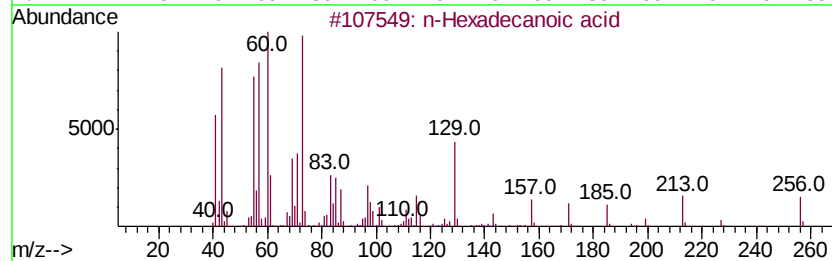
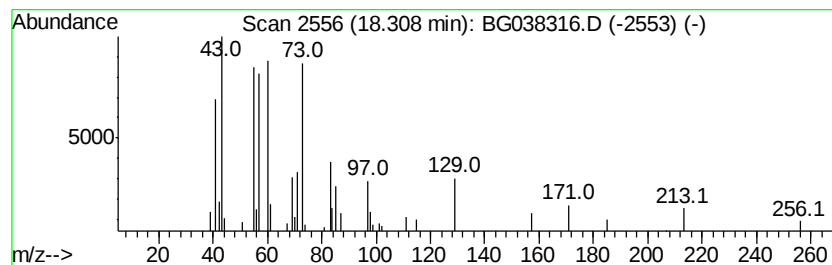
TIC Library : C:\Database\NIST11.L  
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 18.31 | 3.35 ng | 69325 | Phenanthrene-d10 | 17.46 |

| Hit# | of | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------|-----|----------|-------------|------|
| 1    | 5  | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97   |
| 2    |    | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 91   |
| 3    |    | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 81   |
| 4    |    | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 5    |    | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 64   |



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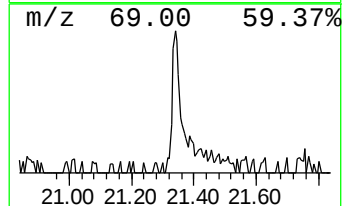
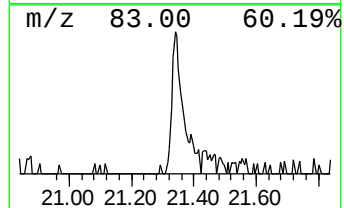
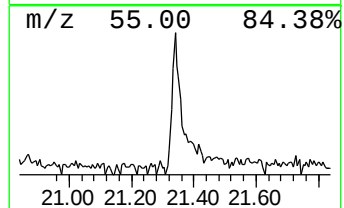
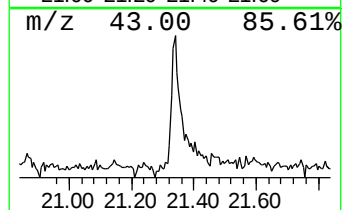
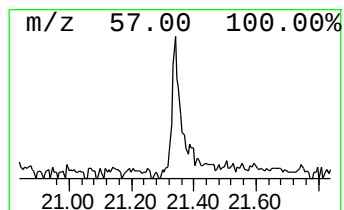
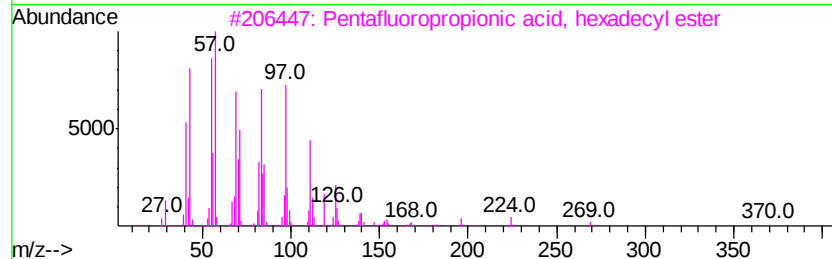
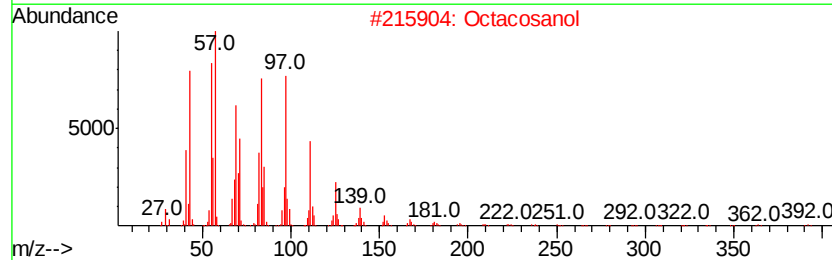
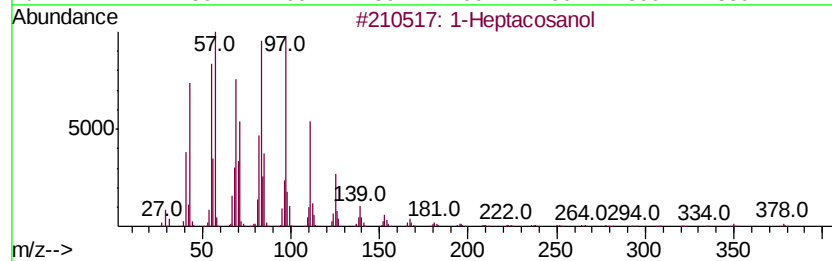
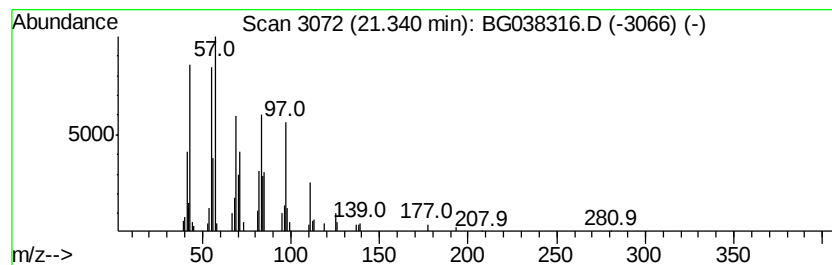
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\*\*\*\*\*  
Peak Number 5 1-Heptacosanol Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD                           |     | R.T.       |             |      |
|-------|---------|-------|--------------------------------------------|-----|------------|-------------|------|
| 21.34 | 2.61 ng | 69948 | Chrysene-d12                               |     | 21.74      |             |      |
| Hit#  | of      | 5     | Tentative ID                               | MW  | MolForm    | CAS#        | Qual |
| 1     |         |       | 1-Heptacosanol                             | 396 | C27H56O    | 002004-39-9 | 91   |
| 2     |         |       | Octacosanol                                | 410 | C28H58O    | 000557-61-9 | 91   |
| 3     |         |       | Pentafluoropropionic acid, hexadecyl ester | 388 | C19H33F5O2 | 006222-07-7 | 91   |
| 4     |         |       | Heptafluorobutyric acid, n-octadecyl ester | 466 | C22H37F7O2 | 000400-57-7 | 91   |
| 5     |         |       | Heptadecyl heptafluorobutyrate             | 452 | C21H35F7O2 | 959085-66-6 | 91   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.16  | 4.0     | ng    | 20227    | 1                     | 8.08  | 99825  | 20.0 |
| unknown7.60          | 7.60  | 80.1    | ng    | 399968   | 1                     | 8.08  | 99825  | 20.0 |
| n-Hexadecanoic acid  | 18.31 | 3.4     | ng    | 69325    | 4                     | 17.46 | 413322 | 20.0 |
| 1-Heptacosanol       | 21.34 | 2.6     | ng    | 69948    | 5                     | 21.74 | 536293 | 20.0 |