

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020719\  
 Data File : BG039386.D  
 Acq On : 7 Feb 2019 17:41  
 Operator : JU/SJ  
 Sample : K1383-04  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 FB-02-05-19

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 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-BG012919.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         | 3.226       | 17            | 23          | 32           | rBV      | 254541         | 473301        | 10.44%          | 2.263%        |
| 2         | 3.303       | 32            | 36          | 50           | rVB      | 196816         | 296106        | 6.53%           | 1.416%        |
| 3         | 5.711       | 438           | 446         | 457          | rBV      | 484913         | 763455        | 16.83%          | 3.650%        |
| 4         | 7.309       | 709           | 718         | 728          | rBV      | 302140         | 514220        | 11.34%          | 2.459%        |
| 5         | 7.703       | 777           | 785         | 794          | rBV      | 886758         | 1509308       | 33.28%          | 7.217%        |
| 6         | 8.178       | 857           | 866         | 876          | rBV      | 189706         | 337785        | 7.45%           | 1.615%        |
| 7         | 8.502       | 911           | 921         | 929          | rBV      | 798194         | 1397065       | 30.80%          | 6.680%        |
| 8         | 9.353       | 1057          | 1066        | 1073         | rBV      | 664324         | 1207623       | 26.63%          | 5.774%        |
| 9         | 10.998      | 1338          | 1346        | 1354         | rBV      | 270603         | 483216        | 10.65%          | 2.310%        |
| 10        | 13.424      | 1748          | 1759        | 1768         | rBV      | 1901183        | 2959894       | 65.26%          | 14.153%       |
| 11        | 14.799      | 1986          | 1993        | 2002         | rVB2     | 439533         | 694531        | 15.31%          | 3.321%        |
| 12        | 16.279      | 2239          | 2245        | 2255         | rBV      | 1422832        | 2178660       | 48.04%          | 10.417%       |
| 13        | 17.542      | 2452          | 2460        | 2470         | rBV      | 588439         | 885844        | 19.53%          | 4.236%        |
| 14        | 19.810      | 2842          | 2846        | 2851         | rVB      | 61958          | 66990         | 1.48%           | 0.320%        |
| 15        | 20.139      | 2895          | 2902        | 2907         | rBV      | 3370270        | 4535370       | 100.00%         | 21.686%       |
| 16        | 20.738      | 3000          | 3004        | 3014         | rBV      | 235559         | 286363        | 6.31%           | 1.369%        |
| 17        | 21.831      | 3182          | 3190        | 3200         | rVB      | 657447         | 1072374       | 23.64%          | 5.128%        |
| 18        | 23.569      | 3479          | 3486        | 3494         | rVB3     | 43954          | 91143         | 2.01%           | 0.436%        |
| 19        | 24.210      | 3589          | 3595        | 3603         | rVB3     | 28933          | 65139         | 1.44%           | 0.311%        |
| 20        | 25.214      | 3754          | 3766        | 3778         | rBV      | 359079         | 1095579       | 24.16%          | 5.239%        |

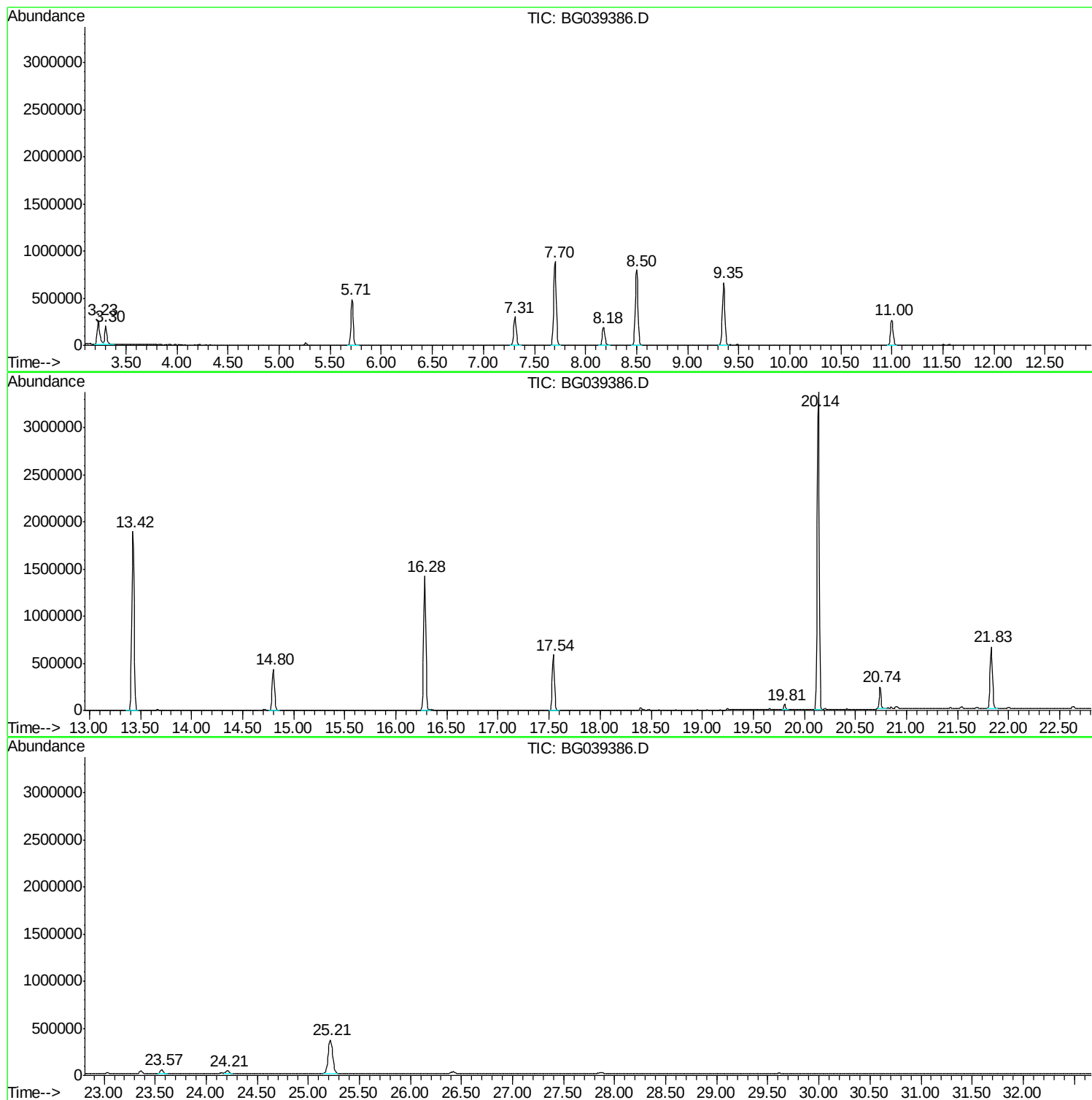
Sum of corrected areas: 20913966

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG012919.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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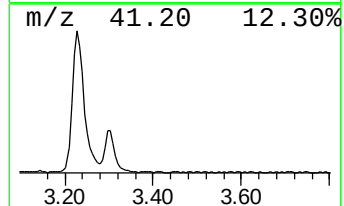
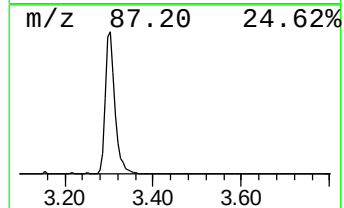
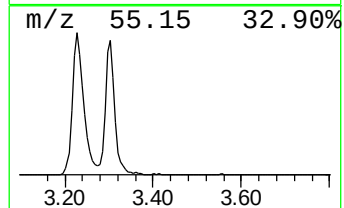
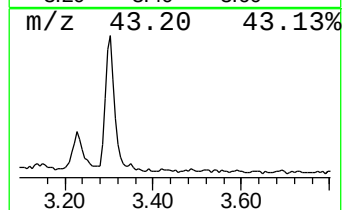
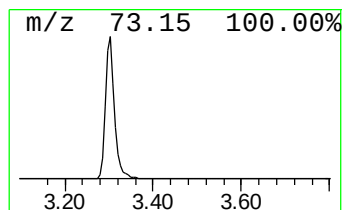
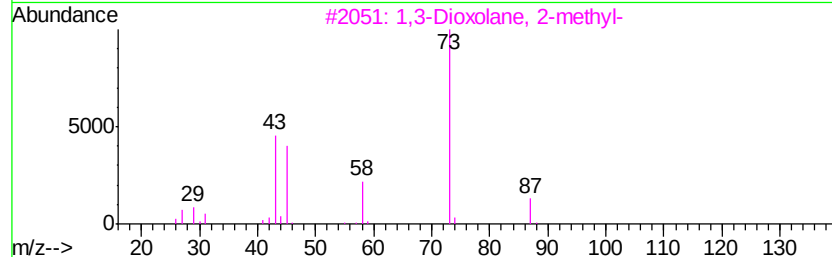
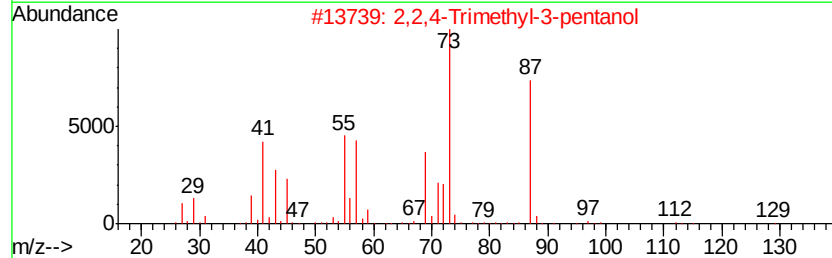
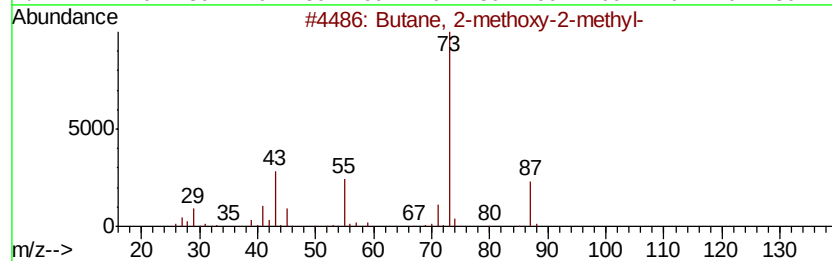
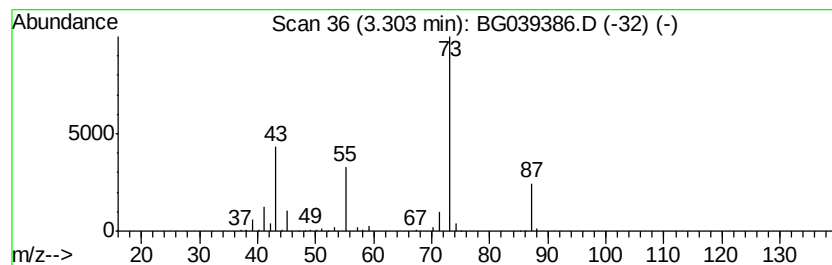
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG012919.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 3.30 | 17.53 ng | 296106 | 1,4-Dichlorobenzene-d4 | 8.18 |

| Hit# | of | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------|-----|---------|-------------|------|
| 1    | 5  | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 74   |
| 2    |    | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 25   |
| 4    |    | 3-Pentanol, 2,4-dimethyl-   | 116 | C7H16O  | 000600-36-2 | 25   |
| 5    |    | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 17   |



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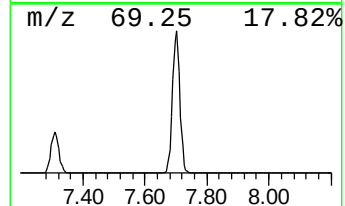
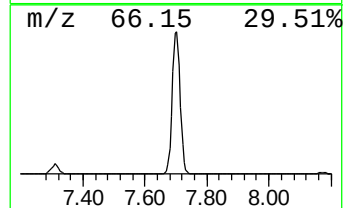
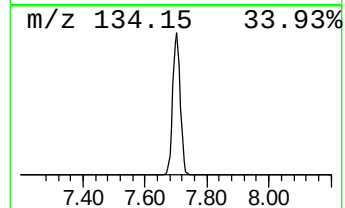
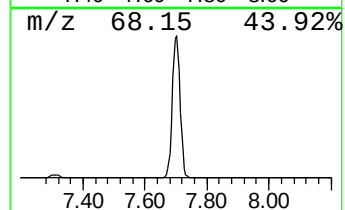
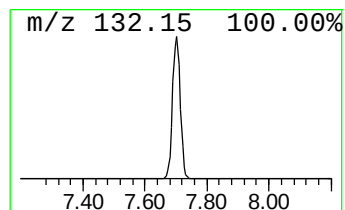
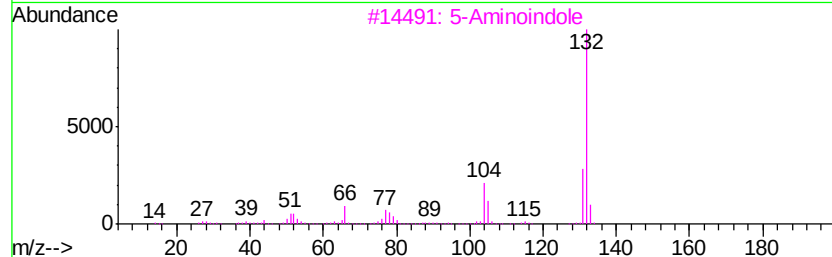
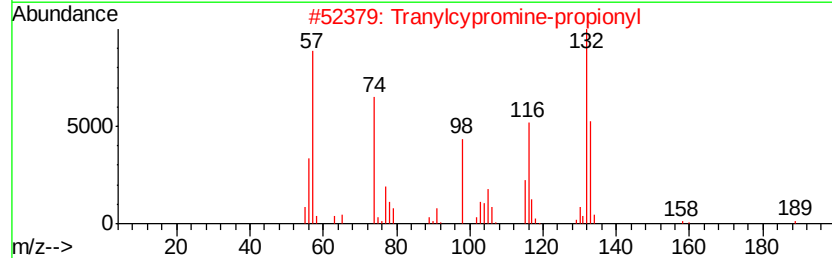
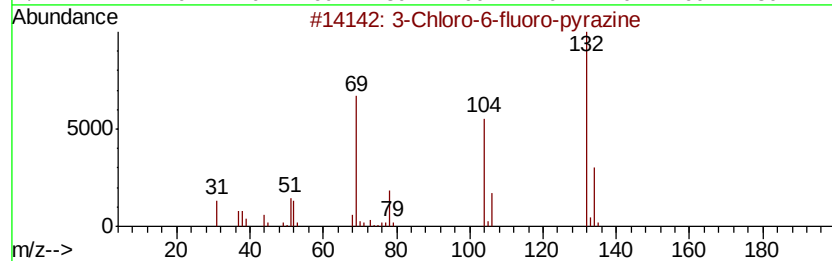
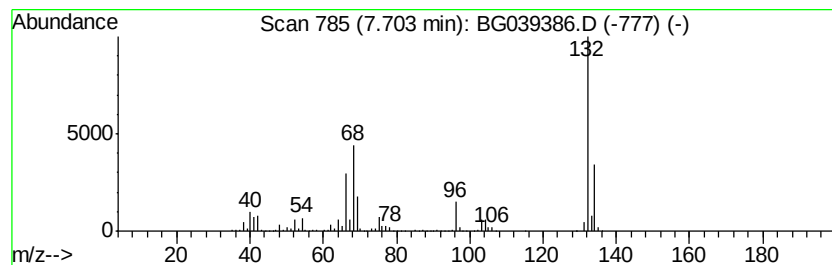
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Peak Number 3 unknown7.70 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.70 | 89.37 ng | 1509310 | 1,4-Dichlorobenzene-d4 | 8.18 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 3    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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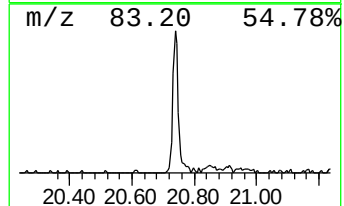
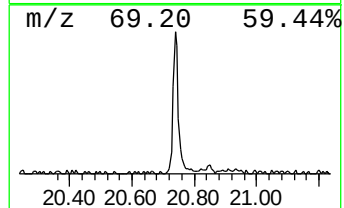
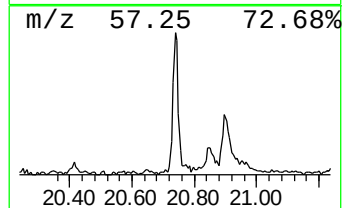
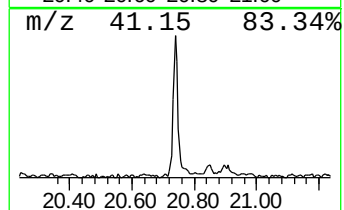
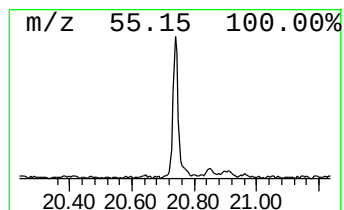
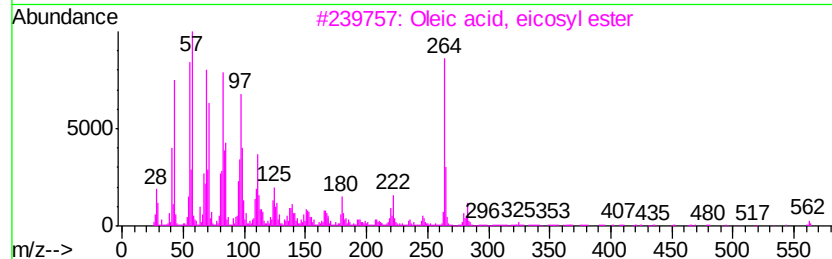
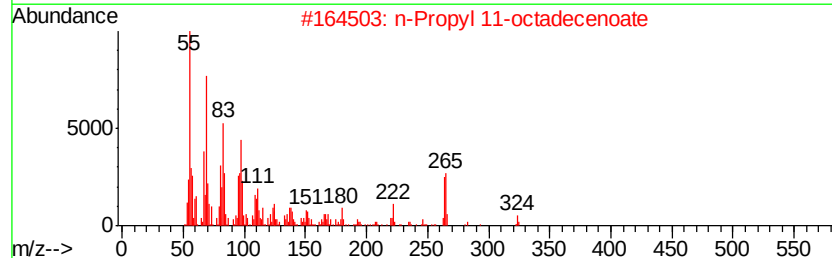
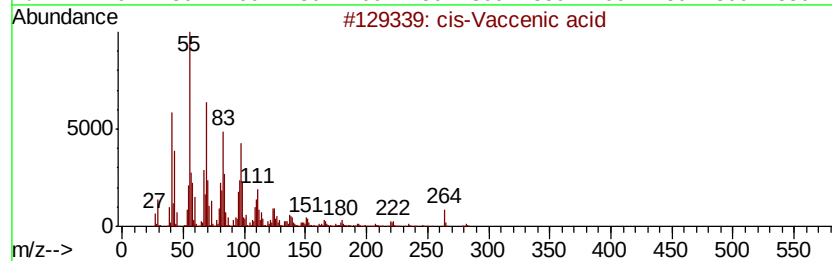
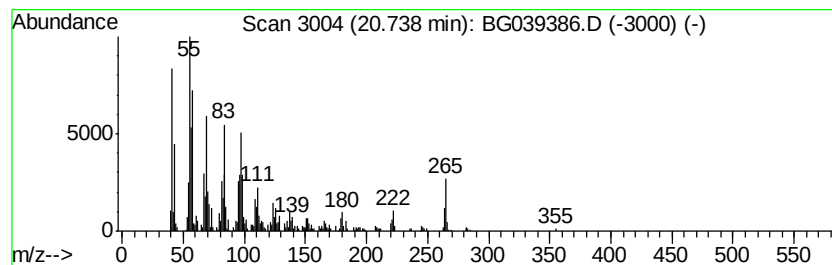
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Peak Number 5 cis-Vaccenic acid Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.74 | 5.34 ng | 286363 | Chrysene-d12     | 21.83 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|---------|---|-------------------------------------|-----|----------|--------------|------|
| 1       |   | cis-Vaccenic acid                   | 282 | C18H34O2 | 000506-17-2  | 94   |
| 2       |   | n-Propyl 11-octadecenoate           | 324 | C21H40O2 | 1000336-71-7 | 91   |
| 3       |   | Oleic acid, eicosyl ester           | 563 | C38H74O2 | 022393-88-0  | 83   |
| 4       |   | 9-Octadecenoic acid (Z)-, octade... | 535 | C36H70O2 | 017673-49-3  | 83   |
| 5       |   | n-Propyl 9-octadecenoate            | 324 | C21H40O2 | 1000336-71-6 | 62   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| Butane, 2-methoxy... | 3.30  | 17.5    | ng    | 296106   | 1                     | 8.18  | 337785  | 20.0 |
| unknown7.70          | 7.70  | 89.4    | ng    | 1509310  | 1                     | 8.18  | 337785  | 20.0 |
| cis-Vaccenic acid    | 20.74 | 5.3     | ng    | 286363   | 5                     | 21.83 | 1072370 | 20.0 |