

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080222\  
 Data File : BM036064.D  
 Acq On : 02 Aug 2022 22:43  
 Operator : CG/JU  
 Sample : N3927-02  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 RVE-76

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\_M\Methods\8270-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036064.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         | 5.434       | 392           | 399         | 414          | rBV      | 5783712        | 8420707       | 40.57%          | 7.960%        |
| 2         | 7.040       | 662           | 672         | 691          | rBV      | 5930572        | 9150575       | 44.09%          | 8.650%        |
| 3         | 7.869       | 802           | 813         | 820          | rBV      | 1292221        | 2006289       | 9.67%           | 1.897%        |
| 4         | 9.040       | 1003          | 1012        | 1026         | rBV      | 3557131        | 5748826       | 27.70%          | 5.435%        |
| 5         | 10.675      | 1281          | 1290        | 1303         | rBV      | 1805350        | 3013207       | 14.52%          | 2.848%        |
| 6         | 13.133      | 1701          | 1708        | 1719         | rBV      | 9366339        | 13625863      | 65.65%          | 12.881%       |
| 7         | 14.504      | 1934          | 1941        | 1953         | rBV      | 2728056        | 3991106       | 19.23%          | 3.773%        |
| 8         | 15.992      | 2186          | 2194        | 2215         | rBV      | 7778300        | 10997995      | 52.99%          | 10.397%       |
| 9         | 17.245      | 2401          | 2407        | 2412         | rBV      | 3411256        | 4710575       | 22.70%          | 4.453%        |
| 10        | 18.145      | 2553          | 2560        | 2570         | rBV      | 586232         | 871738        | 4.20%           | 0.824%        |
| 11        | 19.298      | 2752          | 2756        | 2763         | rBV      | 190403         | 258813        | 1.25%           | 0.245%        |
| 12        | 19.662      | 2813          | 2818        | 2827         | rVB2     | 172962         | 316212        | 1.52%           | 0.299%        |
| 13        | 19.874      | 2848          | 2854        | 2859         | rBV      | 16522685       | 20755235      | 100.00%         | 19.620%       |
| 14        | 21.139      | 3065          | 3069        | 3077         | rBV      | 2532735        | 3299253       | 15.90%          | 3.119%        |
| 15        | 21.421      | 3112          | 3117        | 3122         | rBV      | 4445969        | 5515244       | 26.57%          | 5.214%        |
| 16        | 22.033      | 3218          | 3221        | 3223         | rBV      | 211802         | 273884        | 1.32%           | 0.259%        |
| 17        | 23.068      | 3393          | 3397        | 3402         | rBV2     | 299474         | 455815        | 2.20%           | 0.431%        |
| 18        | 23.786      | 3512          | 3519        | 3531         | rVB2     | 2529654        | 4972276       | 23.96%          | 4.700%        |
| 19        | 24.503      | 3637          | 3641        | 3651         | rVB      | 453641         | 1036151       | 4.99%           | 0.980%        |
| 20        | 26.497      | 3971          | 3980        | 3997         | rVB2     | 1995444        | 6363686       | 30.66%          | 6.016%        |

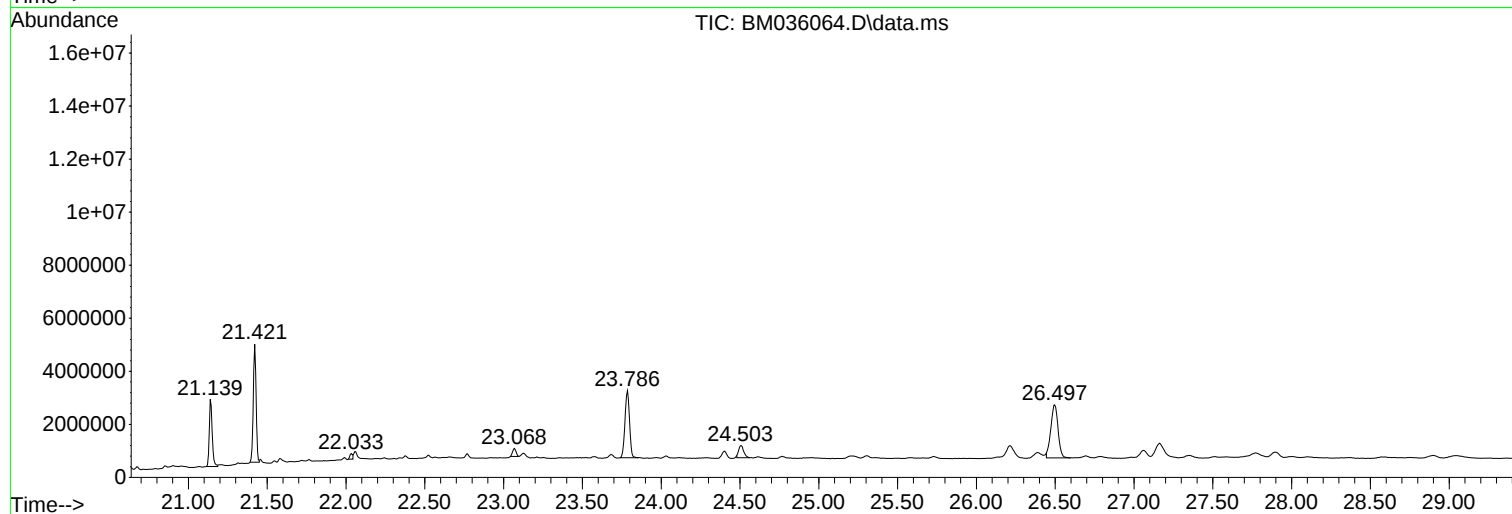
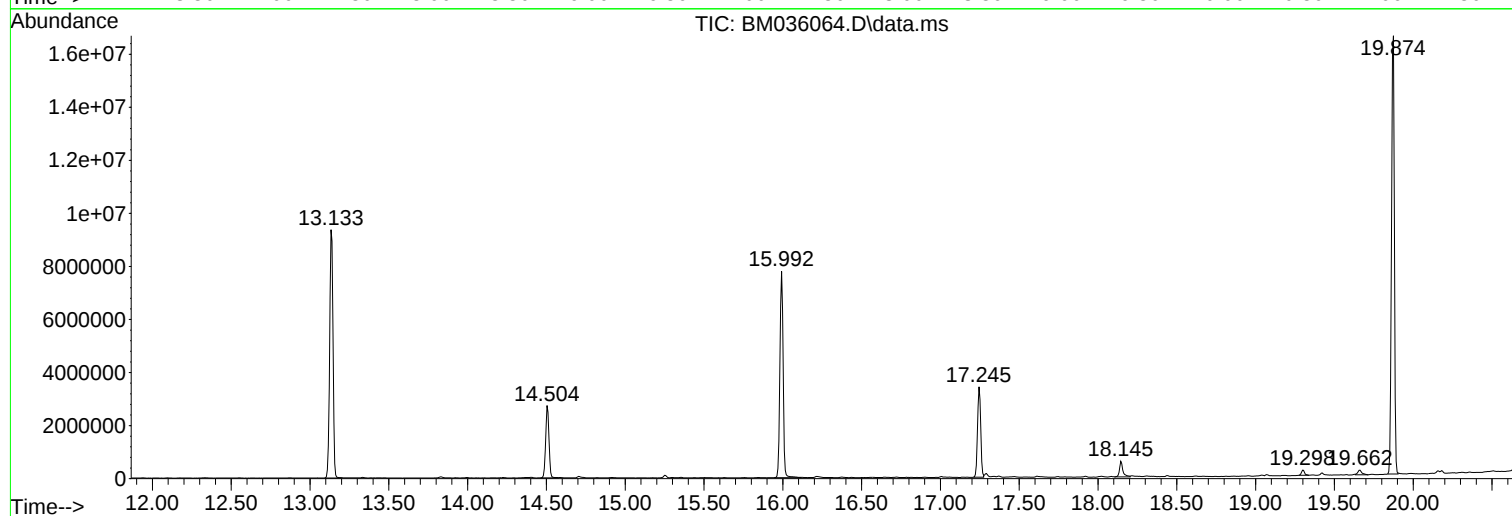
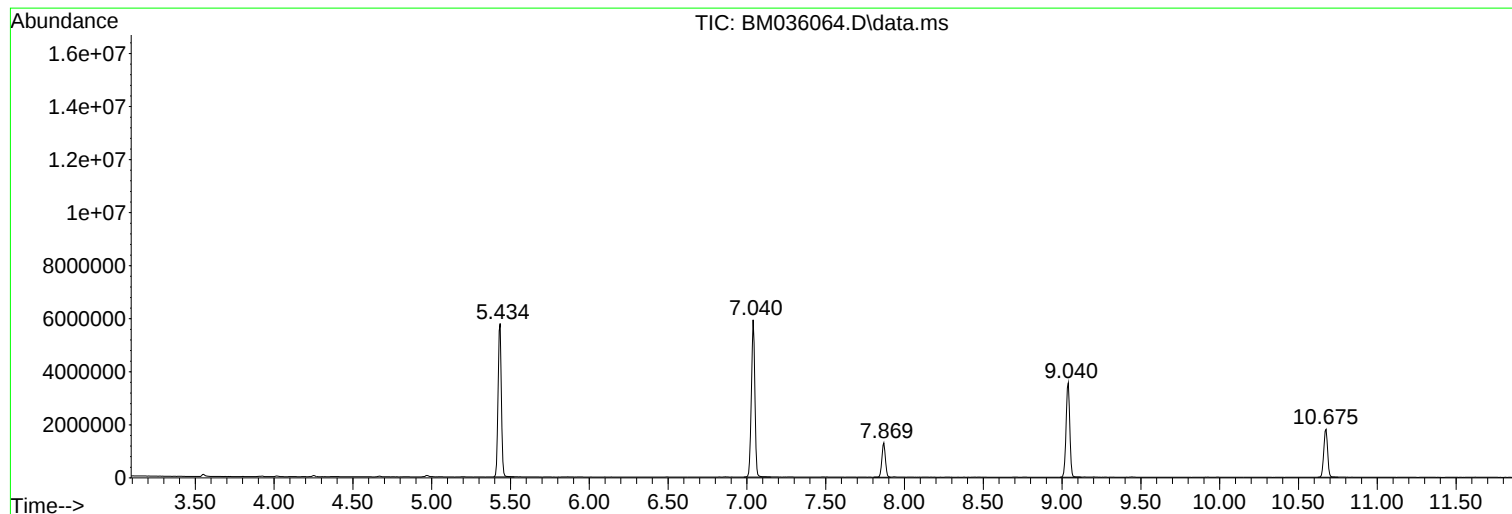
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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM080122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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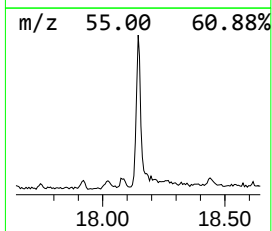
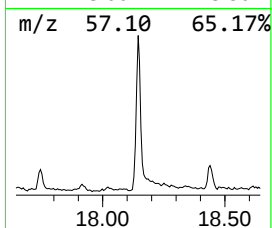
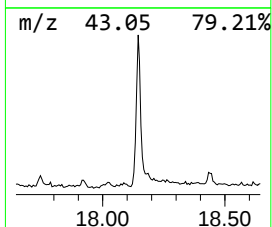
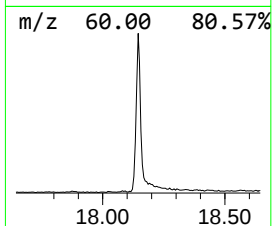
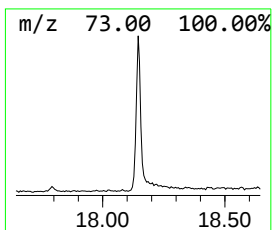
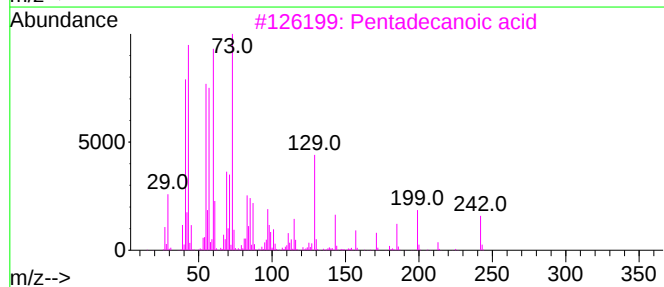
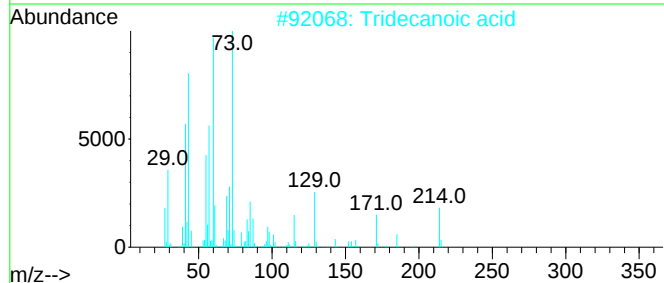
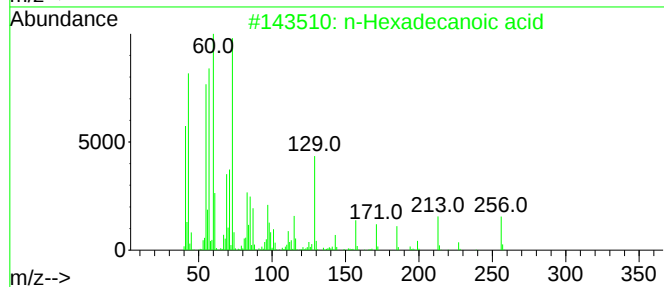
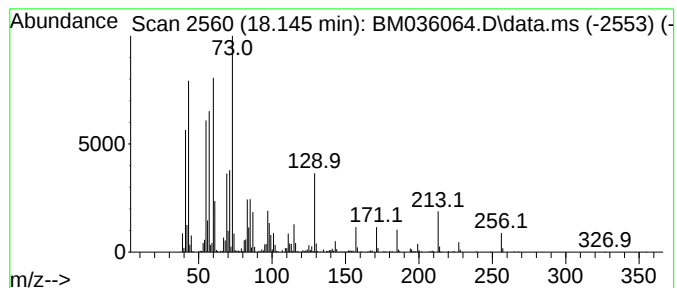
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.145 | 3.70 ng | 871738 | Phenanthrene-d10 | 17.245 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|------|---------------------|-----|----------|-------------|------|
| 1    |      | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |      | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 90   |
| 3    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |      | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 83   |
| 5    |      | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |



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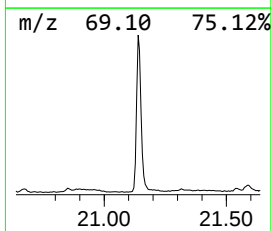
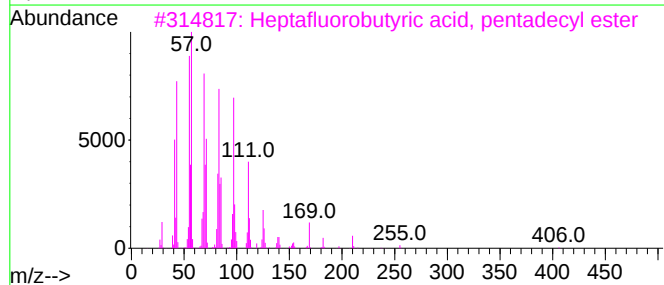
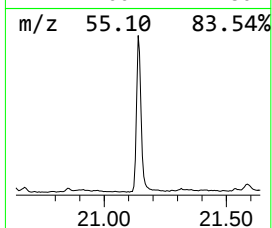
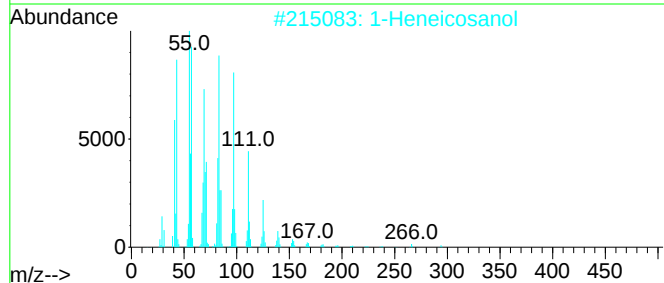
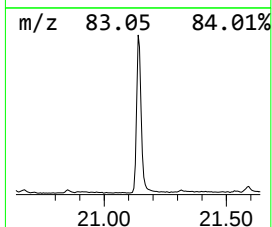
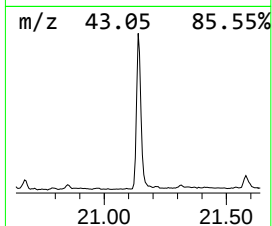
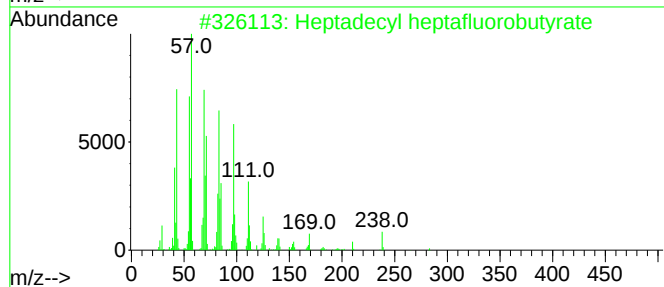
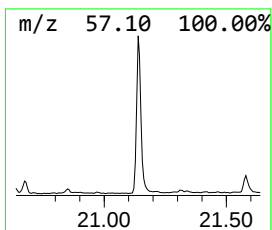
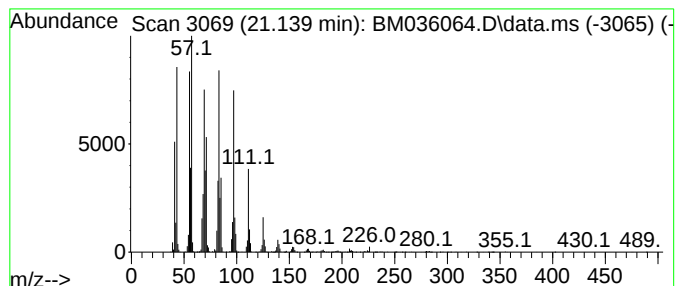
TIC Library : C:\Database\NIST20.L  
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Peak Number 2 Heptadecyl heptafluorobutyrate Concentration Rank 2

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 21.139 | 11.96 ng | 3299250 | Chrysene-d12     | 21.421 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2 | 959085-66-6 | 94   |
| 2    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 91   |
| 3    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 91   |
| 4    |    |   | 1-Hexacosene                        | 364 | C26H52     | 018835-33-1 | 91   |
| 5    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 91   |



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ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :  
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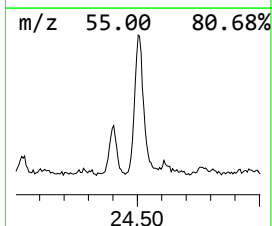
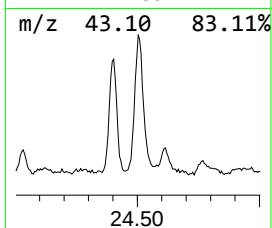
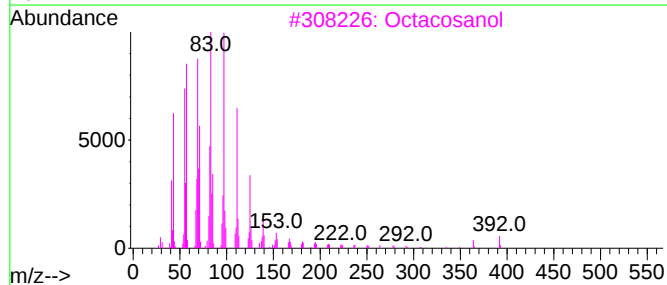
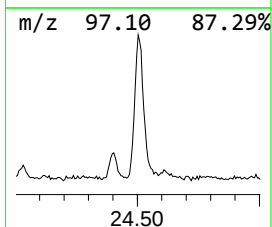
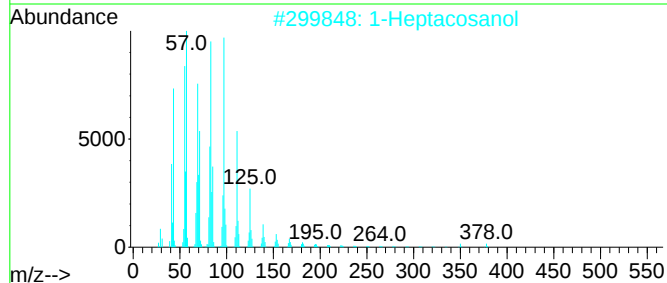
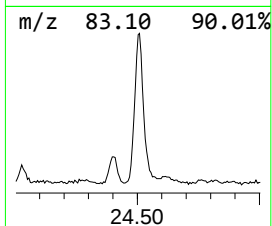
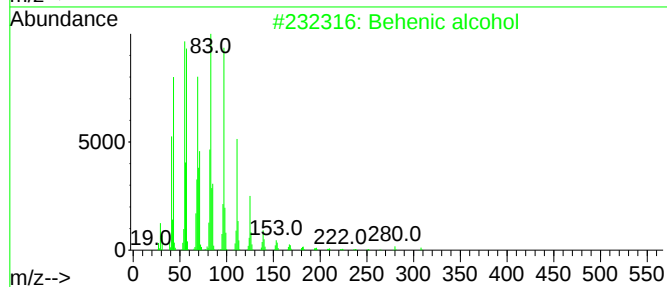
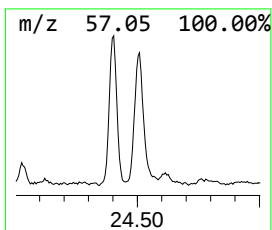
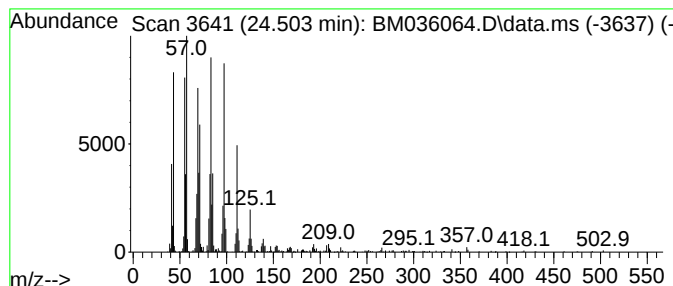
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM080122.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Behenic alcohol Concentration Rank 3

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 24.503 | 4.17 ng | 1036150 | Perylene-d12     | 23.786 |

| Hit# | of 5 | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|------|------|------------------|-----|---------|-------------|------|
| 1    |      | Behenic alcohol  | 326 | C22H46O | 000661-19-8 | 94   |
| 2    |      | 1-Heptacosanol   | 396 | C27H56O | 002004-39-9 | 94   |
| 3    |      | Octacosanol      | 410 | C28H58O | 000557-61-9 | 91   |
| 4    |      | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91   |
| 5    |      | 1-Nonadecene     | 266 | C19H38  | 018435-45-5 | 90   |



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ALS Vial : 13 Sample Multiplier: 1

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RVE-76

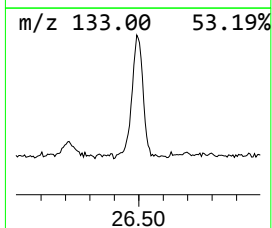
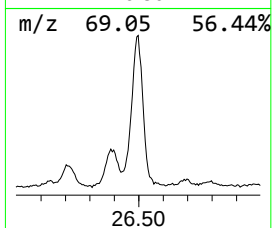
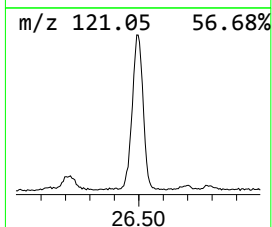
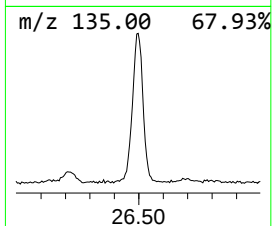
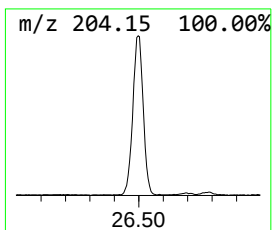
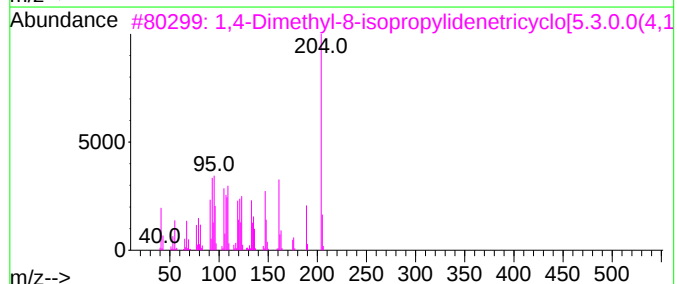
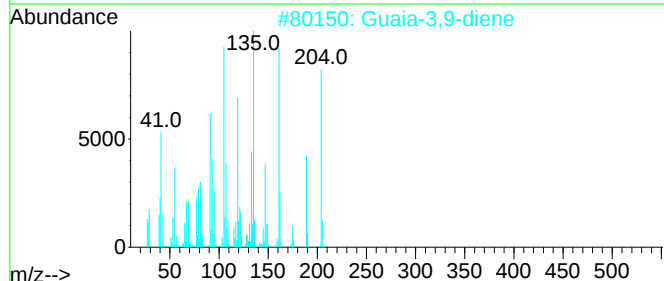
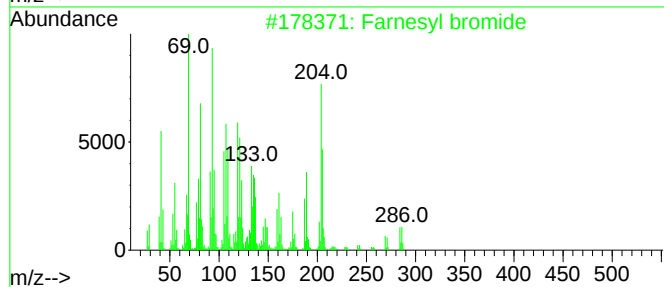
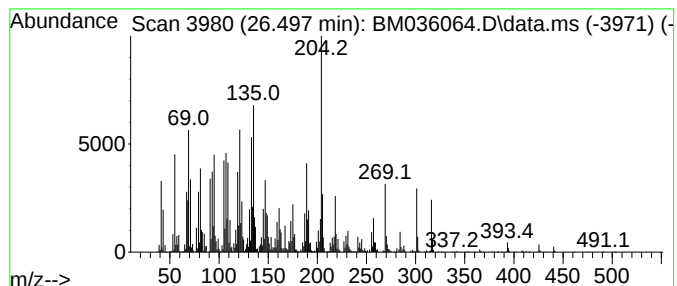
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Peak Number 4 Farnesyl bromide Concentration Rank 1

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 26.497 | 25.60 ng | 6363690 | Perylene-d12     | 23.786 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Farnesyl bromide                    | 284 | C15H25Br | 006874-67-5  | 68   |
| 2    |    |   | Guaia-3,9-diene                     | 204 | C15H24   | 000489-83-8  | 53   |
| 3    |    |   | 1,4-Dimethyl-8-isopropylidenetri... | 204 | C15H24   | 1010140-07-7 | 49   |
| 4    |    |   | 3H-3a,7-Methanoazulene, 2,4,5,6,... | 204 | C15H24   | 002387-78-2  | 49   |
| 5    |    |   | 1,2,4,8-Tetramethylbicyclo[6.3.0... | 204 | C15H24   | 137235-51-9  | 47   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| n-Hexadecanoic ... | 18.145 | 3.7     | ng    | 871738   | 4                     | 17.245 | 4710580 | 20.0 |
| Heptadecyl hept... | 21.139 | 12.0    | ng    | 3299250  | 5                     | 21.421 | 5515240 | 20.0 |
| Behenic alcohol    | 24.503 | 4.2     | ng    | 1036150  | 6                     | 23.786 | 4972280 | 20.0 |
| Farnesyl bromide   | 26.497 | 25.6    | ng    | 6363690  | 6                     | 23.786 | 4972280 | 20.0 |