

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG041422\  
 Data File : BG053154.D  
 Acq On : 14 Apr 2022 13:11  
 Operator : CG/JU  
 Sample : N2334-07  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 MW-19R

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-BG040822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053154.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         | 5.212       | 303           | 310         | 318          | rBV      | 22331          | 36342         | 1.13%           | 0.277%        |
| 2         | 5.687       | 383           | 391         | 405          | rVB      | 356075         | 586096        | 18.26%          | 4.468%        |
| 3         | 7.279       | 652           | 662         | 671          | rBV      | 232451         | 416381        | 12.97%          | 3.175%        |
| 4         | 8.119       | 797           | 805         | 812          | rBV      | 146669         | 253539        | 7.90%           | 1.933%        |
| 5         | 9.283       | 995           | 1003        | 1012         | rBV      | 557335         | 1004934       | 31.32%          | 7.662%        |
| 6         | 10.933      | 1276          | 1284        | 1292         | rVB      | 183760         | 345456        | 10.76%          | 2.634%        |
| 7         | 13.365      | 1688          | 1698        | 1705         | rBV      | 1402334        | 2233876       | 69.61%          | 17.031%       |
| 8         | 14.740      | 1925          | 1932        | 1939         | rBV      | 294436         | 482300        | 15.03%          | 3.677%        |
| 9         | 16.226      | 2178          | 2185        | 2192         | rBV      | 1139291        | 1834194       | 57.16%          | 13.984%       |
| 10        | 17.483      | 2393          | 2399        | 2406         | rBV      | 377957         | 592171        | 18.45%          | 4.515%        |
| 11        | 18.358      | 2544          | 2548        | 2554         | rBV2     | 73544          | 114452        | 3.57%           | 0.873%        |
| 12        | 18.611      | 2586          | 2591        | 2592         | rBV5     | 26527          | 39455         | 1.23%           | 0.301%        |
| 13        | 19.621      | 2760          | 2763        | 2769         | rBV6     | 24083          | 37339         | 1.16%           | 0.285%        |
| 14        | 19.757      | 2779          | 2786        | 2795         | rVB5     | 47083          | 144495        | 4.50%           | 1.102%        |
| 15        | 20.091      | 2836          | 2843        | 2849         | rVB      | 2358535        | 3209107       | 100.00%         | 24.467%       |
| 16        | 21.396      | 3061          | 3065        | 3070         | rBV3     | 57379          | 94207         | 2.94%           | 0.718%        |
| 17        | 21.642      | 3103          | 3107        | 3112         | rVB2     | 63703          | 91704         | 2.86%           | 0.699%        |
| 18        | 21.766      | 3122          | 3128        | 3136         | rBV      | 359013         | 606287        | 18.89%          | 4.622%        |
| 19        | 25.073      | 3681          | 3691        | 3702         | rVB2     | 215161         | 648852        | 20.22%          | 4.947%        |
| 20        | 27.011      | 4014          | 4021        | 4039         | rVB2     | 75180          | 345002        | 10.75%          | 2.630%        |

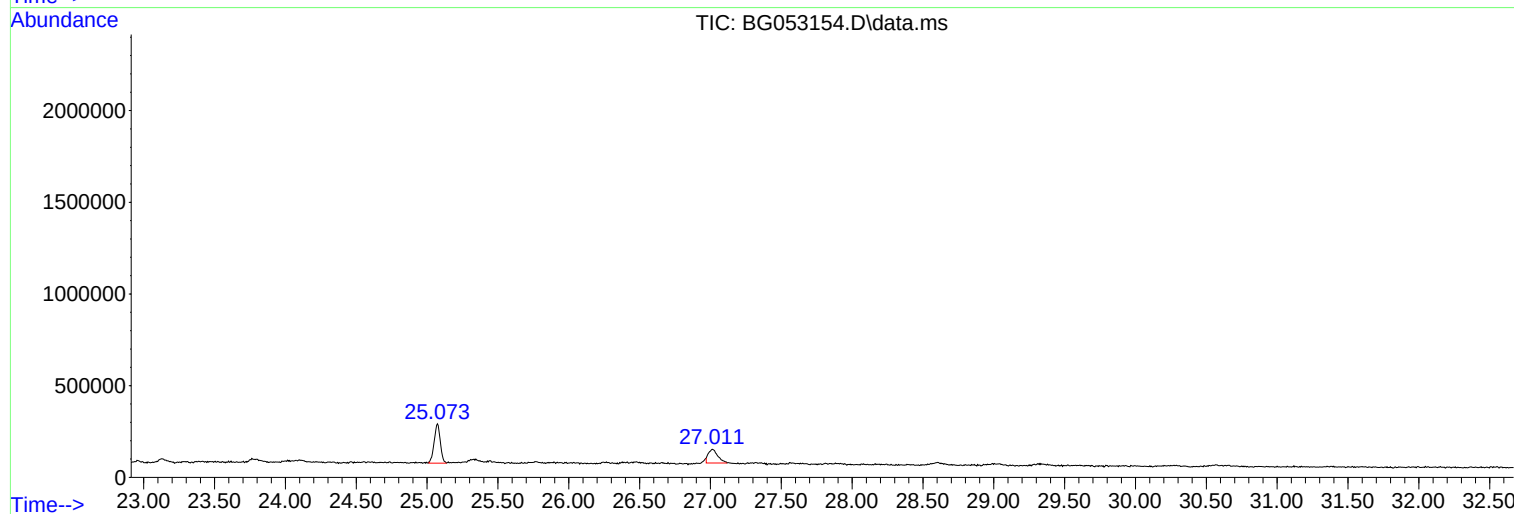
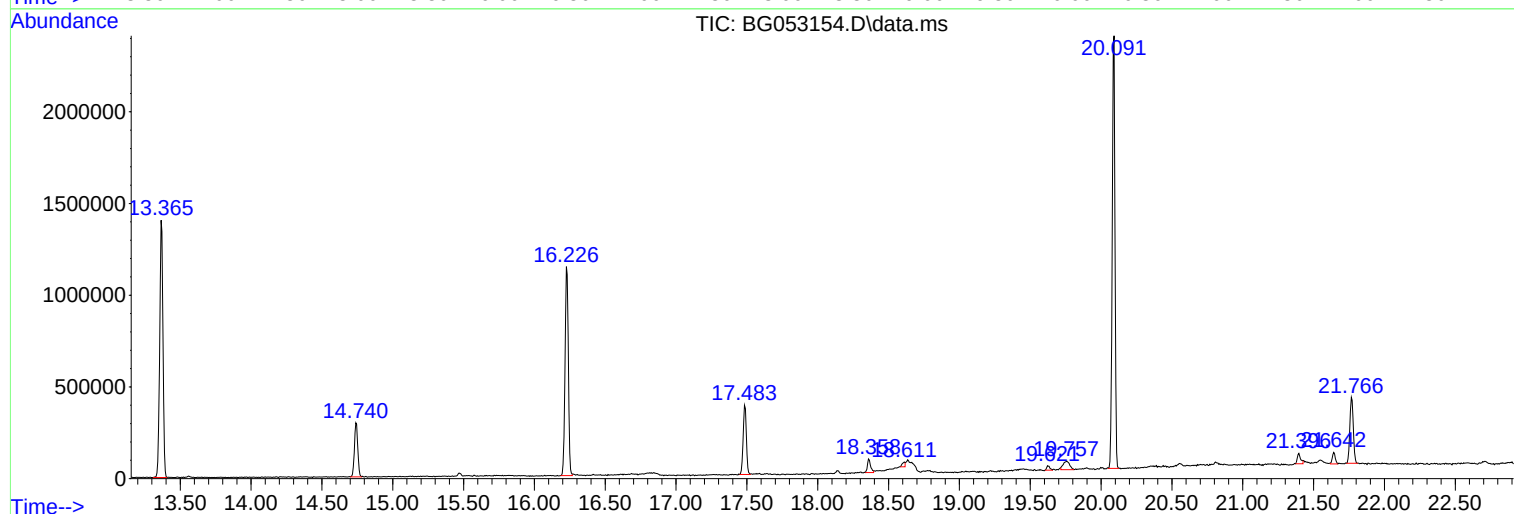
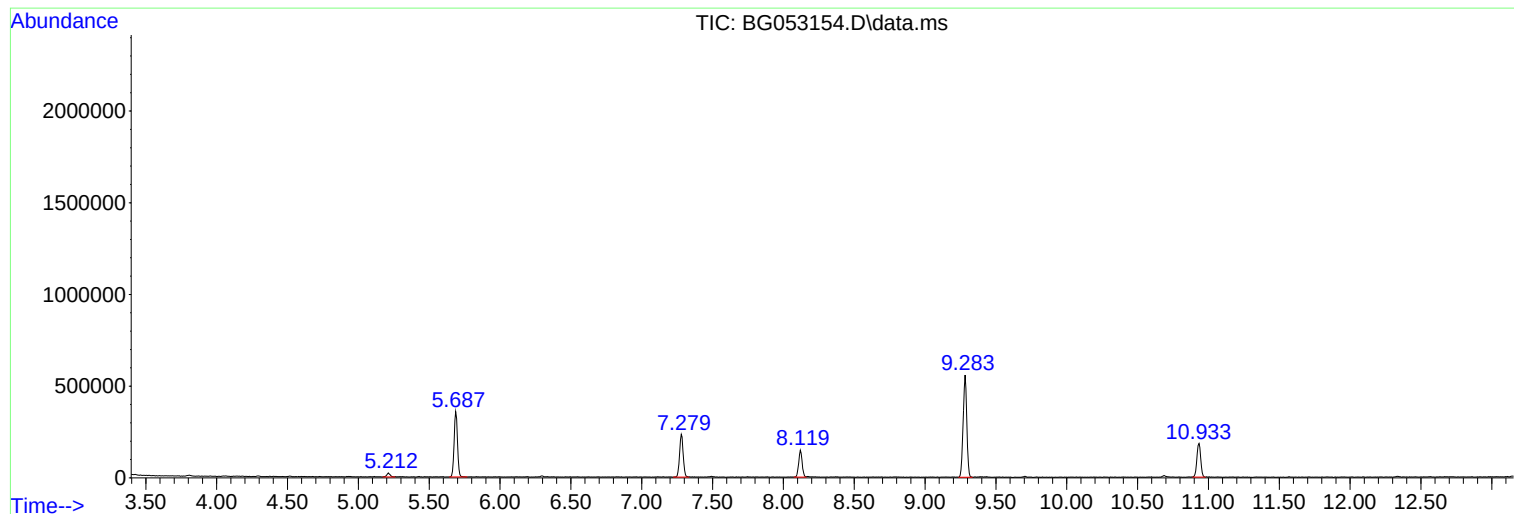
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BNA\_G  
ClientSampleId :  
MW-19R

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG040822.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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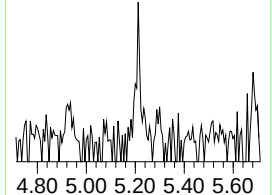
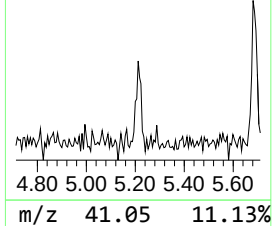
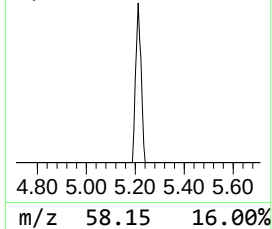
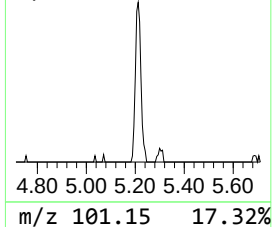
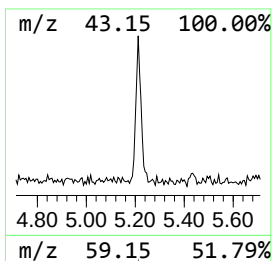
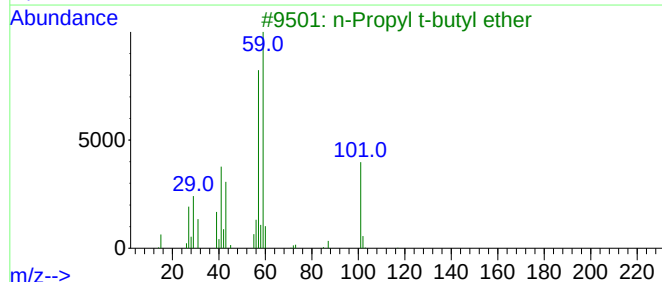
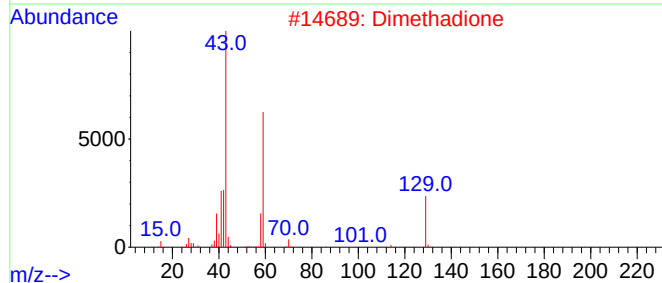
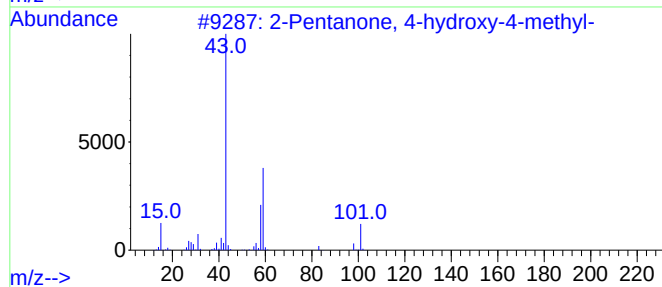
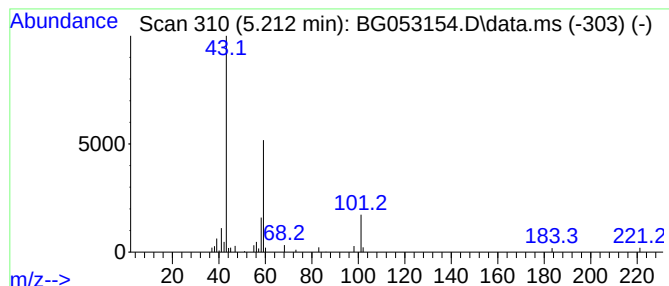
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.212 | 2.87 ng | 36342 | 1,4-Dichlorobenzene-d4 | 8.119 |

| Hit# | of 5 | Tentative ID                     | MW  | MolForm  | CAS#         | Qual |
|------|------|----------------------------------|-----|----------|--------------|------|
| 1    |      | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2  | 000123-42-2  | 42   |
| 2    |      | Dimethadione                     | 129 | C5H7NO3  | 000695-53-4  | 36   |
| 3    |      | n-Propyl t-butyl ether           | 116 | C7H16O   | 1000334-81-9 | 28   |
| 4    |      | Tetraglyme                       | 222 | C10H22O5 | 000143-24-8  | 28   |
| 5    |      | Propane, 1-ethoxy-2-methyl-      | 102 | C6H14O   | 000627-02-1  | 25   |



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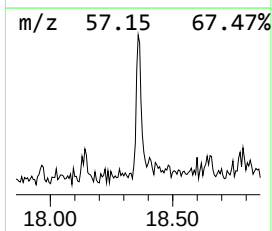
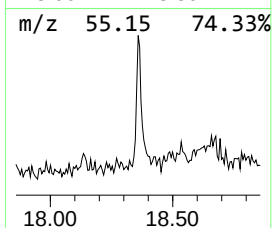
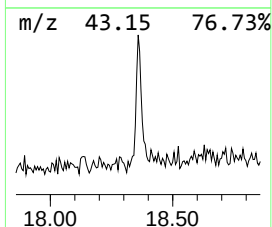
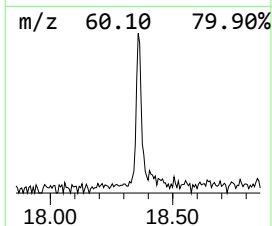
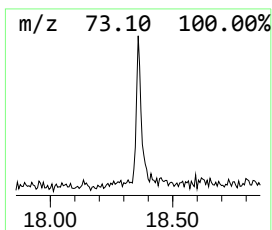
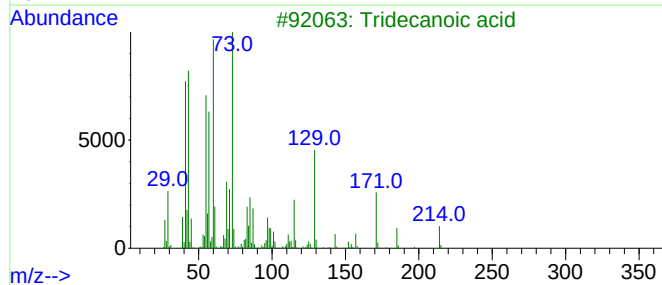
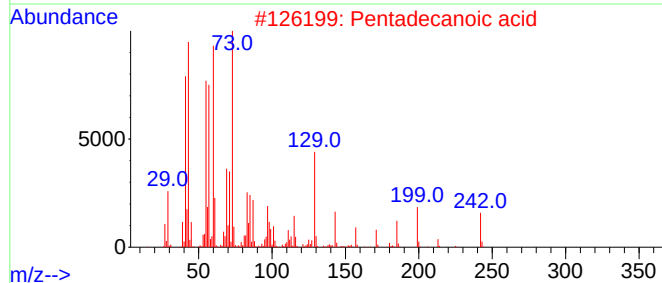
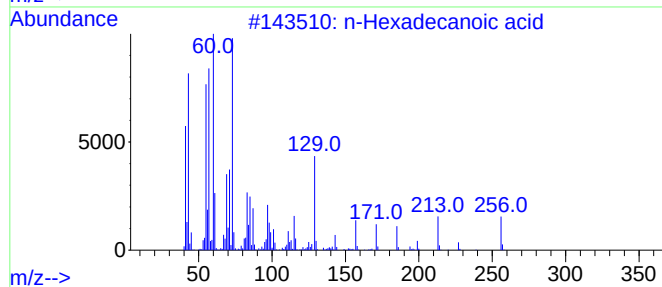
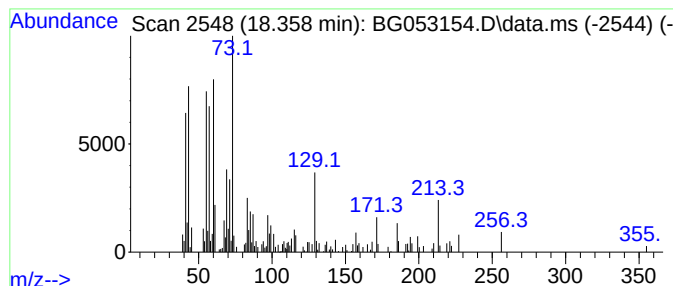
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG040822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.358 | 3.87 ng | 114452 | Phenanthrene-d10 | 17.483 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 96   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 76   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 70   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 60   |
| 5    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 59   |



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ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-19R

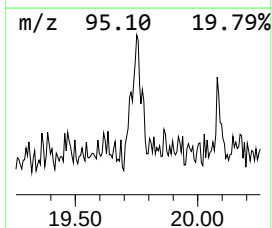
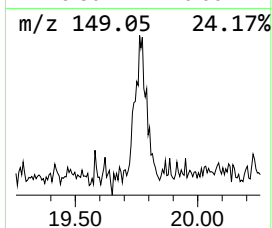
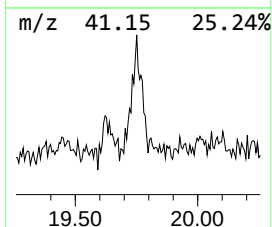
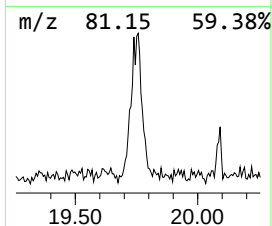
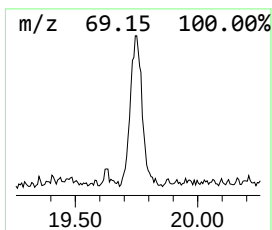
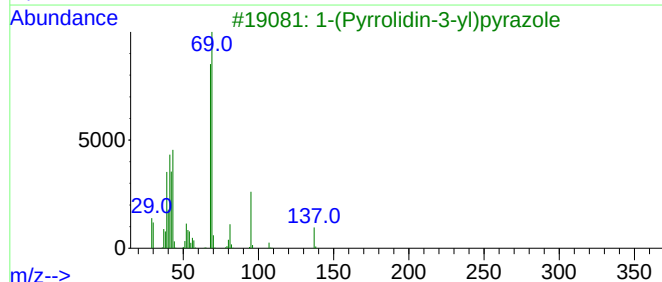
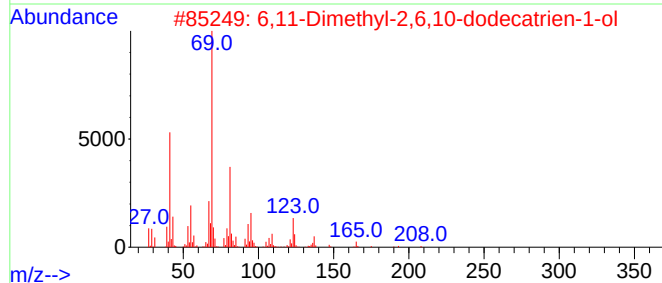
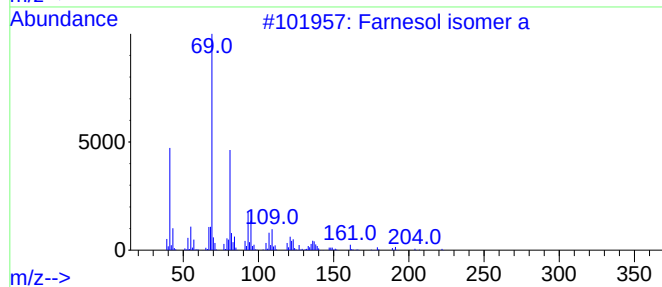
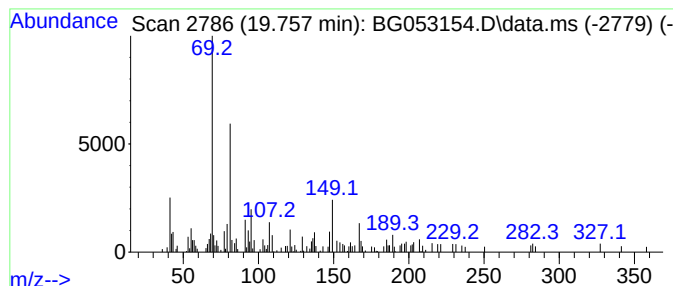
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Peak Number 3 Farnesol isomer a Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.757 | 4.77 ng | 144495 | Chrysene-d12     | 21.766 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Farnesol isomer a                   | 222 | C15H26O | 1000108-92-4 | 50   |
| 2    |    |   | 6,11-Dimethyl-2,6,10-dodecatrien... | 208 | C14H24O | 1000196-53-3 | 50   |
| 3    |    |   | 1-(Pyrrolidin-3-yl)pyrazole         | 137 | C7H11N3 | 1000459-08-8 | 50   |
| 4    |    |   | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4  | 47   |
| 5    |    |   | 3,7,11-Tridecatrienitrile, 4,8...   | 231 | C16H25N | 006006-01-5  | 46   |



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MW-19R

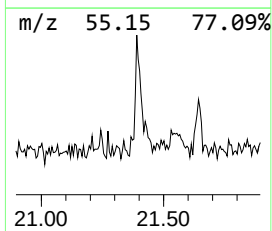
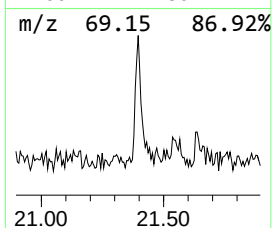
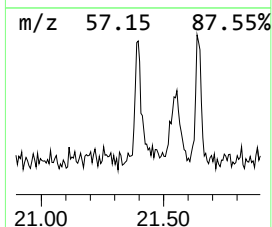
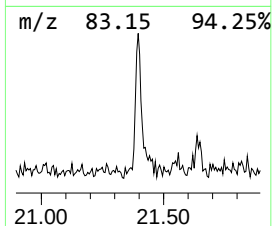
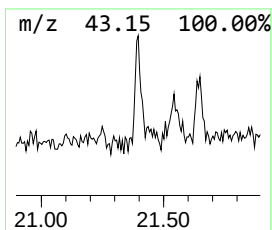
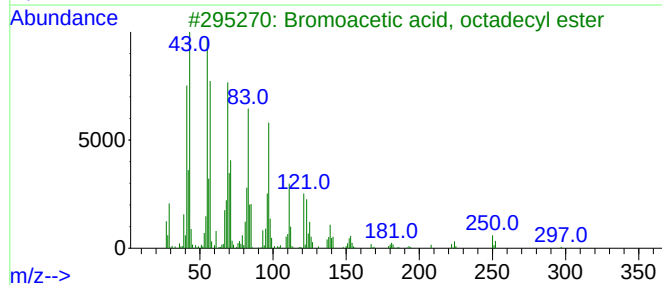
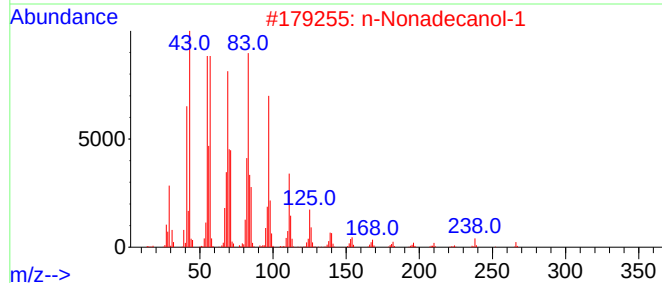
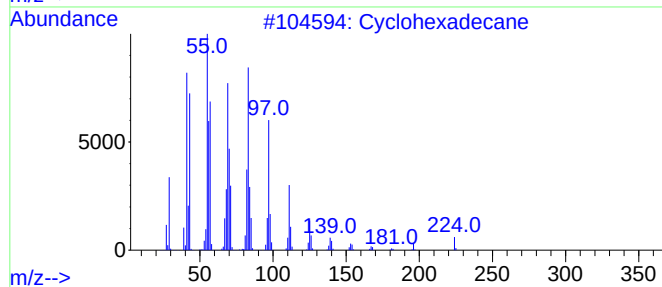
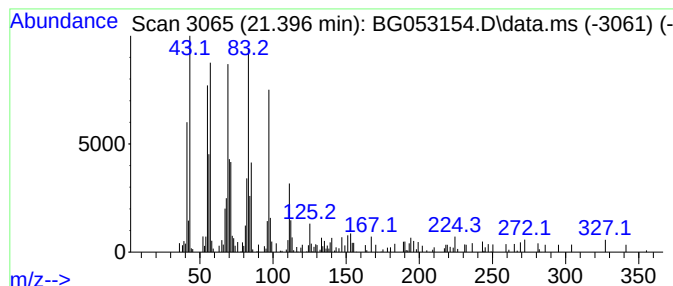
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 Cyclohexadecane Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.395 | 3.11 ng | 94207 | Chrysene-d12     | 21.766 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-----------------------------------|-----|------------|-------------|------|
| 1    |    |   | Cyclohexadecane                   | 224 | C16H32     | 000295-65-8 | 95   |
| 2    |    |   | n-Nonadecanol-1                   | 284 | C19H40O    | 001454-84-8 | 94   |
| 3    |    |   | Bromoacetic acid, octadecyl ester | 390 | C20H39BrO2 | 018992-03-5 | 91   |
| 4    |    |   | Cyclotetradecane                  | 196 | C14H28     | 000295-17-0 | 90   |
| 5    |    |   | Behenic alcohol                   | 326 | C22H46O    | 000661-19-8 | 90   |



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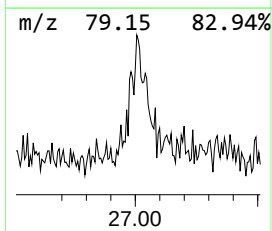
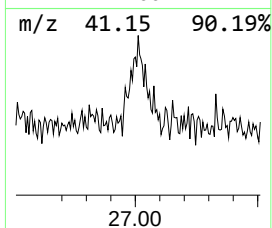
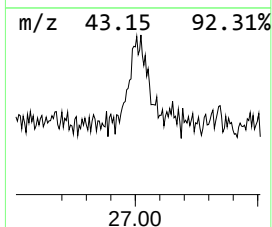
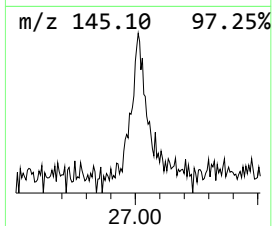
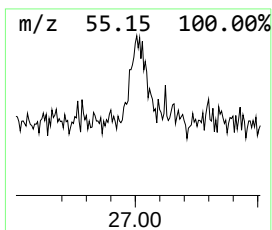
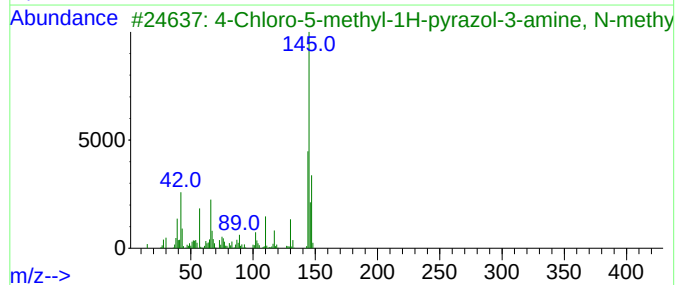
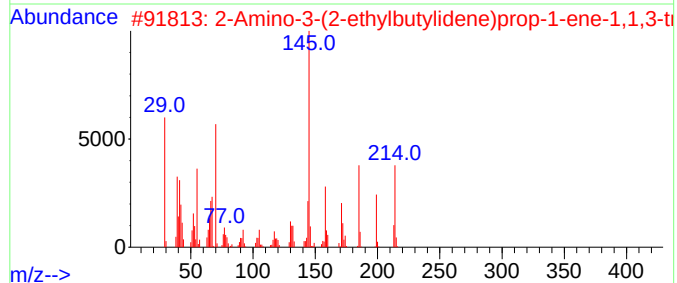
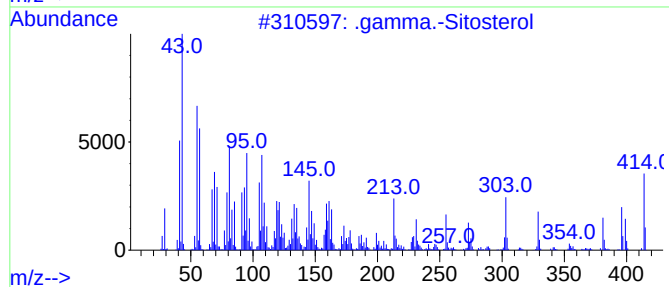
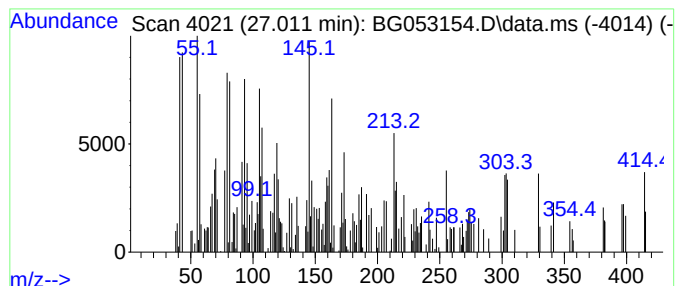
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TIC Library : C:\Database\NIST20.L  
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Peak Number 5 .gamma.-Sitosterol Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 27.012 | 10.63 ng | 345002 | Perylene-d12     | 25.073 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | .gamma.-Sitosterol                  | 414 | C29H50O  | 000083-47-6  | 60   |
| 2    |    |   | 2-Amino-3-(2-ethylbutylidene)pro... | 214 | C12H14N4 | 1000444-22-1 | 43   |
| 3    |    |   | 4-Chloro-5-methyl-1H-pyrazol-3-a... | 145 | C5H8ClN3 | 1000511-78-5 | 38   |
| 4    |    |   | .beta.-Sitosterol                   | 414 | C29H50O  | 000083-46-5  | 35   |
| 5    |    |   | Acetamide, N-phenyl-                | 135 | C8H9NO   | 000103-84-4  | 15   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG041422\  
Data File : BG053154.D  
Acq On : 14 Apr 2022 13:11  
Operator : CG/JU  
Sample : N2334-07  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-19R

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG040822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.212  | 2.9     | ng    | 36342    | 1                     | 8.119  | 253539 | 20.0 |
| n-Hexadecanoic ... | 18.358 | 3.9     | ng    | 114452   | 4                     | 17.483 | 592171 | 20.0 |
| Farnesol isomer a  | 19.757 | 4.8     | ng    | 144495   | 5                     | 21.766 | 606287 | 20.0 |
| Cyclohexadecane    | 21.395 | 3.1     | ng    | 94207    | 5                     | 21.766 | 606287 | 20.0 |
| .gamma.-Sitosterol | 27.012 | 10.6    | ng    | 345002   | 6                     | 25.073 | 648852 | 20.0 |