

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF030524\  
 Data File : BF137505.D  
 Acq On : 05 Mar 2024 17:33  
 Operator : CG\JU  
 Sample : P1674-01  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 1A

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\_F\Methods\8270-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137505.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         | 2.122       | 3             | 6           | 21           | rVB      | 1247982        | 1565489       | 36.76%          | 4.532%        |
| 2         | 2.240       | 22            | 26          | 39           | rVB      | 41938          | 69193         | 1.62%           | 0.200%        |
| 3         | 5.104       | 510           | 513         | 519          | rBV      | 49328          | 62636         | 1.47%           | 0.181%        |
| 4         | 5.498       | 576           | 580         | 599          | rBV      | 4015516        | 4021621       | 94.44%          | 11.642%       |
| 5         | 6.487       | 744           | 748         | 775          | rBV      | 4080122        | 4251117       | 99.82%          | 12.306%       |
| 6         | 6.845       | 806           | 809         | 827          | rBV      | 1169022        | 1112134       | 26.12%          | 3.219%        |
| 7         | 7.404       | 901           | 904         | 926          | rBV      | 2443592        | 2619010       | 61.50%          | 7.582%        |
| 8         | 8.122       | 1023          | 1026        | 1041         | rBV      | 1672619        | 1459860       | 34.28%          | 4.226%        |
| 9         | 9.204       | 1206          | 1210        | 1213         | rBV      | 4710467        | 4258589       | 100.00%         | 12.328%       |
| 10        | 9.880       | 1321          | 1325        | 1339         | rBV      | 1978220        | 1673811       | 39.30%          | 4.845%        |
| 11        | 10.674      | 1456          | 1460        | 1473         | rBV      | 2166636        | 2148028       | 50.44%          | 6.218%        |
| 12        | 11.374      | 1575          | 1579        | 1582         | rBV      | 1876253        | 1605235       | 37.69%          | 4.647%        |
| 13        | 11.398      | 1582          | 1583        | 1589         | rVV      | 297205         | 219806        | 5.16%           | 0.636%        |
| 14        | 11.451      | 1589          | 1592        | 1597         | rVB      | 43137          | 53505         | 1.26%           | 0.155%        |
| 15        | 11.916      | 1668          | 1671        | 1675         | rBV2     | 61973          | 75522         | 1.77%           | 0.219%        |
| 16        | 11.992      | 1681          | 1684        | 1687         | rBV      | 55921          | 59056         | 1.39%           | 0.171%        |
| 17        | 12.433      | 1756          | 1759        | 1762         | rBV      | 45304          | 45953         | 1.08%           | 0.133%        |
| 18        | 12.474      | 1762          | 1766        | 1771         | rVB5     | 24252          | 50186         | 1.18%           | 0.145%        |
| 19        | 12.592      | 1783          | 1786        | 1793         | rBV      | 407894         | 403482        | 9.47%           | 1.168%        |
| 20        | 12.821      | 1820          | 1825        | 1830         | rBV2     | 349506         | 437735        | 10.28%          | 1.267%        |
| 21        | 12.880      | 1833          | 1835        | 1840         | rVB2     | 42980          | 45681         | 1.07%           | 0.132%        |
| 22        | 12.974      | 1847          | 1851        | 1859         | rVB      | 4182886        | 3677836       | 86.36%          | 10.647%       |
| 23        | 13.051      | 1859          | 1864        | 1871         | rVB5     | 40302          | 73642         | 1.73%           | 0.213%        |
| 24        | 13.157      | 1880          | 1882        | 1886         | rVB      | 53533          | 54715         | 1.28%           | 0.158%        |
| 25        | 13.221      | 1890          | 1893        | 1896         | rVV4     | 41214          | 48639         | 1.14%           | 0.141%        |
| 26        | 13.263      | 1896          | 1900        | 1904         | rBV      | 67077          | 75137         | 1.76%           | 0.218%        |
| 27        | 13.563      | 1948          | 1951        | 1954         | rBV      | 52821          | 48901         | 1.15%           | 0.142%        |
| 28        | 13.674      | 1967          | 1970        | 1975         | rVB      | 42171          | 49027         | 1.15%           | 0.142%        |
| 29        | 13.898      | 2003          | 2008        | 2016         | rBV2     | 164304         | 244047        | 5.73%           | 0.706%        |
| 30        | 14.033      | 2024          | 2031        | 2034         | rBV2     | 1164423        | 1294690       | 30.40%          | 3.748%        |
| 31        | 14.063      | 2034          | 2036        | 2044         | rVB      | 194521         | 218519        | 5.13%           | 0.633%        |
| 32        | 14.215      | 2059          | 2062        | 2065         | rVB      | 57970          | 50112         | 1.18%           | 0.145%        |
| 33        | 14.521      | 2111          | 2114        | 2117         | rBV2     | 77716          | 78769         | 1.85%           | 0.228%        |
| 34        | 14.851      | 2166          | 2170        | 2176         | rVB2     | 50019          | 70333         | 1.65%           | 0.204%        |
| 35        | 14.927      | 2180          | 2183        | 2189         | rVB3     | 46750          | 60197         | 1.41%           | 0.174%        |
| 36        | 15.109      | 2209          | 2214        | 2225         | rBV      | 133550         | 290668        | 6.83%           | 0.841%        |

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Sample : P1674-01  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
1A

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\_F\Methods\8270-BF022924.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 15.215 | 2228 | 2232 | 2237 | rVB3 | 89590  | 113256  | 2.66%  | 0.328% |
| 38 | 15.421 | 2264 | 2267 | 2275 | rVB  | 74038  | 100609  | 2.36%  | 0.291% |
| 39 | 15.492 | 2275 | 2279 | 2285 | rBV  | 99534  | 134770  | 3.16%  | 0.390% |
| 40 | 15.557 | 2285 | 2290 | 2299 | rVV  | 792702 | 1081740 | 25.40% | 3.131% |
| 41 | 15.621 | 2299 | 2301 | 2307 | rVB  | 38105  | 54226   | 1.27%  | 0.157% |
| 42 | 16.104 | 2378 | 2383 | 2389 | rVB  | 52064  | 90682   | 2.13%  | 0.263% |
| 43 | 17.127 | 2555 | 2557 | 2565 | rVB4 | 27834  | 54063   | 1.27%  | 0.157% |
| 44 | 18.403 | 2766 | 2774 | 2786 | rVB7 | 85753  | 261364  | 6.14%  | 0.757% |
| 45 | 18.709 | 2822 | 2826 | 2834 | rVB7 | 36699  | 80658   | 1.89%  | 0.233% |

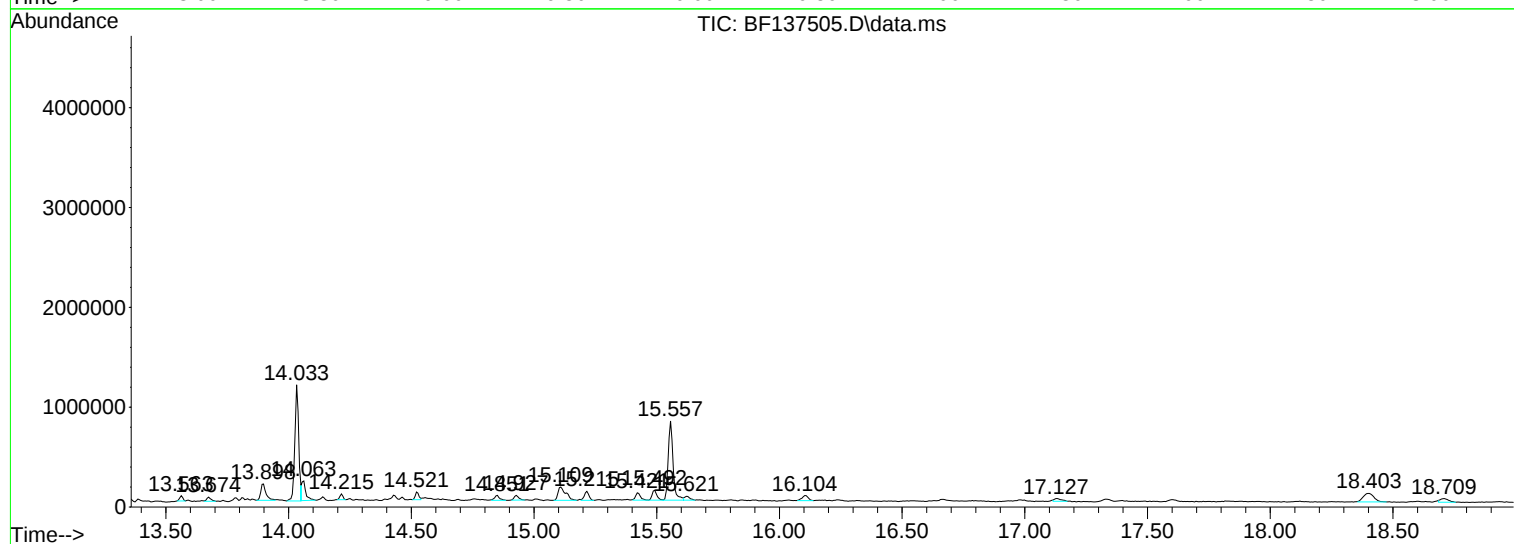
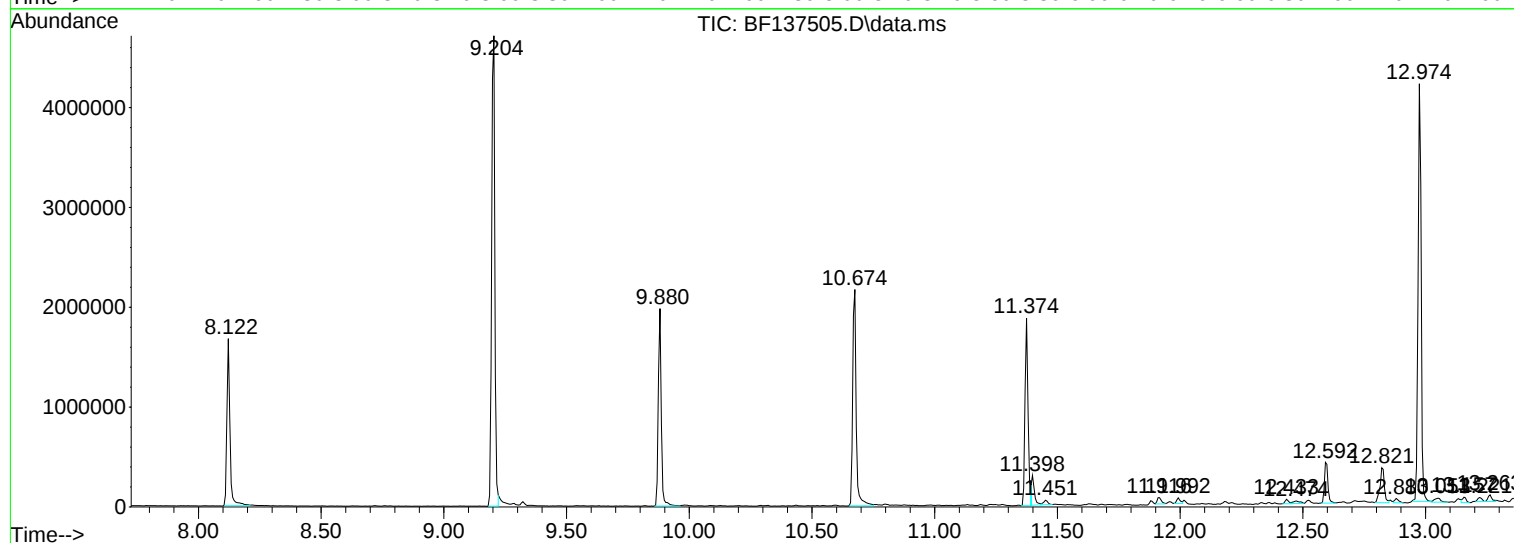
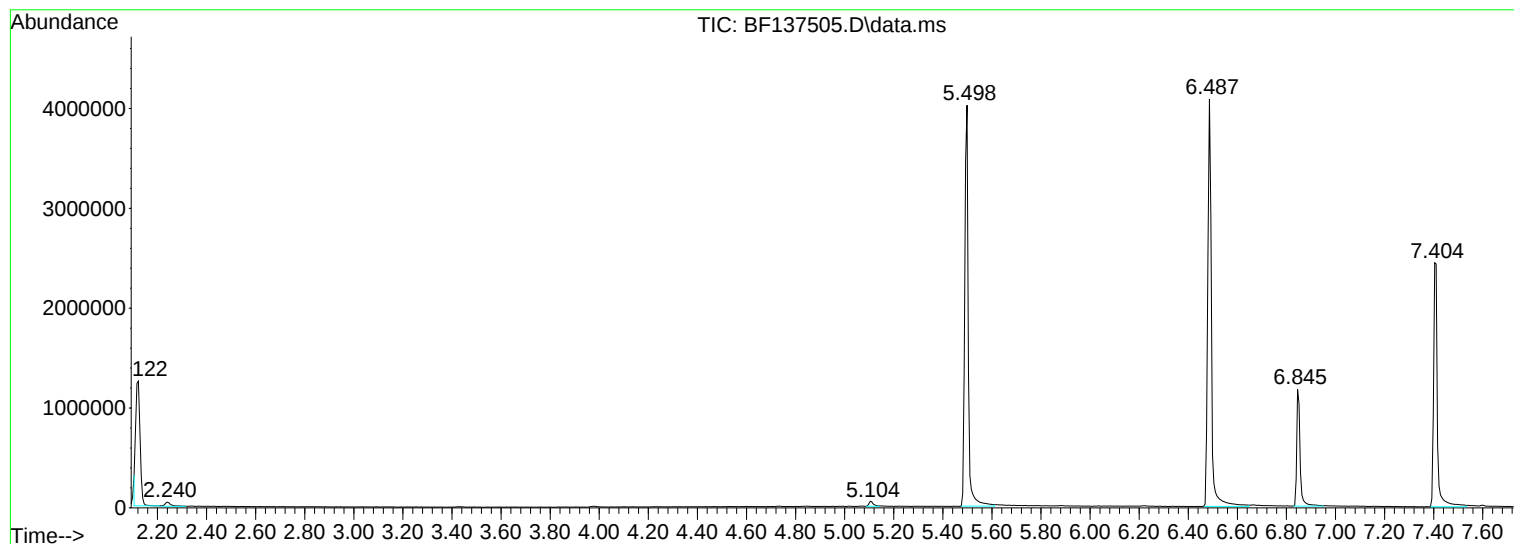
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ALS Vial : 12 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
1A

Quant Title :

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



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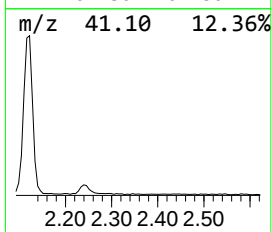
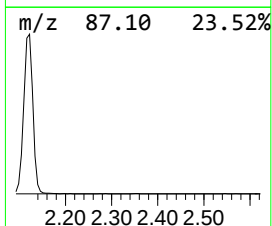
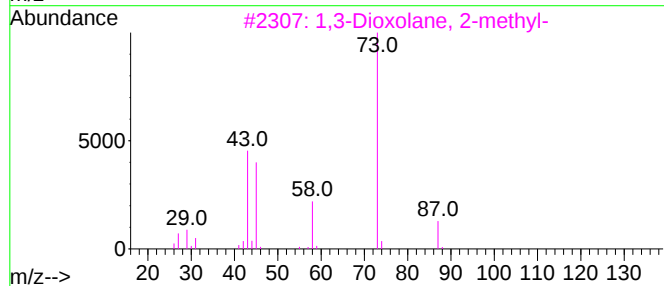
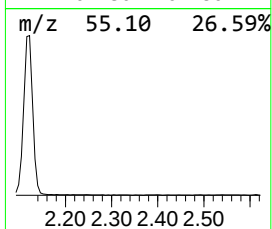
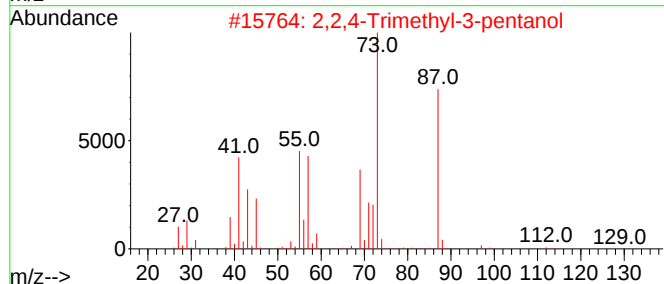
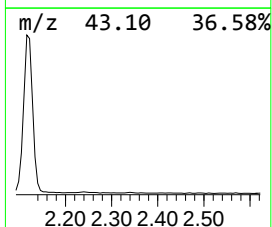
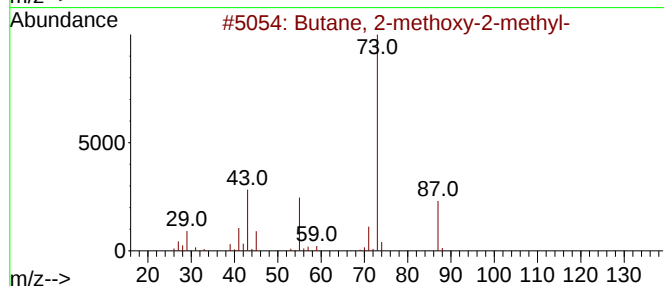
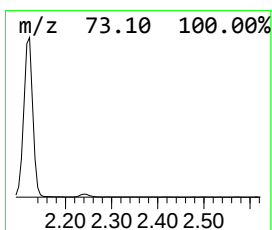
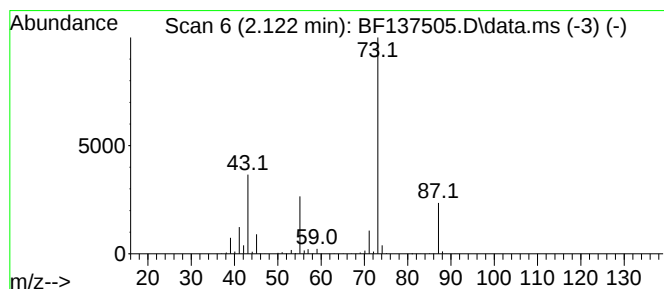
Quant Title :

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.      | EstConc                     | Area    | Relative to ISTD       | R.T.        |      |
|-----------|-----------------------------|---------|------------------------|-------------|------|
| 2.122     | 28.15 ng                    | 1565490 | 1,4-Dichlorobenzene-d4 | 6.845       |      |
| Hit# of 5 | Tentative ID                | MW      | MolForm                | CAS#        | Qual |
| 1         | Butane, 2-methoxy-2-methyl- | 102     | C6H14O                 | 000994-05-8 | 78   |
| 2         | 2,2,4-Trimethyl-3-pentanol  | 130     | C8H18O                 | 005162-48-1 | 40   |
| 3         | 1,3-Dioxolane, 2-methyl-    | 88      | C4H8O2                 | 000497-26-7 | 25   |
| 4         | Pentane, 3-methoxy-         | 102     | C6H14O                 | 036839-67-5 | 17   |
| 5         | Silane, tetramethyl-        | 88      | C4H12Si                | 000075-76-3 | 12   |



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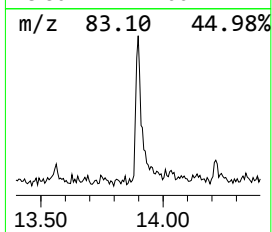
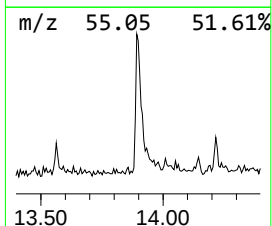
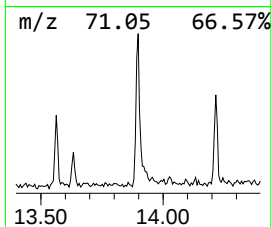
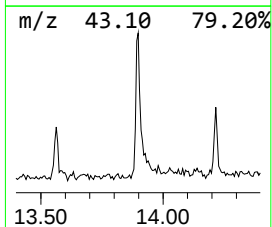
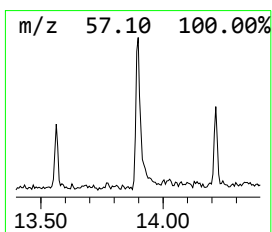
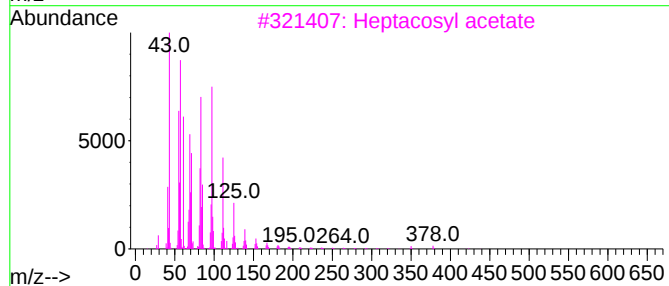
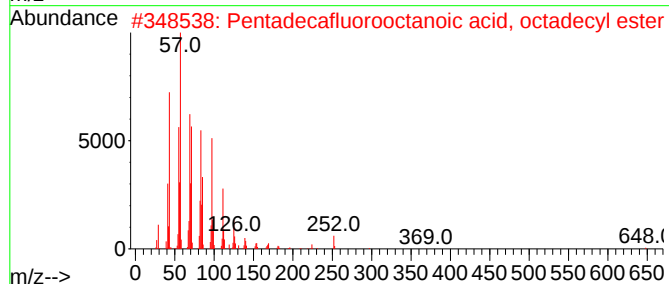
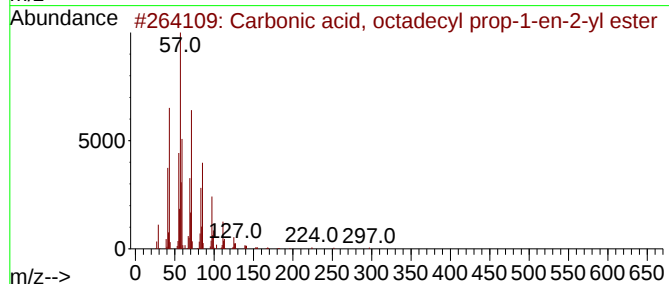
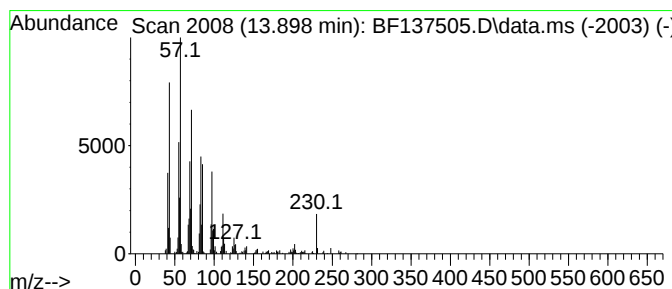
Quant Title :

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

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Peak Number 2 Carbonic acid, octadecyl pr... Concentration Rank 3

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 13.898    | 3.77 ng                             | 244047 | Chrysene-d12     | 14.033       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | Carbonic acid, octadecyl prop-1-... | 354    | C22H42O3         | 1000383-11-5 | 76   |
| 2         | Pentadecafluorooctanoic acid, oc... | 666    | C26H37F15O2      | 1000406-04-8 | 76   |
| 3         | Heptacosyl acetate                  | 438    | C29H58O2         | 1000351-78-2 | 64   |
| 4         | Octacosanol                         | 410    | C28H58O          | 000557-61-9  | 64   |
| 5         | Heptafluorobutyric acid, pentade... | 424    | C19H31F7O2       | 959261-23-5  | 64   |



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BNA\_F  
ClientSampleId :  
1A

Quant Title :

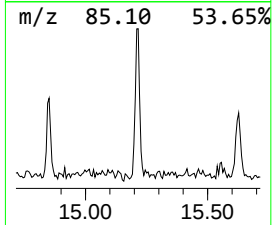
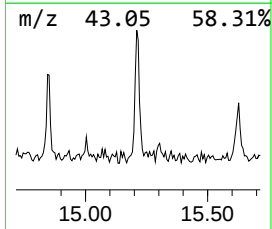
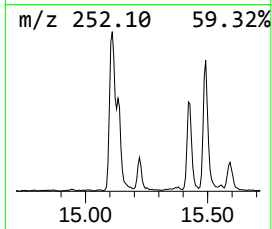
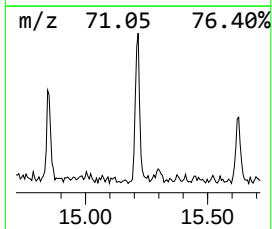
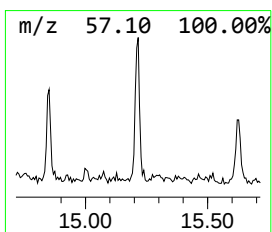
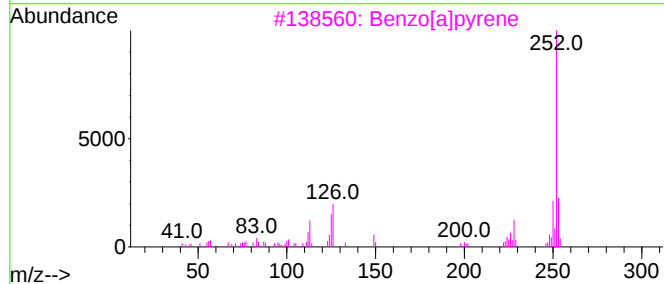
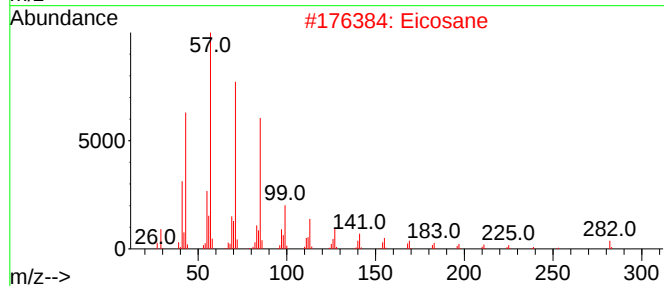
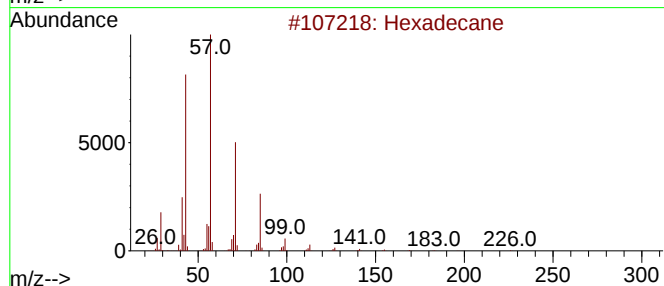
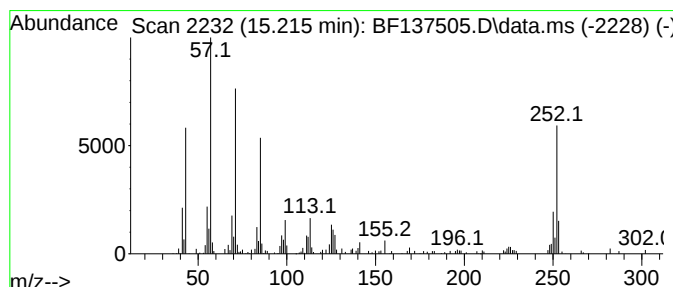
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Hexadecane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.215 | 2.09 ng | 113256 | Perylene-d12     | 15.557 |

| Hit# | of 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|------|----------------------|-----|---------|-------------|------|
| 1    |      | Hexadecane           | 226 | C16H34  | 000544-76-3 | 90   |
| 2    |      | Eicosane             | 282 | C20H42  | 000112-95-8 | 78   |
| 3    |      | Benzo[a]pyrene       | 252 | C20H12  | 000050-32-8 | 70   |
| 4    |      | Benzo[k]fluoranthene | 252 | C20H12  | 000207-08-9 | 55   |
| 5    |      | Benzo[b]fluoranthene | 252 | C20H12  | 000205-99-2 | 55   |



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1A

Quant Title :

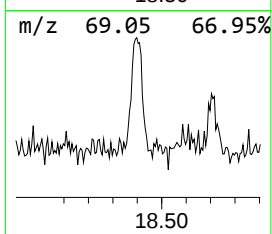
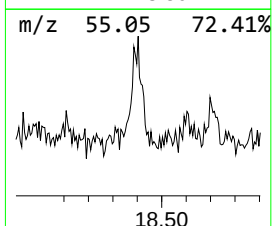
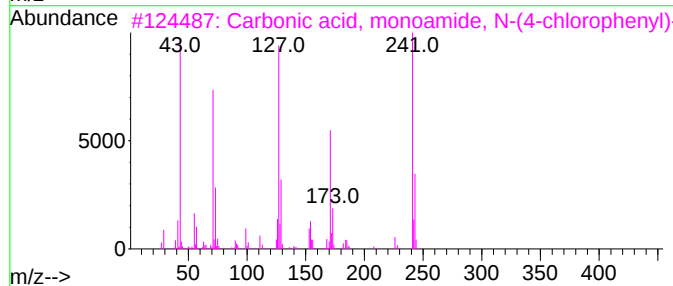
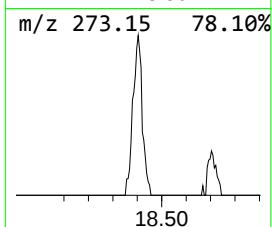
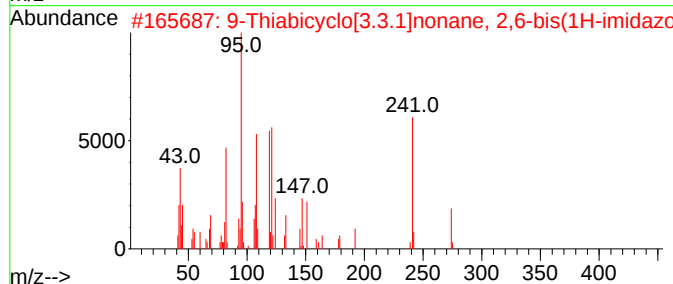
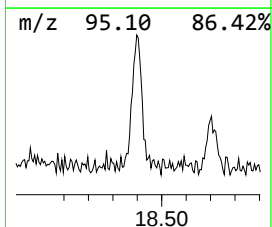
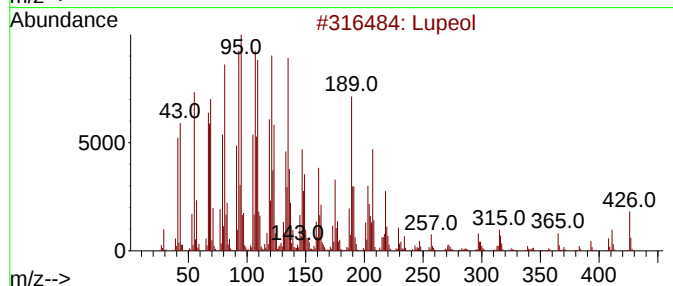
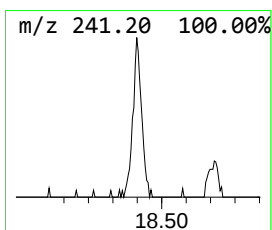
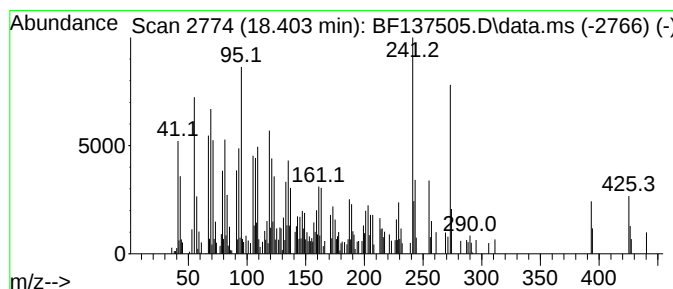
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Lupeol Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.403 | 4.83 ng | 261364 | Perylene-d12     | 15.557 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Lupeol                              | 426 | C30H50O     | 000545-47-1  | 55   |
| 2    |    |   | 9-Thiabicyclo[3.3.1]nonane, 2,6-... | 274 | C14H18N4S   | 1000141-52-1 | 41   |
| 3    |    |   | Carbonic acid, monoamide, N-(4-c... | 241 | C12H16ClNO2 | 1000339-99-7 | 41   |
| 4    |    |   | 9,19-Cyclolanost-24-en-3-ol, (3...  | 426 | C30H50O     | 000469-38-5  | 18   |
| 5    |    |   | Adamantane, 1-(4-methylphenylami... | 241 | C17H23N     | 019984-39-5  | 18   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF030524\  
Data File : BF137505.D  
Acq On : 05 Mar 2024 17:33  
Operator : CG\JU  
Sample : P1674-01  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
1A

Quant Title :

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Butane, 2-metho... | 2.122  | 28.1    | ng    | 1565490  | 1                     | 6.845  | 1112130 | 20.0 |
| Carbonic acid, ... | 13.898 | 3.8     | ng    | 244047   | 5                     | 14.033 | 1294690 | 20.0 |
| Hexadecane         | 15.215 | 2.1     | ng    | 113256   | 6                     | 15.557 | 1081740 | 20.0 |
| Lupeol             | 18.403 | 4.8     | ng    | 261364   | 6                     | 15.557 | 1081740 | 20.0 |