

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF021122\  
 Data File : BF126857.D  
 Acq On : 11 Feb 2022 15:06  
 Operator : CG\JU  
 Sample : N1477-02  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 20220080-BERKELEY-8-COMP

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-BF020922.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126857.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         | 5.193       | 490           | 494         | 502          | rVB      | 40135          | 52853         | 1.20%           | 0.186%        |
| 2         | 5.563       | 551           | 557         | 560          | rBV      | 3627903        | 3755318       | 85.61%          | 13.190%       |
| 3         | 6.563       | 720           | 727         | 730          | rBV      | 3214929        | 3961018       | 90.30%          | 13.913%       |
| 4         | 6.940       | 787           | 791         | 794          | rBV      | 883267         | 698987        | 15.94%          | 2.455%        |
| 5         | 7.504       | 881           | 887         | 890          | rBV      | 2694100        | 2630517       | 59.97%          | 9.239%        |
| 6         | 8.116       | 987           | 991         | 998          | rBV      | 64375          | 72477         | 1.65%           | 0.255%        |
| 7         | 8.222       | 1005          | 1009        | 1012         | rBV      | 1161190        | 951416        | 21.69%          | 3.342%        |
| 8         | 9.298       | 1187          | 1192        | 1195         | rBV      | 4720194        | 4121085       | 93.95%          | 14.475%       |
| 9         | 9.786       | 1271          | 1275        | 1284         | rBV4     | 25515          | 50762         | 1.16%           | 0.178%        |
| 10        | 9.981       | 1304          | 1308        | 1311         | rVB      | 1177204        | 1056493       | 24.09%          | 3.711%        |
| 11        | 10.375      | 1371          | 1375        | 1377         | rBV      | 38794          | 45121         | 1.03%           | 0.158%        |
| 12        | 10.769      | 1437          | 1442        | 1445         | rBV      | 3050557        | 2995312       | 68.29%          | 10.521%       |
| 13        | 11.469      | 1557          | 1561        | 1564         | rBV      | 1401297        | 1126265       | 25.68%          | 3.956%        |
| 14        | 11.980      | 1645          | 1648        | 1652         | rBV      | 99858          | 89552         | 2.04%           | 0.315%        |
| 15        | 13.057      | 1826          | 1831        | 1835         | rBV      | 4185544        | 4386409       | 100.00%         | 15.407%       |
| 16        | 13.274      | 1864          | 1868        | 1872         | rBV      | 63581          | 55857         | 1.27%           | 0.196%        |
| 17        | 13.616      | 1922          | 1926        | 1928         | rBV      | 81927          | 66462         | 1.52%           | 0.233%        |
| 18        | 13.945      | 1977          | 1982        | 1998         | rBV3     | 193025         | 404523        | 9.22%           | 1.421%        |
| 19        | 14.110      | 2007          | 2010        | 2014         | rVB      | 897225         | 800380        | 18.25%          | 2.811%        |
| 20        | 14.263      | 2032          | 2036        | 2039         | rBV      | 121555         | 105582        | 2.41%           | 0.371%        |
| 21        | 14.569      | 2084          | 2088        | 2091         | rBV      | 121390         | 102860        | 2.34%           | 0.361%        |
| 22        | 14.886      | 2138          | 2142        | 2146         | rBV      | 80290          | 78567         | 1.79%           | 0.276%        |
| 23        | 14.968      | 2152          | 2156        | 2161         | rVB      | 93871          | 99903         | 2.28%           | 0.351%        |
| 24        | 15.239      | 2197          | 2202        | 2208         | rBV      | 66793          | 81798         | 1.86%           | 0.287%        |
| 25        | 15.621      | 2261          | 2267        | 2276         | rBV      | 515397         | 681169        | 15.53%          | 2.393%        |

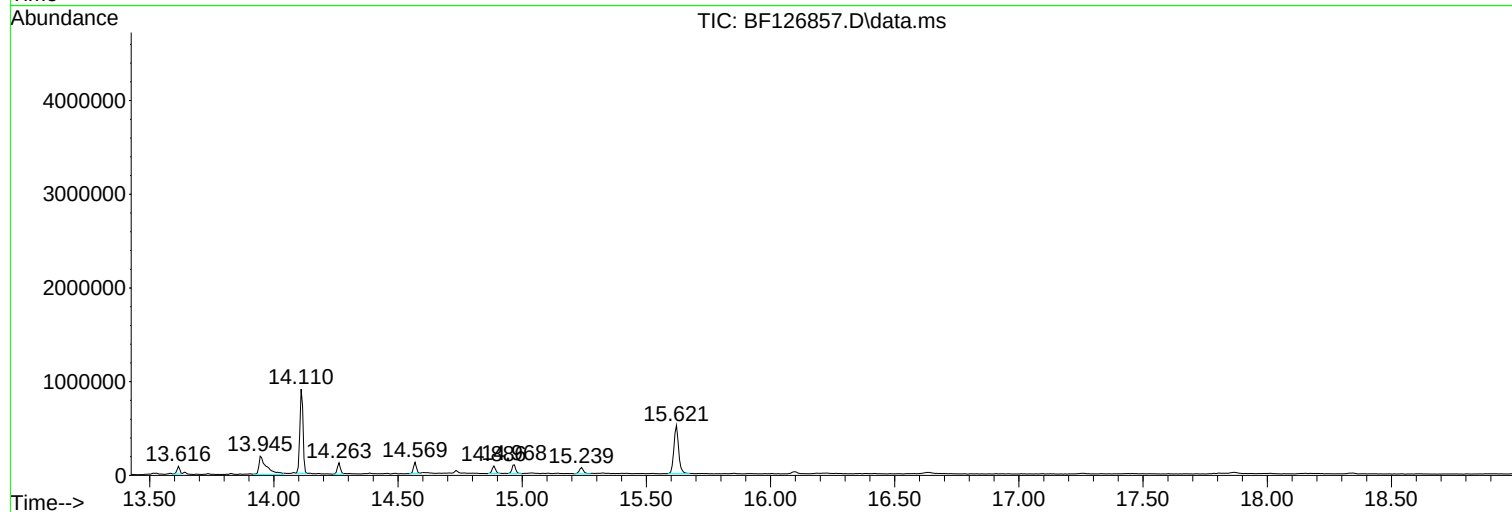
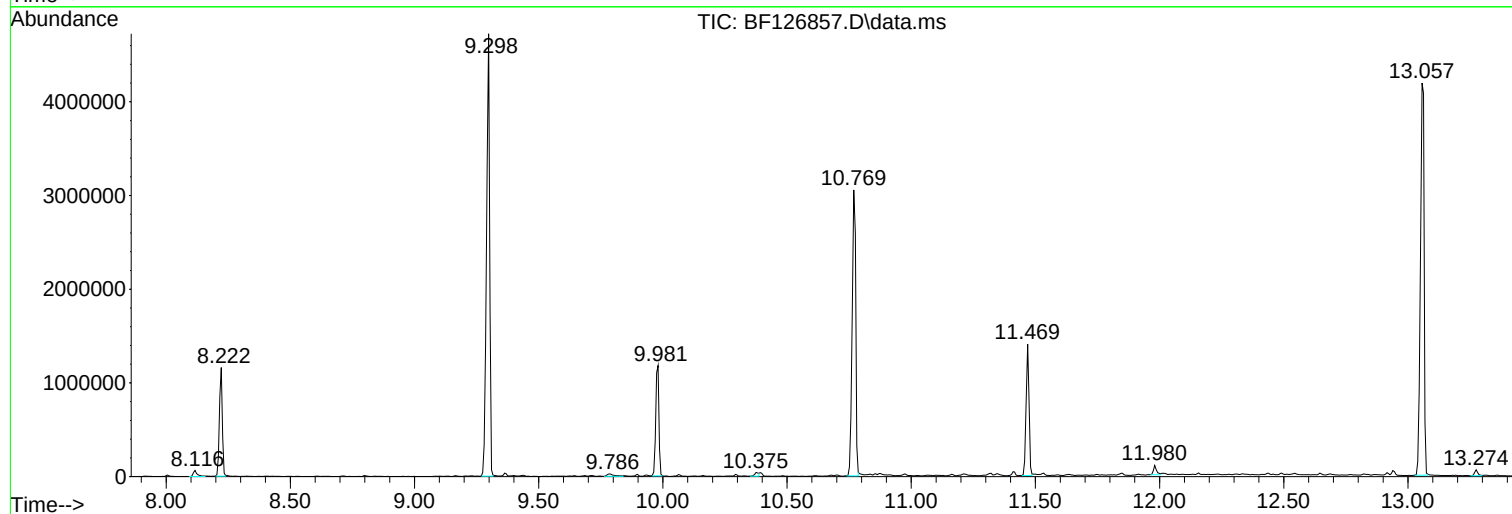
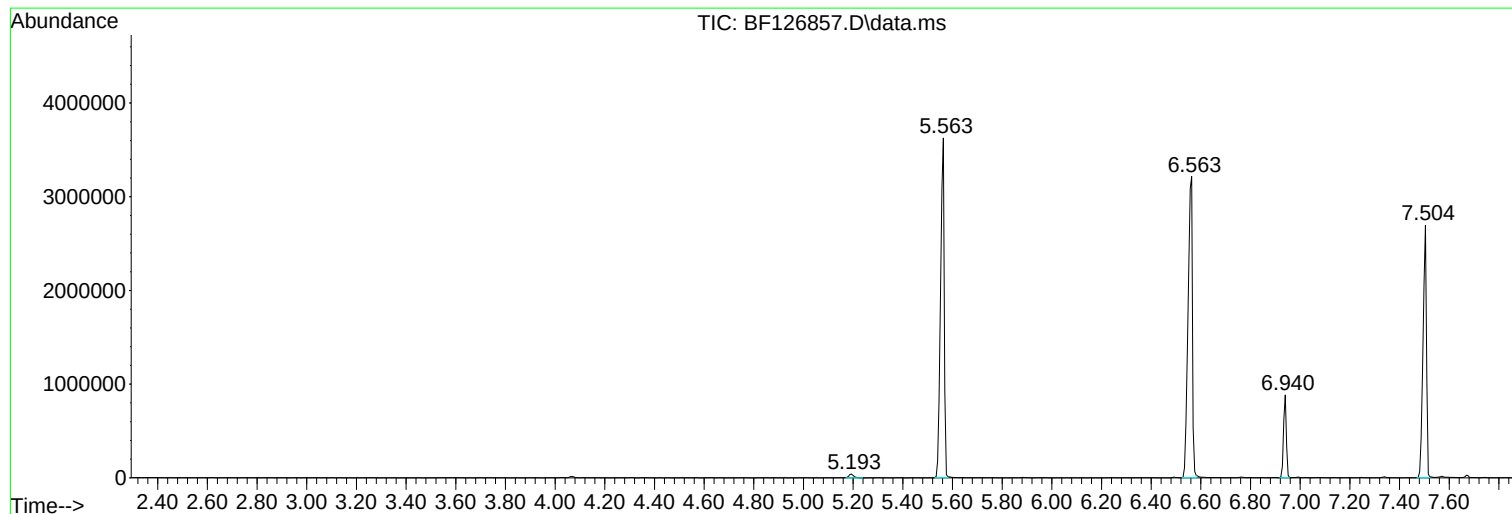
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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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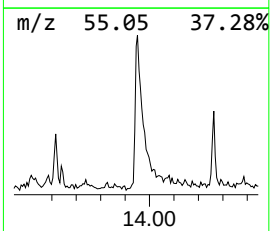
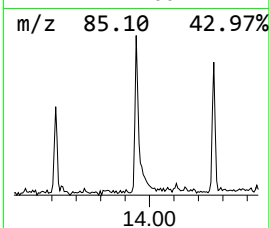
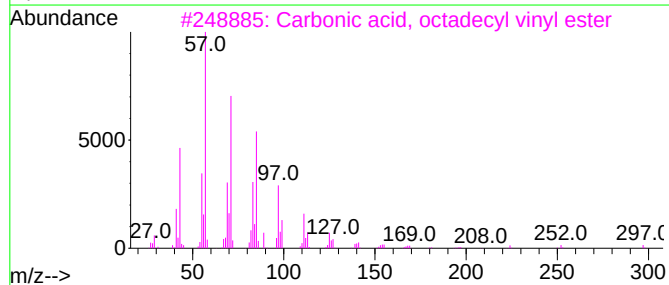
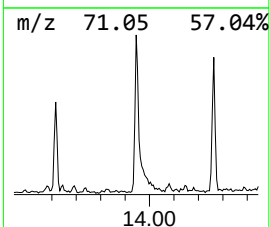
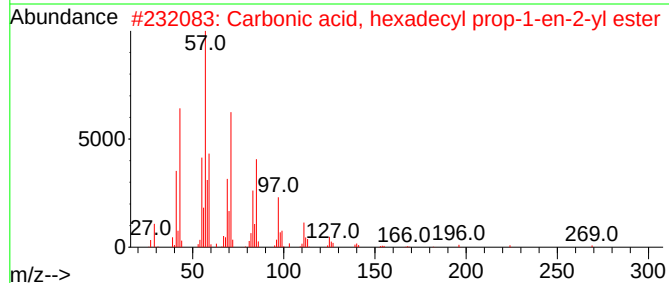
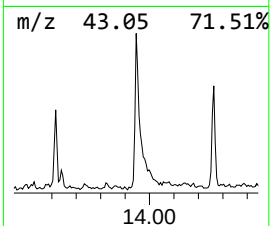
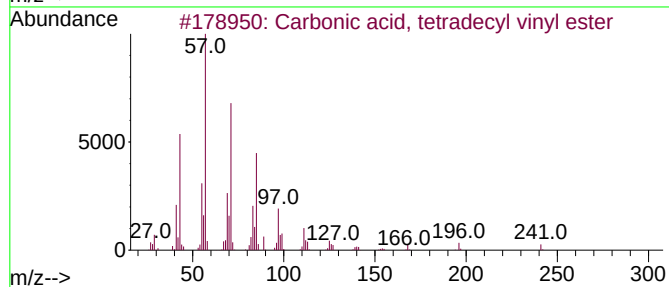
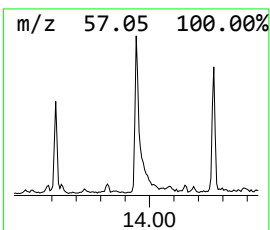
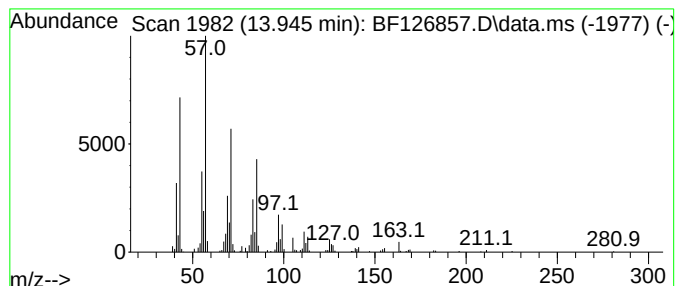
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Carbonic acid, tetradecyl v... Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 13.945 | 10.11 ng | 404523 | Chrysene-d12     | 14.110 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Carbonic acid, tetradecyl vinyl ... | 284 | C17H32O3 | 1000382-54-5 | 91   |
| 2    |    |   | Carbonic acid, hexadecyl prop-1-... | 326 | C20H38O3 | 1000382-90-3 | 90   |
| 3    |    |   | Carbonic acid, octadecyl vinyl e... | 340 | C21H40O3 | 1000382-54-4 | 90   |
| 4    |    |   | Carbonic acid, eicosyl vinyl ester  | 368 | C23H44O3 | 1000382-54-3 | 90   |
| 5    |    |   | Carbonic acid, tridecyl vinyl ester | 270 | C16H30O3 | 1000382-54-7 | 87   |



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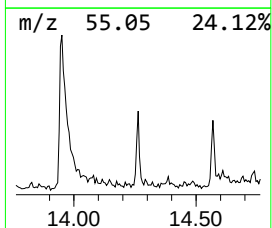
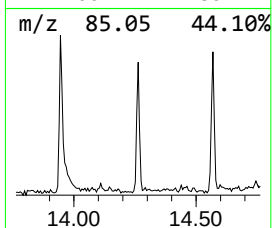
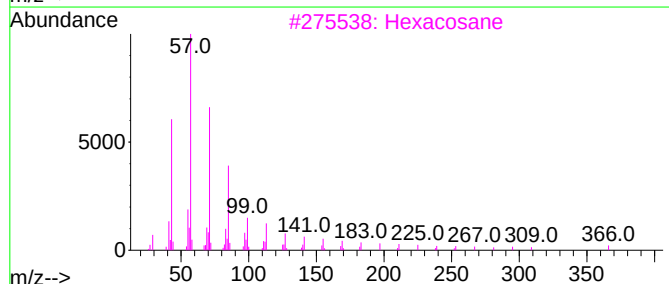
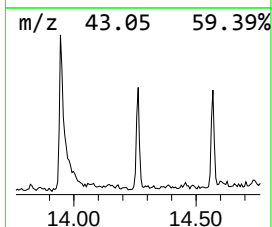
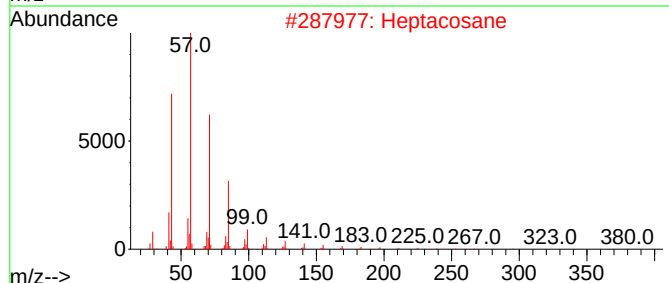
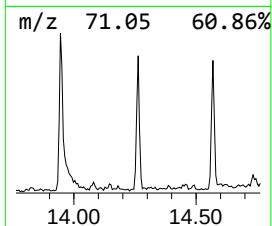
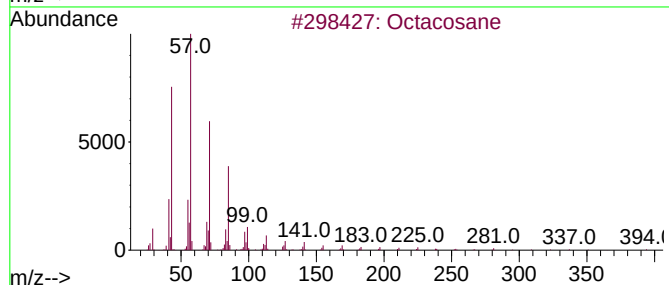
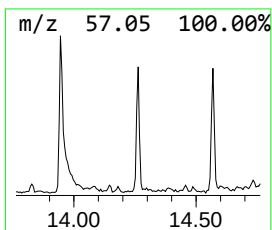
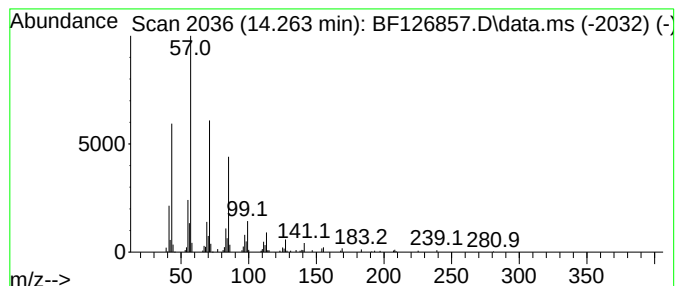
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Octacosane Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.263 | 2.64 ng | 105582 | Chrysene-d12     | 14.110 |

| Hit# | of 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|------|--------------|-----|---------|-------------|------|
| 1    |      | Octacosane   | 394 | C28H58  | 000630-02-4 | 91   |
| 2    |      | Heptacosane  | 380 | C27H56  | 000593-49-7 | 91   |
| 3    |      | Hexacosane   | 366 | C26H54  | 000630-01-3 | 91   |
| 4    |      | Octadecane   | 254 | C18H38  | 000593-45-3 | 91   |
| 5    |      | Nonadecane   | 268 | C19H40  | 000629-92-5 | 91   |



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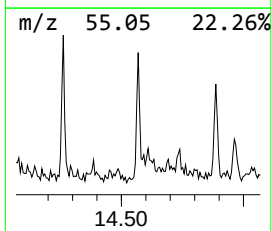
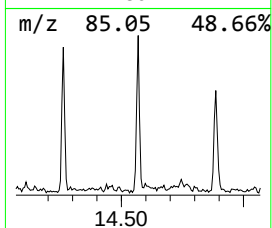
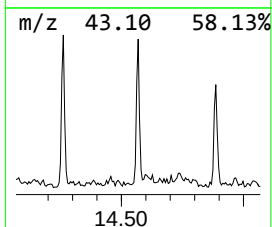
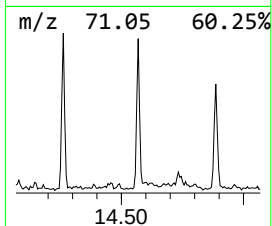
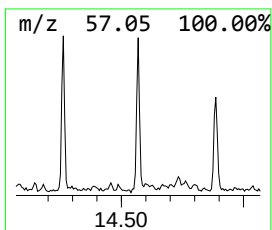
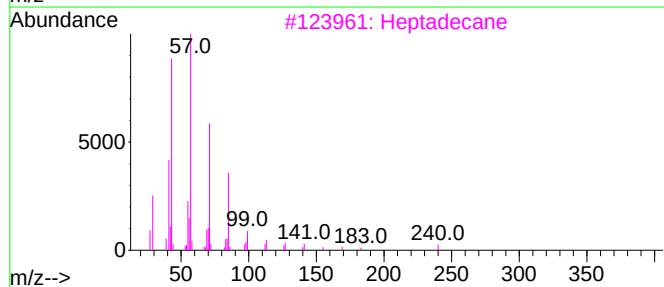
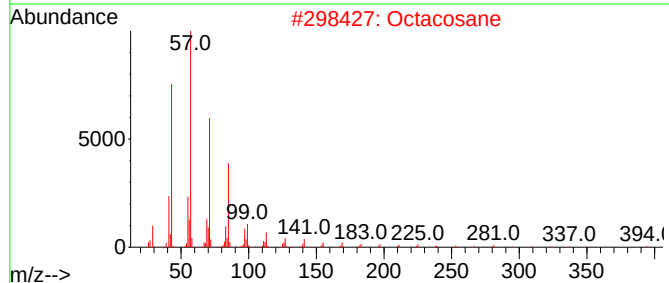
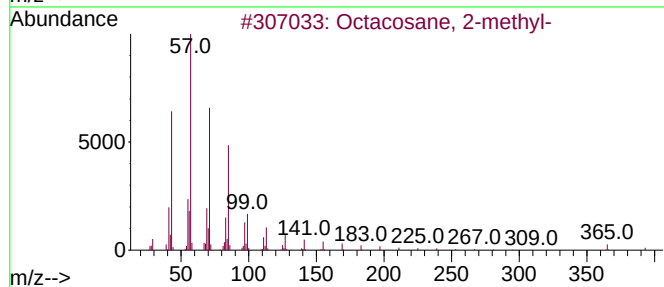
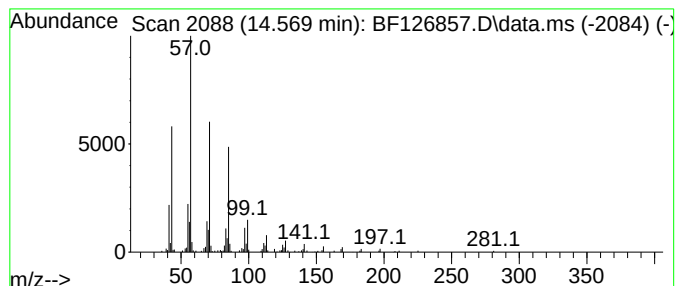
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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Peak Number 3 Octacosane, 2-methyl- Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.569 | 2.57 ng | 102860 | Chrysene-d12     | 14.110 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 91   |
| 2    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 91   |
| 3    |    |   | Heptadecane           | 240 | C17H36  | 000629-78-7 | 87   |
| 4    |    |   | Octadecane            | 254 | C18H38  | 000593-45-3 | 87   |
| 5    |    |   | Nonadecane            | 268 | C19H40  | 000629-92-5 | 87   |



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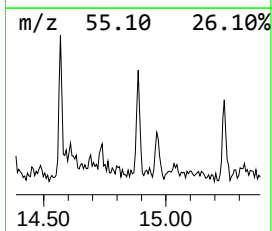
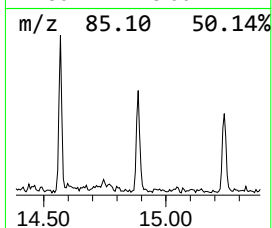
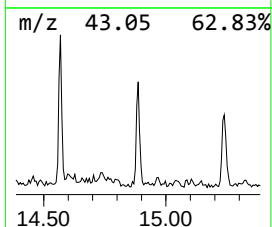
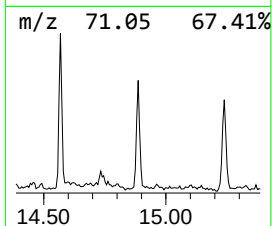
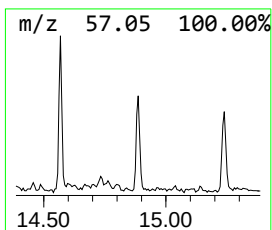
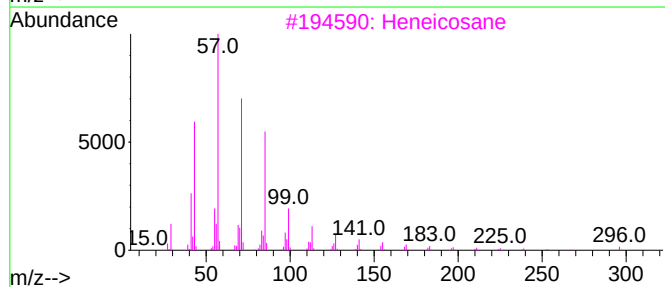
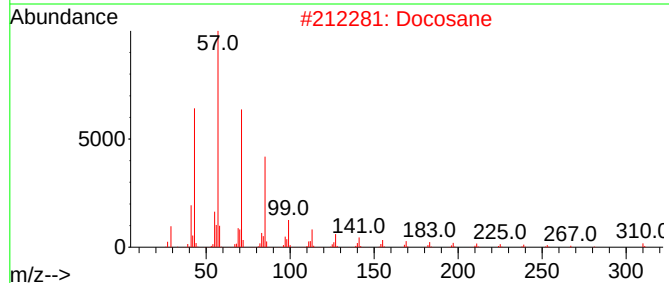
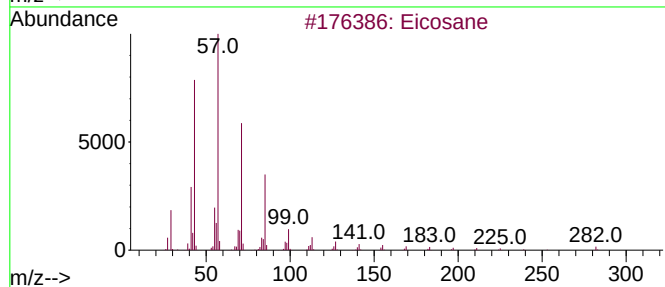
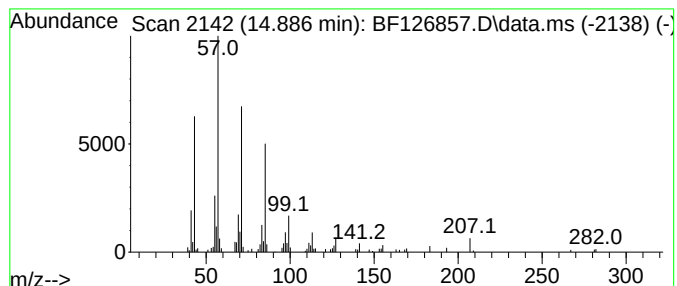
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TIC Library : C:\Database\NIST0.L  
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Peak Number 4 Eicosane Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.886 | 2.31 ng | 78567 | Perylene-d12     | 15.621 |

| Hit# | of | 5 | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------|-----|---------|-------------|------|
| 1    |    |   | Eicosane          | 282 | C20H42  | 000112-95-8 | 92   |
| 2    |    |   | Docosane          | 310 | C22H46  | 000629-97-0 | 86   |
| 3    |    |   | Heneicosane       | 296 | C21H44  | 000629-94-7 | 83   |
| 4    |    |   | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 80   |
| 5    |    |   | Octadecane        | 254 | C18H38  | 000593-45-3 | 80   |



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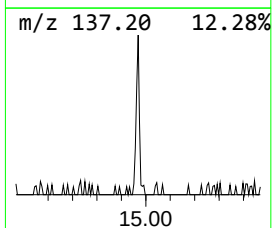
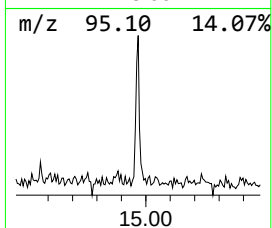
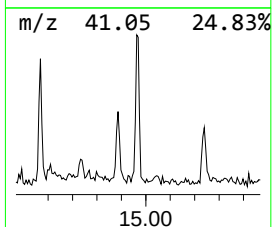
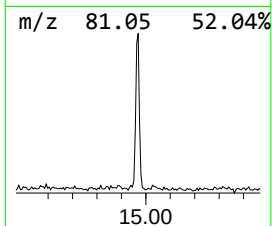
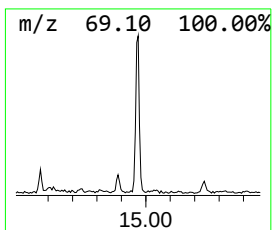
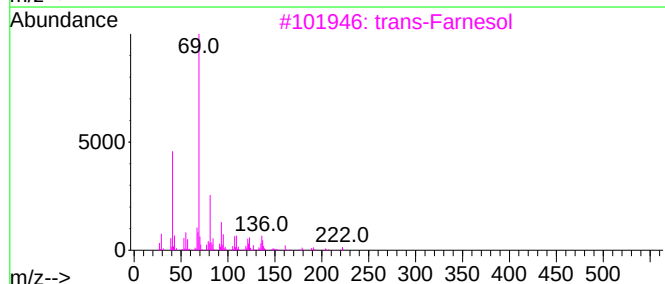
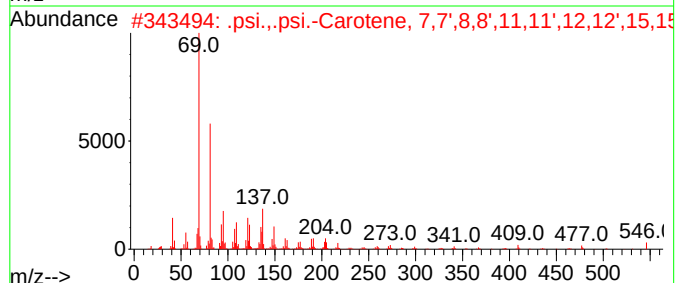
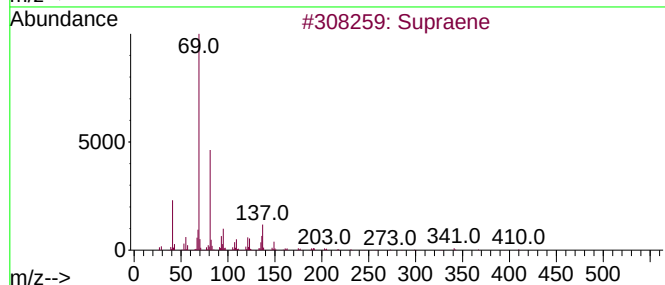
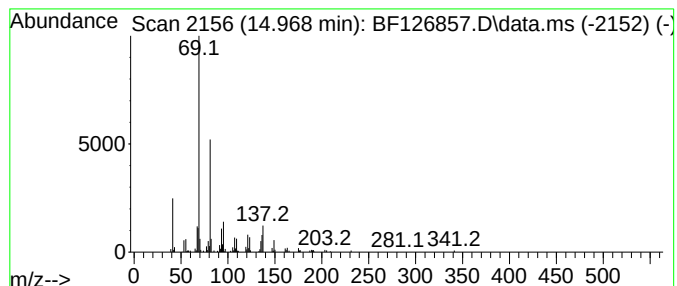
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Supraene Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.969 | 2.93 ng | 99903 | Perylene-d12     | 15.621 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50  | 007683-64-9 | 91   |
| 2    |    |   | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66  | 000502-62-5 | 83   |
| 3    |    |   | trans-Farnesol                      | 222 | C15H26O | 000106-28-5 | 72   |
| 4    |    |   | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 72   |
| 5    |    |   | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 004602-84-0 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF021122\  
Data File : BF126857.D  
Acq On : 11 Feb 2022 15:06  
Operator : CG\JU  
Sample : N1477-02  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20220080-BERKELEY-8-COMP

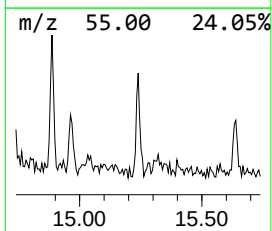
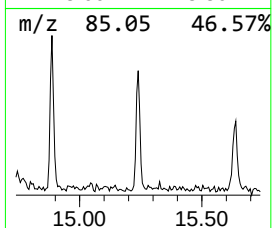
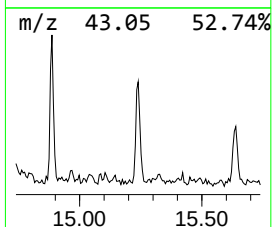
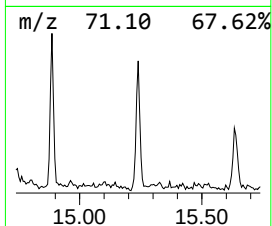
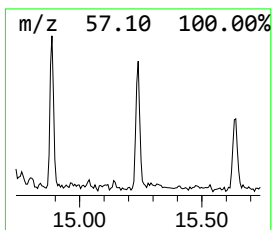
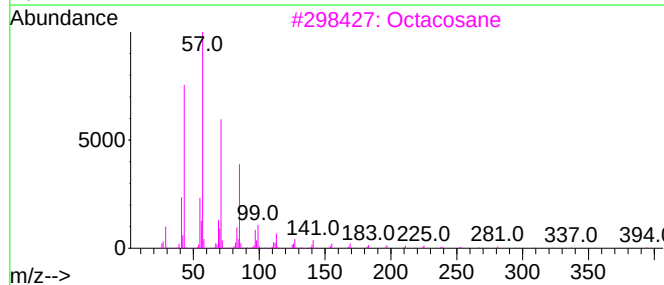
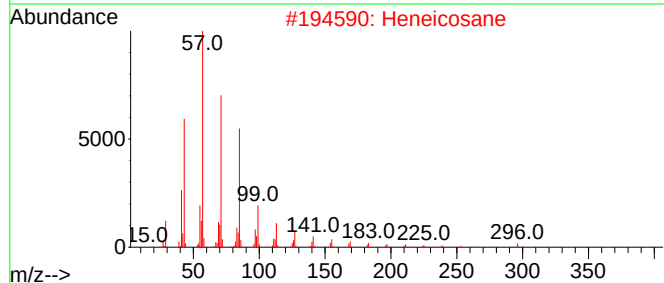
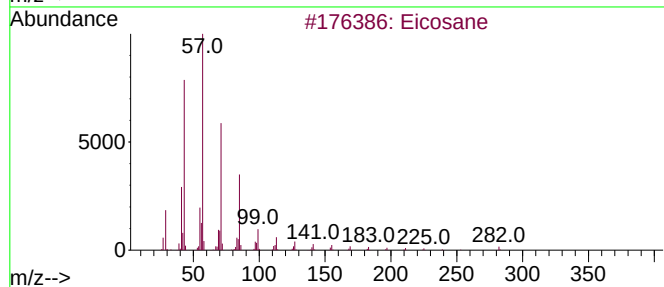
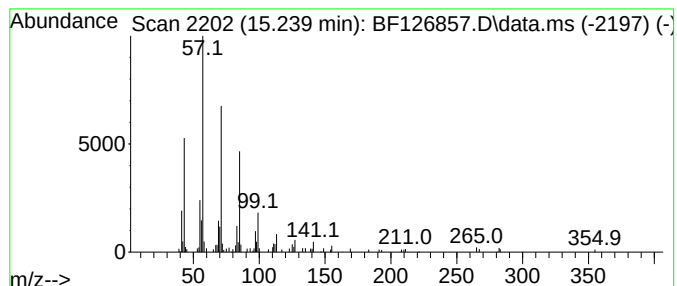
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 Heneicosane Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.239 | 2.40 ng | 81798 | Perylene-d12     | 15.621 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm | CAS#         | Qual |
|------|----|---|----------------------------|-----|---------|--------------|------|
| 1    |    |   | Eicosane                   | 282 | C20H42  | 000112-95-8  | 93   |
| 2    |    |   | Heneicosane                | 296 | C21H44  | 000629-94-7  | 90   |
| 3    |    |   | Octacosane                 | 394 | C28H58  | 000630-02-4  | 87   |
| 4    |    |   | 5-Ethyl-5-methylnonadecane | 310 | C22H46  | 1000360-42-7 | 86   |
| 5    |    |   | Octacosane, 2-methyl-      | 408 | C29H60  | 001560-98-1  | 86   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF021122\  
Data File : BF126857.D  
Acq On : 11 Feb 2022 15:06  
Operator : CG\JU  
Sample : N1477-02  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20220080-BERKELEY-8-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF020922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Carbonic acid, ... | 13.945 | 10.1    | ng    | 404523   | 5                     | 14.110 | 800380 | 20.0 |
| Octacosane         | 14.263 | 2.6     | ng    | 105582   | 5                     | 14.110 | 800380 | 20.0 |
| Octacosane, 2-m... | 14.569 | 2.6     | ng    | 102860   | 5                     | 14.110 | 800380 | 20.0 |
| Eicosane           | 14.886 | 2.3     | ng    | 78567    | 6                     | 15.621 | 681169 | 20.0 |
| Supraene           | 14.969 | 2.9     | ng    | 99903    | 6                     | 15.621 | 681169 | 20.0 |
| Heneicosane        | 15.239 | 2.4     | ng    | 81798    | 6                     | 15.621 | 681169 | 20.0 |