

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF092023\  
 Data File : BF135355.D  
 Acq On : 20 Sep 2023 13:59  
 Operator : CG\JU  
 Sample : 04493-01  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 WC-1

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135355.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         | 4.987       | 490           | 493         | 502          | rVB      | 43498          | 53830         | 2.15%           | 0.265%        |
| 2         | 5.387       | 557           | 561         | 572          | rBV      | 2383568        | 2369495       | 94.83%          | 11.644%       |
| 3         | 6.398       | 729           | 733         | 748          | rBV      | 2360144        | 2498597       | 100.00%         | 12.279%       |
| 4         | 6.757       | 790           | 794         | 805          | rVB      | 1063394        | 864290        | 34.59%          | 4.247%        |
| 5         | 7.122       | 852           | 856         | 859          | rVB      | 56101          | 45163         | 1.81%           | 0.222%        |
| 6         | 7.169       | 861           | 864         | 868          | rBV      | 55309          | 51678         | 2.07%           | 0.254%        |
| 7         | 7.322       | 883           | 890         | 893          | rBV      | 1650289        | 1565718       | 62.66%          | 7.694%        |
| 8         | 7.351       | 893           | 895         | 901          | rVB      | 108854         | 92508         | 3.70%           | 0.455%        |
| 9         | 8.034       | 1007          | 1011        | 1015         | rBV      | 1299142        | 1093523       | 43.77%          | 5.374%        |
| 10        | 9.116       | 1190          | 1195        | 1198         | rBV      | 2723186        | 2480162       | 99.26%          | 12.188%       |
| 11        | 9.234       | 1210          | 1215        | 1222         | rBV      | 41650          | 48967         | 1.96%           | 0.241%        |
| 12        | 9.792       | 1306          | 1310        | 1314         | rBV      | 1325395        | 1118082       | 44.75%          | 5.495%        |
| 13        | 10.198      | 1376          | 1379        | 1381         | rBV      | 29554          | 28017         | 1.12%           | 0.138%        |
| 14        | 10.586      | 1441          | 1445        | 1451         | rBV      | 1434585        | 1359147       | 54.40%          | 6.679%        |
| 15        | 11.128      | 1534          | 1537        | 1540         | rBV      | 165174         | 144989        | 5.80%           | 0.713%        |
| 16        | 11.239      | 1553          | 1556        | 1560         | rBV4     | 49261          | 58314         | 2.33%           | 0.287%        |
| 17        | 11.286      | 1560          | 1564        | 1566         | rVV      | 1168092        | 1080488       | 43.24%          | 5.310%        |
| 18        | 11.310      | 1566          | 1568        | 1572         | rVB      | 123534         | 110180        | 4.41%           | 0.541%        |
| 19        | 11.786      | 1646          | 1649        | 1652         | rBV2     | 133871         | 134374        | 5.38%           | 0.660%        |
| 20        | 11.822      | 1652          | 1655        | 1663         | rVB      | 539132         | 489355        | 19.59%          | 2.405%        |
| 21        | 12.504      | 1768          | 1771        | 1774         | rBV      | 263088         | 223166        | 8.93%           | 1.097%        |
| 22        | 12.610      | 1786          | 1789        | 1794         | rBV3     | 68474          | 79501         | 3.18%           | 0.391%        |
| 23        | 12.733      | 1805          | 1810        | 1813         | rBV      | 203547         | 193404        | 7.74%           | 0.950%        |
| 24        | 12.880      | 1831          | 1835        | 1838         | rBV      | 1918311        | 1585503       | 63.46%          | 7.792%        |
| 25        | 13.739      | 1979          | 1981        | 1986         | rVB      | 56616          | 54239         | 2.17%           | 0.267%        |
| 26        | 13.792      | 1987          | 1990        | 1994         | rVB      | 42535          | 40199         | 1.61%           | 0.198%        |
| 27        | 13.857      | 1996          | 2001        | 2010         | rBV5     | 57706          | 177327        | 7.10%           | 0.871%        |
| 28        | 13.939      | 2010          | 2015        | 2018         | rVV      | 753425         | 791760        | 31.69%          | 3.891%        |
| 29        | 13.963      | 2018          | 2019        | 2026         | rVB      | 111256         | 103510        | 4.14%           | 0.509%        |
| 30        | 14.551      | 2117          | 2119        | 2122         | rVB      | 37774          | 30501         | 1.22%           | 0.150%        |
| 31        | 14.716      | 2145          | 2147        | 2151         | rBV4     | 19084          | 27961         | 1.12%           | 0.137%        |
| 32        | 14.863      | 2170          | 2172        | 2177         | rVB5     | 25752          | 30991         | 1.24%           | 0.152%        |
| 33        | 14.980      | 2188          | 2192        | 2195         | rBV      | 114393         | 162040        | 6.49%           | 0.796%        |
| 34        | 15.057      | 2202          | 2205        | 2208         | rVB2     | 27610          | 29356         | 1.17%           | 0.144%        |
| 35        | 15.280      | 2239          | 2243        | 2250         | rVB      | 71134          | 93409         | 3.74%           | 0.459%        |
| 36        | 15.345      | 2250          | 2254        | 2260         | rVB      | 88186          | 111080        | 4.45%           | 0.546%        |

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Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-1

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-BF091123.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 15.404 | 2260 | 2264 | 2269 | rBV  | 635185 | 838473 | 33.56% | 4.121% |
| 38 | 16.886 | 2512 | 2516 | 2523 | rVB3 | 46690  | 89490  | 3.58%  | 0.440% |

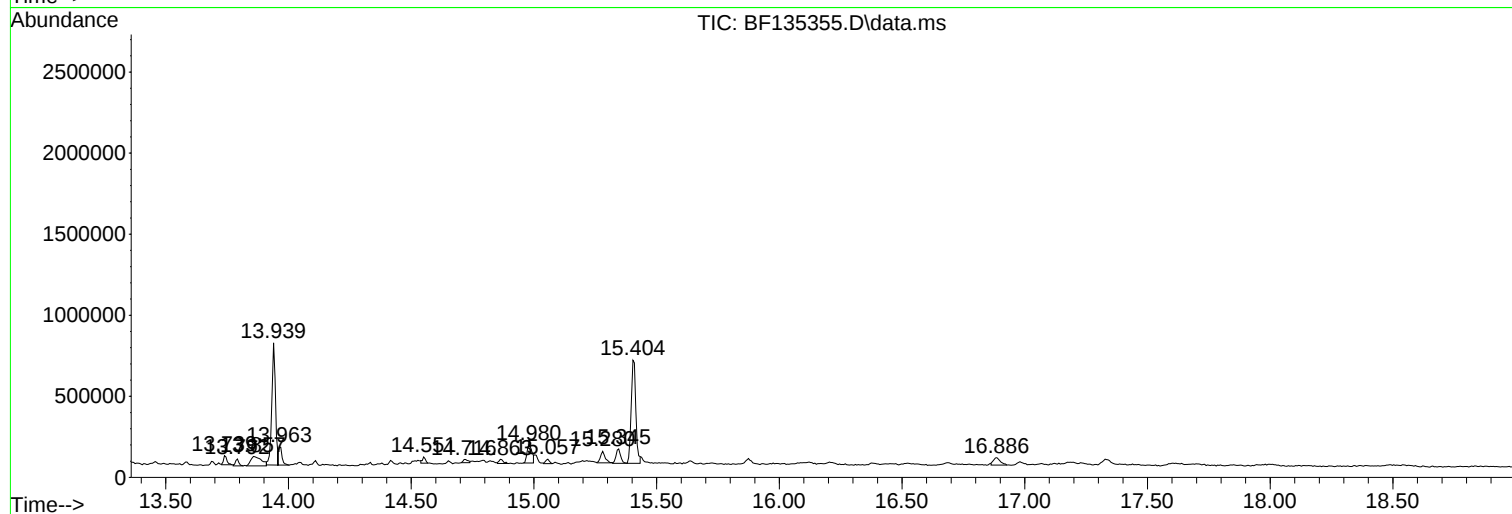
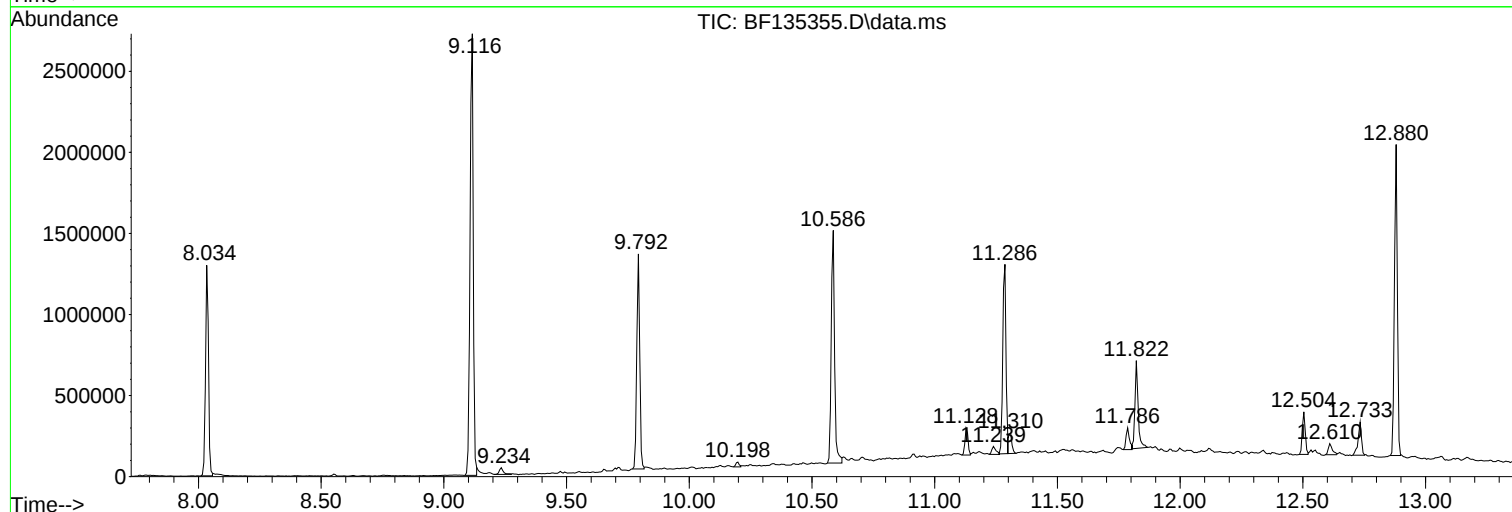
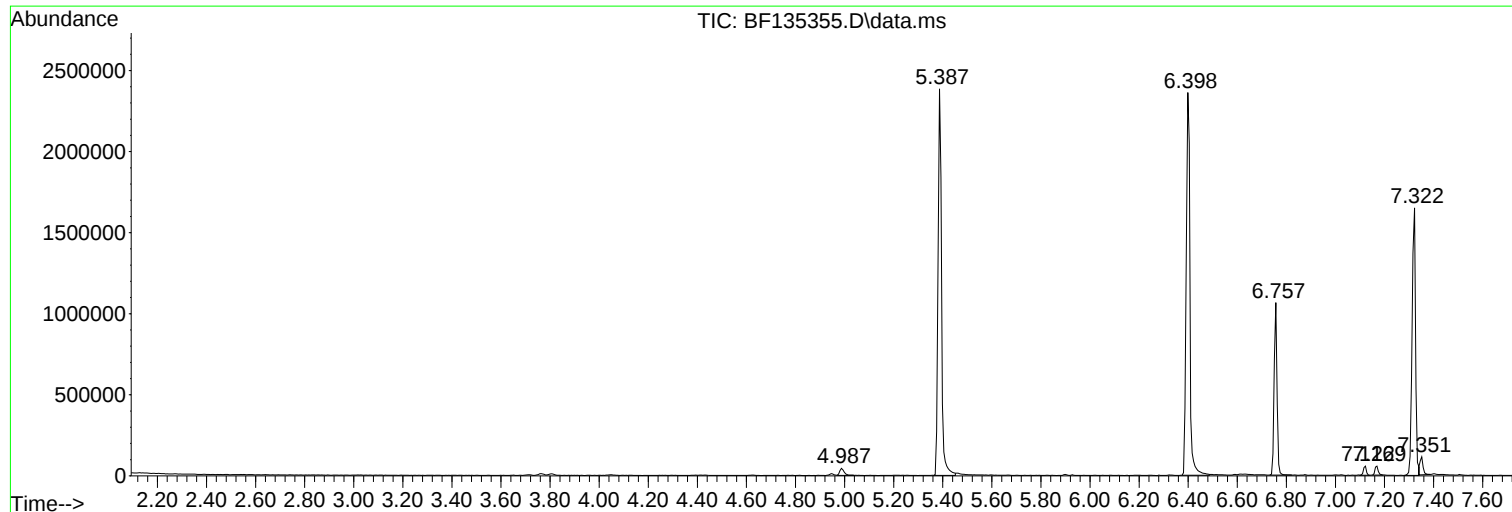
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : 04493-01  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-1

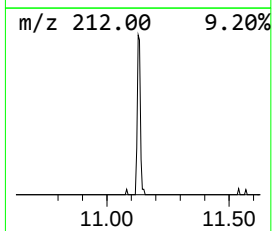
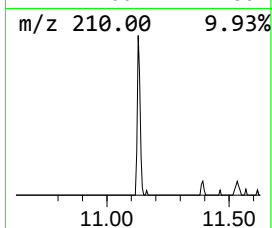
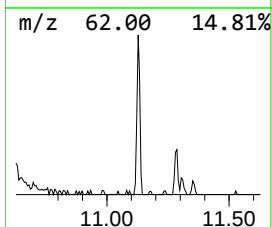
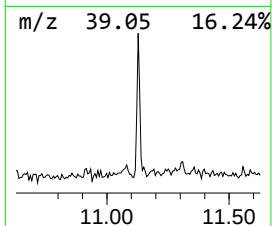
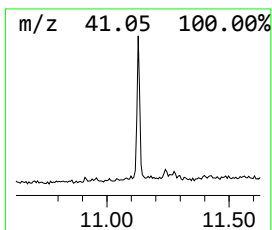
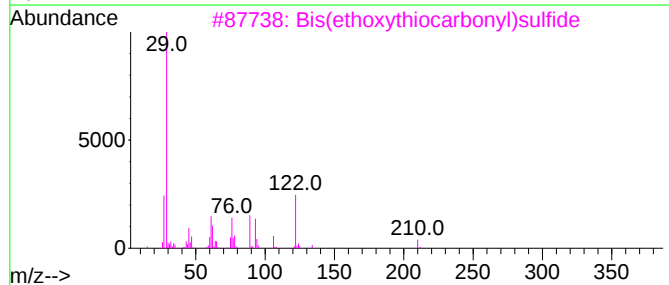
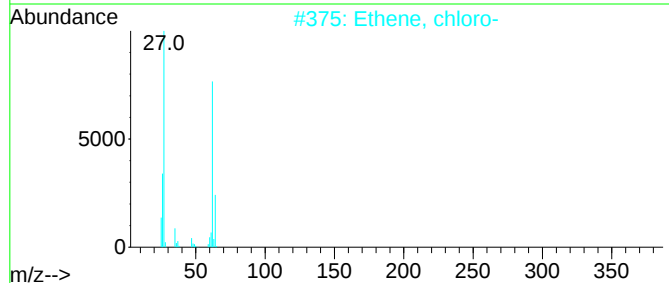
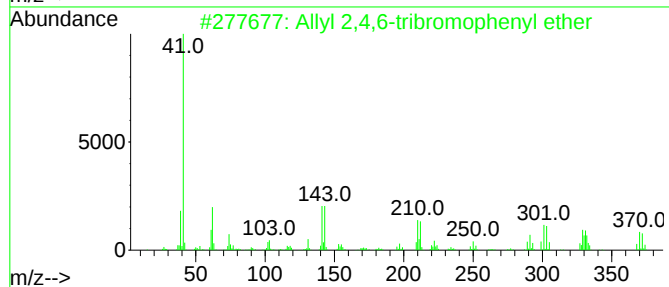
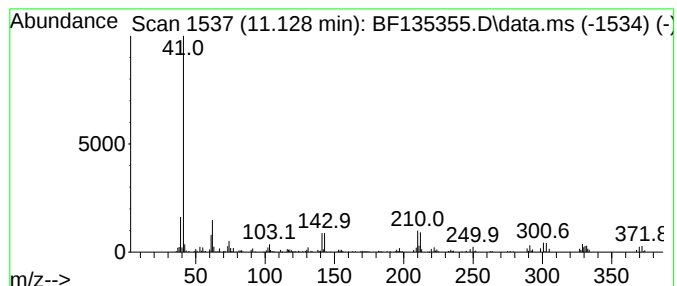
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Allyl 2,4,6-tribromophenyl ... Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.128 | 2.68 ng | 144989 | Phenanthrene-d10 | 11.286 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm   | CAS#        | Qual |
|------|----|---|----------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Allyl 2,4,6-tribromophenyl ether | 368 | C9H7Br3O  | 003278-89-5 | 95   |
| 2    |    |   | Ethene, chloro-                  | 62  | C2H3Cl    | 000075-01-4 | 5    |
| 3    |    |   | Bis(ethoxythiocarbonyl)sulfide   | 210 | C6H10O2S3 | 002905-52-4 | 4    |
| 4    |    |   | Ethanamine, 2-(methylthio)-      | 91  | C3H9NS    | 018542-42-2 | 4    |
| 5    |    |   | tert-Butyl carbamate             | 117 | C5H11NO2  | 004248-19-5 | 4    |



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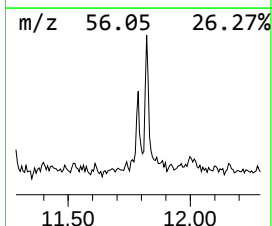
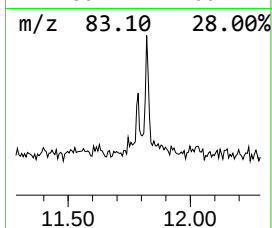
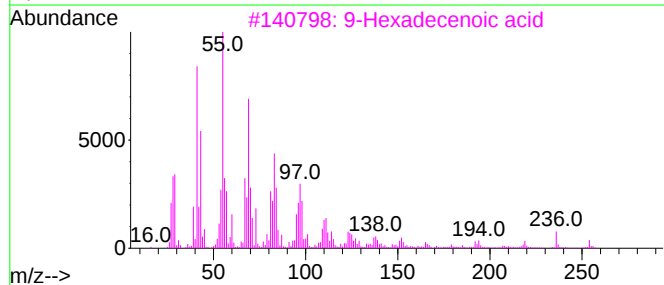
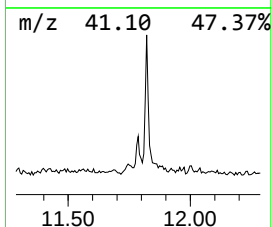
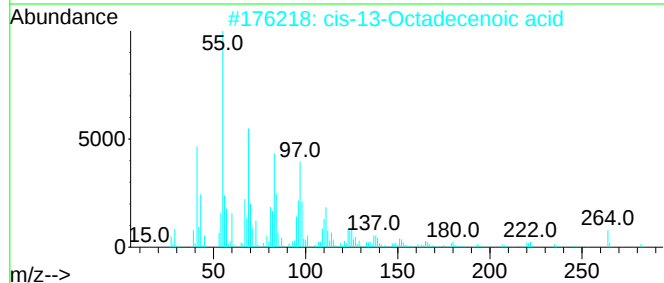
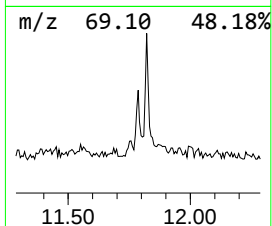
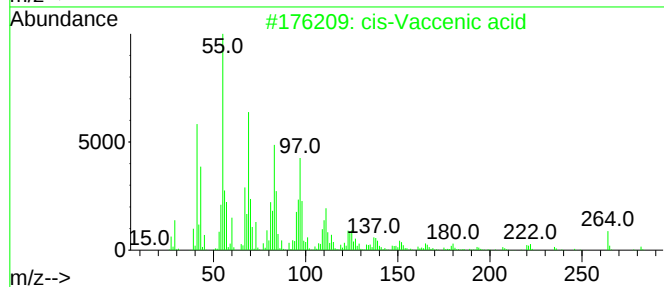
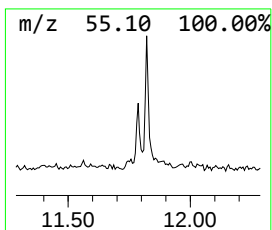
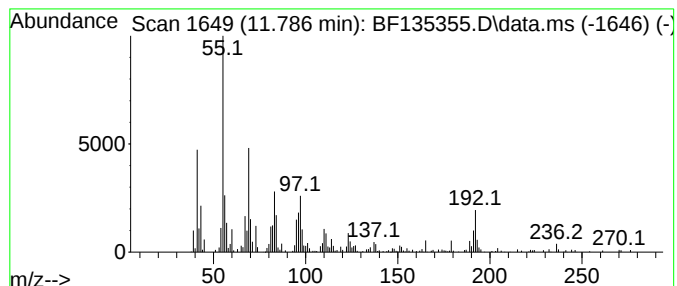
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 cis-Vaccenic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.786 | 2.49 ng | 134374 | Phenanthrene-d10 | 11.286 |

| Hit# | of | 5 | Tentative ID             | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------|-----|----------|-------------|------|
| 1    |    |   | cis-Vaccenic acid        | 282 | C18H34O2 | 000506-17-2 | 52   |
| 2    |    |   | cis-13-Octadecenoic acid | 282 | C18H34O2 | 013126-39-1 | 52   |
| 3    |    |   | 9-Hexadecenoic acid      | 254 | C16H30O2 | 002091-29-4 | 49   |
| 4    |    |   | cis-7-Hexadecenoic acid  | 254 | C16H30O2 | 002416-19-5 | 49   |
| 5    |    |   | Palmitoleic acid         | 254 | C16H30O2 | 000373-49-9 | 47   |



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Instrument :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

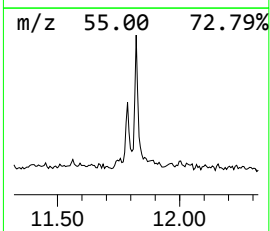
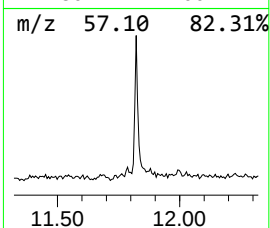
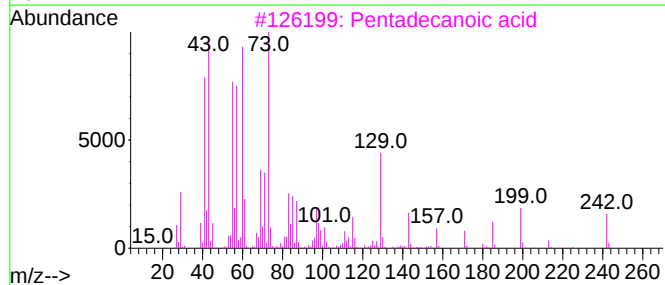
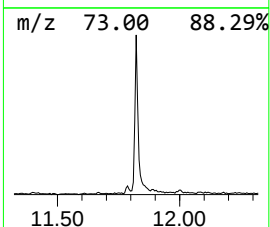
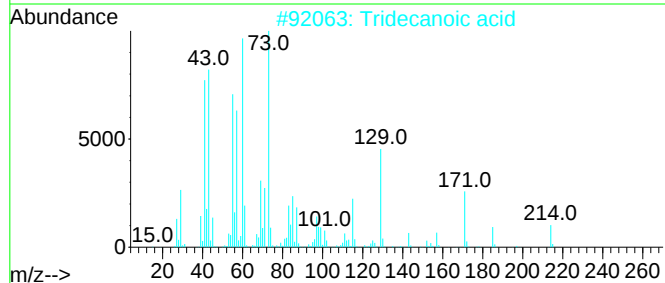
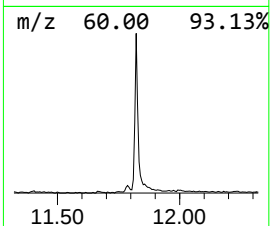
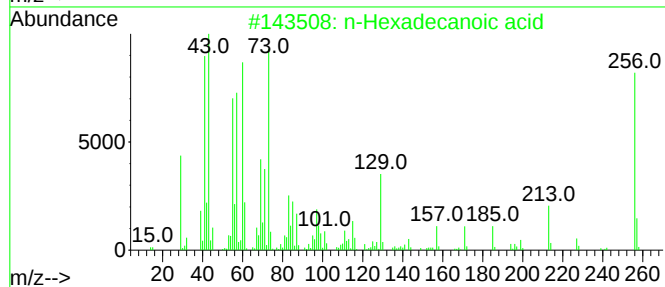
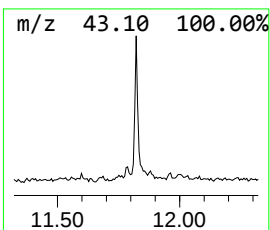
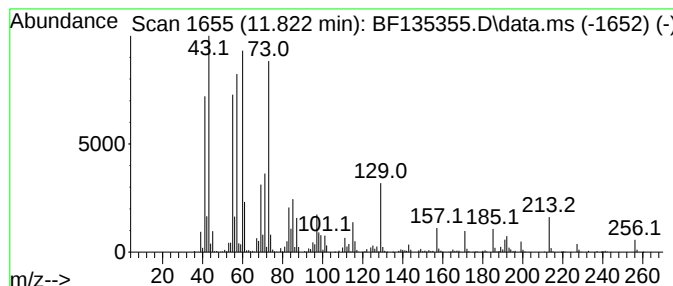
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.822 | 9.06 ng | 489355 | Phenanthrene-d10 | 11.286 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 93   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 86   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 76   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

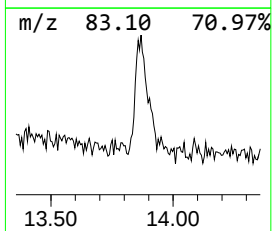
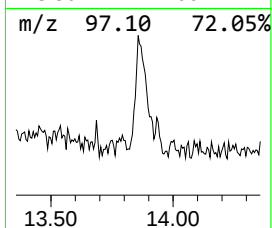
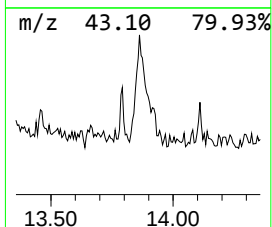
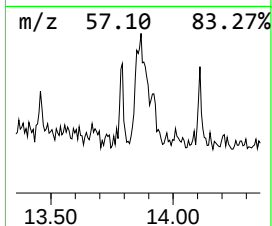
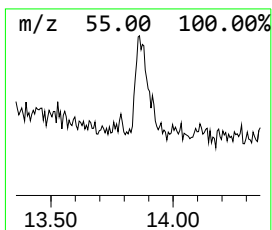
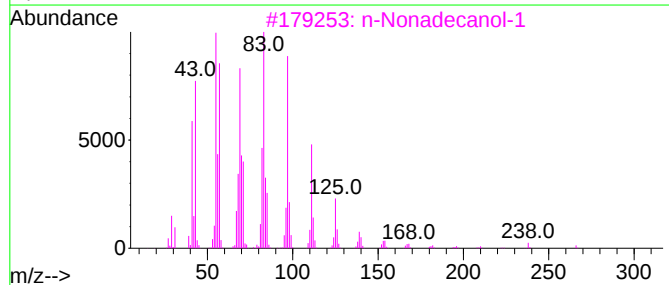
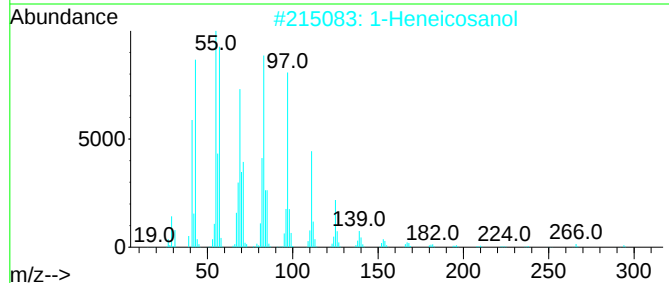
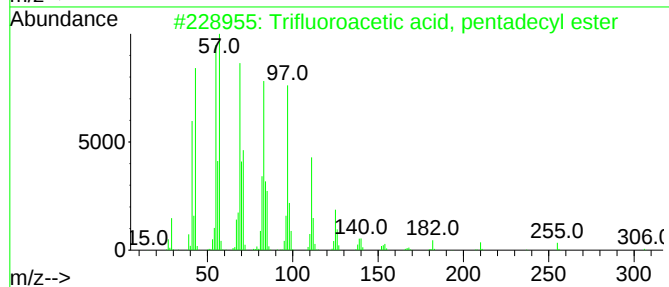
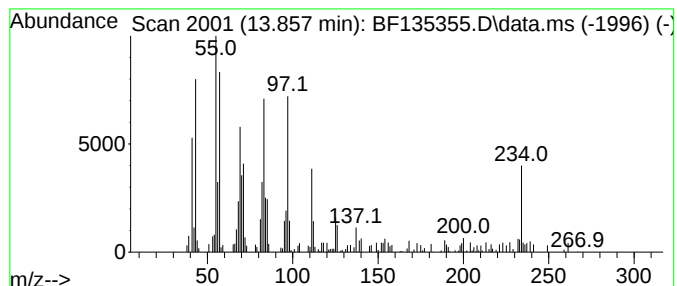
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.857 | 4.48 ng | 177327 | Chrysene-d12     | 13.939 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 93   |
| 2    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 93   |
| 3    |    |   | n-Nonadecanol-1                     | 284 | C19H40O    | 001454-84-8 | 93   |
| 4    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2 | 006222-03-3 | 93   |
| 5    |    |   | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 93   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF092023\  
Data File : BF135355.D  
Acq On : 20 Sep 2023 13:59  
Operator : CG\JU  
Sample : 04493-01  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-1

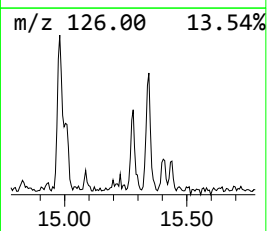
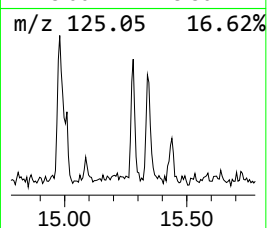
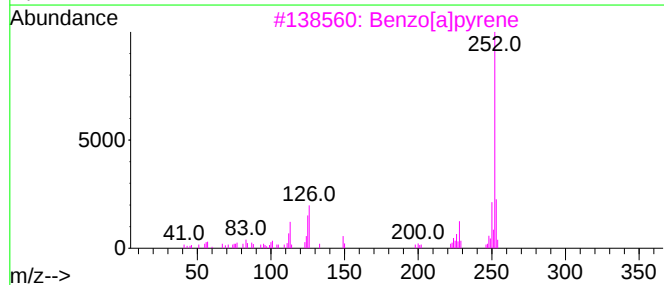
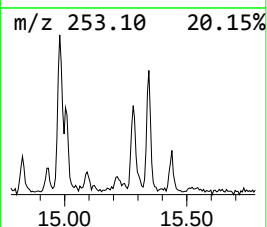
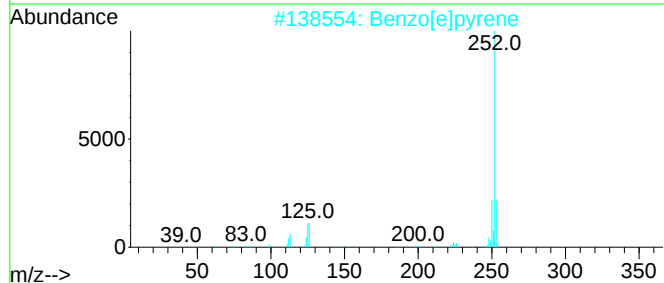
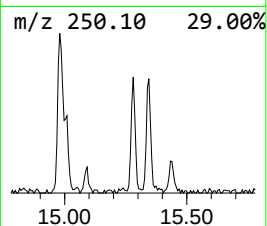
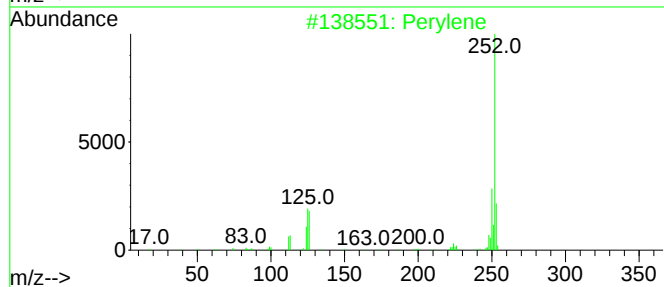
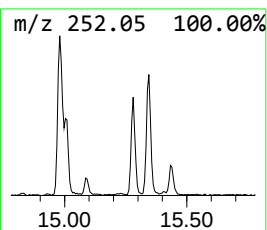
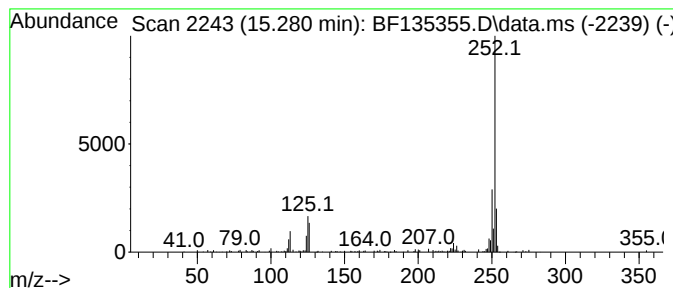
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 Perylene Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.280 | 2.23 ng | 93409 | Perylene-d12     | 15.410 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Perylene             | 252 | C20H12  | 000198-55-0 | 98   |
| 2    |    |   | Benzo[e]pyrene       | 252 | C20H12  | 000192-97-2 | 95   |
| 3    |    |   | Benzo[a]pyrene       | 252 | C20H12  | 000050-32-8 | 93   |
| 4    |    |   | Benzo[k]fluoranthene | 252 | C20H12  | 000207-08-9 | 91   |
| 5    |    |   | Benzo[b]fluoranthene | 252 | C20H12  | 000205-99-2 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF092023\  
Data File : BF135355.D  
Acq On : 20 Sep 2023 13:59  
Operator : CG\JU  
Sample : 04493-01  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-1

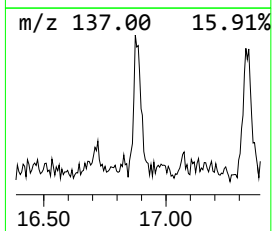
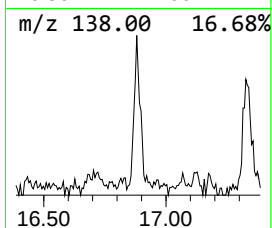
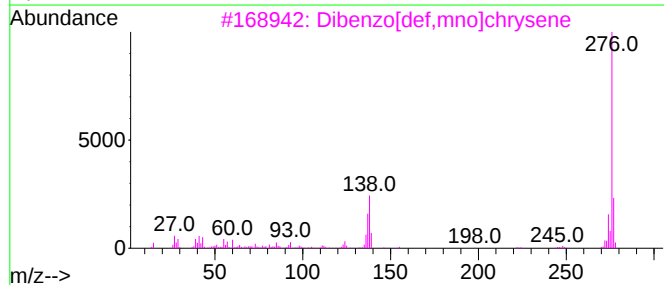
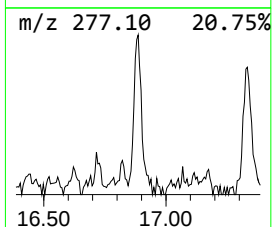
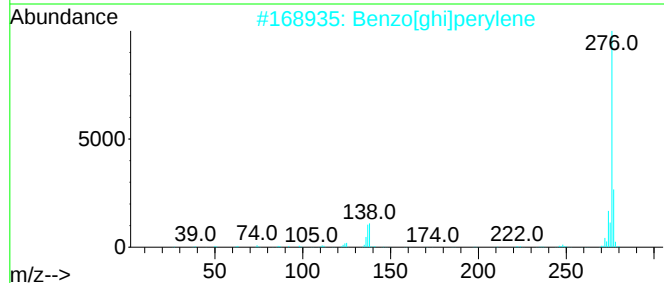
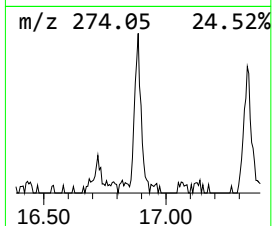
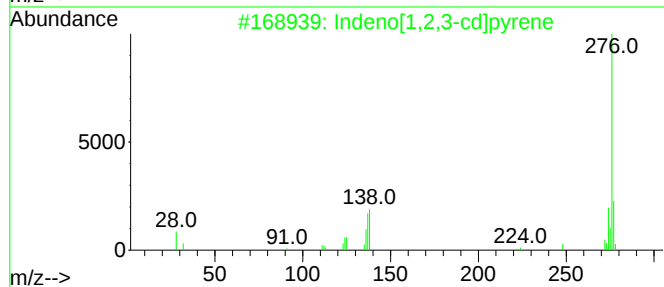
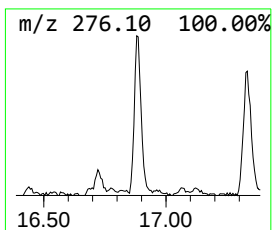
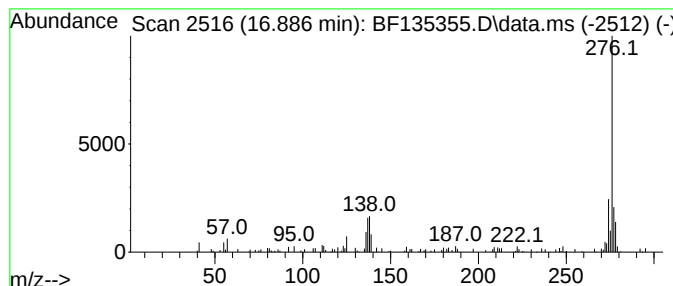
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Dibenzo[def,mno]chrysene Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 16.886 | 2.13 ng | 89490 | Perylene-d12     | 15.410 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Indeno[1,2,3-cd]pyrene              | 276 | C22H12     | 000193-39-5 | 93   |
| 2    |    |   | Benzo[ghi]perylene                  | 276 | C22H12     | 000191-24-2 | 93   |
| 3    |    |   | Dibenzo[def,mno]chrysene            | 276 | C22H12     | 000191-26-4 | 90   |
| 4    |    |   | Indeno[1,2,3-cd]fluoranthene        | 276 | C22H12     | 000193-43-1 | 74   |
| 5    |    |   | 4-(2-(3-Nitrophenyl)ethenyl)quin... | 276 | C17H12N2O2 | 074839-90-0 | 47   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF092023\  
Data File : BF135355.D  
Acq On : 20 Sep 2023 13:59  
Operator : CG\JU  
Sample : 04493-01  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.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 |
| Allyl 2,4,6-tri... | 11.128 | 2.7     | ng    | 144989   | 4                     | 11.286 | 1080490 | 20.0 |
| cis-Vaccenic acid  | 11.786 | 2.5     | ng    | 134374   | 4                     | 11.286 | 1080490 | 20.0 |
| n-Hexadecanoic ... | 11.822 | 9.1     | ng    | 489355   | 4                     | 11.286 | 1080490 | 20.0 |
| Trifluoroacetic... | 13.857 | 4.5     | ng    | 177327   | 5                     | 13.939 | 791760  | 20.0 |
| Perylene           | 15.280 | 2.2     | ng    | 93409    | 6                     | 15.410 | 838473  | 20.0 |
| Dibenzo[def,mno... | 16.886 | 2.1     | ng    | 89490    | 6                     | 15.410 | 838473  | 20.0 |