

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF091124\  
 Data File : BF139338.D  
 Acq On : 11 Sep 2024 20:55  
 Operator : RC/JU  
 Sample : P3930-02  
 Misc :  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 DN-B-34

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-BF090424.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139338.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         | 2.157       | 4             | 11          | 18           | rVB      | 205123         | 311473        | 51.28%          | 5.771%        |
| 2         | 5.087       | 504           | 509         | 515          | rVB      | 19289          | 24717         | 4.07%           | 0.458%        |
| 3         | 5.492       | 573           | 578         | 586          | rBB      | 195595         | 241379        | 39.74%          | 4.472%        |
| 4         | 6.504       | 745           | 750         | 760          | rVB      | 252209         | 316401        | 52.10%          | 5.863%        |
| 5         | 6.887       | 809           | 815         | 820          | rBV      | 362543         | 461802        | 76.04%          | 8.557%        |
| 6         | 7.439       | 902           | 909         | 914          | rBV      | 158566         | 197186        | 32.47%          | 3.654%        |
| 7         | 8.163       | 1027          | 1032        | 1041         | rVB      | 391468         | 504787        | 83.11%          | 9.353%        |
| 8         | 9.239       | 1210          | 1215        | 1220         | rBV      | 246534         | 305976        | 50.38%          | 5.669%        |
| 9         | 9.916       | 1325          | 1330        | 1336         | rBV      | 406592         | 519146        | 85.48%          | 9.619%        |
| 10        | 10.627      | 1446          | 1451        | 1459         | rBV      | 17213          | 21239         | 3.50%           | 0.394%        |
| 11        | 10.704      | 1459          | 1464        | 1469         | rBV      | 150915         | 186061        | 30.64%          | 3.447%        |
| 12        | 10.827      | 1480          | 1485        | 1491         | rVB5     | 3495           | 6695          | 1.10%           | 0.124%        |
| 13        | 11.404      | 1578          | 1583        | 1590         | rBV      | 484273         | 607347        | 100.00%         | 11.253%       |
| 14        | 11.457      | 1590          | 1592        | 1599         | rVB4     | 3955           | 7226          | 1.19%           | 0.134%        |
| 15        | 11.927      | 1663          | 1672        | 1677         | rBV2     | 28749          | 44361         | 7.30%           | 0.822%        |
| 16        | 12.104      | 1697          | 1702        | 1706         | rBV4     | 5010           | 7475          | 1.23%           | 0.139%        |
| 17        | 12.616      | 1785          | 1789        | 1793         | rBV      | 35700          | 49751         | 8.19%           | 0.922%        |
| 18        | 12.710      | 1802          | 1805        | 1810         | rBV5     | 12099          | 17427         | 2.87%           | 0.323%        |
| 19        | 12.845      | 1823          | 1828        | 1835         | rBV      | 28391          | 43726         | 7.20%           | 0.810%        |
| 20        | 12.986      | 1847          | 1852        | 1862         | rVB      | 288360         | 373510        | 61.50%          | 6.921%        |
| 21        | 13.074      | 1863          | 1867        | 1868         | rBV3     | 7737           | 10268         | 1.69%           | 0.190%        |
| 22        | 13.274      | 1898          | 1901        | 1904         | rBV4     | 7159           | 10680         | 1.76%           | 0.198%        |
| 23        | 13.468      | 1931          | 1934        | 1938         | rVB3     | 6860           | 8201          | 1.35%           | 0.152%        |
| 24        | 13.527      | 1940          | 1944        | 1948         | rVV      | 32708          | 40179         | 6.62%           | 0.744%        |
| 25        | 13.892      | 2002          | 2006        | 2013         | rBV4     | 19202          | 43650         | 7.19%           | 0.809%        |
| 26        | 14.039      | 2025          | 2031        | 2040         | rBV      | 247176         | 387400        | 63.79%          | 7.178%        |
| 27        | 15.168      | 2219          | 2223        | 2227         | rBV      | 45410          | 61875         | 10.19%          | 1.146%        |
| 28        | 15.339      | 2242          | 2252        | 2256         | rBV10    | 33544          | 137811        | 22.69%          | 2.553%        |
| 29        | 15.515      | 2277          | 2282        | 2293         | rVB      | 240201         | 379344        | 62.46%          | 7.029%        |
| 30        | 15.998      | 2360          | 2364        | 2368         | rBV      | 21946          | 36263         | 5.97%           | 0.672%        |
| 31        | 16.809      | 2497          | 2502        | 2508         | rBV3     | 16755          | 33638         | 5.54%           | 0.623%        |

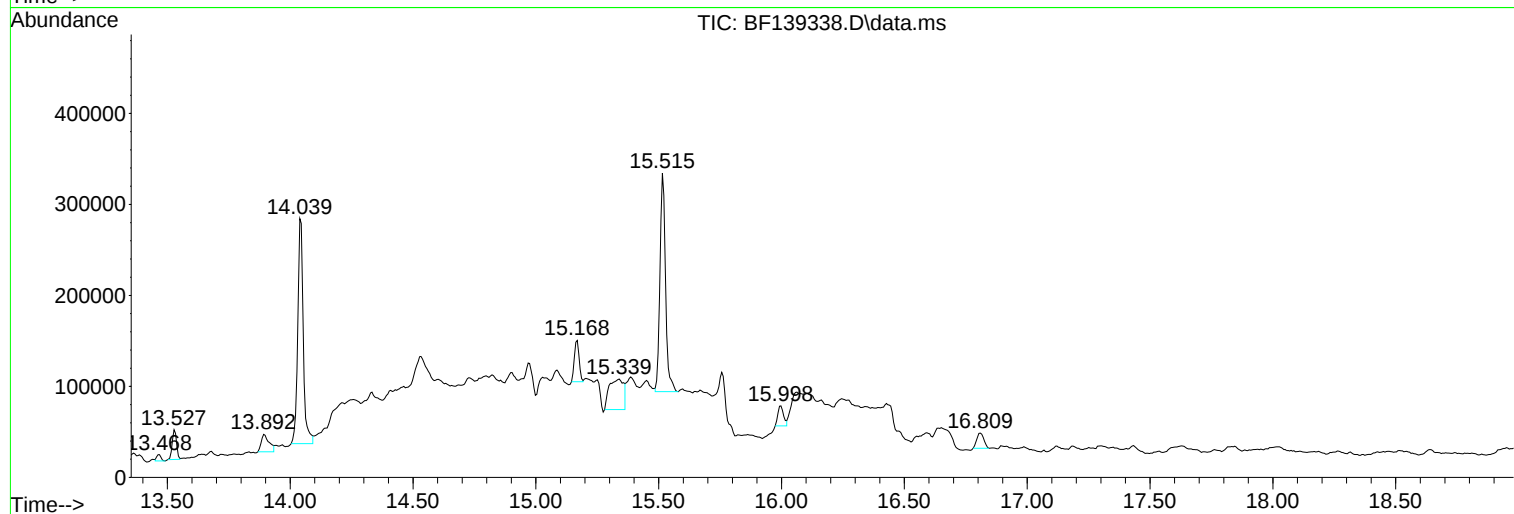
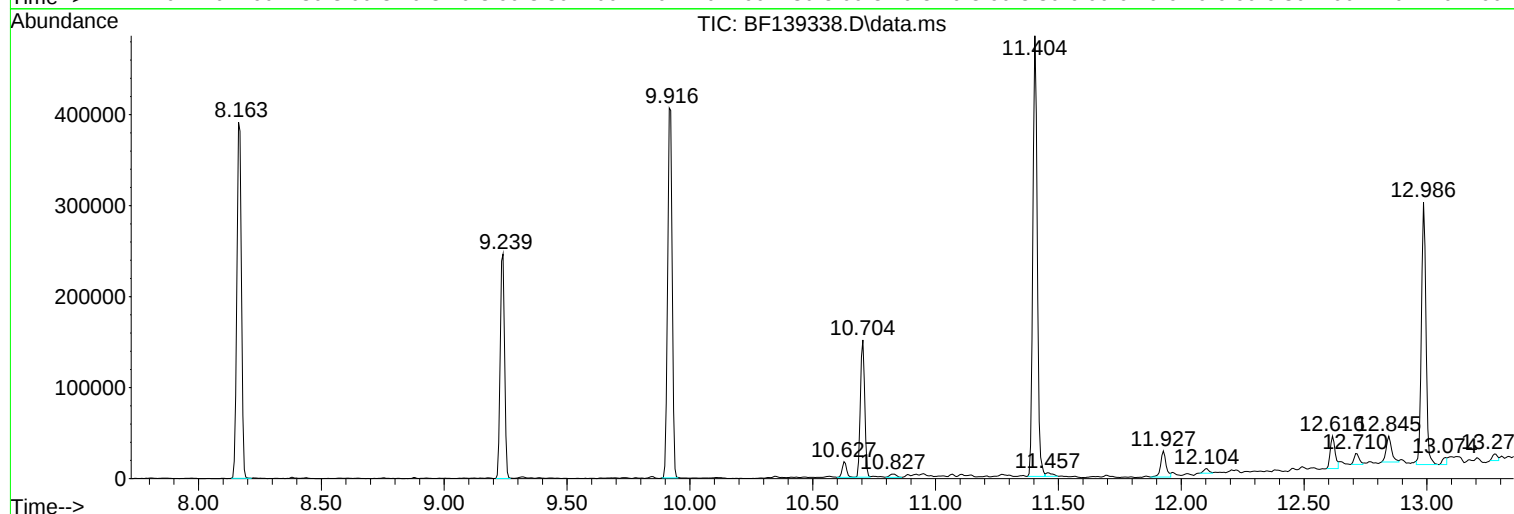
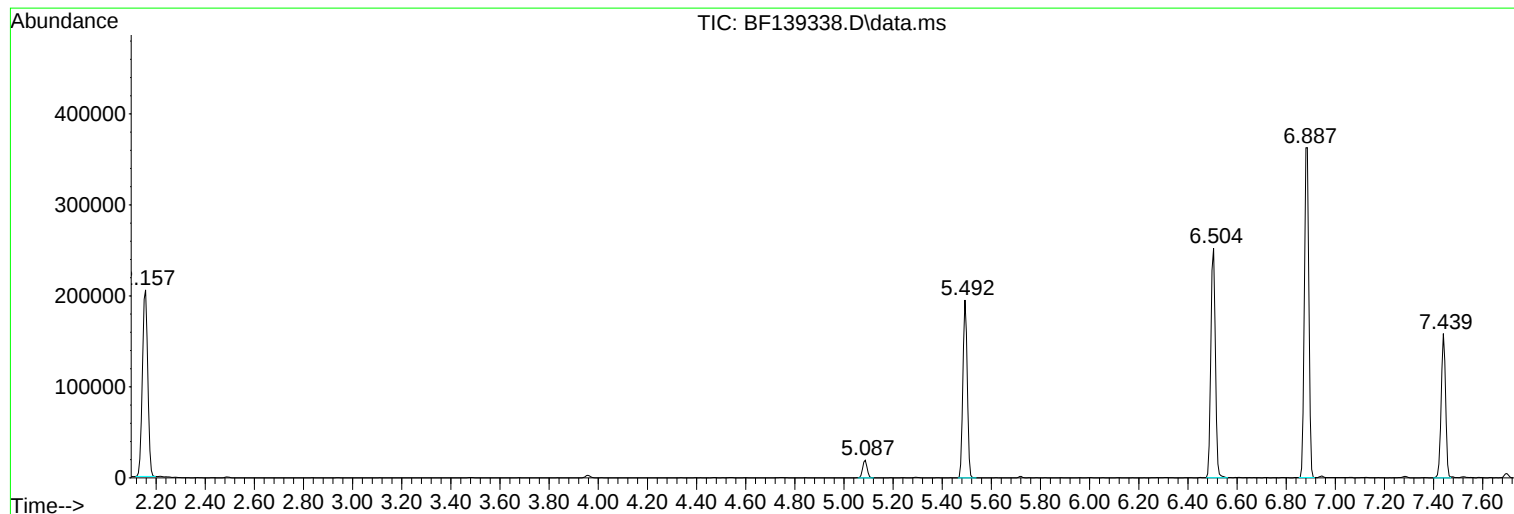
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Misc :  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
DN-B-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF090424.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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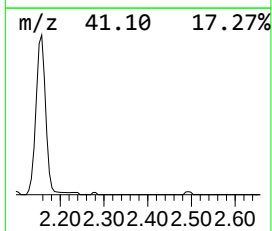
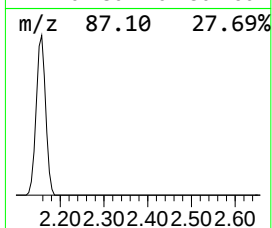
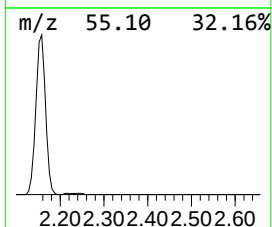
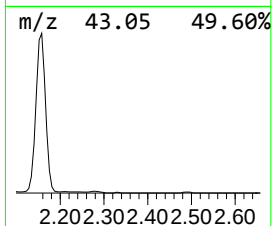
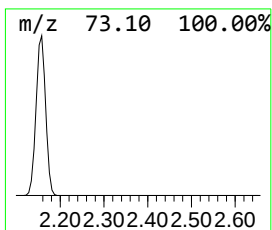
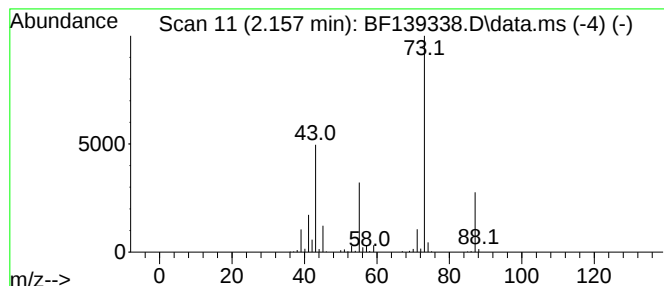
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF090424.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 2.157 | 13.49 ng | 311473 | 1,4-Dichlorobenzene-d4 | 6.887 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 38   |
| 4    |    |   | 3-Pentanol, 3-methyl-       | 102 | C6H14O  | 000077-74-7 | 38   |
| 5    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 9    |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

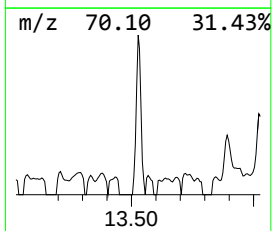
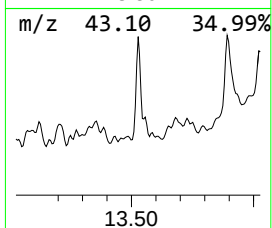
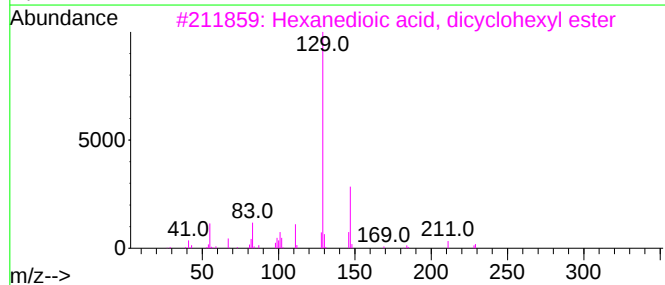
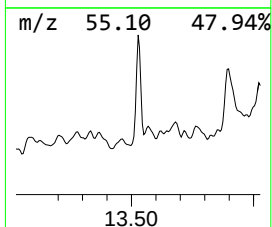
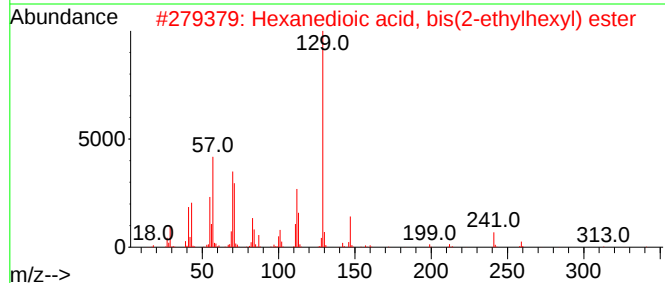
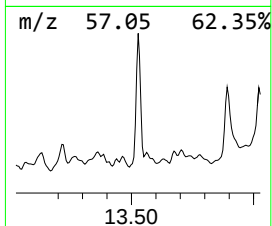
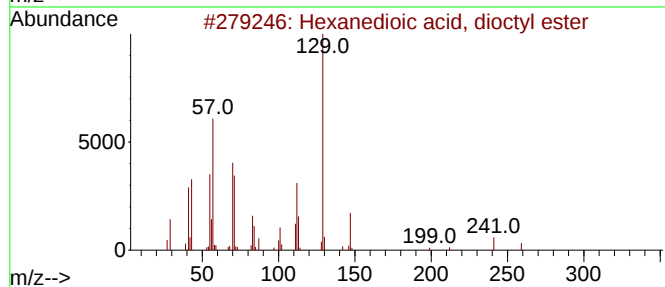
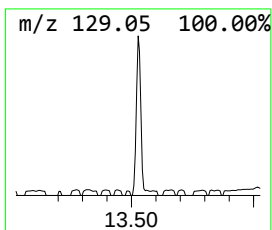
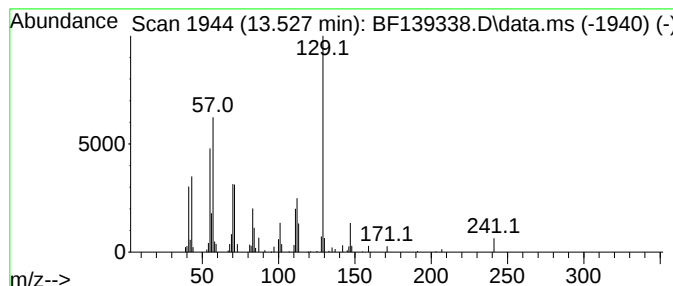
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Hexanedioic acid, dioctyl e... Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 13.527 | 2.07 ng | 40179 | Chrysene-d12     | 14.045 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Hexanedioic acid, dioctyl ester     | 370 | C22H42O4 | 000123-79-5  | 87   |
| 2    |    |   | Hexanedioic acid, bis(2-ethylhex... | 370 | C22H42O4 | 000103-23-1  | 83   |
| 3    |    |   | Hexanedioic acid, dicyclohexyl e... | 310 | C18H30O4 | 000849-99-0  | 47   |
| 4    |    |   | Adipic acid, 2-ethylhexyl isohex... | 342 | C20H38O4 | 1000324-48-3 | 47   |
| 5    |    |   | Adipic acid, isohexyl 3-pentyl e... | 300 | C17H32O4 | 1000324-60-7 | 43   |



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ALS Vial : 25 Sample Multiplier: 1

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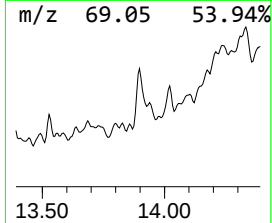
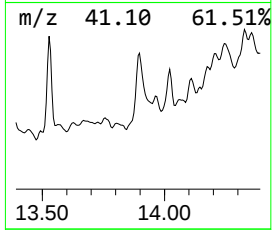
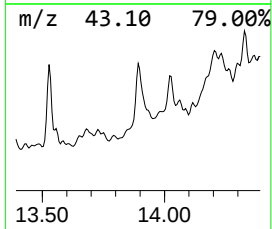
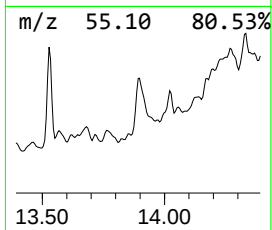
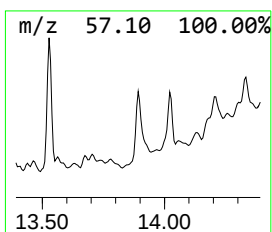
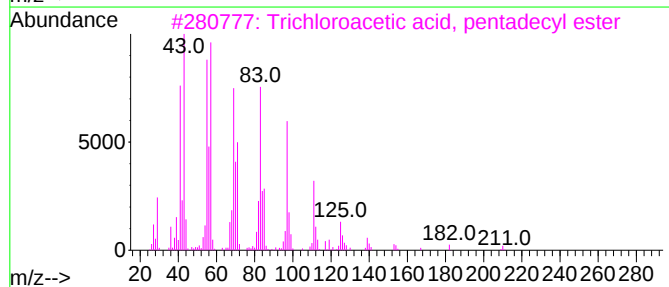
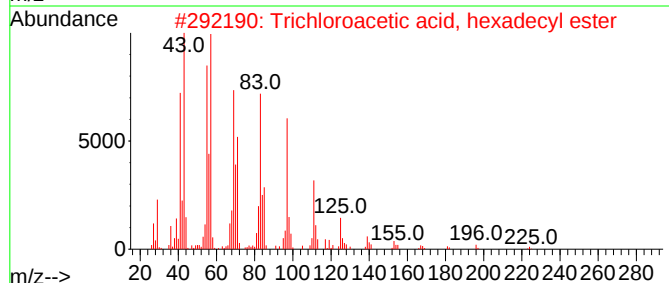
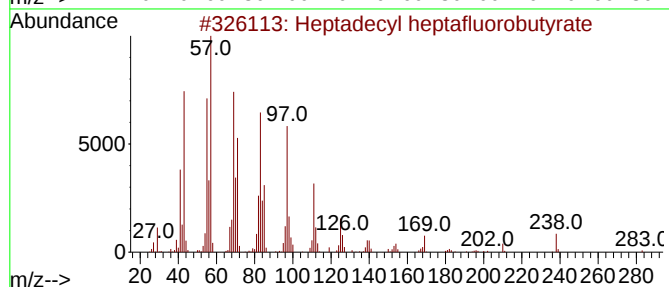
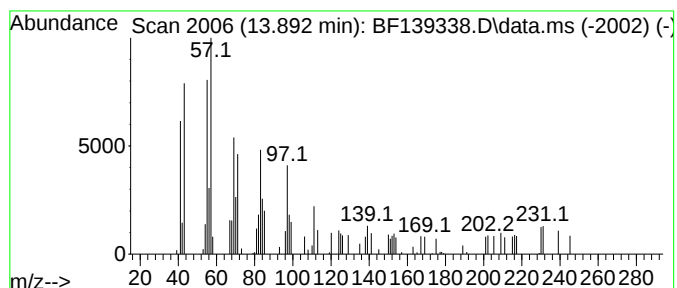
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 5

| R.T.      | EstConc                             | Area  | Relative to ISTD |             | R.T.        |      |
|-----------|-------------------------------------|-------|------------------|-------------|-------------|------|
| 13.892    | 2.25 ng                             | 43650 | Chrysene-d12     |             | 14.045      |      |
| Hit# of 5 | Tentative ID                        |       | MW               | MolForm     | CAS#        | Qual |
| 1         | Heptadecyl heptafluorobutyrate      |       | 452              | C21H35F7O2  | 959085-66-6 | 81   |
| 2         | Trichloroacetic acid, hexadecyl ... |       | 386              | C18H33Cl3O2 | 074339-54-1 | 81   |
| 3         | Trichloroacetic acid, pentadecyl... |       | 372              | C17H31Cl3O2 | 074339-53-0 | 81   |
| 4         | Dichloroacetic acid, tetradecyl ... |       | 324              | C16H30Cl2O2 | 083005-02-1 | 76   |
| 5         | Trichloroacetic acid, tetradecyl... |       | 358              | C16H29Cl3O2 | 074339-52-9 | 76   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF090424.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

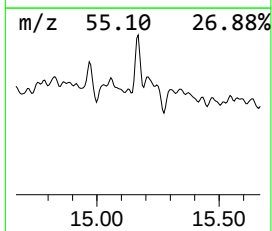
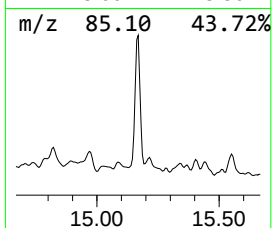
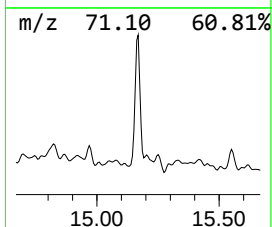
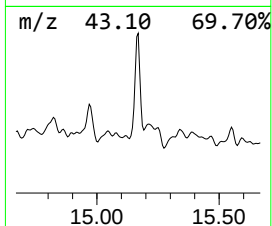
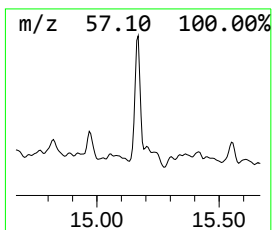
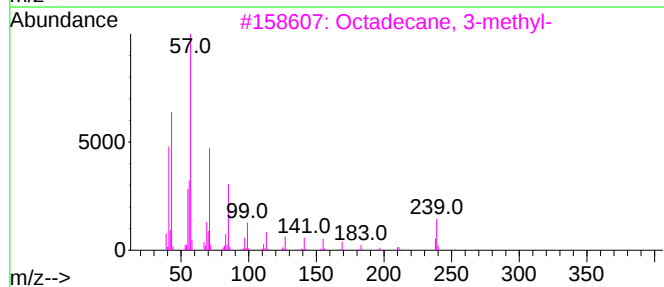
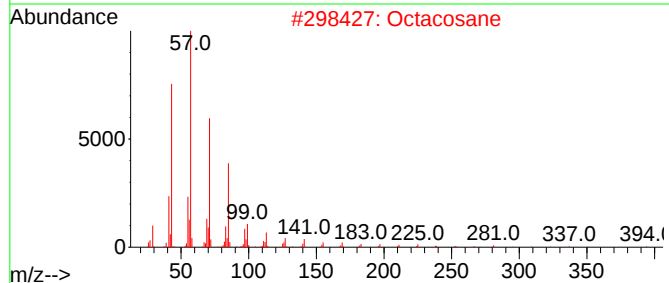
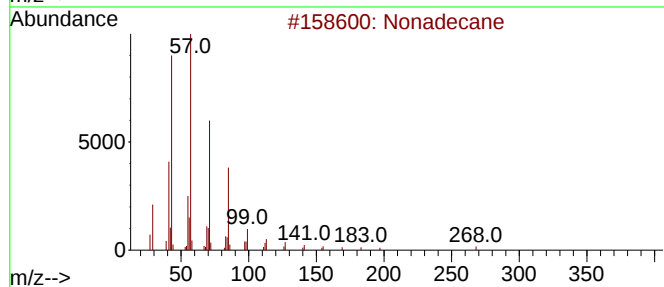
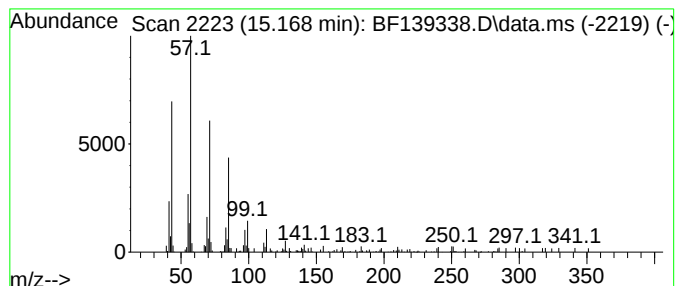
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Nonadecane Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.168 | 3.26 ng | 61875 | Perylene-d12     | 15.515 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Nonadecane            | 268 | C19H40  | 000629-92-5 | 93   |
| 2    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 90   |
| 3    |    |   | Octadecane, 3-methyl- | 268 | C19H40  | 006561-44-0 | 90   |
| 4    |    |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1 | 90   |
| 5    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 87   |



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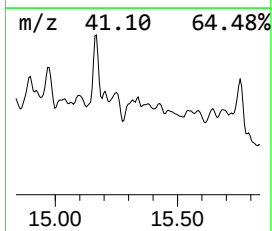
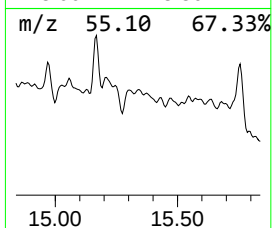
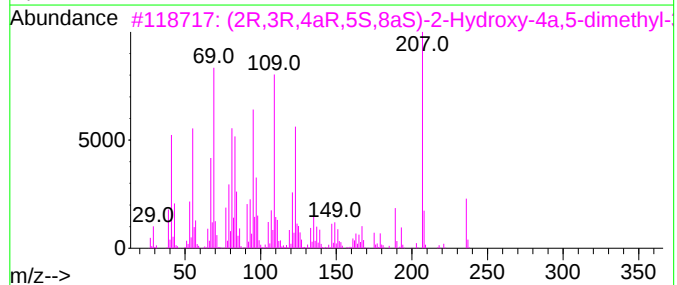
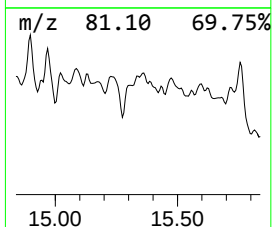
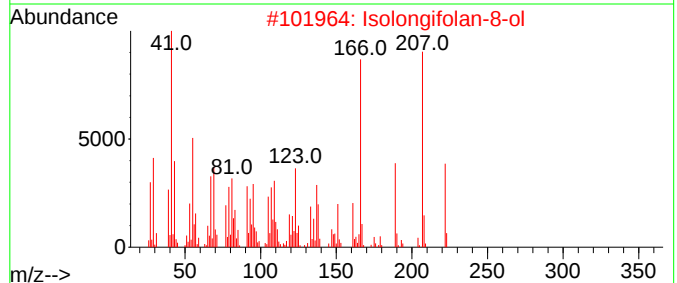
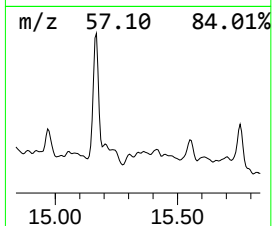
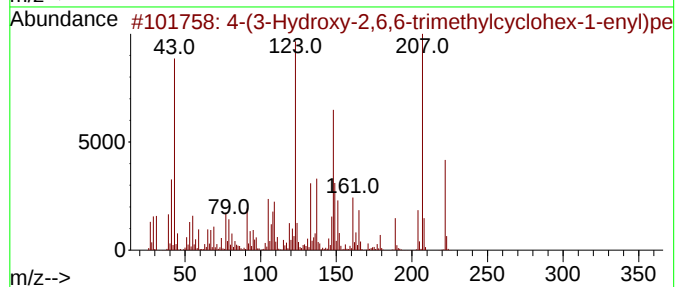
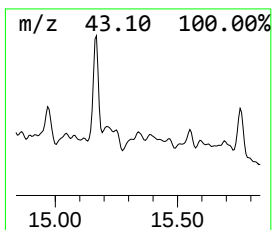
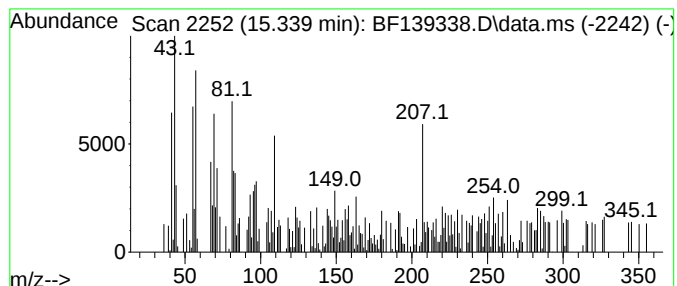
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF090424.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 unknown15.339 Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.339 | 7.27 ng | 137811 | Perylene-d12     | 15.515 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 4-(3-Hydroxy-2,6,6-trimethylcycl... | 222 | C14H22O2     | 097306-57-5  | 45      |      |      |
| 2    | Isolongifolan-8-ol                  | 222 | C15H26O      | 001139-08-8  | 41      |      |      |
| 3    | (2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,... | 236 | C15H24O2     | 066884-74-0  | 38      |      |      |
| 4    | benzamide, N-[4-(heptyloxy)pheny... | 343 | C20H25NO4    | 1000398-24-5 | 30      |      |      |
| 5    | 2H-1,2,3-Triazole-4-carboxylic a... | 207 | C9H6FN3O2    | 051306-44-6  | 25      |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF091124\  
Data File : BF139338.D  
Acq On : 11 Sep 2024 20:55  
Operator : RC/JU  
Sample : P3930-02  
Misc :  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
DN-B-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF090424.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 |
| Butane, 2-metho... | 2.157  | 13.5    | ng    | 311473   | 1                     | 6.887  | 461802 | 20.0 |
| Hexanedioic aci... | 13.527 | 2.1     | ng    | 40179    | 5                     | 14.045 | 387400 | 20.0 |
| Heptadecyl hept... | 13.892 | 2.3     | ng    | 43650    | 5                     | 14.045 | 387400 | 20.0 |
| Nonadecane         | 15.168 | 3.3     | ng    | 61875    | 6                     | 15.515 | 379344 | 20.0 |
| unknown15.339      | 15.339 | 7.3     | ng    | 137811   | 6                     | 15.515 | 379344 | 20.0 |