

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF070122\  
 Data File : BF129093.D  
 Acq On : 01 Jul 2022 15:46  
 Operator : CG\JU  
 Sample : PB145980BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB145980BL

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129093.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         | 2.340       | 3             | 9           | 16           | rVB      | 206415         | 291447        | 2.40%           | 0.389%        |
| 2         | 5.587       | 556           | 561         | 564          | rBV      | 8422672        | 9193367       | 75.67%          | 12.267%       |
| 3         | 6.581       | 723           | 730         | 733          | rBV      | 7895318        | 8943338       | 73.61%          | 11.934%       |
| 4         | 6.957       | 790           | 794         | 797          | rBV      | 2411882        | 2184878       | 17.98%          | 2.915%        |
| 5         | 7.516       | 884           | 889         | 892          | rBV      | 5783292        | 6162162       | 50.72%          | 8.223%        |
| 6         | 8.240       | 1007          | 1012        | 1015         | rBV      | 3061585        | 2960884       | 24.37%          | 3.951%        |
| 7         | 9.316       | 1189          | 1195        | 1198         | rBV      | 11525223       | 11351661      | 93.43%          | 15.147%       |
| 8         | 9.998       | 1305          | 1311        | 1314         | rBV      | 3985488        | 3344818       | 27.53%          | 4.463%        |
| 9         | 10.792      | 1439          | 1446        | 1449         | rBV      | 7534967        | 7326738       | 60.31%          | 9.777%        |
| 10        | 11.492      | 1560          | 1565        | 1568         | rBV      | 3866855        | 3463730       | 28.51%          | 4.622%        |
| 11        | 13.086      | 1830          | 1836        | 1839         | rBV      | 11372705       | 12149295      | 100.00%         | 16.212%       |
| 12        | 14.139      | 2011          | 2015        | 2019         | rBV      | 3454239        | 2975246       | 24.49%          | 3.970%        |
| 13        | 14.233      | 2026          | 2031        | 2038         | rBV      | 567824         | 614362        | 5.06%           | 0.820%        |
| 14        | 14.916      | 2143          | 2147        | 2152         | rBV      | 120637         | 124592        | 1.03%           | 0.166%        |
| 15        | 15.269      | 2204          | 2207        | 2211         | rBV      | 165622         | 184098        | 1.52%           | 0.246%        |
| 16        | 15.663      | 2268          | 2274        | 2284         | rBV      | 2024558        | 2772455       | 22.82%          | 3.699%        |
| 17        | 16.139      | 2350          | 2355        | 2362         | rVB      | 218962         | 345514        | 2.84%           | 0.461%        |
| 18        | 16.680      | 2441          | 2447        | 2453         | rBV      | 189045         | 336817        | 2.77%           | 0.449%        |
| 19        | 17.316      | 2549          | 2555        | 2564         | rVB2     | 107120         | 216475        | 1.78%           | 0.289%        |

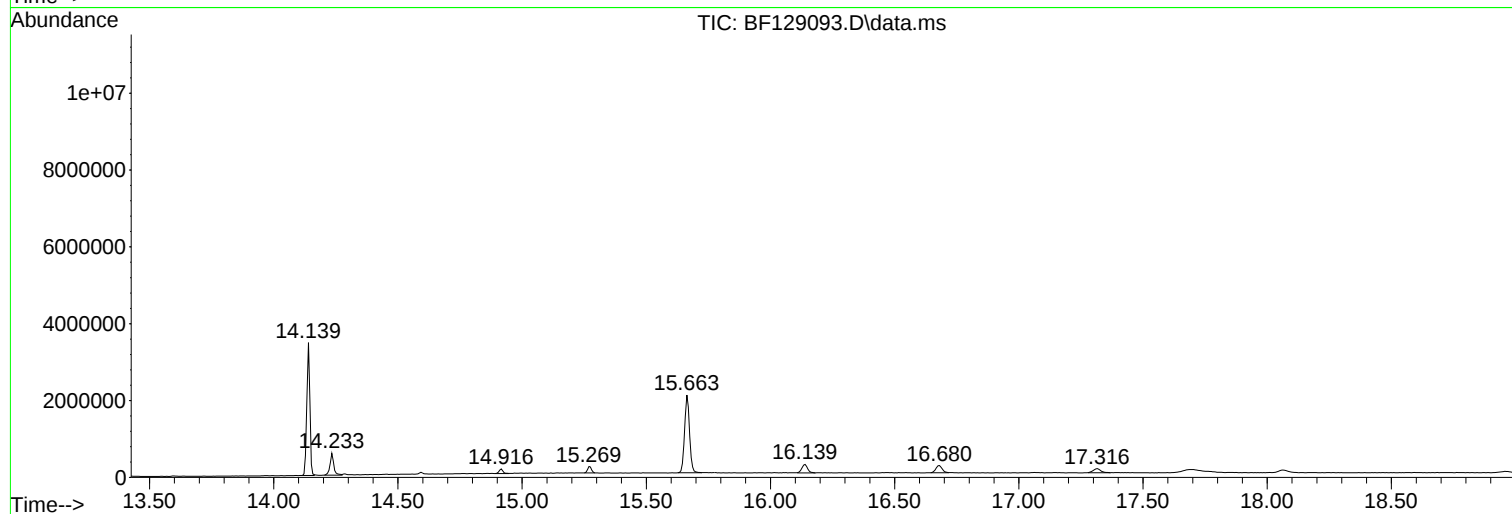
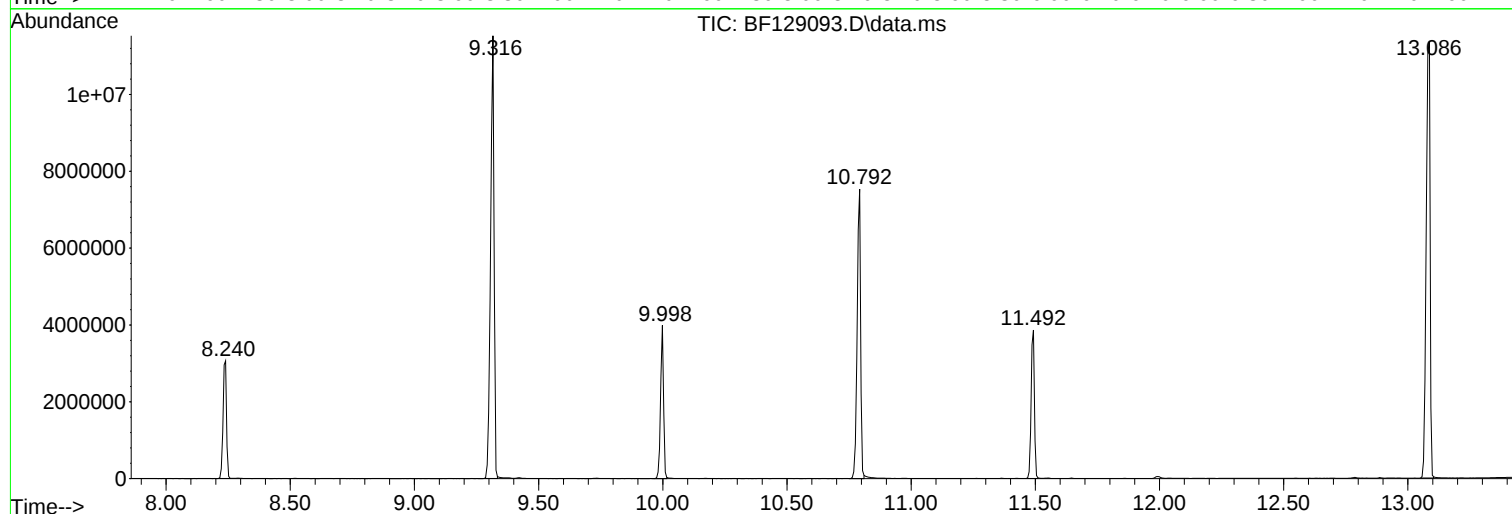
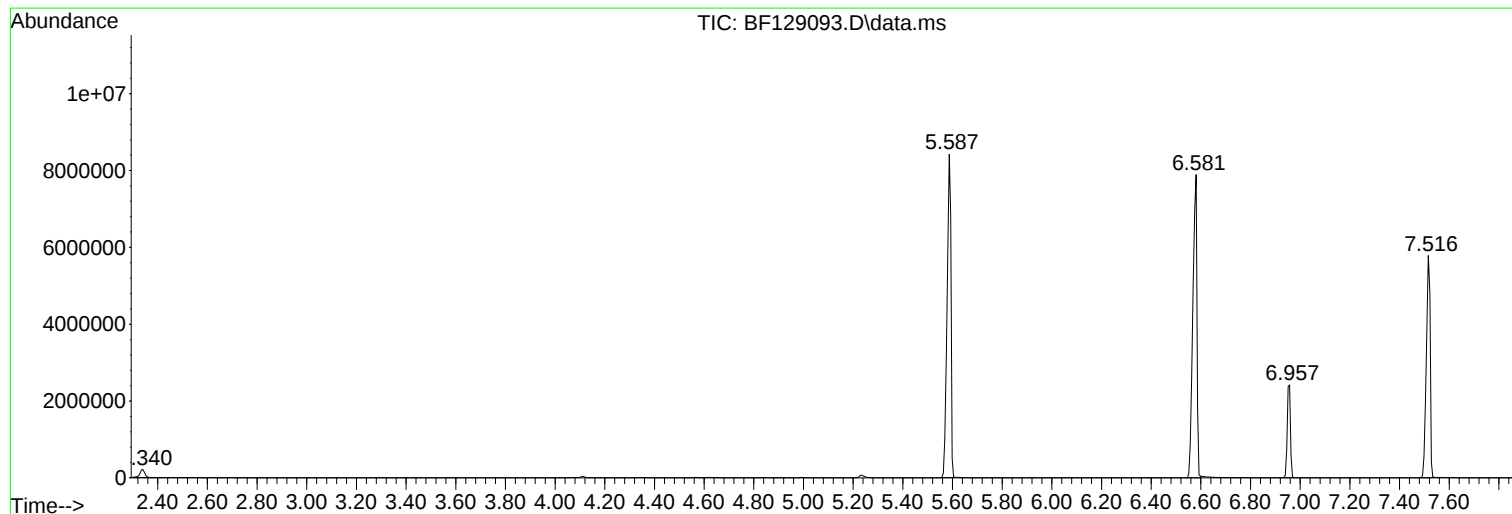
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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB145980BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062922.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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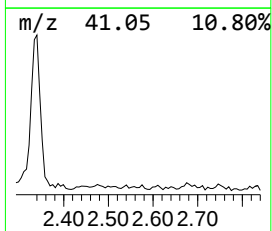
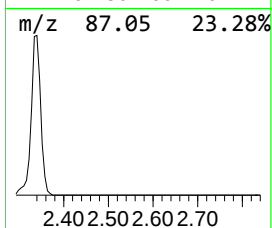
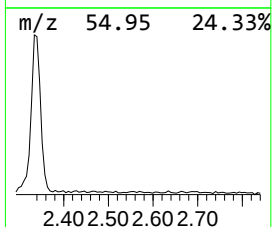
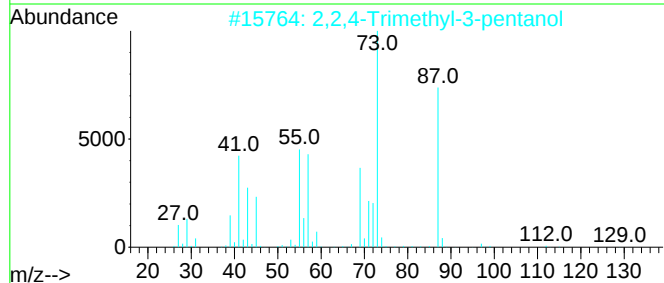
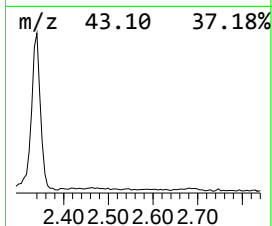
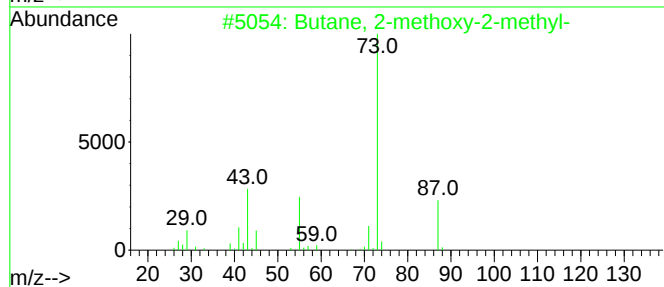
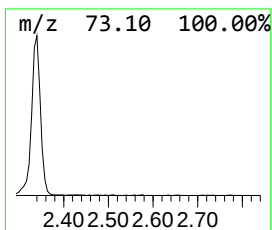
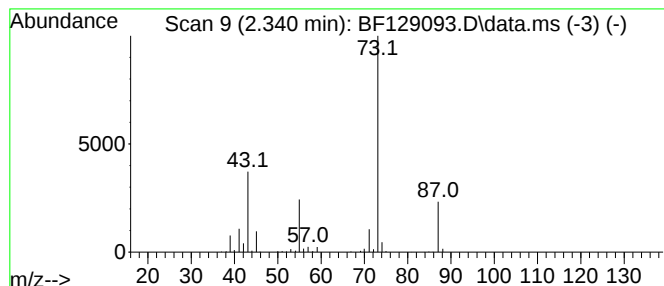
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 2.340 | 2.67 ng | 291447 | 1,4-Dichlorobenzene-d4 | 6.957 |

| 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    |    |   | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB145980BL

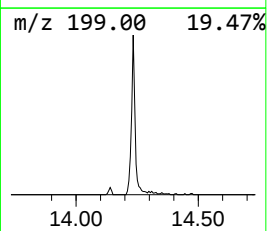
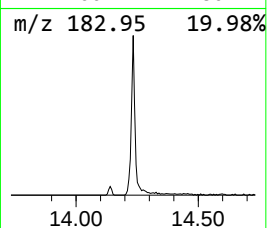
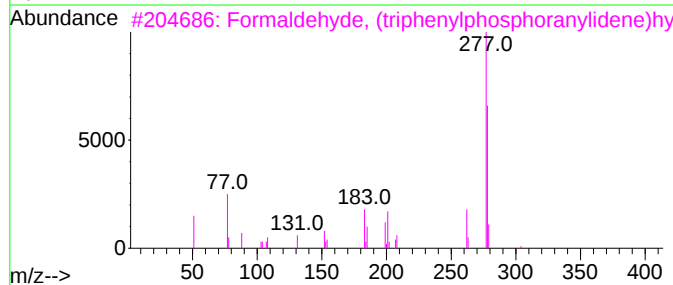
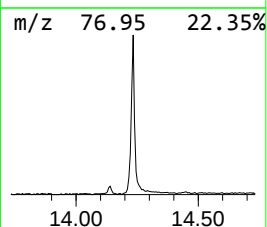
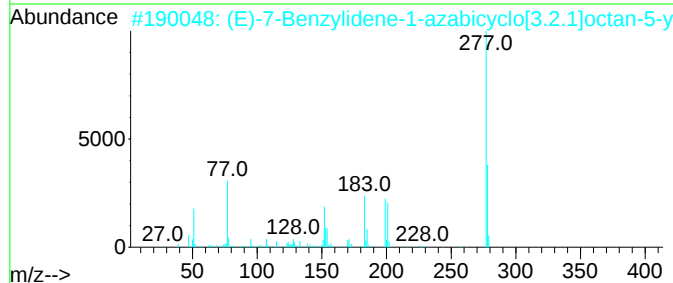
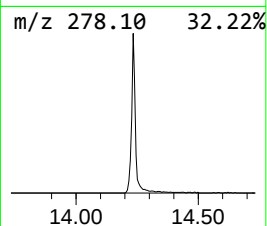
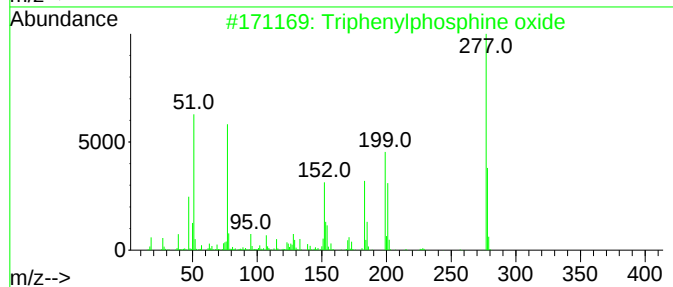
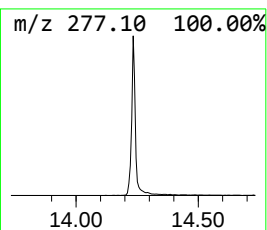
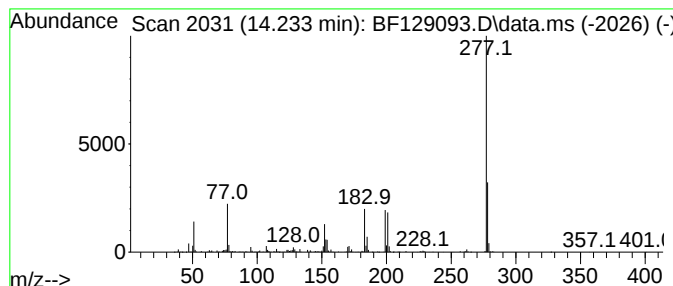
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.233 | 4.13 ng | 614362 | Chrysene-d12     | 14.139 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 92   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S | 1000483-83-4 | 91   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P  | 015990-54-2  | 50   |
| 4    |    |   | Carbazol-1-one, 1,2,3,4-tetrahyd...  | 277 | C18H15NO2  | 299962-12-2  | 38   |
| 5    |    |   | 2-Phenyl-6-(trifluoromethyl)-1H...   | 277 | C15H10F3NO | 1000387-59-3 | 9    |



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ALS Vial : 3 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
PB145980BL

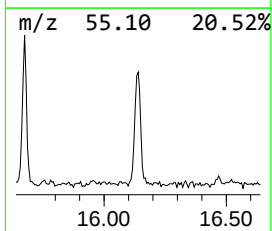
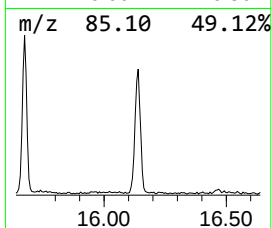
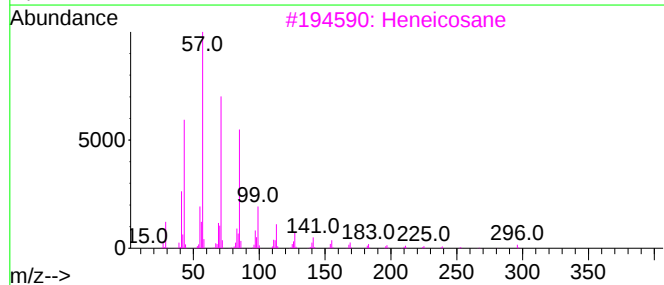
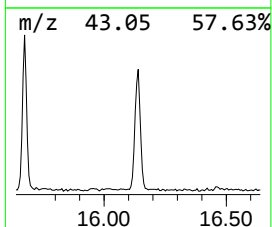
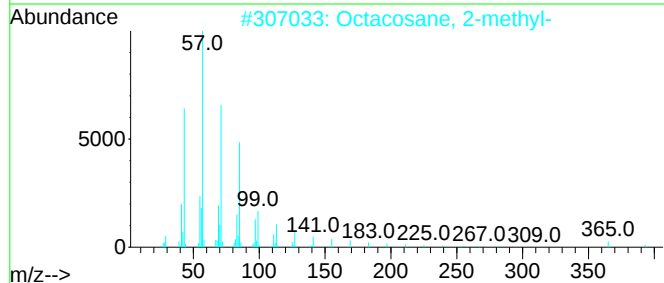
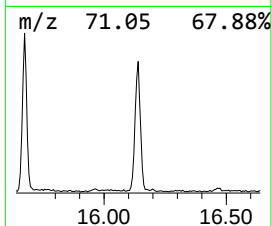
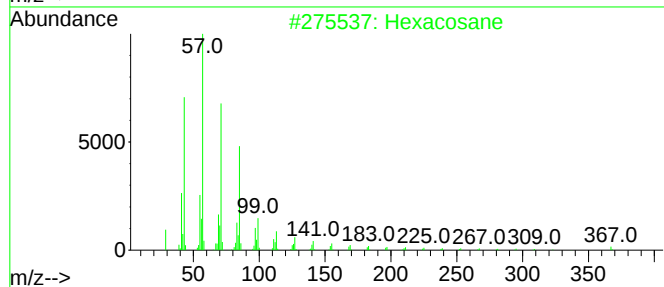
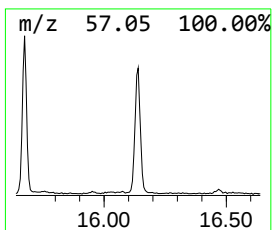
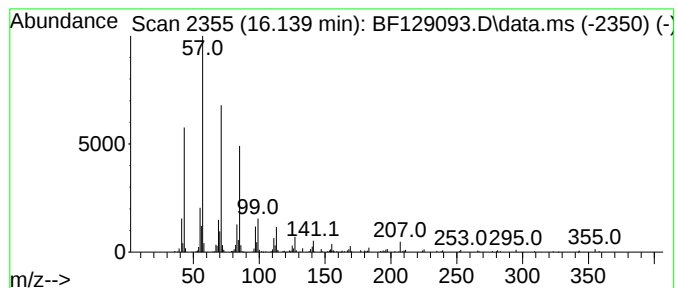
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062922.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Hexacosane Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.139 | 2.49 ng | 345514 | Perylene-d12     | 15.663 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 93   |
| 2    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 90   |
| 3    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 90   |
| 4    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 90   |
| 5    |    |   | Docosane, 11-butyl-   | 366 | C26H54  | 013475-76-8 | 87   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB145980BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

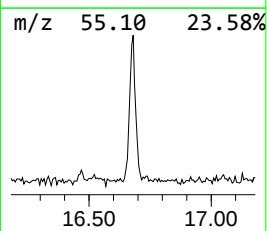
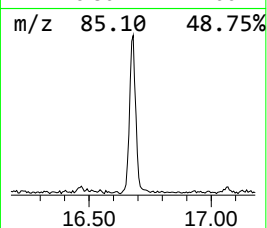
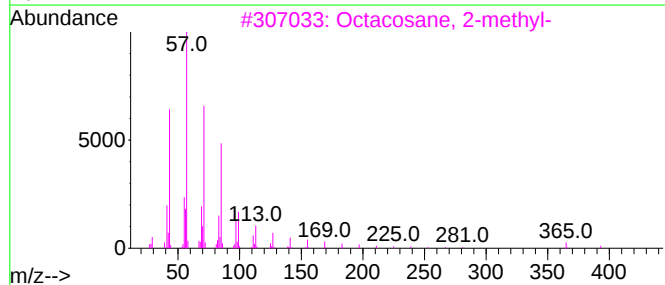
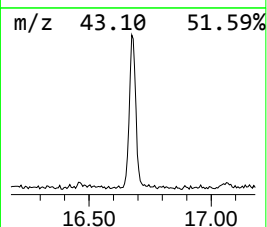
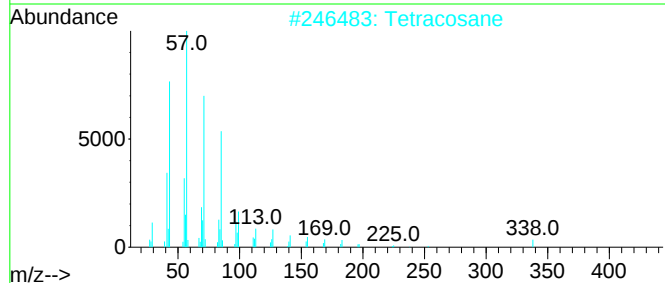
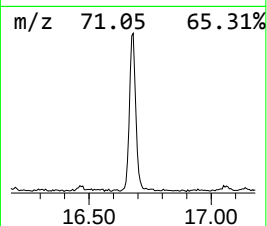
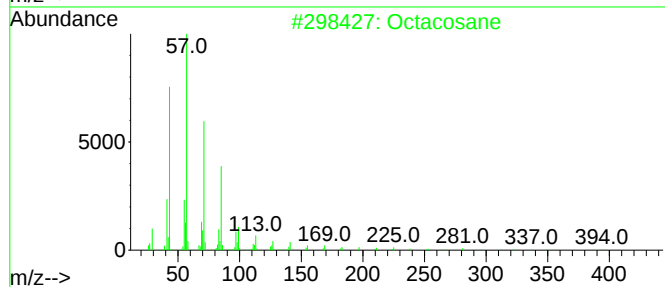
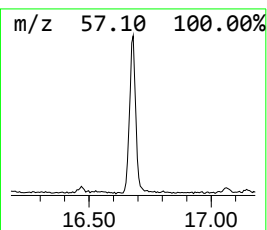
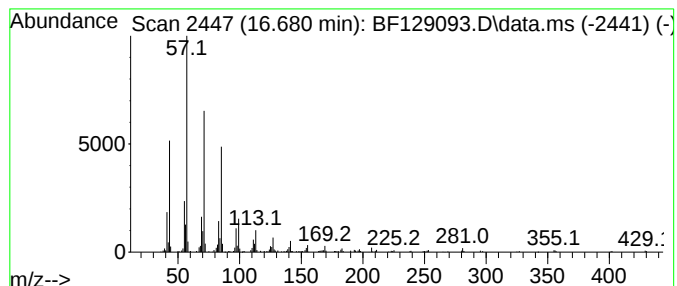
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octacosane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.680 | 2.43 ng | 336817 | Perylene-d12     | 15.663 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#         | Qual |
|------|----|---|-----------------------|-----|---------|--------------|------|
| 1    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4  | 90   |
| 2    |    |   | Tetracosane           | 338 | C24H50  | 000646-31-1  | 90   |
| 3    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1  | 90   |
| 4    |    |   | Triacontane, 1-iodo-  | 548 | C30H61I | 1000406-32-3 | 87   |
| 5    |    |   | Hexacosane, 1-iodo-   | 492 | C26H53I | 1000406-32-1 | 87   |



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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... | 2.340  | 2.7     | ng    | 291447   | 1                     | 6.957  | 2184880 | 20.0 |
| Triphenylphosph... | 14.233 | 4.1     | ng    | 614362   | 5                     | 14.139 | 2975250 | 20.0 |
| Hexacosane         | 16.139 | 2.5     | ng    | 345514   | 6                     | 15.663 | 2772460 | 20.0 |
| Octacosane         | 16.680 | 2.4     | ng    | 336817   | 6                     | 15.663 | 2772460 | 20.0 |