

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082422\  
 Data File : BF129975.D  
 Acq On : 24 Aug 2022 16:43  
 Operator : CG\JU  
 Sample : PB147203BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB147203BL

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-BF081422.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129975.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         | 5.410       | 528           | 531         | 555          | rBV      | 2782478        | 2724470       | 48.36%          | 9.680%        |
| 2         | 6.428       | 700           | 704         | 726          | rBV      | 2817267        | 2737389       | 48.59%          | 9.726%        |
| 3         | 6.763       | 758           | 761         | 771          | rVB      | 868377         | 730958        | 12.97%          | 2.597%        |
| 4         | 7.334       | 854           | 858         | 862          | rBV      | 2388830        | 2608529       | 46.30%          | 9.268%        |
| 5         | 8.045       | 975           | 979         | 987          | rBV      | 1220582        | 1054503       | 18.72%          | 3.747%        |
| 6         | 9.122       | 1157          | 1162        | 1165         | rBV      | 5394628        | 5035787       | 89.39%          | 17.892%       |
| 7         | 9.798       | 1273          | 1277        | 1281         | rBV      | 1443738        | 1246093       | 22.12%          | 4.427%        |
| 8         | 10.598      | 1409          | 1413        | 1416         | rBV      | 2536131        | 2206042       | 39.16%          | 7.838%        |
| 9         | 11.292      | 1527          | 1531        | 1534         | rBV      | 1507002        | 1312831       | 23.30%          | 4.664%        |
| 10        | 12.880      | 1796          | 1801        | 1804         | rBV      | 5801164        | 5633732       | 100.00%         | 20.016%       |
| 11        | 13.939      | 1977          | 1981        | 1988         | rBV      | 1083254        | 1044245       | 18.54%          | 3.710%        |
| 12        | 14.022      | 1990          | 1995        | 2000         | rBV      | 69354          | 80714         | 1.43%           | 0.287%        |
| 13        | 14.674      | 2102          | 2106        | 2109         | rBV      | 60217          | 63202         | 1.12%           | 0.225%        |
| 14        | 14.727      | 2110          | 2115        | 2127         | rVB7     | 27686          | 94036         | 1.67%           | 0.334%        |
| 15        | 14.998      | 2156          | 2161        | 2164         | rBV      | 58662          | 68748         | 1.22%           | 0.244%        |
| 16        | 15.357      | 2217          | 2222        | 2223         | rBV      | 77413          | 87470         | 1.55%           | 0.311%        |
| 17        | 15.386      | 2223          | 2227        | 2237         | rVB      | 625650         | 778518        | 13.82%          | 2.766%        |
| 18        | 15.768      | 2287          | 2292        | 2298         | rVB      | 77153          | 105136        | 1.87%           | 0.374%        |
| 19        | 16.245      | 2368          | 2373        | 2380         | rVB      | 76728          | 126630        | 2.25%           | 0.450%        |
| 20        | 16.604      | 2424          | 2434        | 2446         | rBV6     | 32994          | 147876        | 2.62%           | 0.525%        |
| 21        | 16.810      | 2463          | 2469        | 2475         | rVB2     | 51845          | 101360        | 1.80%           | 0.360%        |
| 22        | 17.468      | 2575          | 2581        | 2588         | rVB2     | 40234          | 87591         | 1.55%           | 0.311%        |
| 23        | 18.257      | 2709          | 2715        | 2725         | rVB4     | 24921          | 70392         | 1.25%           | 0.250%        |

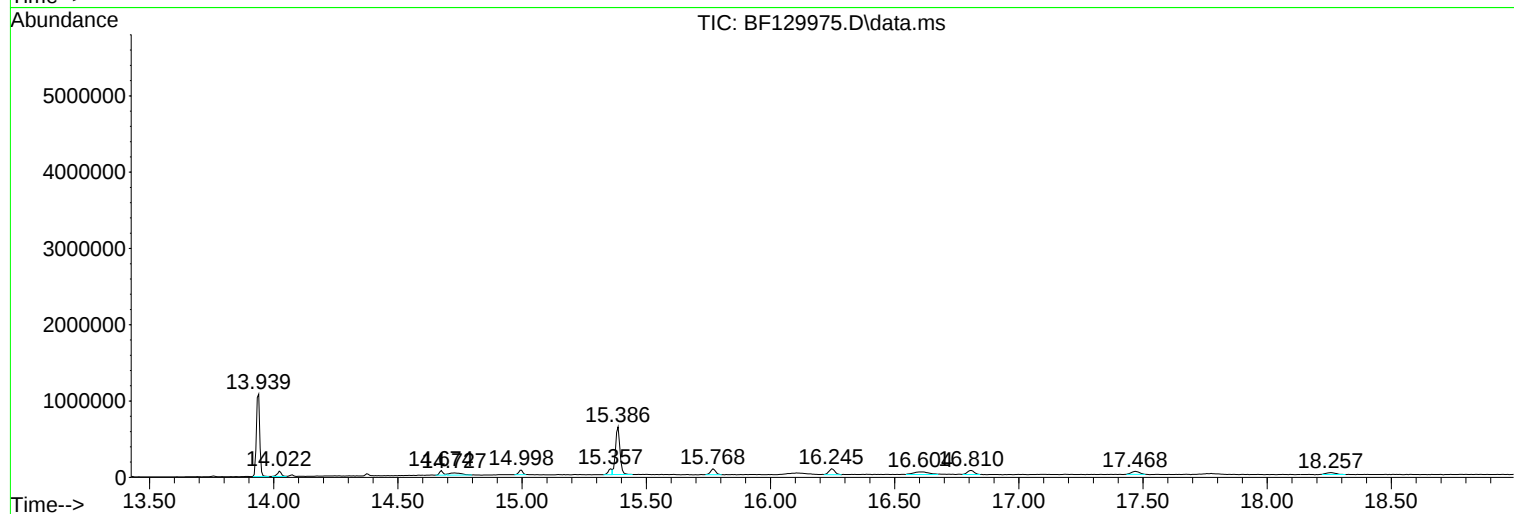
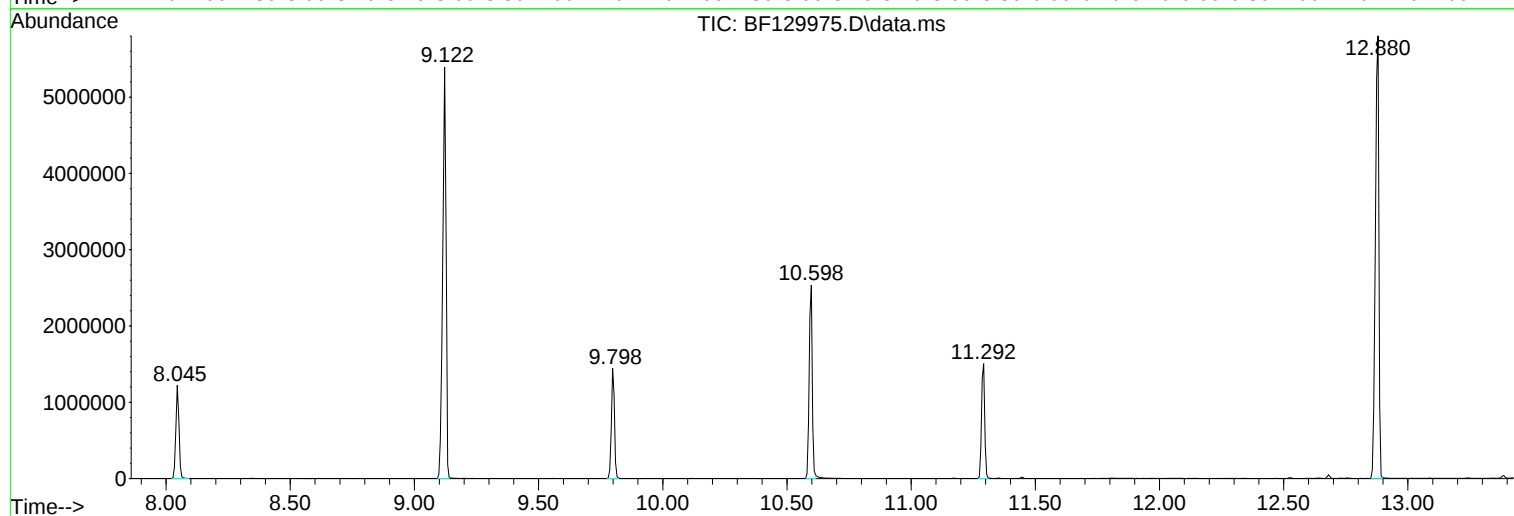
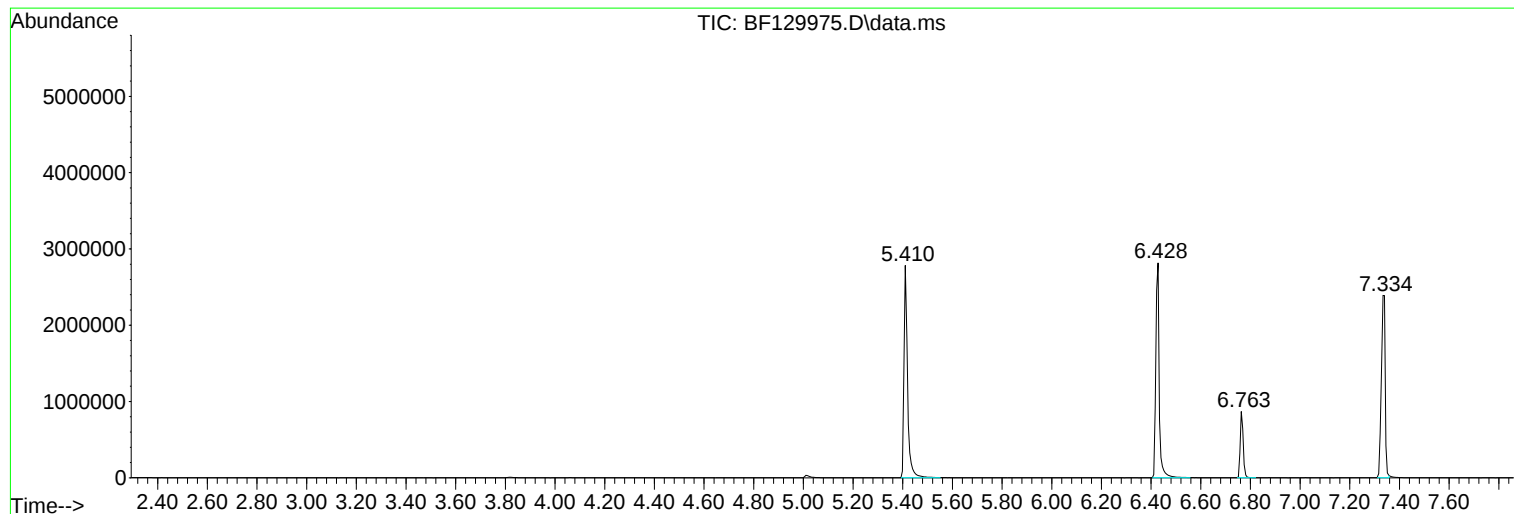
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ALS Vial : 3 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
PB147203BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF081422.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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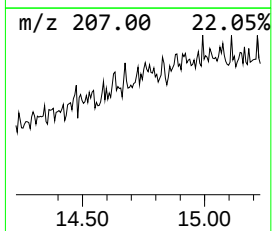
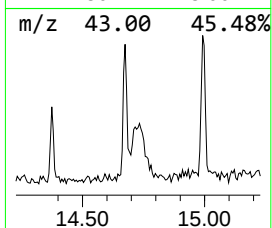
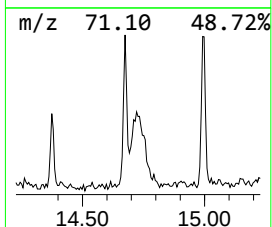
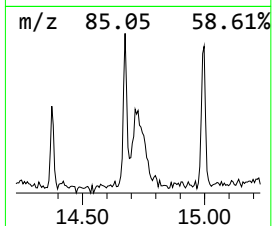
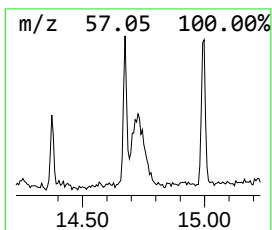
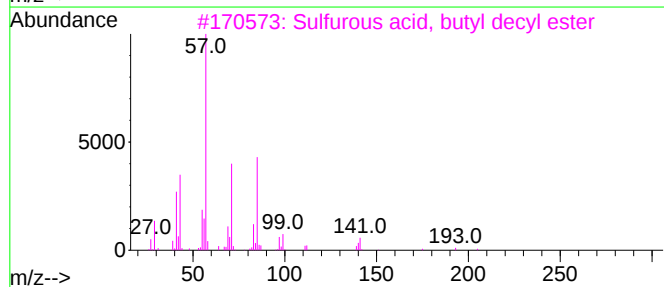
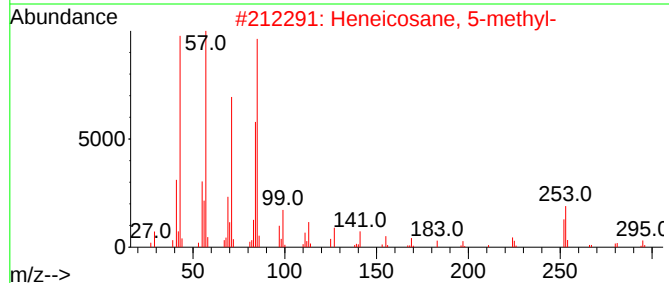
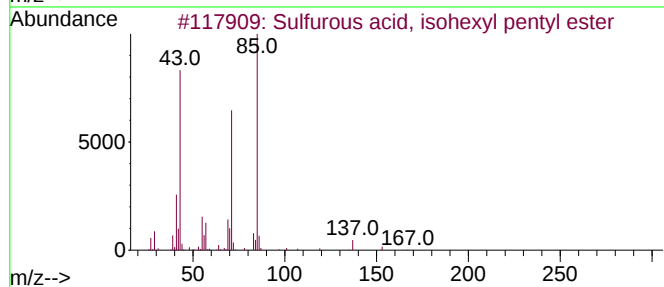
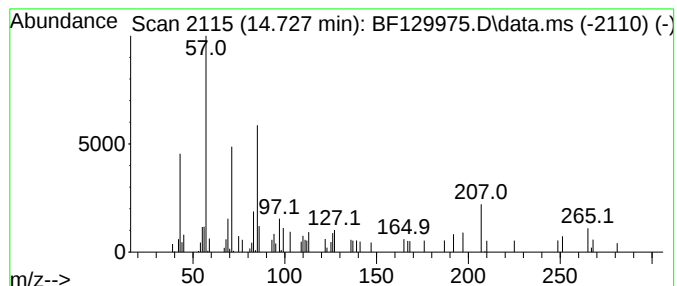
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown14.727 Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.727 | 2.42 ng | 94036 | Perylene-d12     | 15.386 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|------|-------------------------------------|-----|-----------|--------------|------|
| 1    |      | Sulfurous acid, isohexyl pentyl ... | 236 | C11H24O3S | 1000309-14-0 | 43   |
| 2    |      | Heneicosane, 5-methyl-              | 310 | C22H46    | 025117-37-7  | 43   |
| 3    |      | Sulfurous acid, butyl decyl ester   | 278 | C14H30O3S | 1000309-17-7 | 43   |
| 4    |      | Hentriacontane                      | 437 | C31H64    | 000630-04-6  | 38   |
| 5    |      | Nonadecane                          | 268 | C19H40    | 000629-92-5  | 35   |



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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF081422.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

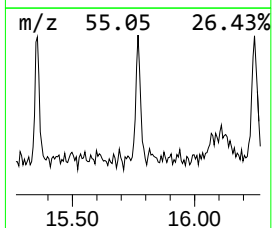
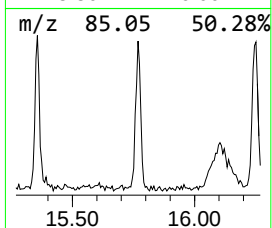
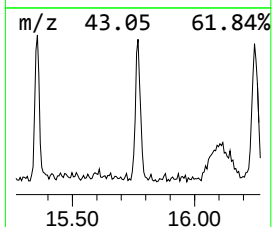
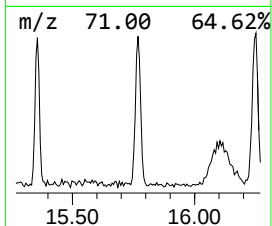
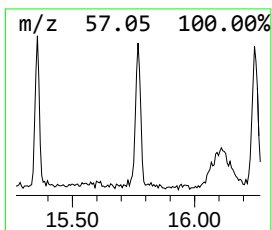
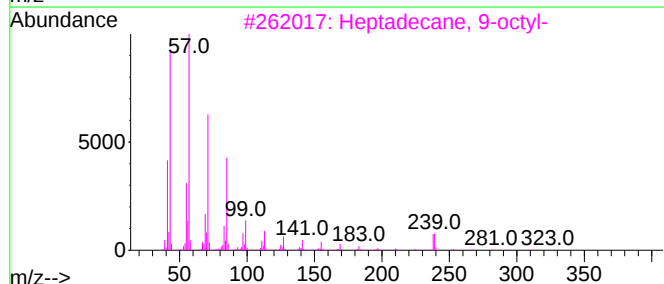
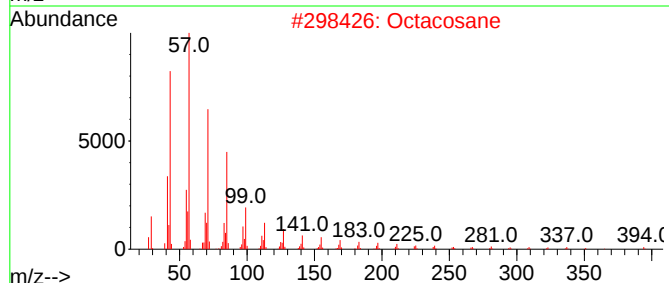
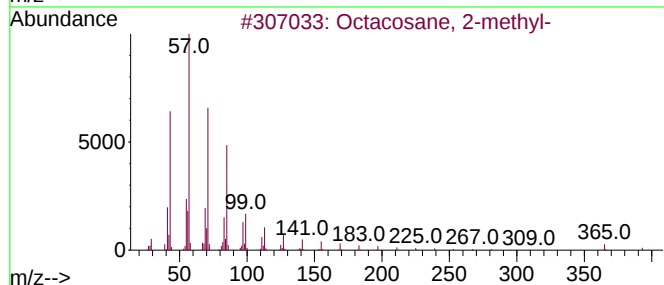
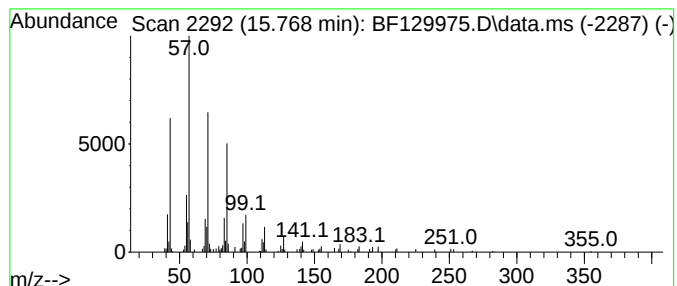
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Octacosane, 2-methyl- Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.769 | 2.70 ng | 105136 | Perylene-d12     | 15.386 |

| 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, 9-octyl-  | 352 | C25H52  | 007225-64-1  | 91   |
| 4    |      | Tetracosane            | 338 | C24H50  | 000646-31-1  | 91   |
| 5    |      | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 90   |



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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB147203BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF081422.M  
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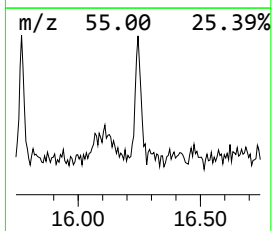
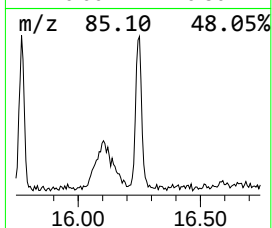
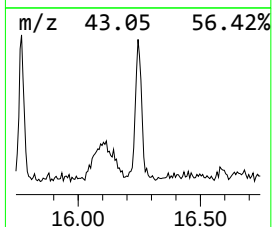
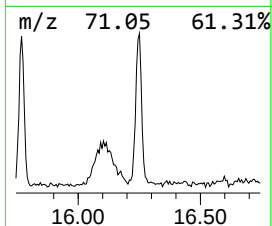
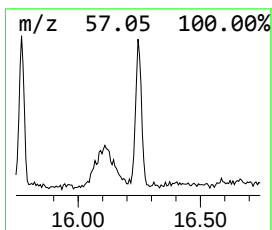
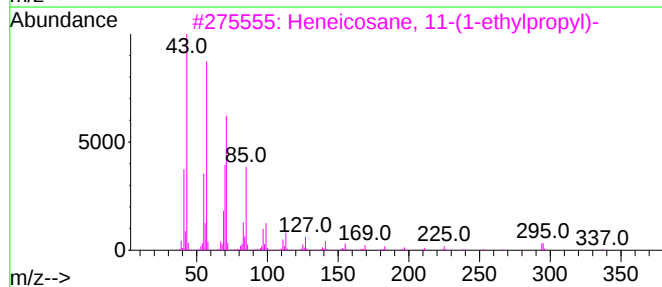
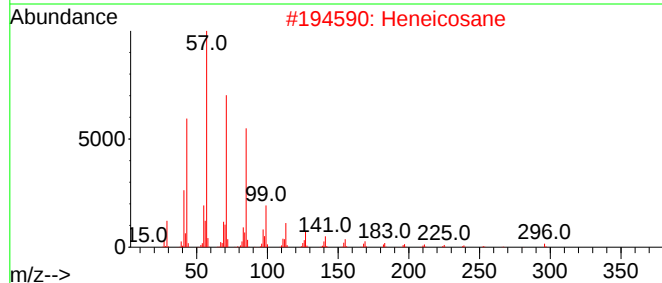
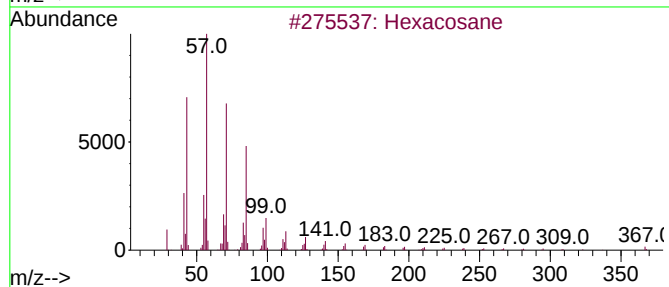
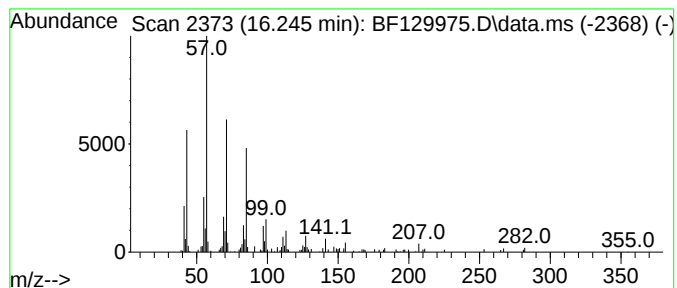
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Hexacosane Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.245 | 3.25 ng | 126630 | Perylene-d12     | 15.386 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------|-----|---------|-------------|------|
| 1    |    |   | Hexacosane                       | 366 | C26H54  | 000630-01-3 | 93   |
| 2    |    |   | Heneicosane                      | 296 | C21H44  | 000629-94-7 | 90   |
| 3    |    |   | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54  | 055282-11-6 | 87   |
| 4    |    |   | Eicosane, 2-methyl-              | 296 | C21H44  | 001560-84-5 | 87   |
| 5    |    |   | Heptadecane, 9-octyl-            | 352 | C25H52  | 007225-64-1 | 87   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
PB147203BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF081422.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

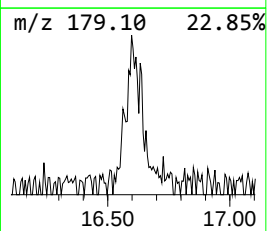
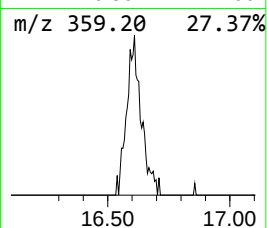
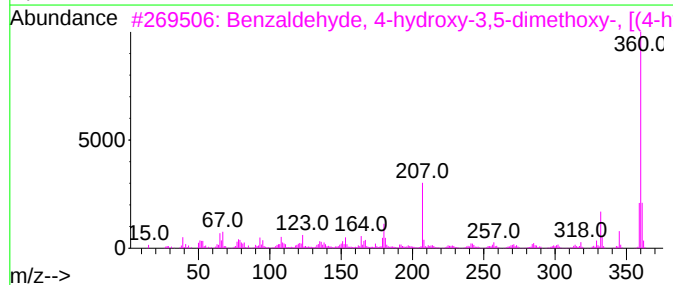
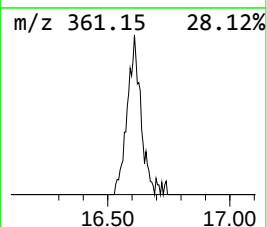
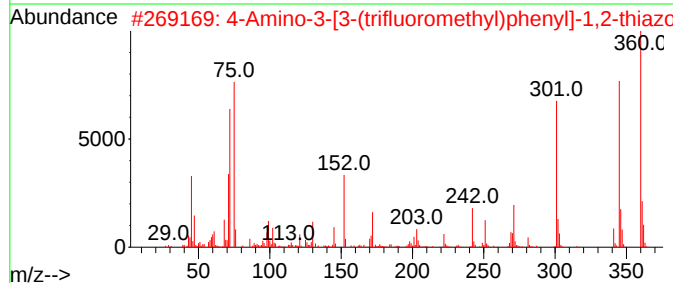
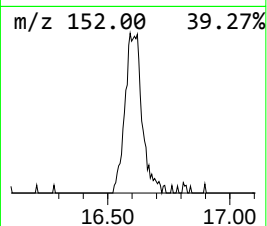
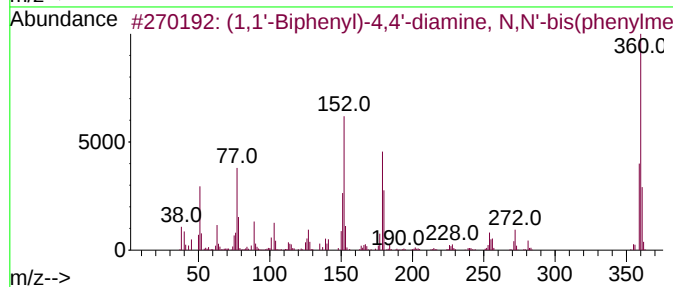
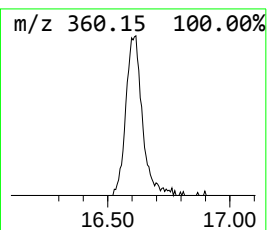
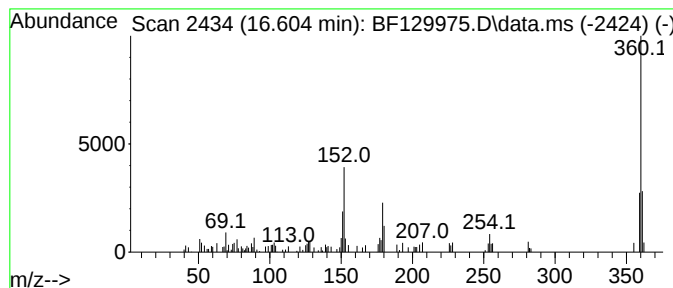
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.604 | 3.80 ng | 147876 | Perylene-d12     | 15.386 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm         | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------------|--------------|------|
| 1    |    |   | (1,1'-Biphenyl)-4,4'-diamine, N,... | 360 | C26H20N2        | 006311-48-4  | 87   |
| 2    |    |   | 4-Amino-3-[3-(trifluoromethyl)ph... | 360 | C14H15F3N2O2SSi | 1010500-98-0 | 50   |
| 3    |    |   | Benzaldehyde, 4-hydroxy-3,5-dime... | 360 | C18H20N2O6      | 014414-32-5  | 50   |
| 4    |    |   | 1,10-Phenanthroline, 2,9-dimethy... | 360 | C26H20N2        | 004733-39-5  | 49   |
| 5    |    |   | Jaceidin                            | 360 | C18H16O8        | 010173-01-0  | 47   |



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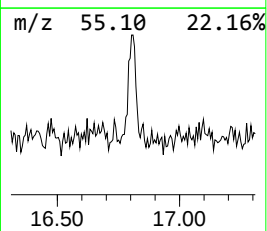
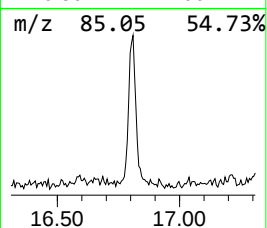
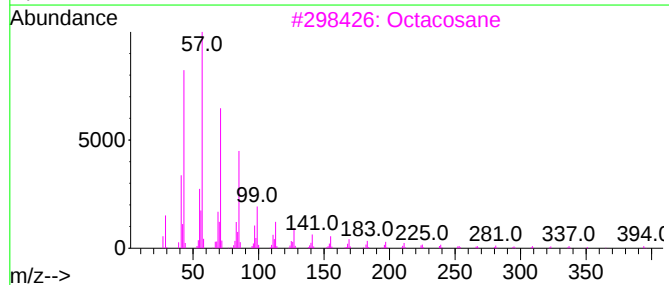
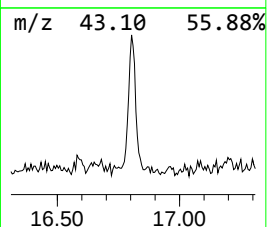
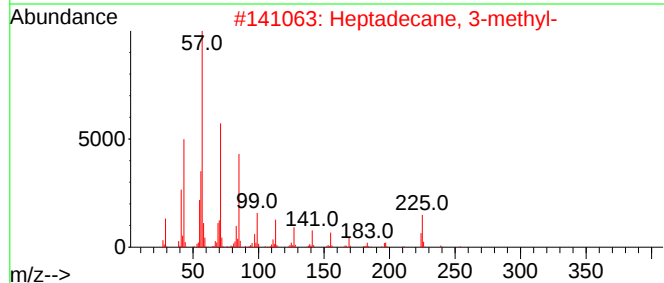
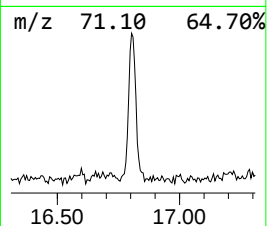
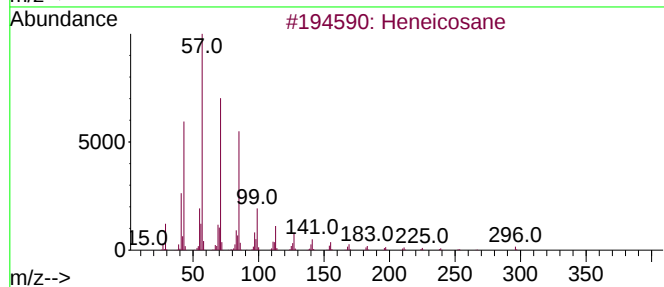
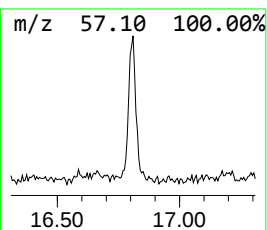
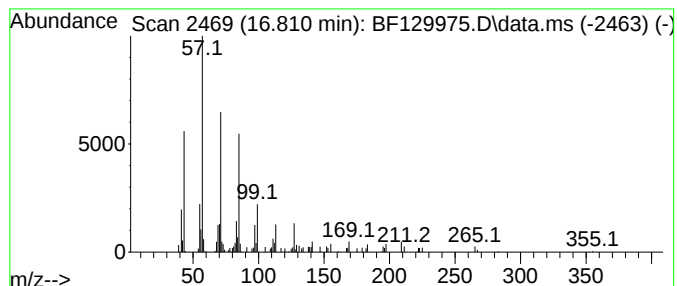
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Peak Number 5 Heneicosane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.810 | 2.60 ng | 101360 | Perylene-d12     | 15.386 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm | CAS#         | Qual |
|------|----|---|------------------------|-----|---------|--------------|------|
| 1    |    |   | Heneicosane            | 296 | C21H44  | 000629-94-7  | 90   |
| 2    |    |   | Heptadecane, 3-methyl- | 254 | C18H38  | 006418-44-6  | 87   |
| 3    |    |   | Octacosane             | 394 | C28H58  | 000630-02-4  | 87   |
| 4    |    |   | Docosane, 1-iodo-      | 436 | C22H45I | 1000406-31-9 | 87   |
| 5    |    |   | Octacosane, 2-methyl-  | 408 | C29H60  | 001560-98-1  | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082422\  
Data File : BF129975.D  
Acq On : 24 Aug 2022 16:43  
Operator : CG\JU  
Sample : PB147203BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB147203BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF081422.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

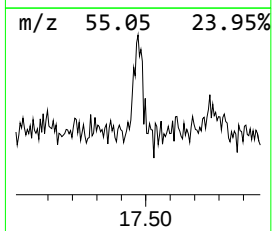
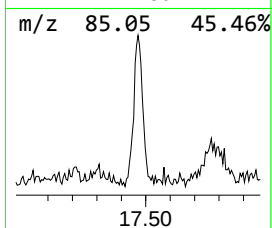
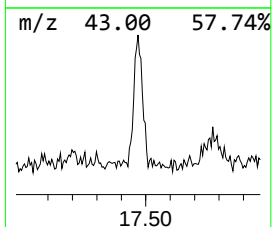
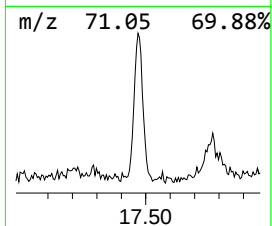
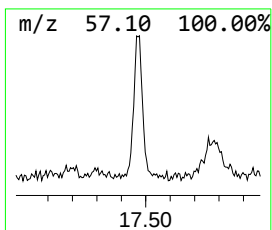
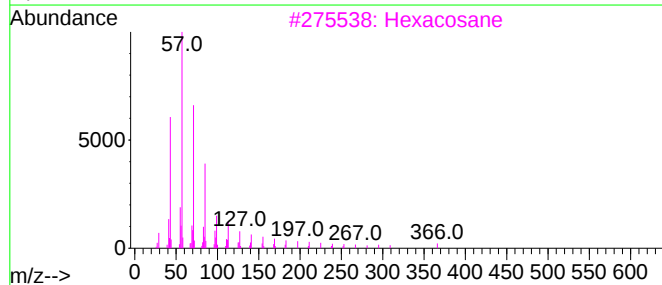
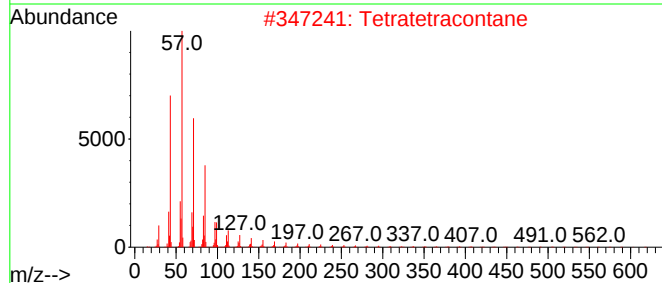
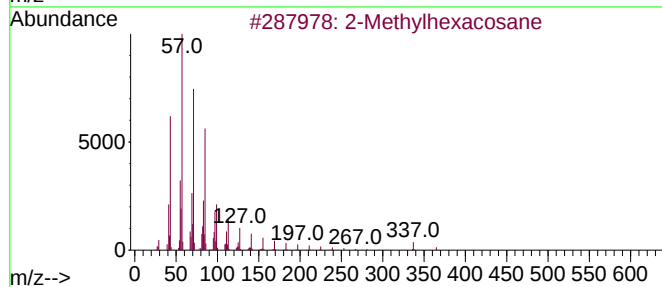
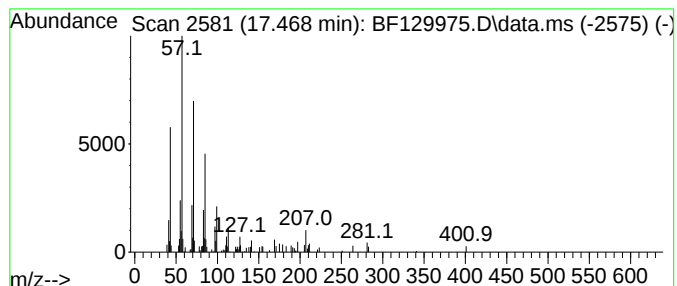
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 2-Methylhexacosane Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 17.468 | 2.25 ng | 87591 | Perylene-d12     | 15.386 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 2-Methylhexacosane                  | 380 | C27H56    | 001561-02-0  | 86   |
| 2    |    |   | Tetratetracontane                   | 619 | C44H90    | 007098-22-8  | 80   |
| 3    |    |   | Hexacosane                          | 366 | C26H54    | 000630-01-3  | 80   |
| 4    |    |   | Sulfurous acid, butyl tetradecyl... | 334 | C18H38O3S | 1010309-18-1 | 72   |
| 5    |    |   | Heptadecane, 9-octyl-               | 352 | C25H52    | 007225-64-1  | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF082422\  
Data File : BF129975.D  
Acq On : 24 Aug 2022 16:43  
Operator : CG\JU  
Sample : PB147203BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB147203BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF081422.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 |
| unknown14.727      | 14.727 | 2.4     | ng    | 94036    | 6                     | 15.386 | 778518 | 20.0 |
| Octacosane, 2-m... | 15.769 | 2.7     | ng    | 105136   | 6                     | 15.386 | 778518 | 20.0 |
| Hexacosane         | 16.245 | 3.3     | ng    | 126630   | 6                     | 15.386 | 778518 | 20.0 |
| (1,1'-Biphenyl)... | 16.604 | 3.8     | ng    | 147876   | 6                     | 15.386 | 778518 | 20.0 |
| Heneicosane        | 16.810 | 2.6     | ng    | 101360   | 6                     | 15.386 | 778518 | 20.0 |
| 2-Methylhexacosane | 17.468 | 2.3     | ng    | 87591    | 6                     | 15.386 | 778518 | 20.0 |