

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030519\  
 Data File : BM019054.D  
 Acq On : 06 Mar 2019 03:03  
 Operator : JU/SJ  
 Sample : K1704-08  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PST-028-SW002-022719

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA\_M\METHODS\8270-BM021119.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 5.269       | 365           | 371         | 388          | rBV      | 3646680        | 5273530       | 54.13%          | 7.596%        |
| 2         | 6.851       | 633           | 640         | 658          | rBV      | 3622939        | 5722810       | 58.74%          | 8.244%        |
| 3         | 7.204       | 692           | 700         | 718          | rBV      | 3673237        | 5944881       | 61.02%          | 8.564%        |
| 4         | 7.675       | 773           | 780         | 788          | rBV      | 815925         | 1314918       | 13.50%          | 1.894%        |
| 5         | 7.986       | 825           | 833         | 842          | rBV      | 2572977        | 4109343       | 42.18%          | 5.919%        |
| 6         | 8.839       | 971           | 978         | 996          | rBV      | 1942238        | 3333683       | 34.22%          | 4.802%        |
| 7         | 10.457      | 1246          | 1253        | 1268         | rBV      | 955305         | 1752909       | 17.99%          | 2.525%        |
| 8         | 12.939      | 1668          | 1675        | 1697         | rBV      | 4535680        | 6666371       | 68.43%          | 9.603%        |
| 9         | 13.792      | 1815          | 1820        | 1833         | rBV      | 162674         | 260911        | 2.68%           | 0.376%        |
| 10        | 14.327      | 1904          | 1911        | 1928         | rBV2     | 1437641        | 2273335       | 23.34%          | 3.275%        |
| 11        | 15.827      | 2159          | 2166        | 2185         | rBV      | 3815742        | 5990474       | 61.49%          | 8.629%        |
| 12        | 17.080      | 2373          | 2379        | 2384         | rBV      | 1942013        | 2790538       | 28.64%          | 4.020%        |
| 13        | 17.121      | 2384          | 2386        | 2396         | rVB      | 214040         | 281392        | 2.89%           | 0.405%        |
| 14        | 17.968      | 2525          | 2530        | 2535         | rBV      | 439571         | 652935        | 6.70%           | 0.941%        |
| 15        | 19.145      | 2725          | 2730        | 2738         | rVB      | 318721         | 462210        | 4.74%           | 0.666%        |
| 16        | 19.256      | 2744          | 2749        | 2753         | rBV      | 148223         | 206373        | 2.12%           | 0.297%        |
| 17        | 19.480      | 2783          | 2787        | 2789         | rBV2     | 84439          | 110557        | 1.13%           | 0.159%        |
| 18        | 19.509      | 2789          | 2792        | 2801         | rVB      | 325685         | 484124        | 4.97%           | 0.697%        |
| 19        | 19.715      | 2821          | 2827        | 2839         | rVB      | 8070667        | 9742020       | 100.00%         | 14.033%       |
| 20        | 20.009      | 2875          | 2877        | 2881         | rVB2     | 106382         | 125048        | 1.28%           | 0.180%        |
| 21        | 20.386      | 2938          | 2941        | 2948         | rVB9     | 68561          | 115068        | 1.18%           | 0.166%        |
| 22        | 20.509      | 2959          | 2962        | 2966         | rBV      | 129503         | 143156        | 1.47%           | 0.206%        |
| 23        | 20.974      | 3037          | 3041        | 3052         | rBV      | 1194308        | 1555784       | 15.97%          | 2.241%        |
| 24        | 21.274      | 3086          | 3092        | 3097         | rBV      | 2899168        | 4036123       | 41.43%          | 5.814%        |
| 25        | 21.415      | 3112          | 3116        | 3125         | rBV2     | 230285         | 372691        | 3.83%           | 0.537%        |
| 26        | 21.844      | 3186          | 3189        | 3191         | rBV      | 201688         | 249196        | 2.56%           | 0.359%        |
| 27        | 21.868      | 3191          | 3193        | 3202         | rVB5     | 295342         | 447244        | 4.59%           | 0.644%        |
| 28        | 22.303      | 3264          | 3267        | 3272         | rVB      | 239950         | 286765        | 2.94%           | 0.413%        |
| 29        | 22.809      | 3349          | 3353        | 3356         | rBV      | 268540         | 367115        | 3.77%           | 0.529%        |
| 30        | 23.374      | 3446          | 3449        | 3453         | rVB      | 178218         | 240622        | 2.47%           | 0.347%        |
| 31        | 23.521      | 3467          | 3474        | 3489         | rVB      | 1891082        | 3622727       | 37.19%          | 5.219%        |
| 32        | 24.109      | 3571          | 3574        | 3587         | rVB3     | 227499         | 485777        | 4.99%           | 0.700%        |

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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\_M\METHODS\8270-BM021119.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

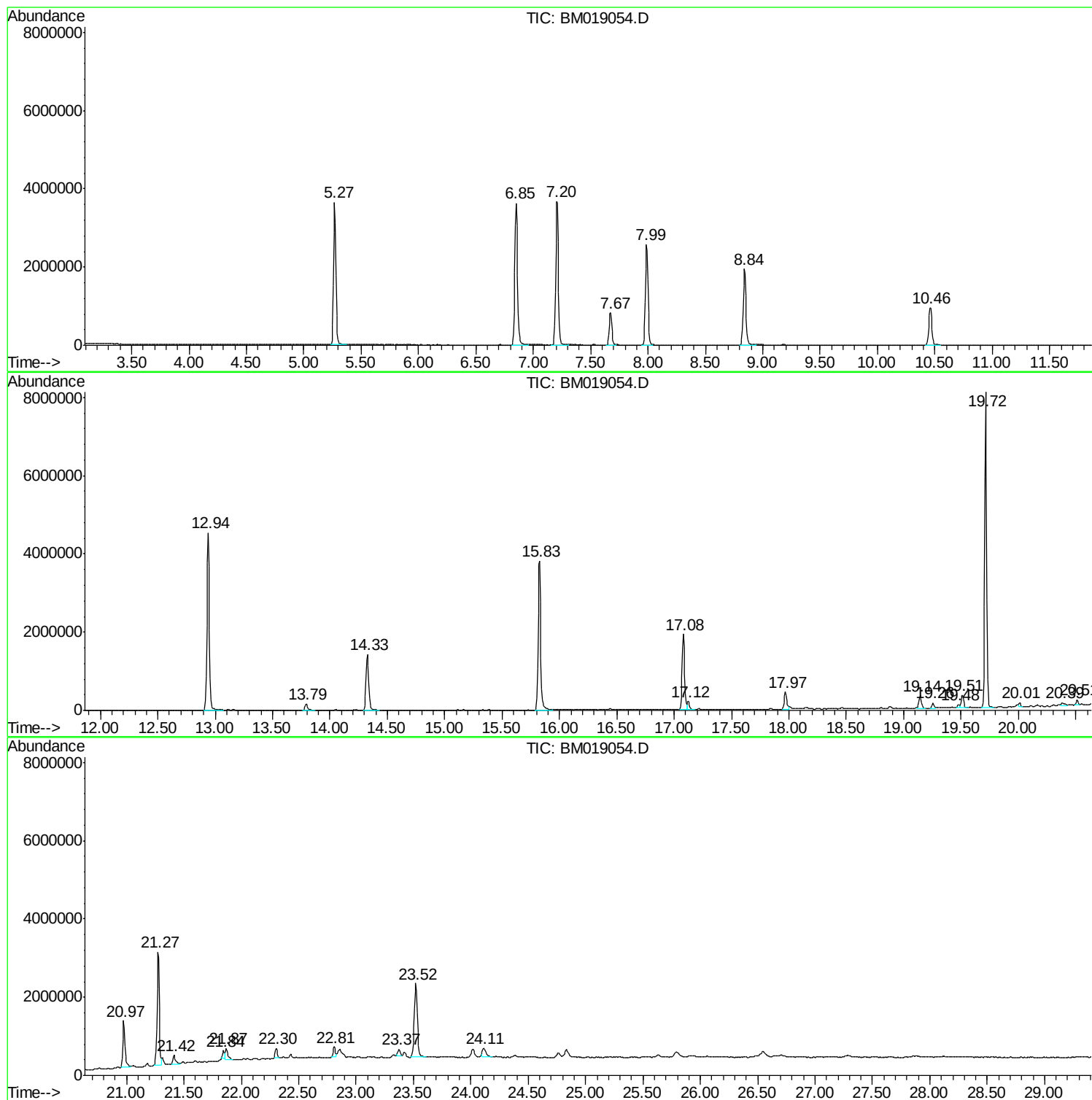
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M  
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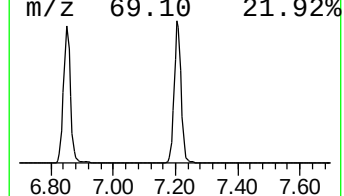
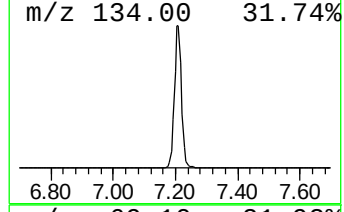
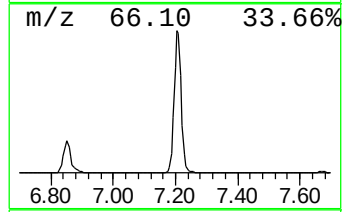
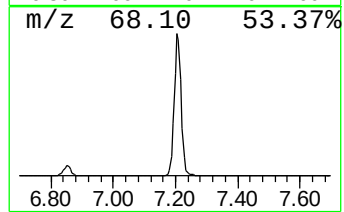
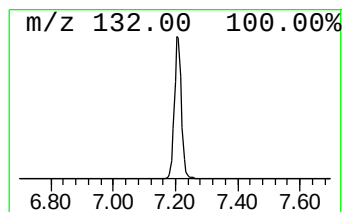
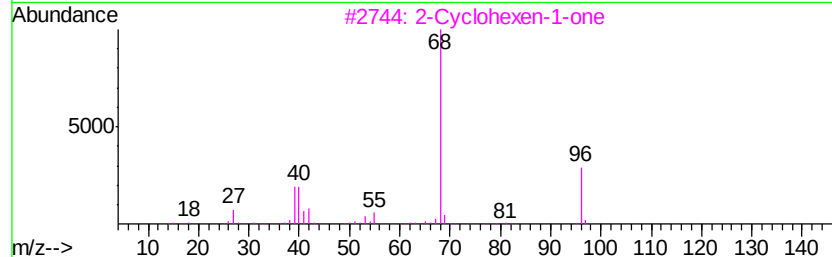
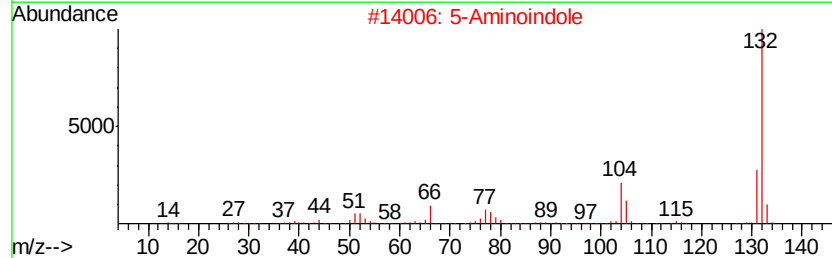
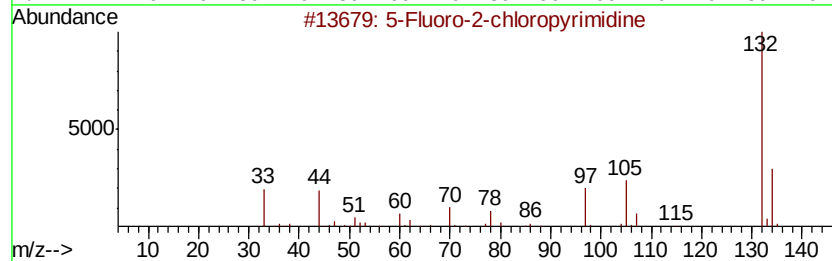
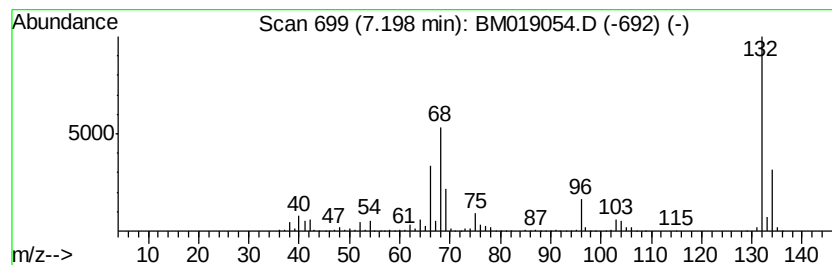
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown7.20 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.20 | 90.42 ng | 5944880 | 1,4-Dichlorobenzene-d4 | 7.67 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#        | Qual |
|------|----|----------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0 | 12   |
| 2    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0 | 10   |
| 3    |    | 2-Cyclohexen-1-one               | 96  | C6H8O     | 000930-68-7 | 10   |
| 4    |    | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12    | 005379-20-4 | 9    |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5 | 9    |



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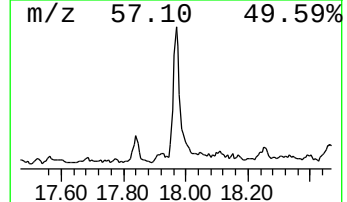
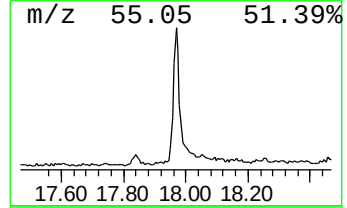
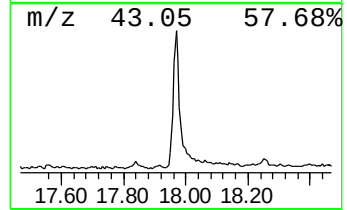
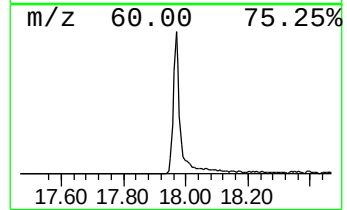
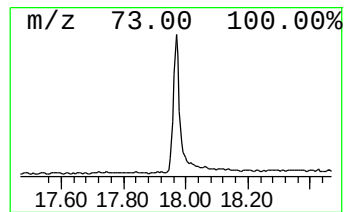
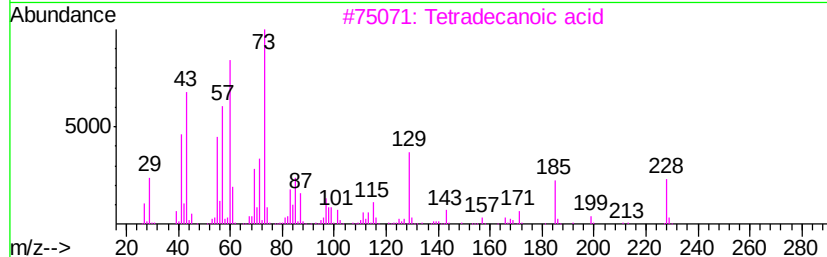
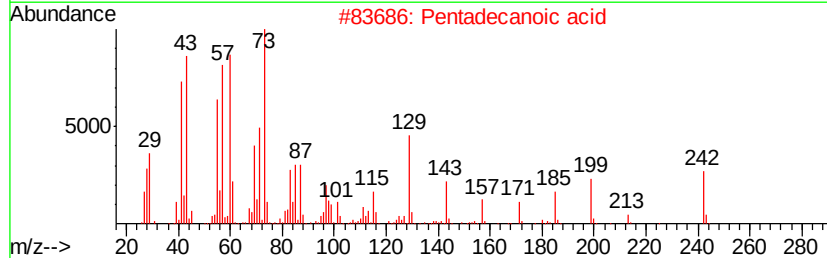
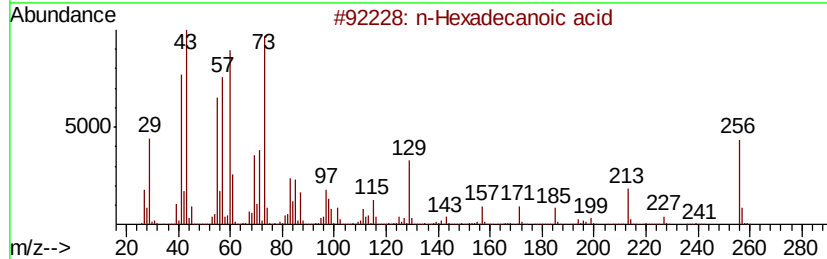
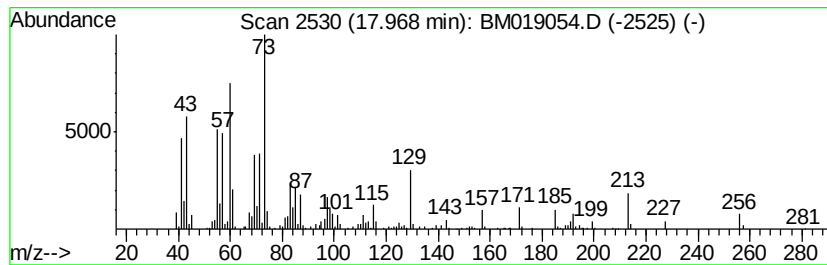
Instrument :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T.      | EstConc             | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------|--------|------------------|-------------|------|
| 17.97     | 4.68 ng             | 652935 | Phenanthrene-d10 | 17.08       |      |
| Hit# of 5 | Tentative ID        | MW     | MolForm          | CAS#        | Qual |
| 1         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 98   |
| 2         | Pentadecanoic acid  | 242    | C15H30O2         | 001002-84-2 | 83   |
| 3         | Tetradecanoic acid  | 228    | C14H28O2         | 000544-63-8 | 64   |
| 4         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 64   |
| 5         | n-Decanoic acid     | 172    | C10H20O2         | 000334-48-5 | 59   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M  
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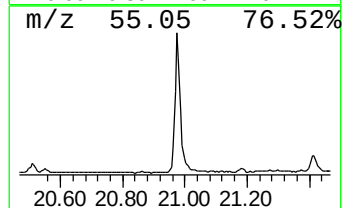
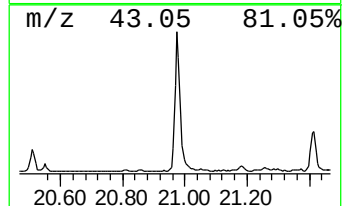
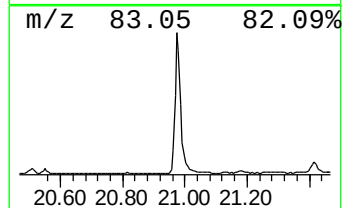
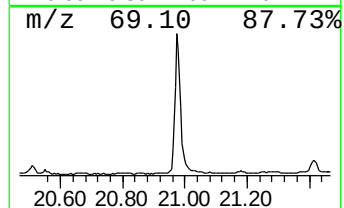
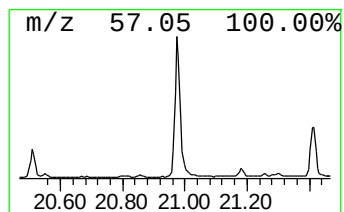
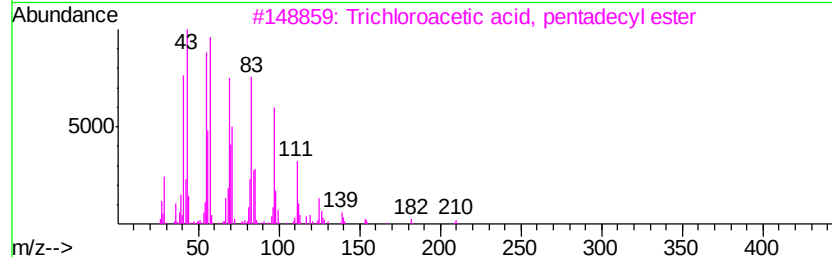
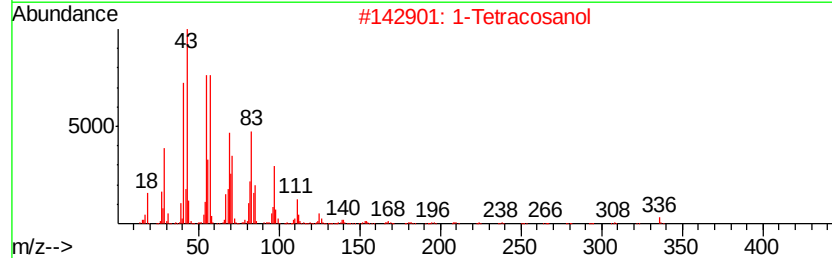
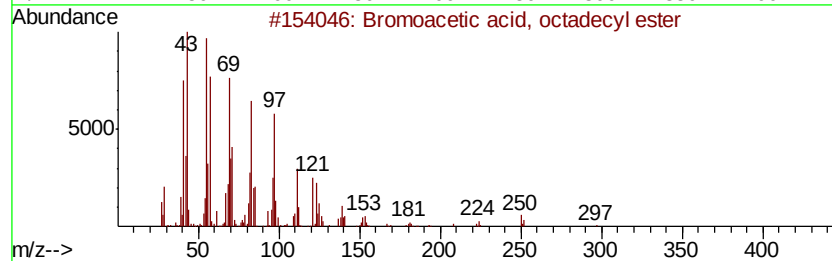
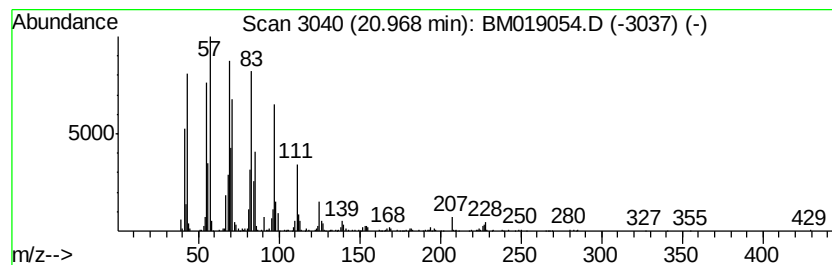
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Bromoacetic acid, octadecyl... Concentration Rank 3

| R.T.  | EstConc | Area    | Relative to ISTD | R.T.  |
|-------|---------|---------|------------------|-------|
| 20.97 | 7.71 ng | 1555780 | Chrysene-d12     | 21.27 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|-------------------------------------|-----|-------------|-------------|------|
| 1    | 5  | Bromoacetic acid, octadecyl ester   | 390 | C20H39BrO2  | 018992-03-5 | 91   |
| 2    |    | 1-Tetracosanol                      | 354 | C24H50O     | 000506-51-4 | 91   |
| 3    |    | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91   |
| 4    |    | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91   |
| 5    |    | 3-Eicosene, (E)-                    | 280 | C20H40      | 074685-33-9 | 90   |



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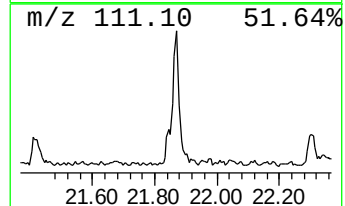
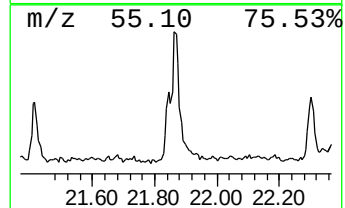
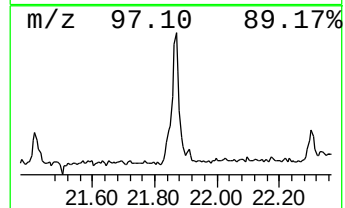
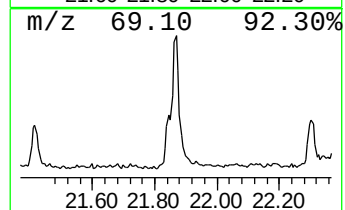
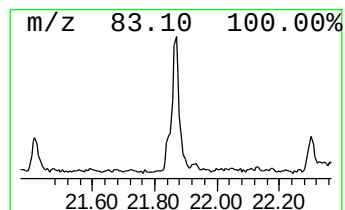
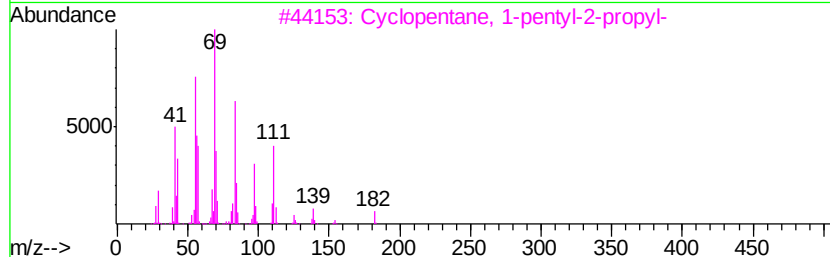
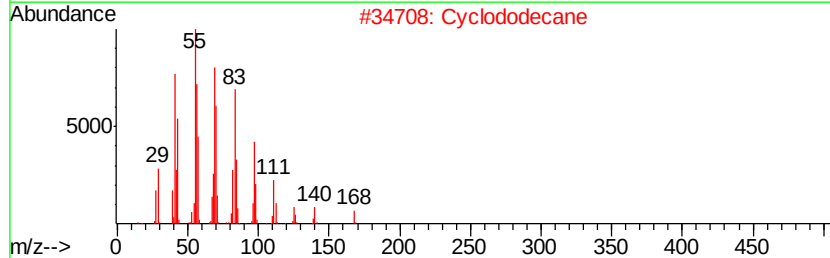
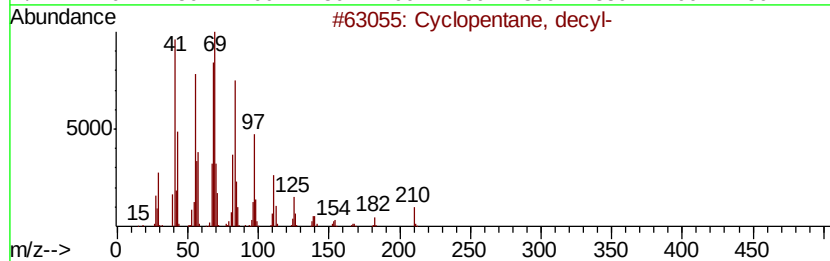
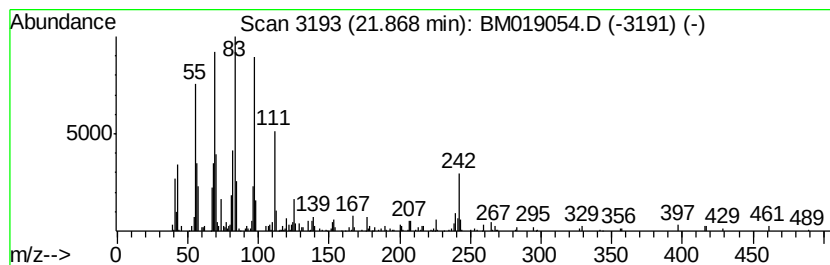
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Cyclopentane, decyl- Concentration Rank 6

| R.T.    | EstConc | Area                             | Relative to ISTD | R.T.           |
|---------|---------|----------------------------------|------------------|----------------|
| 21.87   | 2.22 ng | 447244                           | Chrysene-d12     | 21.27          |
| Hit# of | 5       | Tentative ID                     | MW MolForm       | CAS# Qual      |
| 1       |         | Cyclopentane, decyl-             | 210 C15H30       | 001795-21-7 64 |
| 2       |         | Cyclododecane                    | 168 C12H24       | 000294-62-2 64 |
| 3       |         | Cyclopentane, 1-pentyl-2-propyl- | 182 C13H26       | 062199-51-3 55 |
| 4       |         | 1-Hexadecanol                    | 242 C16H34O      | 036653-82-4 52 |
| 5       |         | Cyclopentane, nonyl-             | 196 C14H28       | 002882-98-6 49 |



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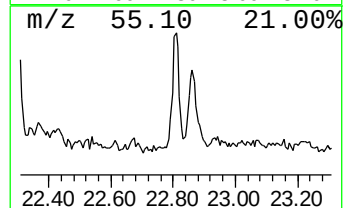
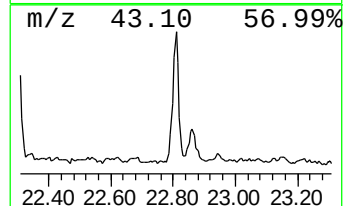
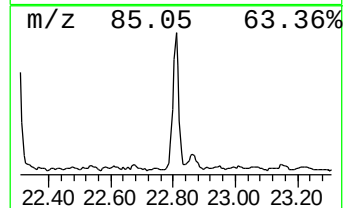
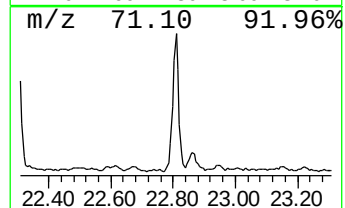
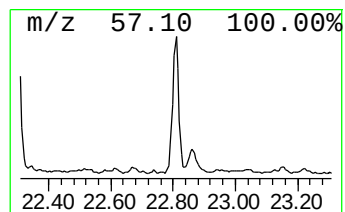
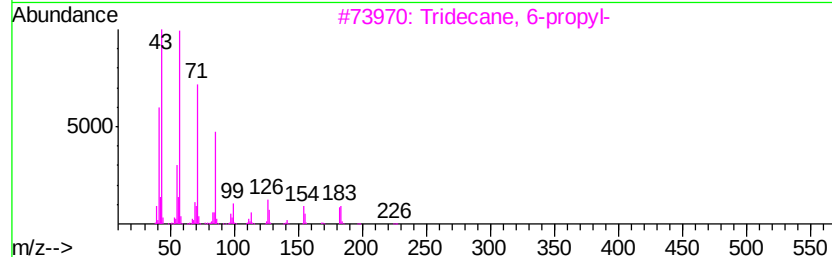
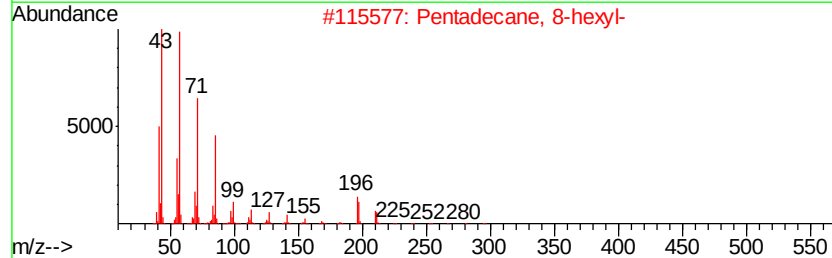
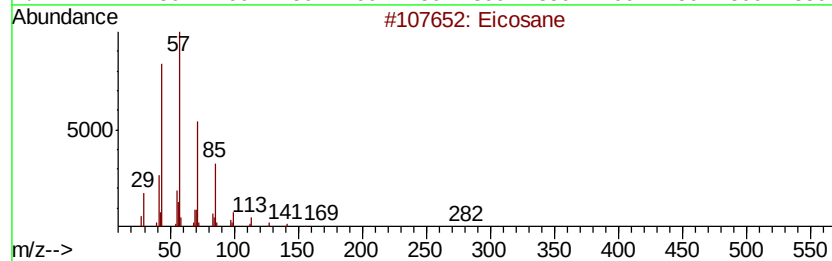
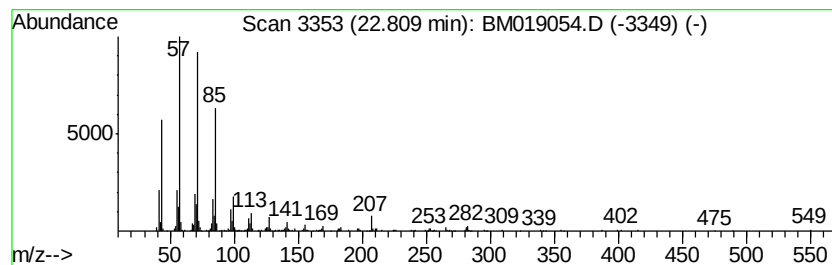
Instrument :  
BNA\_M  
ClientSampleId :  
PST-028-SW002-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 Eicosane Concentration Rank 7

| R.T.      | EstConc                          | Area   | Relative to ISTD | R.T.        |      |
|-----------|----------------------------------|--------|------------------|-------------|------|
| 22.81     | 2.03 ng                          | 367115 | Perylene-d12     | 23.52       |      |
| Hit# of 5 | Tentative ID                     | MW     | MolForm          | CAS#        | Qual |
| 1         | Eicosane                         | 282    | C20H42           | 000112-95-8 | 93   |
| 2         | Pentadecane, 8-hexyl-            | 296    | C21H44           | 013475-75-7 | 91   |
| 3         | Tridecane, 6-propyl-             | 226    | C16H34           | 055045-10-8 | 91   |
| 4         | Heneicosane, 11-(1-ethylpropyl)- | 366    | C26H54           | 055282-11-6 | 91   |
| 5         | Hexadecane                       | 226    | C16H34           | 000544-76-3 | 83   |





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030519\  
Data File : BM019054.D  
Acq On : 06 Mar 2019 03:03  
Operator : JU/SJ  
Sample : K1704-08  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

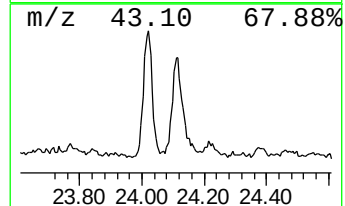
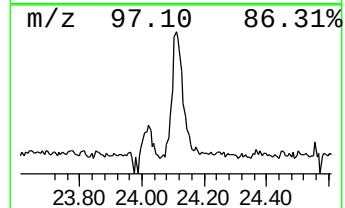
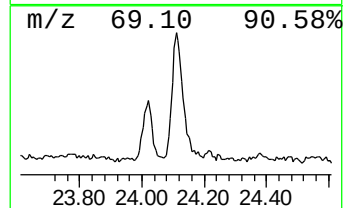
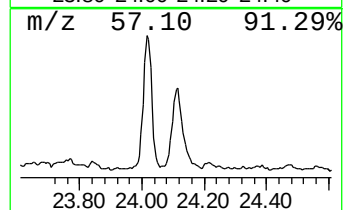
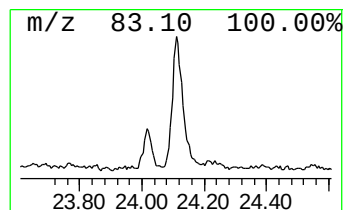
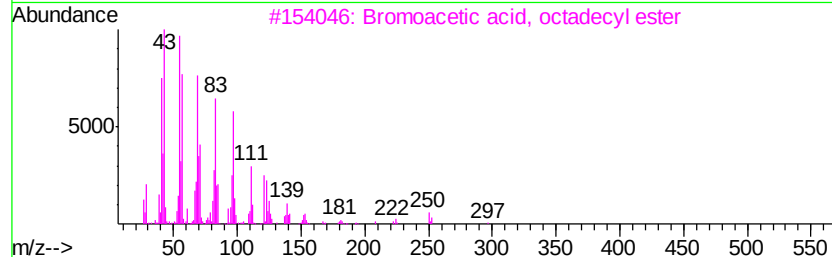
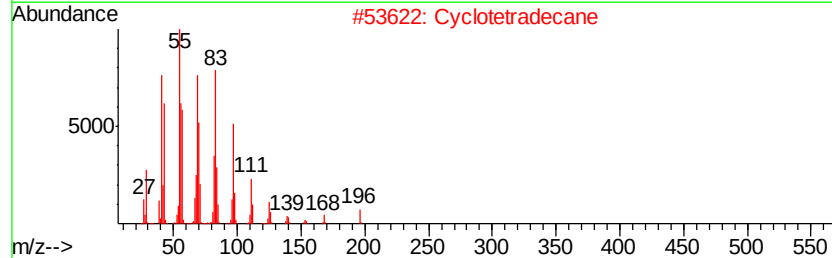
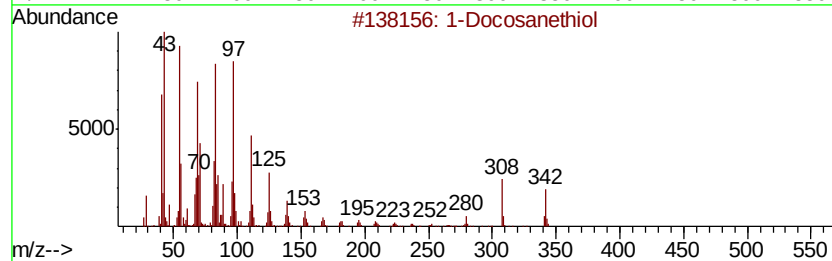
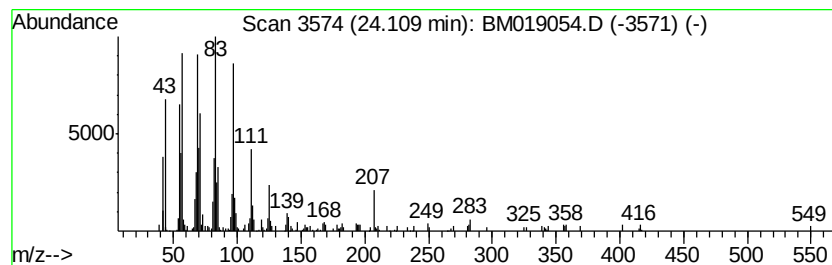
Instrument :  
BNA\_M  
ClientSampleId :  
PST-028-SW002-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 1-Docosanethiol Concentration Rank 5

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|-------------|------|
| 24.11     | 2.68 ng                             | 485777 | Perylene-d12     | 23.52       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#        | Qual |
| 1         | 1-Docosanethiol                     | 342    | C22H46S          | 007773-83-3 | 91   |
| 2         | Cyclotetradecane                    | 196    | C14H28           | 000295-17-0 | 90   |
| 3         | Bromoacetic acid, octadecyl ester   | 390    | C20H39BrO2       | 018992-03-5 | 87   |
| 4         | 3-Eicosene, (E)-                    | 280    | C20H40           | 074685-33-9 | 83   |
| 5         | 2- Chloropropionic acid, octadec... | 360    | C21H41ClO2       | 088104-31-8 | 83   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_M\DATA\BM030519\  
Data File : BM019054.D  
Acq On : 06 Mar 2019 03:03  
Operator : JU/SJ  
Sample : K1704-08  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PST-028-SW002-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_M\METHODS\8270-BM021119.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| unknown7.20          | 7.20  | 90.4    | ng    | 5944880  | 1                     | 7.67  | 1314920 | 20.0 |
| n-Hexadecanoic acid  | 17.97 | 4.7     | ng    | 652935   | 4                     | 17.08 | 2790540 | 20.0 |
| Bromoacetic acid,... | 20.97 | 7.7     | ng    | 1555780  | 5                     | 21.27 | 4036120 | 20.0 |
| Cyclopentane, decyl- | 21.87 | 2.2     | ng    | 447244   | 5                     | 21.27 | 4036120 | 20.0 |
| Eicosane             | 22.81 | 2.0     | ng    | 367115   | 6                     | 23.52 | 3622730 | 20.0 |
| 1-Docosanethiol      | 24.11 | 2.7     | ng    | 485777   | 6                     | 23.52 | 3622730 | 20.0 |