

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF070623\  
 Data File : BF134110.D  
 Acq On : 06 Jul 2023 22:28  
 Operator : CG\JU  
 Sample : 03475-03  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 ALDENE-COMP-2

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134110.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         | 2.193       | 11            | 18          | 28           | rVB      | 803183         | 1149672       | 45.48%          | 6.140%        |
| 2         | 2.310       | 34            | 38          | 45           | rVB3     | 22311          | 33097         | 1.31%           | 0.177%        |
| 3         | 5.098       | 508           | 512         | 521          | rVB      | 88573          | 122928        | 4.86%           | 0.656%        |
| 4         | 5.487       | 573           | 578         | 581          | rBV      | 2428122        | 2190052       | 86.63%          | 11.696%       |
| 5         | 6.481       | 742           | 747         | 750          | rBV      | 2317234        | 2215187       | 87.63%          | 11.830%       |
| 6         | 6.845       | 805           | 809         | 817          | rBV      | 741226         | 598216        | 23.66%          | 3.195%        |
| 7         | 7.410       | 900           | 905         | 908          | rBV      | 1461538        | 1445303       | 57.17%          | 7.718%        |
| 8         | 8.122       | 1023          | 1026        | 1038         | rVB      | 888274         | 770866        | 30.49%          | 4.117%        |
| 9         | 9.204       | 1205          | 1210        | 1213         | rBV      | 2870882        | 2527916       | 100.00%         | 13.500%       |
| 10        | 9.880       | 1321          | 1325        | 1335         | rBV      | 1017324        | 846328        | 33.48%          | 4.520%        |
| 11        | 10.598      | 1443          | 1447        | 1456         | rBV      | 202958         | 168537        | 6.67%           | 0.900%        |
| 12        | 10.675      | 1456          | 1460        | 1472         | rBV      | 2029278        | 1816821       | 71.87%          | 9.702%        |
| 13        | 11.374      | 1575          | 1579        | 1587         | rBV      | 997019         | 881422        | 34.87%          | 4.707%        |
| 14        | 11.904      | 1666          | 1669        | 1674         | rBV      | 132540         | 126780        | 5.02%           | 0.677%        |
| 15        | 12.974      | 1846          | 1851        | 1854         | rBV      | 2876758        | 2527606       | 99.99%          | 13.498%       |
| 16        | 13.921      | 2007          | 2012        | 2024         | rBV6     | 36969          | 109671        | 4.34%           | 0.586%        |
| 17        | 14.033      | 2027          | 2031        | 2039         | rVB      | 713482         | 655585        | 25.93%          | 3.501%        |
| 18        | 15.539      | 2281          | 2287        | 2297         | rBV      | 387984         | 539519        | 21.34%          | 2.881%        |

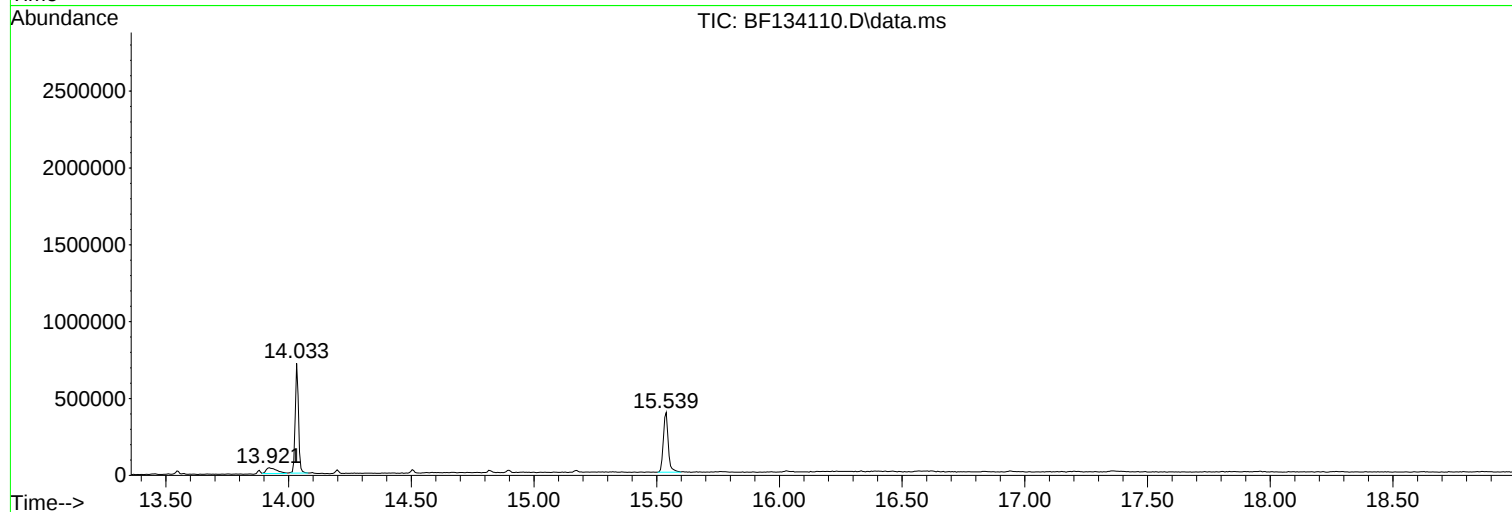
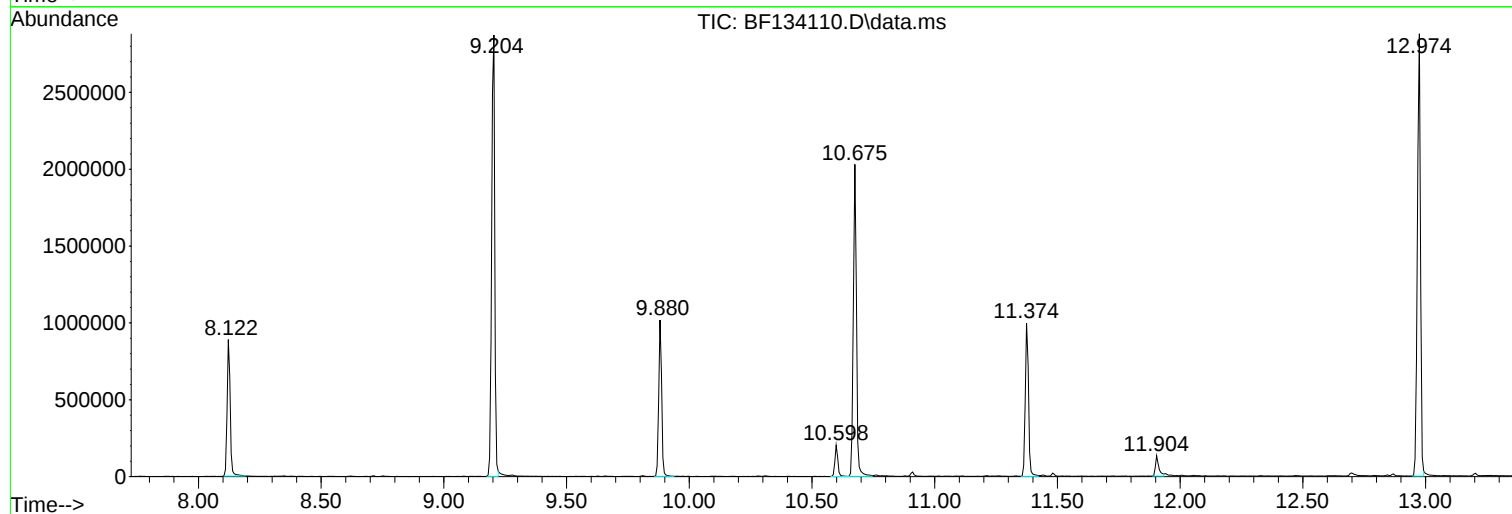
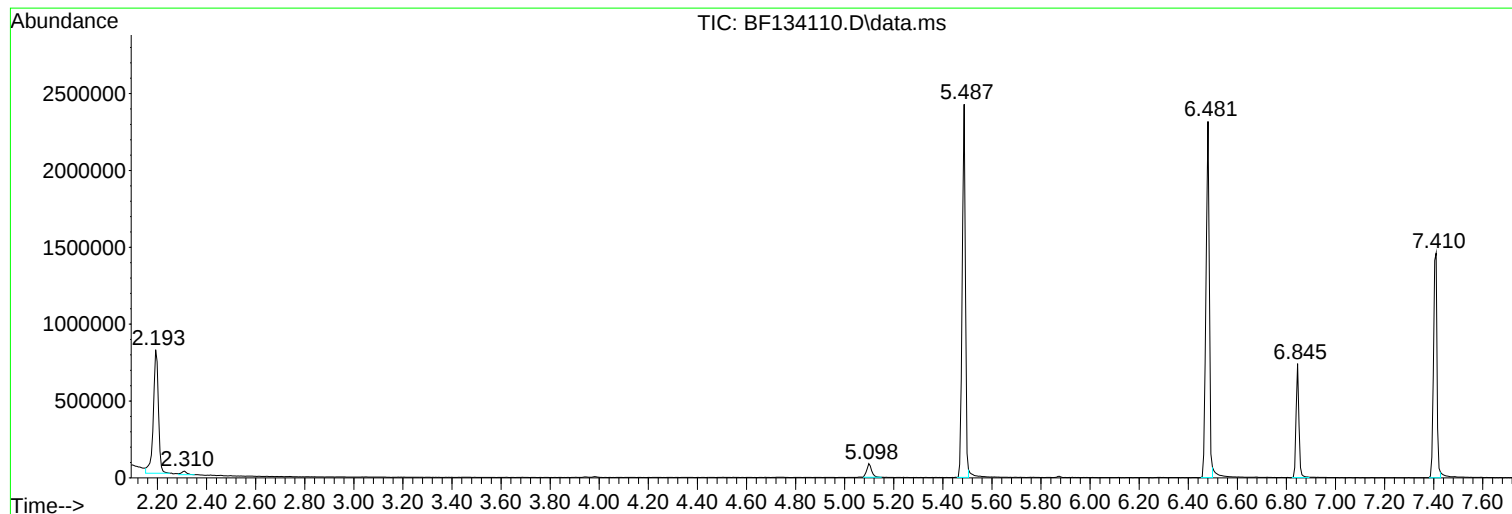
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BNA\_F  
ClientSampleId :  
ALDENE-COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062623.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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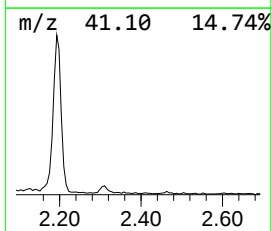
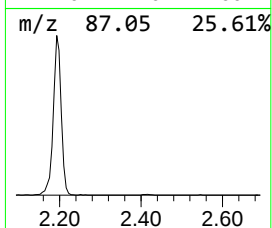
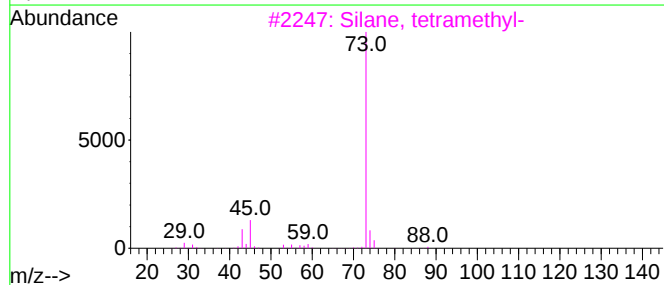
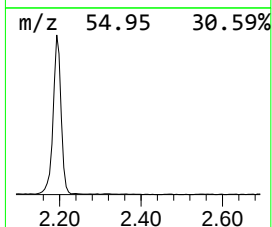
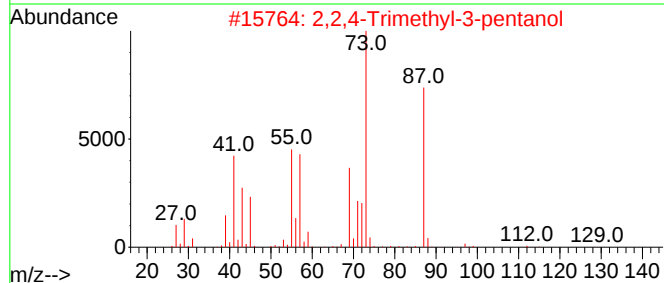
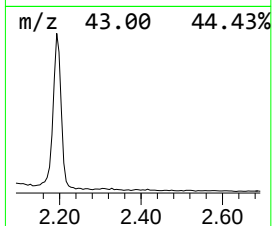
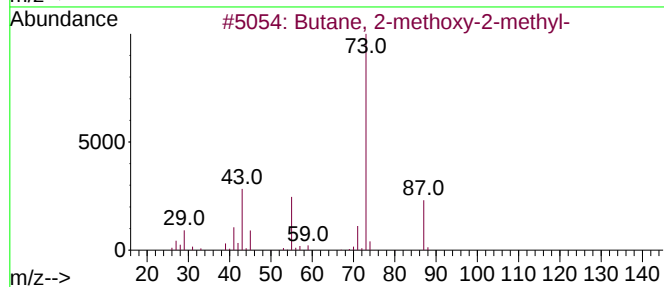
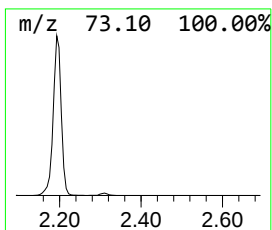
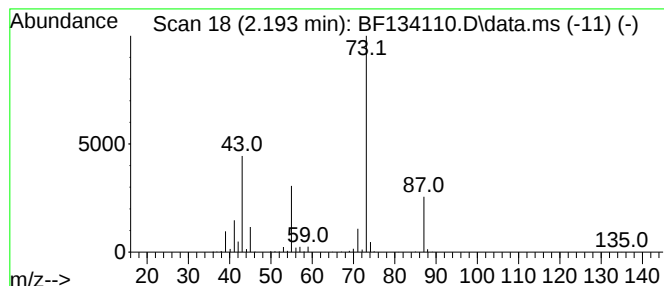
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.193 | 38.44 ng | 1149670 | 1,4-Dichlorobenzene-d4 | 6.845 |

| 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 | 39   |
| 3    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 38   |
| 4    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 25   |
| 5    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

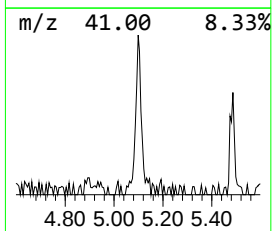
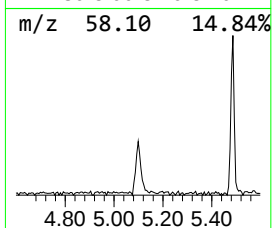
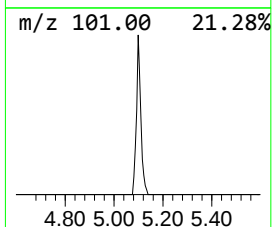
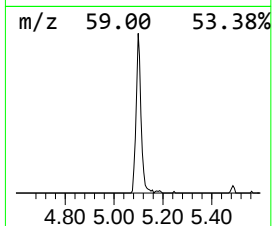
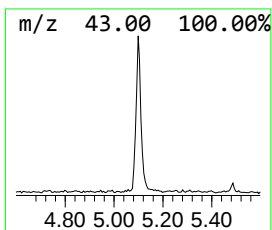
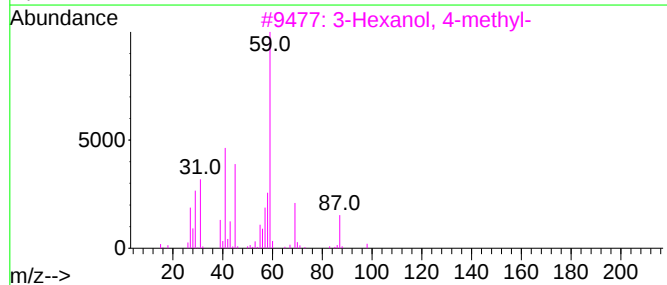
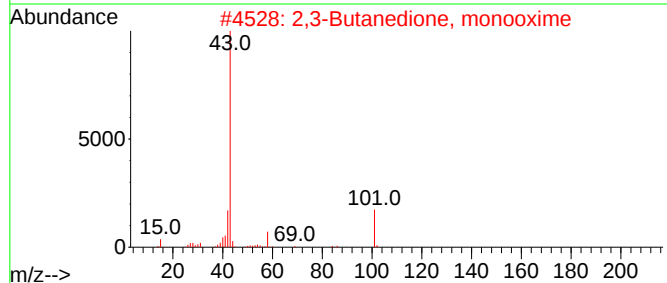
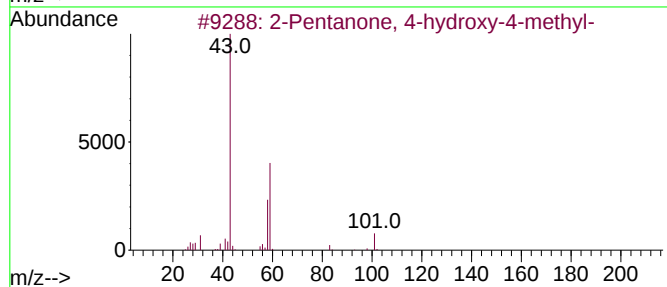
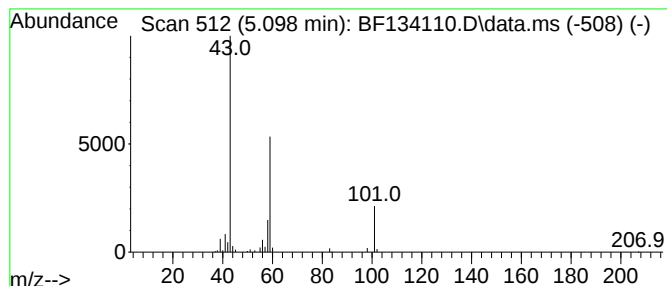
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.098 | 4.11 ng | 122928 | 1,4-Dichlorobenzene-d4 | 6.845 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 35      |      |      |
| 3    | 3-Hexanol, 4-methyl-                | 116 | C7H16O       | 000615-29-2 | 28      |      |      |
| 4    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 23      |      |      |
| 5    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |



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ClientSampleId :  
ALDENE-COMP-2

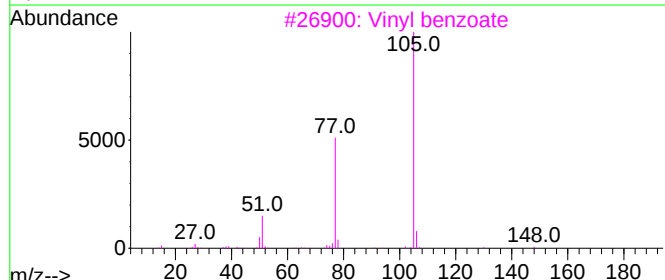
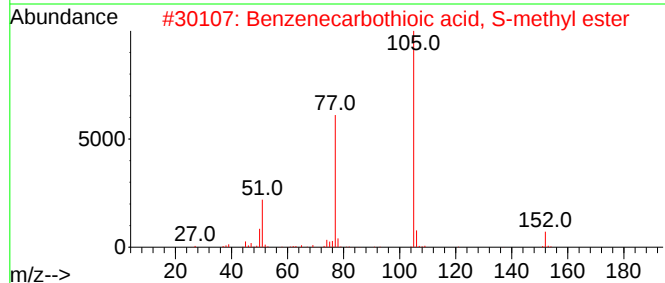
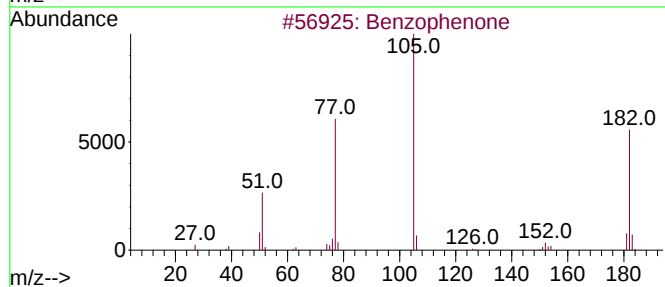
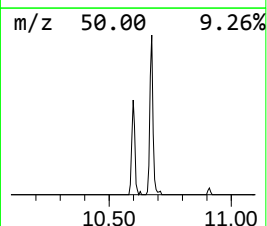
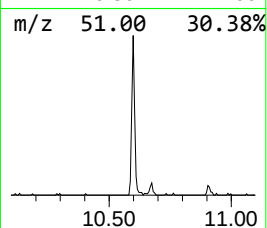
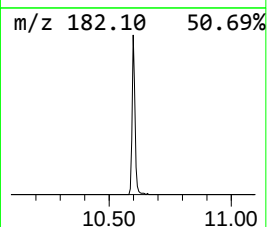
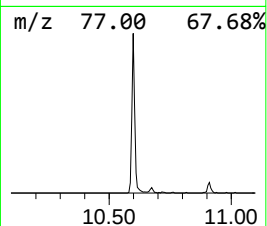
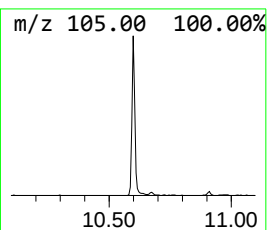
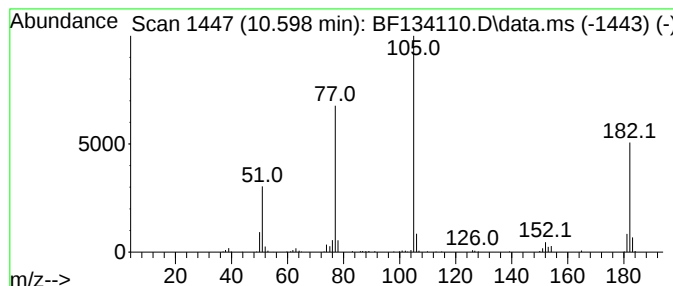
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Benzophenone Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.598 | 3.98 ng | 168537 | Acenaphthene-d10 | 9.880 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O    | 000119-61-9  | 96   |
| 2    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS     | 005925-68-8  | 52   |
| 3    |    |   | Vinyl benzoate                      | 148 | C9H8O2     | 000769-78-8  | 50   |
| 4    |    |   | acetic acid, 2-bromo-, 2-oxo-2-p... | 256 | C10H9BrO3  | 1000401-50-0 | 50   |
| 5    |    |   | Disulfide, dibenzoyl                | 274 | C14H10O2S2 | 000644-32-6  | 50   |



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ALDENE-COMP-2

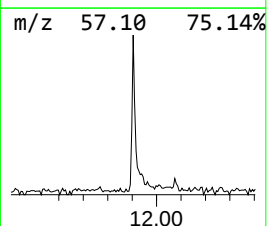
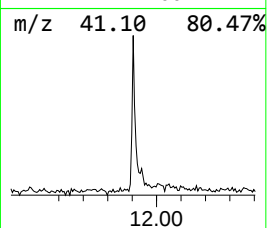
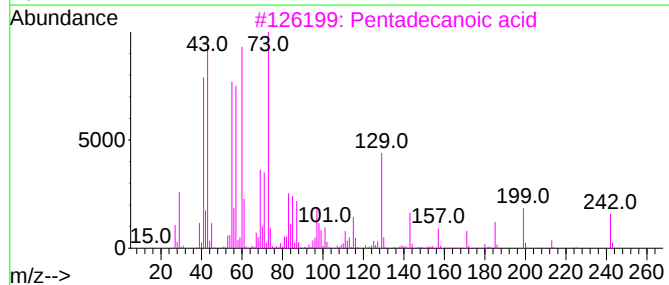
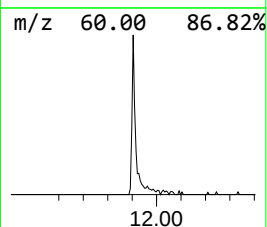
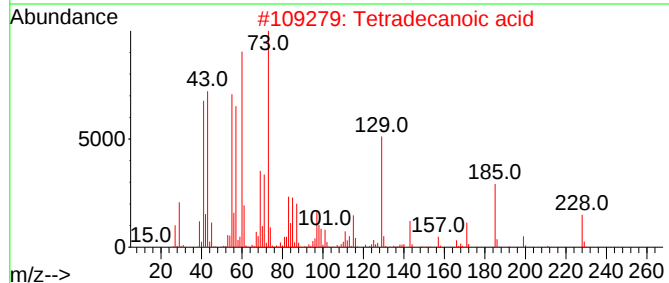
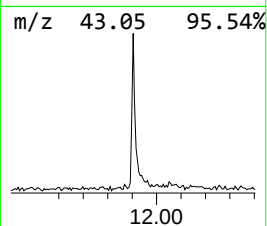
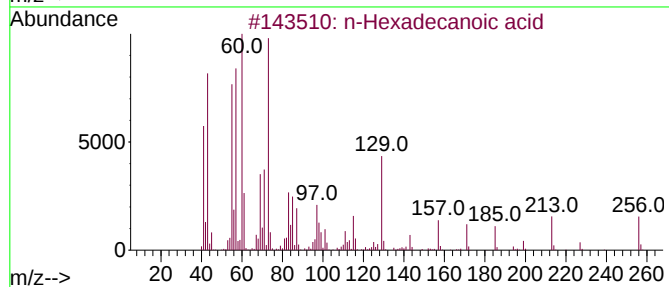
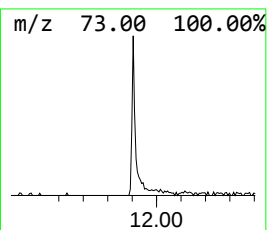
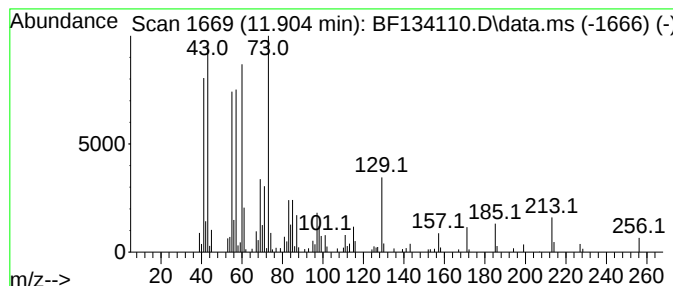
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.904 | 2.88 ng | 126780 | Phenanthrene-d10 | 11.374 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|------|---------------------|-----|----------|-------------|------|
| 1    |      | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |      | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 94   |
| 3    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |      | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 80   |
| 5    |      | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 72   |



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ALDENE-COMP-2

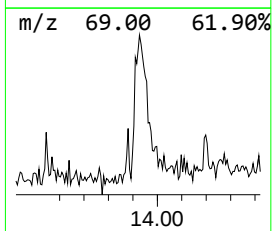
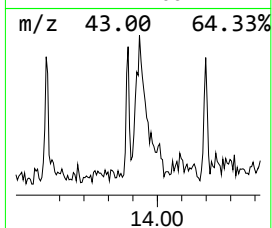
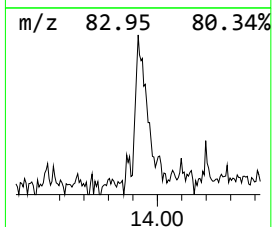
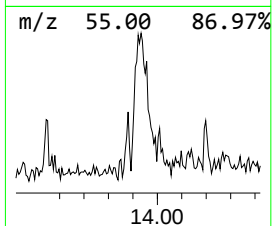
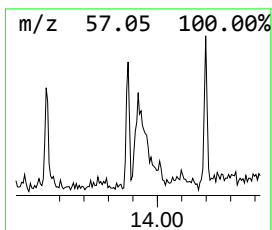
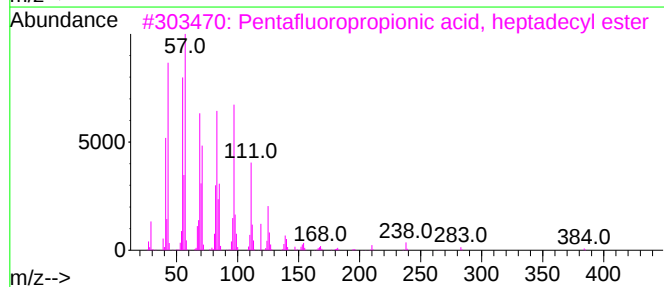
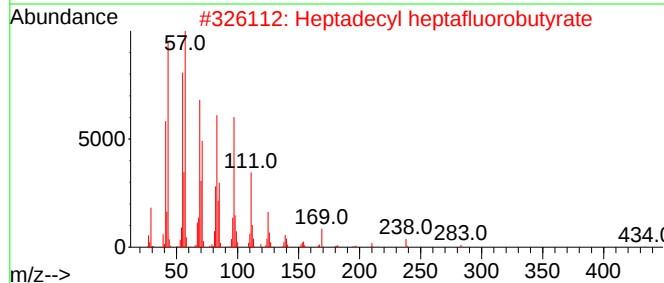
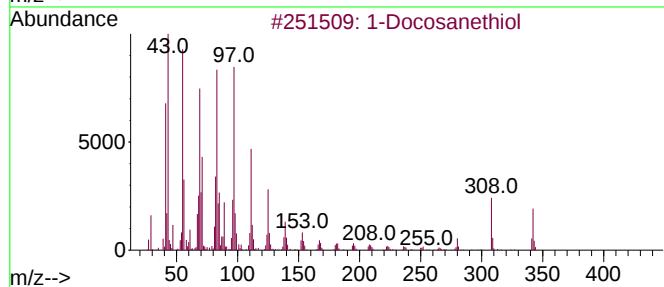
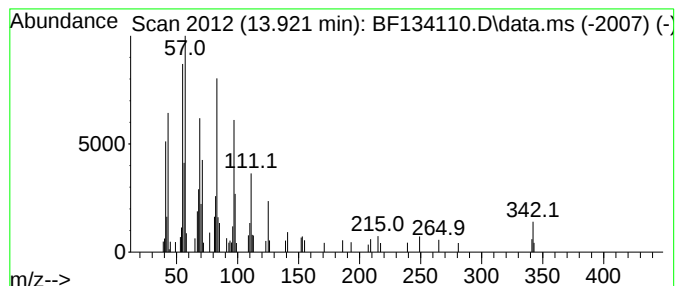
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Peak Number 5 1-Docosanethiol Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.921 | 3.35 ng | 109671 | Chrysene-d12     | 14.033 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 1-Docosanethiol                     | 342 | C22H46S    | 007773-83-3  | 89   |
| 2    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2 | 959085-66-6  | 58   |
| 3    |    |   | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1  | 52   |
| 4    |    |   | Tricosyl trifluoroacetate           | 436 | C25H47F3O2 | 1000351-75-1 | 52   |
| 5    |    |   | 17-Pentatriacontene                 | 491 | C35H70     | 006971-40-0  | 52   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF070623\  
Data File : BF134110.D  
Acq On : 06 Jul 2023 22:28  
Operator : CG\JU  
Sample : 03475-03  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
ALDENE-COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062623.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... | 2.193  | 38.4    | ng    | 1149670  | 1                     | 6.845  | 598216 | 20.0 |
| 2-Pentanone, 4-... | 5.098  | 4.1     | ng    | 122928   | 1                     | 6.845  | 598216 | 20.0 |
| Benzophenone       | 10.598 | 4.0     | ng    | 168537   | 3                     | 9.880  | 846328 | 20.0 |
| n-Hexadecanoic ... | 11.904 | 2.9     | ng    | 126780   | 4                     | 11.374 | 881422 | 20.0 |
| 1-Docosanethiol    | 13.921 | 3.4     | ng    | 109671   | 5                     | 14.033 | 655585 | 20.0 |