

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
 Data File : BM041233.D  
 Acq On : 01 Aug 2023 20:15  
 Operator : MA/JU  
 Sample : 03715-11  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 T843-CT-01

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\_M\Methods\8270-BM072823.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041233.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         | 5.375       | 365           | 372         | 383          | rBV      | 3205597        | 4445849       | 47.49%          | 5.892%        |
| 2         | 6.987       | 636           | 646         | 662          | rBV      | 3022757        | 4772758       | 50.98%          | 6.325%        |
| 3         | 7.798       | 777           | 784         | 791          | rBV      | 736806         | 1104118       | 11.79%          | 1.463%        |
| 4         | 8.975       | 976           | 984         | 996          | rBV      | 1767359        | 2907913       | 31.06%          | 3.854%        |
| 5         | 10.604      | 1254          | 1261        | 1267         | rBV      | 840119         | 1399290       | 14.95%          | 1.854%        |
| 6         | 13.086      | 1675          | 1683        | 1697         | rBV      | 4165439        | 6228873       | 66.54%          | 8.255%        |
| 7         | 13.927      | 1820          | 1826        | 1840         | rVB      | 158919         | 239254        | 2.56%           | 0.317%        |
| 8         | 14.116      | 1851          | 1858        | 1875         | rBV      | 435904         | 782706        | 8.36%           | 1.037%        |
| 9         | 14.463      | 1911          | 1917        | 1927         | rVB      | 1059465        | 1553854       | 16.60%          | 2.059%        |
| 10        | 14.892      | 1984          | 1990        | 2001         | rBV      | 95141          | 140132        | 1.50%           | 0.186%        |
| 11        | 15.839      | 2141          | 2151        | 2162         | rBV      | 2541558        | 3363826       | 35.93%          | 4.458%        |
| 12        | 15.968      | 2167          | 2173        | 2179         | rBV      | 3674656        | 4939978       | 52.77%          | 6.547%        |
| 13        | 17.227      | 2381          | 2387        | 2392         | rBV      | 1251642        | 1767858       | 18.88%          | 2.343%        |
| 14        | 17.821      | 2482          | 2488        | 2497         | rBV2     | 44819          | 151963        | 1.62%           | 0.201%        |
| 15        | 18.133      | 2535          | 2541        | 2550         | rBV      | 2874178        | 4020675       | 42.95%          | 5.328%        |
| 16        | 19.262      | 2729          | 2733        | 2735         | rBV      | 145413         | 187881        | 2.01%           | 0.249%        |
| 17        | 19.292      | 2735          | 2738        | 2746         | rVB      | 162297         | 301781        | 3.22%           | 0.400%        |
| 18        | 19.409      | 2754          | 2758        | 2778         | rBV      | 2365874        | 3386659       | 36.18%          | 4.488%        |
| 19        | 19.686      | 2799          | 2805        | 2810         | rVV      | 377114         | 617287        | 6.59%           | 0.818%        |
| 20        | 19.739      | 2810          | 2814        | 2829         | rVB      | 550697         | 1004368       | 10.73%          | 1.331%        |
| 21        | 19.862      | 2830          | 2835        | 2840         | rBV      | 7946990        | 9361509       | 100.00%         | 12.406%       |
| 22        | 20.162      | 2882          | 2886        | 2890         | rVB      | 230421         | 252462        | 2.70%           | 0.335%        |
| 23        | 20.562      | 2951          | 2954        | 2961         | rVB4     | 86434          | 110082        | 1.18%           | 0.146%        |
| 24        | 20.662      | 2967          | 2971        | 2974         | rBV      | 357671         | 413434        | 4.42%           | 0.548%        |
| 25        | 21.127      | 3046          | 3050        | 3057         | rBV      | 880298         | 1164026       | 12.43%          | 1.543%        |
| 26        | 21.333      | 3082          | 3085        | 3088         | rBV      | 143497         | 142543        | 1.52%           | 0.189%        |
| 27        | 21.427      | 3097          | 3101        | 3109         | rVB      | 1704639        | 2069161       | 22.10%          | 2.742%        |
| 28        | 21.568      | 3121          | 3125        | 3129         | rVB      | 496894         | 569901        | 6.09%           | 0.755%        |
| 29        | 22.021      | 3198          | 3202        | 3206         | rBV      | 545309         | 662539        | 7.08%           | 0.878%        |
| 30        | 22.509      | 3282          | 3285        | 3294         | rVB      | 481034         | 696268        | 7.44%           | 0.923%        |
| 31        | 23.050      | 3374          | 3377        | 3383         | rVB      | 369579         | 532546        | 5.69%           | 0.706%        |
| 32        | 23.803      | 3499          | 3505        | 3513         | rVB      | 1129498        | 2199735       | 23.50%          | 2.915%        |
| 33        | 24.238      | 3572          | 3579        | 3588         | rVB      | 2932155        | 5801386       | 61.97%          | 7.688%        |
| 34        | 28.221      | 4245          | 4256        | 4269         | rVB      | 2233164        | 8164731       | 87.22%          | 10.820%       |

Sum of corrected areas: 75457346

**Instrument :**

BNA\_M

**ClientSampleId :**

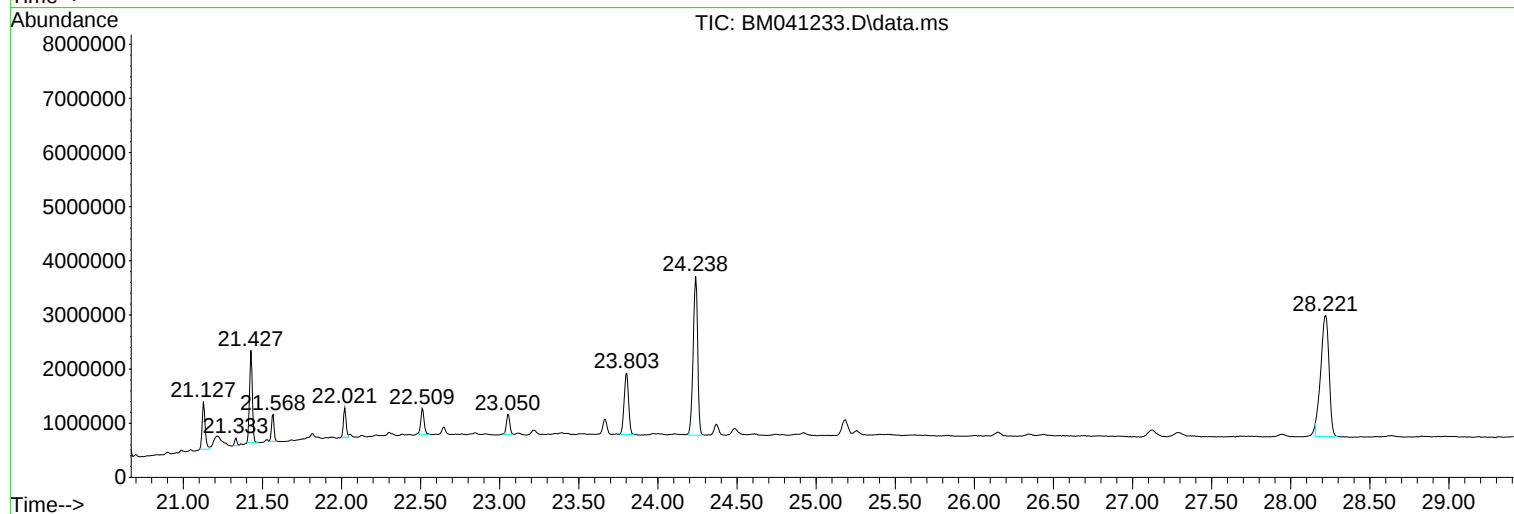
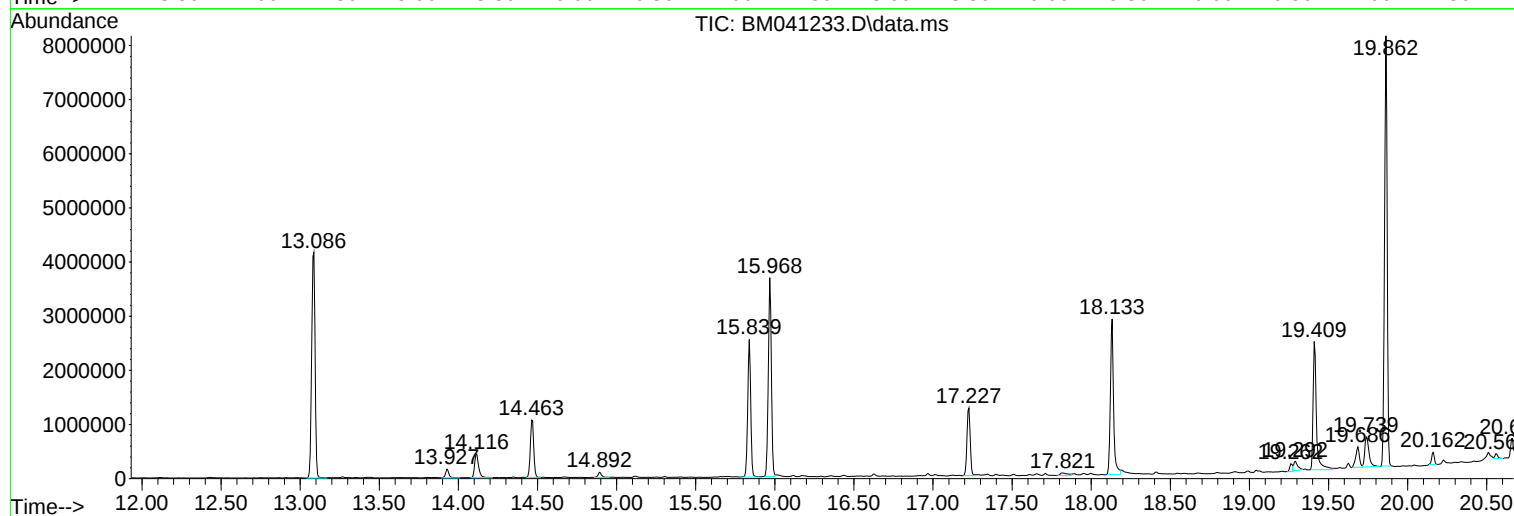
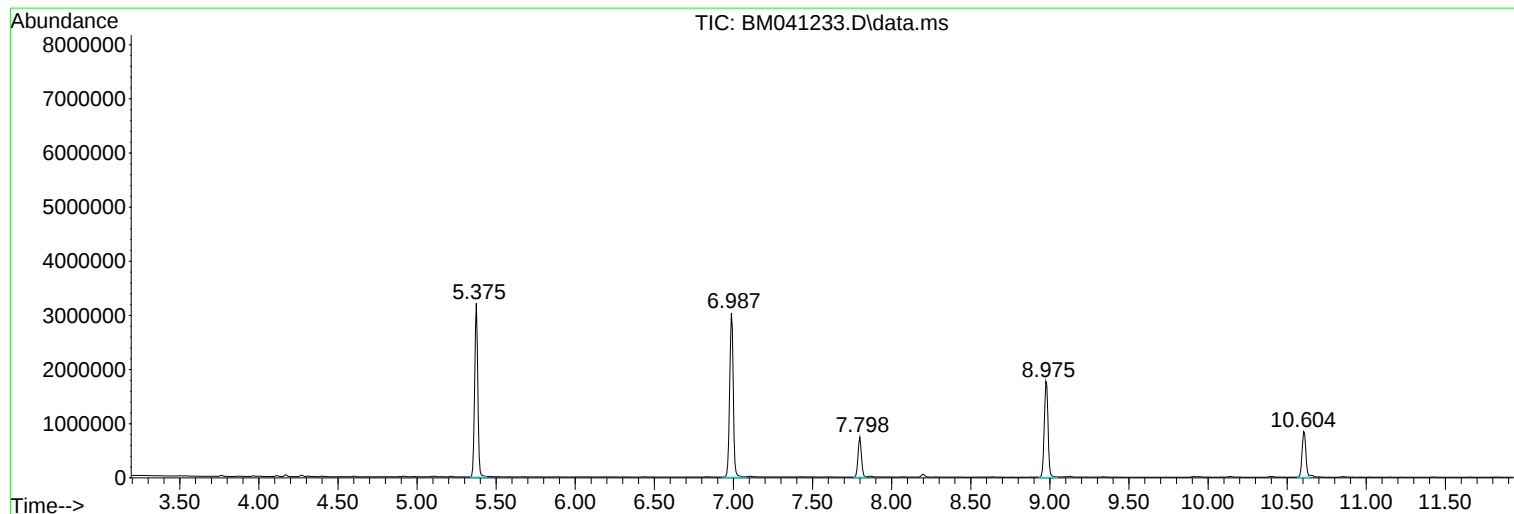
T843-CT-01

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

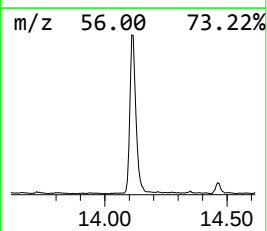
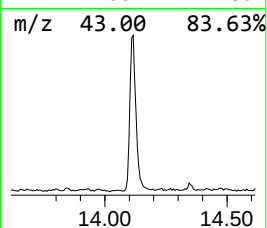
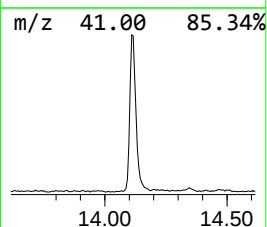
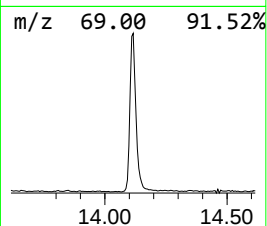
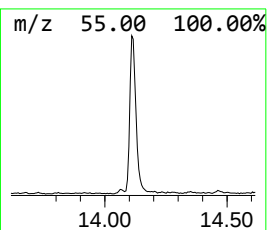
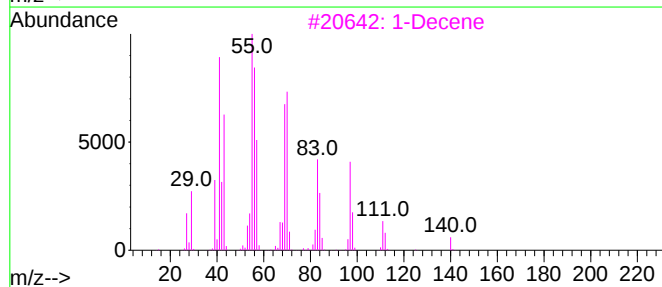
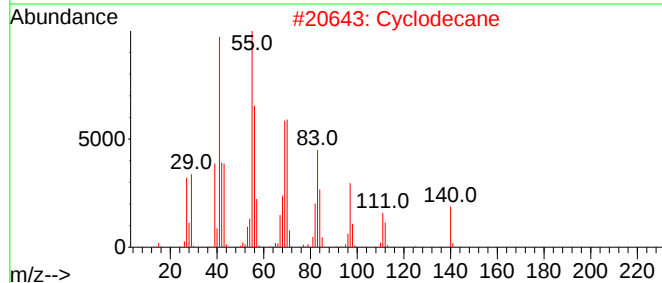
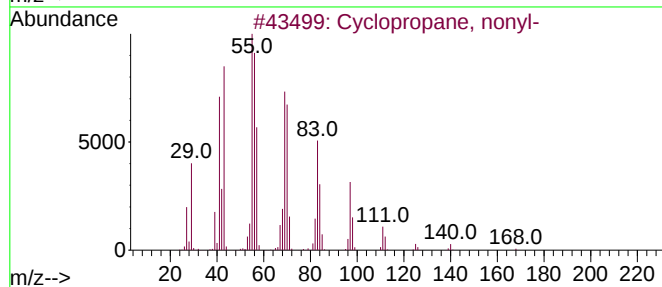
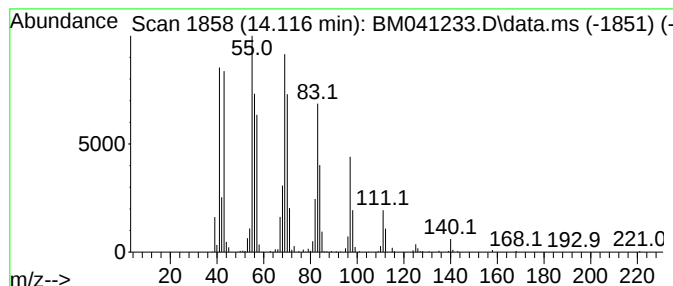
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 1 Cyclopropane, nonyl- Concentration Rank 7

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 14.116 | 10.07 ng | 782706 | Acenaphthene-d10 | 14.463 |

| Hit# | of 5 | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|------|----------------------------|-----|---------|-------------|------|
| 1    |      | Cyclopropane, nonyl-       | 168 | C12H24  | 074663-85-7 | 95   |
| 2    |      | Cyclodecane                | 140 | C10H20  | 000293-96-9 | 94   |
| 3    |      | 1-Decene                   | 140 | C10H20  | 000872-05-9 | 94   |
| 4    |      | Cyclooctane, 1,2-dimethyl- | 140 | C10H20  | 013151-94-5 | 91   |
| 5    |      | 1-Undecanol                | 172 | C11H24O | 000112-42-5 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

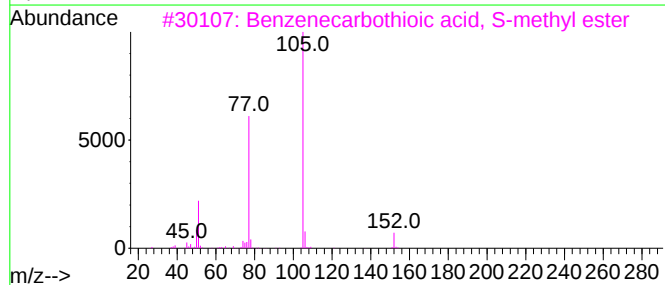
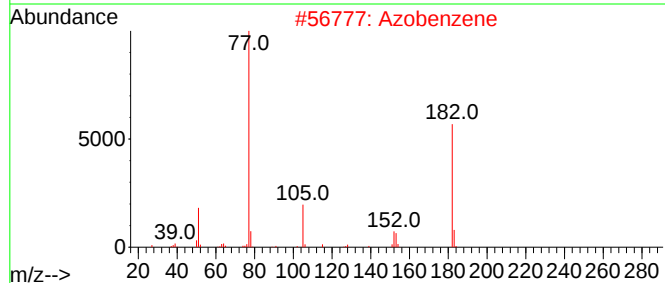
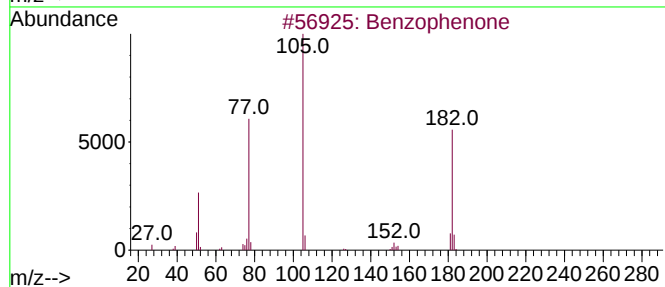
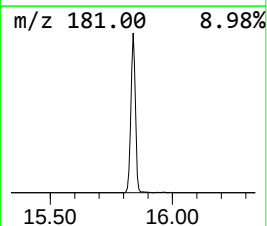
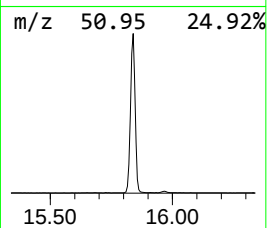
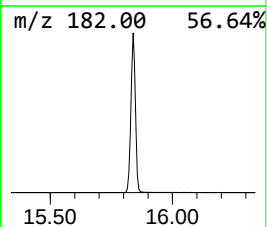
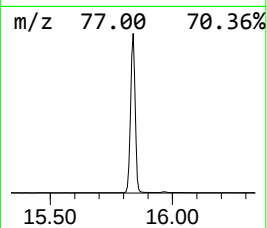
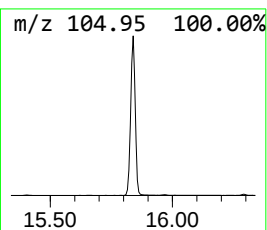
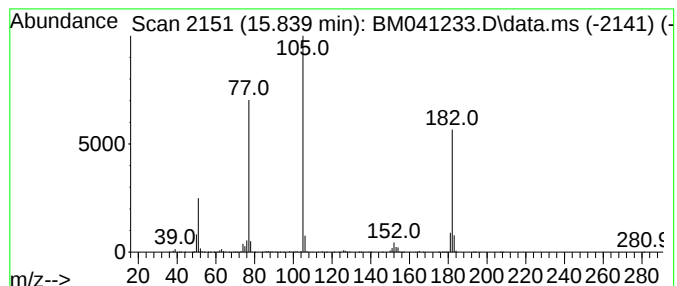
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 Benzophenone Concentration Rank 4

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 15.839 | 43.30 ng | 3363830 | Acenaphthene-d10 | 14.463 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | Azobenzene                          | 182 | C12H10N2 | 000103-33-3 | 72   |
| 3    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS   | 005925-68-8 | 50   |
| 4    |    |   | Acetophenone, 2-chloro-             | 154 | C8H7ClO  | 000532-27-4 | 49   |
| 5    |    |   | Benzenebutanoic acid, .gamma.-oxo-  | 178 | C10H10O3 | 002051-95-8 | 47   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

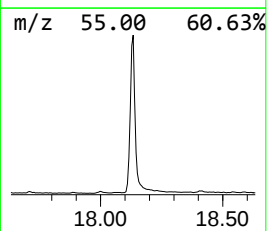
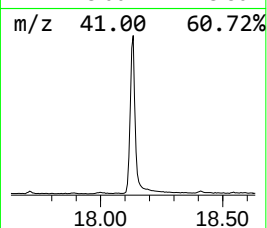
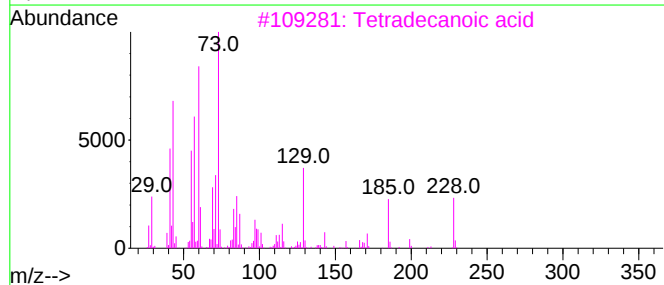
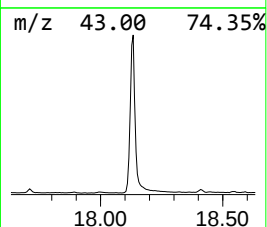
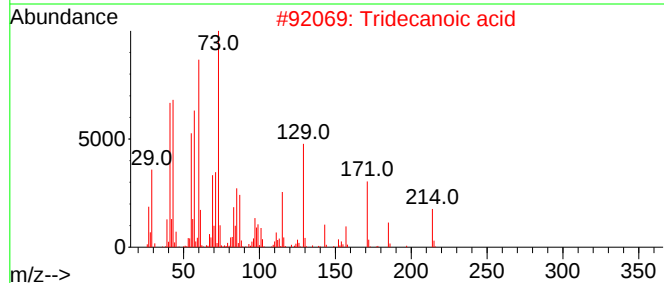
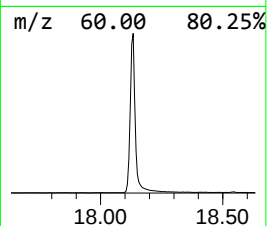
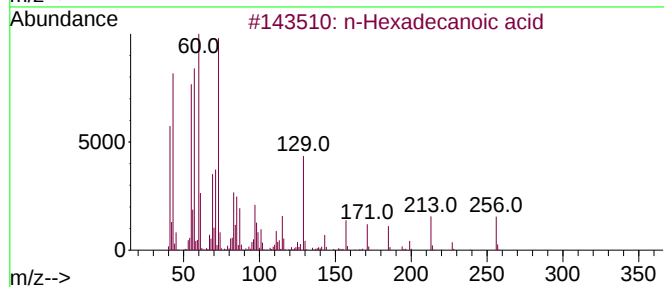
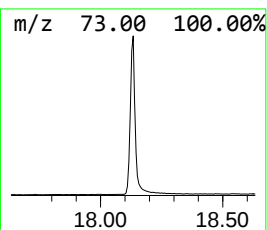
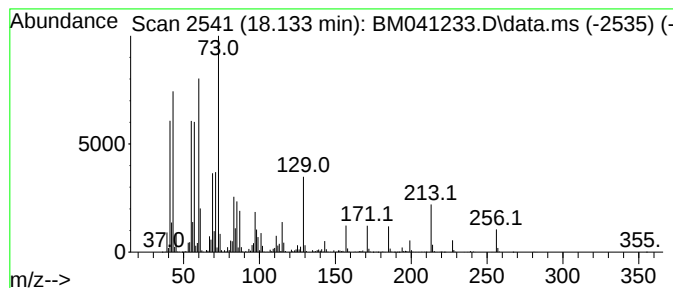
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 18.133 | 45.49 ng | 4020680 | Phenanthrene-d10 | 17.227 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 94   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 93   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

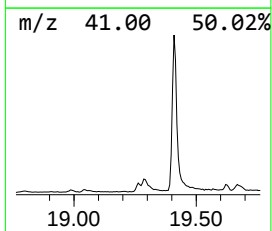
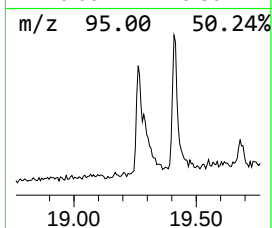
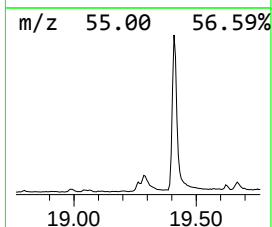
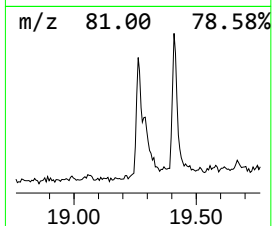
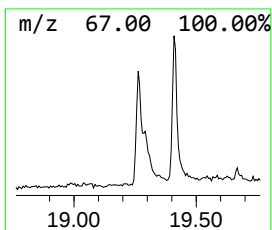
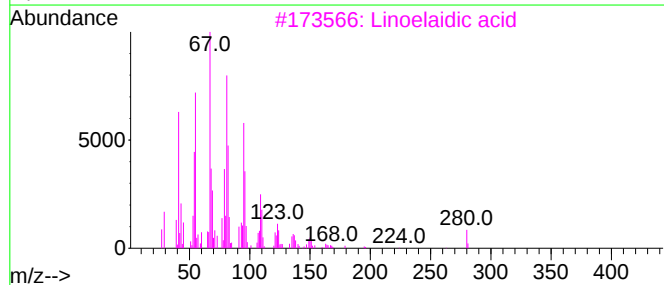
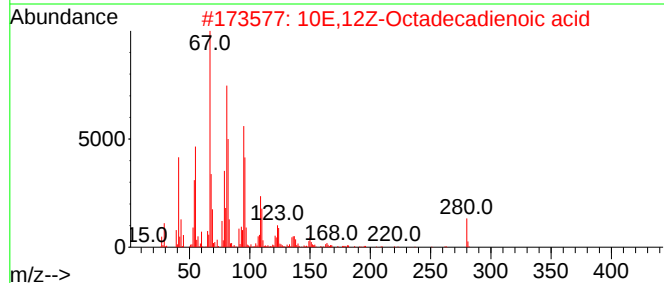
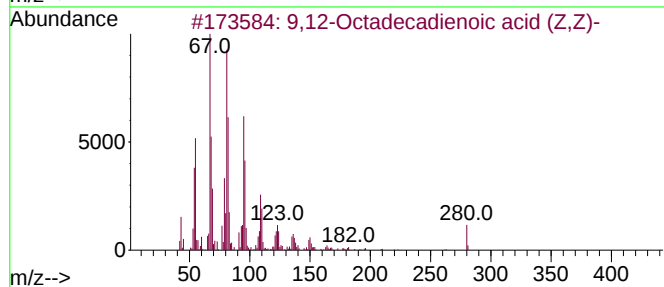
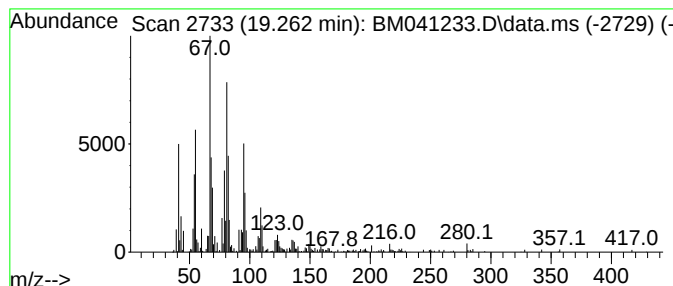
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 17

| R.T.      | EstConc                          | Area   | Relative to ISTD | R.T.        |      |
|-----------|----------------------------------|--------|------------------|-------------|------|
| 19.262    | 2.13 ng                          | 187881 | Phenanthrene-d10 | 17.227      |      |
| Hit# of 5 | Tentative ID                     | MW     | MolForm          | CAS#        | Qual |
| 1         | 9,12-Octadecadienoic acid (Z,Z)- | 280    | C18H32O2         | 000060-33-3 | 99   |
| 2         | 10E,12Z-Octadecadienoic acid     | 280    | C18H32O2         | 002420-56-6 | 92   |
| 3         | Linoleic acid                    | 280    | C18H32O2         | 000506-21-8 | 91   |
| 4         | 2-Chloroethyl linoleate          | 342    | C20H35ClO2       | 025525-76-2 | 91   |
| 5         | Cyclooctane, ethenyl-            | 138    | C10H18           | 061142-41-4 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

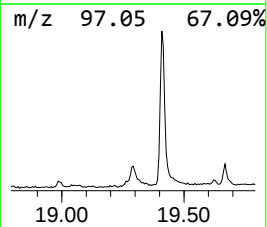
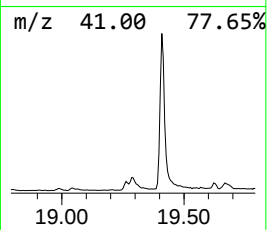
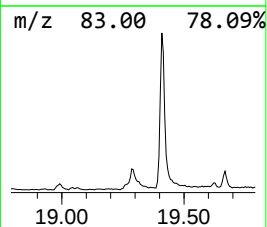
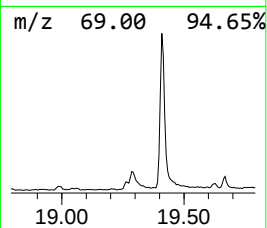
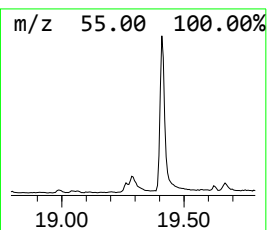
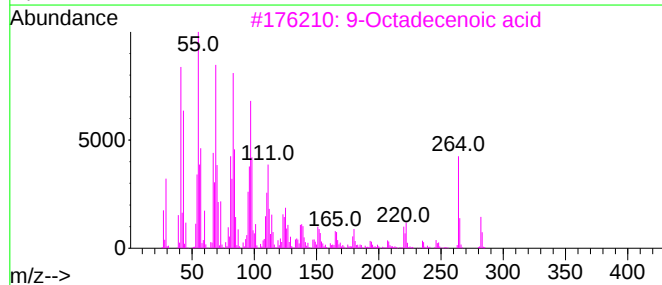
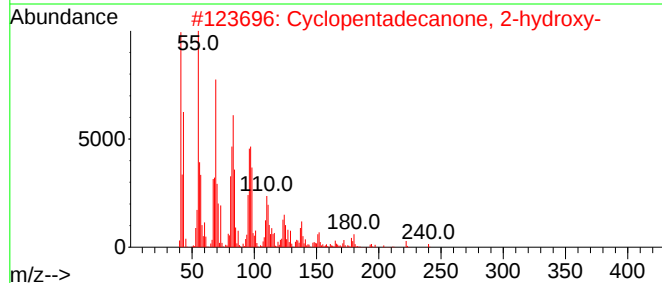
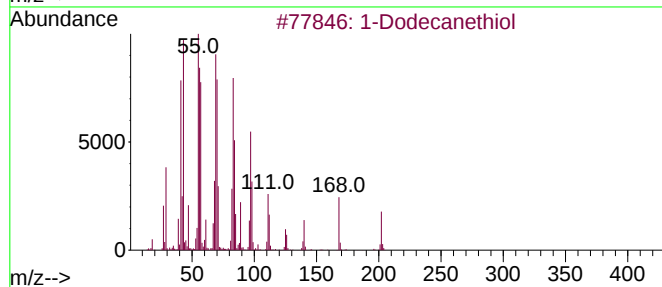
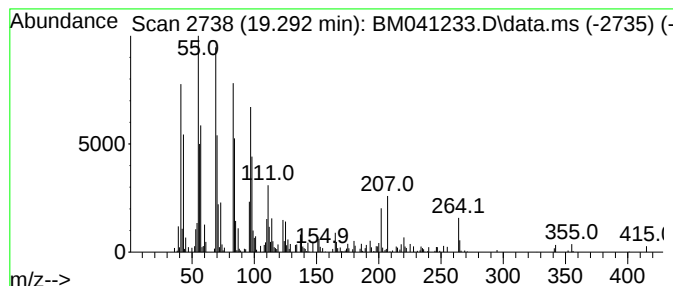
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 5 1-Dodecanethiol Concentration Rank 15

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.292 | 3.41 ng | 301781 | Phenanthrene-d10 | 17.227 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 1-Dodecanethiol                     | 202 | C12H26S    | 000112-55-0 | 83   |
| 2    |    |   | Cyclopentadecanone, 2-hydroxy-      | 240 | C15H28O2   | 004727-18-8 | 81   |
| 3    |    |   | 9-Octadecenoic acid                 | 282 | C18H34O2   | 002027-47-6 | 80   |
| 4    |    |   | Acetic acid, trifluoro-, undecyl... | 268 | C13H23F3O2 | 053800-01-4 | 76   |
| 5    |    |   | 9-Octadecenoic acid, (E)-           | 282 | C18H34O2   | 000112-79-8 | 74   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

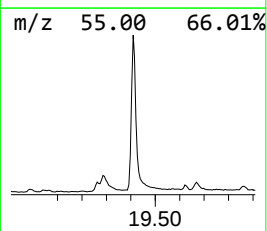
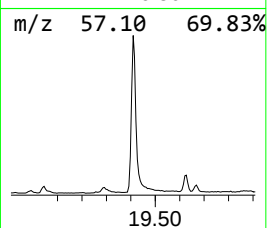
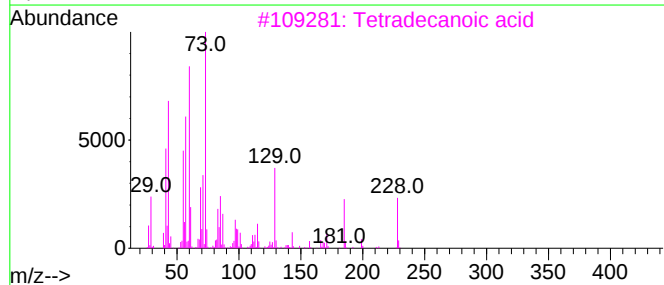
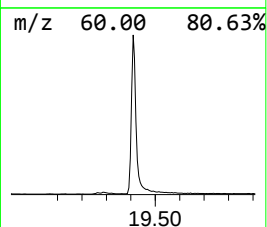
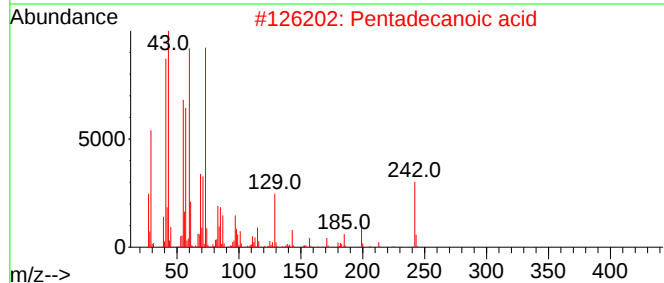
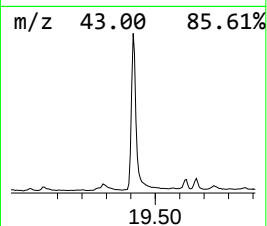
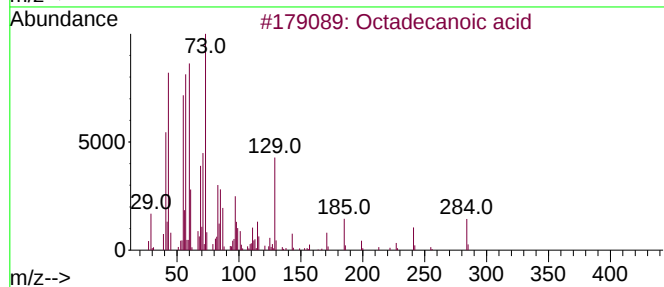
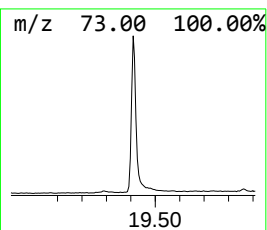
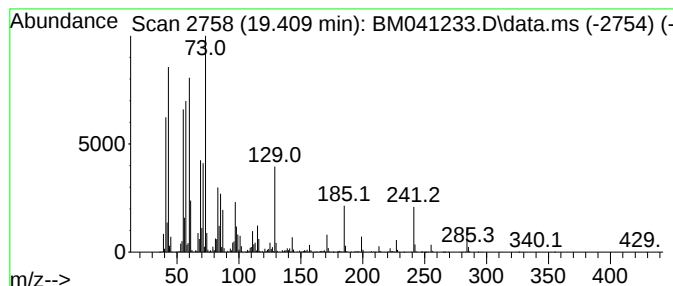
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 Octadecanoic acid Concentration Rank 5

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 19.409 | 32.73 ng | 3386660 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4  | 99   |
| 2    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2  | 91   |
| 3    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8  | 87   |
| 4    |    |   | n-Decanoic acid                     | 172 | C10H20O2 | 000334-48-5  | 62   |
| 5    |    |   | Oxalic acid, propyl tetradecyl e... | 328 | C19H36O4 | 1000309-26-7 | 30   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

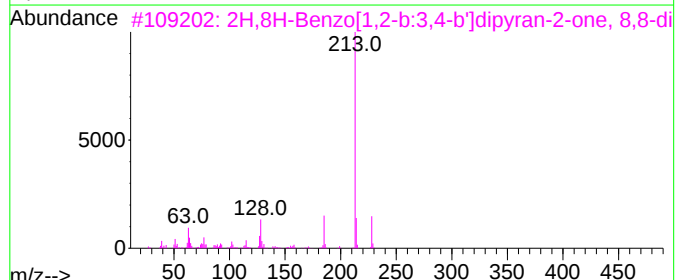
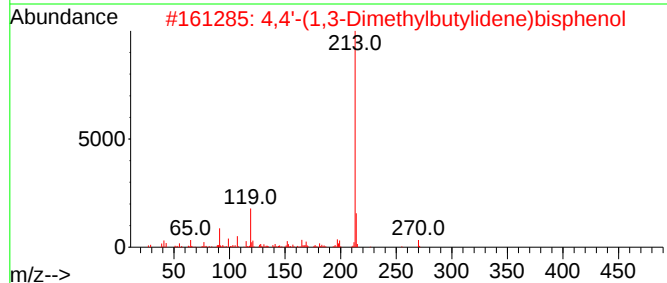
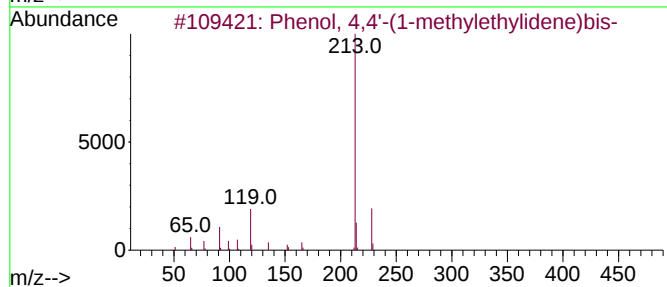
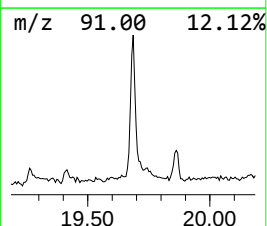
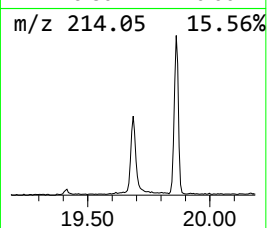
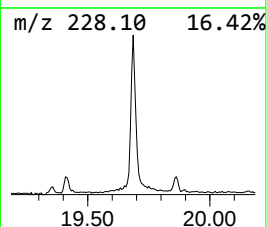
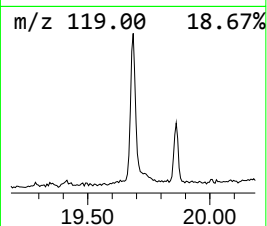
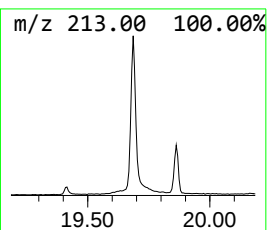
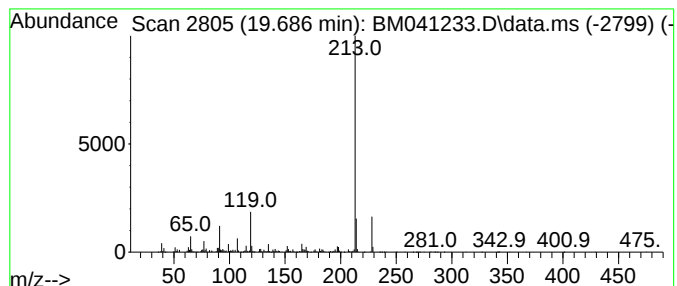
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 11

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.686 | 5.97 ng | 617287 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Phenol, 4,4'-(1-methylethylidene... | 228 | C15H16O2  | 000080-05-7 | 97   |
| 2    |    |   | 4,4'-(1,3-Dimethylbutylidene)bis... | 270 | C18H22O2  | 006807-17-6 | 80   |
| 3    |    |   | 2H,8H-Benzo[1,2-b:3,4-b']dipyr...   | 228 | C14H12O3  | 000523-59-1 | 59   |
| 4    |    |   | 3,4'-Isopropylidenediphenol         | 228 | C15H16O2  | 046765-25-7 | 55   |
| 5    |    |   | Carbanilic acid, p-phenyl-          | 213 | C13H11NO2 | 004474-53-7 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

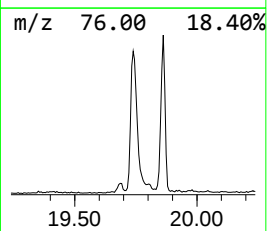
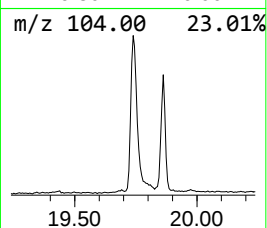
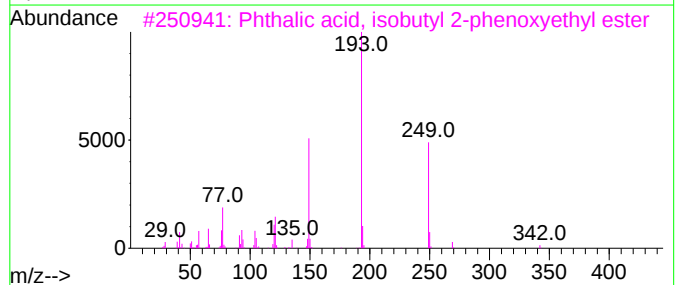
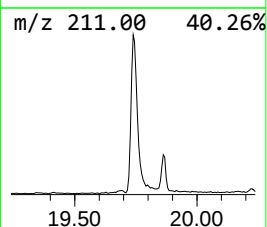
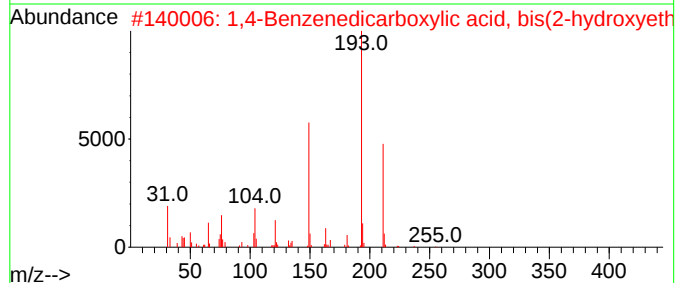
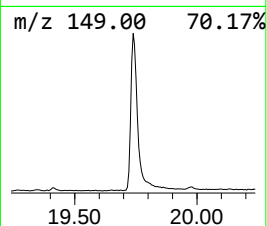
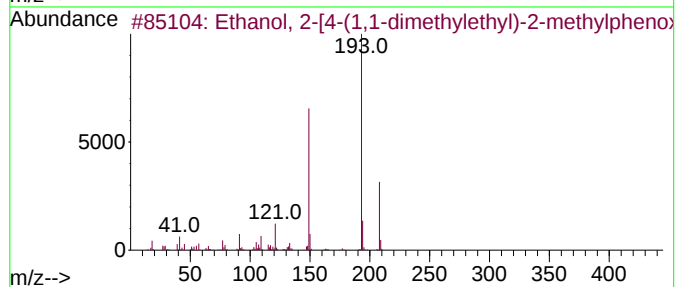
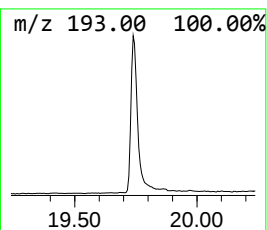
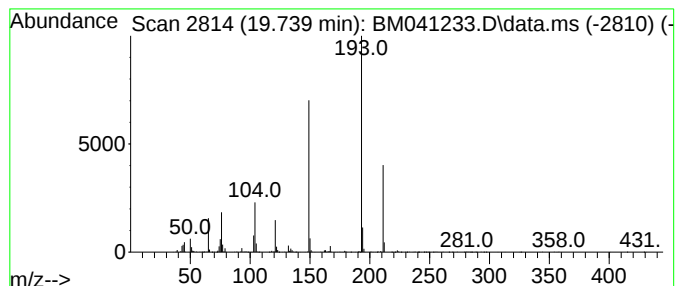
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 8 Ethanol, 2-[4-(1,1-dimethyl... Concentration Rank 8

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 19.739 | 9.71 ng | 1004370 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm   | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Ethanol, 2-[4-(1,1-dimethylethyl...] | 208 | C13H20O2  | 054934-87-1  | 50   |
| 2    |    |   | 1,4-Benzenedicarboxylic acid, bi...  | 254 | C12H14O6  | 000959-26-2  | 43   |
| 3    |    |   | Phthalic acid, isobutyl 2-phenox...  | 342 | C20H22O5  | 1000382-47-9 | 42   |
| 4    |    |   | Phthalic acid, isobutyl 2-(4-nit...  | 387 | C20H21NO7 | 1000382-57-3 | 42   |
| 5    |    |   | 2,4,6-Trimethoxybenzonitrile         | 193 | C10H11NO3 | 002571-54-2  | 37   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

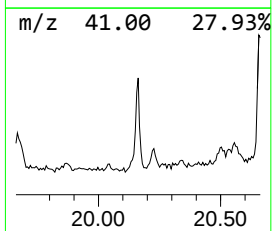
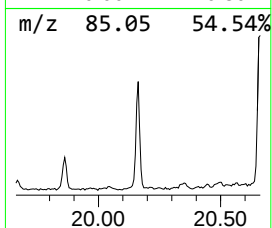
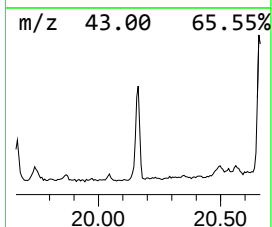
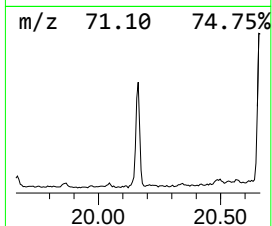
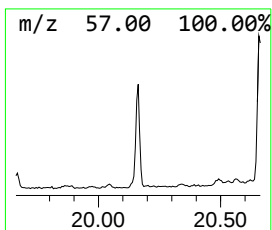
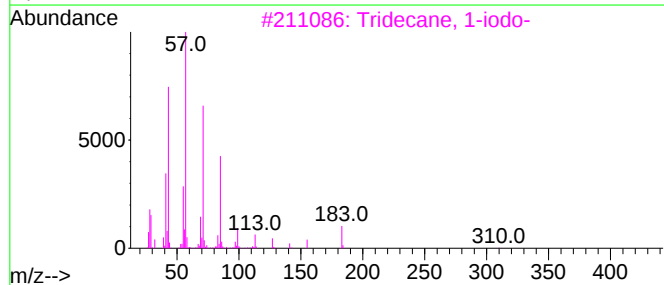
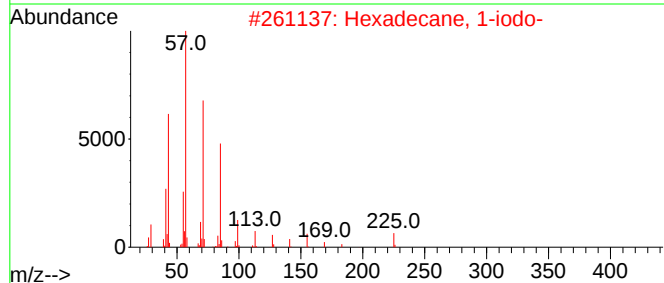
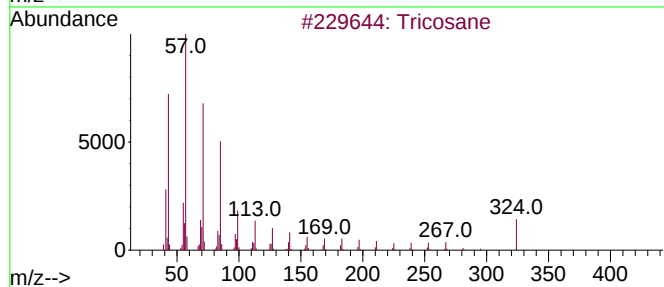
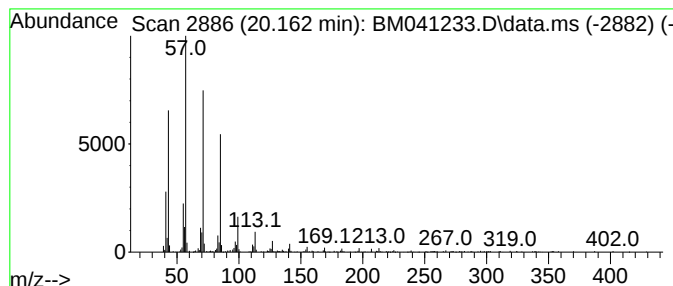
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 9 Tricosane Concentration Rank 16

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 20.162 | 2.44 ng | 252462 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Tricosane            | 324 | C23H48  | 000638-67-5 | 94   |
| 2    |    |   | Hexadecane, 1-iodo-  | 352 | C16H33I | 000544-77-4 | 91   |
| 3    |    |   | Tridecane, 1-iodo-   | 310 | C13H27I | 035599-77-0 | 91   |
| 4    |    |   | Octadecane, 1-iodo-  | 380 | C18H37I | 000629-93-6 | 90   |
| 5    |    |   | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

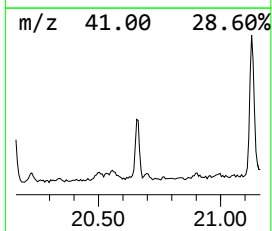
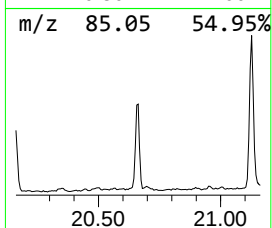
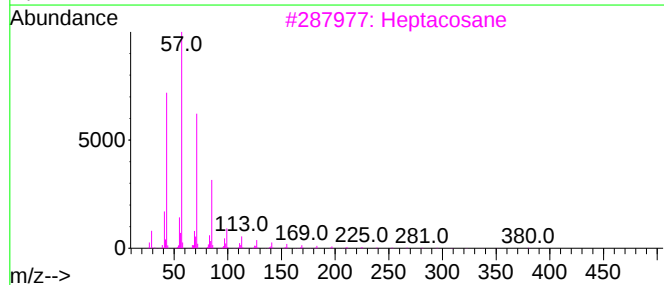
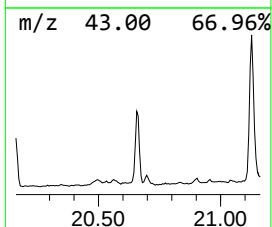
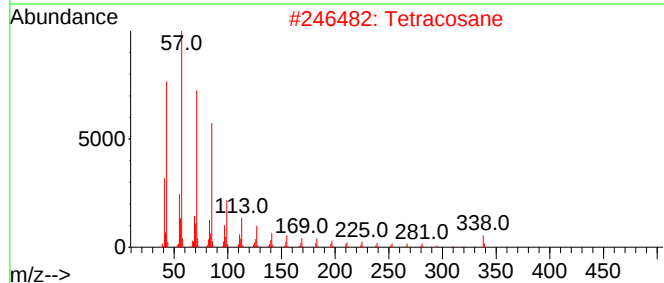
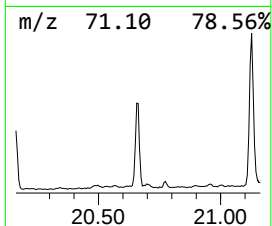
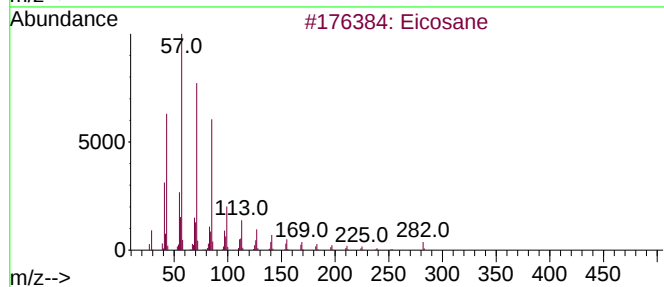
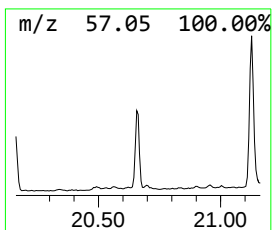
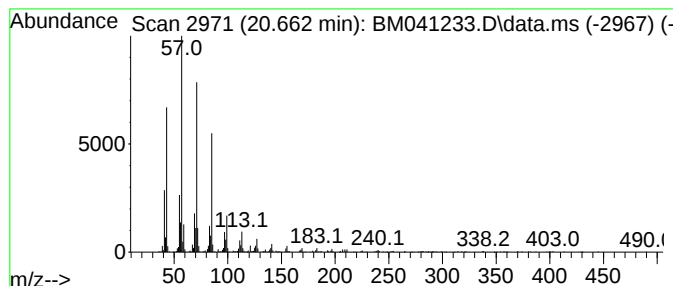
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 10 Eicosane Concentration Rank 14

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 20.662 | 4.00 ng | 413434 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Eicosane                       | 282 | C20H42  | 000112-95-8 | 96   |
| 2    |    |   | Tetracosane                    | 338 | C24H50  | 000646-31-1 | 96   |
| 3    |    |   | Heptacosane                    | 380 | C27H56  | 000593-49-7 | 94   |
| 4    |    |   | Tetradecane, 2,6,10-trimethyl- | 240 | C17H36  | 014905-56-7 | 87   |
| 5    |    |   | Heneicosane                    | 296 | C21H44  | 000629-94-7 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

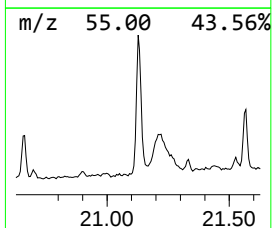
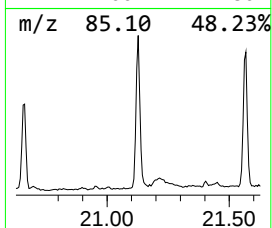
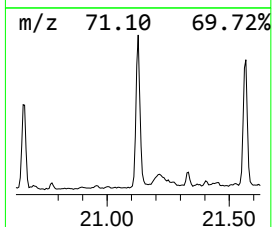
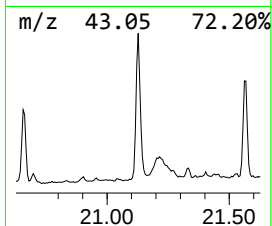
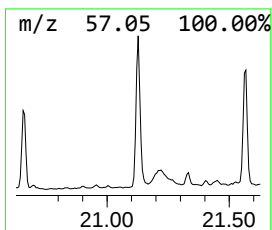
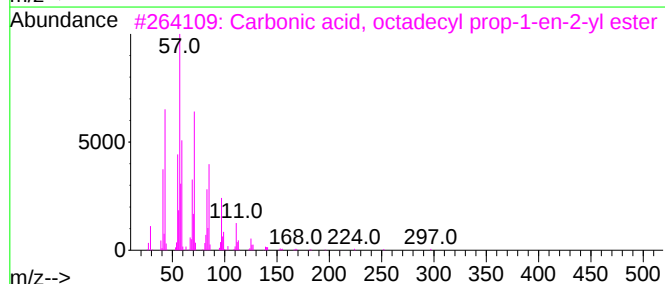
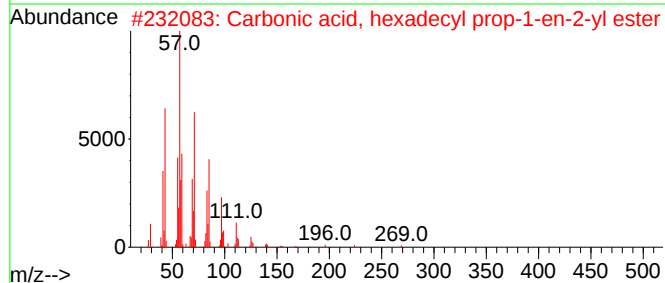
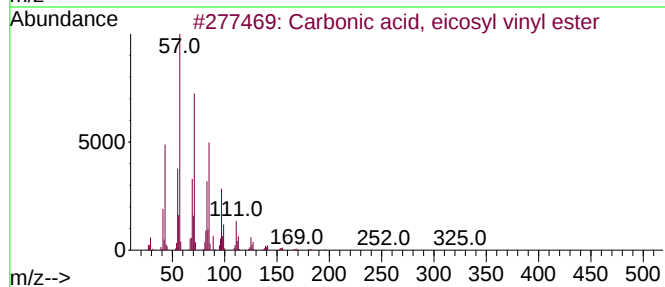
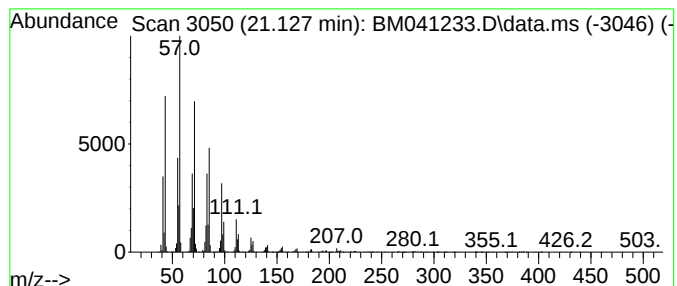
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 11 Carbonic acid, eicosyl vinyl... Concentration Rank 6

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 21.127 | 11.25 ng | 1164030 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Carbonic acid, eicosyl vinyl ester  | 368 | C23H44O3  | 1000382-54-3 | 95   |
| 2    |    |   | Carbonic acid, hexadecyl prop-1-... | 326 | C20H38O3  | 1000382-90-3 | 91   |
| 3    |    |   | Carbonic acid, octadecyl prop-1-... | 354 | C22H42O3  | 1000383-11-5 | 91   |
| 4    |    |   | Carbonic acid, octadecyl vinyl e... | 340 | C21H40O3  | 1000382-54-4 | 90   |
| 5    |    |   | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

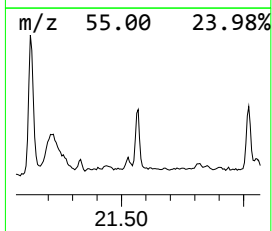
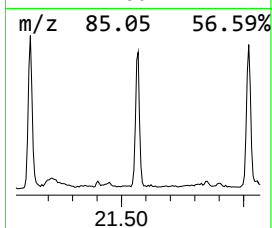
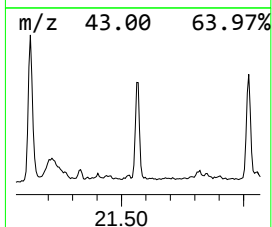
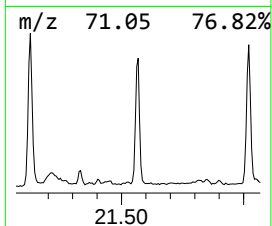
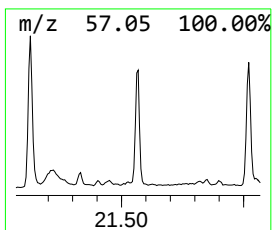
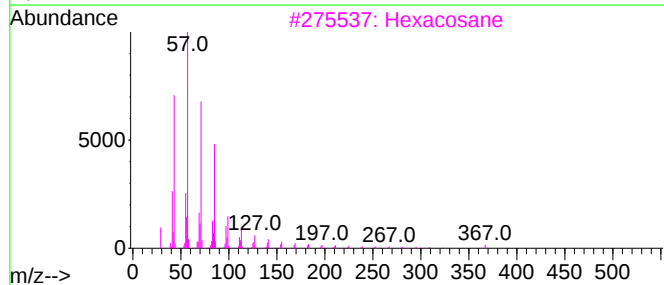
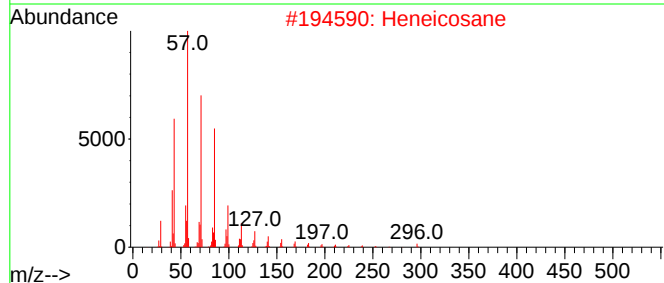
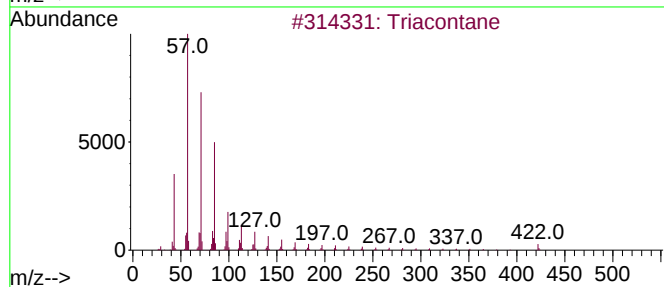
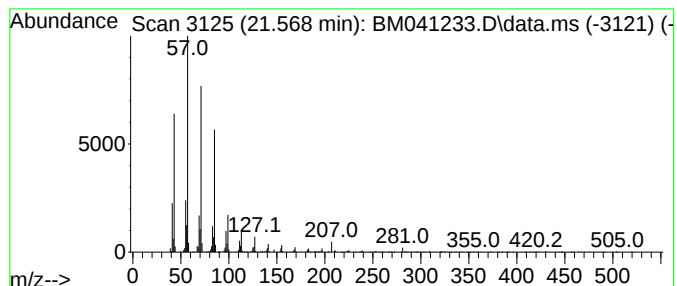
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

Peak Number 12 Triacontane Concentration Rank 12

| R.T.      | EstConc            | Area   | Relative to ISTD | R.T.        |      |
|-----------|--------------------|--------|------------------|-------------|------|
| 21.568    | 5.51 ng            | 569901 | Chrysene-d12     | 21.427      |      |
| Hit# of 5 | Tentative ID       | MW     | MolForm          | CAS#        | Qual |
| 1         | Triacontane        | 422    | C30H62           | 000638-68-6 | 93   |
| 2         | Heneicosane        | 296    | C21H44           | 000629-94-7 | 91   |
| 3         | Hexacosane         | 366    | C26H54           | 000630-01-3 | 91   |
| 4         | Octacosane         | 394    | C28H58           | 000630-02-4 | 91   |
| 5         | Docosane, 7-hexyl- | 394    | C28H58           | 055373-86-9 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

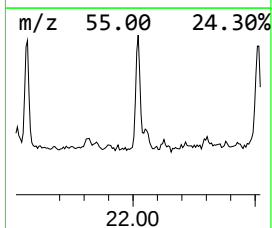
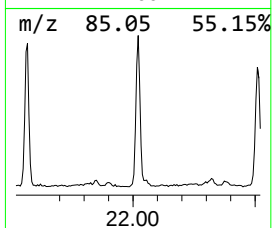
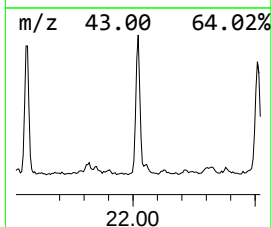
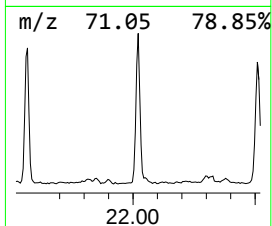
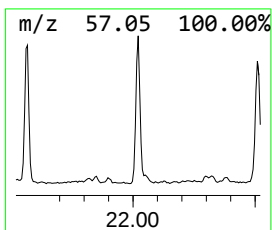
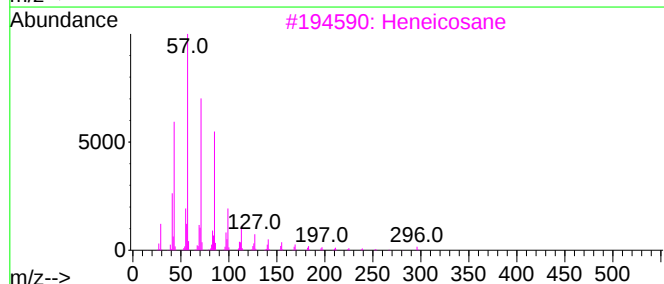
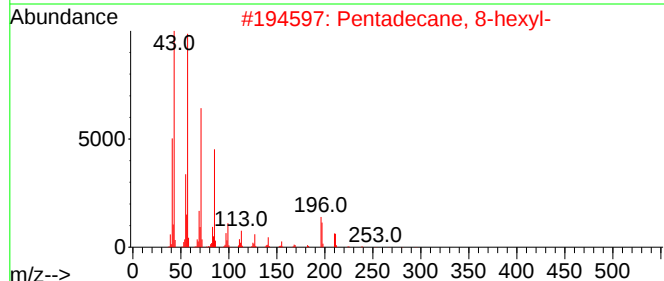
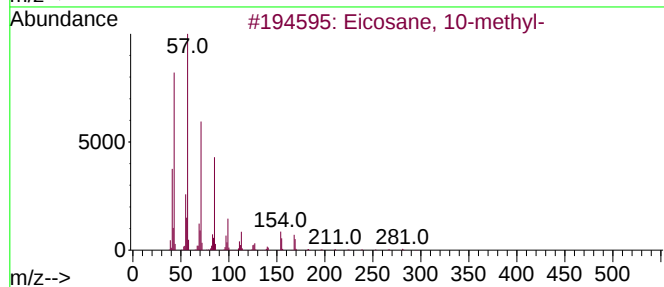
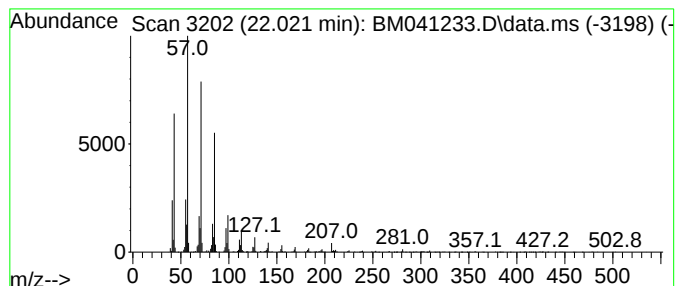
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 13 Eicosane, 10-methyl- Concentration Rank 10

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 22.021 | 6.40 ng | 662539 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Eicosane, 10-methyl-  | 296 | C21H44  | 054833-23-7 | 93   |
| 2    |    |   | Pentadecane, 8-hexyl- | 296 | C21H44  | 013475-75-7 | 93   |
| 3    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 91   |
| 4    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 91   |
| 5    |    |   | Octadecane            | 254 | C18H38  | 000593-45-3 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

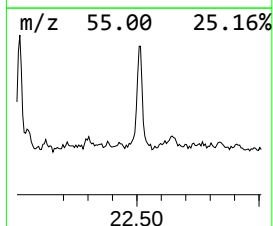
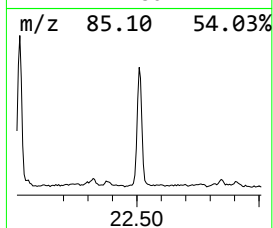
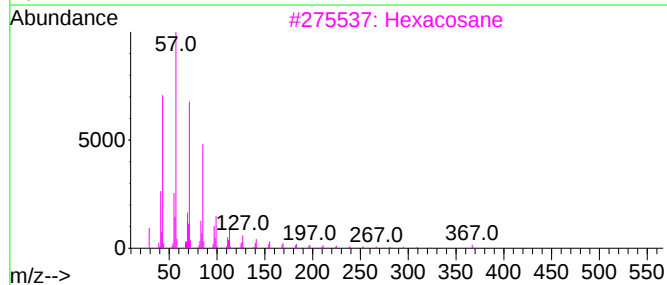
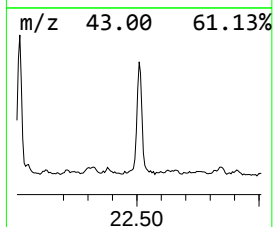
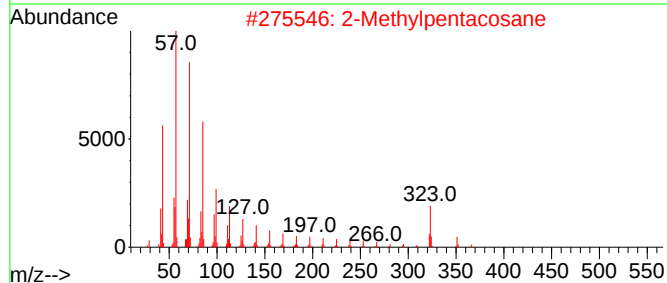
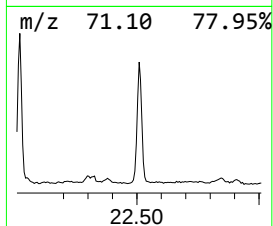
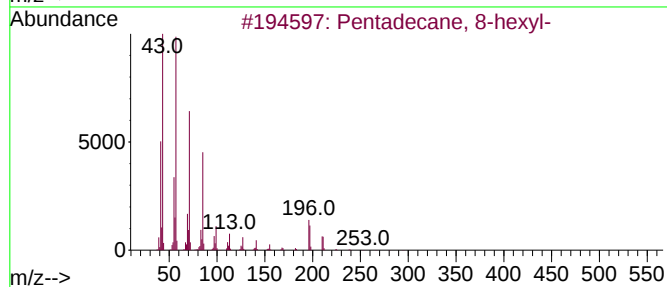
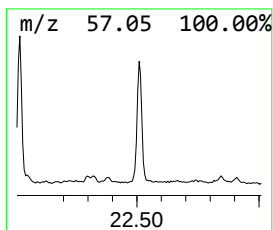
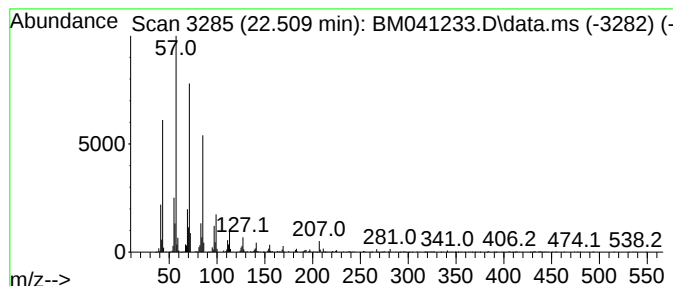
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 14 Pentadecane, 8-hexyl- Concentration Rank 9

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 22.509 | 6.73 ng | 696268 | Chrysene-d12     | 21.427 |

| Hit# | of 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|------|-----------------------|-----|---------|-------------|------|
| 1    |      | Pentadecane, 8-hexyl- | 296 | C21H44  | 013475-75-7 | 94   |
| 2    |      | 2-Methylpentacosane   | 366 | C26H54  | 000629-87-8 | 94   |
| 3    |      | Hexacosane            | 366 | C26H54  | 000630-01-3 | 91   |
| 4    |      | Heneicosane           | 296 | C21H44  | 000629-94-7 | 91   |
| 5    |      | Eicosane, 7-hexyl-    | 366 | C26H54  | 055333-99-8 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

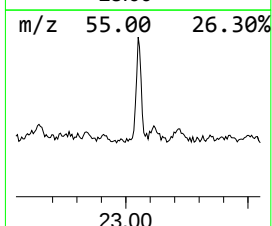
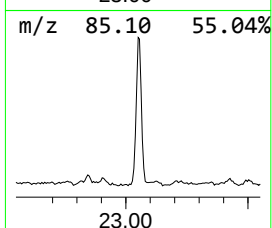
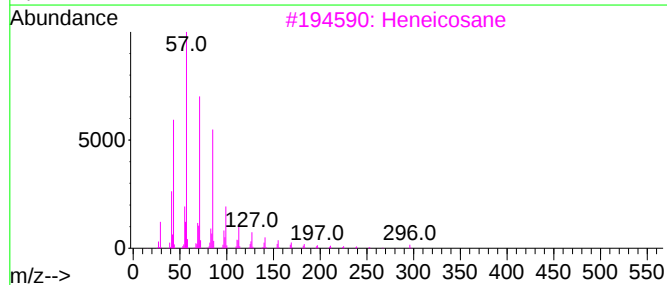
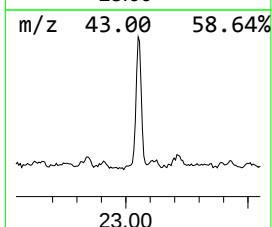
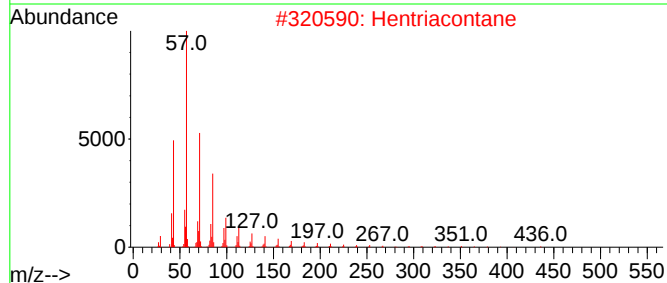
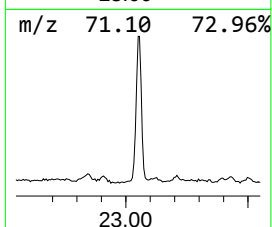
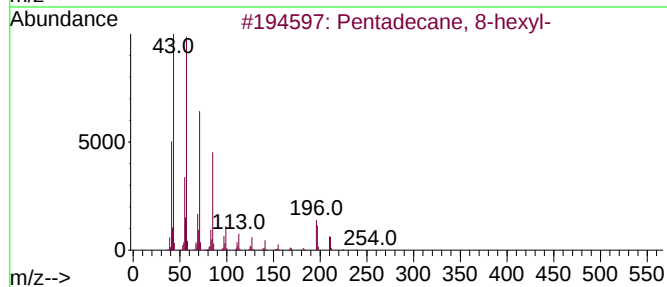
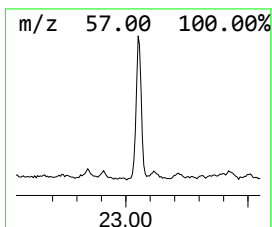
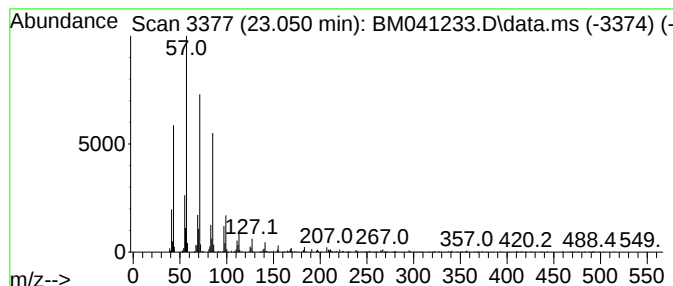
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

Peak Number 15 Hentriacontane Concentration Rank 13

| R.T.      | EstConc               | Area   | Relative to ISTD | R.T.        |      |
|-----------|-----------------------|--------|------------------|-------------|------|
| 23.050    | 4.84 ng               | 532546 | Perylene-d12     | 23.803      |      |
| Hit# of 5 | Tentative ID          | MW     | MolForm          | CAS#        | Qual |
| 1         | Pentadecane, 8-hexyl- | 296    | C21H44           | 013475-75-7 | 93   |
| 2         | Hentriacontane        | 437    | C31H64           | 000630-04-6 | 90   |
| 3         | Heneicosane           | 296    | C21H44           | 000629-94-7 | 90   |
| 4         | Docosane, 9-butyl-    | 366    | C26H54           | 055282-14-9 | 90   |
| 5         | 2-Methyltetracosane   | 352    | C25H52           | 001560-78-7 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

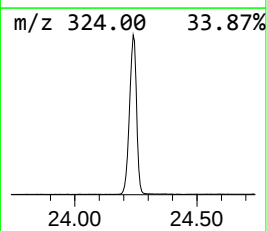
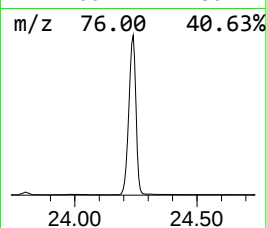
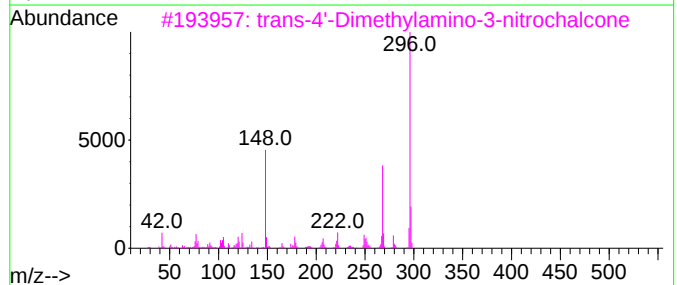
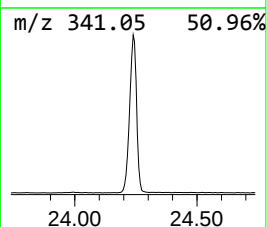
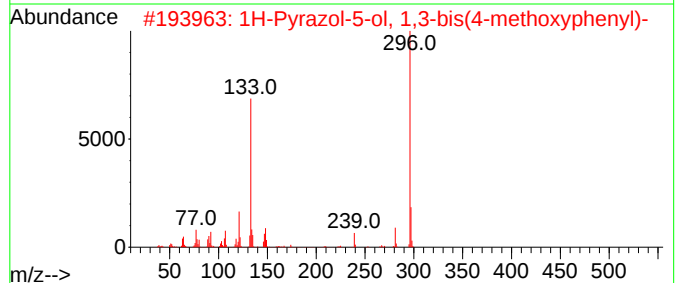
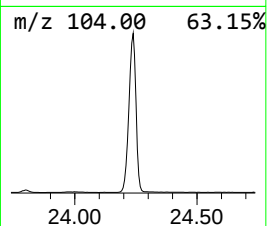
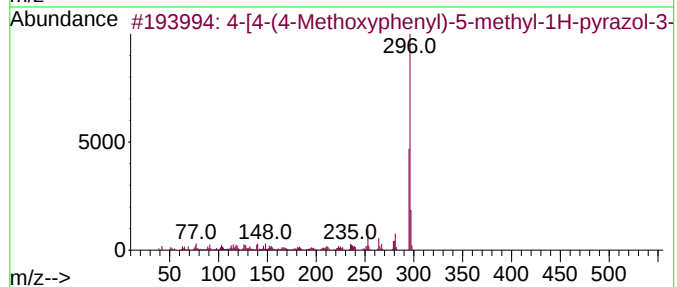
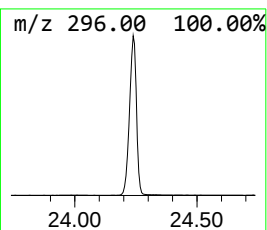
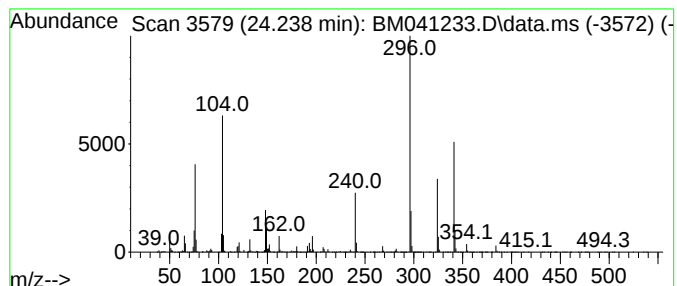
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 16 unknown24.238 Concentration Rank 2

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 24.238 | 52.75 ng | 5801390 | Perylene-d12     | 23.803 |

| Hit# | of                                  | 5                                 | Tentative ID | MW           | MolForm     | CAS# | Qual |
|------|-------------------------------------|-----------------------------------|--------------|--------------|-------------|------|------|
| 1    | 4-                                  | [4-(4-Methoxyphenyl)-5-methyl-... | 296          | C17H16N2O3   | 394237-61-7 | 22   |      |
| 2    | 1H-Pyrazol-5-ol, 1,3-bis(4-metho... | 296                               | C17H16N2O3   | 1000337-80-1 | 22          |      |      |
| 3    | trans-4'-Dimethylamino-3-nitroch... | 296                               | C17H16N2O3   | 1000234-56-7 | 16          |      |      |
| 4    | N,N'-Bis(2-hydroxy-alpha-methylb... | 296                               | C18H20N2O2   | 005464-60-8  | 16          |      |      |
| 5    | (2S,7R,Z)-2-Ethyl-1-methyl-3-pen... | 325                               | C20H27N3O    | 1000482-33-2 | 16          |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
Data File : BM041233.D  
Acq On : 01 Aug 2023 20:15  
Operator : MA/JU  
Sample : 03715-11  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
T843-CT-01

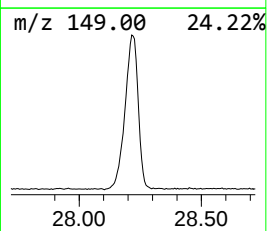
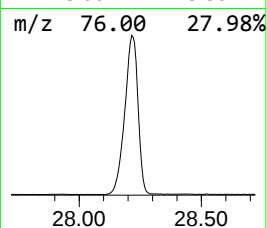
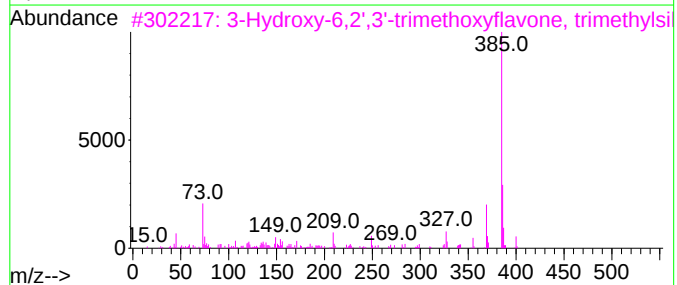
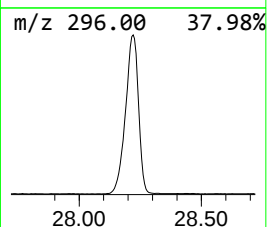
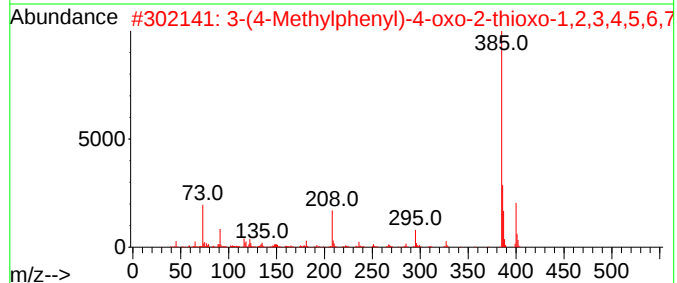
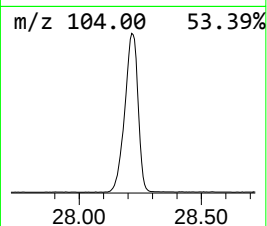
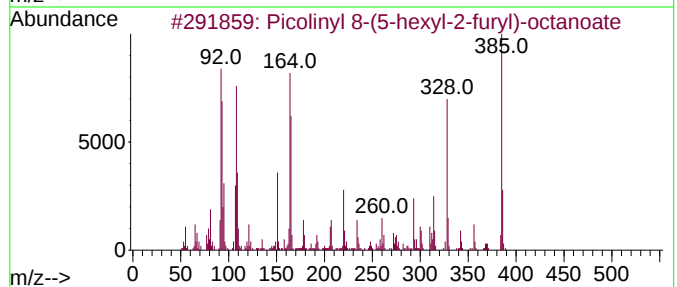
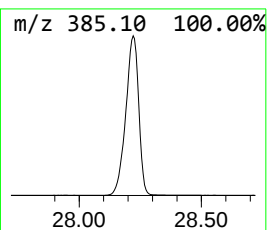
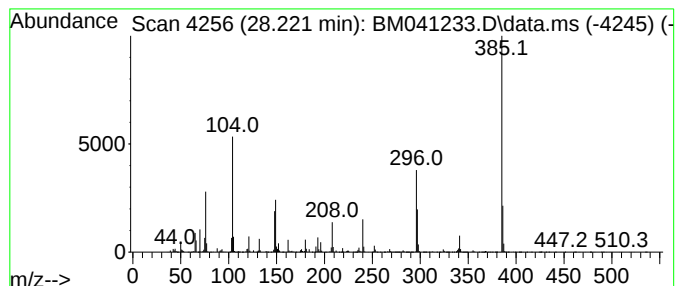
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 17 unknown28.221 Concentration Rank 1

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 28.221 | 74.23 ng | 8164730 | Perylene-d12     | 23.803 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm       | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------------|--------------|------|
| 1    |    |   | Picolinyl 8-(5-hexyl-2-furyl)-oc... | 385 | C24H35NO3     | 1000335-93-0 | 42   |
| 2    |    |   | 3-(4-Methylphenyl)-4-oxo-2-thiox... | 400 | C20H24N2OS2Si | 1000512-11-8 | 17   |
| 3    |    |   | 3-Hydroxy-6,2',3'-trimethoxyflav... | 400 | C21H24O6Si    | 1000448-94-4 | 16   |
| 4    |    |   | 2,3-Dibenzyl-5,8-dimethoxy-6-ami... | 385 | C24H23N3O2    | 056393-28-3  | 16   |
| 5    |    |   | 3-Hydroxy-6,3',4'-trimethoxyflav... | 400 | C21H24O6Si    | 1000448-94-7 | 16   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080123\  
 Data File : BM041233.D  
 Acq On : 01 Aug 2023 20:15  
 Operator : MA/JU  
 Sample : 03715-11  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 T843-CT-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.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 |
| Cyclopropane, n... | 14.116 | 10.1    | ng    | 782706   | 3                     | 14.463 | 1553850 | 20.0 |
| Benzophenone       | 15.839 | 43.3    | ng    | 3363830  | 3                     | 14.463 | 1553850 | 20.0 |
| n-Hexadecanoic ... | 18.133 | 45.5    | ng    | 4020680  | 4                     | 17.227 | 1767860 | 20.0 |
| 9,12-Octadecadi... | 19.262 | 2.1     | ng    | 187881   | 4                     | 17.227 | 1767860 | 20.0 |
| 1-Dodecanethiol    | 19.292 | 3.4     | ng    | 301781   | 4                     | 17.227 | 1767860 | 20.0 |
| Octadecanoic acid  | 19.409 | 32.7    | ng    | 3386660  | 5                     | 21.427 | 2069160 | 20.0 |
| Phenol, 4,4'-(1... | 19.686 | 6.0     | ng    | 617287   | 5                     | 21.427 | 2069160 | 20.0 |
| Ethanol, 2-[4-(... | 19.739 | 9.7     | ng    | 1004370  | 5                     | 21.427 | 2069160 | 20.0 |
| Tricosane          | 20.162 | 2.4     | ng    | 252462   | 5                     | 21.427 | 2069160 | 20.0 |
| Eicosane           | 20.662 | 4.0     | ng    | 413434   | 5                     | 21.427 | 2069160 | 20.0 |
| Carbonic acid, ... | 21.127 | 11.3    | ng    | 1164030  | 5                     | 21.427 | 2069160 | 20.0 |
| Triacontane        | 21.568 | 5.5     | ng    | 569901   | 5                     | 21.427 | 2069160 | 20.0 |
| Eicosane, 10-me... | 22.021 | 6.4     | ng    | 662539   | 5                     | 21.427 | 2069160 | 20.0 |
| Pentadecane, 8-... | 22.509 | 6.7     | ng    | 696268   | 5                     | 21.427 | 2069160 | 20.0 |
| Hentriacontane     | 23.050 | 4.8     | ng    | 532546   | 6                     | 23.803 | 2199740 | 20.0 |
| unknown24.238      | 24.238 | 52.8    | ng    | 5801390  | 6                     | 23.803 | 2199740 | 20.0 |
| unknown28.221      | 28.221 | 74.2    | ng    | 8164730  | 6                     | 23.803 | 2199740 | 20.0 |