

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM020323\  
 Data File : BM038686.D  
 Acq On : 03 Feb 2023 19:24  
 Operator : CG/JU  
 Sample : 01414-04  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 SASP2-123-2(55-62)

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038686.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         | 5.016       | 305           | 311         | 319          | rVB      | 284345         | 372307        | 12.44%          | 2.549%        |
| 2         | 5.487       | 385           | 391         | 404          | rBV      | 815160         | 1137456       | 38.00%          | 7.789%        |
| 3         | 7.104       | 658           | 666         | 678          | rBV      | 758138         | 1148355       | 38.36%          | 7.863%        |
| 4         | 7.922       | 799           | 805         | 812          | rVB      | 209042         | 327764        | 10.95%          | 2.244%        |
| 5         | 9.098       | 997           | 1005        | 1014         | rBV      | 440454         | 691713        | 23.11%          | 4.736%        |
| 6         | 10.734      | 1272          | 1283        | 1289         | rBV      | 249622         | 397879        | 13.29%          | 2.724%        |
| 7         | 13.186      | 1694          | 1700        | 1714         | rBV      | 1407536        | 1988342       | 66.42%          | 13.615%       |
| 8         | 14.563      | 1928          | 1934        | 1942         | rBV      | 407777         | 591001        | 19.74%          | 4.047%        |
| 9         | 15.921      | 2158          | 2165        | 2171         | rBV      | 48789          | 64200         | 2.14%           | 0.440%        |
| 10        | 16.057      | 2181          | 2188        | 2197         | rBV      | 1141683        | 1628958       | 54.42%          | 11.154%       |
| 11        | 17.304      | 2394          | 2400        | 2411         | rBV      | 519781         | 721518        | 24.10%          | 4.941%        |
| 12        | 18.192      | 2546          | 2551        | 2563         | rBV      | 237390         | 366982        | 12.26%          | 2.513%        |
| 13        | 19.468      | 2763          | 2768        | 2780         | rBV      | 92853          | 159972        | 5.34%           | 1.095%        |
| 14        | 19.921      | 2840          | 2845        | 2852         | rBV      | 2513556        | 2993415       | 100.00%         | 20.497%       |
| 15        | 21.174      | 3054          | 3058        | 3066         | rBV      | 215930         | 286432        | 9.57%           | 1.961%        |
| 16        | 21.486      | 3106          | 3111        | 3117         | rBV      | 626464         | 802595        | 26.81%          | 5.496%        |
| 17        | 23.880      | 3512          | 3518        | 3529         | rVB2     | 466637         | 925260        | 30.91%          | 6.336%        |

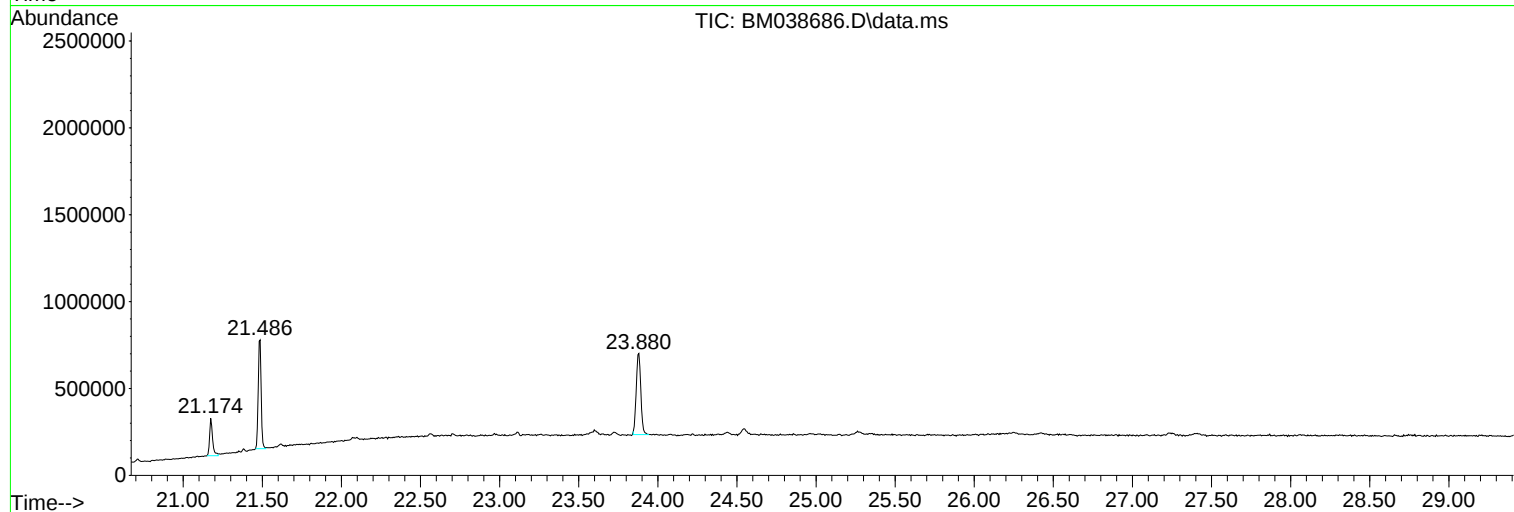
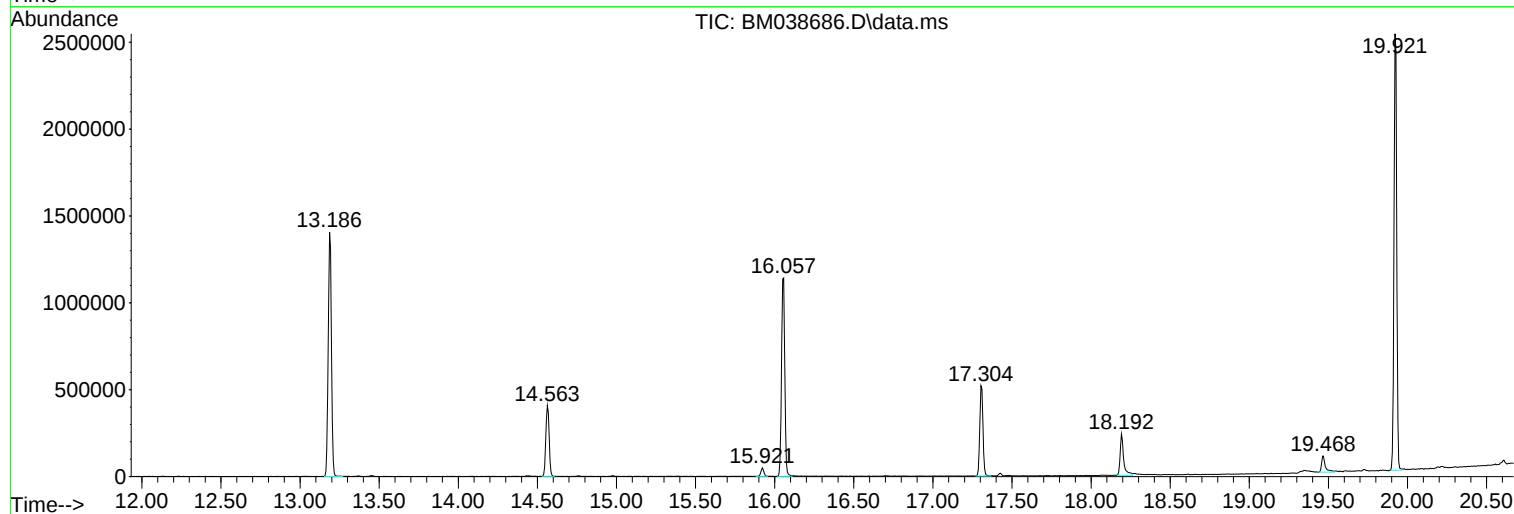
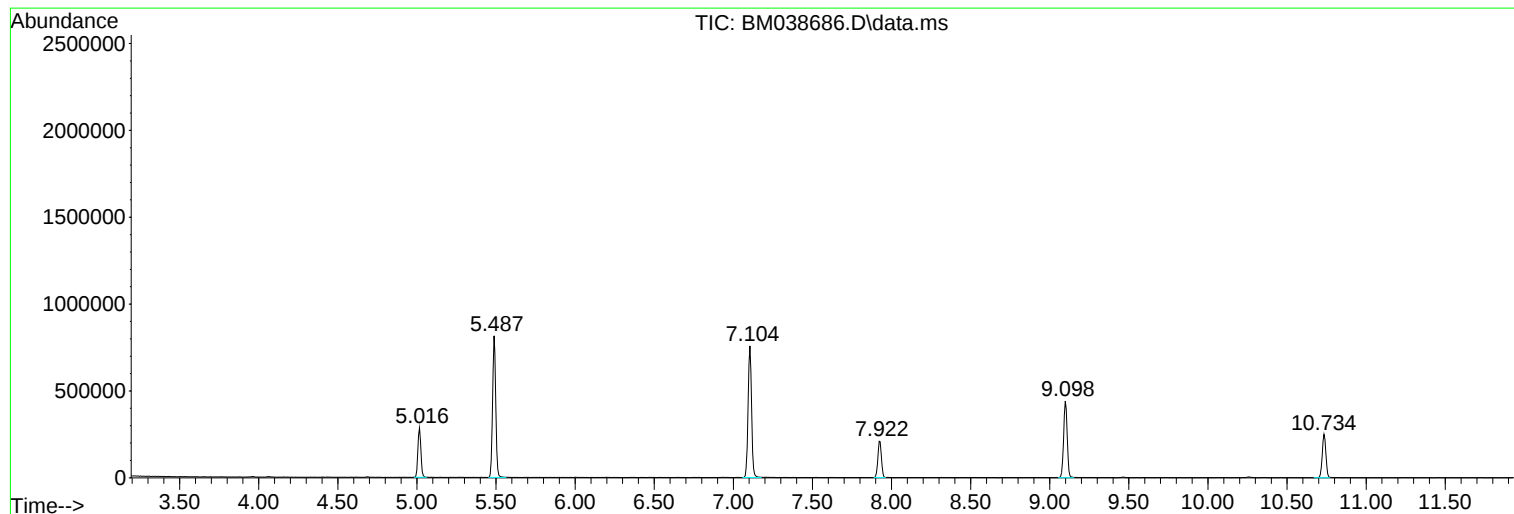
Sum of corrected areas: 14604149

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM020323\  
Data File : BM038686.D  
Acq On : 03 Feb 2023 19:24  
Operator : CG/JU  
Sample : 01414-04  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
SASP2-123-2(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM020123.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\BM020323\  
Data File : BM038686.D  
Acq On : 03 Feb 2023 19:24  
Operator : CG/JU  
Sample : 01414-04  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
SASP2-123-2(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM020123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

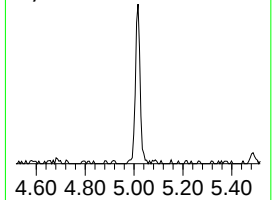
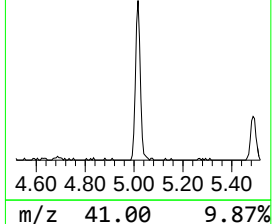
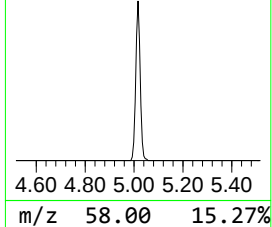
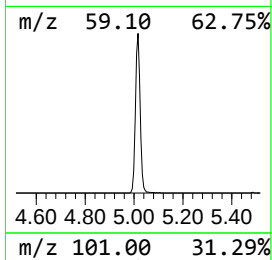
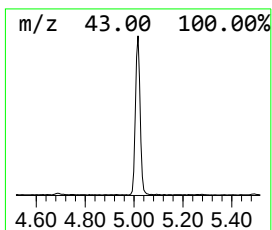
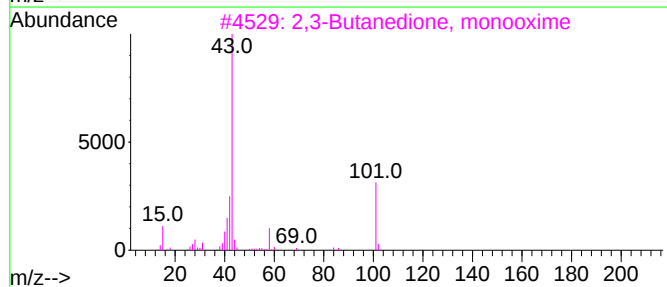
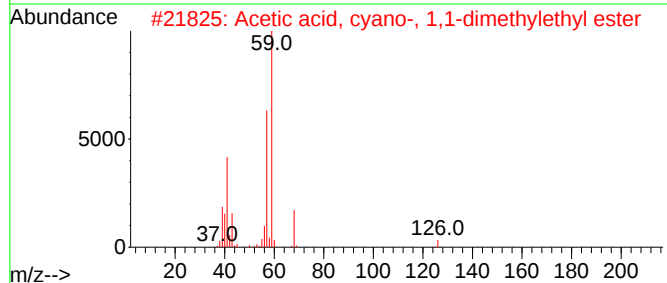
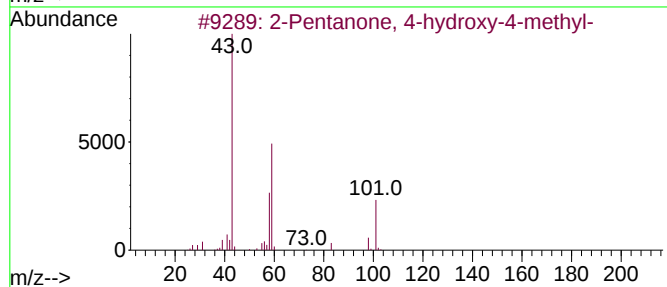
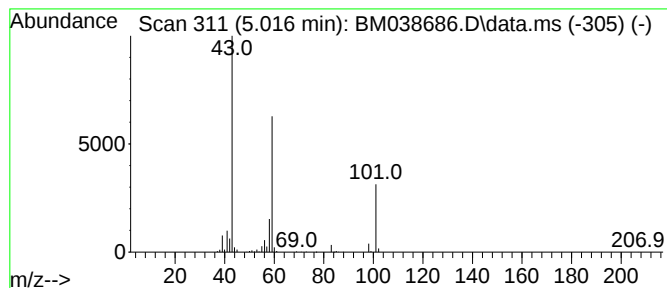
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.016 | 22.72 ng | 372307 | 1,4-Dichlorobenzene-d4 | 7.922 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 72      |      |      |
| 2    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 25      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 17      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Propanenitrile, 3-ethoxy-           | 99  | C5H9NO       | 002141-62-0 | 9       |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM020323\  
Data File : BM038686.D  
Acq On : 03 Feb 2023 19:24  
Operator : CG/JU  
Sample : 01414-04  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

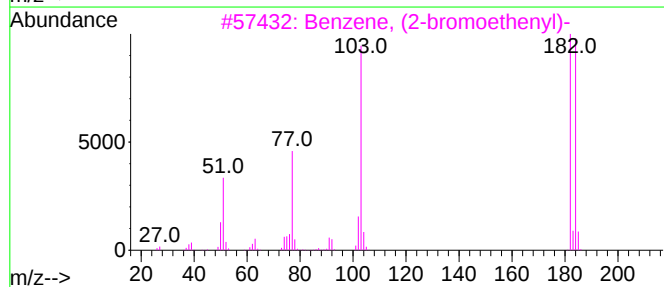
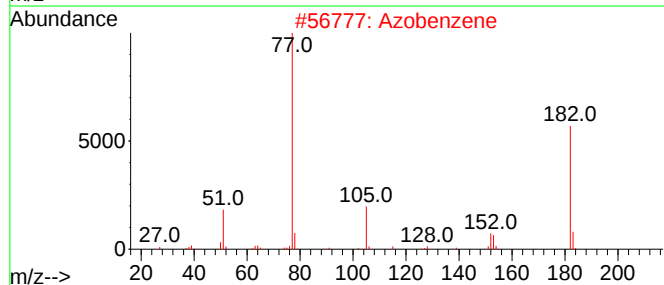
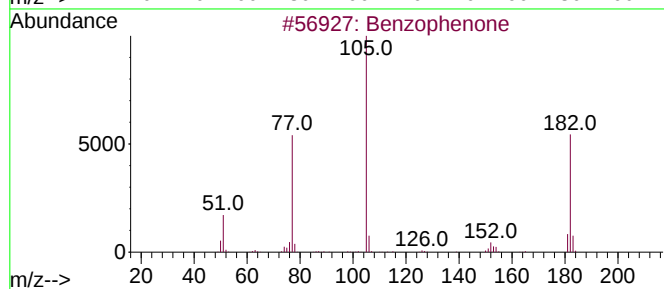
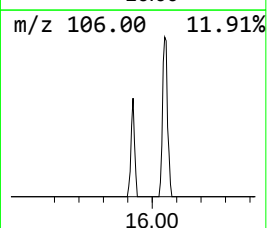
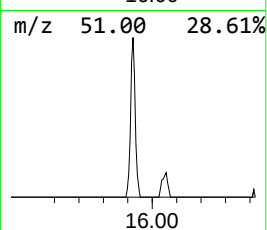
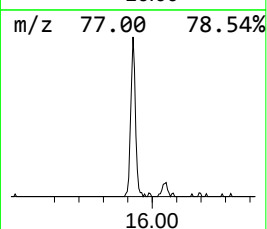
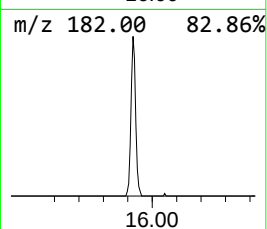
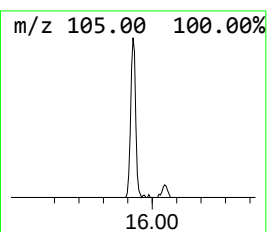
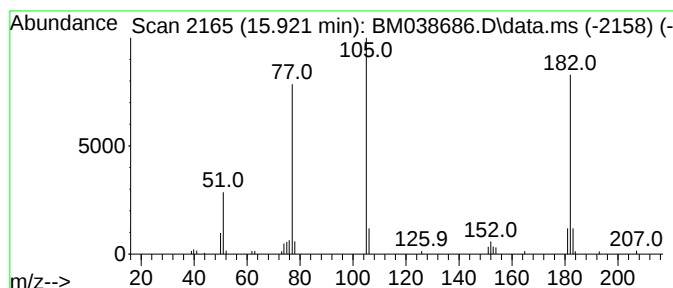
Instrument :  
BNA\_M  
ClientSampleId :  
SASP2-123-2(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM020123.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 5

| R.T.      | EstConc                      | Area  | Relative to ISTD |          | R.T.         |      |
|-----------|------------------------------|-------|------------------|----------|--------------|------|
| 15.922    | 2.17 ng                      | 64200 | Acenaphthene-d10 |          | 14.563       |      |
| Hit# of 5 | Tentative ID                 |       | MW               | MolForm  | CAS#         | Qual |
| 1         | Benzophenone                 |       | 182              | C13H10O  | 000119-61-9  | 95   |
| 2         | Azobenzene                   |       | 182              | C12H10N2 | 000103-33-3  | 43   |
| 3         | Benzene, (2-bromoethenyl)-   |       | 182              | C8H7Br   | 000103-64-0  | 43   |
| 4         | Phenylglyoxal                |       | 134              | C8H6O2   | 001074-12-0  | 38   |
| 5         | 5-Oxo-5-phenylpentanenitrile |       | 173              | C11H11NO | 1000486-83-7 | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM020323\  
Data File : BM038686.D  
Acq On : 03 Feb 2023 19:24  
Operator : CG/JU  
Sample : 01414-04  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
SASP2-123-2(55-62)

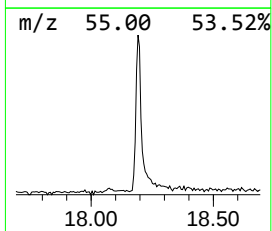
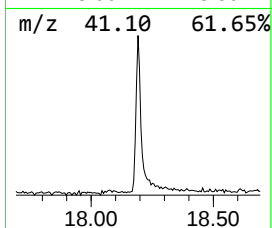
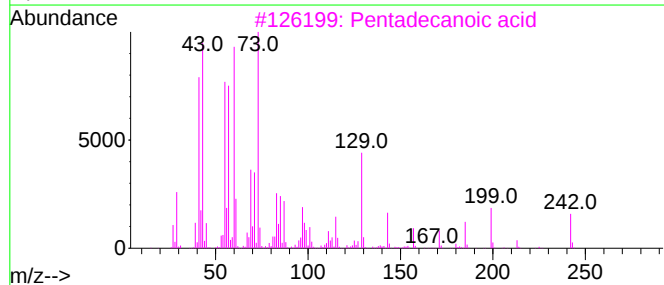
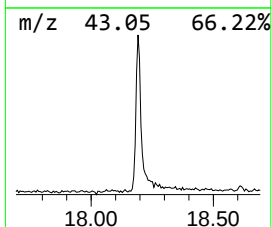
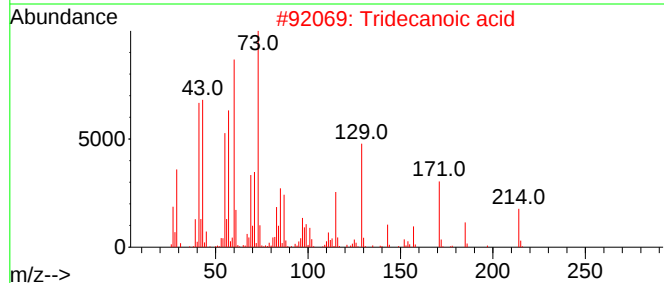
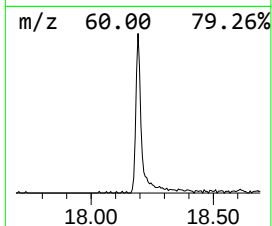
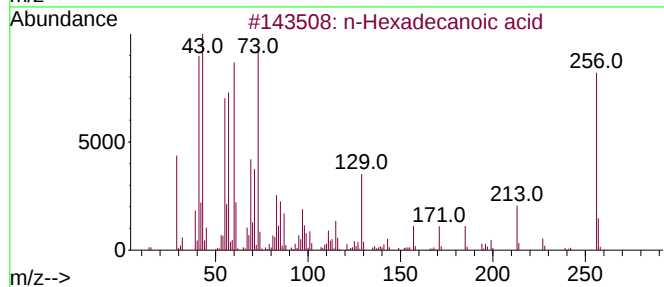
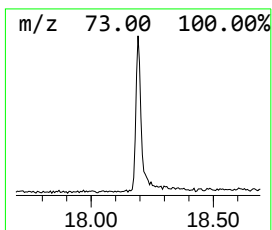
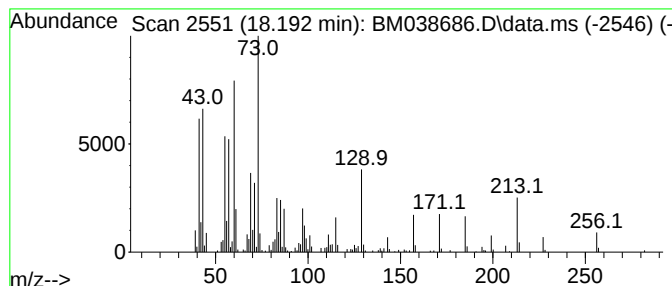
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM020123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T.      | EstConc             | Area   | Relative to ISTD |          | R.T.        |      |
|-----------|---------------------|--------|------------------|----------|-------------|------|
| 18.192    | 10.17 ng            | 366982 | Phenanthrene-d10 |          | 17.304      |      |
| Hit# of 5 | Tentative ID        |        | MW               | MolForm  | CAS#        | Qual |
| 1         | n-Hexadecanoic acid |        | 256              | C16H32O2 | 000057-10-3 | 97   |
| 2         | Tridecanoic acid    |        | 214              | C13H26O2 | 000638-53-9 | 93   |
| 3         | Pentadecanoic acid  |        | 242              | C15H30O2 | 001002-84-2 | 74   |
| 4         | Tetradecanoic acid  |        | 228              | C14H28O2 | 000544-63-8 | 64   |
| 5         | n-Decanoic acid     |        | 172              | C10H20O2 | 000334-48-5 | 58   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM020323\  
Data File : BM038686.D  
Acq On : 03 Feb 2023 19:24  
Operator : CG/JU  
Sample : 01414-04  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
SASP2-123-2(55-62)

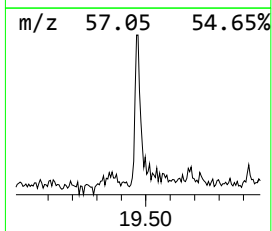
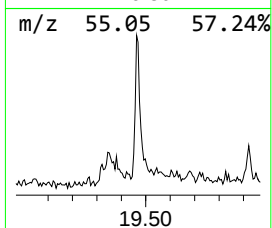
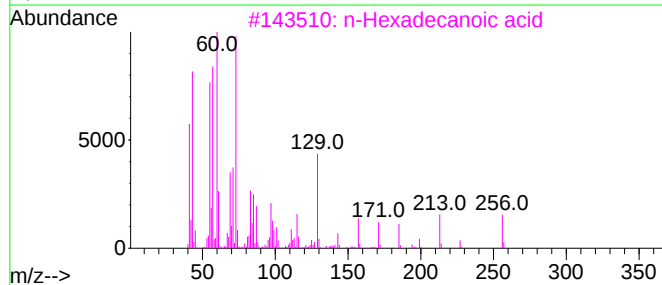
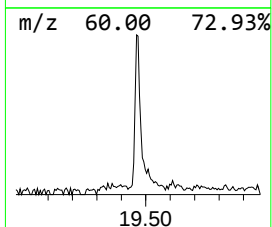
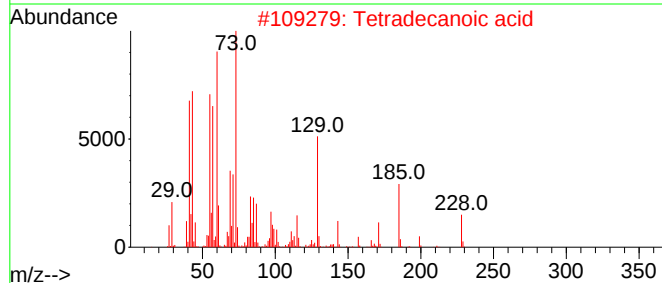
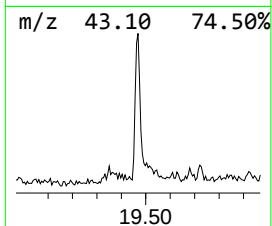
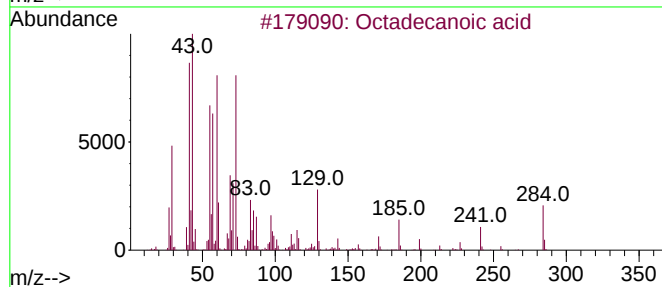
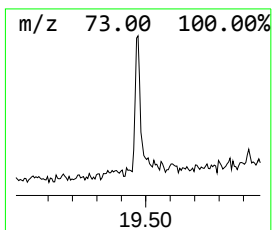
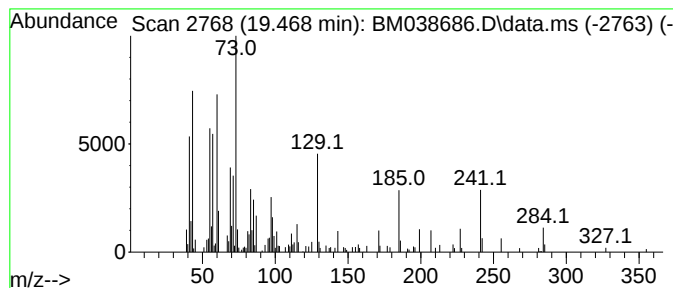
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM020123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 4 Octadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.468 | 3.99 ng | 159972 | Chrysene-d12     | 21.486 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 98   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 76   |
| 3    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 68   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 64   |
| 5    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 58   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM020323\  
Data File : BM038686.D  
Acq On : 03 Feb 2023 19:24  
Operator : CG/JU  
Sample : 01414-04  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
SASP2-123-2(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM020123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

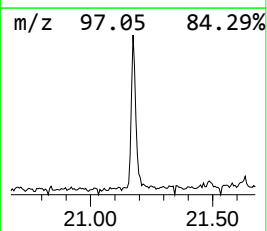
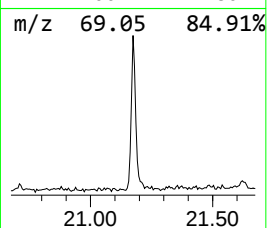
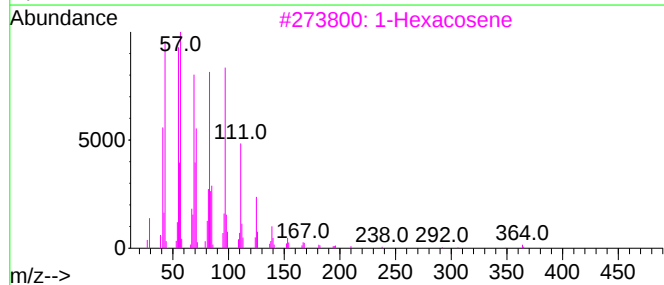
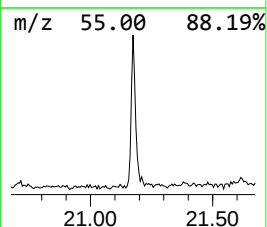
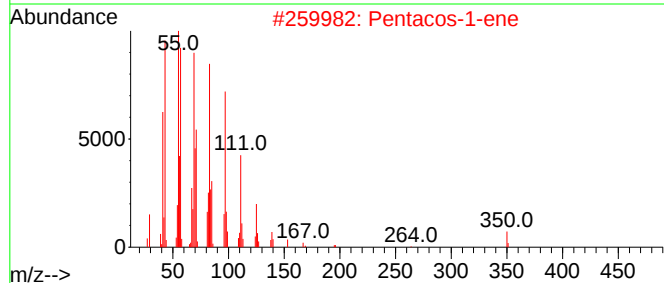
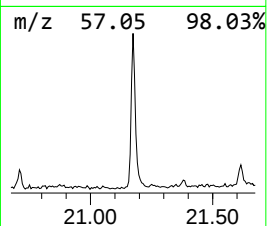
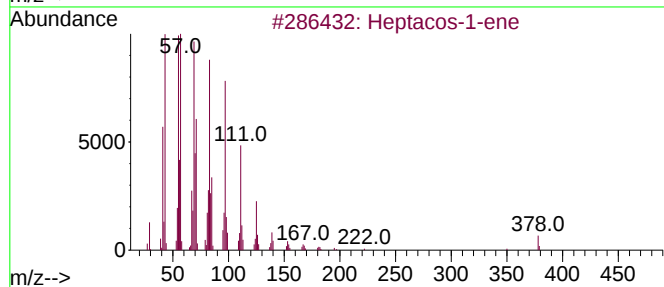
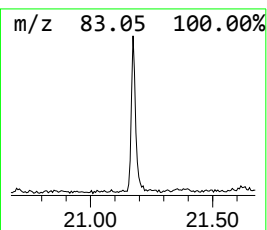
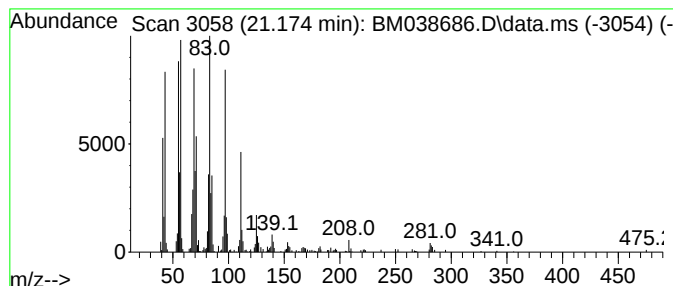
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 5 Heptacos-1-ene Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.174 | 7.14 ng | 286432 | Chrysene-d12     | 21.486 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|----------------------|-----|----------|-------------|------|
| 1    |    |   | Heptacos-1-ene       | 378 | C27H54   | 015306-27-1 | 94   |
| 2    |    |   | Pentacos-1-ene       | 350 | C25H50   | 016980-85-1 | 94   |
| 3    |    |   | 1-Hexacosene         | 364 | C26H52   | 018835-33-1 | 93   |
| 4    |    |   | 1-Heneicosanol       | 312 | C21H44O  | 015594-90-8 | 93   |
| 5    |    |   | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM020323\  
Data File : BM038686.D  
Acq On : 03 Feb 2023 19:24  
Operator : CG/JU  
Sample : 01414-04  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
SASP2-123-2(55-62)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM020123.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 |
| 2-Pentanone, 4-... | 5.016  | 22.7    | ng    | 372307   | 1                     | 7.922  | 327764 | 20.0 |
| Benzophenone       | 15.922 | 2.2     | ng    | 64200    | 3                     | 14.563 | 591001 | 20.0 |
| n-Hexadecanoic ... | 18.192 | 10.2    | ng    | 366982   | 4                     | 17.304 | 721518 | 20.0 |
| Octadecanoic acid  | 19.468 | 4.0     | ng    | 159972   | 5                     | 21.486 | 802595 | 20.0 |
| Heptacos-1-ene     | 21.174 | 7.1     | ng    | 286432   | 5                     | 21.486 | 802595 | 20.0 |