

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF053023\  
 Data File : BF133524.D  
 Acq On : 30 May 2023 16:17  
 Operator : CG\JU  
 Sample : 02957-01  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-9-0A

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-BF052523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133524.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         | 2.116       | 3             | 5           | 11           | rVB      | 398557         | 456256        | 12.03%          | 1.655%        |
| 2         | 5.057       | 496           | 505         | 512          | rBV      | 112666         | 144054        | 3.80%           | 0.523%        |
| 3         | 5.446       | 566           | 571         | 574          | rBV      | 3094044        | 3350292       | 88.36%          | 12.152%       |
| 4         | 6.457       | 737           | 743         | 746          | rBV      | 3088885        | 3442988       | 90.80%          | 12.488%       |
| 5         | 6.828       | 803           | 806         | 810          | rBV      | 999784         | 870893        | 22.97%          | 3.159%        |
| 6         | 7.398       | 897           | 903         | 905          | rBV      | 2114712        | 2126574       | 56.09%          | 7.713%        |
| 7         | 8.116       | 1021          | 1025        | 1027         | rBV      | 1376488        | 1178751       | 31.09%          | 4.275%        |
| 8         | 8.134       | 1027          | 1028        | 1032         | rVB      | 319161         | 189879        | 5.01%           | 0.689%        |
| 9         | 8.828       | 1142          | 1146        | 1149         | rBV      | 110149         | 94132         | 2.48%           | 0.341%        |
| 10        | 8.922       | 1158          | 1162        | 1167         | rVB      | 58312          | 51694         | 1.36%           | 0.188%        |
| 11        | 9.192       | 1204          | 1208        | 1211         | rVB      | 4147542        | 3598822       | 94.91%          | 13.053%       |
| 12        | 9.869       | 1319          | 1323        | 1326         | rVV      | 1558300        | 1206613       | 31.82%          | 4.377%        |
| 13        | 9.898       | 1326          | 1328        | 1332         | rVB      | 104218         | 84346         | 2.22%           | 0.306%        |
| 14        | 10.069      | 1354          | 1357        | 1361         | rVB      | 100205         | 88411         | 2.33%           | 0.321%        |
| 15        | 10.416      | 1412          | 1416        | 1419         | rVB      | 98667          | 77103         | 2.03%           | 0.280%        |
| 16        | 10.586      | 1441          | 1445        | 1448         | rBV      | 334574         | 270991        | 7.15%           | 0.983%        |
| 17        | 10.657      | 1453          | 1457        | 1461         | rBV      | 2658326        | 2480333       | 65.41%          | 8.996%        |
| 18        | 11.357      | 1572          | 1576        | 1578         | rBV      | 1554861        | 1300606       | 34.30%          | 4.717%        |
| 19        | 11.375      | 1578          | 1579        | 1583         | rVB      | 115717         | 93121         | 2.46%           | 0.338%        |
| 20        | 11.886      | 1663          | 1666        | 1671         | rBV      | 287262         | 263847        | 6.96%           | 0.957%        |
| 21        | 12.569      | 1776          | 1782        | 1784         | rBV      | 44312          | 40508         | 1.07%           | 0.147%        |
| 22        | 12.675      | 1794          | 1800        | 1809         | rBV3     | 46450          | 60930         | 1.61%           | 0.221%        |
| 23        | 12.951      | 1842          | 1847        | 1850         | rBV      | 3906703        | 3791691       | 100.00%         | 13.753%       |
| 24        | 13.851      | 1996          | 2000        | 2015         | rBV2     | 191677         | 330210        | 8.71%           | 1.198%        |
| 25        | 13.998      | 2020          | 2025        | 2028         | rBV      | 1257892        | 1104958       | 29.14%          | 4.008%        |
| 26        | 14.763      | 2151          | 2155        | 2158         | rBV2     | 76734          | 89402         | 2.36%           | 0.324%        |
| 27        | 15.457      | 2267          | 2273        | 2277         | rBV      | 635853         | 782709        | 20.64%          | 2.839%        |

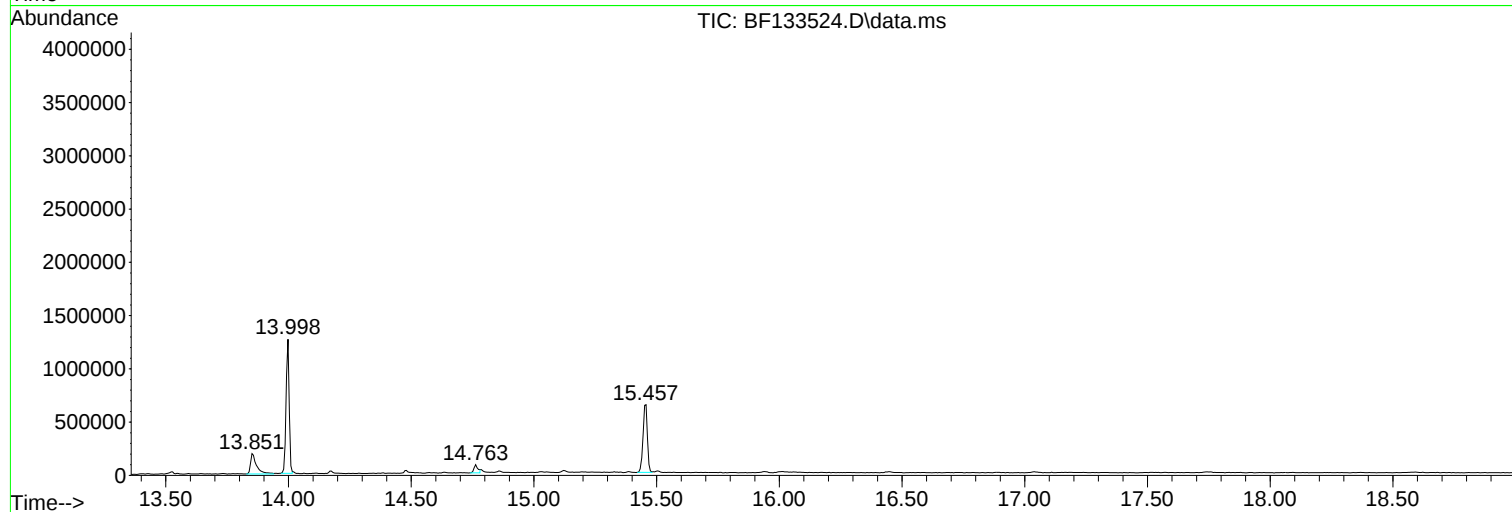
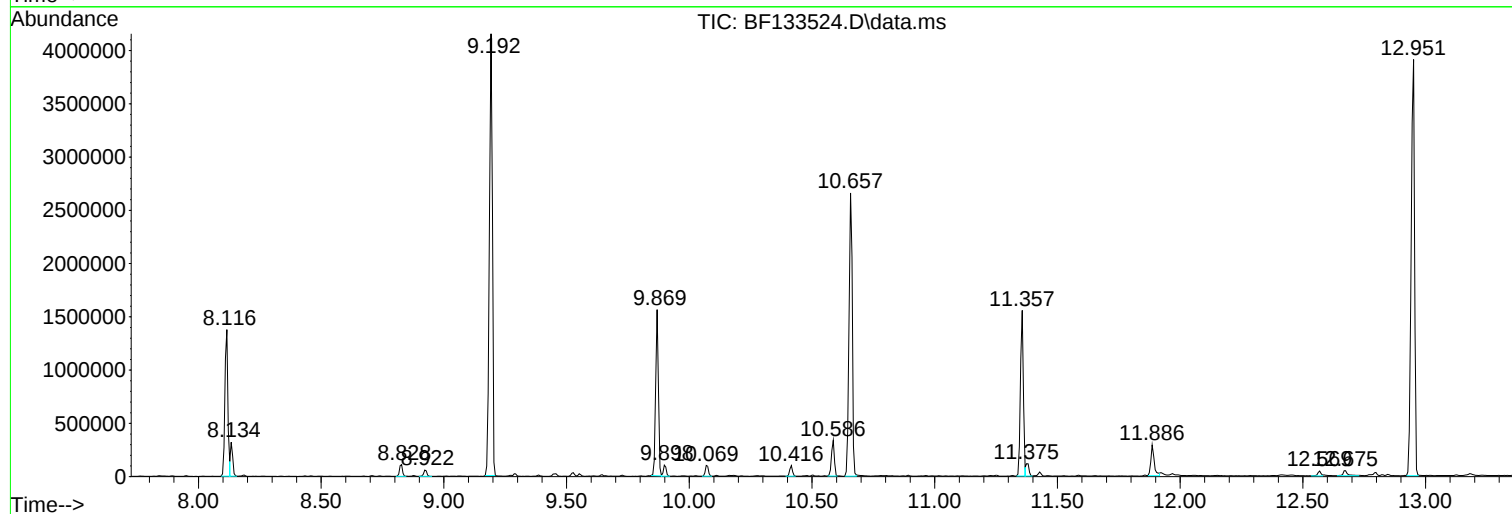
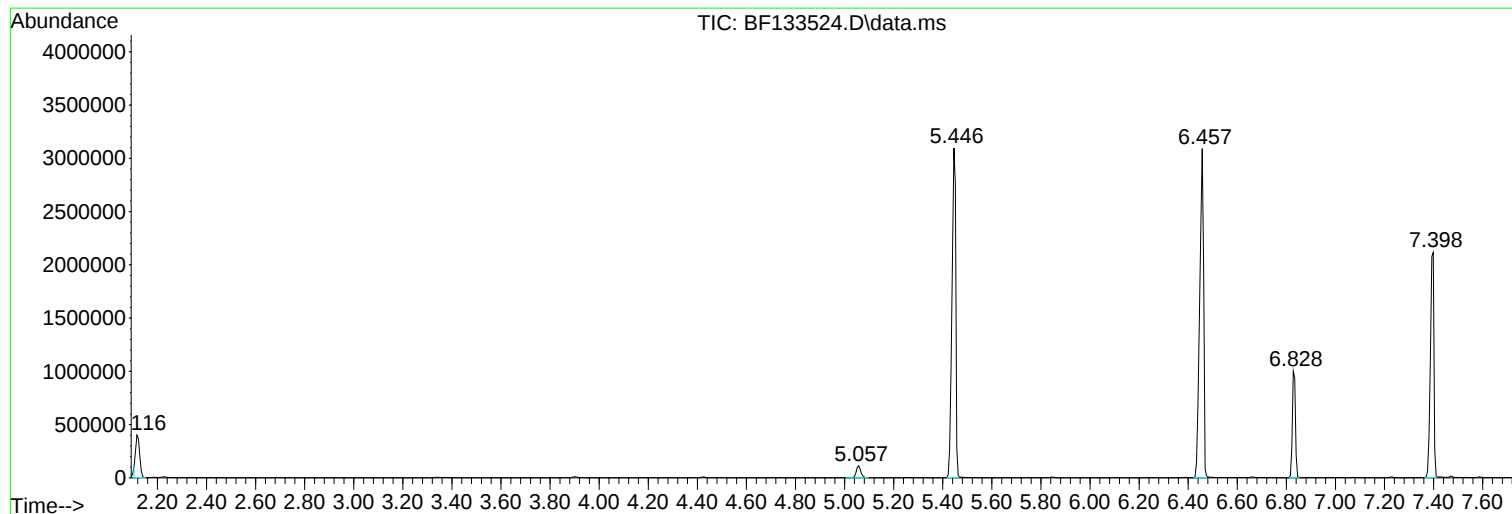
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TP-9-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052523.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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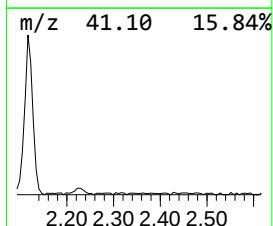
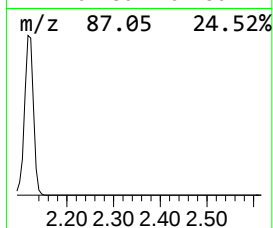
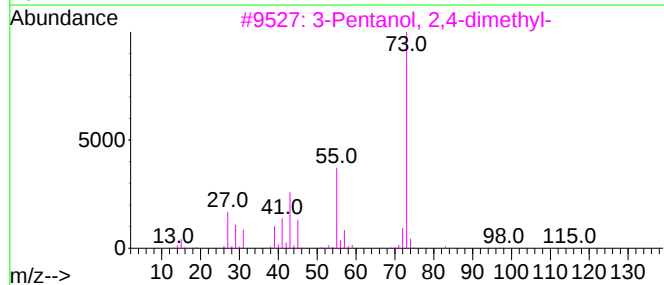
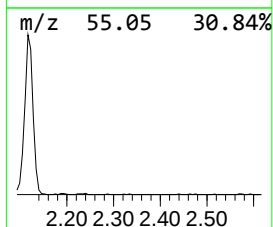
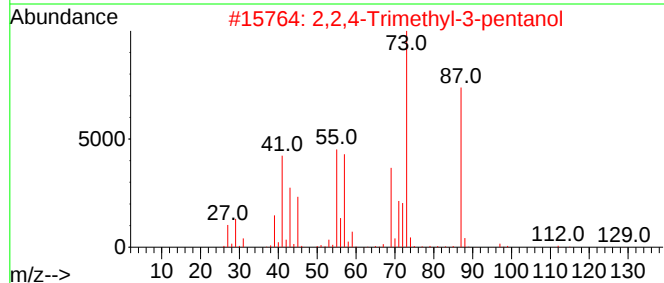
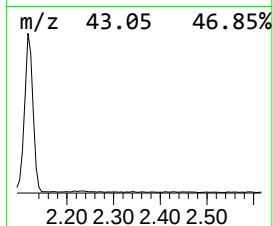
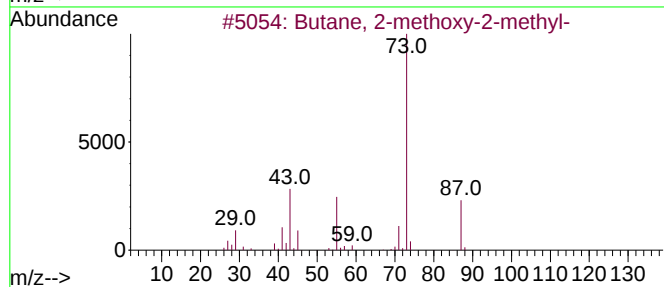
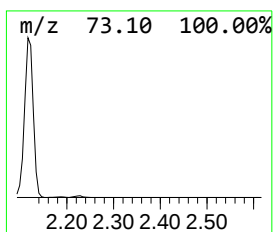
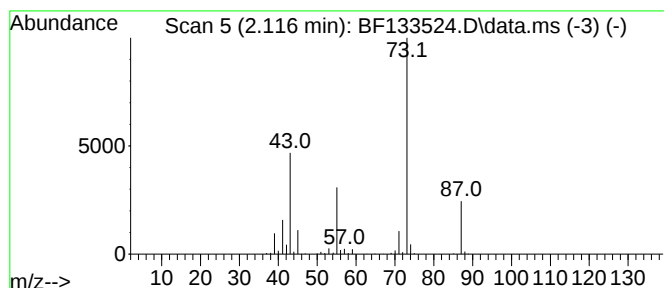
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052523.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|----------|--------|------------------------|-------|
| 2.116 | 10.48 ng | 456256 | 1,4-Dichlorobenzene-d4 | 6.834 |

| 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    |    |   | 3-Pentanol, 2,4-dimethyl-   | 116 | C7H16O  | 000600-36-2 | 37   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 35   |
| 5    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 25   |



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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
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TP-9-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052523.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

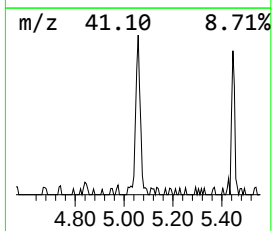
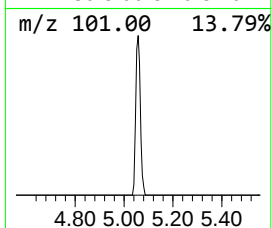
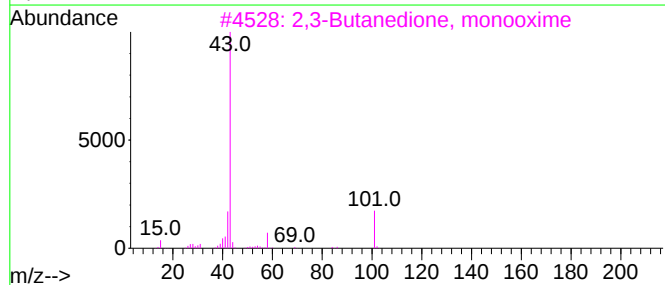
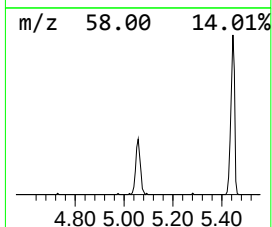
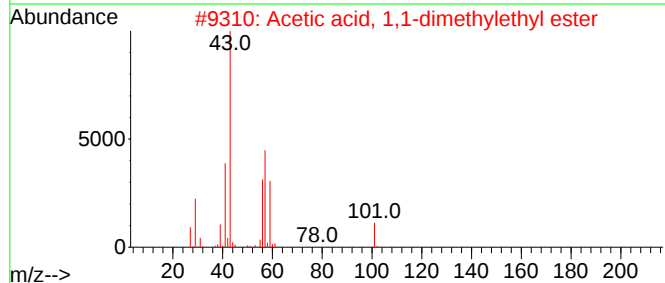
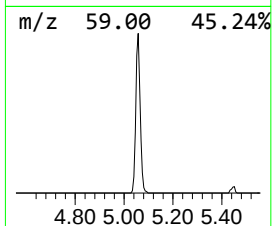
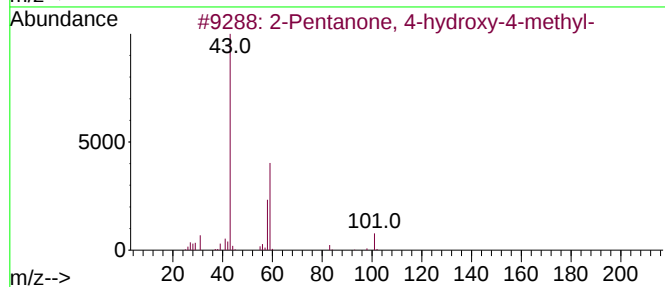
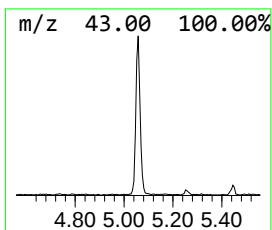
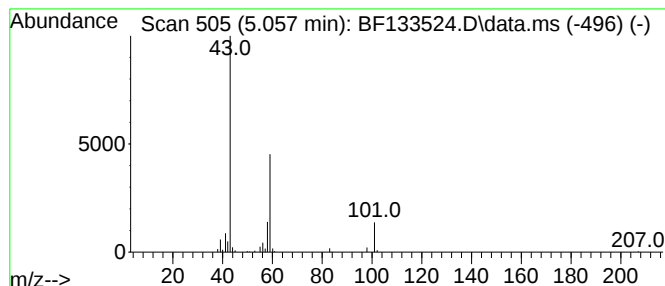
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.057 | 3.31 ng | 144054 | 1,4-Dichlorobenzene-d4 | 6.834 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2      | 000540-88-5 | 28      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 27      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 12      |      |      |
| 5    | 4-Penten-2-one, 4-methyl-           | 98  | C6H10O       | 003744-02-3 | 9       |      |      |



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Sample : 02957-01  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-9-0A

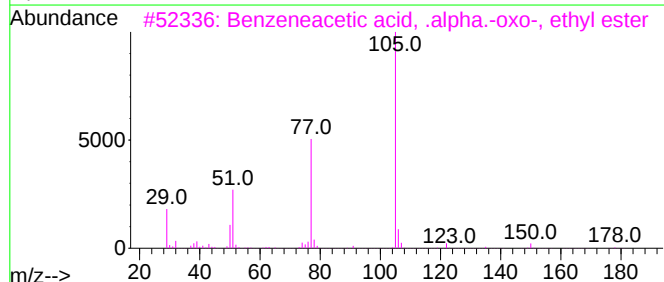
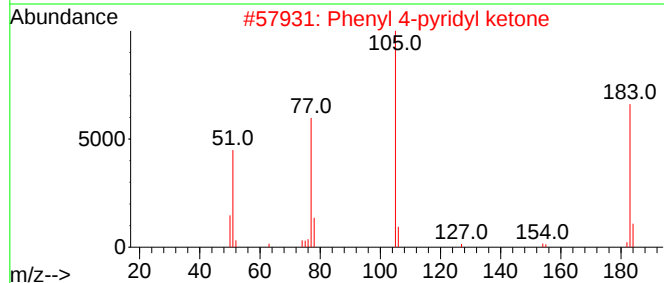
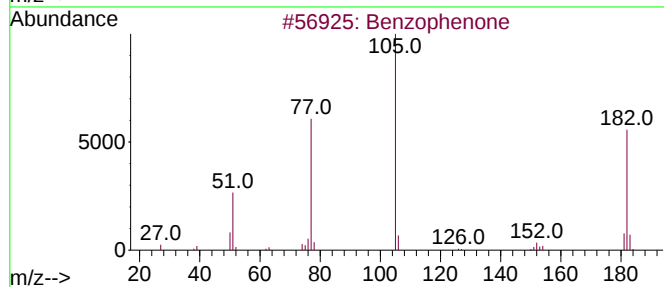
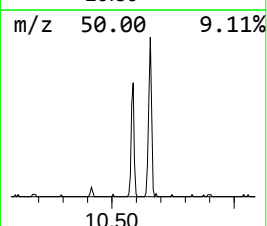
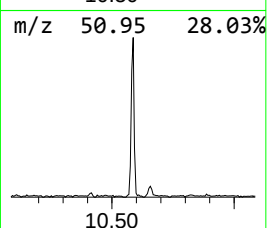
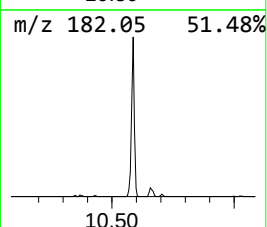
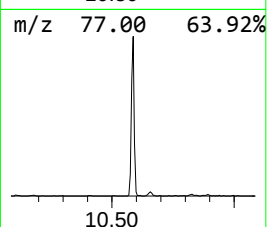
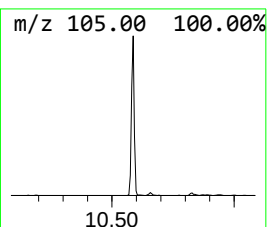
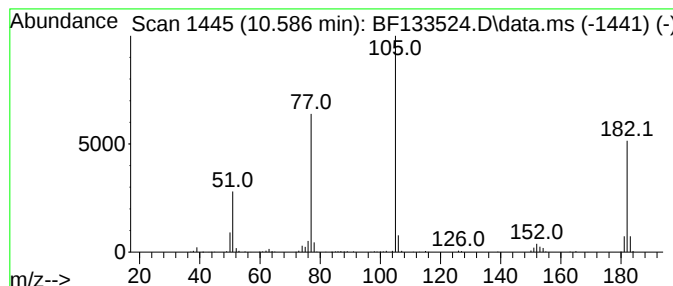
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Benzophenone Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.586 | 4.49 ng | 270991 | Acenaphthene-d10 | 9.869 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | Phenyl 4-pyridyl ketone             | 183 | C12H9NO  | 014548-46-0 | 50   |
| 3    |    |   | Benzeneacetic acid, .alpha.-oxo-... | 178 | C10H10O3 | 001603-79-8 | 50   |
| 4    |    |   | N-Methoxy-N-methylbenzamide         | 165 | C9H11NO2 | 006919-61-5 | 50   |
| 5    |    |   | 1-Propanone, 3-chloro-1-phenyl-     | 168 | C9H9ClO  | 000936-59-4 | 50   |



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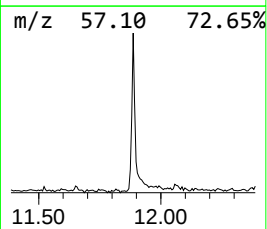
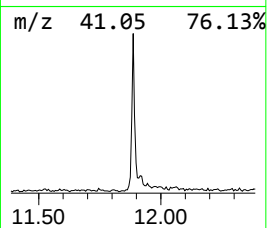
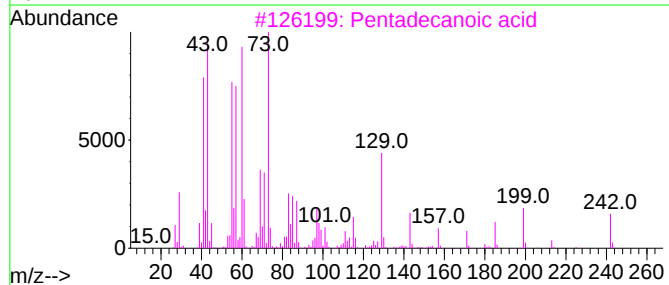
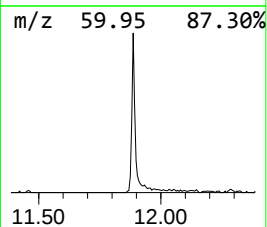
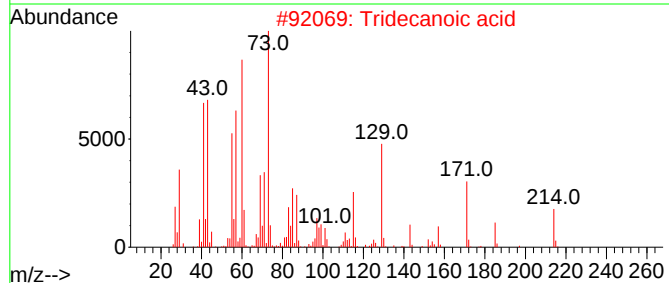
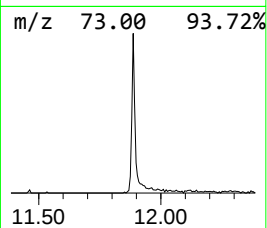
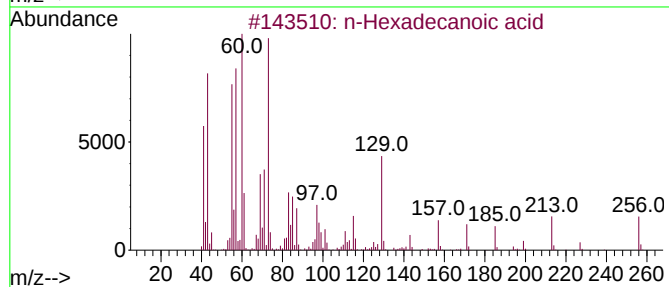
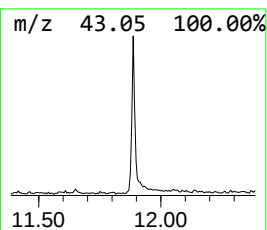
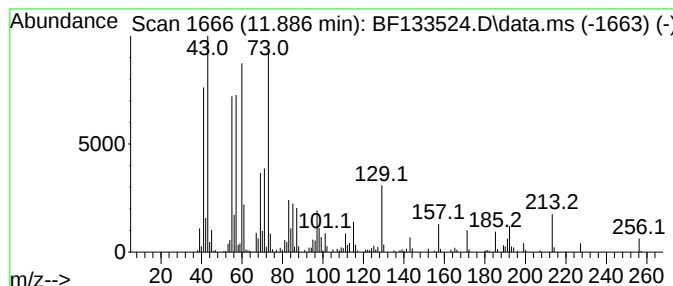
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.886 | 4.06 ng | 263847 | Phenanthrene-d10 | 11.357 |

| 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 | 95   |
| 3    |    |   | Pentadecanoic acid    | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |    |   | Tetradecanoic acid    | 228 | C14H28O2 | 000544-63-8 | 80   |
| 5    |    |   | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 64   |



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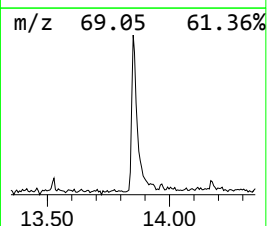
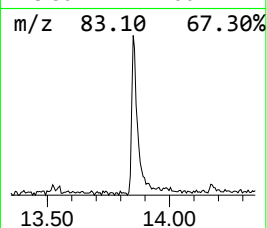
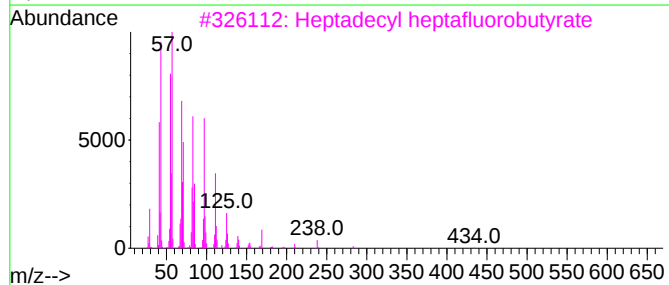
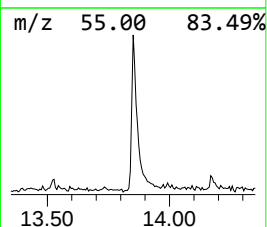
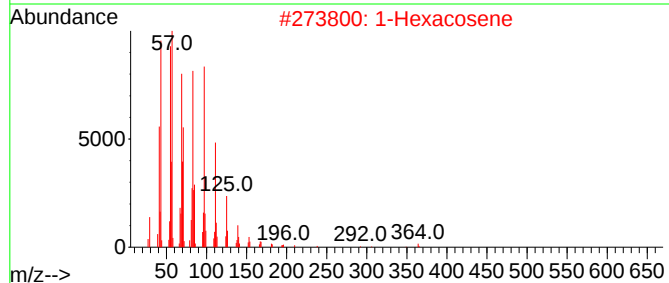
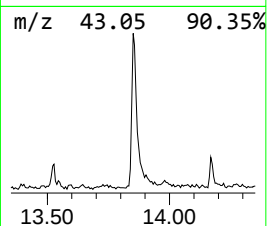
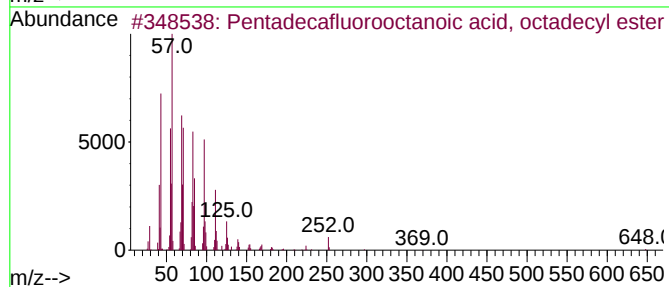
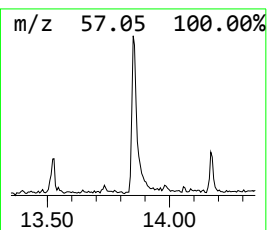
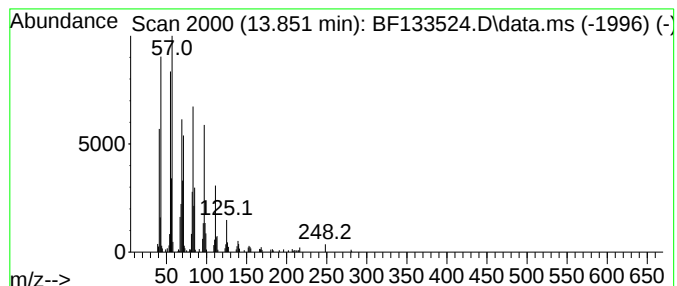
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.851 | 5.98 ng | 330210 | Chrysene-d12     | 13.998 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 94   |
| 2    |    |   | 1-Hexacosene                        | 364 | C26H52      | 018835-33-1  | 94   |
| 3    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2  | 959085-66-6  | 94   |
| 4    |    |   | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2  | 006385-15-5  | 91   |
| 5    |    |   | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2  | 000400-57-7  | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF053023\  
Data File : BF133524.D  
Acq On : 30 May 2023 16:17  
Operator : CG\JU  
Sample : 02957-01  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-9-0A

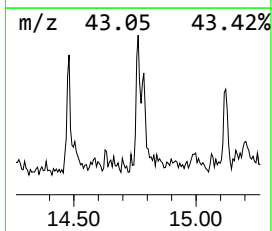
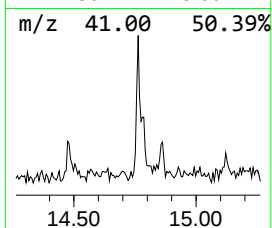
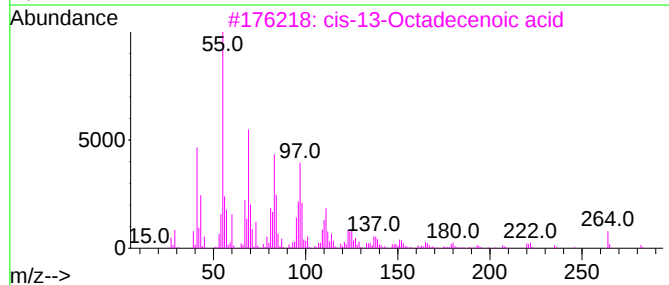
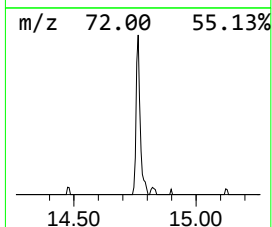
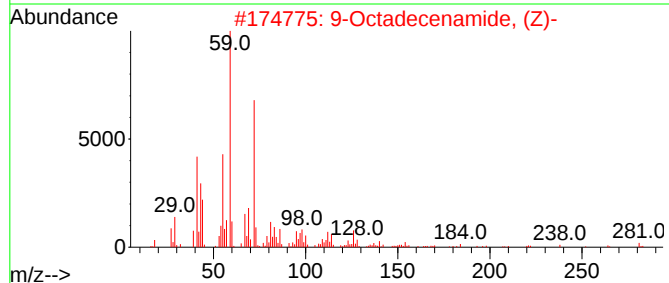
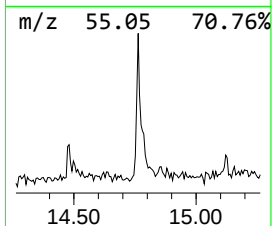
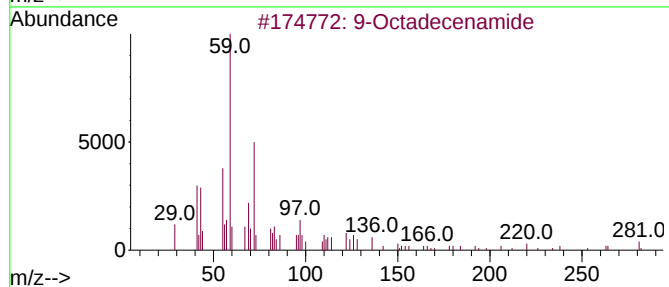
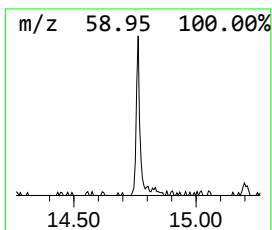
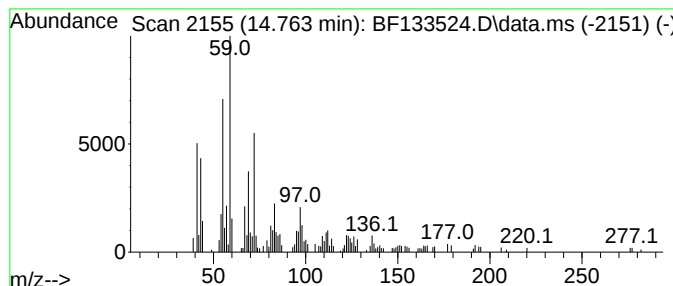
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052523.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 9-Octadecenamide Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.763 | 2.28 ng | 89402 | Perylene-d12     | 15.457 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 9-Octadecenamide                    | 281 | C18H35NO | 003322-62-1  | 68   |
| 2    |    |   | 9-Octadecenamide, (Z)-              | 281 | C18H35NO | 000301-02-0  | 64   |
| 3    |    |   | cis-13-Octadecenoic acid            | 282 | C18H34O2 | 013126-39-1  | 38   |
| 4    |    |   | Palmitoleamide                      | 253 | C16H31NO | 106010-22-4  | 38   |
| 5    |    |   | 2-Hydroxy-2,4-dimethyl-hept-6-en... | 156 | C9H16O2  | 1000192-56-0 | 30   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF053023\  
Data File : BF133524.D  
Acq On : 30 May 2023 16:17  
Operator : CG\JU  
Sample : 02957-01  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-9-0A

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052523.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 |
| Butane, 2-metho... | 2.116  | 10.5    | ng    | 456256   | 1                     | 6.834  | 870893  | 20.0 |
| 2-Pentanone, 4-... | 5.057  | 3.3     | ng    | 144054   | 1                     | 6.834  | 870893  | 20.0 |
| Benzophenone       | 10.586 | 4.5     | ng    | 270991   | 3                     | 9.869  | 1206610 | 20.0 |
| n-Hexadecanoic ... | 11.886 | 4.1     | ng    | 263847   | 4                     | 11.357 | 1300610 | 20.0 |
| Pentadecafluoro... | 13.851 | 6.0     | ng    | 330210   | 5                     | 13.998 | 1104960 | 20.0 |
| 9-Octadecenamide   | 14.763 | 2.3     | ng    | 89402    | 6                     | 15.457 | 782709  | 20.0 |