LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131410.D
Acq On : 25 Nov 2022 22:57
Operator : CG\JU
Sample : N5742-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-43

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-BF112122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131410.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.263 | 23 | 30 | 35 | rVB | 1658021 | 2184326 | 74.43% | 11.879% |
| 2 | 5.169 | 520 | 524 | 529 | rBV | 115588 | 126508 | 4.31% | 0.688% |
| 3 | 5.563 | 586 | 591 | 594 | rBV | 1428281 | 1254979 | 42.76% | 6.825% |
| 4 | 6.563 | 757 | 761 | 764 | rBV | 950847 | 793460 | 27.04% | 4.315% |
| 5 | 6.951 | 824 | 827 | 831 | rBV | 667215 | 569126 | 19.39% | 3.095% |
| 6 | 7.522 | 911 | 924 | 927 | rBV | 1789037 | 1688502 | 57.54% | 9.183% |
| 7 | 8.245 | 1038 | 1047 | 1050 | rBV | 826752 | 771031 | 26.27% | 4.193% |
| 8 | 9.328 | 1225 | 1231 | 1234 | rBV | 3295149 | 2934628 | 100.00% | 15.960% |
| 9 | 10.010 | 1343 | 1347 | 1350 | rBV | 1041384 | 845714 | 28.82% | 4.599% |
| 10 | 10.804 | 1477 | 1482 | 1485 | rBV | 2087249 | 1932350 | 65.85% | 10.509% |
| 11 | 11.504 | 1597 | 1601 | 1605 | rBV | 1019177 | 842555 | 28.71% | 4.582% |
| 12 | 12.027 | 1684 | 1690 | 1698 | rBV | 195185 | 217368 | 7.41% | 1.182% |
| 13 | 12.816 | 1819 | 1824 | 1831 | rBV | 60916 | 71274 | 2.43% | 0.388% |
| 14 | 13.104 | 1868 | 1873 | 1876 | rBV | 2642330 | 2487769 | 84.77% | 13.530% |
| 15 | 14.004 | 2022 | 2026 | 2033 | rBV | 235908 | 327886 | 11.17% | 1.783% |
| 16 | 14.163 | 2049 | 2053 | 2056 | rVB | 621904 | 526886 | 17.95% | 2.865% |
| 17 | 14.263 | 2065 | 2070 | 2077 | rBV | 77310 | 94184 | 3.21% | 0.512% |
| 18 | 15.039 | 2199 | 2202 | 2207 | rVB | 60753 | 61023 | 2.08% | 0.332% |
| 19 | 15.698 | 2309 | 2314 | 2318 | rBV | 371137 | 486196 | 16.57% | 2.644% |
| 20 | 15.733 | 2318 | 2320 | 2325 | rVB2 | 37292 | 41858 | 1.43% | 0.228% |
| 21 | 16.210 | 2396 | 2401 | 2406 | rVB | 33649 | 50741 | 1.73% | 0.276% |
| 22 | 16.757 | 2490 | 2494 | 2499 | rBV2 | 26219 | 38951 | 1.33% | 0.212% |
| 23 | 17.410 | 2599 | 2605 | 2613 | rVB5 | 19553 | 40238 | 1.37% | 0.219% |

Sum of corrected areas: 18387553

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**ClientSampleId :**
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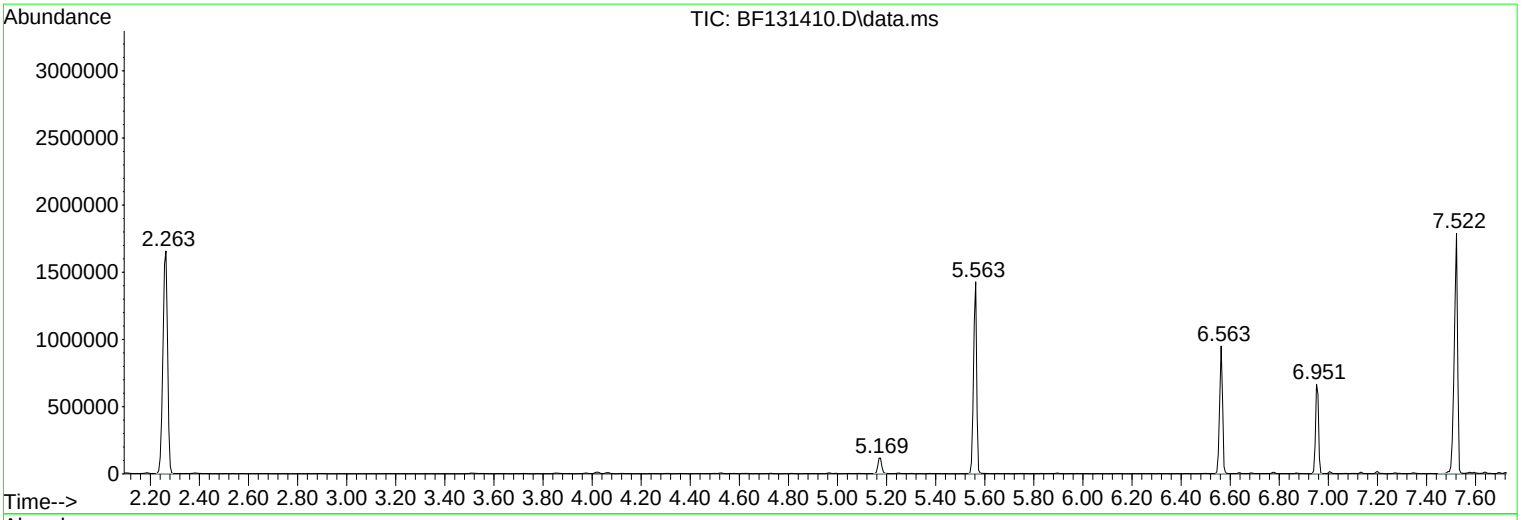
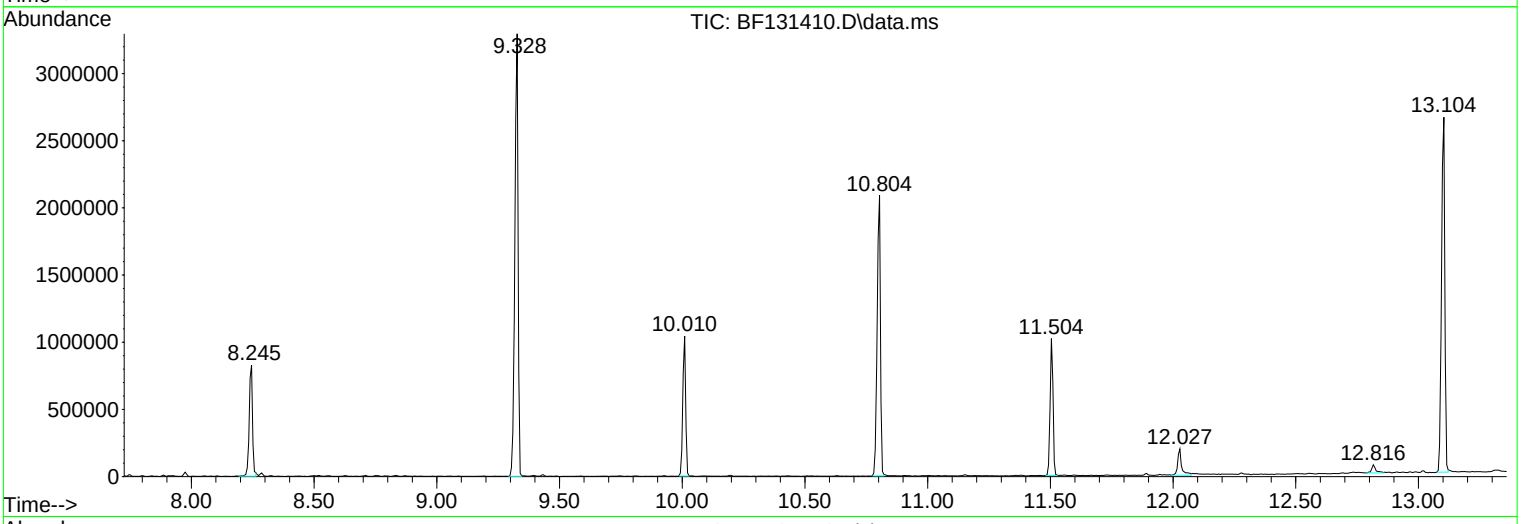
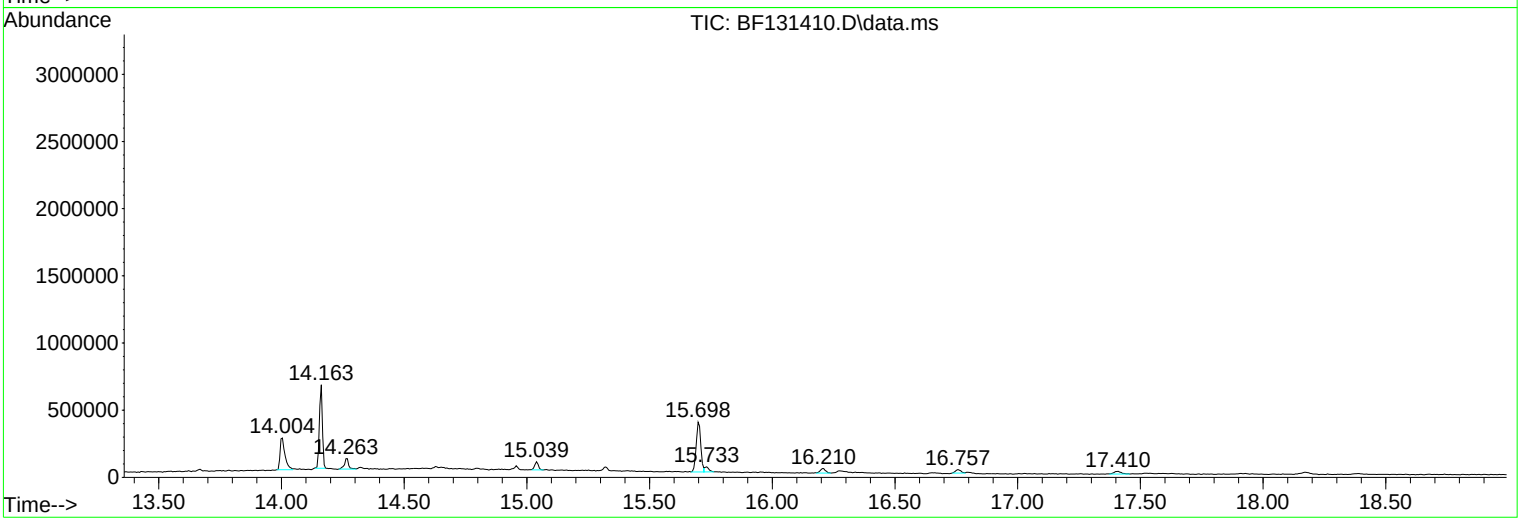
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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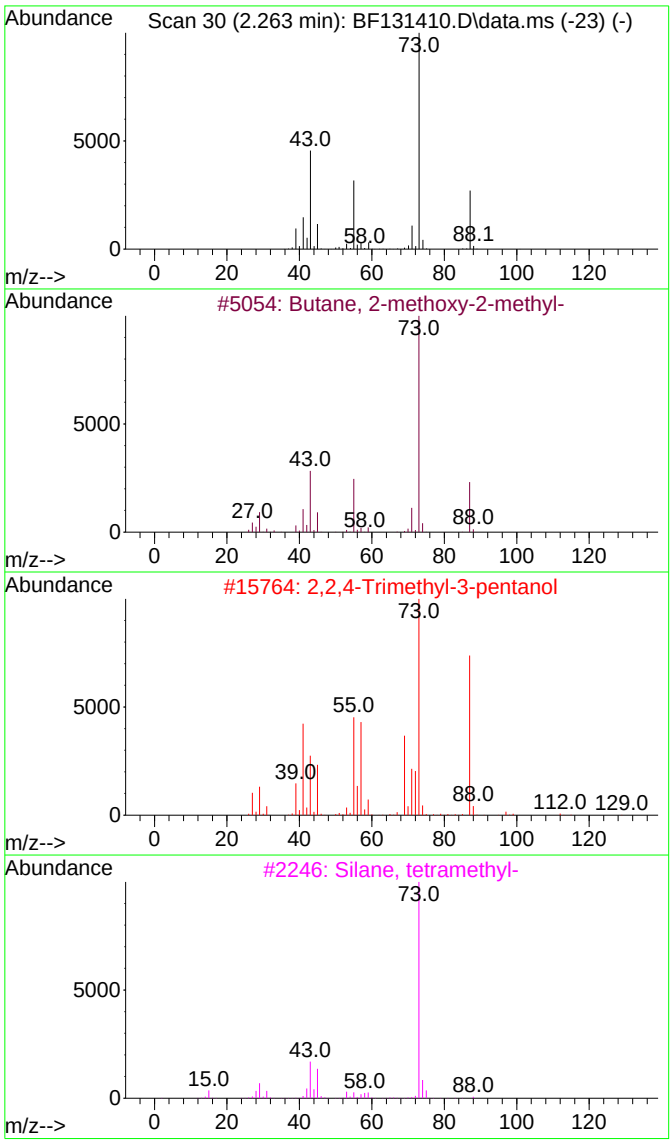
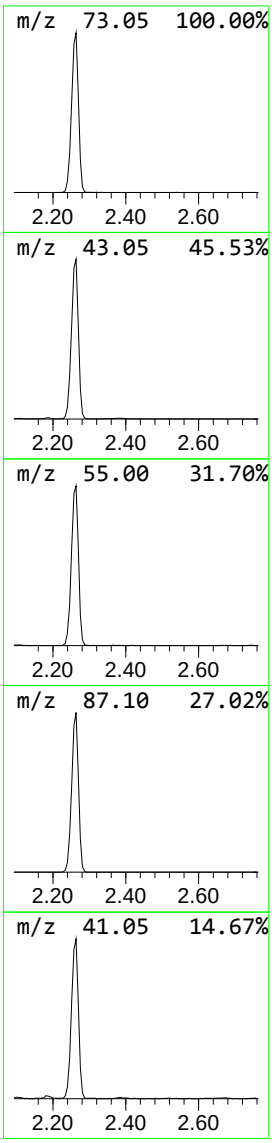
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.263 | 76.76 ng | 2184330 | 1,4-Dichlorobenzene-d4 | 6.957 |

| 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 | 40 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



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Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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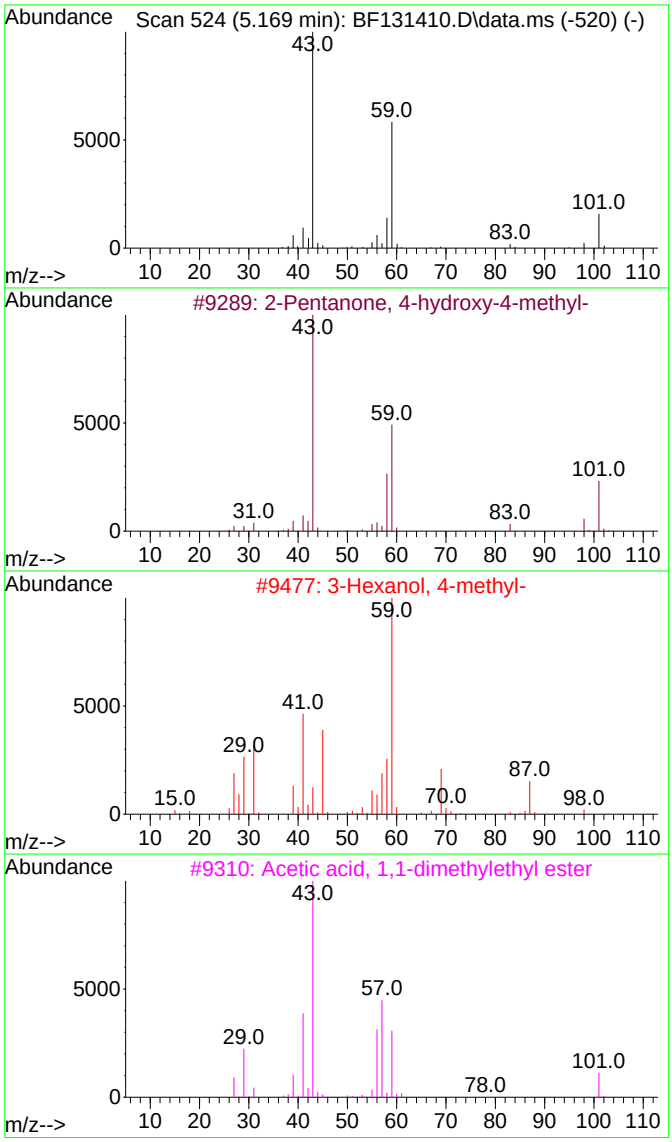
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

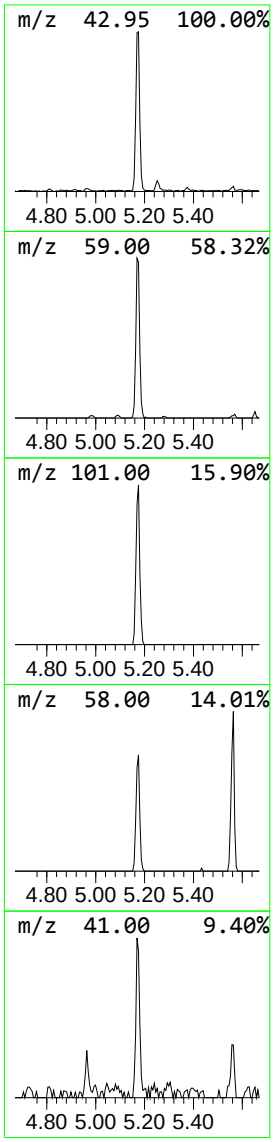
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.169 | 4.45 ng | 126508 | 1,4-Dichlorobenzene-d4 | 6.957 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 28 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131410.D
Acq On : 25 Nov 2022 22:57
Operator : CG\JU
Sample : N5742-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-43

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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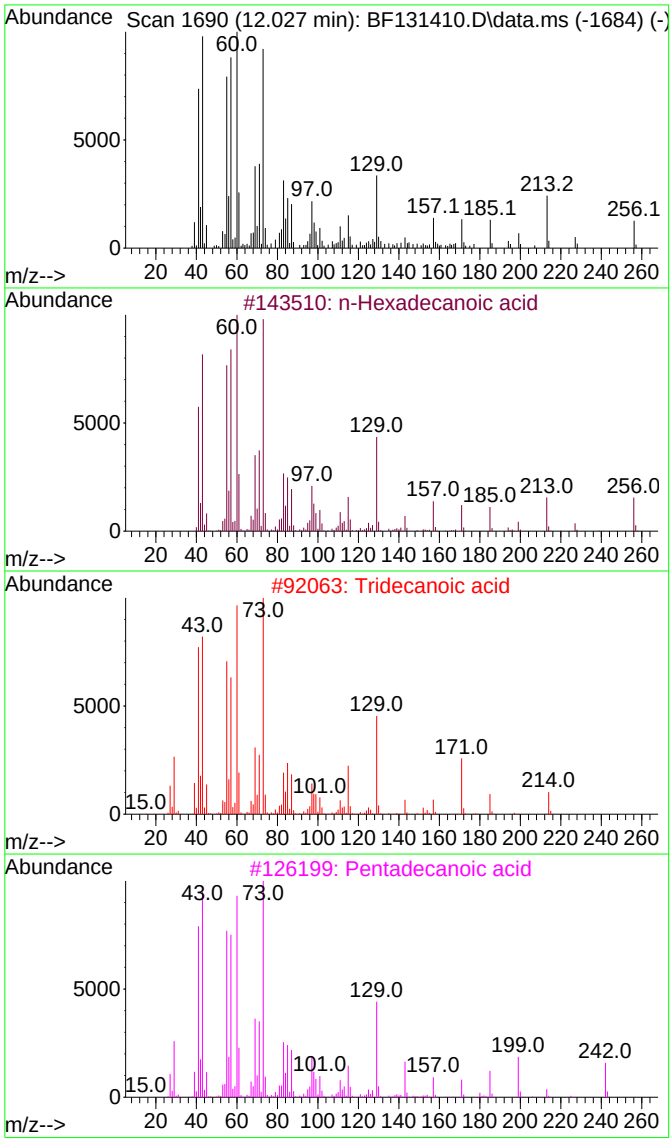
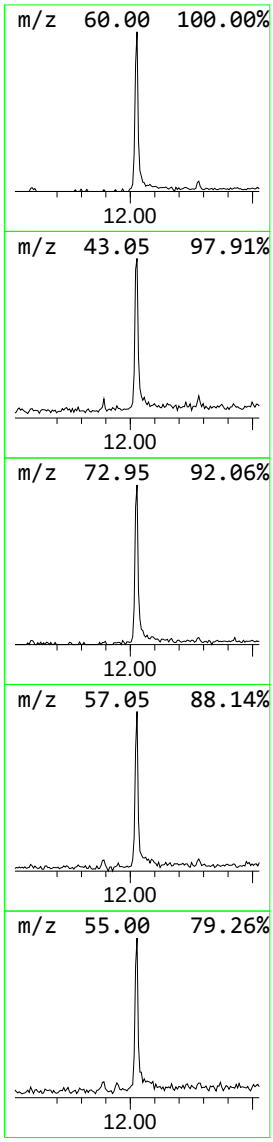
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.028 | 5.16 ng | 217368 | Phenanthrene-d10 | 11.504 |

| 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 | 93 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 62 |



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Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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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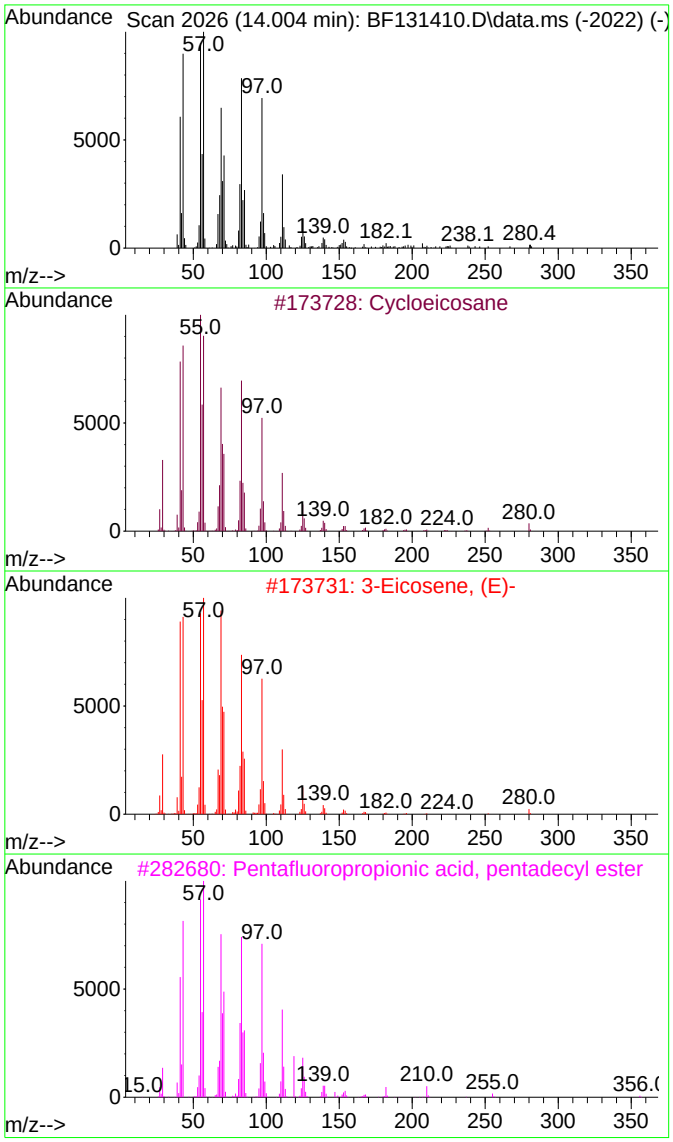
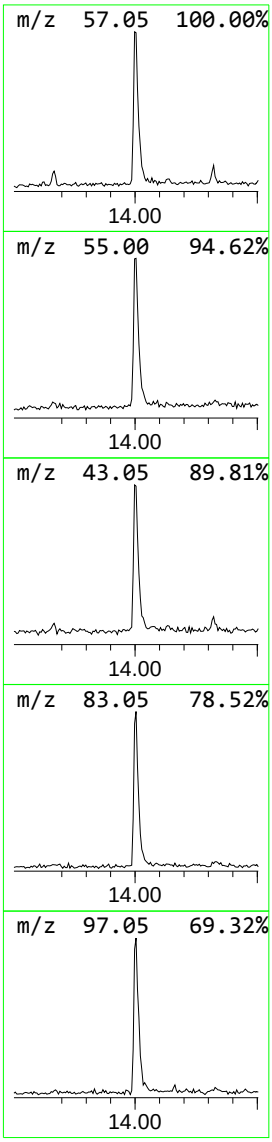
Peak Number 4 Cycloeicosane Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.004 | 12.45 ng | 327886 | Chrysene-d12 | 14.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 95 |
| 2 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 95 |
| 3 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94 |
| 4 | 1-Heptadecene | 238 | C17H34 | 006765-39-5 | 93 |
| 5 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |



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Sample : N5742-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-43

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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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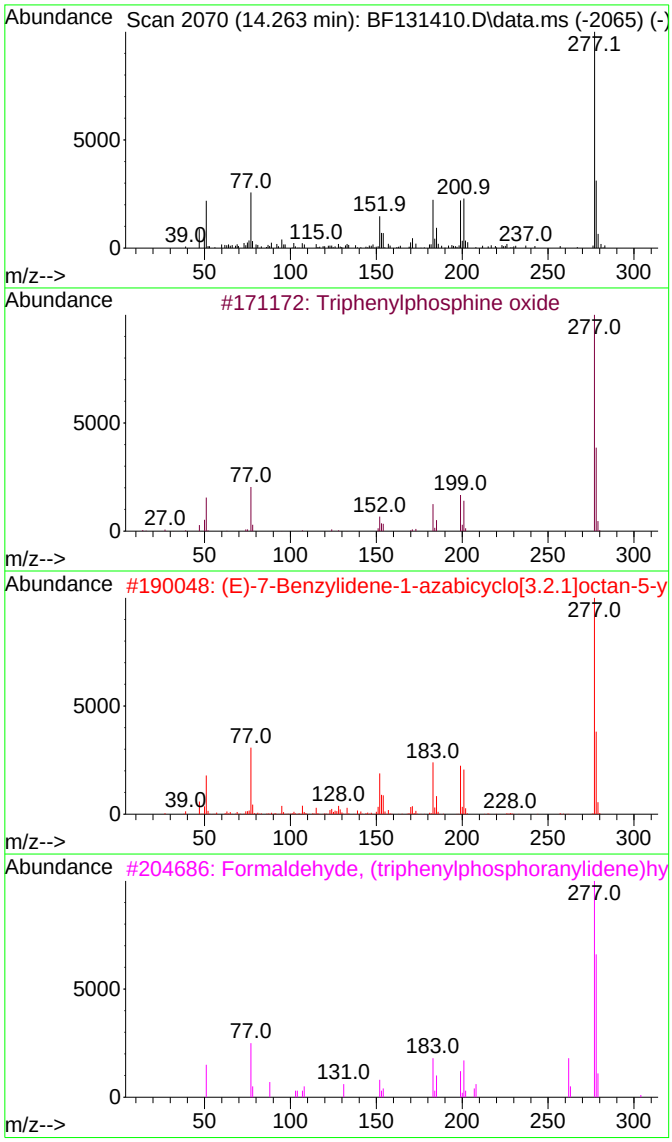
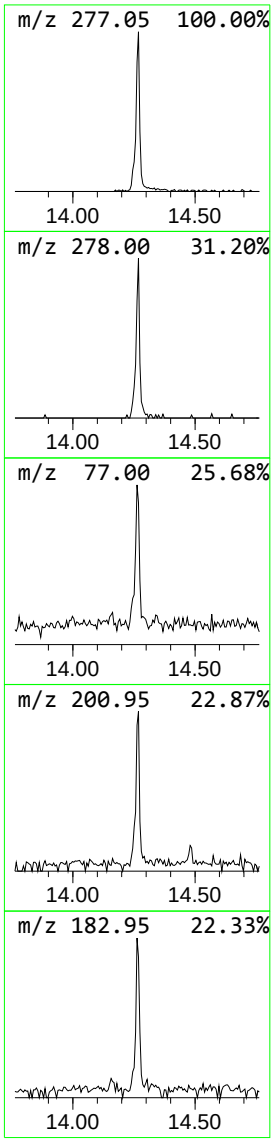
Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.263 | 3.58 ng | 94184 | Chrysene-d12 | 14.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 97 |
| 2 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 91 |
| 3 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 50 |
| 4 | Vanadium, cycloheptatrienyl-(pen... | 277 | C17H22V | 1000155-20-5 | 46 |
| 5 | 2-Methoxy-5-amino-4,6-diphenylpy... | 277 | C17H15N3O | 076891-83-3 | 23 |



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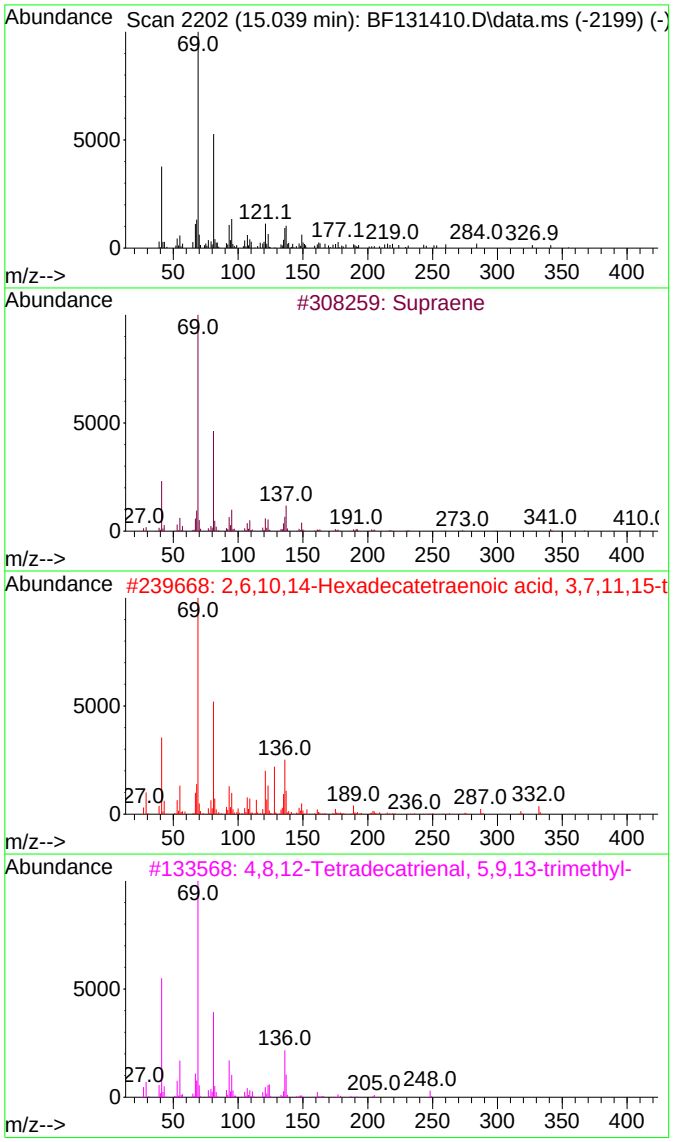
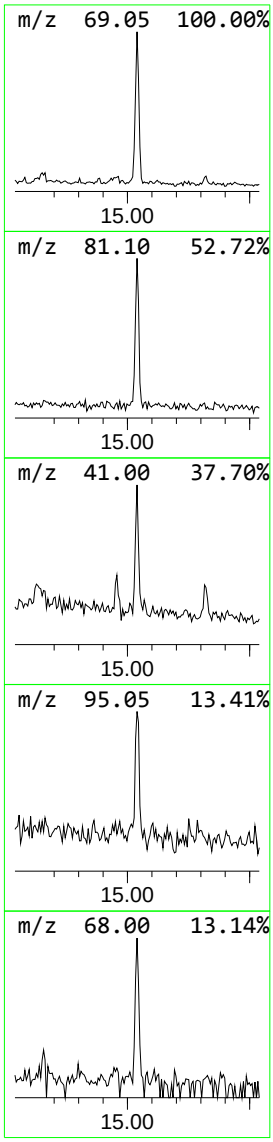
Peak Number 6 Supraene Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.039 | 2.51 ng | 61023 | Perylene-d12 | 15.698 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 87 |
| 2 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 72 |
| 3 | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O | 066408-55-7 | 64 |
| 4 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 64 |
| 5 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 64 |



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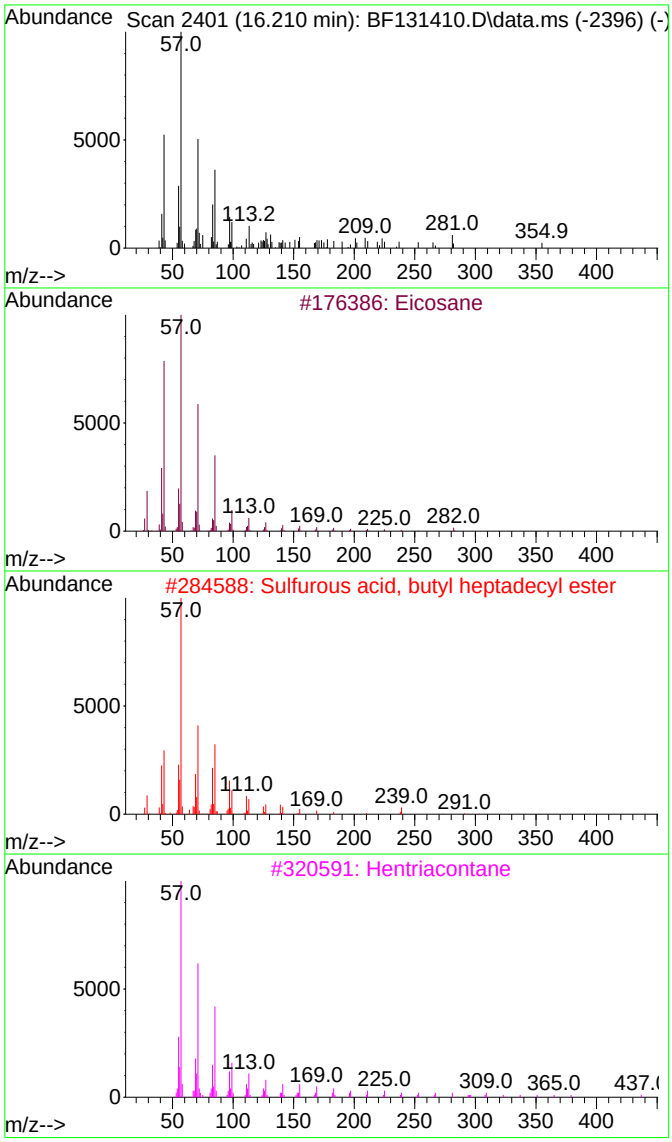
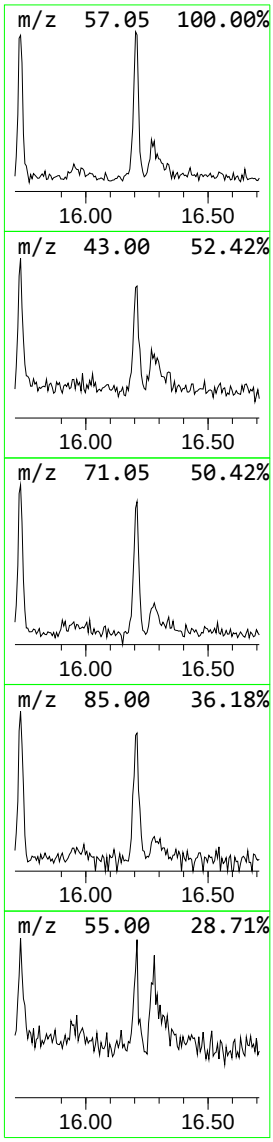
Peak Number 7 Eicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.210 | 2.09 ng | 50741 | Perylene-d12 | 15.698 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 89 |
| 2 | Sulfurous acid, butyl heptadecyl... | 376 | C21H44O3S | 1000309-18-4 | 86 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 80 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 72 |
| 5 | Tetracosane, 11-decyl- | 479 | C34H70 | 055429-84-0 | 68 |



Tentatively Identified Compound (LSC) summary

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| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 2.263 | 76.8 | ng | 2184330 | 1 | 6.957 | 569126 | 20.0 |
| 2-Pentanone, 4-... | 5.169 | 4.5 | ng | 126508 | 1 | 6.957 | 569126 | 20.0 |
| n-Hexadecanoic ... | 12.028 | 5.2 | ng | 217368 | 4 | 11.504 | 842555 | 20.0 |
| Cycloeicosane | 14.004 | 12.4 | ng | 327886 | 5 | 14.163 | 526886 | 20.0 |
| Triphenylphosph... | 14.263 | 3.6 | ng | 94184 | 5 | 14.163 | 526886 | 20.0 |
| Supraene | 15.039 | 2.5 | ng | 61023 | 6 | 15.698 | 486196 | 20.0 |
| Eicosane | 16.210 | 2.1 | ng | 50741 | 6 | 15.698 | 486196 | 20.0 |