LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102722\
Data File : BF130811.D
Acq On : 27 Oct 2022 22:24
Operator : CG\JU
Sample : PB148576BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB148576BL

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130811.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.322 | 32 | 40 | 46 | rVB | 80421 | 112207 | 2.85% | 0.483% |
| 2 | 5.198 | 521 | 529 | 539 | rBV | 246268 | 344884 | 8.77% | 1.485% |
| 3 | 5.575 | 587 | 593 | 596 | rBV | 2780974 | 2835880 | 72.09% | 12.209% |
| 4 | 6.569 | 755 | 762 | 765 | rBV | 2617542 | 2912797 | 74.04% | 12.540% |
| 5 | 6.951 | 823 | 827 | 831 | rVB | 772108 | 616041 | 15.66% | 2.652% |
| 6 | 7.516 | 917 | 923 | 926 | rBV | 1880965 | 1837081 | 46.70% | 7.909% |
| 7 | 8.239 | 1041 | 1046 | 1049 | rVB | 873554 | 830008 | 21.10% | 3.573% |
| 8 | 9.316 | 1223 | 1229 | 1232 | rBV | 3679050 | 3448753 | 87.67% | 14.847% |
| 9 | 9.998 | 1340 | 1345 | 1348 | rBV | 1196327 | 973291 | 24.74% | 4.190% |
| 10 | 10.786 | 1473 | 1479 | 1483 | rBV | 2277382 | 2304234 | 58.57% | 9.920% |
| 11 | 11.492 | 1595 | 1599 | 1602 | rVB | 1201978 | 1066079 | 27.10% | 4.590% |
| 12 | 13.086 | 1864 | 1870 | 1873 | rBV | 4053136 | 3933993 | 100.00% | 16.936% |
| 13 | 14.133 | 2044 | 2048 | 2052 | rBV | 1015787 | 937275 | 23.83% | 4.035% |
| 14 | 15.292 | 2241 | 2245 | 2250 | rVB | 44432 | 52098 | 1.32% | 0.224% |
| 15 | 15.657 | 2301 | 2307 | 2311 | rBV | 537036 | 671169 | 17.06% | 2.889% |
| 16 | 15.698 | 2311 | 2314 | 2320 | rVB | 63462 | 80790 | 2.05% | 0.348% |
| 17 | 16.168 | 2388 | 2394 | 2401 | rBV2 | 46324 | 76366 | 1.94% | 0.329% |
| 18 | 16.715 | 2479 | 2487 | 2495 | rBV3 | 40405 | 81691 | 2.08% | 0.352% |
| 19 | 17.362 | 2590 | 2597 | 2605 | rBV3 | 23890 | 54101 | 1.38% | 0.233% |
| 20 | 18.127 | 2718 | 2727 | 2738 | rBV6 | 19979 | 59360 | 1.51% | 0.256% |

Sum of corrected areas: 23228098

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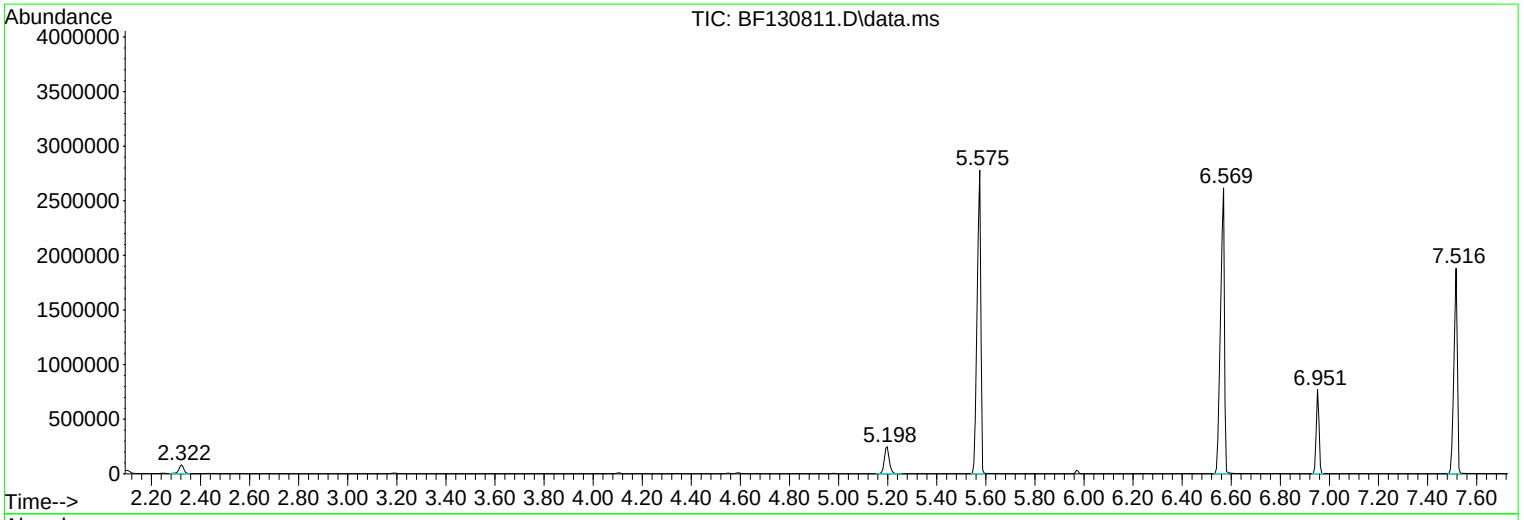
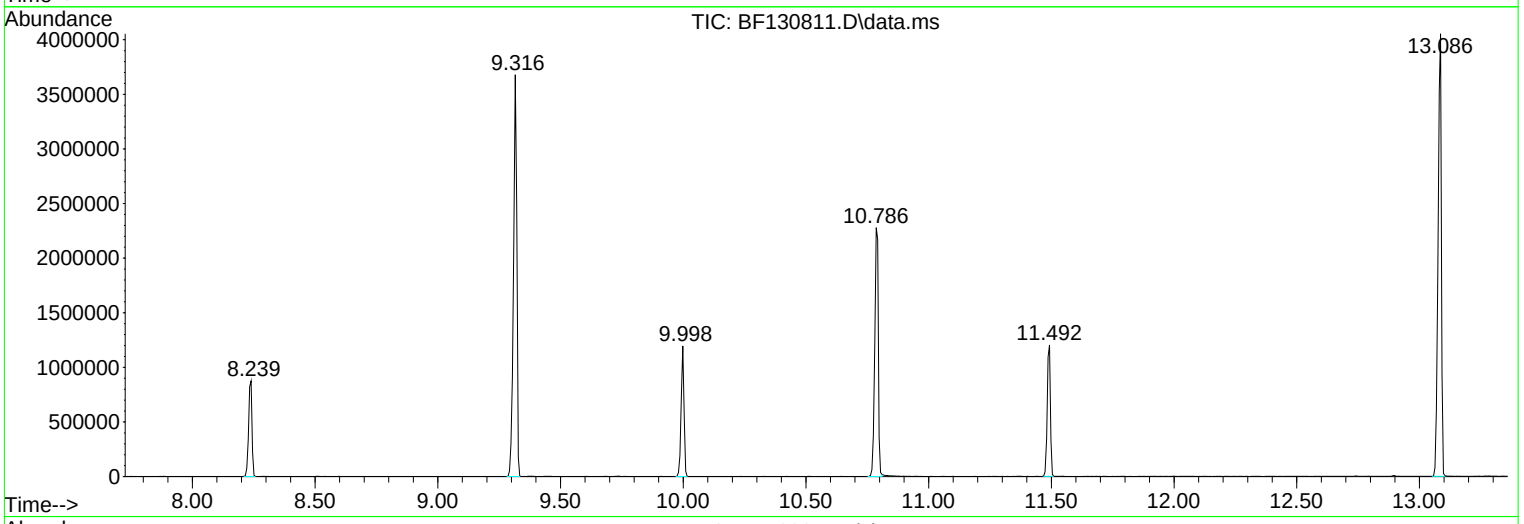
ALS Vial : 14 Sample Multiplier: 1

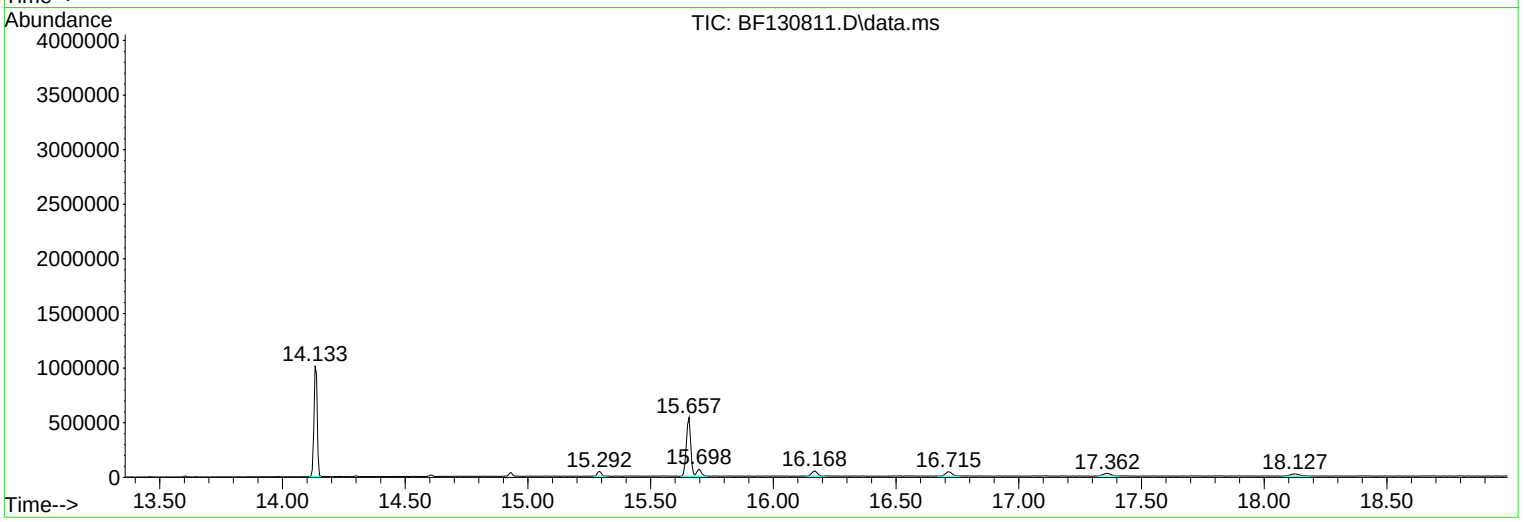
**Instrument :**
BNA_F
**ClientSampleId :**
PB148576BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

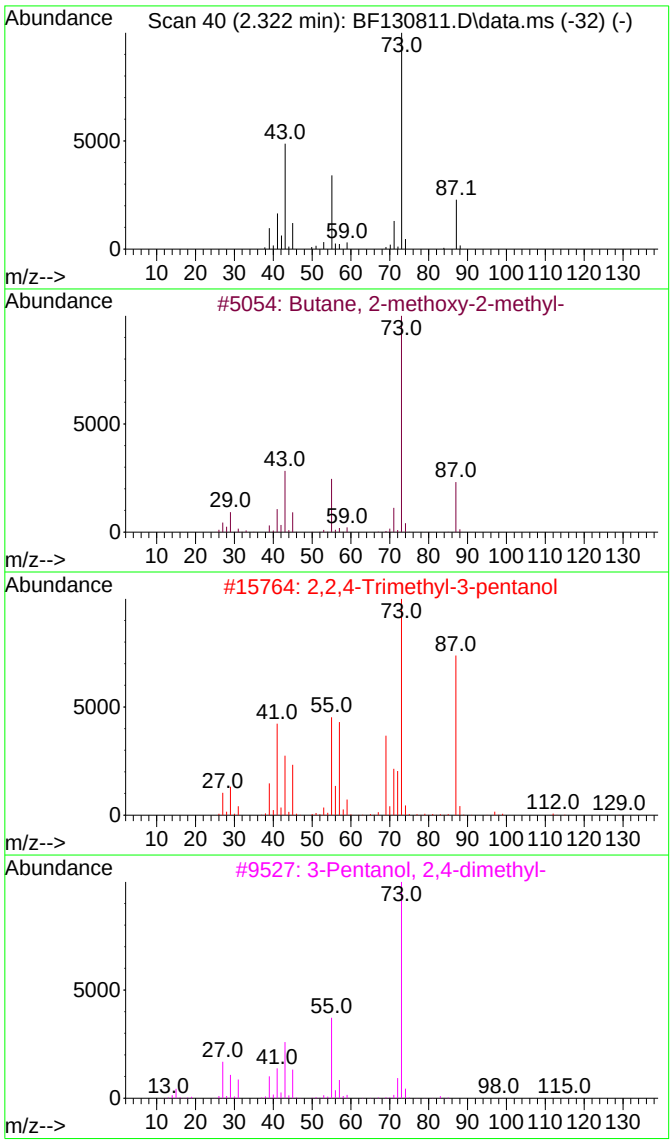
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

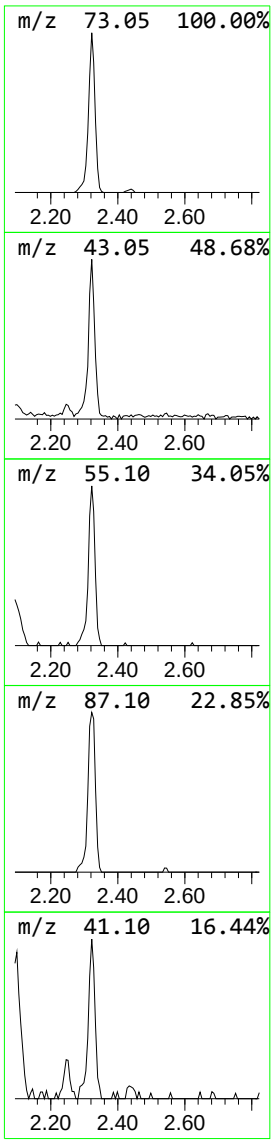
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.322 | 3.64 ng | 112207 | 1,4-Dichlorobenzene-d4 | 6.951 |

| 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 | 25 |
| 4 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 23 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |



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ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB148576BL

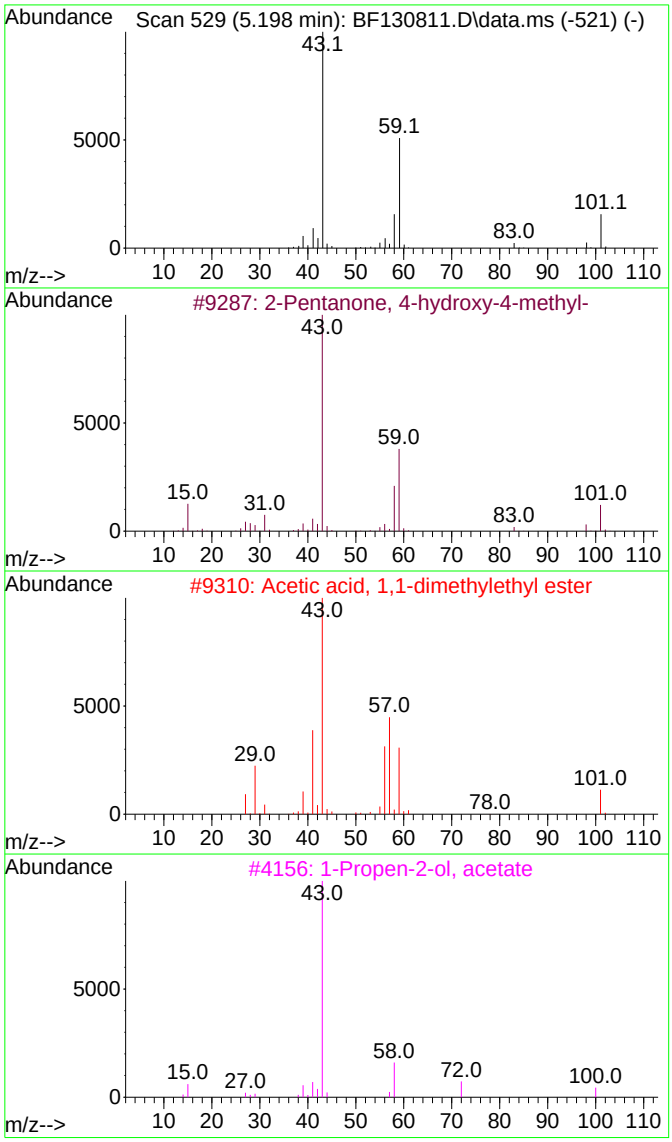
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

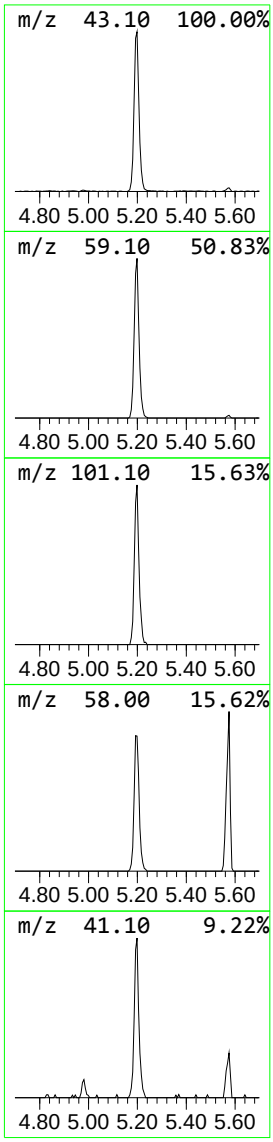
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.198 | 11.20 ng | 344884 | 1,4-Dichlorobenzene-d4 | 6.951 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 28 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 9 |



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Operator : CG\JU
Sample : PB148576BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB148576BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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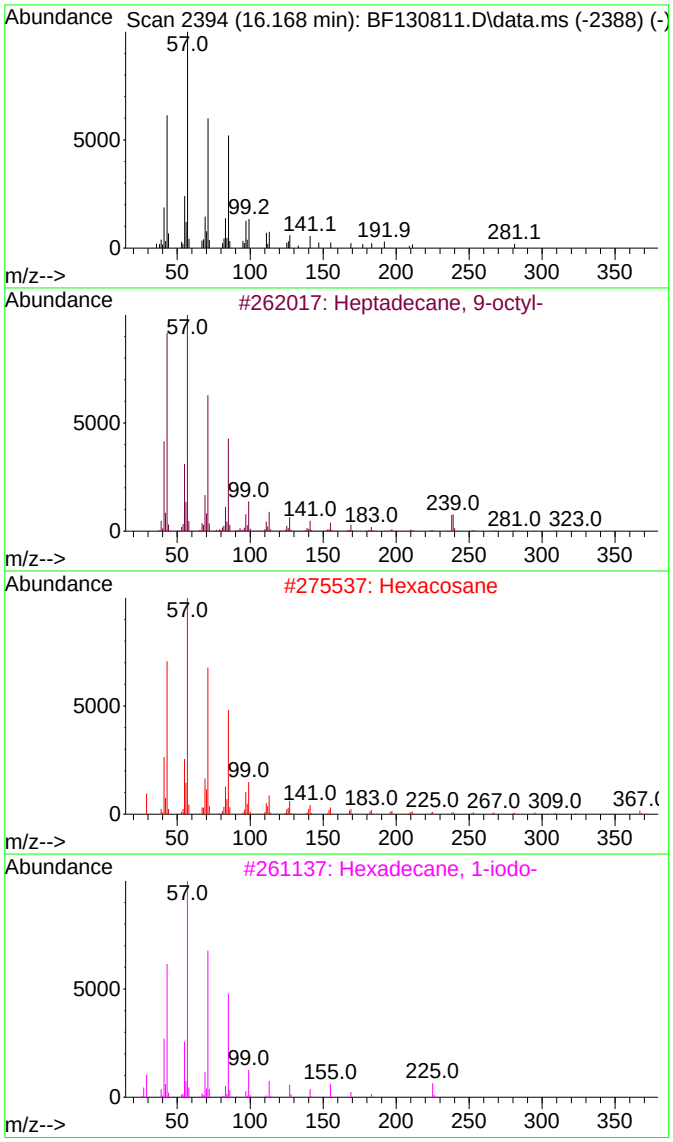
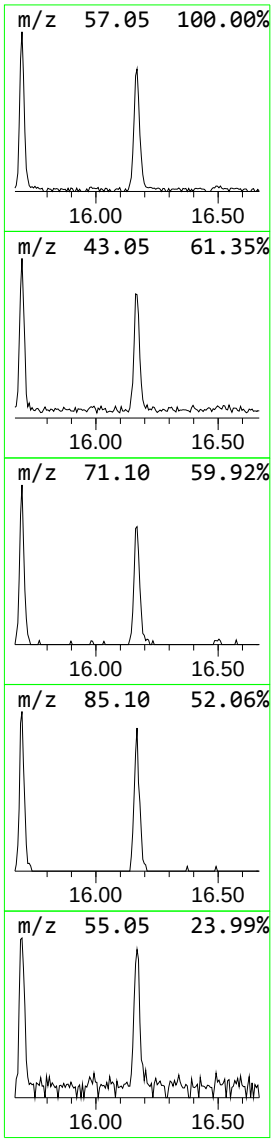
Peak Number 3 Heptadecane, 9-octyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.168 | 2.28 ng | 76366 | Perylene-d12 | 15.656 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 3 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 87 |
| 4 | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 86 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 86 |



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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-BF102722.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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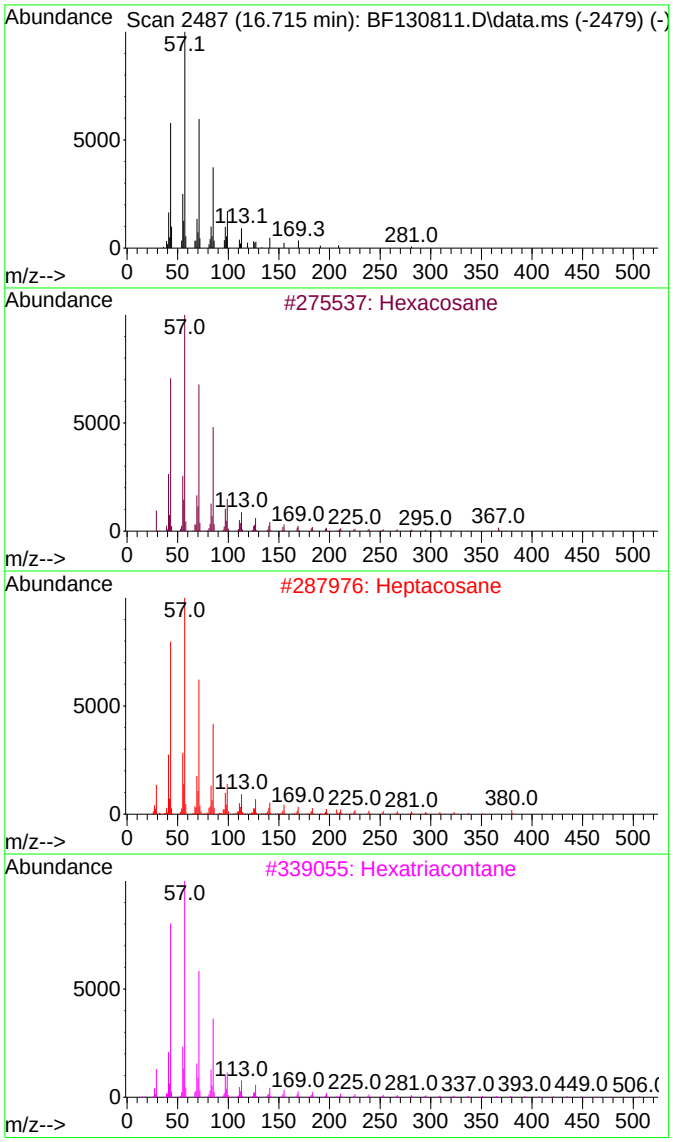
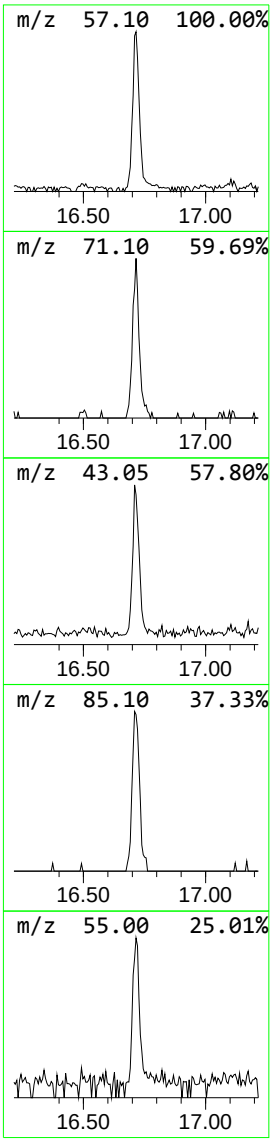
Peak Number 4 Hexacosane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.715 | 2.43 ng | 81691 | Perylene-d12 | 15.656 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 3 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 90 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 86 |



Tentatively Identified Compound (LSC) summary

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Data File : BF130811.D
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Operator : CG\JU
Sample : PB148576BL
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
PB148576BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 2.322 | 3.6 | ng | 112207 | 1 | 6.951 | 616041 | 20.0 |
| 2-Pentanone, 4-... | 5.198 | 11.2 | ng | 344884 | 1 | 6.951 | 616041 | 20.0 |
| Heptadecane, 9-... | 16.168 | 2.3 | ng | 76366 | 6 | 15.656 | 671169 | 20.0 |
| Hexacosane | 16.715 | 2.4 | ng | 81691 | 6 | 15.656 | 671169 | 20.0 |