LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087548.D
Acq On : 30 May 2016 13:37
Operator : UM/SJ
Sample : H3317-02
Misc :
ALS Vial : 68 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-21

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:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.776 | 276 | 279 | 295 | rBV2 | 19988 | 122816 | 2.92% | 0.455% |
| 2 | 5.393 | 330 | 333 | 355 | rBV | 413550 | 1409702 | 33.51% | 5.217% |
| 3 | 7.050 | 476 | 478 | 483 | rBV | 294244 | 740181 | 17.60% | 2.739% |
| 4 | 7.130 | 483 | 485 | 502 | rVB | 1593518 | 3347414 | 79.58% | 12.388% |
| 5 | 7.473 | 513 | 515 | 527 | rBV | 336346 | 775970 | 18.45% | 2.872% |
| 6 | 7.702 | 533 | 535 | 552 | rVB | 1987376 | 2786195 | 66.24% | 10.311% |
| 7 | 8.387 | 593 | 595 | 607 | rBV | 1366356 | 2372162 | 56.40% | 8.779% |
| 8 | 9.508 | 691 | 693 | 715 | rBV4 | 386427 | 990915 | 23.56% | 3.667% |
| 9 | 11.279 | 846 | 848 | 866 | rBV | 3196020 | 4206192 | 100.00% | 15.566% |
| 10 | 12.331 | 938 | 940 | 955 | rBV | 601132 | 1000215 | 23.78% | 3.702% |
| 11 | 13.622 | 1051 | 1053 | 1074 | rBV | 1240287 | 2355685 | 56.01% | 8.718% |
| 12 | 14.754 | 1150 | 1152 | 1173 | rBV | 358933 | 951970 | 22.63% | 3.523% |
| 13 | 16.925 | 1340 | 1342 | 1345 | rBV | 414147 | 456069 | 10.84% | 1.688% |
| 14 | 17.040 | 1350 | 1352 | 1354 | rVB | 53128 | 55282 | 1.31% | 0.205% |
| 15 | 17.085 | 1354 | 1356 | 1373 | rBV | 2748989 | 3532054 | 83.97% | 13.071% |
| 16 | 17.851 | 1421 | 1423 | 1426 | rBV2 | 221451 | 281021 | 6.68% | 1.040% |
| 17 | 18.331 | 1462 | 1465 | 1468 | rBV | 37025 | 44759 | 1.06% | 0.166% |
| 18 | 18.468 | 1476 | 1477 | 1492 | rBV | 240566 | 680765 | 16.18% | 2.519% |
| 19 | 18.731 | 1498 | 1500 | 1503 | rVB | 44194 | 50199 | 1.19% | 0.186% |
| 20 | 19.486 | 1563 | 1566 | 1569 | rBV | 49120 | 52972 | 1.26% | 0.196% |
| 21 | 19.840 | 1595 | 1597 | 1600 | rBV | 47350 | 52864 | 1.26% | 0.196% |
| 22 | 20.160 | 1622 | 1625 | 1643 | rBV2 | 177056 | 653563 | 15.54% | 2.419% |
| 23 | 20.526 | 1654 | 1657 | 1661 | rBV | 34185 | 48892 | 1.16% | 0.181% |
| 24 | 20.914 | 1686 | 1691 | 1694 | rBV2 | 27035 | 53894 | 1.28% | 0.199% |

Sum of corrected areas: 27021751

LSC Report - Integrated Chromatogram

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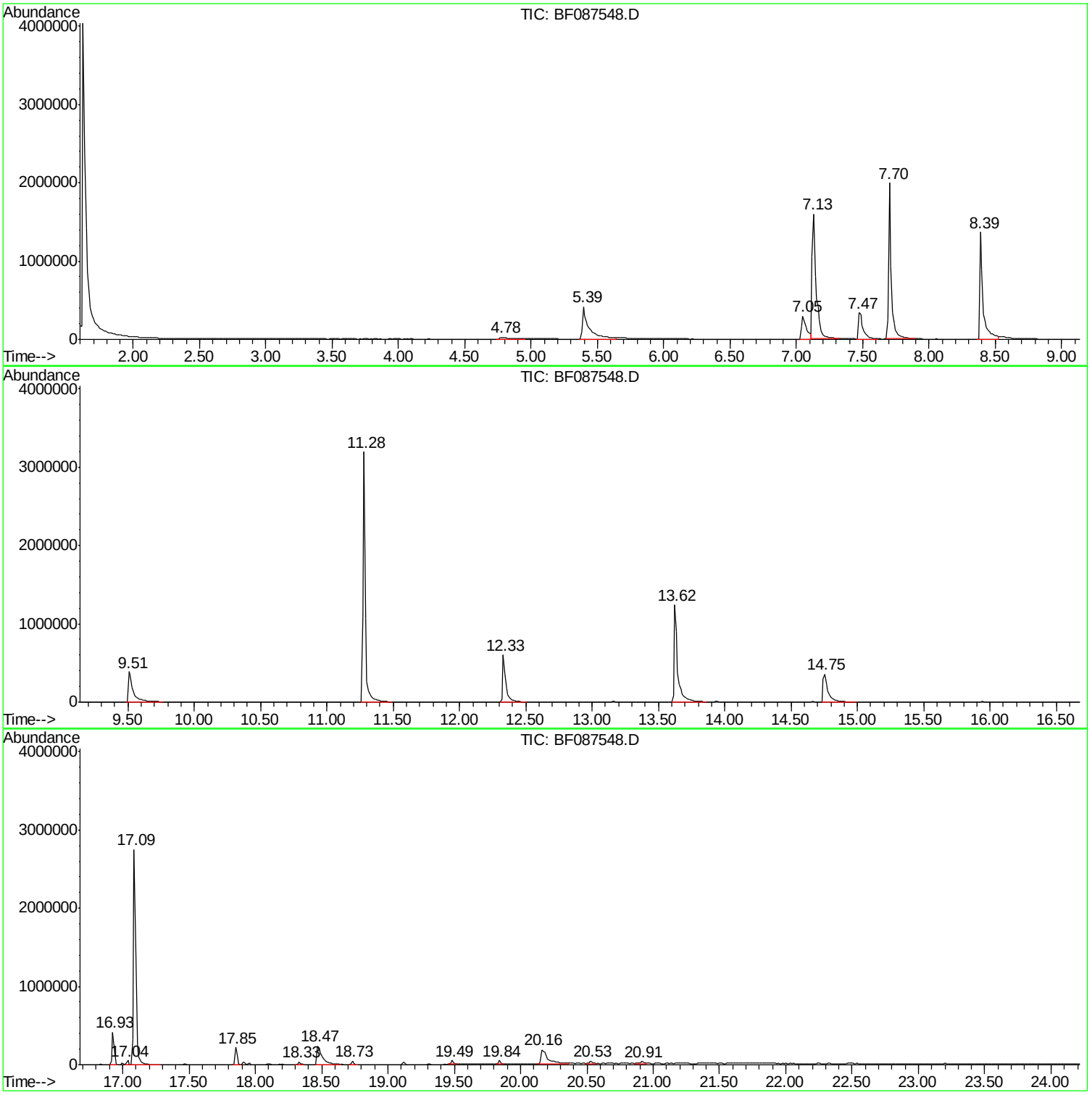
Operator : UM/SJ
Sample : H3317-02
Misc :
ALS Vial : 68 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
Data File : BF087548.D
Acq On : 30 May 2016 13:37
Operator : UM/SJ
Sample : H3317-02
Misc :
ALS Vial : 68 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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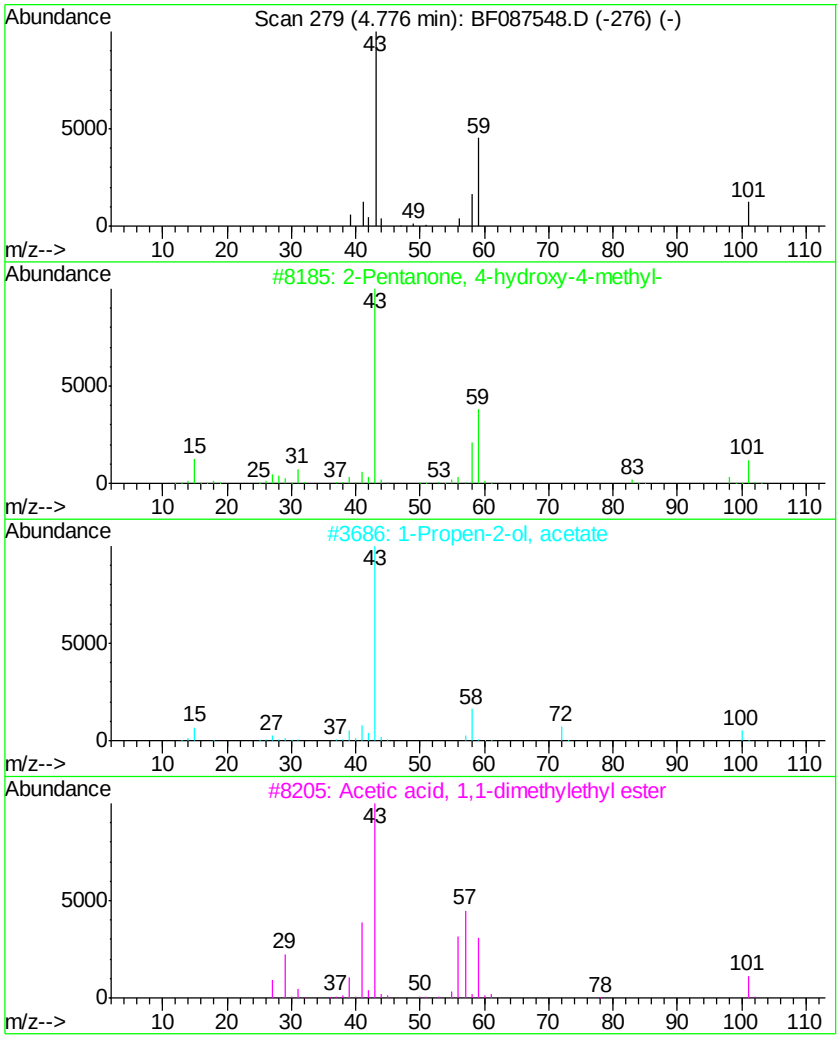
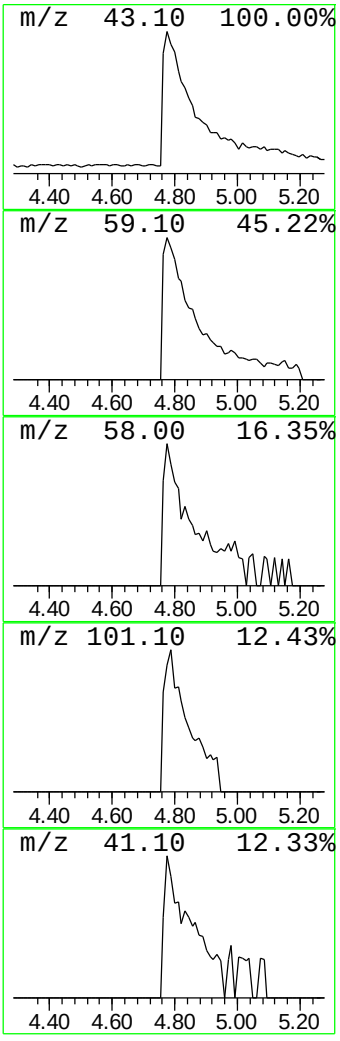
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.78 | 3.17 ng | 122816 | 1,4-Dichlorobenzene-d4 | 7.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 2 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |
| 3 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |
| 4 | 1,3,4-Oxadiazole, 2-(acetyloxy)-... | 172 | C7H12N2O3 | 066398-57-0 | 9 |
| 5 | Diacetamide | 101 | C4H7NO2 | 000625-77-4 | 7 |



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Operator : UM/SJ
Sample : H3317-02
Misc :
ALS Vial : 68 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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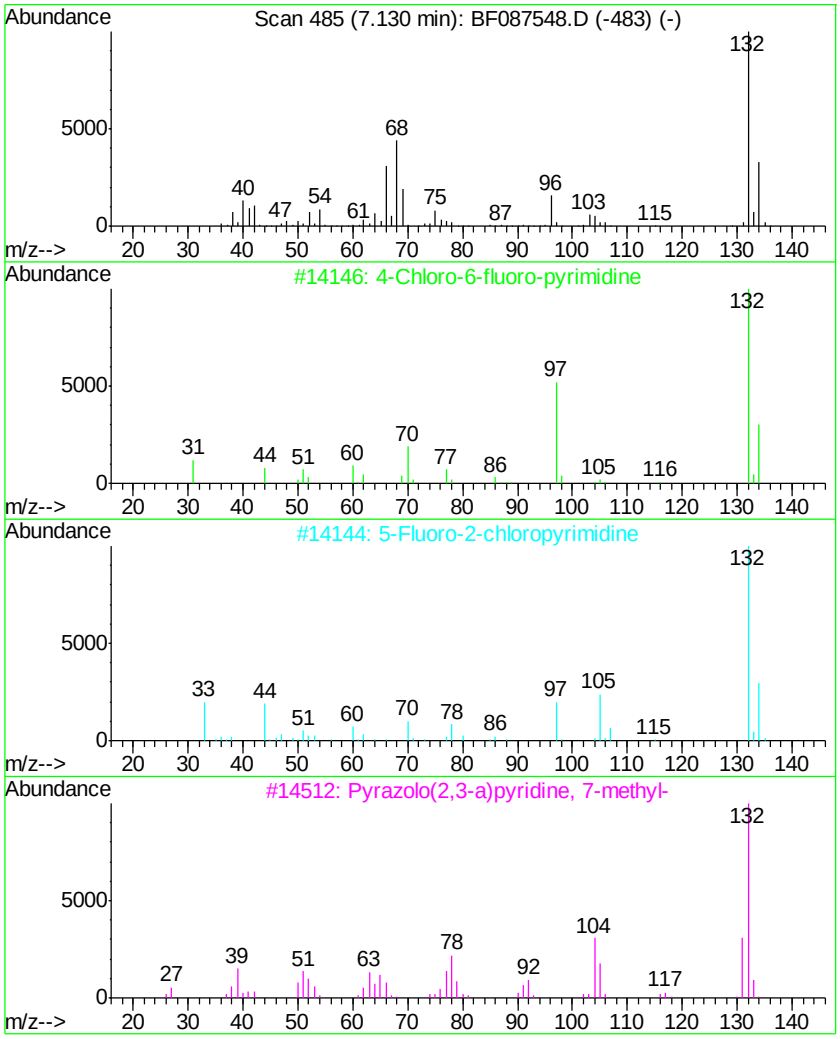
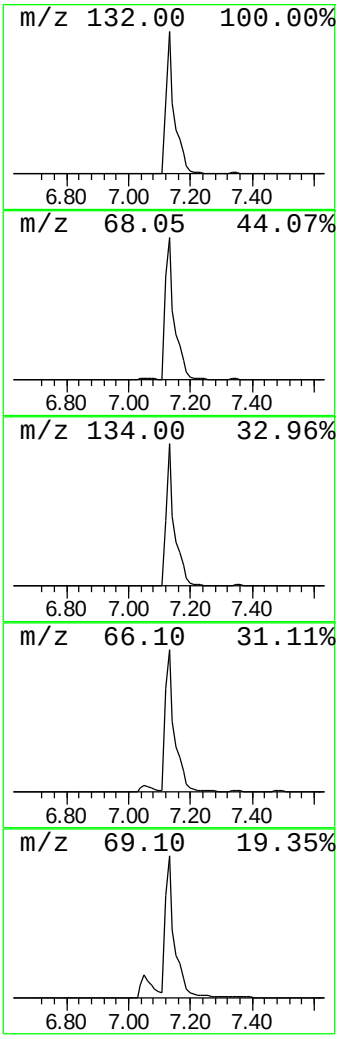
Peak Number 2 unknown7.13 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.13 | 86.28 ng | 3347410 | 1,4-Dichlorobenzene-d4 | 7.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | Pyrazolo(2,3-a)pyridine, 7-methyl- | 132 | C8H8N2 | 034760-58-2 | 10 |
| 4 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



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Operator : UM/SJ
Sample : H3317-02
Misc :
ALS Vial : 68 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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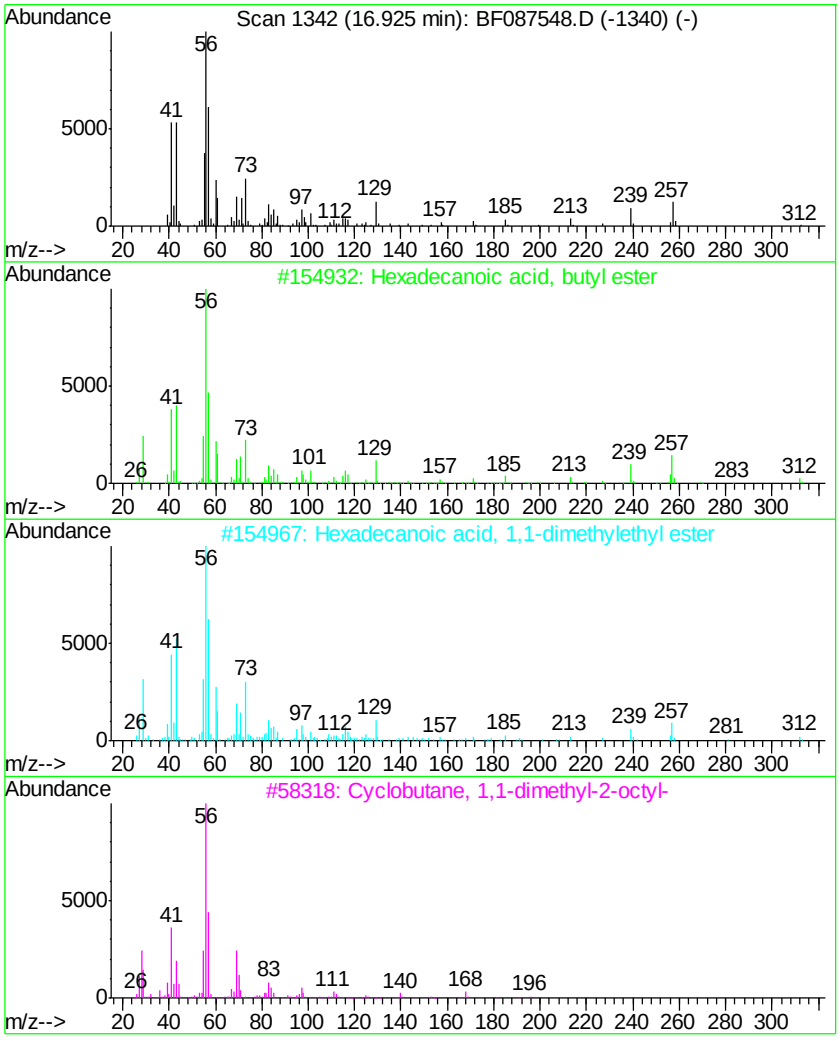
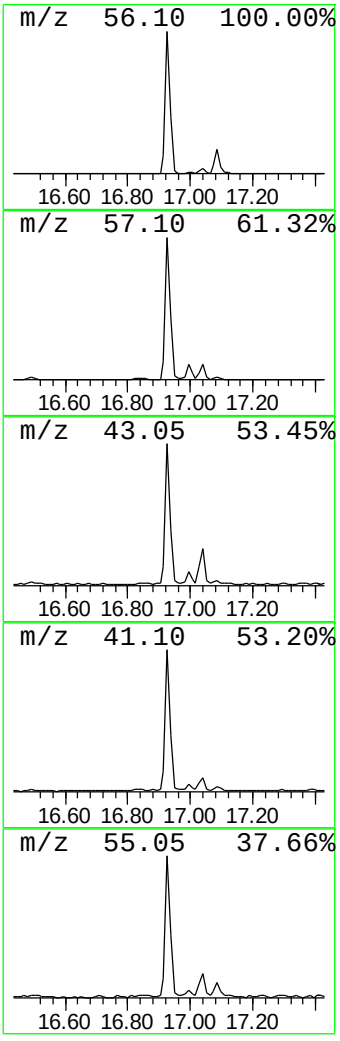
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.93 | 13.40 ng | 456069 | Chrysene-d12 | 18.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 91 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 58 |
| 3 | Cyclobutane, 1,1-dimethyl-2-octyl- | 196 | C14H28 | 062338-30-1 | 35 |
| 4 | 1-Pentadecene, 2-methyl- | 224 | C16H32 | 029833-69-0 | 35 |
| 5 | 2-Isopropyl-3-vinyloxirane | 112 | C7H12O | 070777-23-0 | 35 |



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Sample : H3317-02
Misc :
ALS Vial : 68 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
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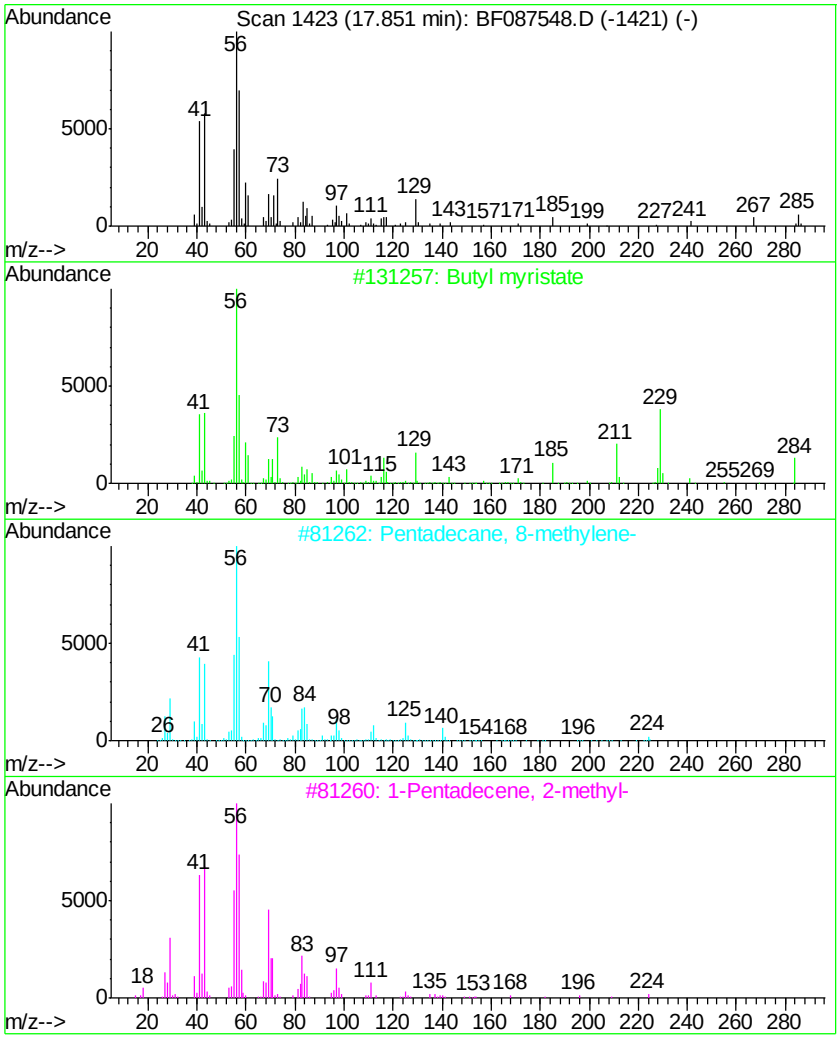
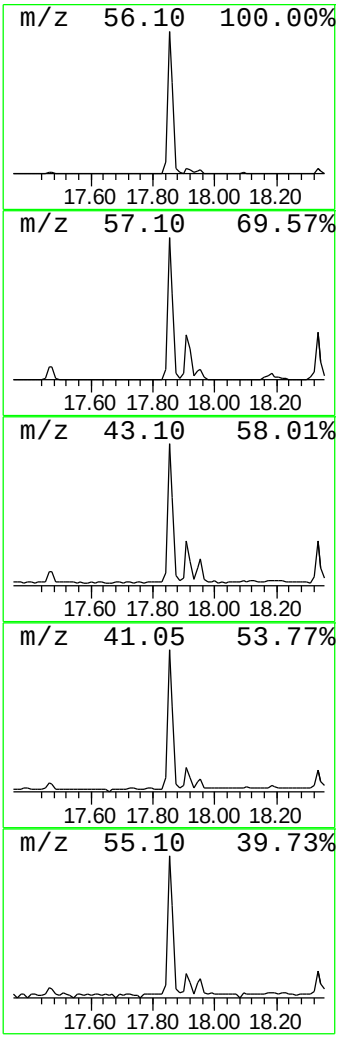
Peak Number 5 Butyl myristate Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.85 | 8.26 ng | 281021 | Chrysene-d12 | 18.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butyl myristate | 284 | C18H36O2 | 000110-36-1 | 90 |
| 2 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 43 |
| 3 | 1-Pentadecene, 2-methyl- | 224 | C16H32 | 029833-69-0 | 43 |
| 4 | 1-Hexanol, 3,5,5-trimethyl- | 144 | C9H20O | 003452-97-9 | 43 |
| 5 | 4-Aminocyclohexanol acetate (ester) | 157 | C8H15NO2 | 1000130-62-8 | 38 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
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Sample : H3317-02
Misc :
ALS Vial : 68 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.78 | 3.2 | ng | 122816 | 1 | 7.48 | 775970 | 20.0 |
| unknown7.13 | 7.13 | 86.3 | ng | 3347410 | 1 | 7.48 | 775970 | 20.0 |
| Hexadecanoic acid... | 16.93 | 13.4 | ng | 456069 | 5 | 18.47 | 680765 | 20.0 |
| Butyl myristate | 17.85 | 8.3 | ng | 281021 | 5 | 18.47 | 680765 | 20.0 |