LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135432.D
Acq On : 25 Sep 2023 17:52
Operator : CG\JU
Sample : 04540-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
EMBRIDGE-M-R-HEATER

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135432.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.381 | 557 | 560 | 571 | rBV | 1491816 | 1561780 | 3.10% | 2.014% |
| 2 | 6.398 | 729 | 733 | 752 | rVB | 912069 | 1003845 | 1.99% | 1.294% |
| 3 | 6.751 | 790 | 793 | 802 | rVB | 1291204 | 1061679 | 2.10% | 1.369% |
| 4 | 7.322 | 884 | 890 | 893 | rBV | 2832565 | 2916214 | 5.78% | 3.760% |
| 5 | 8.033 | 1004 | 1011 | 1014 | rBV | 1510608 | 1407631 | 2.79% | 1.815% |
| 6 | 8.627 | 1107 | 1112 | 1117 | rBV | 1092466 | 893019 | 1.77% | 1.151% |
| 7 | 9.110 | 1189 | 1194 | 1197 | rBV | 4599129 | 4514537 | 8.95% | 5.821% |
| 8 | 9.233 | 1211 | 1215 | 1222 | rBV | 1420796 | 1394031 | 2.76% | 1.797% |
| 9 | 9.522 | 1260 | 1264 | 1267 | rBV | 1638487 | 1382781 | 2.74% | 1.783% |
| 10 | 9.786 | 1305 | 1309 | 1313 | rBV | 1726664 | 1562896 | 3.10% | 2.015% |
| 11 | 10.133 | 1332 | 1368 | 1370 | rBV | 6581534 | 50449692 | 100.00% | 65.046% |
| 12 | 10.586 | 1441 | 1445 | 1449 | rBV | 2379977 | 2464087 | 4.88% | 3.177% |
| 13 | 11.280 | 1559 | 1563 | 1567 | rBV | 1675939 | 1423338 | 2.82% | 1.835% |
| 14 | 11.815 | 1651 | 1654 | 1667 | rBV | 445547 | 551819 | 1.09% | 0.711% |
| 15 | 12.880 | 1830 | 1835 | 1838 | rBV | 3413656 | 3326684 | 6.59% | 4.289% |
| 16 | 13.939 | 2011 | 2015 | 2019 | rVB | 741244 | 718481 | 1.42% | 0.926% |
| 17 | 15.404 | 2259 | 2264 | 2275 | rBV | 737263 | 927677 | 1.84% | 1.196% |

Sum of corrected areas: 77560191

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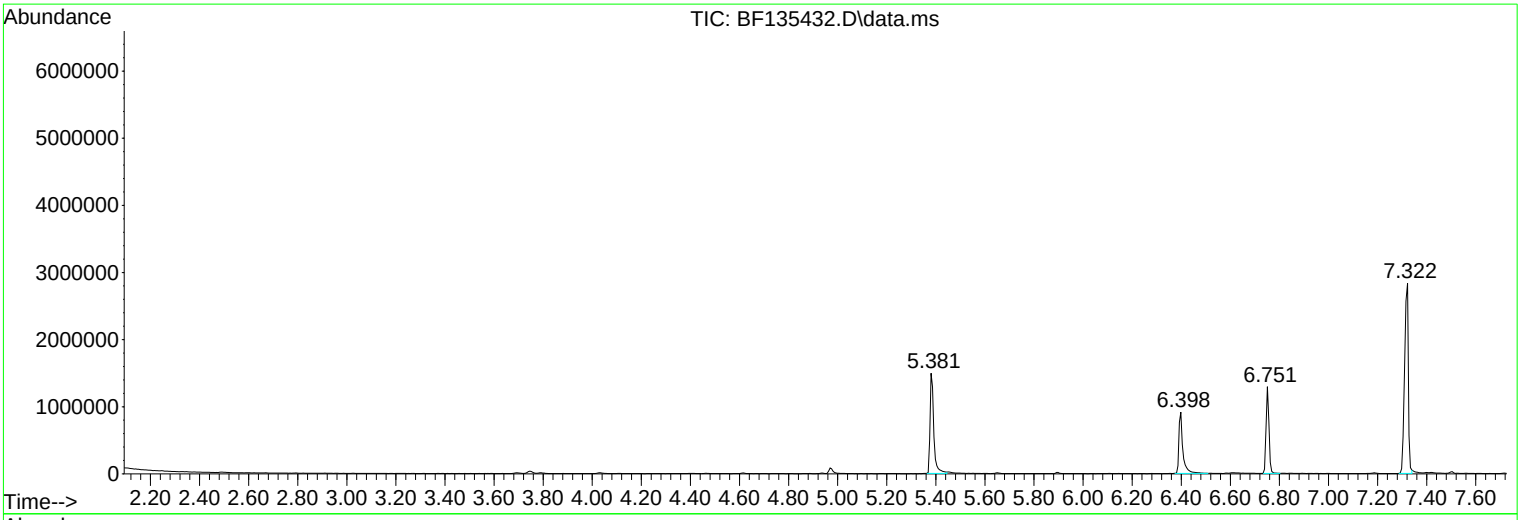
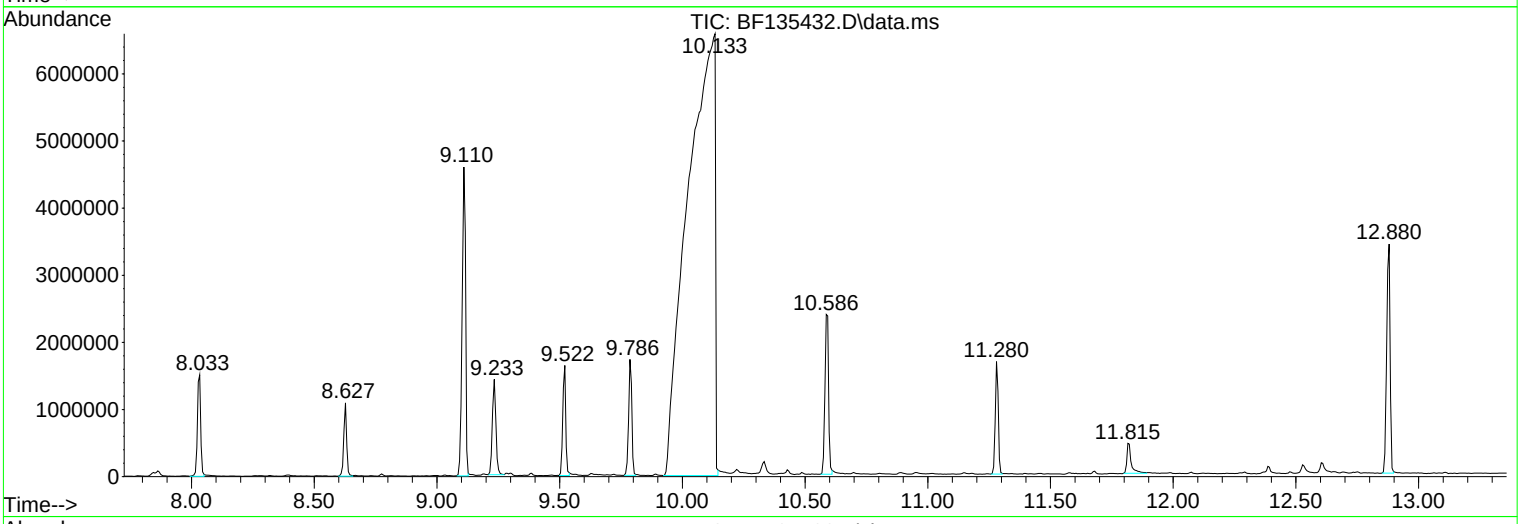
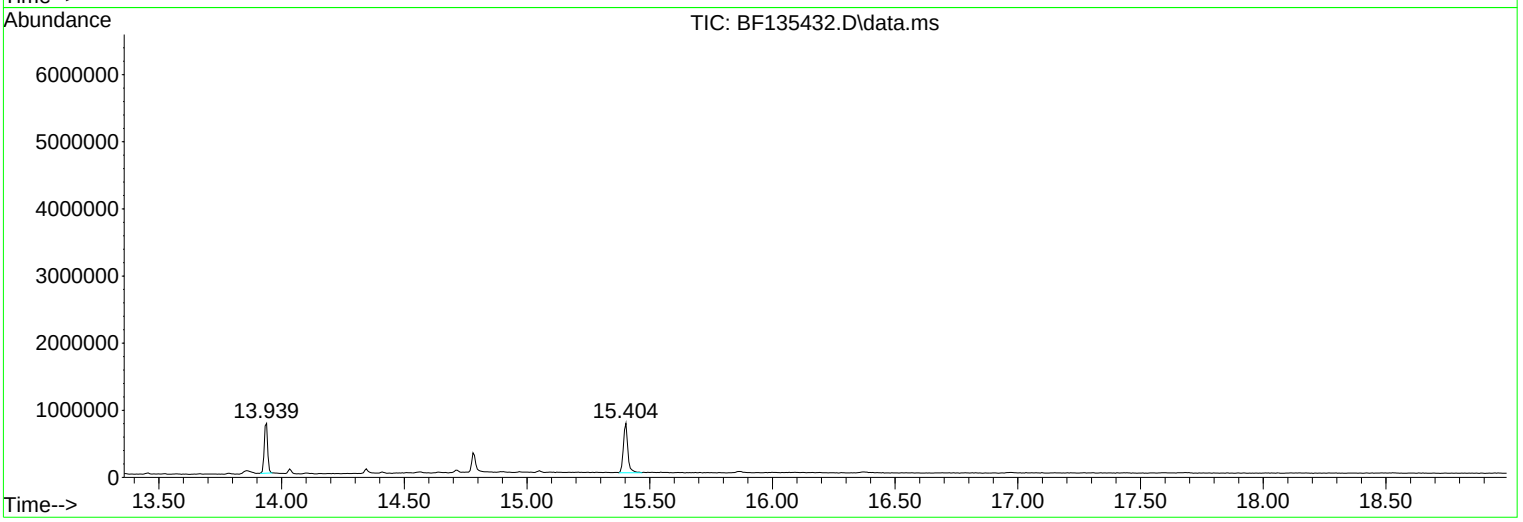
**Instrument :**
BNA_F
**ClientSampleId :**
EMBRIDGE-M-R-HEATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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Data File : BF135432.D
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Operator : CG\JU
Sample : 04540-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
EMBRIDGE-M-R-HEATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

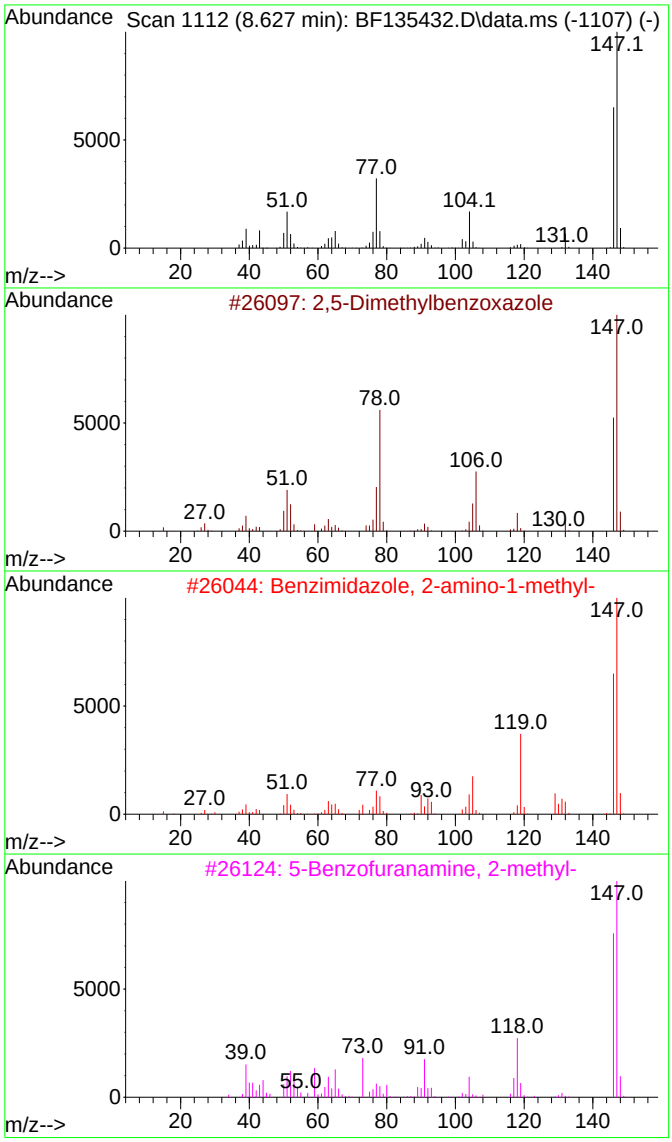
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

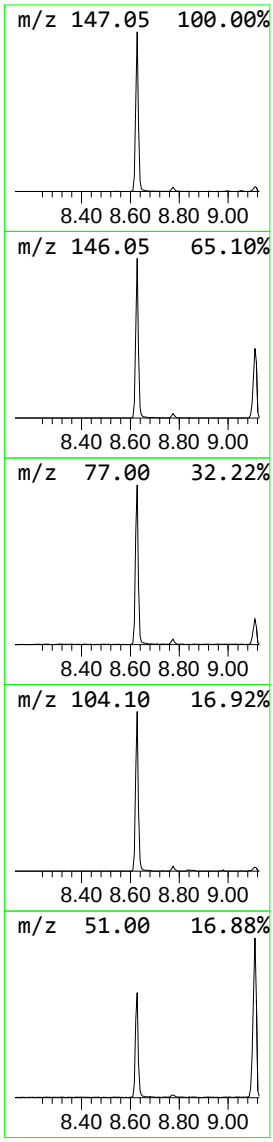
**********

Peak Number 1 2,5-Dimethylbenzoxazole Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.627 | 12.69 ng | 893019 | Naphthalene-d8 | 8.033 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,5-Dimethylbenzoxazole | 147 | C9H9NO | 005676-58-4 | 80 |
| 2 | Benzimidazole, 2-amino-1-methyl- | 147 | C8H9N3 | 001622-57-7 | 64 |
| 3 | 5-Benzofuranamine, 2-methyl- | 147 | C9H9NO | 1000327-45-8 | 58 |
| 4 | 2H-Indazol-3-amine, 2-methyl- | 147 | C8H9N3 | 097990-19-7 | 53 |
| 5 | 2-Methyl-4-indolol | 147 | C9H9NO | 035320-67-3 | 53 |



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Sample : 04540-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
EMBRIDGE-M-R-HEATER

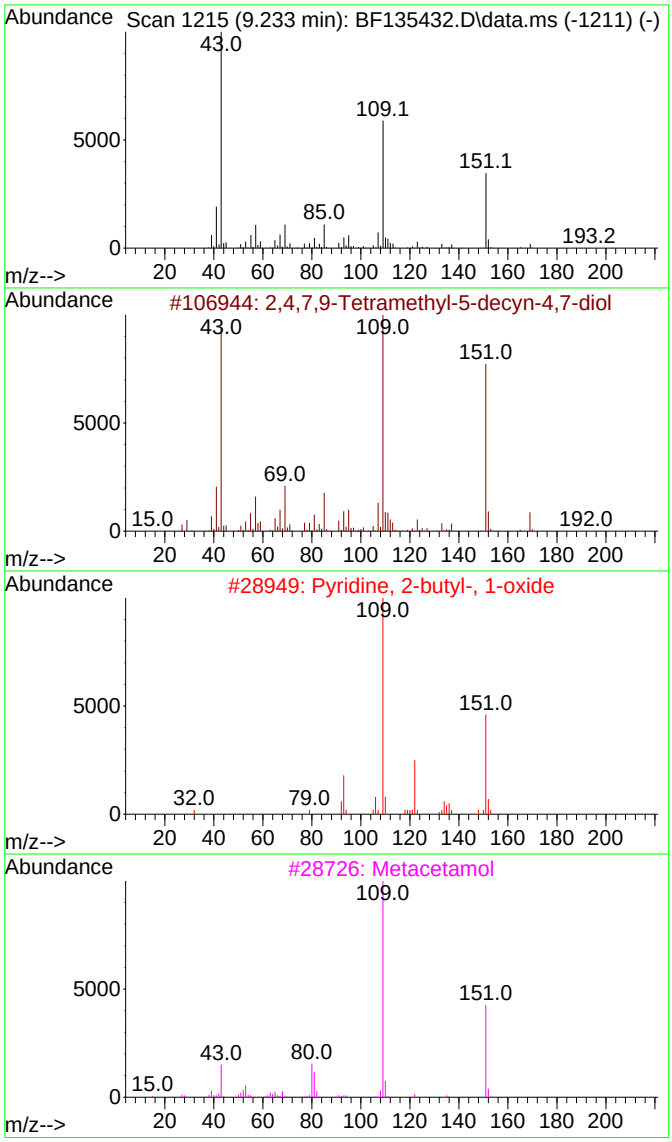
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

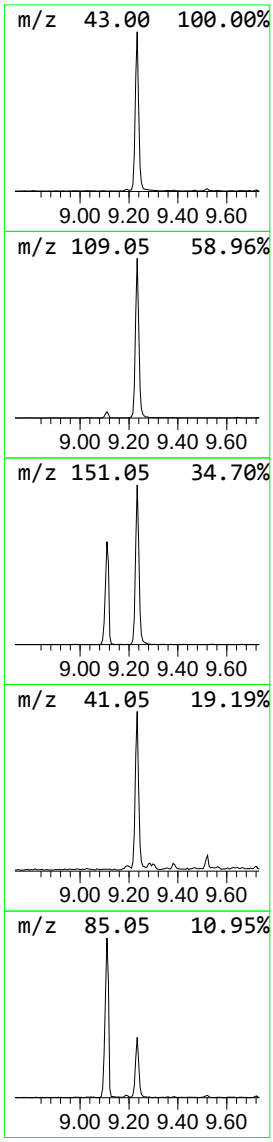
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.233 | 17.84 ng | 1394030 | Acenaphthene-d10 | 9.786 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,7,9-Tetramethyl-5-decyn-4,7-... | 226 | C14H26O2 | 000126-86-3 | 87 |
| 2 | Pyridine, 2-butyl-, 1-oxide | 151 | C9H13NO | 031396-32-4 | 53 |
| 3 | Metacetamol | 151 | C8H9NO2 | 000621-42-1 | 47 |
| 4 | Butanamide, N-acetyl-N-(4-hydrox... | 221 | C12H15NO3 | 1000107-08-7 | 47 |
| 5 | Cyclohexanol, 3,3,5-trimethyl- | 142 | C9H18O | 000116-02-9 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135432.D
Acq On : 25 Sep 2023 17:52
Operator : CG\JU
Sample : 04540-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
EMBRIDGE-M-R-HEATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

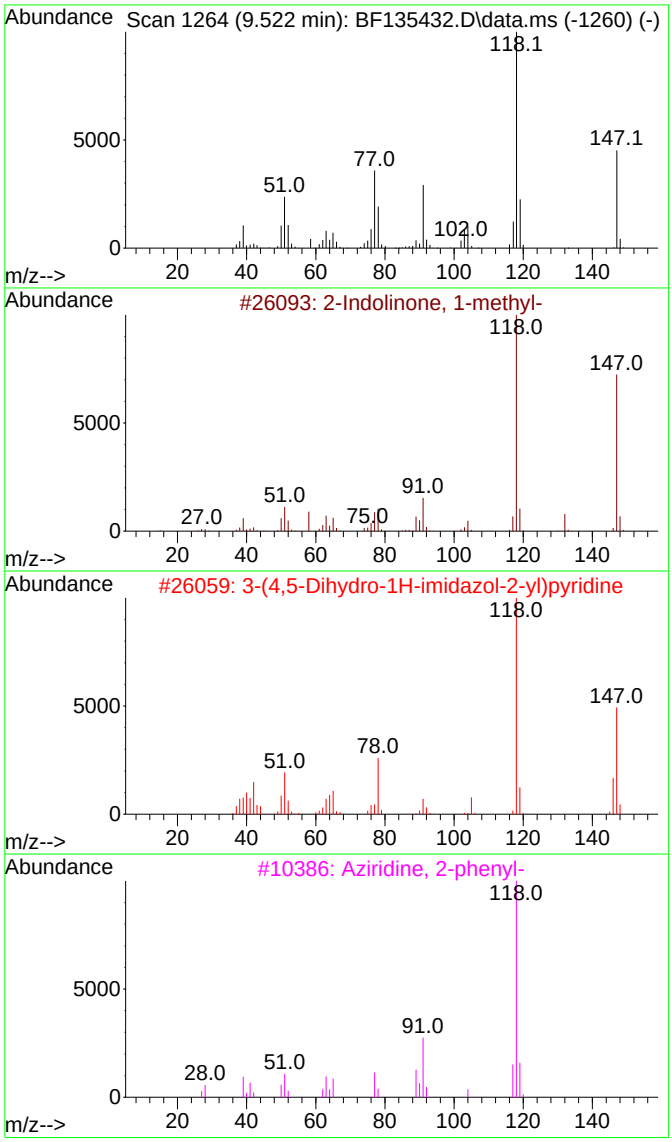
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

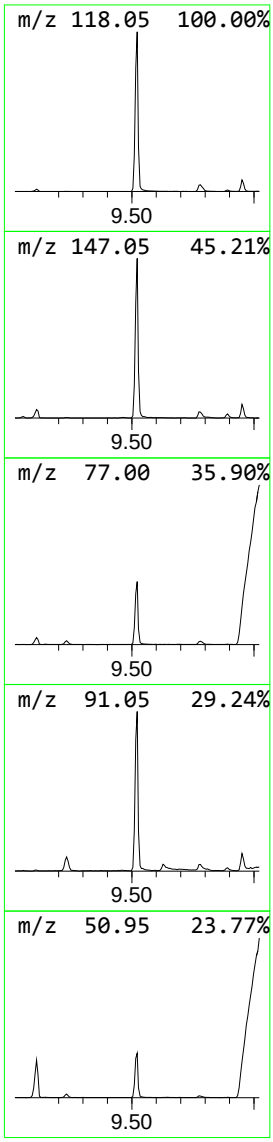
**********

Peak Number 3 2-Indolinone, 1-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.522 | 17.70 ng | 1382780 | Acenaphthene-d10 | 9.786 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Indolinone, 1-methyl- | 147 | C9H9NO | 000061-70-1 | 80 |
| 2 | 3-(4,5-Dihydro-1H-imidazol-2-yl)... | 147 | C8H9N3 | 006302-53-0 | 53 |
| 3 | Aziridine, 2-phenyl- | 119 | C8H9N | 001499-00-9 | 47 |
| 4 | 4-(4,5-Dihydro-1H-imidazol-2-yl)... | 147 | C8H9N3 | 021381-61-3 | 46 |
| 5 | 3-Pyridineacetonitrile | 118 | C7H6N2 | 006443-85-2 | 38 |



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Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
EMBRIDGE-M-R-HEATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

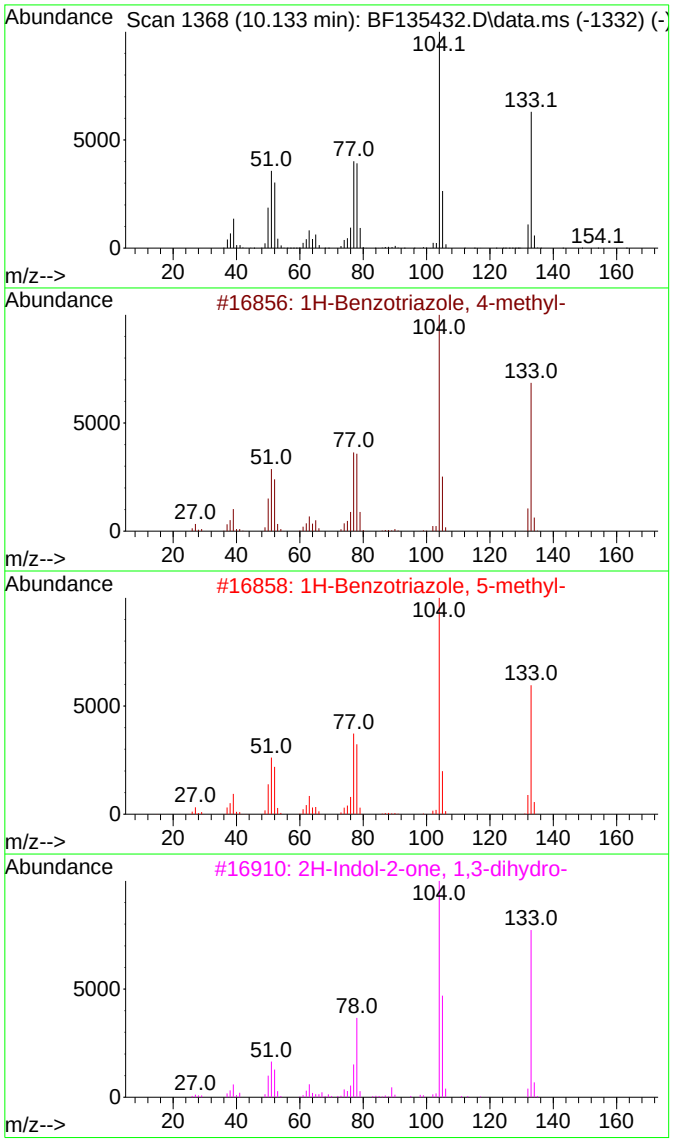
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

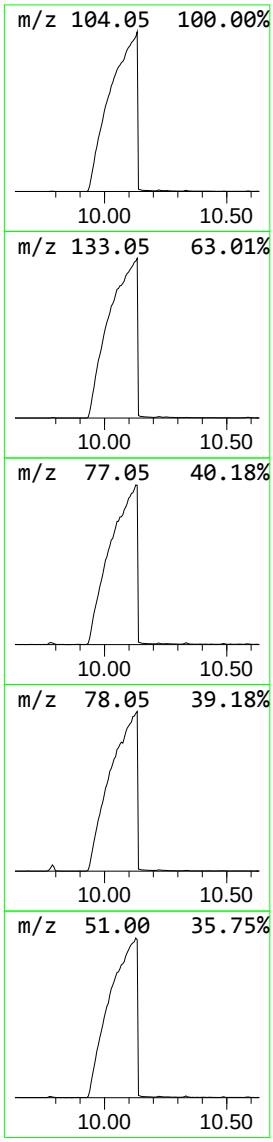
**********

Peak Number 4 1H-Benzotriazole, 4-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.133 | 645.59 ng | 50449700 | Acenaphthene-d10 | 9.786 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Benzotriazole, 4-methyl- | 133 | C7H7N3 | 029878-31-7 | 98 |
| 2 | 1H-Benzotriazole, 5-methyl- | 133 | C7H7N3 | 000136-85-6 | 97 |
| 3 | 2H-Indol-2-one, 1,3-dihydro- | 133 | C8H7NO | 000059-48-3 | 72 |
| 4 | Benzene, 1-azido-2-methyl- | 133 | C7H7N3 | 031656-92-5 | 64 |
| 5 | 1H-Indol-4-ol | 133 | C8H7NO | 002380-94-1 | 58 |



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ALS Vial : 13 Sample Multiplier: 1

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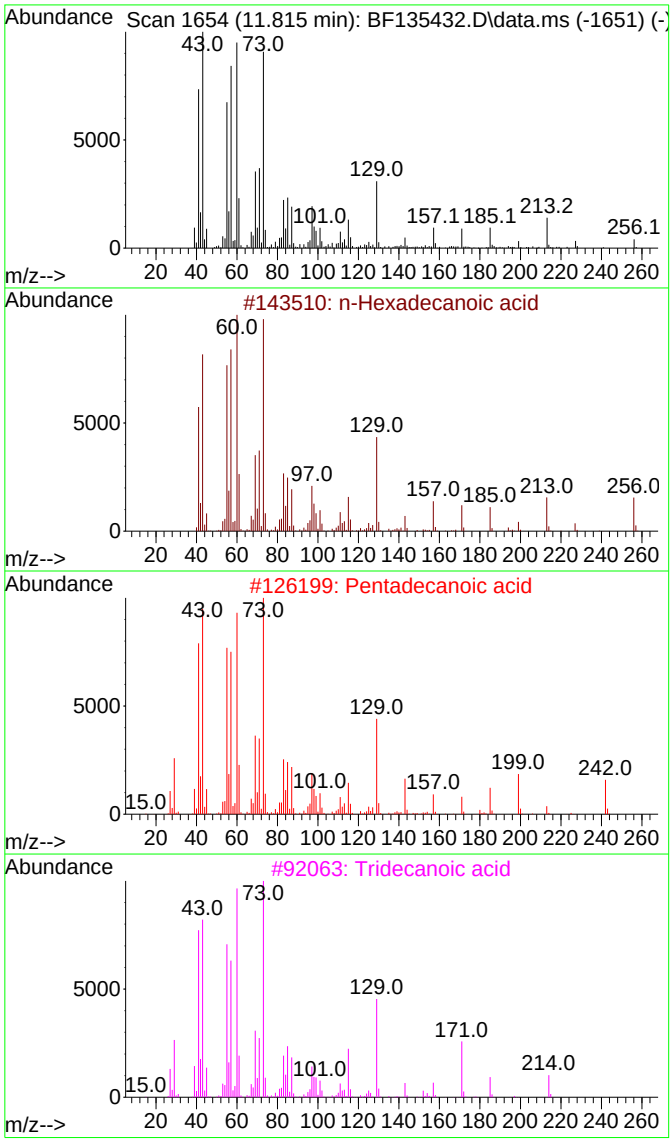
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

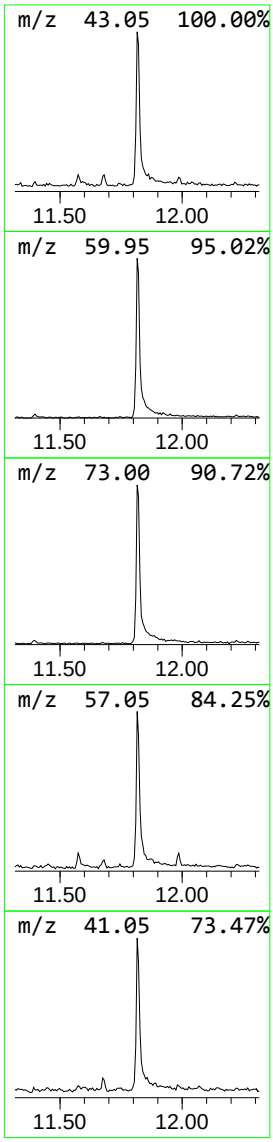
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.816 | 7.75 ng | 551819 | Phenanthrene-d10 | 11.280 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 94 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 72 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135432.D
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Operator : CG\JU
Sample : 04540-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
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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 |
| 2,5-Dimethylben... | 8.627 | 12.7 | ng | 893019 | 2 | 8.033 | 1407630 | 20.0 |
| 2,4,7,9-Tetrame... | 9.233 | 17.8 | ng | 1394030 | 3 | 9.786 | 1562900 | 20.0 |
| 2-Indolinone, 1... | 9.522 | 17.7 | ng | 1382780 | 3 | 9.786 | 1562900 | 20.0 |
| 1H-Benzotriazol... | 10.133 | 645.6 | ng | 50449700 | 3 | 9.786 | 1562900 | 20.0 |
| n-Hexadecanoic ... | 11.816 | 7.8 | ng | 551819 | 4 | 11.280 | 1423340 | 20.0 |