LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099458.D
Acq On : 13 Oct 2017 23:57
Operator : SJ/JU
Sample : I5819-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3910-SPP3

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-BF092317.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 | 2.134 | 3 | 8 | 19 | rVB | 206985 | 267512 | 9.38% | 1.345% |
| 2 | 5.075 | 506 | 508 | 525 | rVB | 158825 | 194952 | 6.83% | 0.980% |
| 3 | 5.475 | 573 | 576 | 594 | rBV | 1394235 | 1432296 | 50.20% | 7.203% |
| 4 | 6.487 | 744 | 748 | 760 | rBV | 994368 | 862075 | 30.22% | 4.336% |
| 5 | 6.628 | 767 | 772 | 775 | rBV | 2564467 | 2317374 | 81.23% | 11.655% |
| 6 | 6.851 | 807 | 810 | 814 | rBV | 671362 | 543531 | 19.05% | 2.734% |
| 7 | 7.010 | 833 | 837 | 840 | rBV | 2498719 | 2259184 | 79.19% | 11.362% |
| 8 | 7.422 | 902 | 907 | 910 | rBV | 1793643 | 1713693 | 60.07% | 8.619% |
| 9 | 8.134 | 1024 | 1028 | 1035 | rBV | 860519 | 692384 | 24.27% | 3.482% |
| 10 | 8.416 | 1072 | 1076 | 1092 | rBV | 1377770 | 1175194 | 41.19% | 5.910% |
| 11 | 9.210 | 1206 | 1211 | 1214 | rBV | 3204710 | 2852922 | 100.00% | 14.348% |
| 12 | 9.886 | 1323 | 1326 | 1337 | rVB2 | 720446 | 645520 | 22.63% | 3.246% |
| 13 | 10.680 | 1457 | 1461 | 1470 | rBV | 1395037 | 1268153 | 44.45% | 6.378% |
| 14 | 10.928 | 1500 | 1503 | 1506 | rBV | 46985 | 44875 | 1.57% | 0.226% |
| 15 | 11.375 | 1576 | 1579 | 1583 | rBV | 627618 | 515371 | 18.06% | 2.592% |
| 16 | 12.110 | 1700 | 1704 | 1716 | rBV | 42981 | 79084 | 2.77% | 0.398% |
| 17 | 12.957 | 1844 | 1848 | 1852 | rBV | 1911784 | 1916813 | 67.19% | 9.640% |
| 18 | 13.980 | 2019 | 2022 | 2025 | rBV | 59029 | 45947 | 1.61% | 0.231% |
| 19 | 14.016 | 2025 | 2028 | 2034 | rBV | 498269 | 473968 | 16.61% | 2.384% |
| 20 | 15.492 | 2274 | 2279 | 2288 | rVB | 442349 | 546456 | 19.15% | 2.748% |
| 21 | 15.915 | 2347 | 2351 | 2355 | rVB2 | 25289 | 36548 | 1.28% | 0.184% |

Sum of corrected areas: 19883852

LSC Report - Integrated Chromatogram

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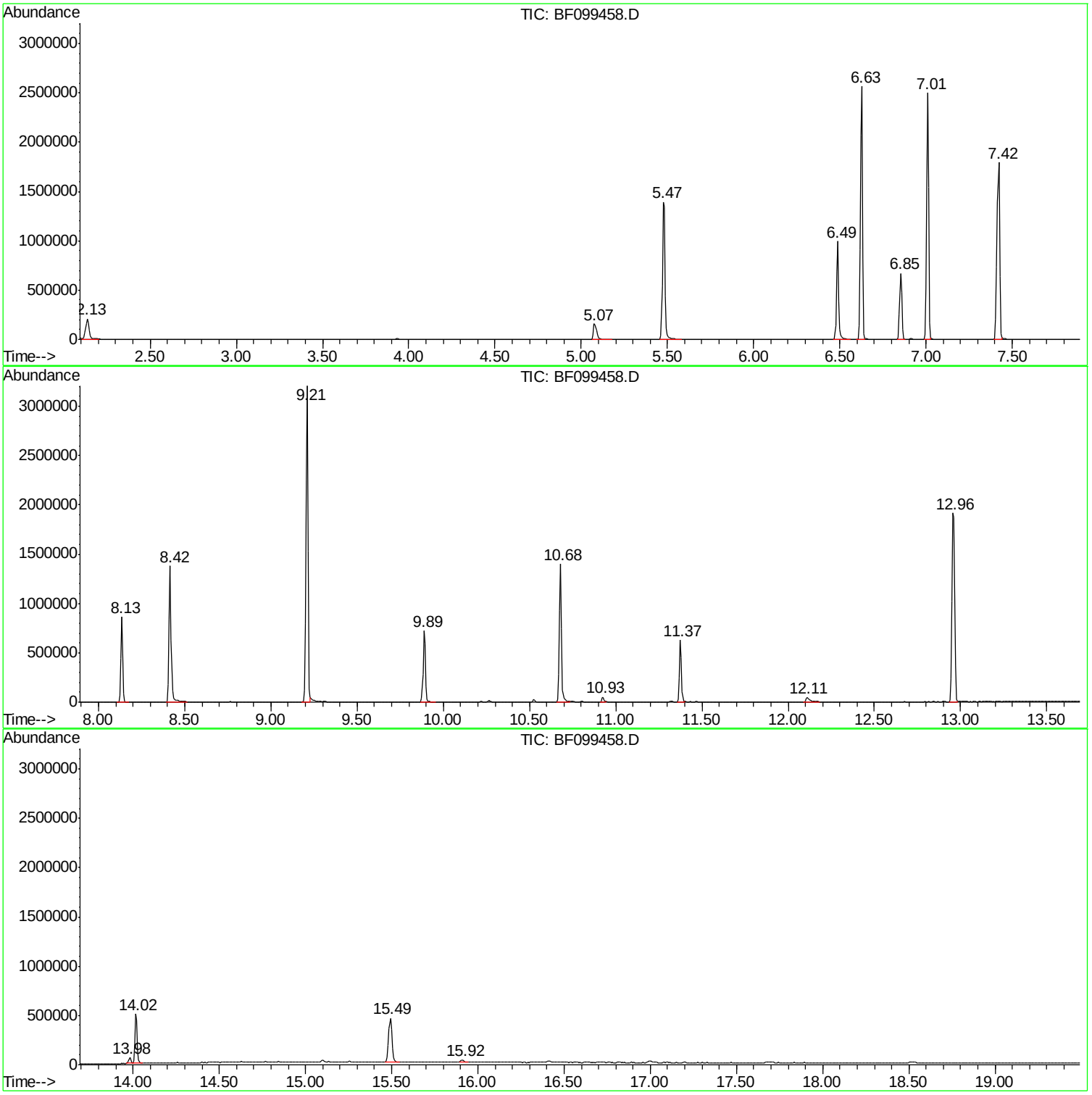
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3910-SPP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Sample : I5819-09
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**Instrument :** BNA_F
**ClientSampleId :** 3910-SPP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

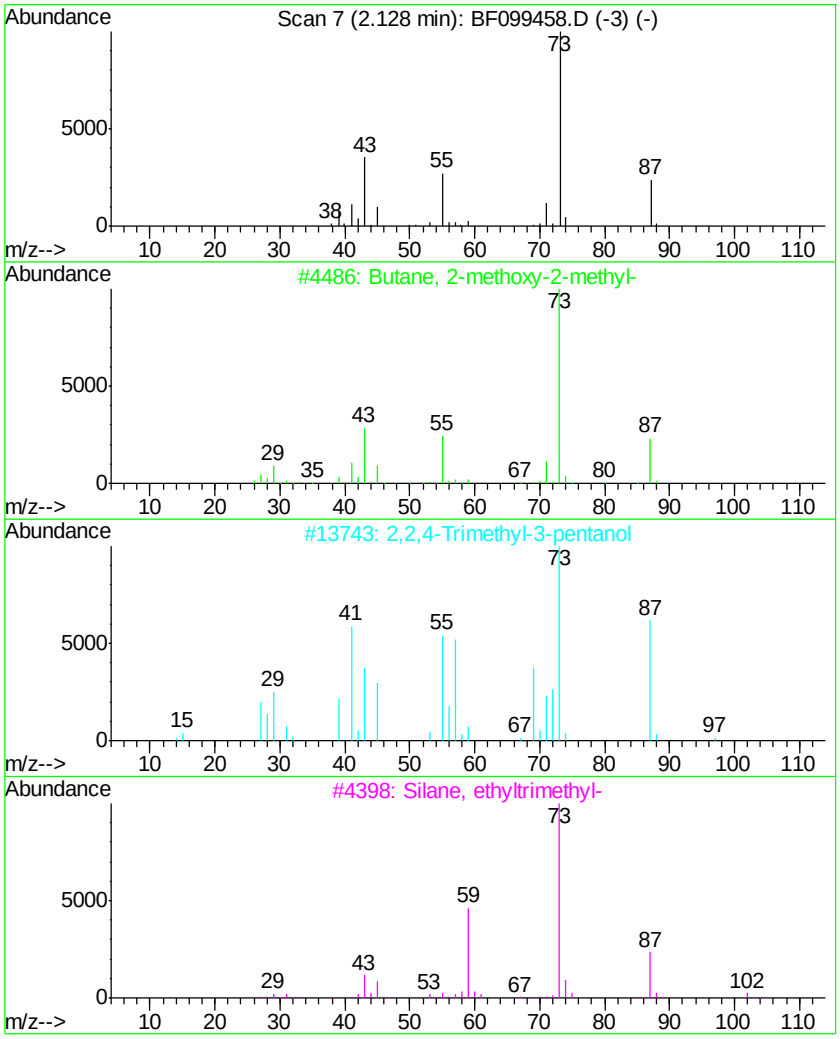
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

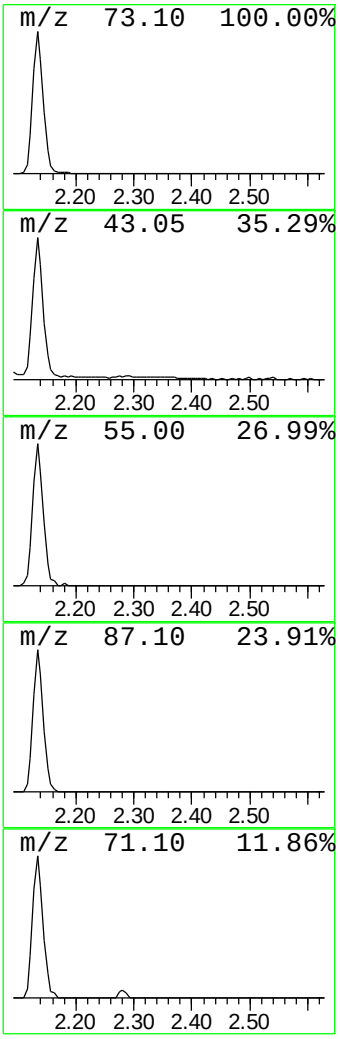
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.13 | 9.84 ng | 267512 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | Silane, ethyltrimethyl- | 102 | C5H14Si | 003439-38-1 | 36 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 10 |



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Sample : I5819-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3910-SPP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Integration Parameters: LSCINT.P

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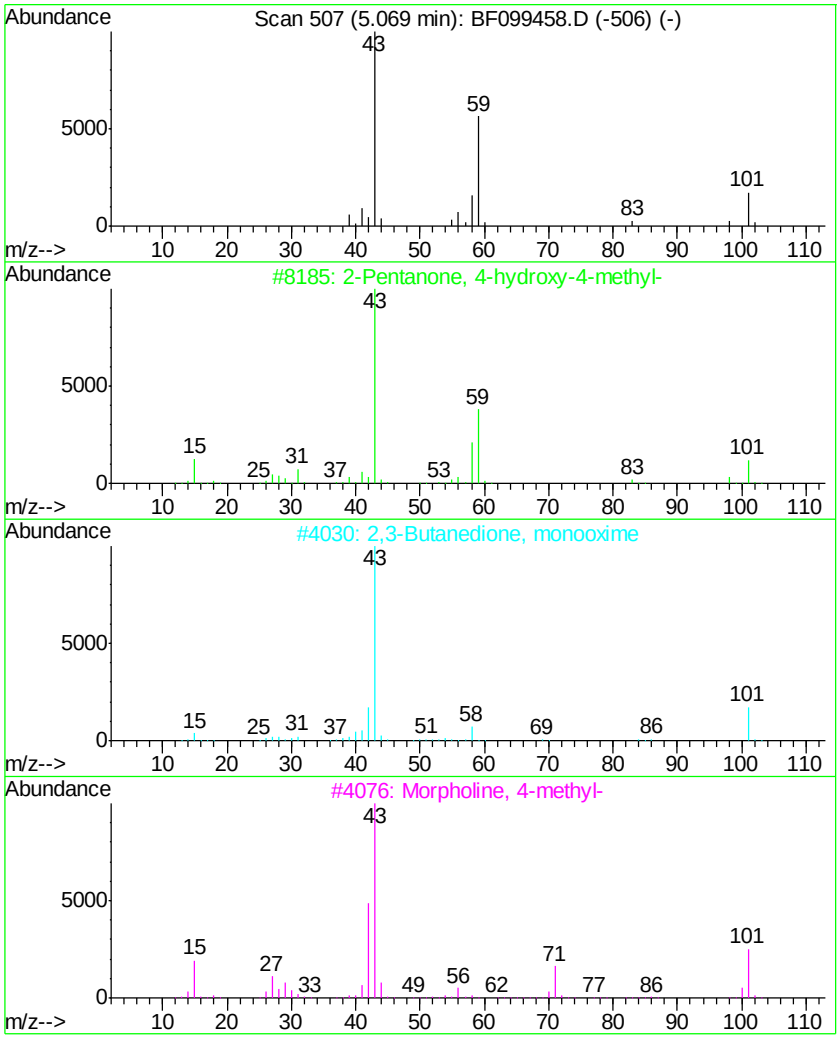
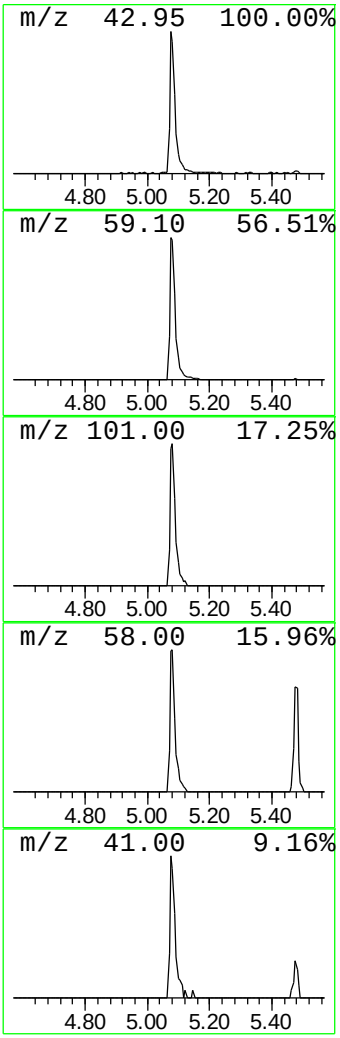
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.07 | 7.17 ng | 194952 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 9 |



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Operator : SJ/JU
Sample : I5819-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3910-SPP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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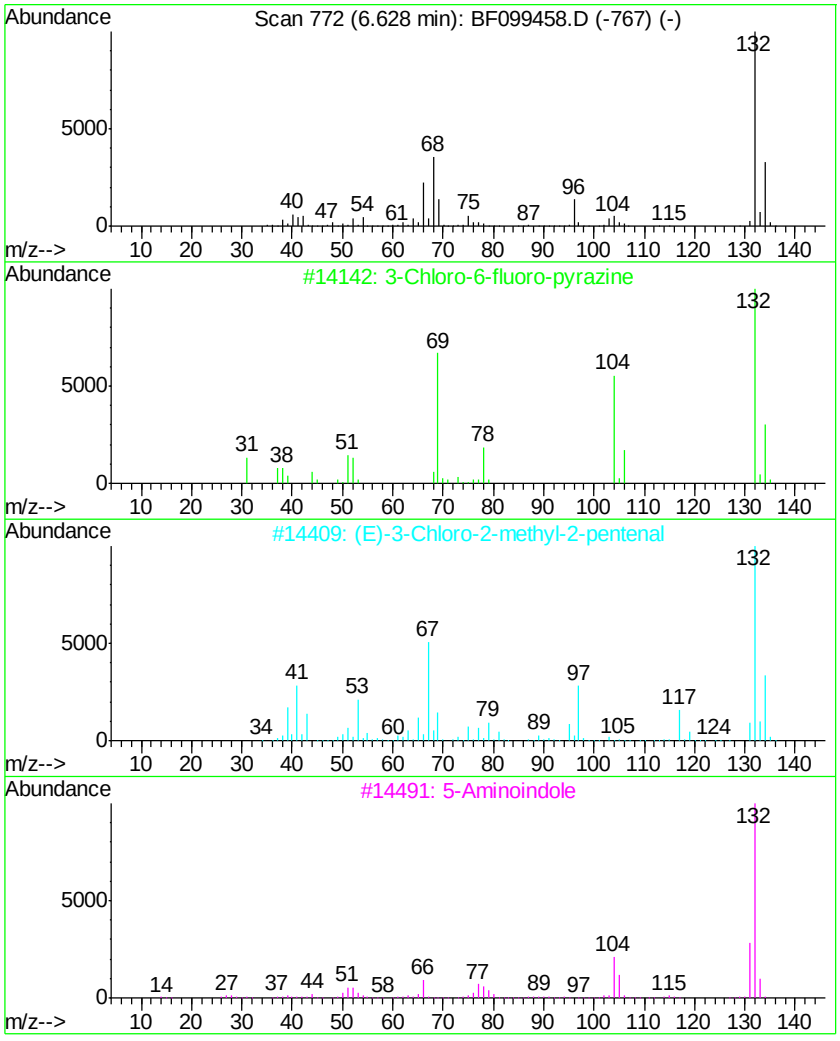
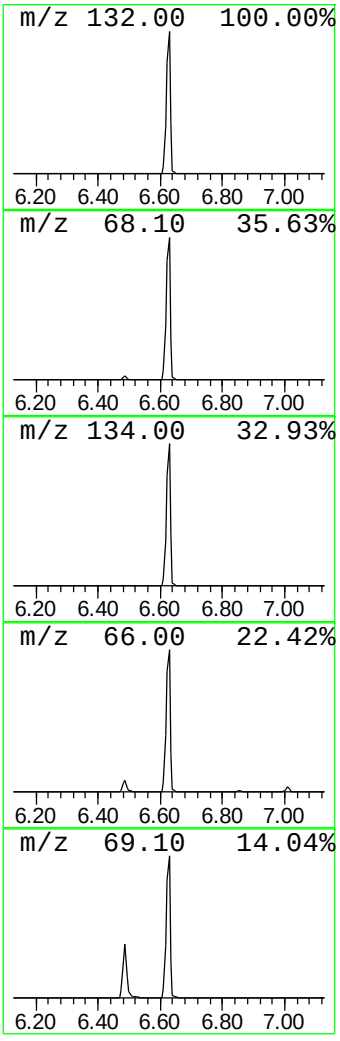
Peak Number 3 unknown6.63 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 85.27 ng | 2317370 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



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Sample : I5819-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3910-SPP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Integration Parameters: LSCINT.P

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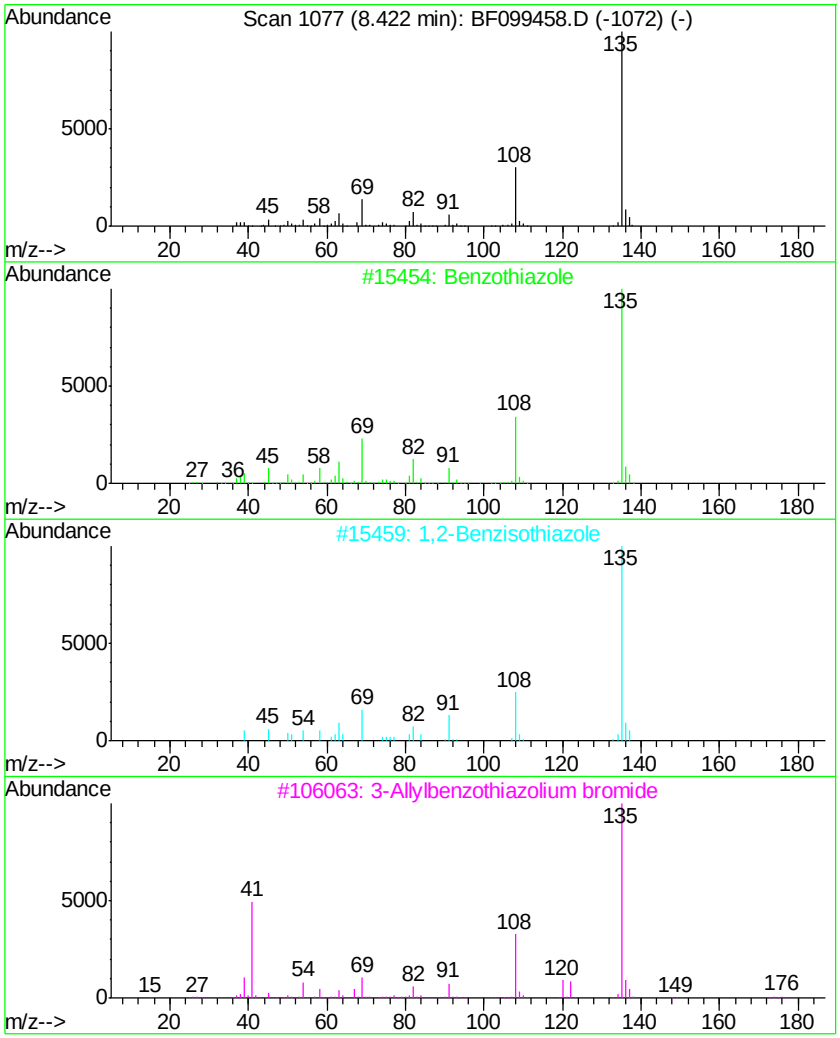
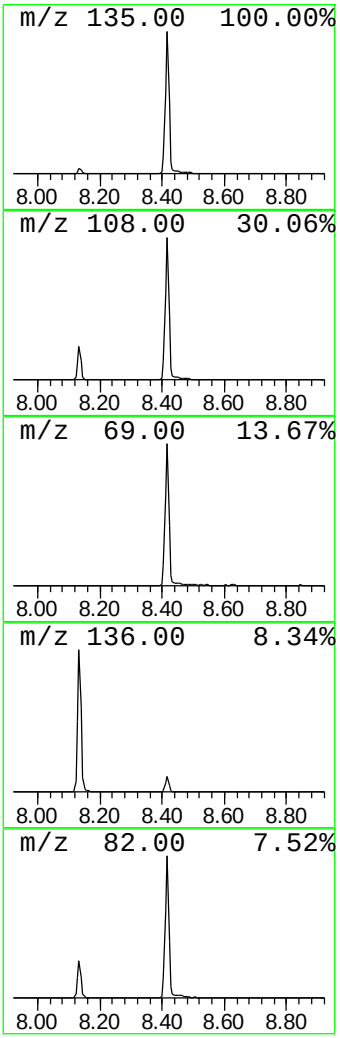
Peak Number 5 Benzothiazole Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.42 | 33.95 ng | 1175190 | Naphthalene-d8 | 8.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzothiazole | 135 | C7H5NS | 000095-16-9 | 95 |
| 2 | 1,2-Benzisothiazole | 135 | C7H5NS | 000272-16-2 | 90 |
| 3 | 3-Allylbenzothiazolium bromide | 255 | C10H10BrNS | 016407-55-9 | 90 |
| 4 | Thieno[2,3-c]pyridine | 135 | C7H5NS | 000272-12-8 | 72 |
| 5 | 1H-Pyrazolo[3,4-d]pyrimidin-4-amine | 135 | C5H5N5 | 002380-63-4 | 59 |



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Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3910-SPP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Integration Parameters: LSCINT.P

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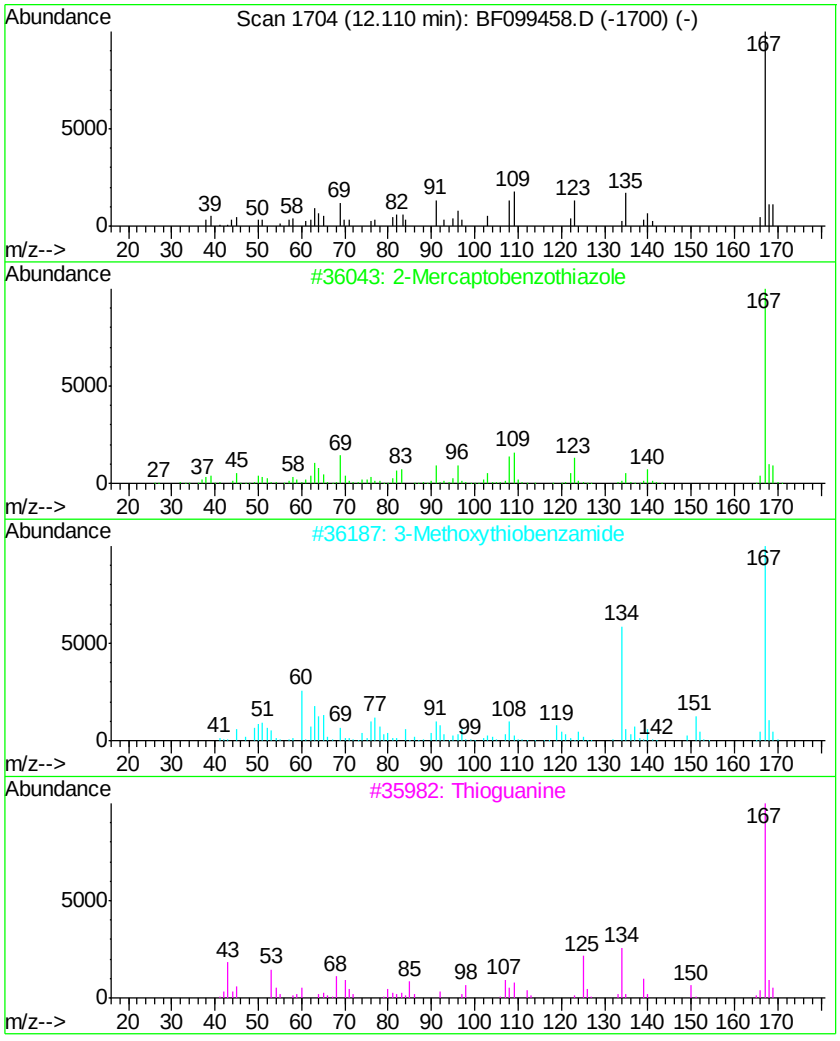
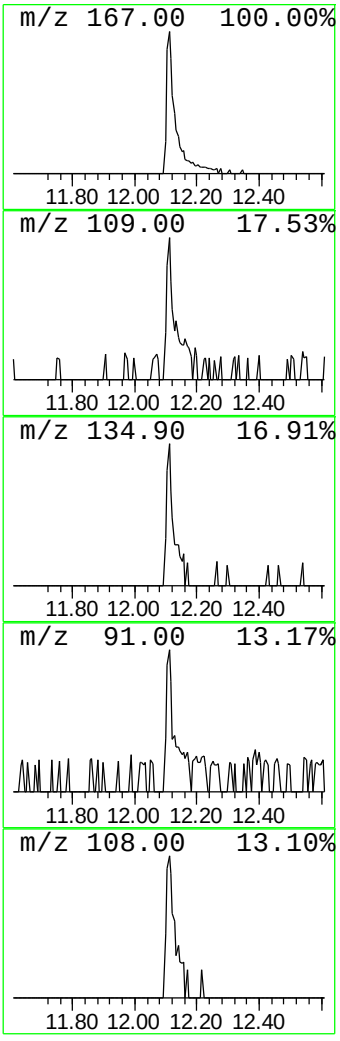
Peak Number 6 2-Mercaptobenzothiazole Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.11 | 3.07 ng | 79084 | Phenanthrene-d10 | 11.37 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Mercaptobenzothiazole | 167 | C7H5NS2 | 000149-30-4 | 96 |
| 2 | 3-Methoxythiobenzamide | 167 | C8H9NOS | 064559-06-4 | 59 |
| 3 | Thioguanine | 167 | C5H5N5S | 000154-42-7 | 59 |
| 4 | Phenol, 2,6-dimethyl-4-nitro- | 167 | C8H9NO3 | 002423-71-4 | 59 |
| 5 | 4-Amino-6-mercaptopyrazolo(3,4-d... | 167 | C5H5N5S | 023771-52-0 | 53 |



# Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 2.13 | 9.8 | ng | 267512 | 1 | 6.85 | 543531 | 20.0 |
| 2-Pentanone, 4-hy... | 5.07 | 7.2 | ng | 194952 | 1 | 6.85 | 543531 | 20.0 |
| unknown6.63 | 6.63 | 85.3 | ng | 2317370 | 1 | 6.85 | 543531 | 20.0 |
| Benzothiazole | 8.42 | 34.0 | ng | 1175190 | 2 | 8.13 | 692384 | 20.0 |
| 2-Mercaptobenzoth... | 12.11 | 3.1 | ng | 79084 | 4 | 11.37 | 515371 | 20.0 |