LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099451.D
Acq On : 13 Oct 2017 20:40
Operator : SJ/JU
Sample : I5819-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3903-PP1-DUP

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 | 2.128 | 3 | 7 | 30 | rVB | 216310 | 411834 | 13.63% | 2.139% |
| 2 | 5.075 | 505 | 508 | 520 | rBV | 155341 | 179169 | 5.93% | 0.931% |
| 3 | 5.475 | 572 | 576 | 592 | rBV | 1399228 | 1291028 | 42.73% | 6.706% |
| 4 | 6.481 | 744 | 747 | 759 | rBV | 792815 | 755606 | 25.01% | 3.925% |
| 5 | 6.628 | 767 | 772 | 775 | rBV | 2372482 | 2272989 | 75.23% | 11.806% |
| 6 | 6.851 | 807 | 810 | 814 | rBV | 673936 | 550721 | 18.23% | 2.861% |
| 7 | 7.010 | 833 | 837 | 840 | rBV | 2558659 | 2293733 | 75.91% | 11.914% |
| 8 | 7.422 | 902 | 907 | 910 | rBV | 1821613 | 1764522 | 58.40% | 9.165% |
| 9 | 8.133 | 1024 | 1028 | 1035 | rBV | 882573 | 712295 | 23.57% | 3.700% |
| 10 | 8.416 | 1072 | 1076 | 1091 | rBV | 287033 | 267886 | 8.87% | 1.391% |
| 11 | 9.210 | 1206 | 1211 | 1214 | rBV | 3275960 | 3021507 | 100.00% | 15.694% |
| 12 | 9.886 | 1323 | 1326 | 1334 | rVB2 | 779556 | 678002 | 22.44% | 3.522% |
| 13 | 10.680 | 1457 | 1461 | 1472 | rBV | 1409204 | 1324892 | 43.85% | 6.882% |
| 14 | 11.374 | 1575 | 1579 | 1587 | rBV | 636936 | 546291 | 18.08% | 2.838% |
| 15 | 12.957 | 1844 | 1848 | 1852 | rBV | 2111772 | 2038399 | 67.46% | 10.588% |
| 16 | 13.980 | 2019 | 2022 | 2025 | rBV | 67127 | 52390 | 1.73% | 0.272% |
| 17 | 14.015 | 2025 | 2028 | 2036 | rVV | 570085 | 512731 | 16.97% | 2.663% |
| 18 | 15.492 | 2273 | 2279 | 2288 | rBV | 446022 | 578097 | 19.13% | 3.003% |

Sum of corrected areas: 19252092

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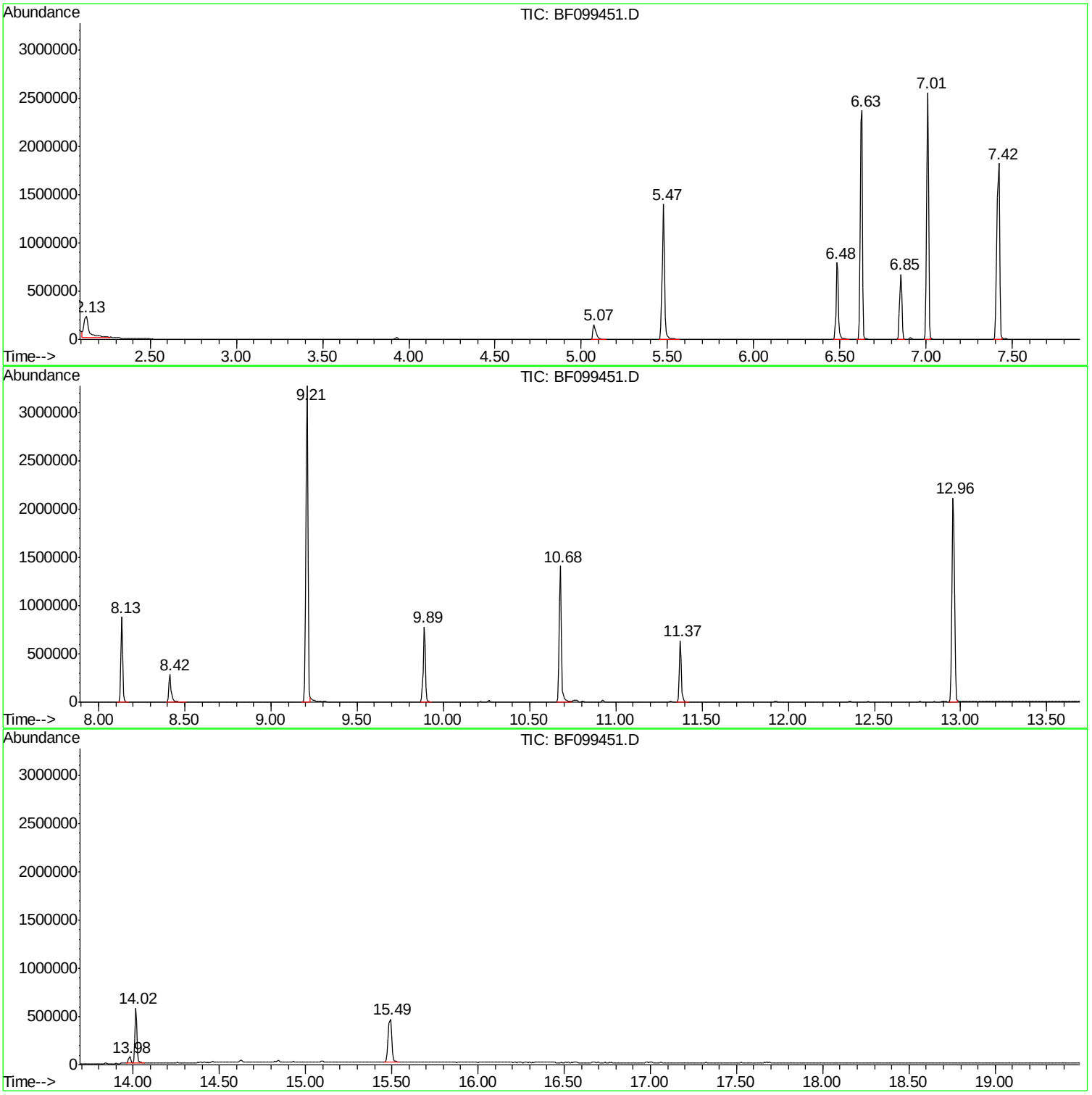
**Instrument :** BNA_F
**ClientSampleId :** 3903-PP1-DUP

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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TIC Integration Parameters: LSCINT.P

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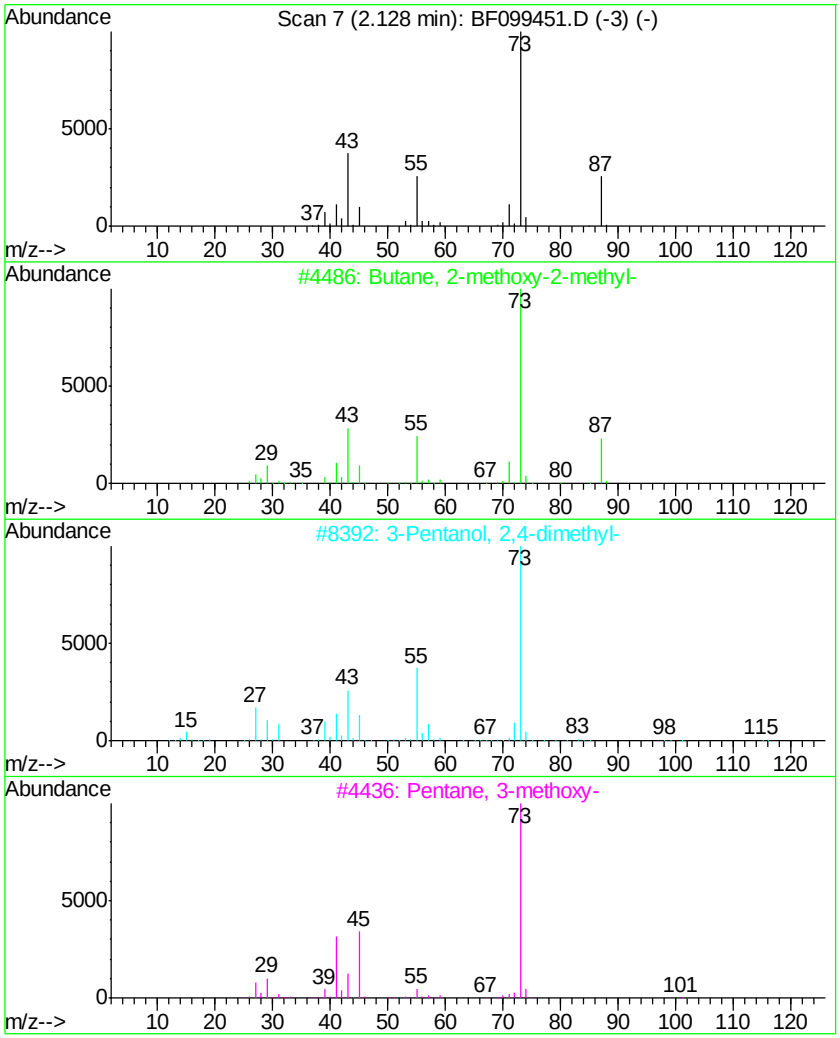
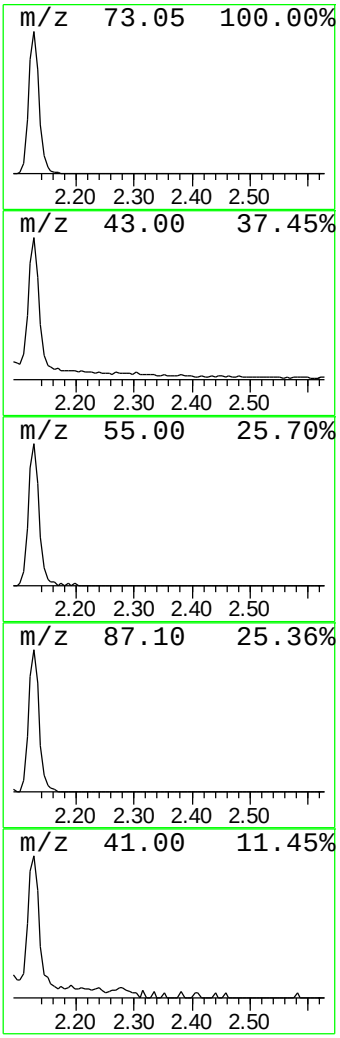
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.13 | 14.96 ng | 411834 | 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 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 37 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 4 | 3-Hexanol, 2-methyl- | 116 | C7H16O | 000617-29-8 | 16 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |



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Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3903-PP1-DUP

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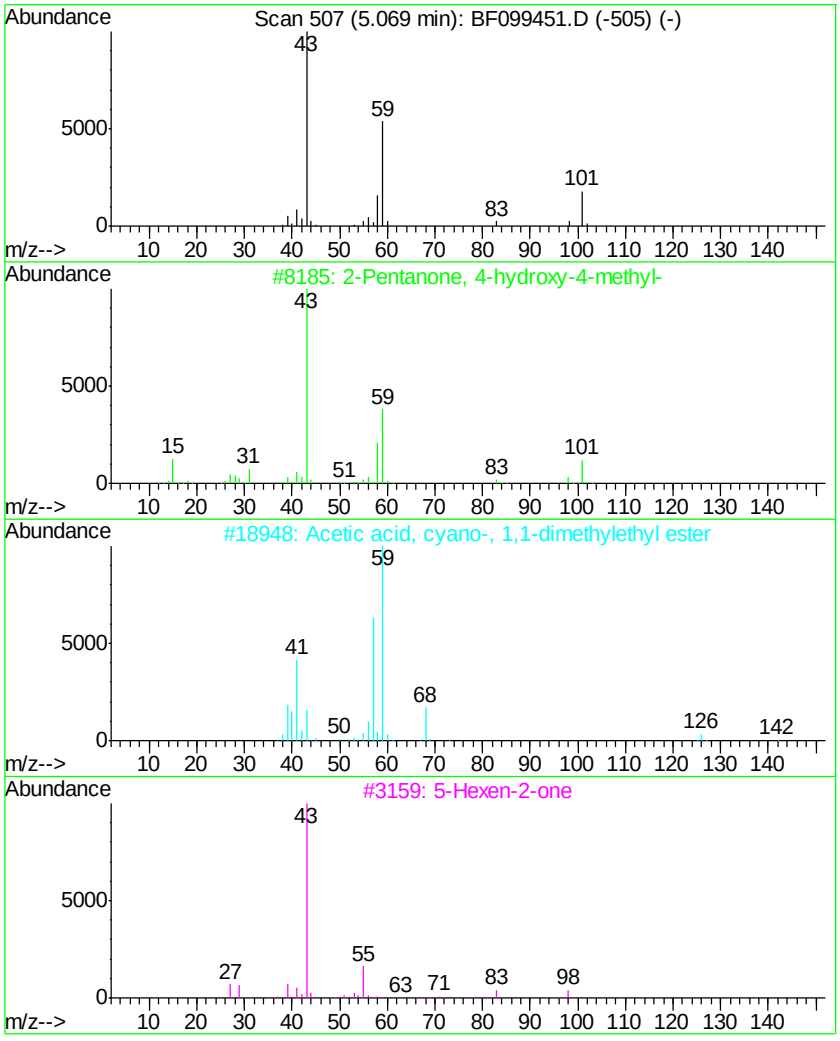
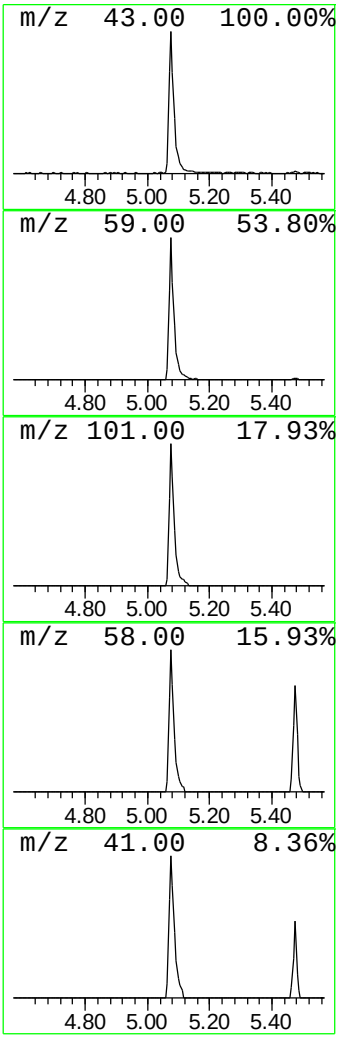
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.07 | 6.51 ng | 179169 | 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 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 4 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



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Operator : SJ/JU
Sample : I5819-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3903-PP1-DUP

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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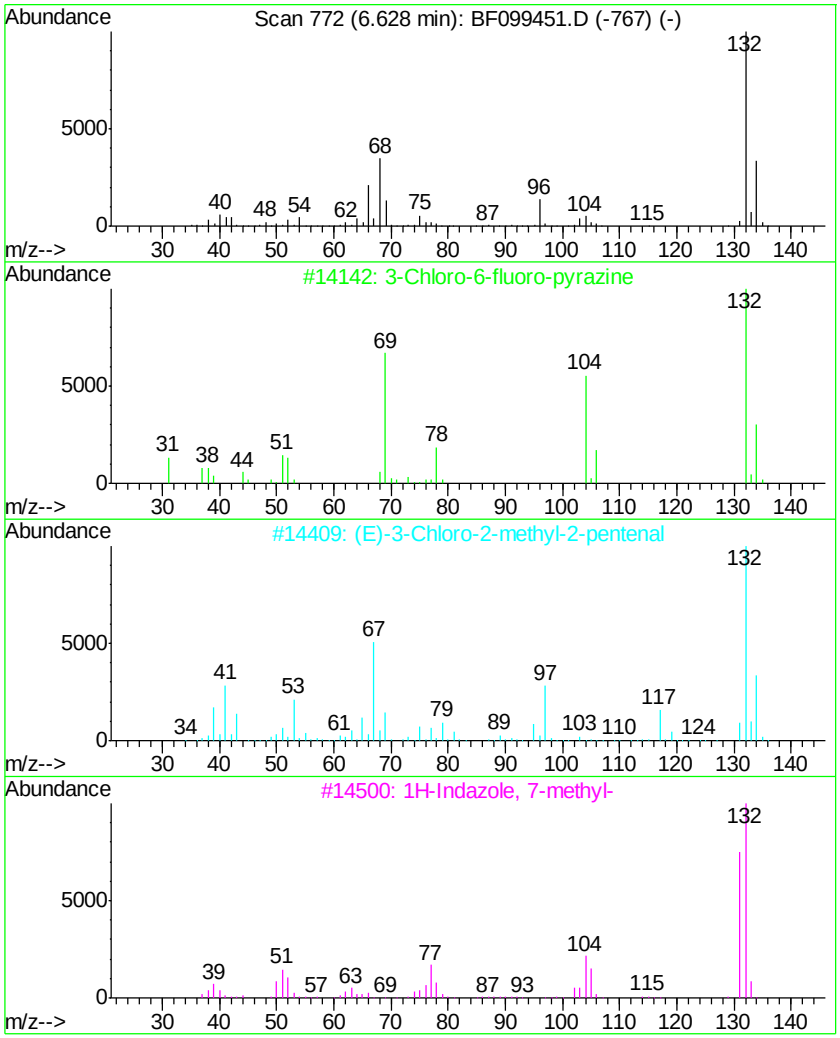
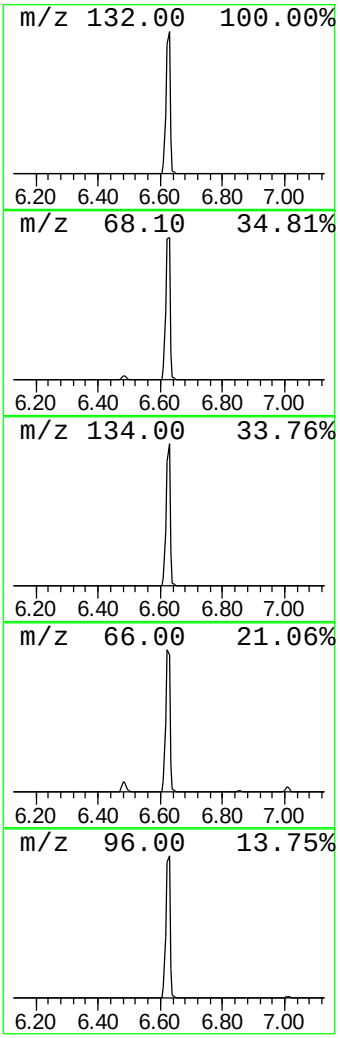
Peak Number 3 unknown6.63 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 82.55 ng | 2272990 | 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 | 1H-Indazole, 7-methyl- | 132 | C8H8N2 | 1000316-00-7 | 10 |
| 4 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



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Acq On : 13 Oct 2017 20:40
Operator : SJ/JU
Sample : I5819-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 3903-PP1-DUP

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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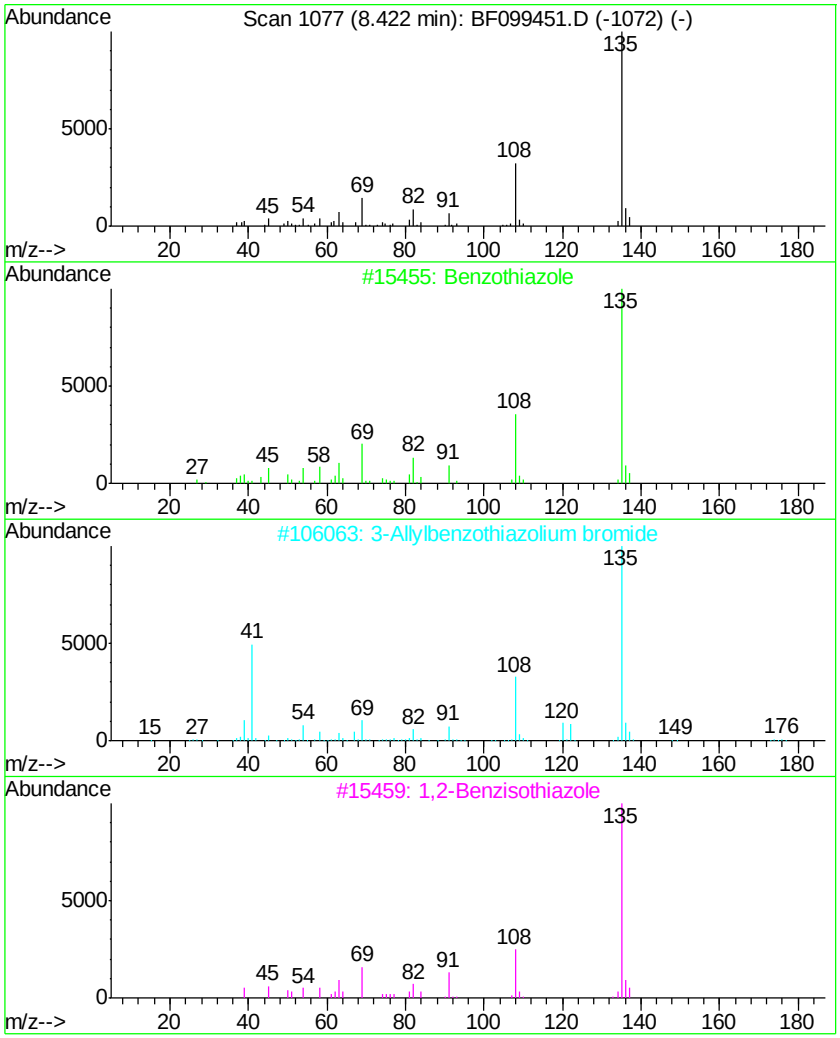
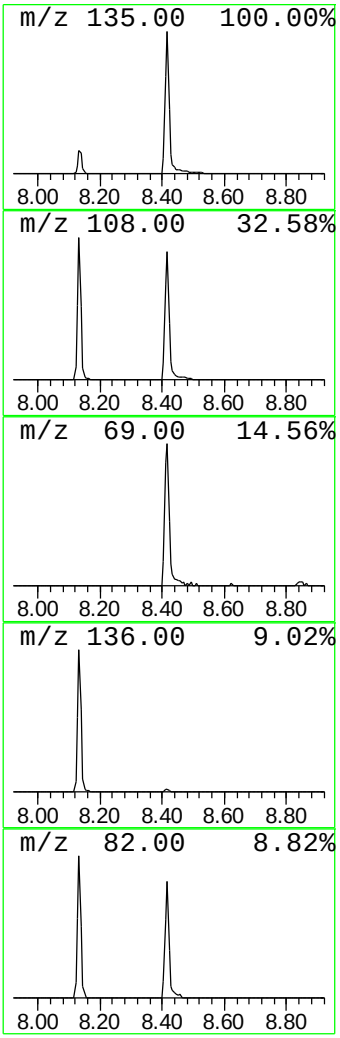
Peak Number 5 Benzothiazole Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.42 | 7.52 ng | 267886 | Naphthalene-d8 | 8.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzothiazole | 135 | C7H5NS | 000095-16-9 | 94 |
| 2 | 3-Allylbenzothiazolium bromide | 255 | C10H10BrNS | 016407-55-9 | 90 |
| 3 | 1,2-Benzisothiazole | 135 | C7H5NS | 000272-16-2 | 78 |
| 4 | 1H-Pyrazolo[3,4-d]pyrimidin-4-amine | 135 | C5H5N5 | 002380-63-4 | 64 |
| 5 | Thieno[2,3-c]pyridine | 135 | C7H5NS | 000272-12-8 | 64 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101317\
Data File : BF099451.D
Acq On : 13 Oct 2017 20:40
Operator : SJ/JU
Sample : I5819-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
3903-PP1-DUP

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 2.13 | 15.0 | ng | 411834 | 1 | 6.85 | 550721 | 20.0 |
| 2-Pentanone, 4-hy... | 5.07 | 6.5 | ng | 179169 | 1 | 6.85 | 550721 | 20.0 |
| unknown6.63 | 6.63 | 82.5 | ng | 2272990 | 1 | 6.85 | 550721 | 20.0 |
| Benzothiazole | 8.42 | 7.5 | ng | 267886 | 2 | 8.13 | 712295 | 20.0 |