LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099983.D
Acq On : 31 Oct 2017 2:28
Operator : SJ/JU
Sample : I6083-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 102017-TIFR-F-U-M

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-BF102317.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 | 4.998 | 492 | 495 | 509 | rBV | 68589 | 101796 | 3.74% | 0.629% |
| 2 | 5.410 | 562 | 565 | 588 | rBV | 566344 | 755342 | 27.73% | 4.670% |
| 3 | 6.428 | 736 | 738 | 754 | rBV | 353074 | 534519 | 19.62% | 3.305% |
| 4 | 6.557 | 757 | 760 | 771 | rVB | 1518609 | 1398430 | 51.33% | 8.647% |
| 5 | 6.786 | 796 | 799 | 810 | rBV | 557090 | 497341 | 18.26% | 3.075% |
| 6 | 6.939 | 822 | 825 | 838 | rBV | 1963913 | 1894625 | 69.55% | 11.715% |
| 7 | 7.363 | 892 | 897 | 916 | rBV | 1370428 | 1439155 | 52.83% | 8.899% |
| 8 | 8.069 | 1014 | 1017 | 1036 | rBV | 796105 | 679485 | 24.94% | 4.201% |
| 9 | 8.633 | 1110 | 1113 | 1119 | rBV | 40956 | 42379 | 1.56% | 0.262% |
| 10 | 9.145 | 1195 | 1200 | 1203 | rBV | 3025885 | 2724172 | 100.00% | 16.844% |
| 11 | 9.539 | 1265 | 1267 | 1274 | rBV | 50908 | 48221 | 1.77% | 0.298% |
| 12 | 9.804 | 1309 | 1312 | 1313 | rBV | 45980 | 37599 | 1.38% | 0.232% |
| 13 | 9.822 | 1313 | 1315 | 1324 | rVB | 835587 | 736830 | 27.05% | 4.556% |
| 14 | 10.492 | 1426 | 1429 | 1434 | rBB | 43228 | 36148 | 1.33% | 0.224% |
| 15 | 10.539 | 1434 | 1437 | 1447 | rBV | 197673 | 159130 | 5.84% | 0.984% |
| 16 | 10.621 | 1447 | 1451 | 1466 | rBV | 1057871 | 1003896 | 36.85% | 6.207% |
| 17 | 11.321 | 1566 | 1570 | 1579 | rBV | 731697 | 719794 | 26.42% | 4.451% |
| 18 | 12.910 | 1835 | 1840 | 1843 | rBV | 2455985 | 2337372 | 85.80% | 14.452% |
| 19 | 13.786 | 1986 | 1989 | 2000 | rBV | 31451 | 45298 | 1.66% | 0.280% |
| 20 | 13.974 | 2018 | 2021 | 2032 | rBV | 548608 | 523752 | 19.23% | 3.238% |
| 21 | 15.462 | 2269 | 2274 | 2291 | rVB | 319511 | 457704 | 16.80% | 2.830% |

Sum of corrected areas: 16172988

LSC Report - Integrated Chromatogram

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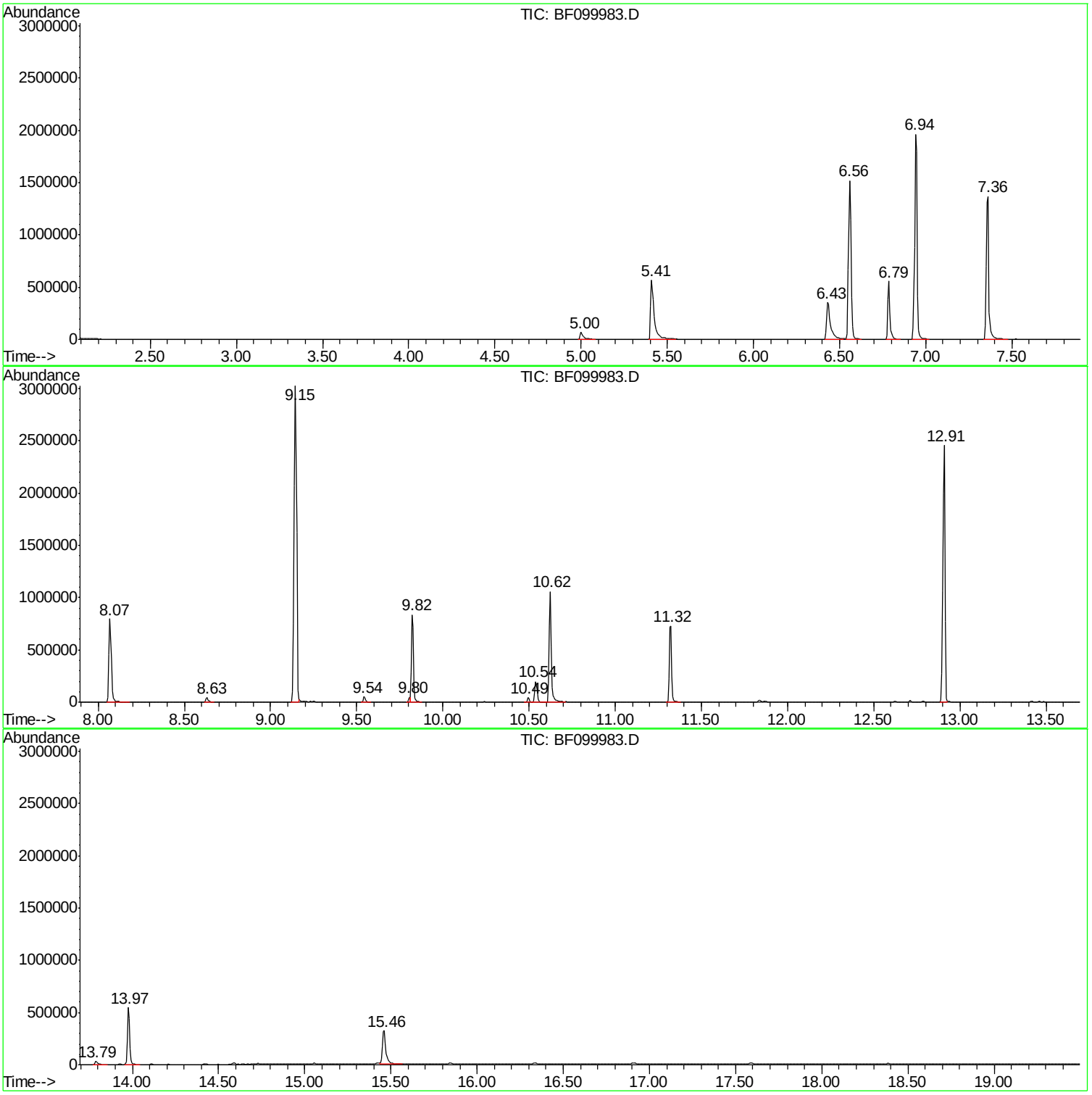
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 102017-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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\BF103017\
Data File : BF099983.D
Acq On : 31 Oct 2017 2:28
Operator : SJ/JU
Sample : I6083-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 102017-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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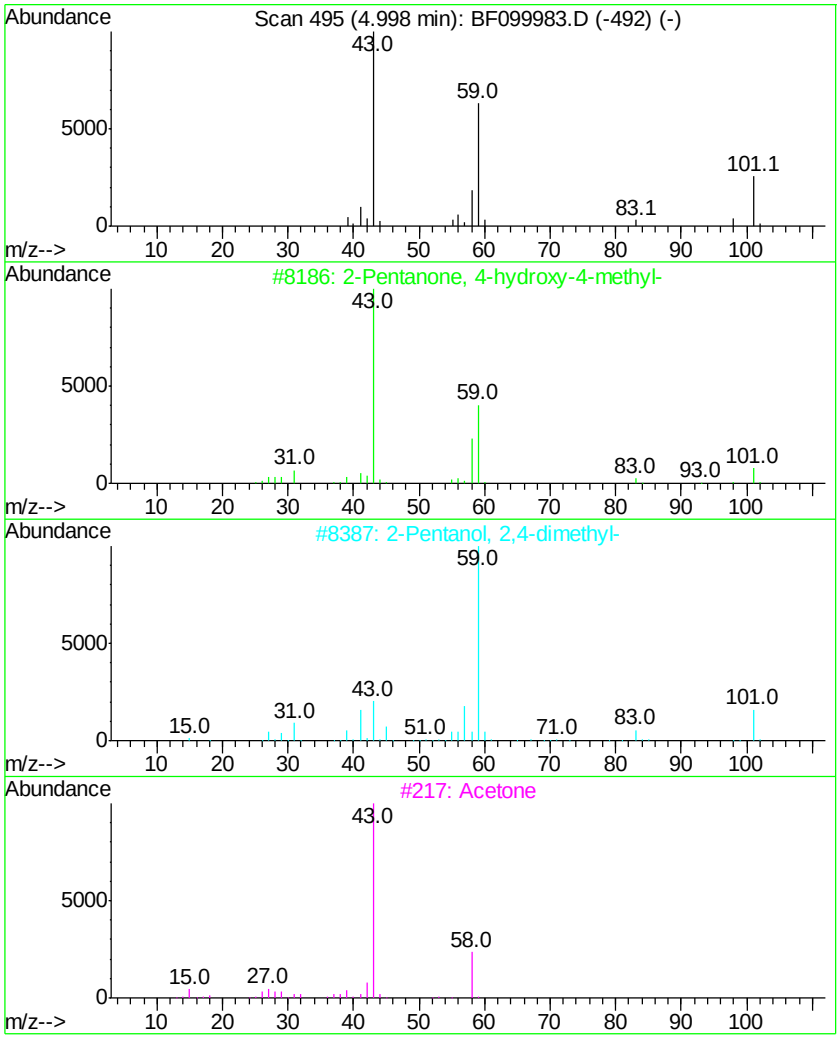
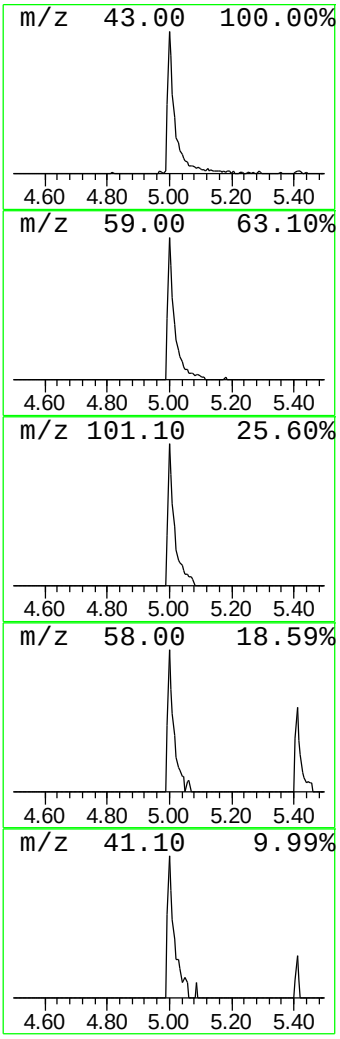
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.00 | 4.09 ng | 101796 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 40 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



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ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 102017-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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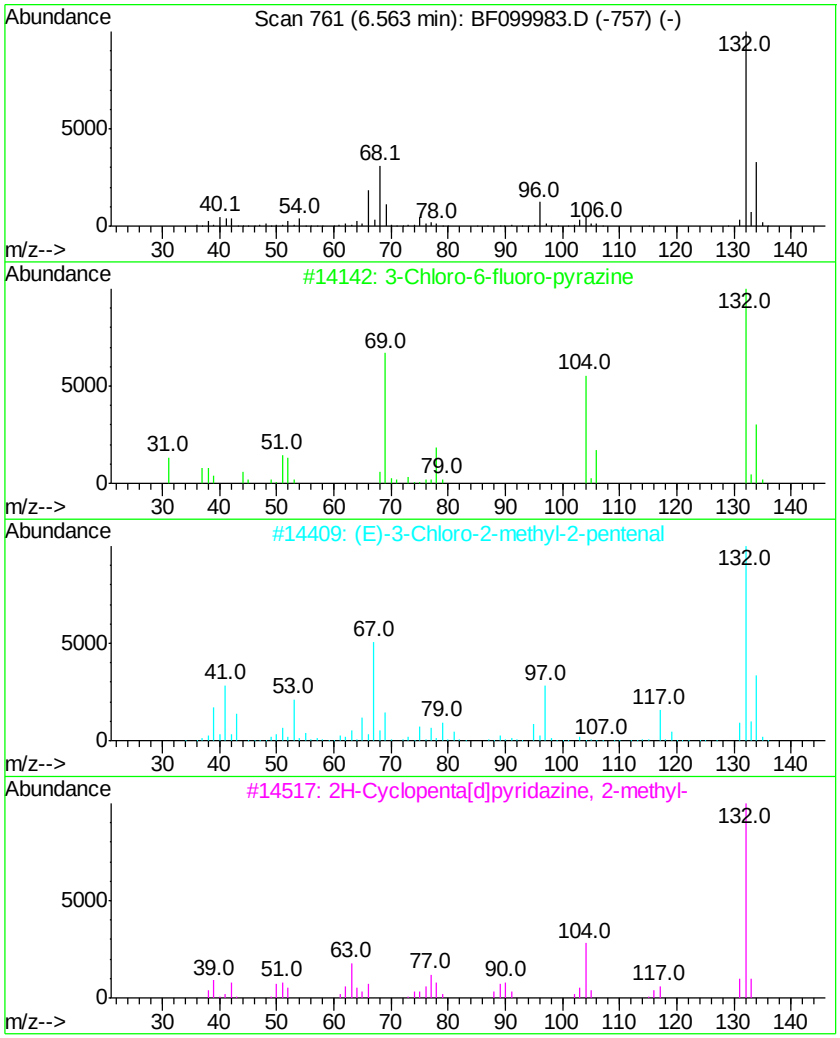
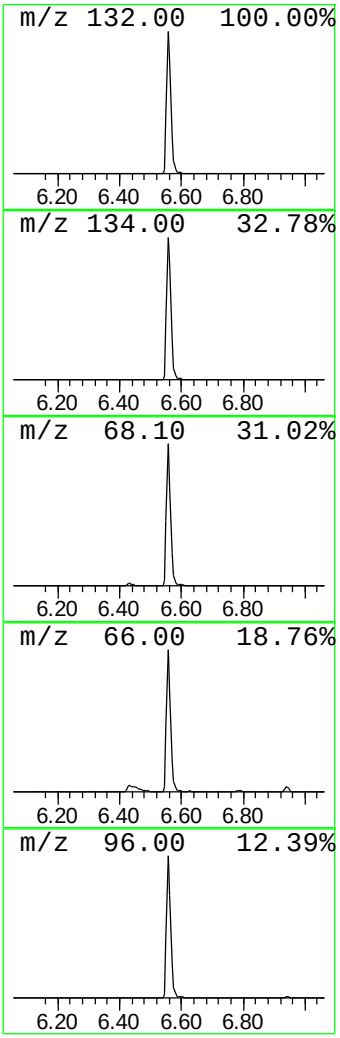
Peak Number 2 unknown6.56 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.56 | 56.24 ng | 1398430 | 1,4-Dichlorobenzene-d4 | 6.79 |

| 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 | 17 |
| 3 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 9 |
| 5 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



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Operator : SJ/JU
Sample : I6083-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 102017-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Integration Parameters: LSCINT.P

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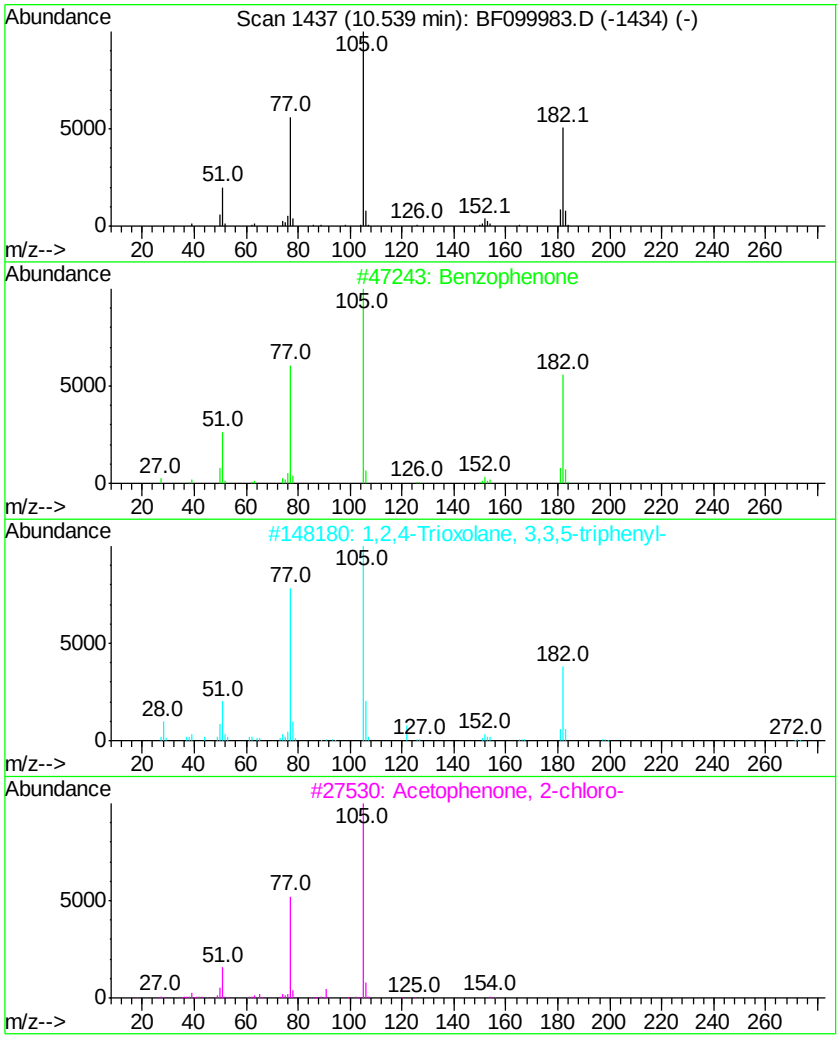
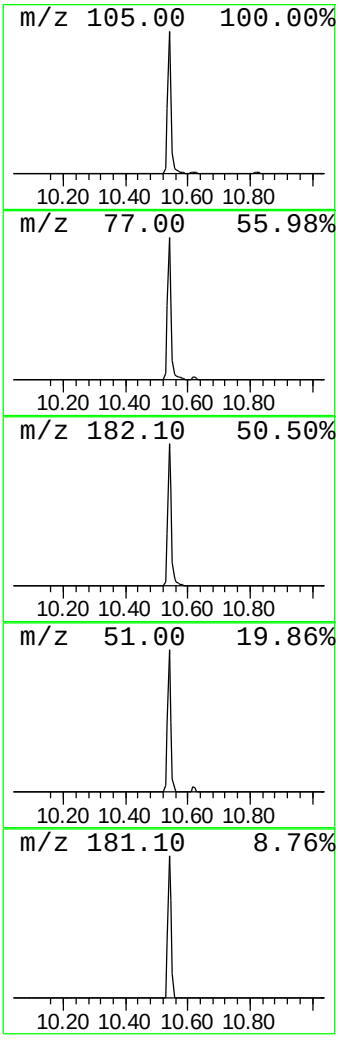
Peak Number 4 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.54 | 4.32 ng | 159130 | Acenaphthene-d10 | 9.82 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | 1,2,4-Trioxolane, 3,3,5-triphenyl- | 304 | C20H16O3 | 023246-12-0 | 64 |
| 3 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 49 |
| 4 | Benzeneacetic acid, .alpha.-oxo-... | 164 | C9H8O3 | 015206-55-0 | 47 |
| 5 | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 47 |



Tentatively Identified Compound (LSC) summary

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Sample : I6083-09
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.00 | 4.1 | ng | 101796 | 1 | 6.79 | 497341 | 20.0 |
| unknown6.56 | 6.56 | 56.2 | ng | 1398430 | 1 | 6.79 | 497341 | 20.0 |
| Benzophenone | 10.54 | 4.3 | ng | 159130 | 3 | 9.82 | 736830 | 20.0 |