LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111321\
Data File : BF126182.D
Acq On : 13 Nov 2021 22:34
Operator : JU/CG
Sample : M4595-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CMC-OF4-001-002

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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126182.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.210 | 16 | 21 | 31 | rVB2 | 74452 | 112259 | 1.53% | 0.251% |
| 2 | 5.039 | 498 | 502 | 509 | rVB | 268369 | 322679 | 4.39% | 0.723% |
| 3 | 5.445 | 566 | 571 | 574 | rBV | 5546875 | 5293687 | 72.07% | 11.853% |
| 4 | 6.457 | 738 | 743 | 746 | rBV | 5450722 | 6164935 | 83.93% | 13.804% |
| 5 | 6.828 | 803 | 806 | 810 | rBV | 1959484 | 1604668 | 21.85% | 3.593% |
| 6 | 7.392 | 897 | 902 | 905 | rBV | 4298185 | 3998532 | 54.44% | 8.953% |
| 7 | 8.016 | 1005 | 1008 | 1020 | rBV | 1530133 | 1534082 | 20.89% | 3.435% |
| 8 | 8.116 | 1020 | 1025 | 1028 | rBV | 2334435 | 2064439 | 28.11% | 4.623% |
| 9 | 9.192 | 1203 | 1208 | 1211 | rBV | 8683785 | 7345195 | 100.00% | 16.447% |
| 10 | 9.310 | 1224 | 1228 | 1231 | rVB | 113981 | 99084 | 1.35% | 0.222% |
| 11 | 9.869 | 1319 | 1323 | 1326 | rBV | 2949303 | 2335304 | 31.79% | 5.229% |
| 12 | 10.657 | 1453 | 1457 | 1460 | rBV | 4517951 | 3924754 | 53.43% | 8.788% |
| 13 | 11.351 | 1571 | 1575 | 1579 | rBV | 1883759 | 1652986 | 22.50% | 3.701% |
| 14 | 11.421 | 1581 | 1587 | 1590 | rVV5 | 98638 | 117878 | 1.60% | 0.264% |
| 15 | 11.751 | 1640 | 1643 | 1646 | rBV | 149846 | 122034 | 1.66% | 0.273% |
| 16 | 12.339 | 1740 | 1743 | 1747 | rBV3 | 73361 | 103803 | 1.41% | 0.232% |
| 17 | 12.457 | 1760 | 1763 | 1766 | rBV | 190709 | 169230 | 2.30% | 0.379% |
| 18 | 12.792 | 1818 | 1820 | 1823 | rBV2 | 96018 | 116848 | 1.59% | 0.262% |
| 19 | 12.945 | 1841 | 1846 | 1849 | rBV | 4549605 | 4461353 | 60.74% | 9.990% |
| 20 | 13.180 | 1884 | 1886 | 1888 | rBV2 | 101638 | 91128 | 1.24% | 0.204% |
| 21 | 13.992 | 2021 | 2024 | 2028 | rBV | 1246039 | 1080551 | 14.71% | 2.420% |
| 22 | 15.456 | 2269 | 2273 | 2277 | rBV | 1240640 | 1438456 | 19.58% | 3.221% |
| 23 | 16.168 | 2390 | 2394 | 2406 | rVB2 | 255512 | 505421 | 6.88% | 1.132% |

Sum of corrected areas: 44659306

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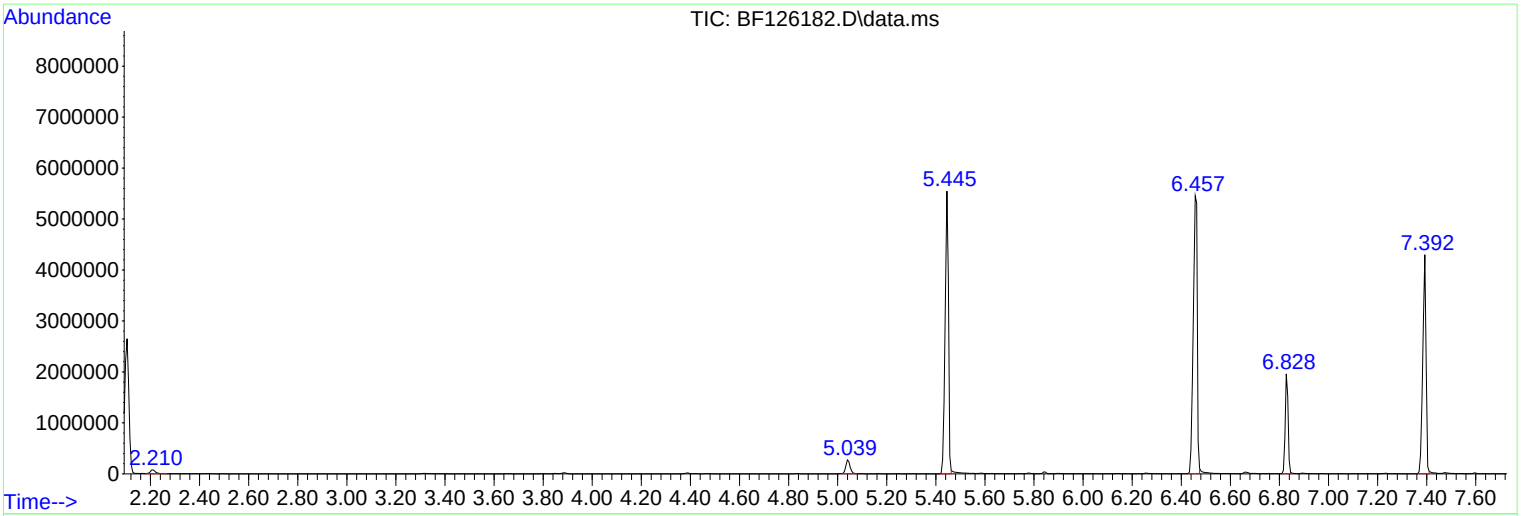
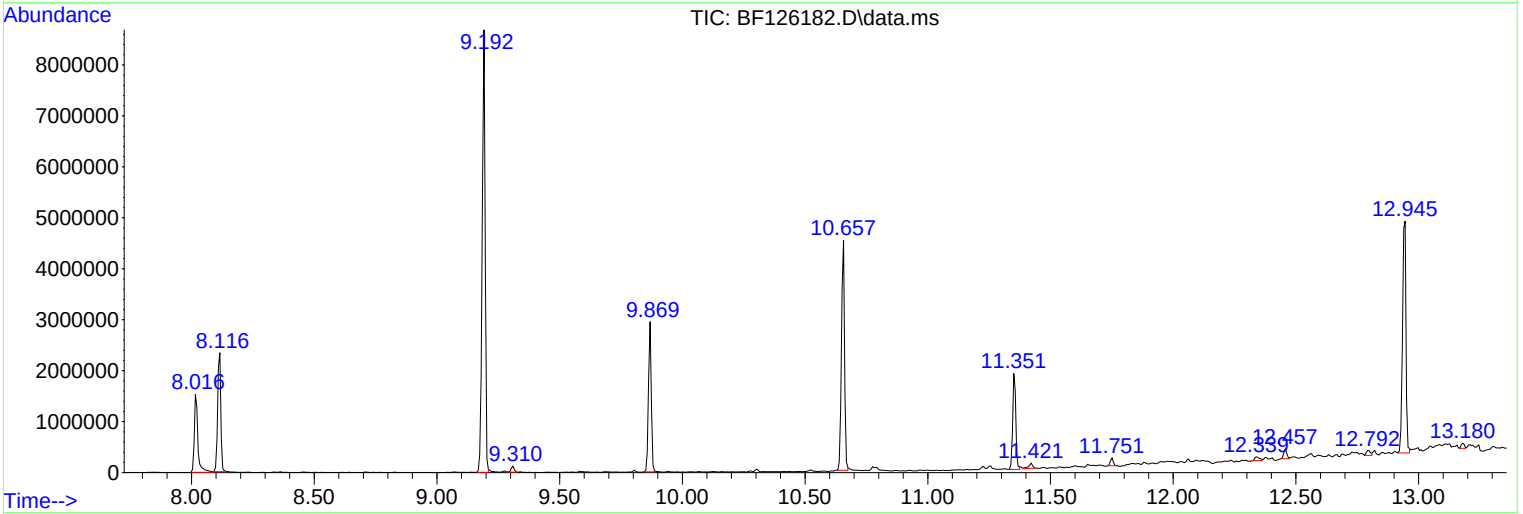
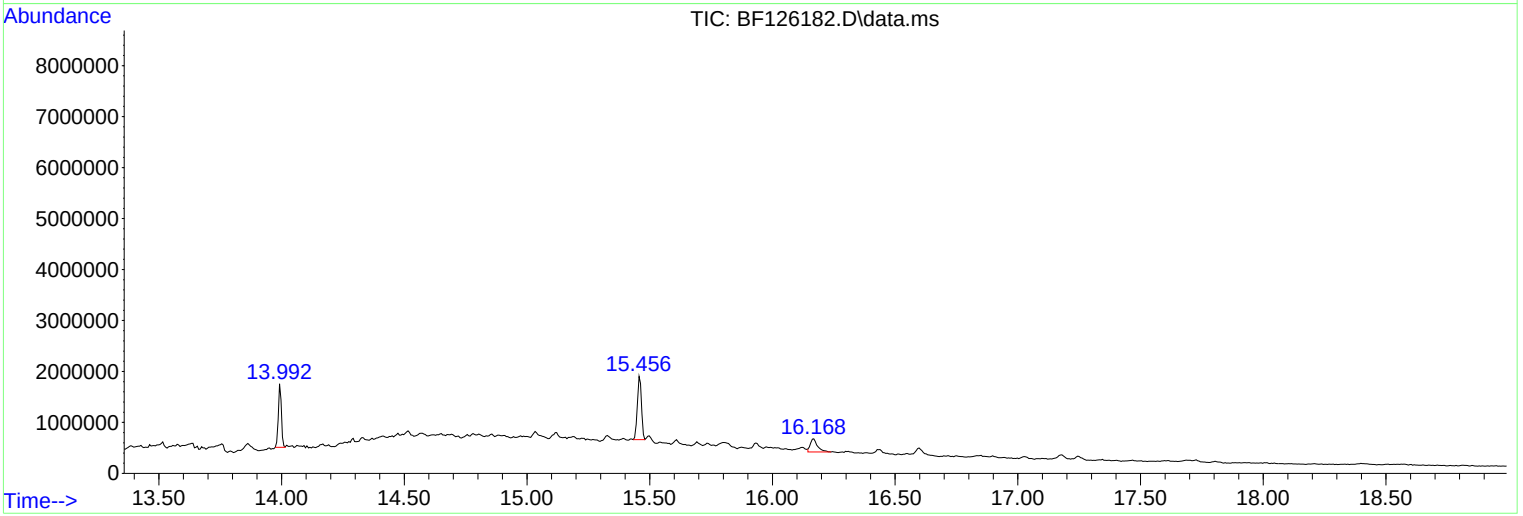
BNA_F
**ClientSampleId :**
CMC-OF4-001-002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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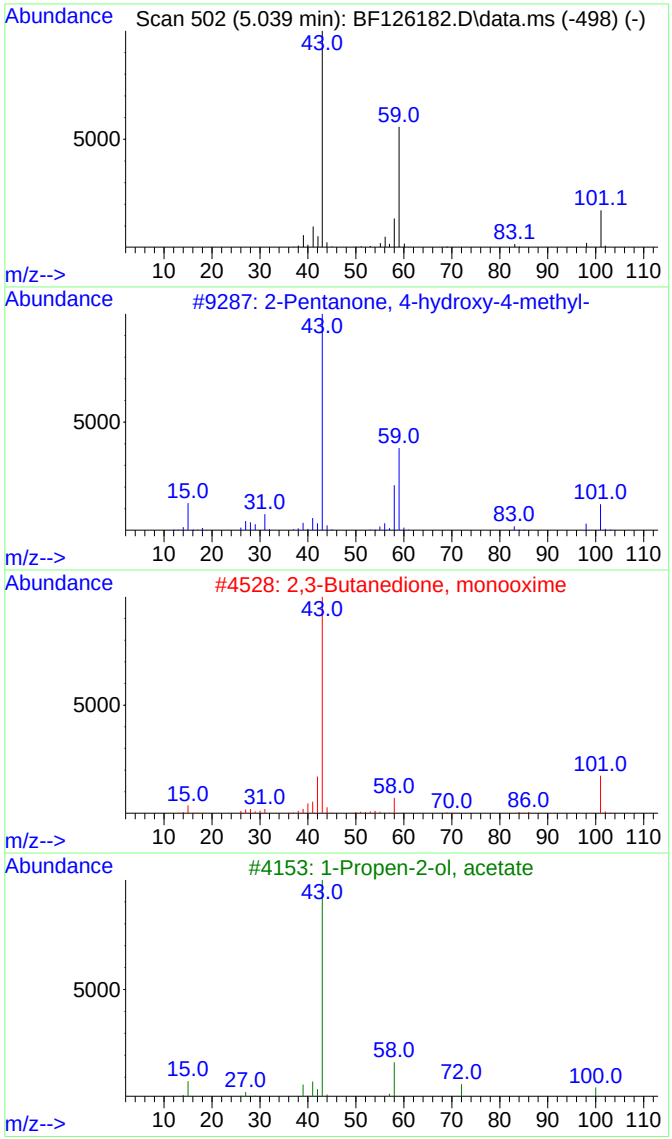
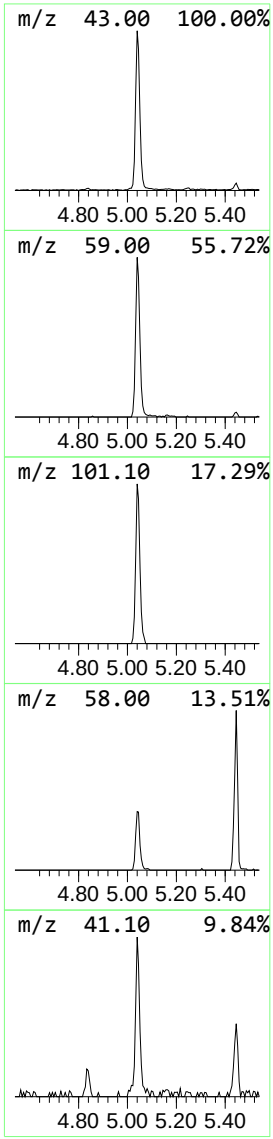
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.039 | 4.02 ng | 322679 | 1,4-Dichlorobenzene-d4 | 6.828 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |
| 4 | 2-Propanone, 1-(1-methylethoxy)- | 116 | C6H12O2 | 042781-12-4 | 9 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 9 |



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Sample : M4595-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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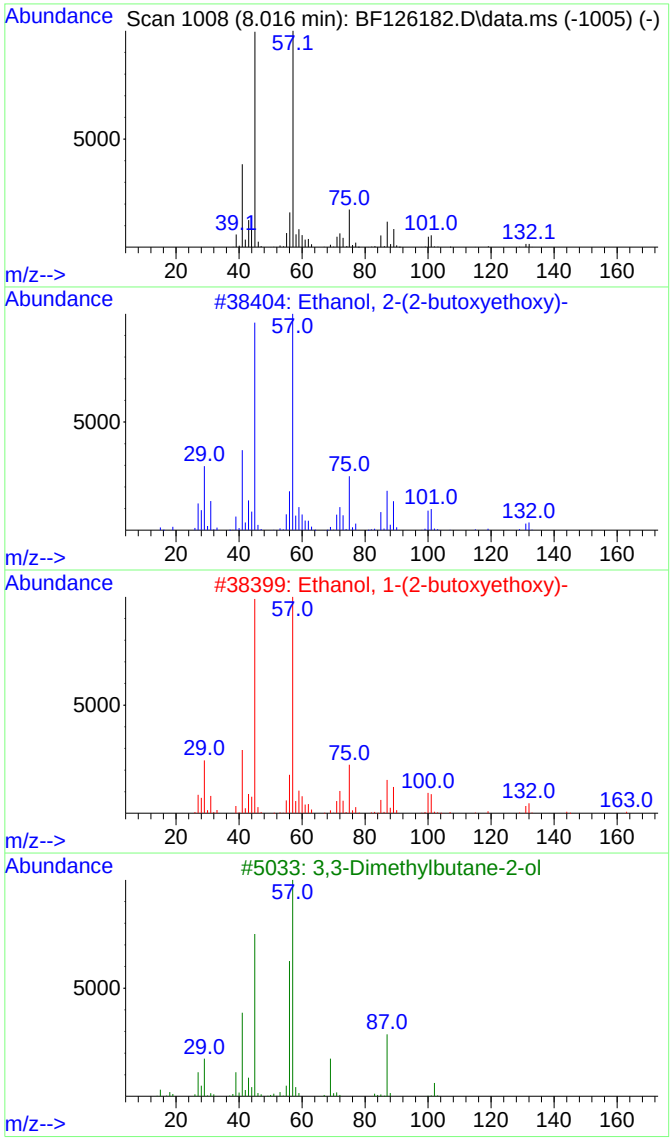
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

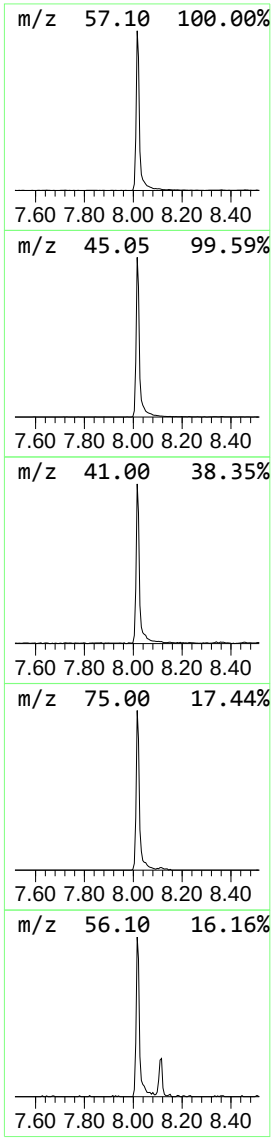
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.016 | 14.86 ng | 1534080 | Naphthalene-d8 | 8.116 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 90 |
| 2 | Ethanol, 1-(2-butoxyethoxy)- | 162 | C8H18O3 | 054446-78-5 | 90 |
| 3 | 3,3-Dimethylbutane-2-ol | 102 | C6H14O | 000464-07-3 | 53 |
| 4 | Di-sec-Butyl ether | 130 | C8H18O | 006863-58-7 | 53 |
| 5 | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 50 |



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**Instrument :**
BNA_F
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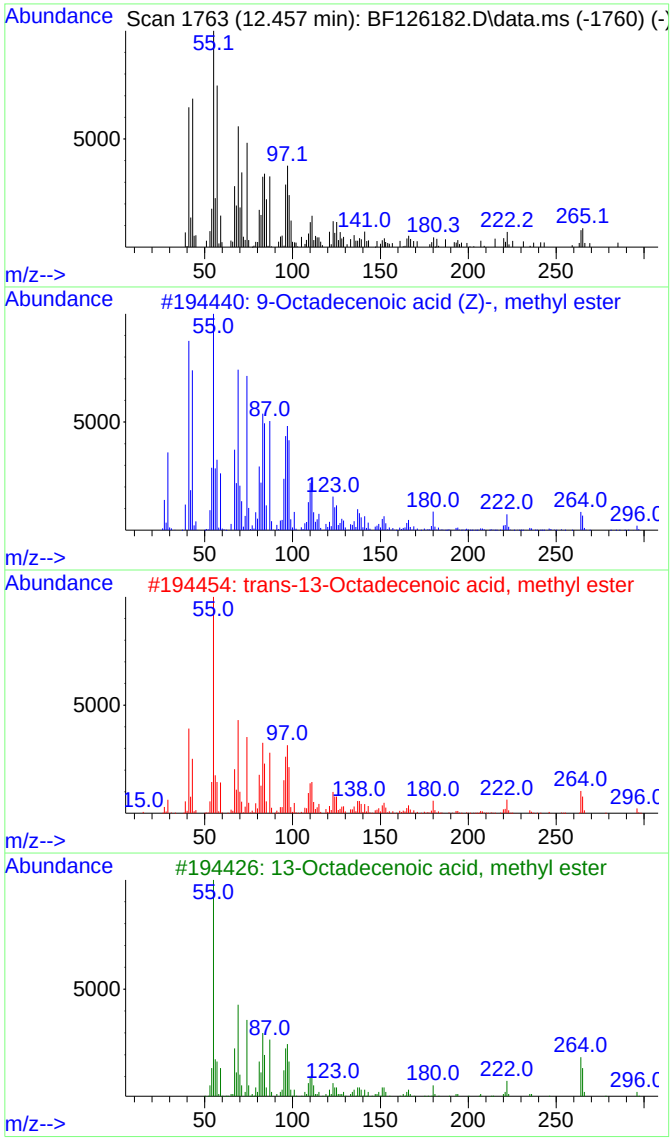
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

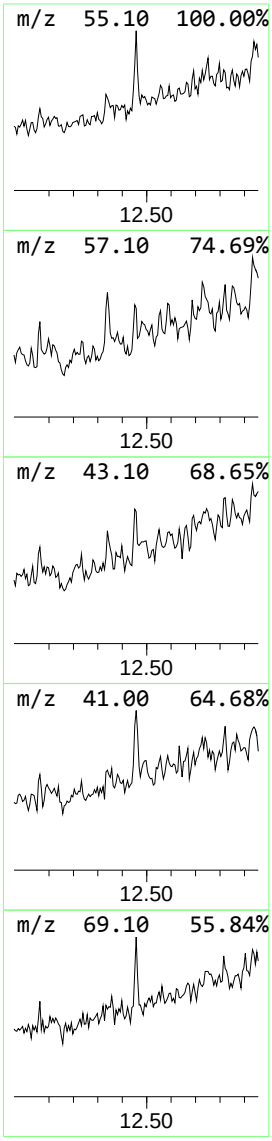
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.457 | 2.05 ng | 169230 | Phenanthrene-d10 | 11.351 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 87 |
| 2 | trans-13-Octadecenoic acid, meth... | 296 | C19H36O2 | 1000333-61-3 | 87 |
| 3 | 13-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-47-3 | 83 |
| 4 | 10-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 013481-95-3 | 74 |
| 5 | 9-Hexadecenoic acid, methyl este... | 268 | C17H32O2 | 001120-25-8 | 46 |



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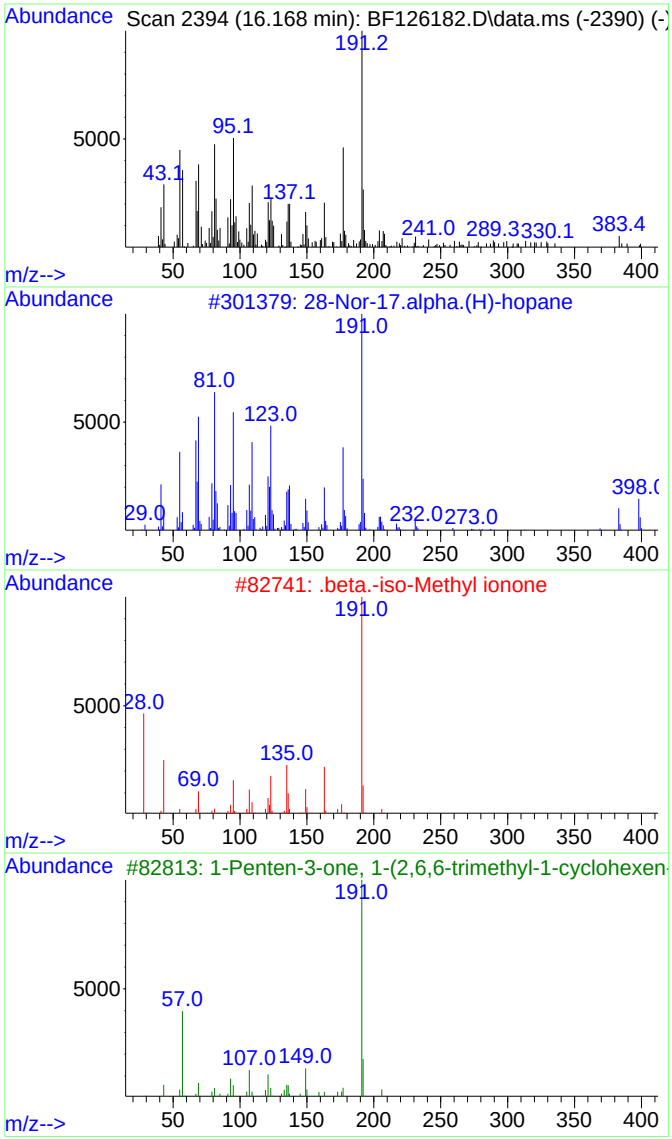
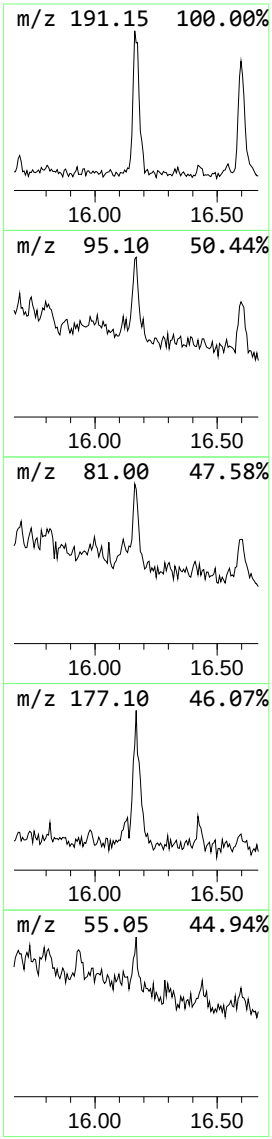
**********
Peak Number 5 28-Nor-17.alpha.(H)-hopane Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.168 | 7.03 ng | 505421 | Perylene-d12 | 15.456 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 28-Nor-17.alpha.(H)-hopane | 398 | C29H50 | 053584-60-4 | 80 |
| 2 | .beta.-iso-Methyl ionone | 206 | C14H22O | 1000285-40-2 | 43 |
| 3 | 1-Penten-3-one, 1-(2,6,6-trimeth... | 206 | C14H22O | 000127-43-5 | 27 |
| 4 | 3-([4-(4-Fluorophenyl)-5-methyl-... | 289 | C14H12FN3O3 | 1000388-71-0 | 25 |
| 5 | 6-Fluoro-2-trifluoromethylbenzoi... | 250 | C11H10F4O2 | 1000338-97-6 | 22 |



Tentatively Identified Compound (LSC) summary

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| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-... | 5.039 | 4.0 | ng | 322679 | 1 | 6.828 | 1604670 | 20.0 |
| Ethanol, 2-(2-b... | 8.016 | 14.9 | ng | 1534080 | 2 | 8.116 | 2064440 | 20.0 |
| 9-Octadecenoic ... | 12.457 | 2.0 | ng | 169230 | 4 | 11.351 | 1652990 | 20.0 |
| 28-Nor-17.alpha... | 16.168 | 7.0 | ng | 505421 | 6 | 15.456 | 1438460 | 20.0 |