LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033964.D
Acq On : 24 Apr 2018 21:20
Operator : SJ/JU
Sample : J2512-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-7-9

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_G\METHODS\8270-BG041918.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 | 4.992 | 284 | 290 | 296 | rVB | 96468 | 143866 | 3.51% | 0.562% |
| 2 | 5.438 | 359 | 366 | 378 | rVB | 1171856 | 1887328 | 46.04% | 7.378% |
| 3 | 7.001 | 623 | 632 | 644 | rBV | 1173441 | 2058157 | 50.20% | 8.045% |
| 4 | 7.365 | 686 | 694 | 702 | rBV | 1186340 | 2000305 | 48.79% | 7.819% |
| 5 | 7.829 | 766 | 773 | 780 | rBV | 297551 | 490253 | 11.96% | 1.916% |
| 6 | 8.147 | 818 | 827 | 835 | rBV | 860814 | 1480604 | 36.12% | 5.788% |
| 7 | 8.975 | 960 | 968 | 976 | rBV | 684983 | 1199103 | 29.25% | 4.687% |
| 8 | 10.609 | 1236 | 1246 | 1257 | rBV | 389649 | 696708 | 16.99% | 2.723% |
| 9 | 13.082 | 1659 | 1667 | 1675 | rVB | 1717110 | 2614603 | 63.78% | 10.220% |
| 10 | 13.916 | 1804 | 1809 | 1815 | rBV | 197706 | 273776 | 6.68% | 1.070% |
| 11 | 14.381 | 1882 | 1888 | 1893 | rBV2 | 33063 | 46022 | 1.12% | 0.180% |
| 12 | 14.457 | 1893 | 1901 | 1911 | rVB2 | 610383 | 955662 | 23.31% | 3.736% |
| 13 | 15.332 | 2045 | 2050 | 2056 | rVB | 44880 | 55104 | 1.34% | 0.215% |
| 14 | 15.949 | 2148 | 2155 | 2166 | rBV | 1526145 | 2276573 | 55.53% | 8.899% |
| 15 | 16.196 | 2192 | 2197 | 2201 | rBV2 | 40527 | 56394 | 1.38% | 0.220% |
| 16 | 17.207 | 2363 | 2369 | 2378 | rBV2 | 816696 | 1252300 | 30.55% | 4.895% |
| 17 | 18.123 | 2520 | 2525 | 2540 | rBV2 | 123154 | 206066 | 5.03% | 0.806% |
| 18 | 19.404 | 2738 | 2743 | 2754 | rBV4 | 33666 | 66206 | 1.61% | 0.259% |
| 19 | 19.845 | 2812 | 2818 | 2824 | rBV | 3180283 | 4099677 | 100.00% | 16.026% |
| 20 | 20.544 | 2931 | 2937 | 2946 | rBV | 83635 | 109600 | 2.67% | 0.428% |
| 21 | 21.155 | 3036 | 3041 | 3050 | rBV2 | 115246 | 181233 | 4.42% | 0.708% |
| 22 | 21.466 | 3087 | 3094 | 3102 | rBV | 1042840 | 1625483 | 39.65% | 6.354% |
| 23 | 23.129 | 3372 | 3377 | 3386 | rVB | 81823 | 140826 | 3.44% | 0.550% |
| 24 | 24.522 | 3602 | 3614 | 3625 | rBV2 | 605140 | 1615920 | 39.42% | 6.317% |
| 25 | 29.592 | 4469 | 4477 | 4482 | rBV10 | 15398 | 50375 | 1.23% | 0.197% |

Sum of corrected areas: 25582144

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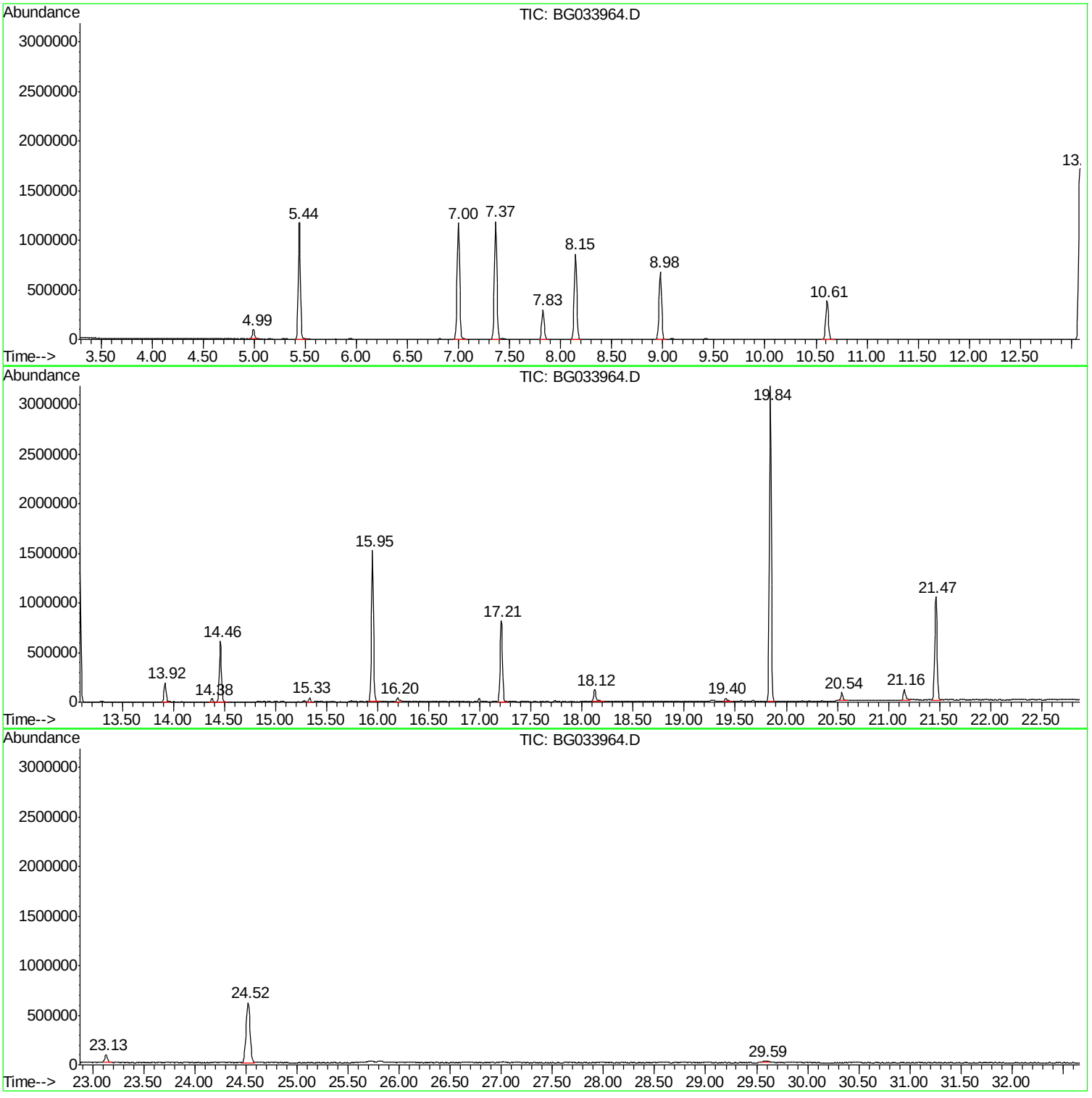
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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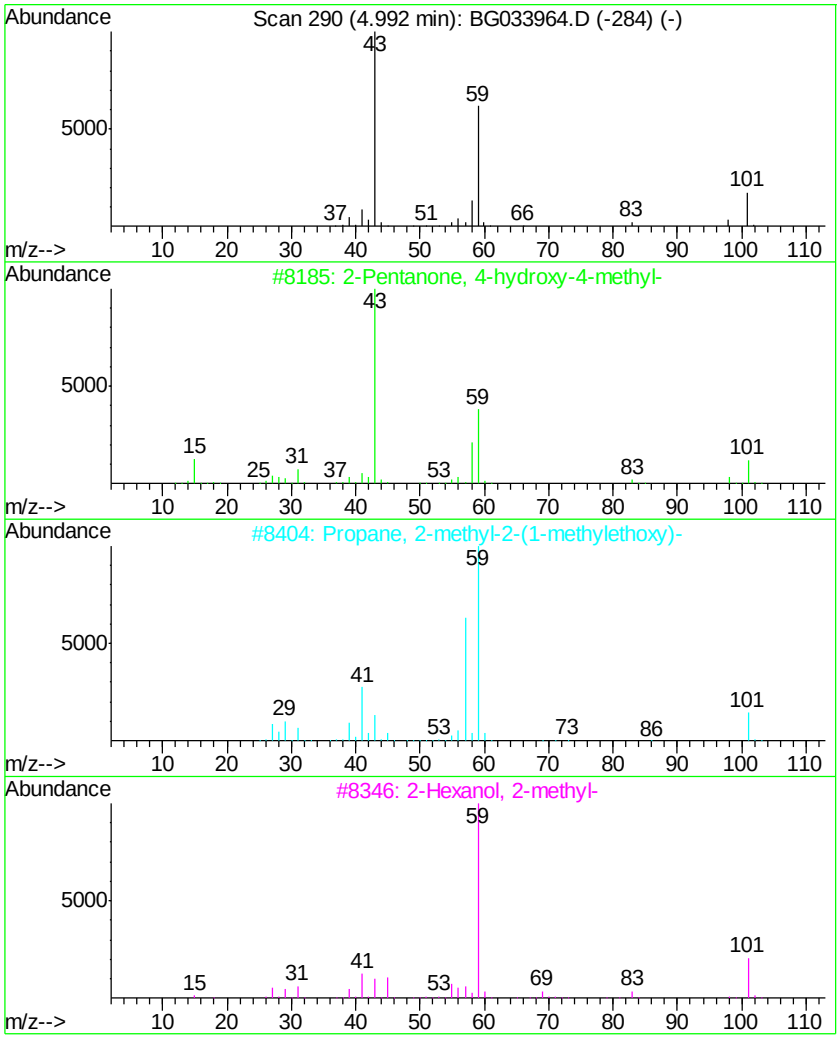
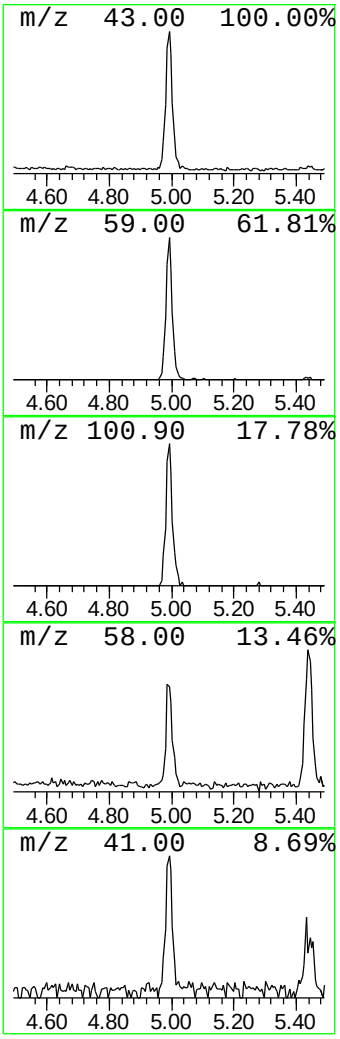
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.99 | 5.87 ng | 143866 | 1,4-Dichlorobenzene-d4 | 7.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 53 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 4 | 3-Octanol | 130 | C8H18O | 000589-98-0 | 28 |
| 5 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 23 |



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Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
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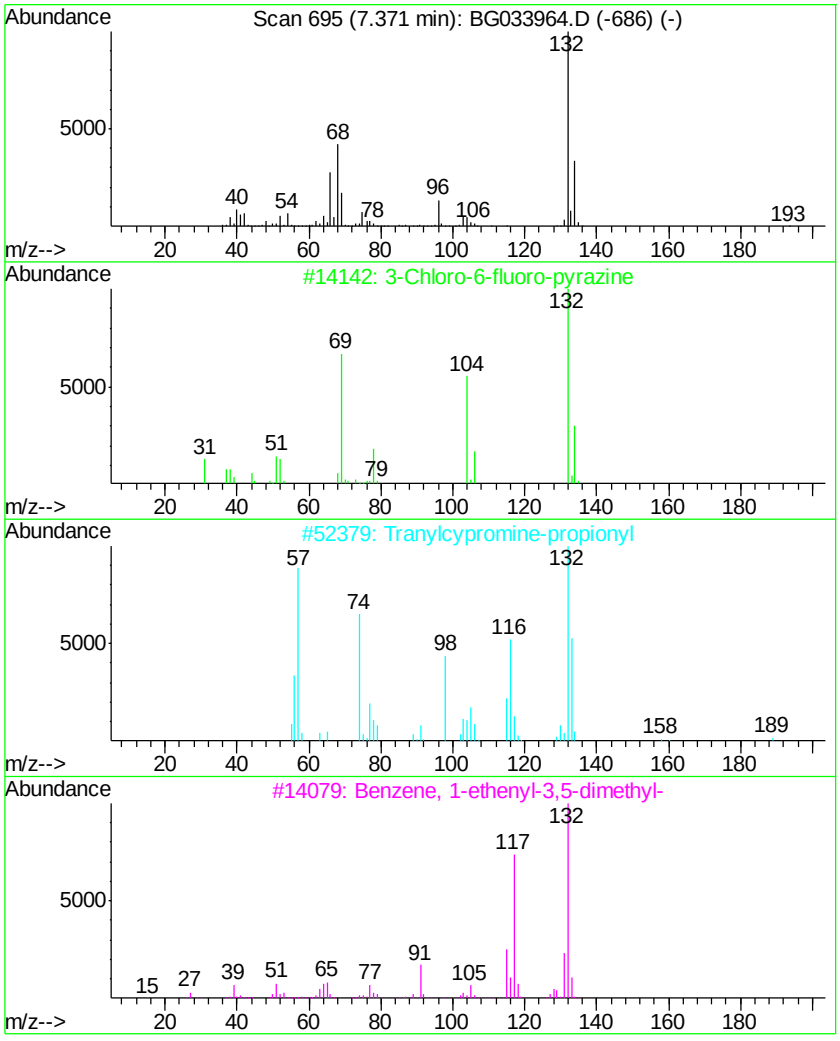
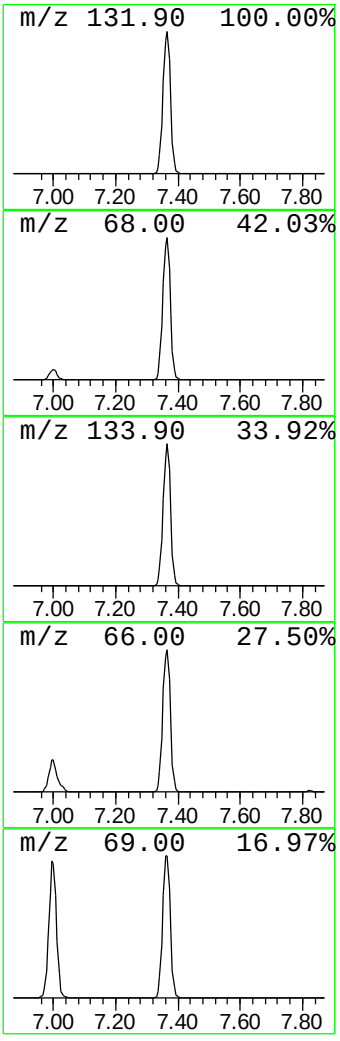
Peak Number 2 unknown7.37 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.37 | 81.60 ng | 2000310 | 1,4-Dichlorobenzene-d4 | 7.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



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Sample : J2512-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
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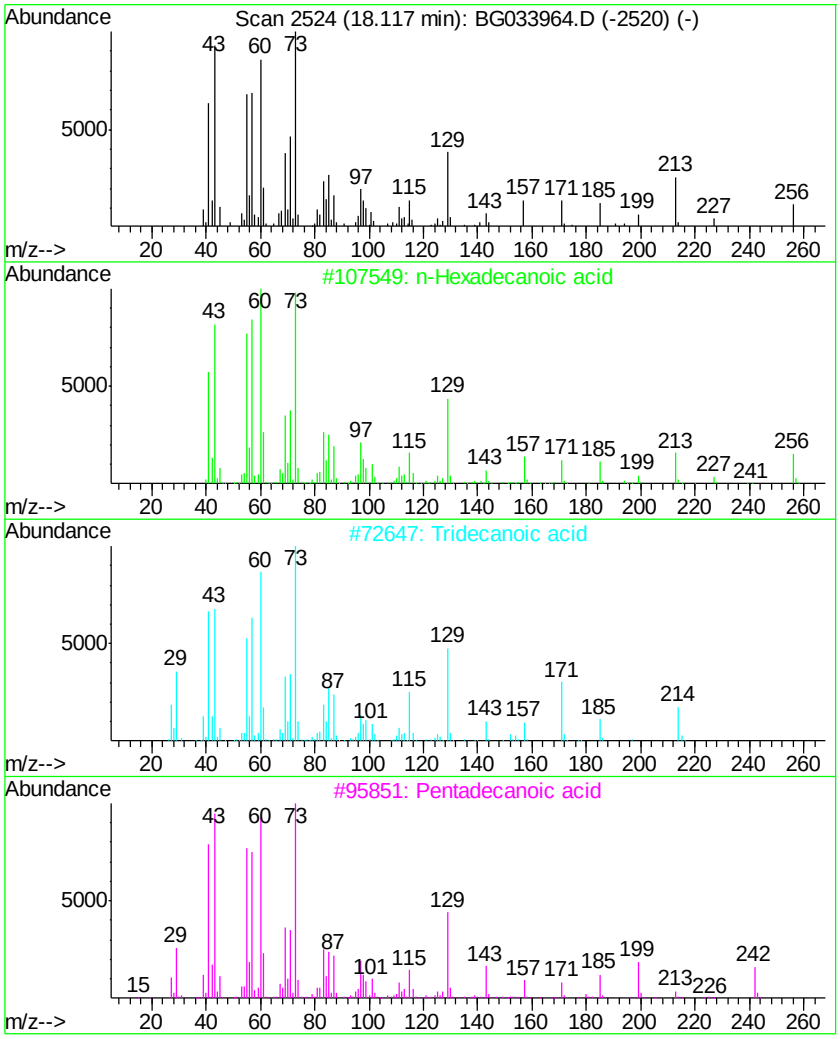
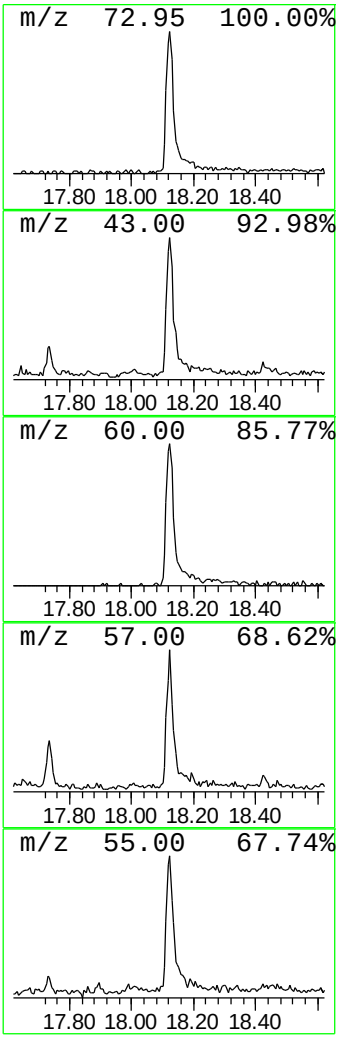
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.12 | 3.29 ng | 206066 | Phenanthrene-d10 | 17.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 76 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 64 |



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Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-5-7-9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
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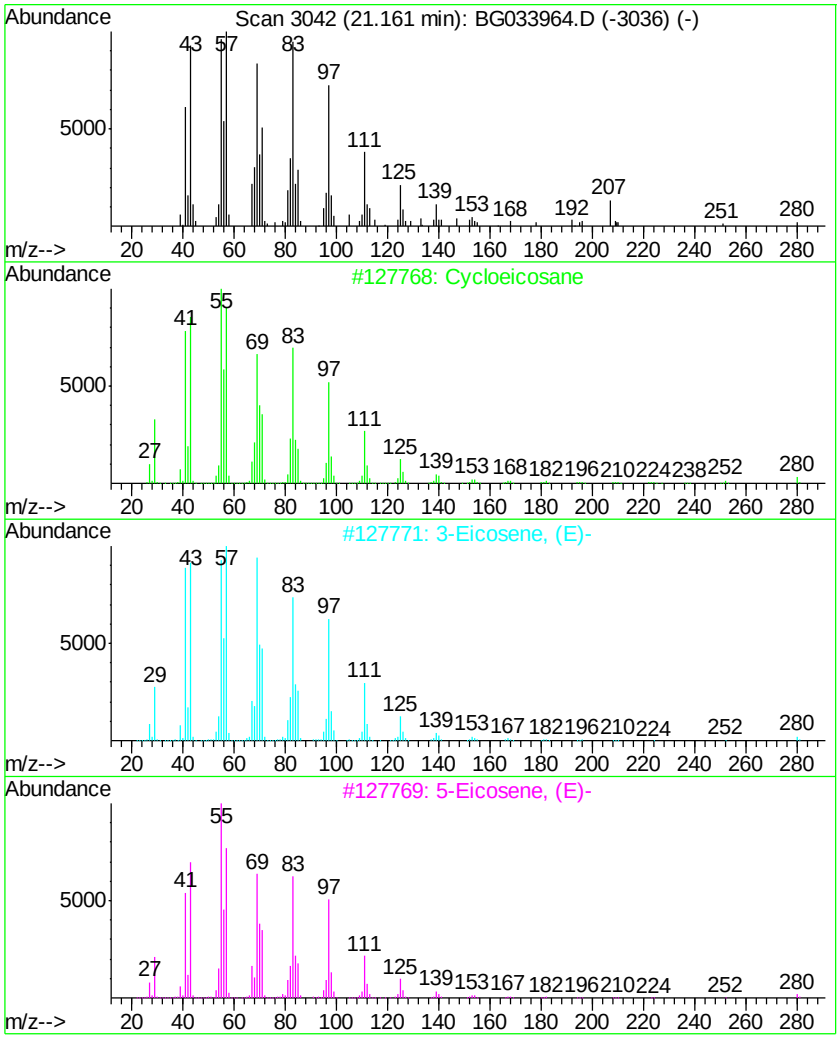
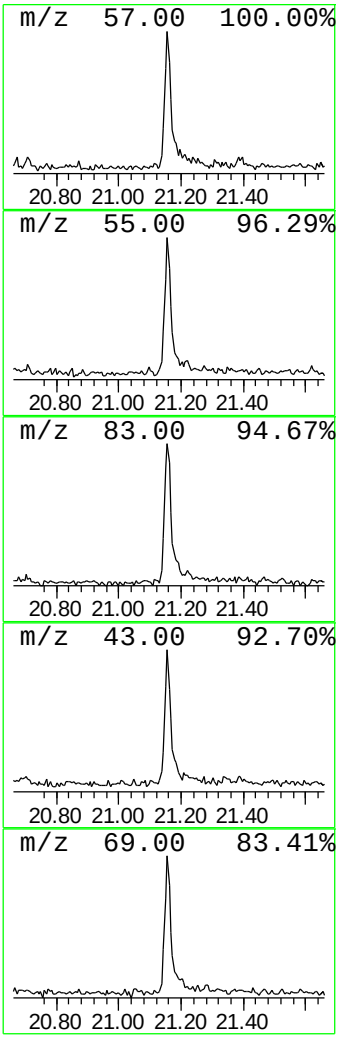
Peak Number 5 Cycloeicosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.16 | 2.23 ng | 181233 | Chrysene-d12 | 21.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 99 |
| 2 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 96 |
| 3 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 96 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 5 | Cyclohexadecane, 1,2-diethyl- | 280 | C20H40 | 1000155-85-3 | 94 |



# 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-hy... | 4.99 | 5.9 | ng | 143866 | 1 | 7.83 | 490253 | 20.0 |
| unknown7.37 | 7.37 | 81.6 | ng | 2000310 | 1 | 7.83 | 490253 | 20.0 |
| n-Hexadecanoic acid | 18.12 | 3.3 | ng | 206066 | 4 | 17.21 | 1252300 | 20.0 |
| Cycloeicosane | 21.16 | 2.2 | ng | 181233 | 5 | 21.47 | 1625480 | 20.0 |