# LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030916\
Data File : BF085304.D
Acq On : 9 Mar 2016 17:43
Operator : UM/SJ
Sample : H1623-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HSR-WC-34-022516

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-BF030316.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 | 2.892 | 51 | 53 | 58 | rVB | 202998 | 262557 | 4.67% | 0.526% |
| 2 | 4.447 | 186 | 189 | 192 | rVB | 160001 | 184567 | 3.28% | 0.370% |
| 3 | 4.538 | 195 | 197 | 200 | rVB | 119086 | 131934 | 2.35% | 0.264% |
| 4 | 4.733 | 212 | 214 | 218 | rVB | 48515 | 60296 | 1.07% | 0.121% |
| 5 | 5.167 | 249 | 252 | 261 | rVB | 910926 | 1556054 | 27.66% | 3.117% |
| 6 | 5.567 | 284 | 287 | 290 | rBV | 3783835 | 4241766 | 75.41% | 8.496% |
| 7 | 6.584 | 372 | 376 | 378 | rVB | 3522082 | 4707999 | 83.70% | 9.429% |
| 8 | 6.721 | 385 | 388 | 390 | rBV | 4539418 | 5114749 | 90.93% | 10.244% |
| 9 | 6.950 | 406 | 408 | 410 | rVB | 1091197 | 1143490 | 20.33% | 2.290% |
| 10 | 7.110 | 419 | 422 | 424 | rVB | 3241166 | 4252633 | 75.61% | 8.517% |
| 11 | 7.510 | 454 | 457 | 459 | rBV | 2752487 | 2957067 | 52.57% | 5.923% |
| 12 | 7.956 | 488 | 496 | 500 | rVB3 | 45921 | 94834 | 1.69% | 0.190% |
| 13 | 8.230 | 517 | 520 | 522 | rBV | 1558749 | 1460751 | 25.97% | 2.926% |
| 14 | 8.562 | 547 | 549 | 553 | rBV2 | 82609 | 117541 | 2.09% | 0.235% |
| 15 | 9.305 | 611 | 614 | 617 | rVB | 4221034 | 5624679 | 100.00% | 11.265% |
| 16 | 9.990 | 671 | 674 | 676 | rBV | 1393717 | 1546668 | 27.50% | 3.098% |
| 17 | 10.516 | 717 | 720 | 724 | rVB | 45787 | 68529 | 1.22% | 0.137% |
| 18 | 10.779 | 740 | 743 | 745 | rBV | 3334323 | 3546758 | 63.06% | 7.104% |
| 19 | 11.476 | 801 | 804 | 806 | rBV | 1675262 | 1712365 | 30.44% | 3.430% |
| 20 | 12.002 | 846 | 850 | 852 | rBV | 728234 | 887745 | 15.78% | 1.778% |
| 21 | 12.711 | 908 | 912 | 915 | rBV2 | 87976 | 209232 | 3.72% | 0.419% |
| 22 | 12.791 | 916 | 919 | 926 | rVV | 1951551 | 2212546 | 39.34% | 4.431% |
| 23 | 13.065 | 940 | 943 | 945 | rBV | 5164556 | 5481611 | 97.46% | 10.979% |
| 24 | 14.105 | 1032 | 1034 | 1037 | rBV | 1064399 | 1413461 | 25.13% | 2.831% |
| 25 | 15.568 | 1159 | 1162 | 1165 | rBV | 654897 | 938708 | 16.69% | 1.880% |

Sum of corrected areas: 49928540

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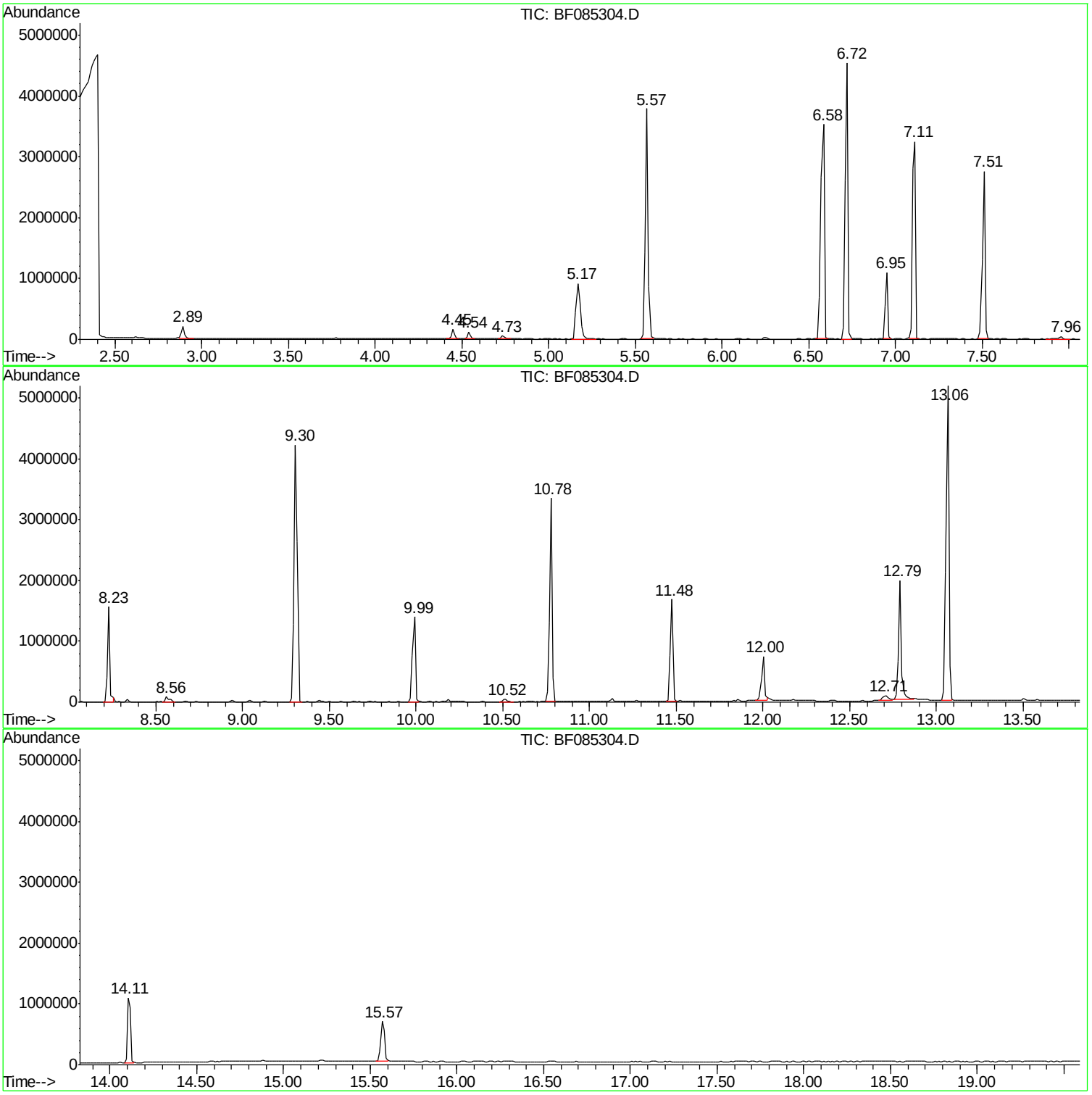
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HSR-WC-34-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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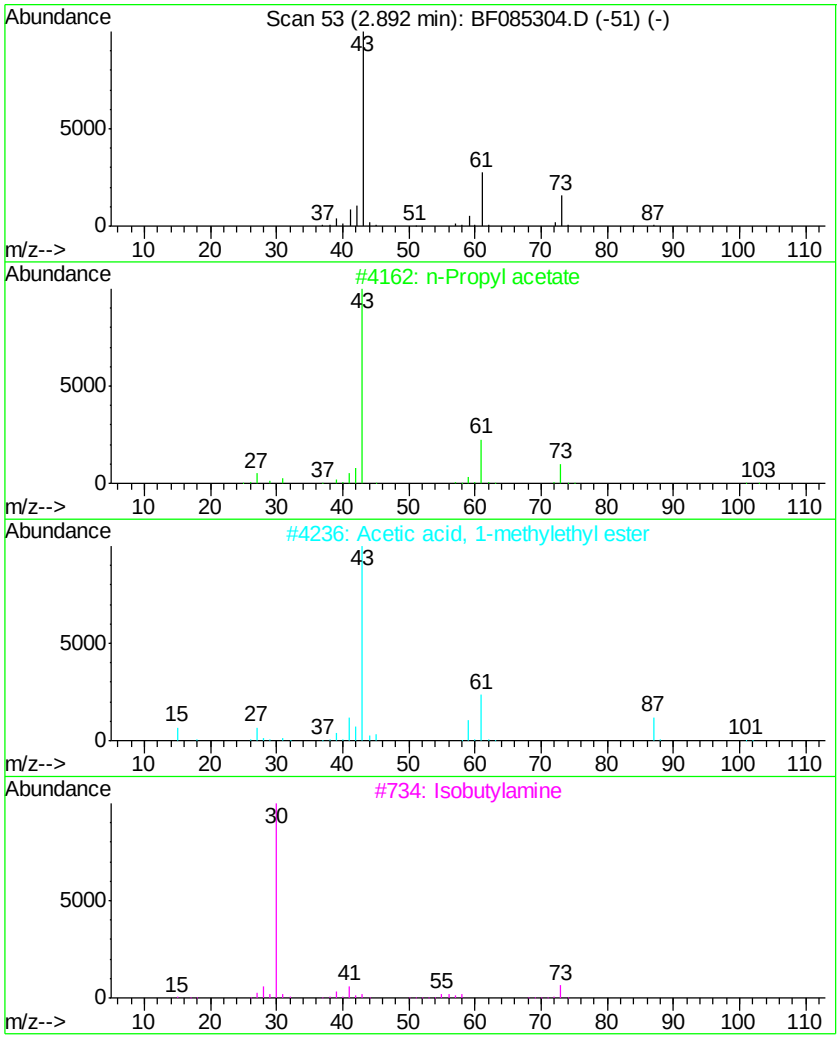
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

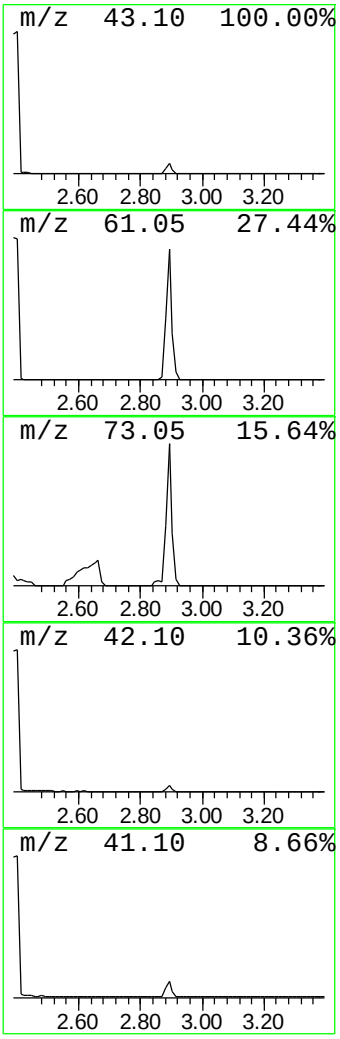
**********

Peak Number 1 n-Propyl acetate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.89 | 4.59 ng | 262557 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Propyl acetate | 102 | C5H10O2 | 000109-60-4 | 83 |
| 2 | Acetic acid, 1-methylethyl ester | 102 | C5H10O2 | 000108-21-4 | 9 |
| 3 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 5 |
| 4 | 1-Butanamine | 73 | C4H11N | 000109-73-9 | 5 |
| 5 | Pentane | 72 | C5H12 | 000109-66-0 | 4 |



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Sample : H1623-07
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ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HSR-WC-34-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

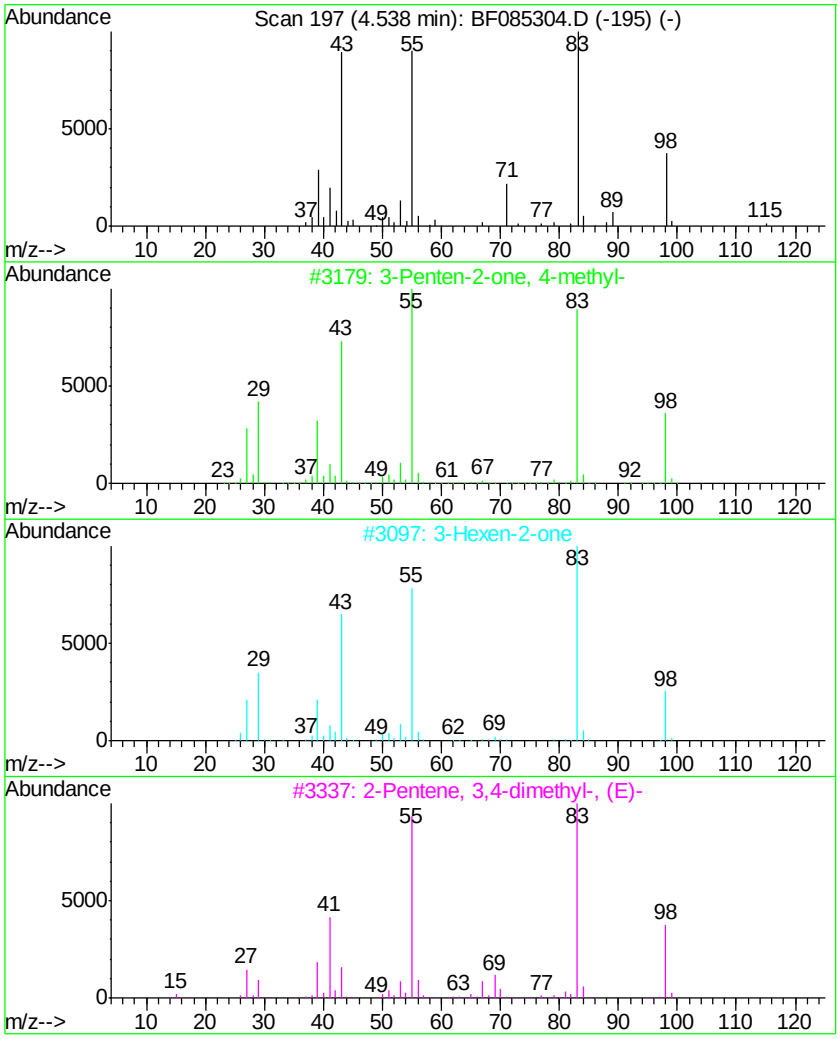
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

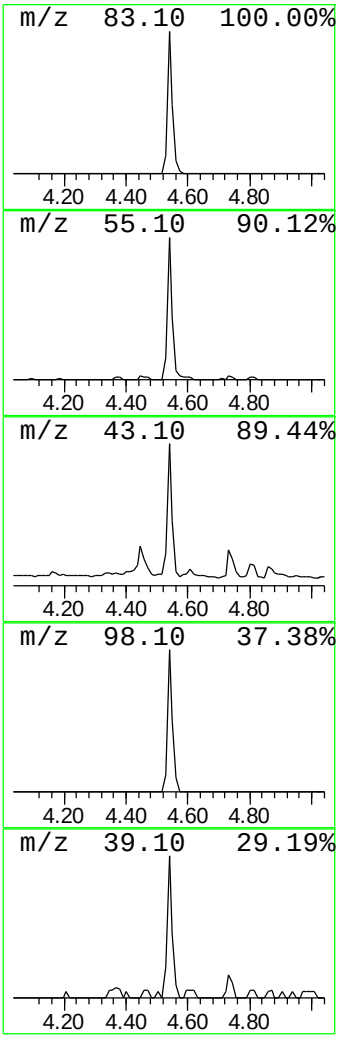
**********

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.54 | 2.31 ng | 131934 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 87 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 72 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 64 |
| 4 | 2-Pentene, 2,3-dimethyl- | 98 | C7H14 | 010574-37-5 | 64 |
| 5 | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14 | 000762-63-0 | 59 |



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Sample : H1623-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HSR-WC-34-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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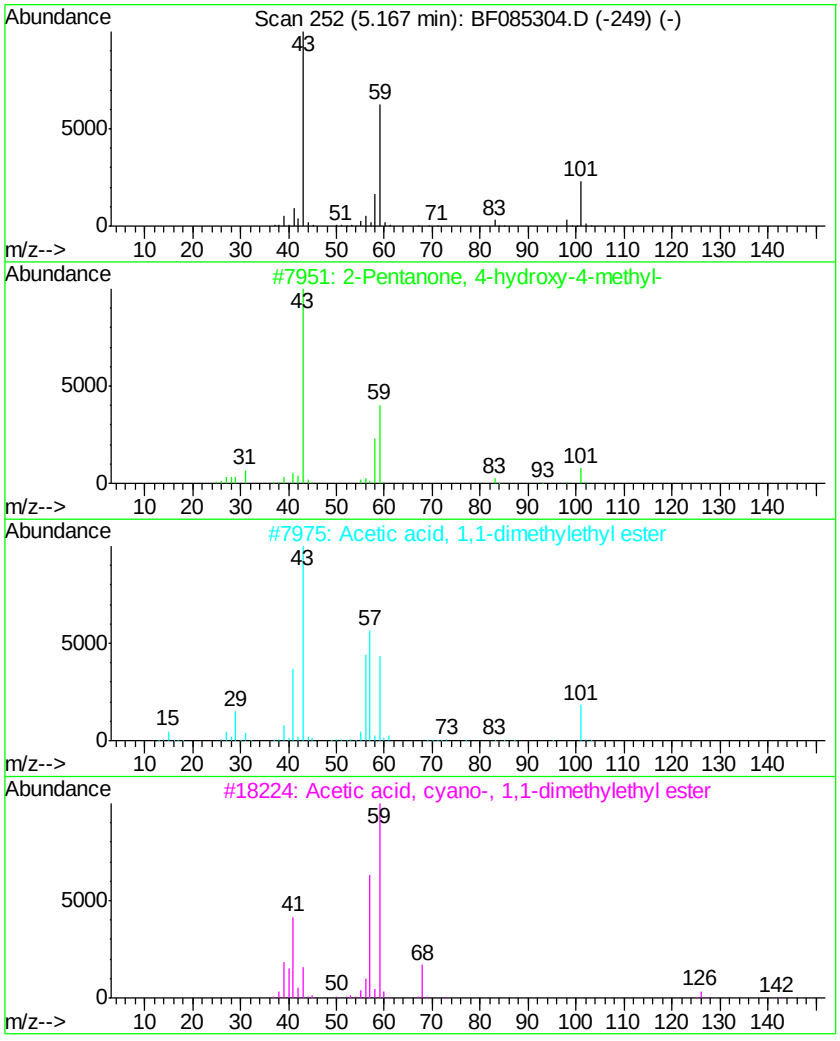
TIC Integration Parameters: LSCINT.P

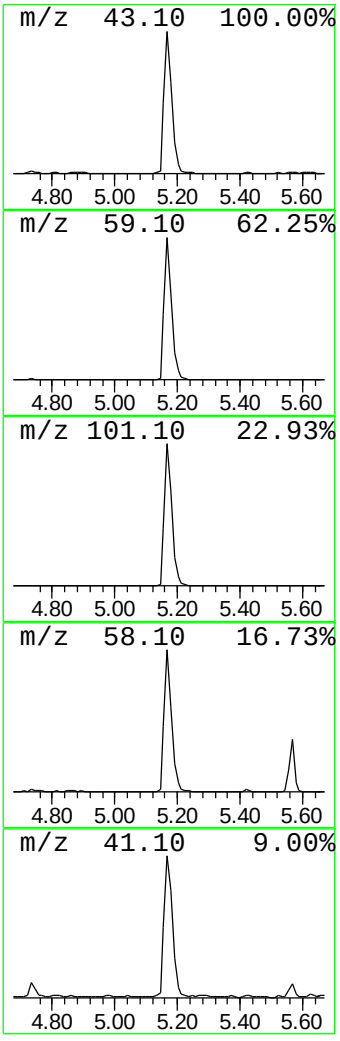
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.17 | 27.22 ng | 1556050 | 1,4-Dichlorobenzene-d4 | 6.95 |

| 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, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



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Operator : UM/SJ
Sample : H1623-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HSR-WC-34-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
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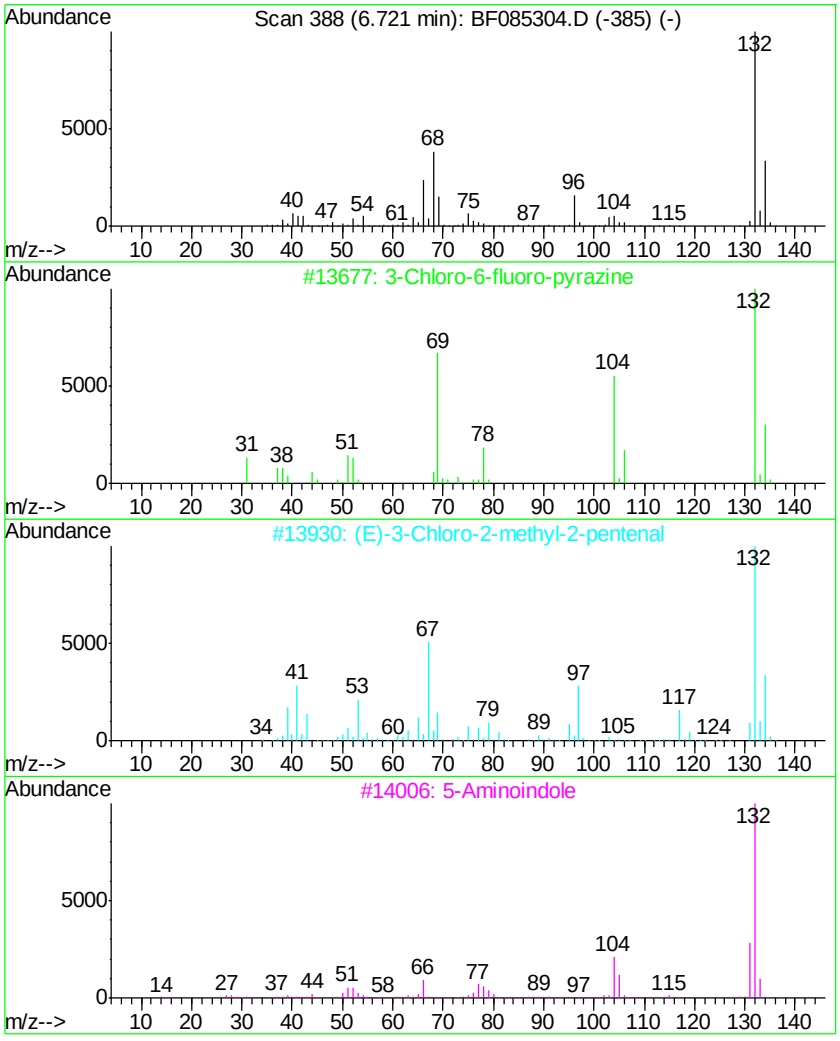
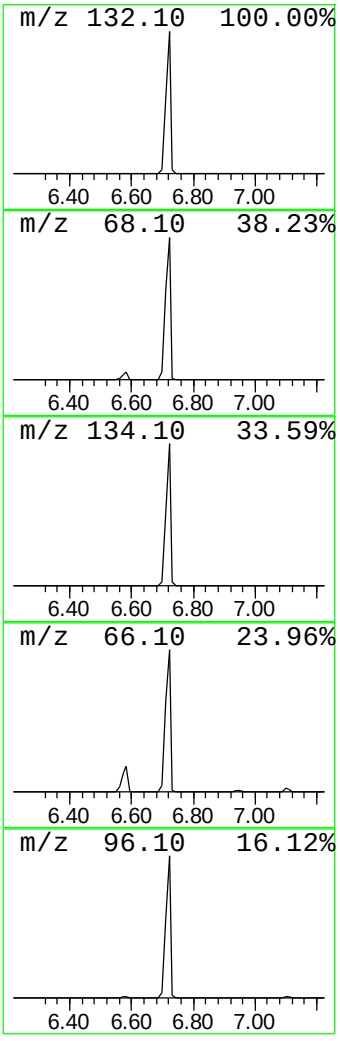
**********

Peak Number 5 unknown6.72 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.72 | 89.46 ng | 5114750 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 10 |



# Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HSR-WC-34-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

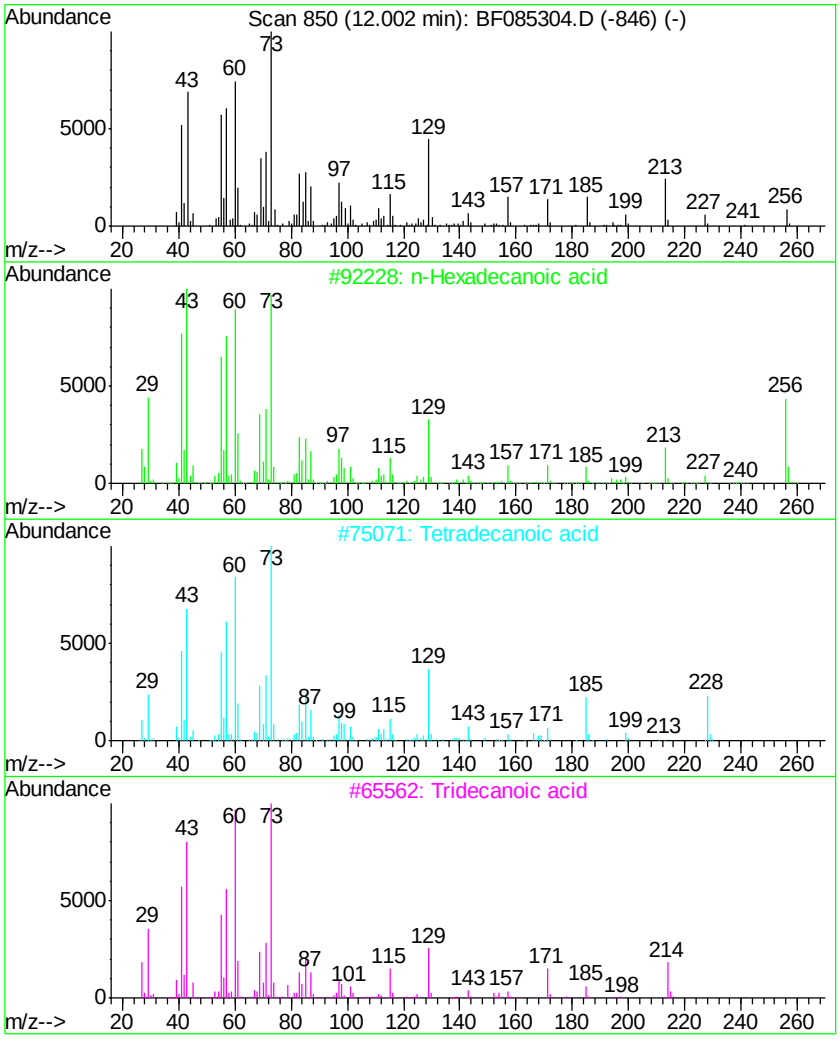
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

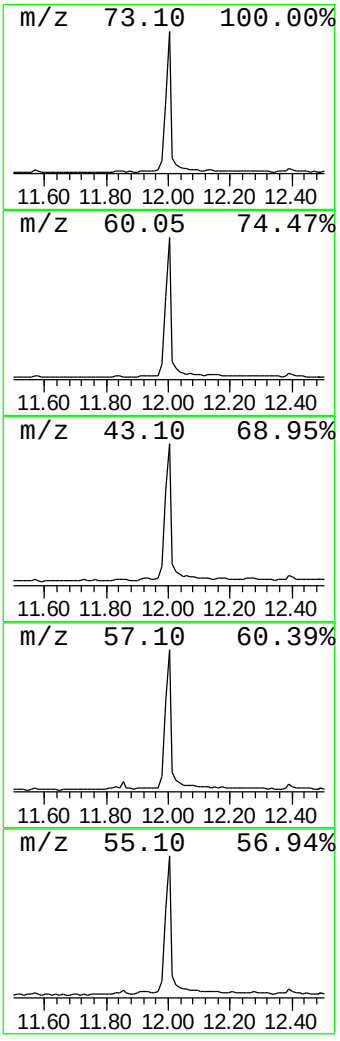
**********

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.00 | 10.37 ng | 887745 | Phenanthrene-d10 | 11.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 93 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 91 |
| 4 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 83 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 76 |



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Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
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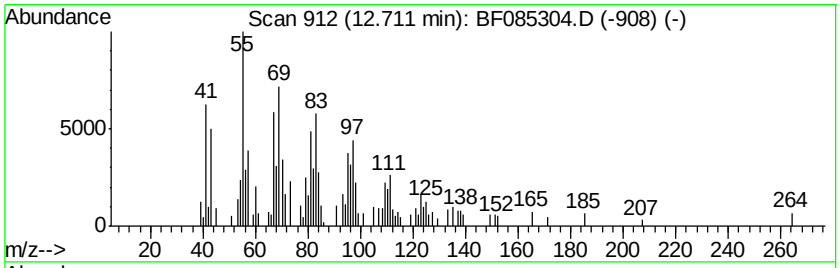
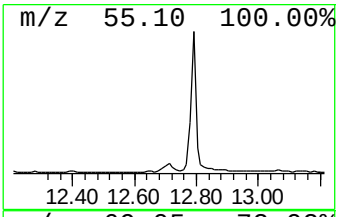
**********

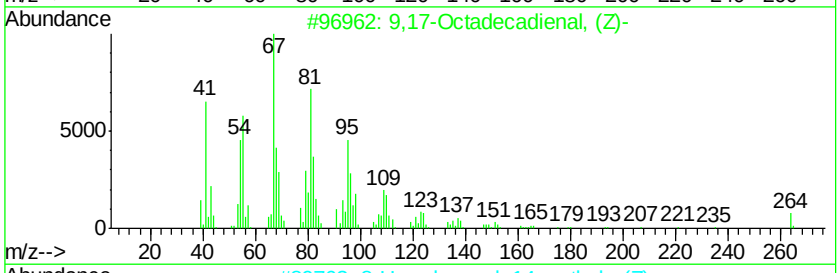
Peak Number 8 9,17-Octadecadienal, (Z)- Concentration Rank 8

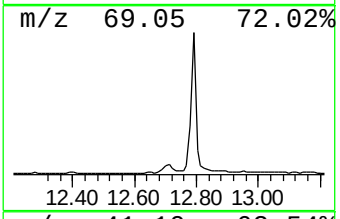
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.71 | 2.44 ng | 209232 | Phenanthrene-d10 | 11.48 |

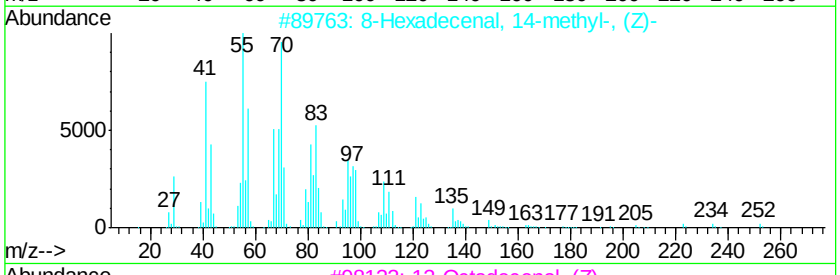
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,17-Octadecadienal, (Z)- | 264 | C18H32O | 056554-35-9 | 95 |
| 2 | 8-Hexadecenal, 14-methyl-, (Z)- | 252 | C17H32O | 060609-53-2 | 83 |
| 3 | 13-Octadecenal, (Z)- | 266 | C18H34O | 058594-45-9 | 58 |
| 4 | Oleic Acid | 282 | C18H34O2 | 000112-80-1 | 52 |
| 5 | 9-Hexadecenoic acid | 254 | C16H30O2 | 002091-29-4 | 52 |

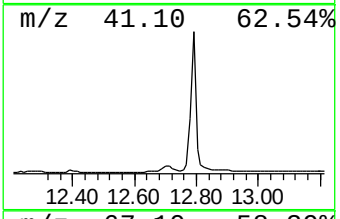


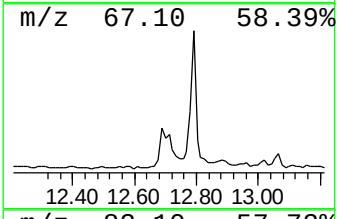



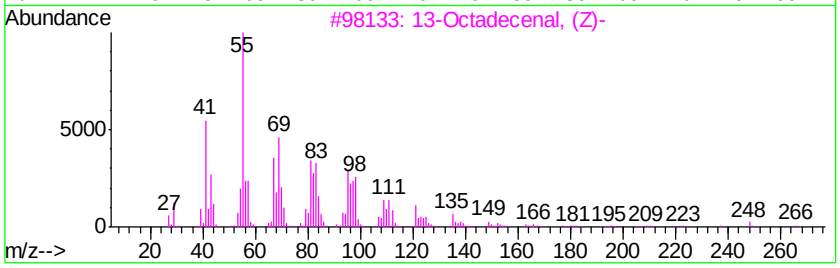



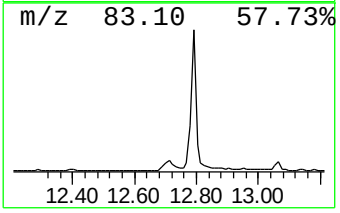



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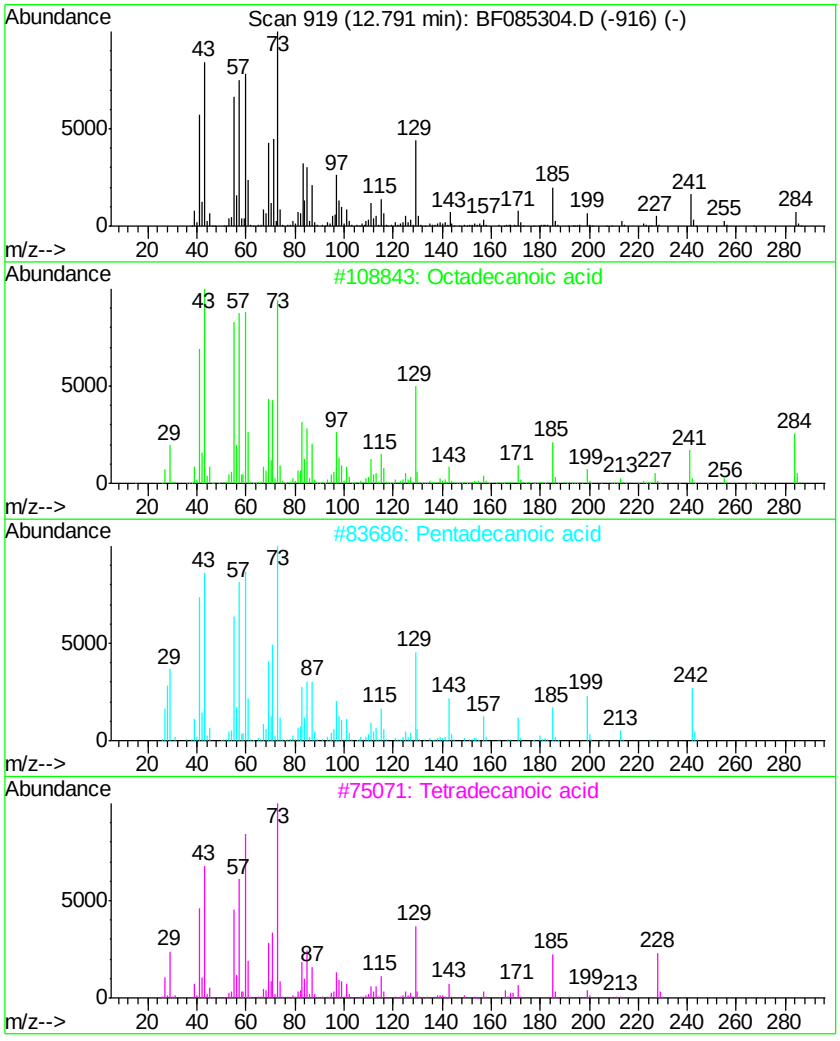
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

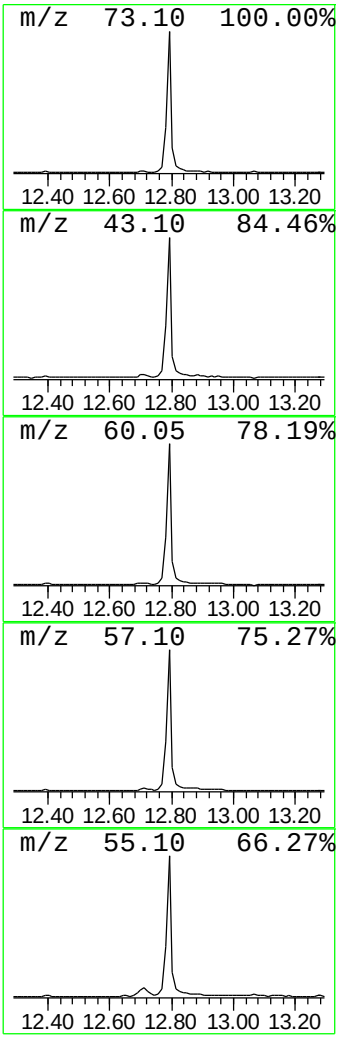
**********

Peak Number 9 Octadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.79 | 25.84 ng | 2212550 | Phenanthrene-d10 | 11.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 76 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 68 |



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 |
| n-Propyl acetate | 2.89 | 4.6 | ng | 262557 | 1 | 6.95 | 1143490 | 20.0 |
| 3-Penten-2-one, 4... | 4.54 | 2.3 | ng | 131934 | 1 | 6.95 | 1143490 | 20.0 |
| 2-Pentanone, 4-hy... | 5.17 | 27.2 | ng | 1556050 | 1 | 6.95 | 1143490 | 20.0 |
| unknown6.72 | 6.72 | 89.5 | ng | 5114750 | 1 | 6.95 | 1143490 | 20.0 |
| n-Hexadecanoic acid | 12.00 | 10.4 | ng | 887745 | 4 | 11.48 | 1712370 | 20.0 |
| 9,17-Octadecadien... | 12.71 | 2.4 | ng | 209232 | 4 | 11.48 | 1712370 | 20.0 |
| Octadecanoic acid | 12.79 | 25.8 | ng | 2212550 | 4 | 11.48 | 1712370 | 20.0 |