LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081721\
Data File : BP006701.D
Acq On : 17 Aug 2021 01:28
Operator : CG/JU
Sample : M3389-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** CRT-18

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_P\Methods\8270E-BP080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006701.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.858 | 297 | 301 | 309 | rVB | 137336 | 199808 | 2.73% | 0.474% |
| 2 | 5.305 | 371 | 377 | 385 | rBV | 2738069 | 3848293 | 52.57% | 9.122% |
| 3 | 6.887 | 639 | 646 | 660 | rVB | 2679450 | 4139187 | 56.55% | 9.812% |
| 4 | 7.705 | 779 | 785 | 793 | rVB | 755588 | 1187888 | 16.23% | 2.816% |
| 5 | 8.864 | 975 | 982 | 994 | rVB | 1702925 | 2713505 | 37.07% | 6.432% |
| 6 | 10.287 | 1219 | 1224 | 1235 | rBV | 62536 | 117862 | 1.61% | 0.279% |
| 7 | 10.487 | 1251 | 1258 | 1270 | rVB | 1078930 | 1733830 | 23.69% | 4.110% |
| 8 | 12.969 | 1672 | 1680 | 1694 | rBV | 3760919 | 5460839 | 74.60% | 12.945% |
| 9 | 14.346 | 1906 | 1914 | 1921 | rBV | 1459442 | 2103935 | 28.74% | 4.987% |
| 10 | 15.840 | 2158 | 2168 | 2182 | rBV | 2976549 | 4036899 | 55.15% | 9.569% |
| 11 | 17.098 | 2376 | 2382 | 2387 | rBV | 1648878 | 2371546 | 32.40% | 5.622% |
| 12 | 17.140 | 2387 | 2389 | 2396 | rVB | 71140 | 92685 | 1.27% | 0.220% |
| 13 | 18.016 | 2533 | 2538 | 2547 | rBV2 | 312404 | 455192 | 6.22% | 1.079% |
| 14 | 19.122 | 2720 | 2726 | 2734 | rBV | 144426 | 231489 | 3.16% | 0.549% |
| 15 | 19.251 | 2744 | 2748 | 2756 | rBV | 253515 | 352652 | 4.82% | 0.836% |
| 16 | 19.475 | 2778 | 2786 | 2789 | rBV | 133810 | 198169 | 2.71% | 0.470% |
| 17 | 19.681 | 2816 | 2821 | 2827 | rBV | 6361746 | 7319912 | 100.00% | 17.352% |
| 18 | 20.933 | 3031 | 3034 | 3040 | rBV | 240805 | 340825 | 4.66% | 0.808% |
| 19 | 21.204 | 3075 | 3080 | 3084 | rBV | 2124207 | 2602569 | 35.55% | 6.169% |
| 20 | 21.369 | 3106 | 3108 | 3113 | rVB | 95081 | 87552 | 1.20% | 0.208% |
| 21 | 23.516 | 3467 | 3473 | 3481 | rVB2 | 1378207 | 2591201 | 35.40% | 6.142% |

Sum of corrected areas: 42185838

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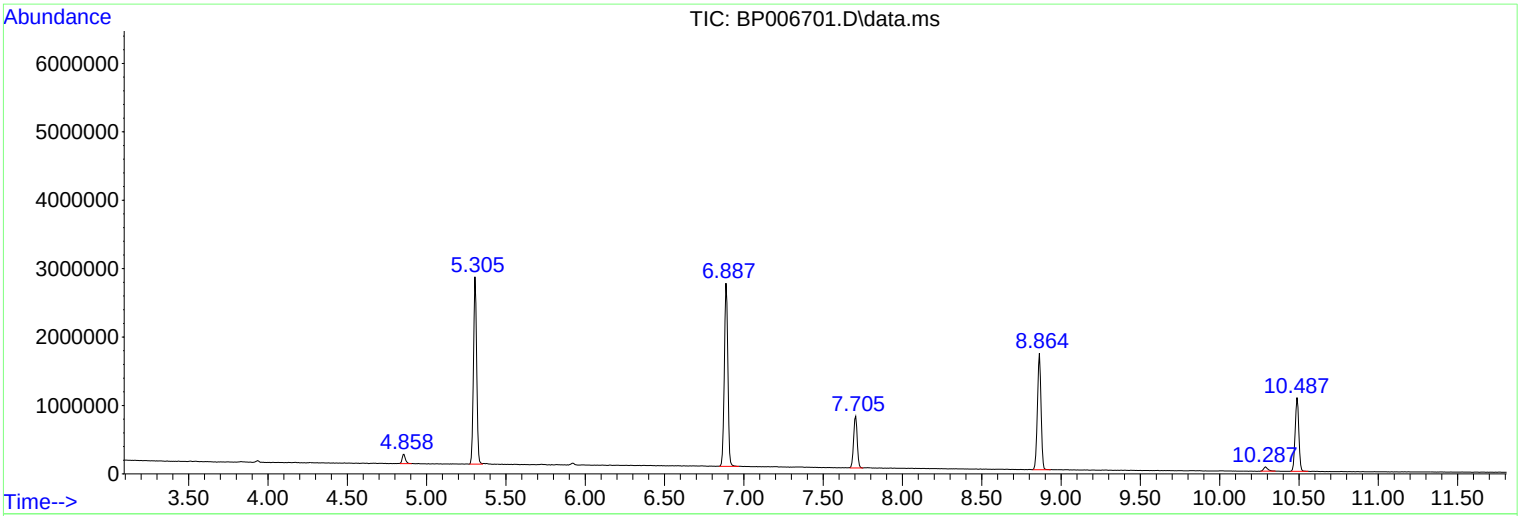
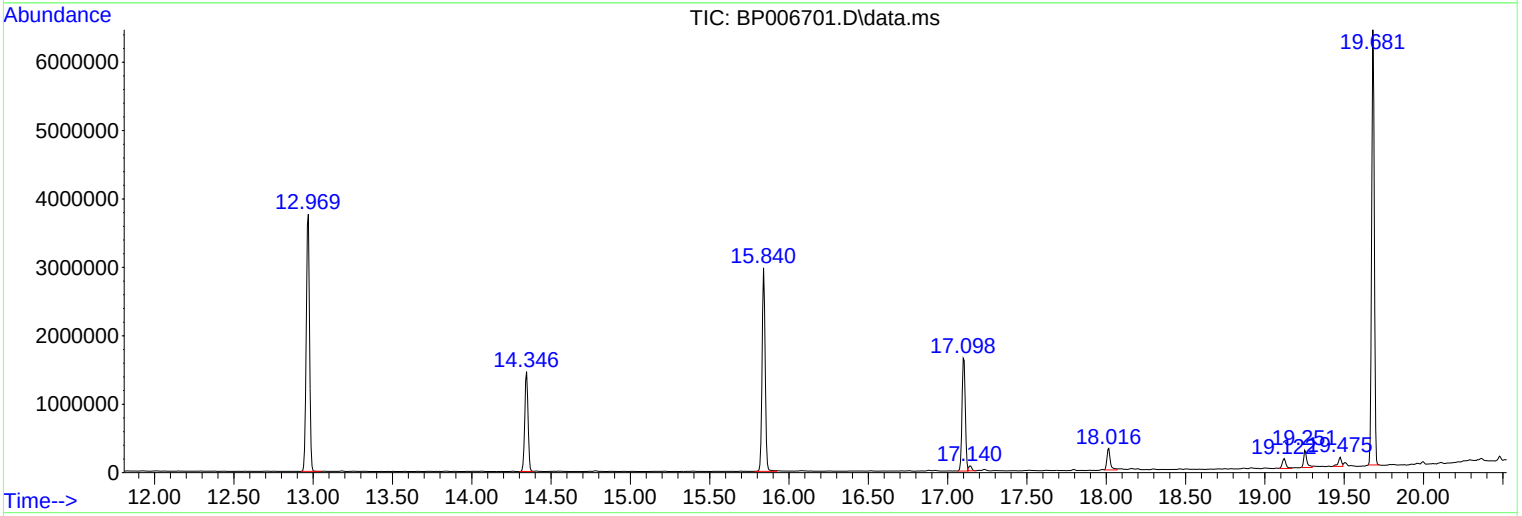
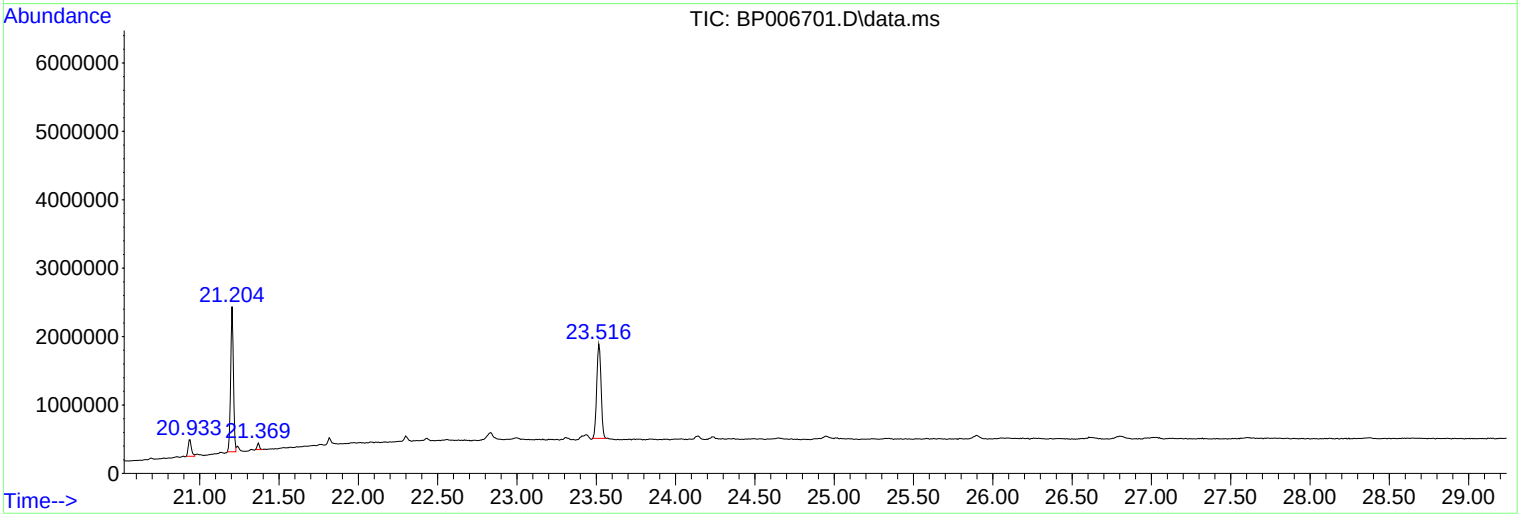
BNA_P
**ClientSampleId :**
CRT-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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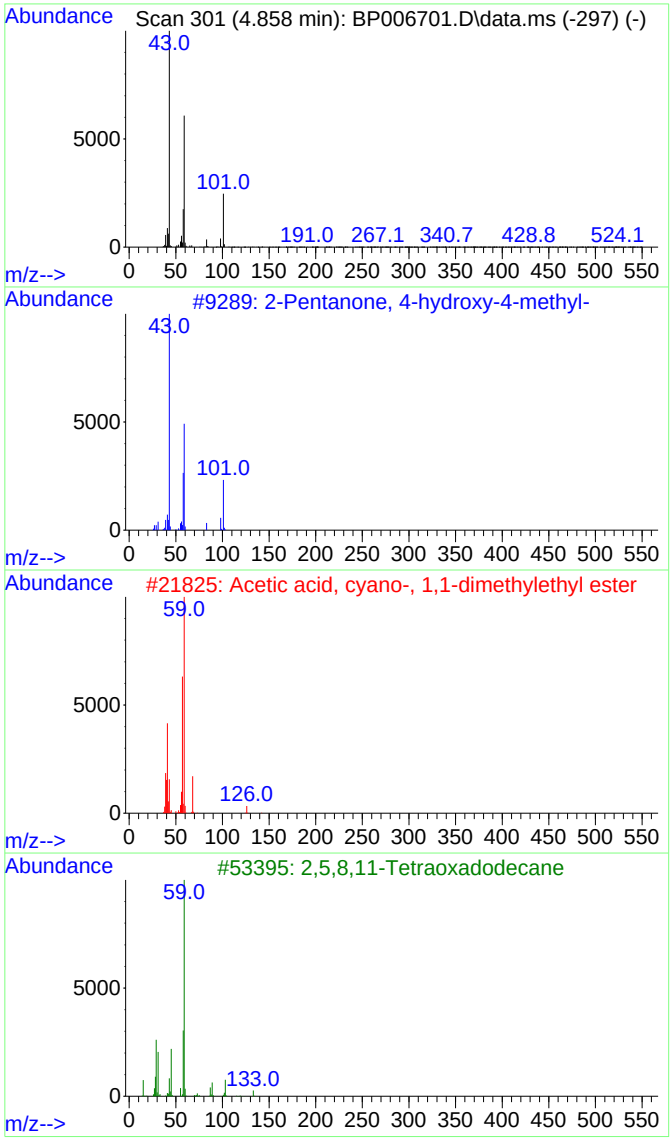
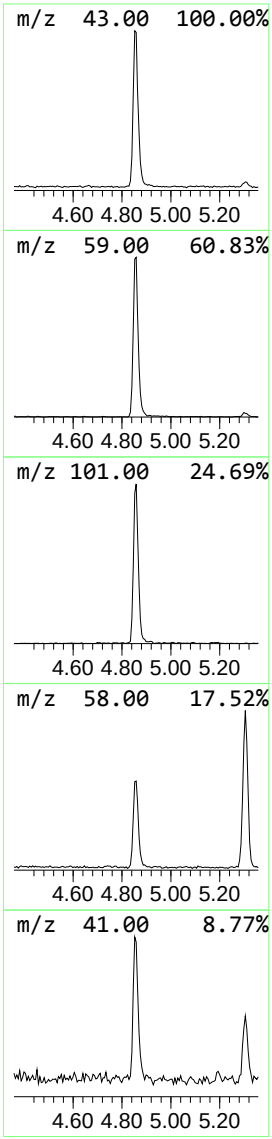
**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.858 | 3.36 ng | 199808 | 1,4-Dichlorobenzene-d4 | 7.705 |

| 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 | 2,5,8,11-Tetraoxadodecane | 178 | C8H18O4 | 000112-49-2 | 17 |
| 4 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 12 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



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BNA_P
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CRT-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
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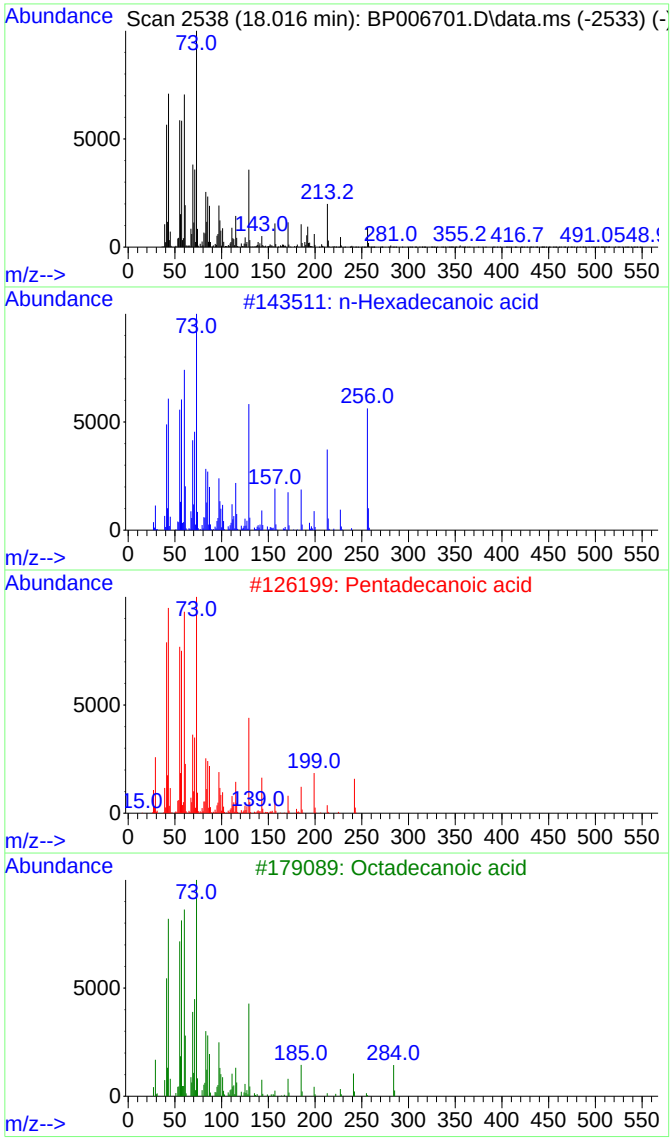
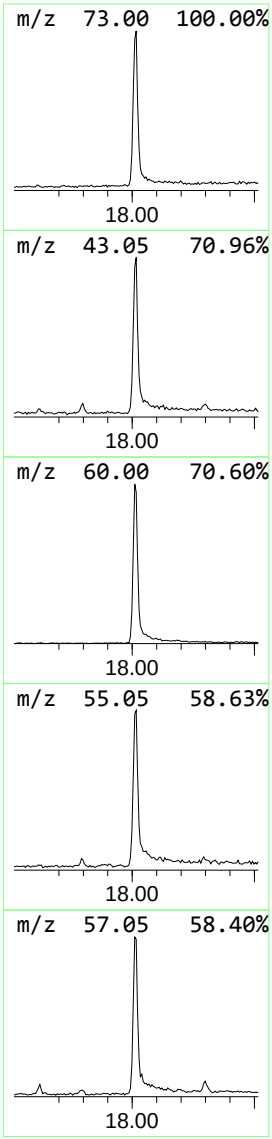
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.016 | 3.84 ng | 455192 | Phenanthrene-d10 | 17.098 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 81 |
| 4 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 49 |
| 5 | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 46 |



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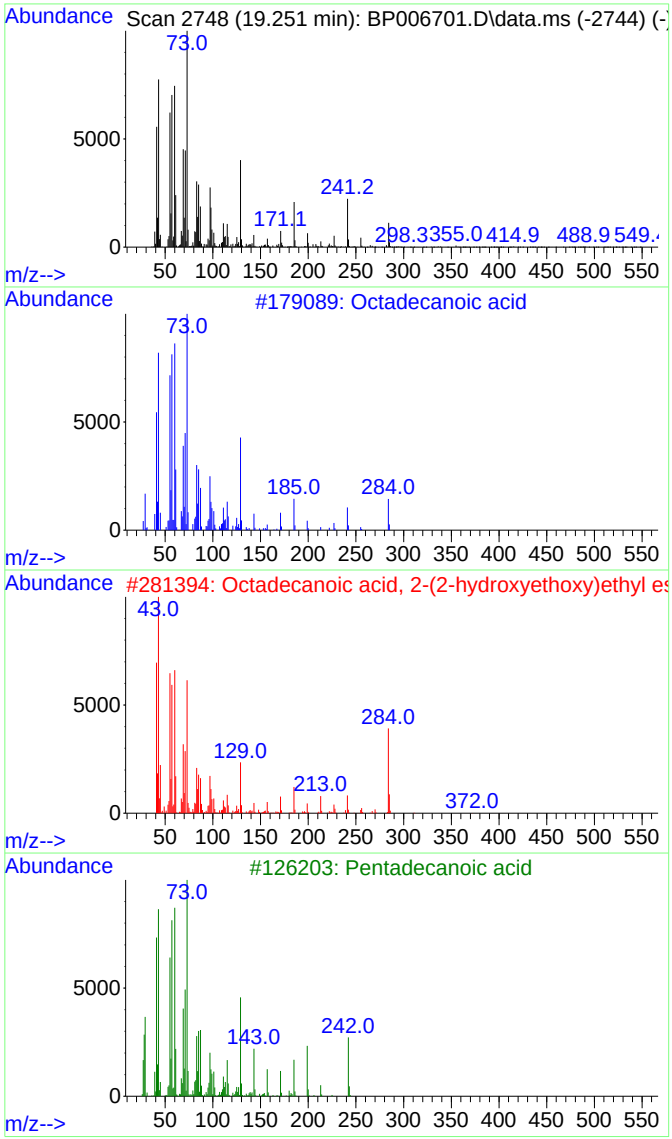
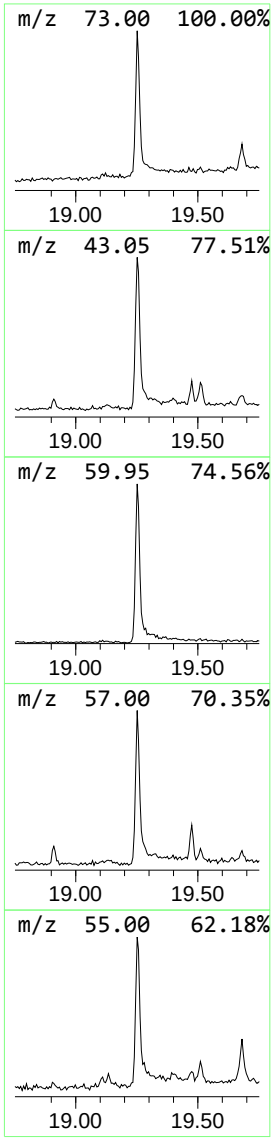
**********

Peak Number 3 Octadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.251 | 2.71 ng | 352652 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 90 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 72 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 58 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |



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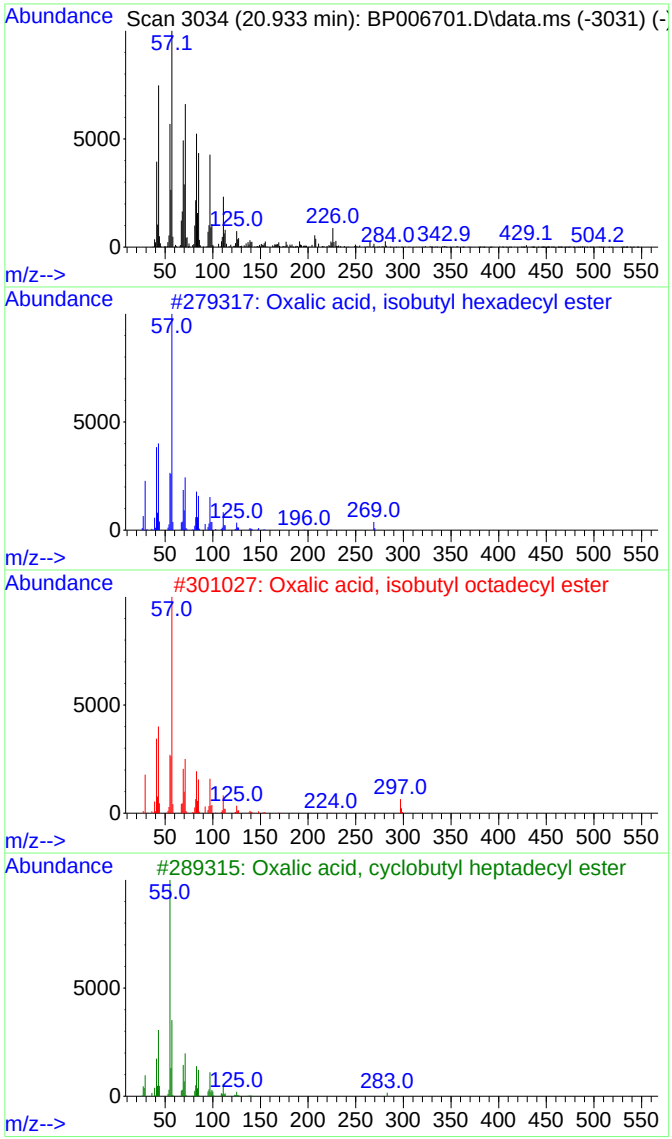
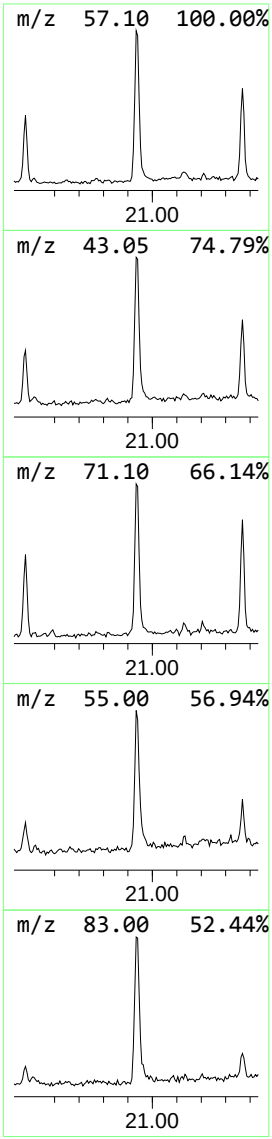
**********
Peak Number 4 Oxalic acid, isobutyl hexad... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.933 | 2.62 ng | 340825 | Chrysene-d12 | 21.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4 | 1000309-38-1 | 91 |
| 2 | Oxalic acid, isobutyl octadecyl ... | 398 | C24H46O4 | 1000309-38-3 | 91 |
| 3 | Oxalic acid, cyclobutyl heptadec... | 382 | C23H42O4 | 1000309-70-7 | 91 |
| 4 | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 87 |
| 5 | Pentadecafluorooctanoic acid, he... | 638 | C24H33F15O2 | 1000406-04-6 | 76 |



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-... | 4.858 | 3.4 | ng | 199808 | 1 | 7.705 | 1187890 | 20.0 |
| n-Hexadecanoic ... | 18.016 | 3.8 | ng | 455192 | 4 | 17.098 | 2371550 | 20.0 |
| Octadecanoic acid | 19.251 | 2.7 | ng | 352652 | 5 | 21.204 | 2602570 | 20.0 |
| Oxalic acid, is... | 20.933 | 2.6 | ng | 340825 | 5 | 21.204 | 2602570 | 20.0 |