LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110921\
Data File : BP007887.D
Acq On : 09 Nov 2021 12:33
Operator : CG/JU
Sample : M4540-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
TP-6

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-BP110221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007887.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.452 | 361 | 368 | 381 | rBV | 2875131 | 4132800 | 49.45% | 10.325% |
| 2 | 7.040 | 630 | 638 | 649 | rBV | 2491027 | 4016143 | 48.05% | 10.033% |
| 3 | 7.863 | 771 | 778 | 786 | rBV | 481472 | 754259 | 9.02% | 1.884% |
| 4 | 9.022 | 967 | 975 | 985 | rBV | 1451376 | 2434159 | 29.13% | 6.081% |
| 5 | 10.446 | 1210 | 1217 | 1228 | rBV | 263126 | 421753 | 5.05% | 1.054% |
| 6 | 10.663 | 1246 | 1254 | 1263 | rBV | 567758 | 946321 | 11.32% | 2.364% |
| 7 | 13.122 | 1665 | 1672 | 1681 | rBV | 3679576 | 5321004 | 63.67% | 13.293% |
| 8 | 14.498 | 1899 | 1906 | 1914 | rVB | 847698 | 1217313 | 14.57% | 3.041% |
| 9 | 15.992 | 2153 | 2160 | 2181 | rVB | 3121448 | 4608494 | 55.14% | 11.513% |
| 10 | 17.251 | 2368 | 2374 | 2381 | rBV | 1044215 | 1495522 | 17.89% | 3.736% |
| 11 | 17.375 | 2389 | 2395 | 2401 | rVB5 | 65242 | 102291 | 1.22% | 0.256% |
| 12 | 18.151 | 2522 | 2527 | 2534 | rBV | 305090 | 436665 | 5.22% | 1.091% |
| 13 | 19.380 | 2733 | 2736 | 2745 | rBV | 124459 | 192323 | 2.30% | 0.480% |
| 14 | 19.816 | 2805 | 2810 | 2819 | rVB | 6886859 | 8357477 | 100.00% | 20.879% |
| 15 | 20.451 | 2914 | 2918 | 2922 | rBV | 523139 | 608500 | 7.28% | 1.520% |
| 16 | 20.569 | 2934 | 2938 | 2948 | rBV | 346503 | 408832 | 4.89% | 1.021% |
| 17 | 21.057 | 3018 | 3021 | 3030 | rBV | 356919 | 452318 | 5.41% | 1.130% |
| 18 | 21.345 | 3065 | 3070 | 3075 | rBV | 1508005 | 1963517 | 23.49% | 4.905% |
| 19 | 23.763 | 3475 | 3481 | 3489 | rVB2 | 1057712 | 2158276 | 25.82% | 5.392% |

Sum of corrected areas: 40027967

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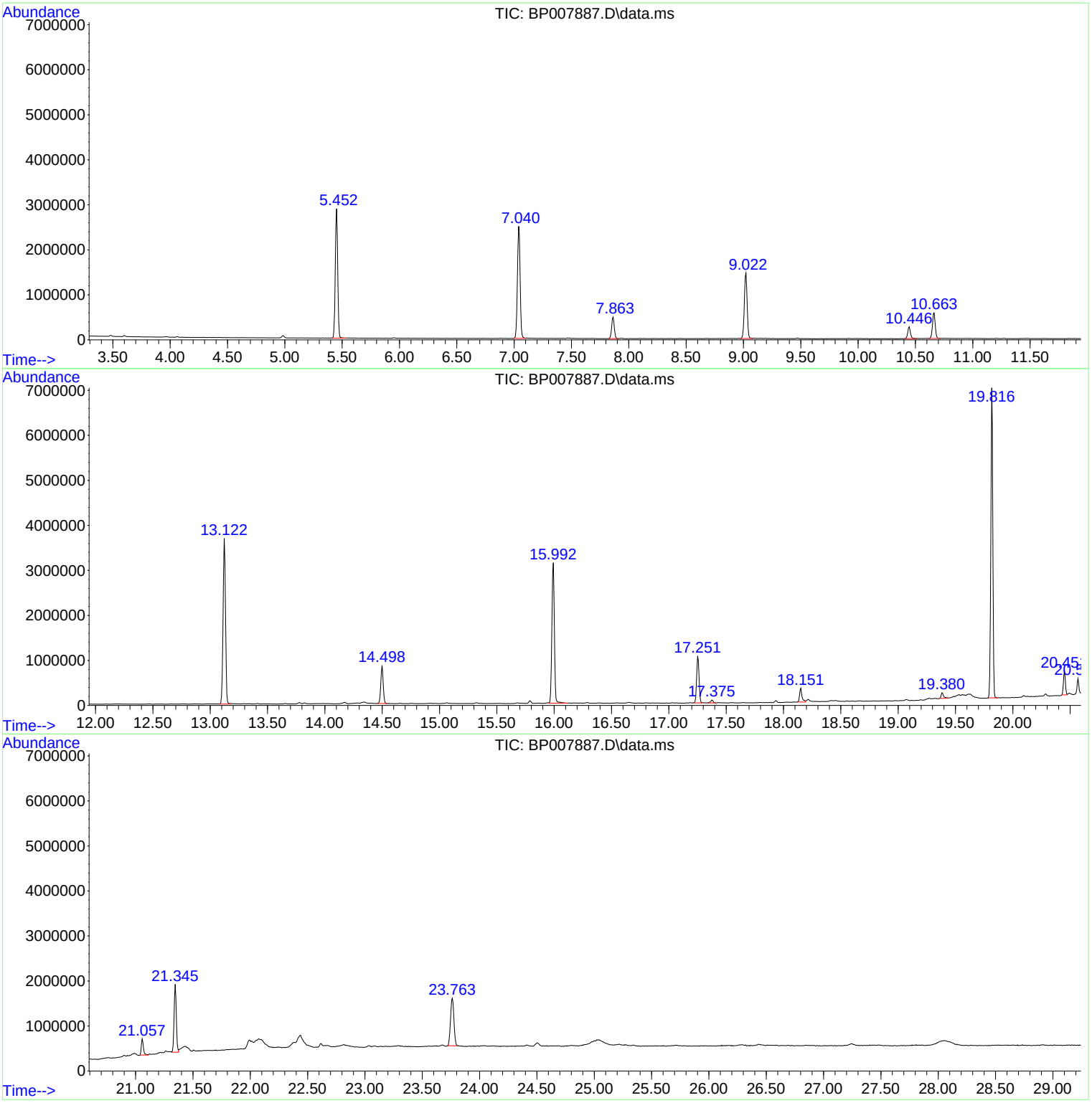
**Instrument :**
BNA_P
**ClientSampleId :**
TP-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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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Data File : BP007887.D
Acq On : 09 Nov 2021 12:33
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**Instrument :**
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
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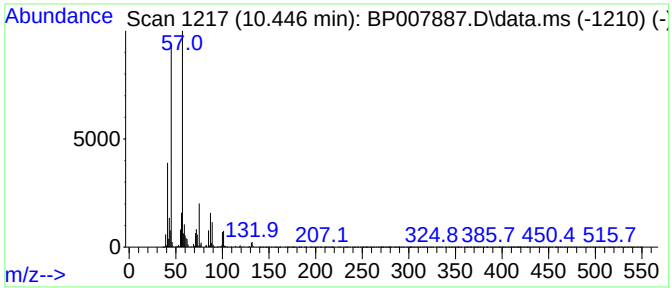
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

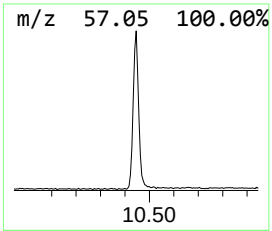
**********

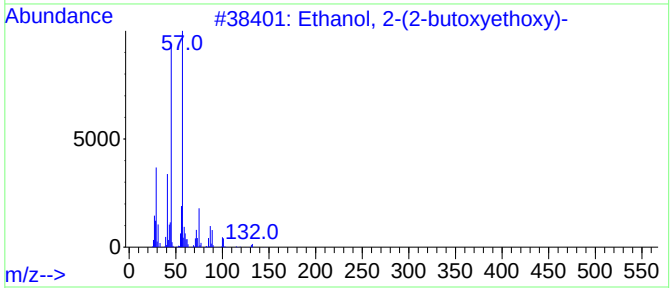
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

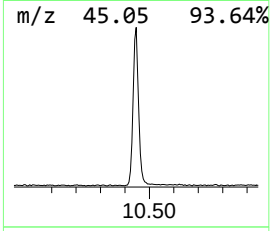
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.446 | 8.91 ng | 421753 | Naphthalene-d8 | 10.663 |

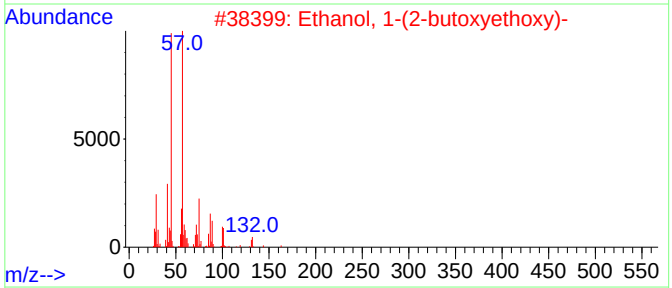
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 90 |
| 2 | Ethanol, 1-(2-butoxyethoxy)- | 162 | C8H18O3 | 054446-78-5 | 83 |
| 3 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 64 |
| 4 | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 64 |
| 5 | Di-sec-Butyl ether | 130 | C8H18O | 006863-58-7 | 50 |

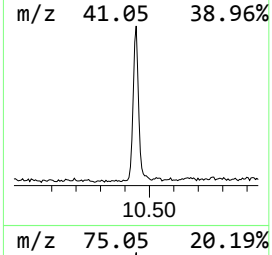


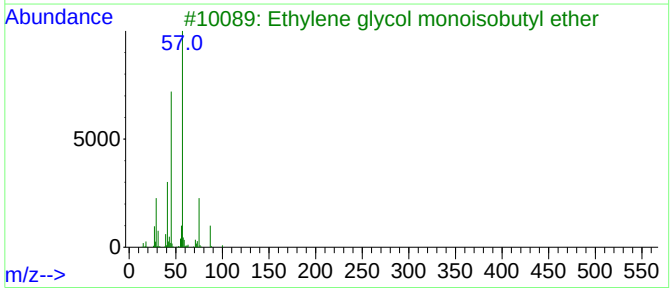



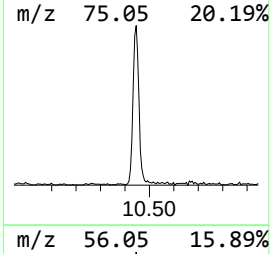



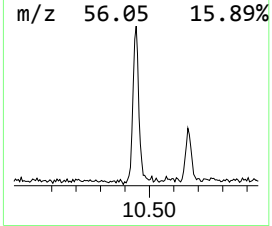



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ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
TP-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

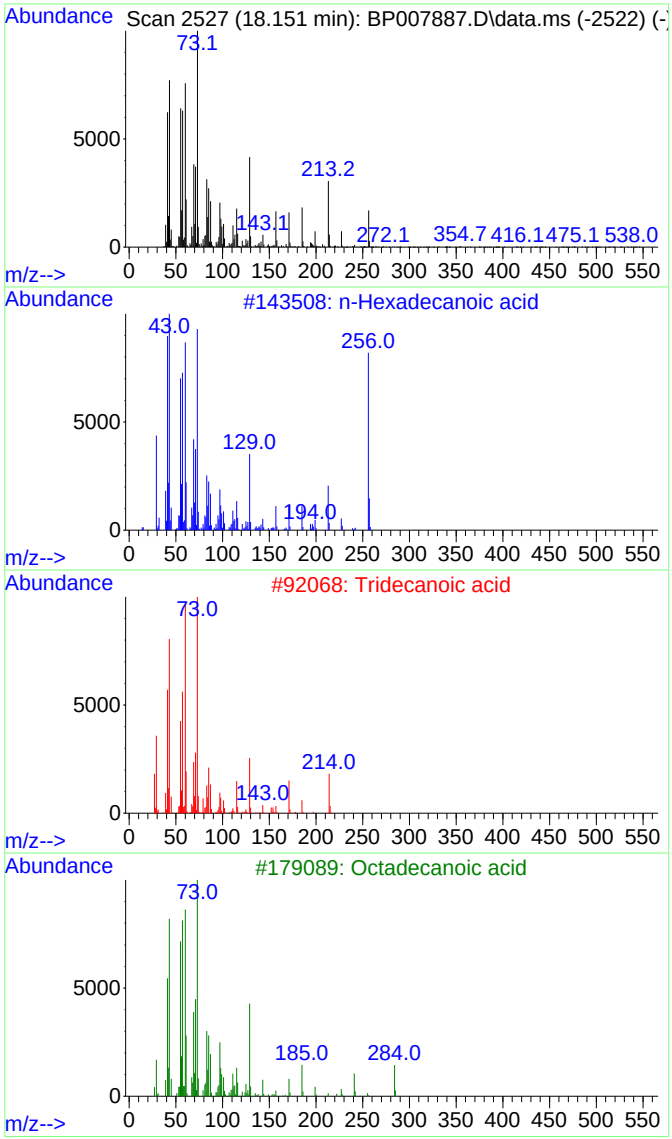
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

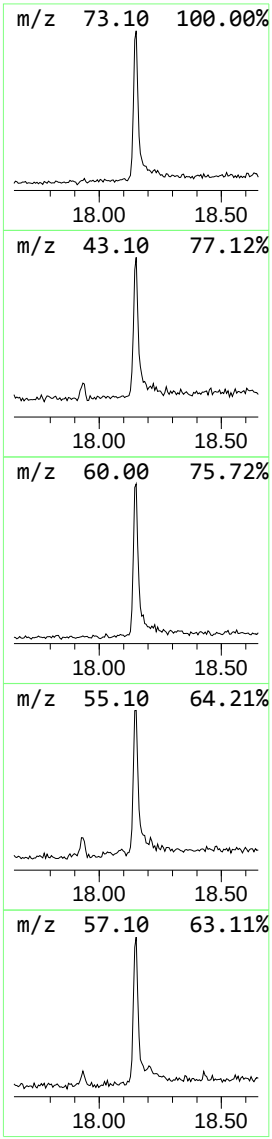
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.151 | 5.84 ng | 436665 | Phenanthrene-d10 | 17.251 |

| 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 | 89 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 87 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 83 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |



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Data File : BP007887.D
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Sample : M4540-11
Misc :
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**Instrument :**
BNA_P
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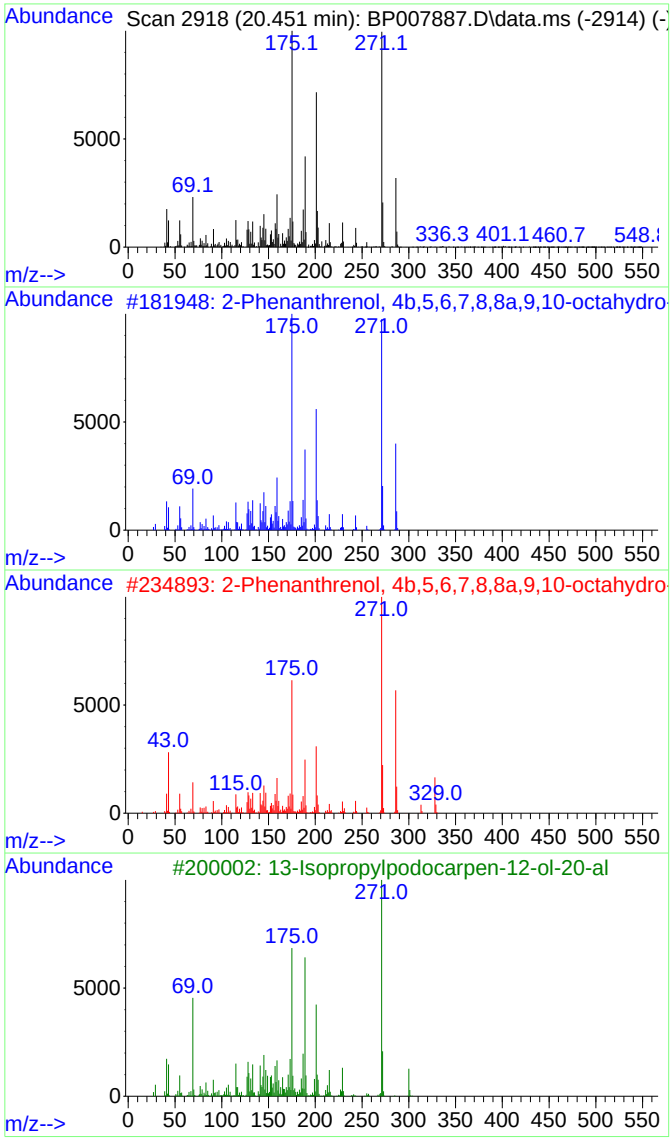
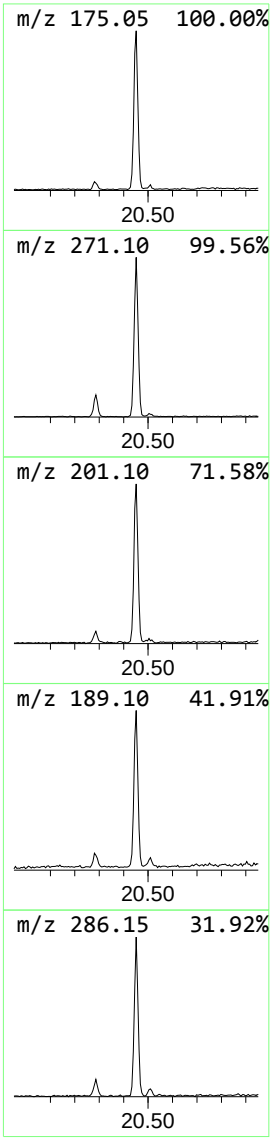
**********
Peak Number 3 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.451 | 6.20 ng | 608500 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Phenanthrenol, 4b,5,6,7,8,8a,9... | 286 | C20H30O | 000511-15-9 | 99 |
| 2 | 2-Phenanthrenol, 4b,5,6,7,8,8a,9... | 328 | C22H32O2 | 015340-82-6 | 91 |
| 3 | 13-Isopropylpodocarpen-12-ol-20-al | 300 | C20H28O2 | 024035-37-8 | 49 |
| 4 | Pisiferol | 302 | C20H30O2 | 024035-36-7 | 49 |
| 5 | 5-Androstene, 4,4-dimethyl- | 286 | C21H34 | 1000194-15-4 | 35 |



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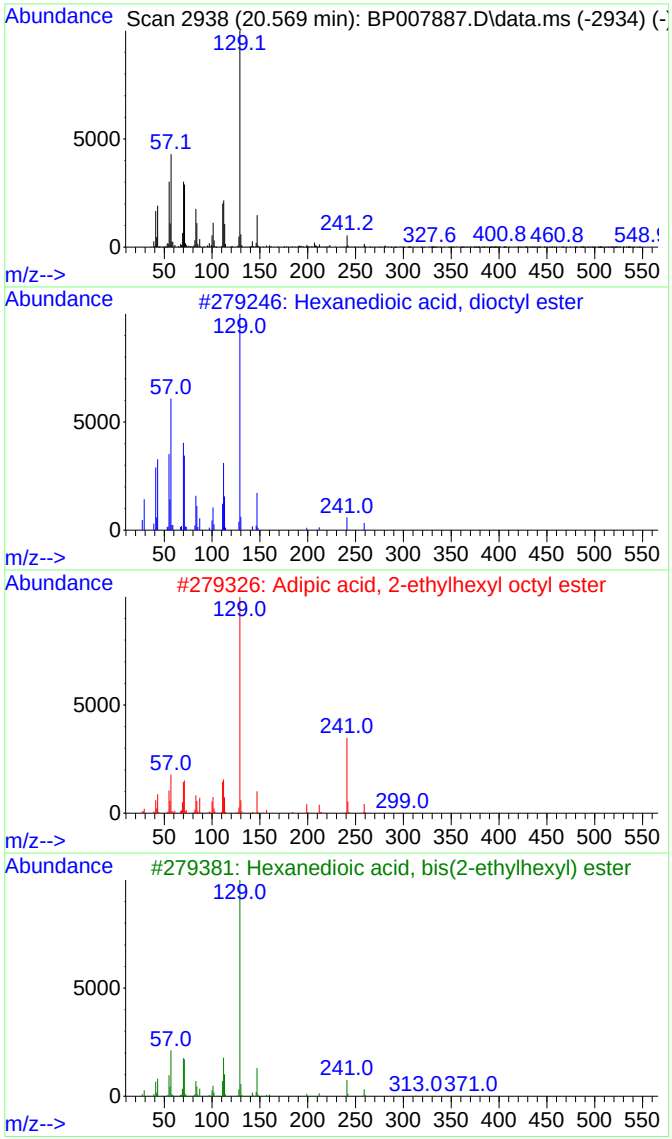
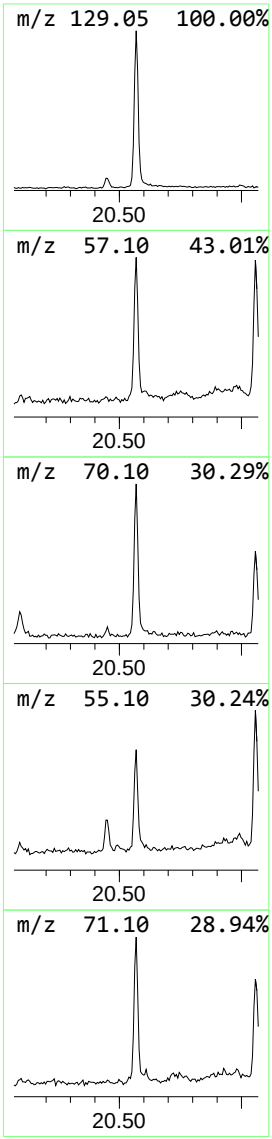
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Hexanedioic acid, dioctyl e... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.569 | 4.16 ng | 408832 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanedioic acid, dioctyl ester | 370 | C22H42O4 | 000123-79-5 | 90 |
| 2 | Adipic acid, 2-ethylhexyl octyl ... | 370 | C22H42O4 | 1000324-48-6 | 90 |
| 3 | Hexanedioic acid, bis(2-ethylhex... | 370 | C22H42O4 | 000103-23-1 | 87 |
| 4 | Adipic acid, 2-ethylhexyl isobut... | 314 | C18H34O4 | 1010324-48-0 | 64 |
| 5 | Hexanedioic acid, mono(2-ethylhe... | 258 | C14H26O4 | 004337-65-9 | 50 |



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Sample : M4540-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_P
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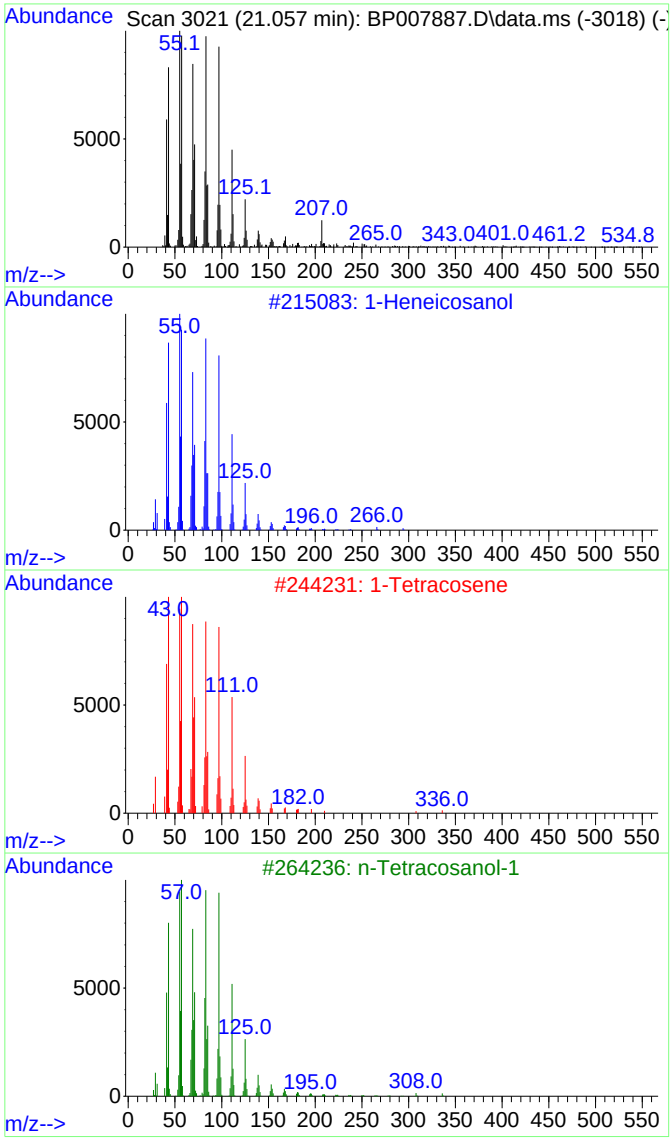
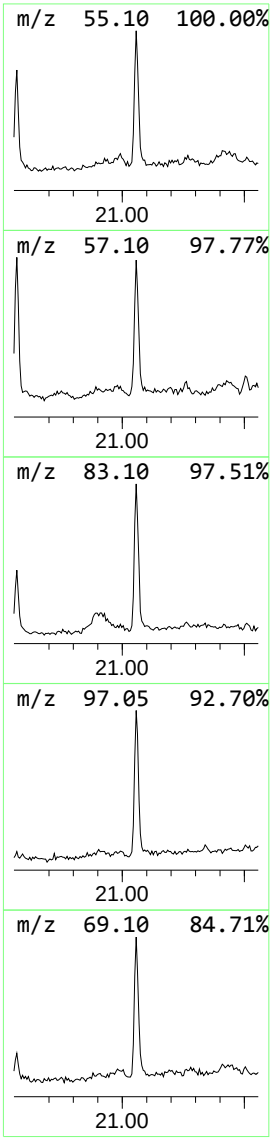
**********

Peak Number 5 1-Heneicosanol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.057 | 4.61 ng | 452318 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 2 | 1-Tetracosene | 336 | C24H48 | 010192-32-2 | 95 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 94 |
| 5 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 94 |



Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
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**ClientSampleId :**
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TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Ethanol, 2-(2-b... | 10.446 | 8.9 | ng | 421753 | 2 | 10.663 | 946321 | 20.0 |
| n-Hexadecanoic ... | 18.151 | 5.8 | ng | 436665 | 4 | 17.251 | 1495520 | 20.0 |
| 2-Phenanthrenol... | 20.451 | 6.2 | ng | 608500 | 5 | 21.345 | 1963520 | 20.0 |
| Hexanedioic aci... | 20.569 | 4.2 | ng | 408832 | 5 | 21.345 | 1963520 | 20.0 |
| 1-Heneicosanol | 21.057 | 4.6 | ng | 452318 | 5 | 21.345 | 1963520 | 20.0 |