LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009055.D
Acq On : 08 Feb 2022 13:17
Operator : CG/JU
Sample : N1362-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RO-341

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-BP020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009055.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.017 | 3 | 5 | 16 | rVB | 239021 | 264435 | 1.30% | 0.395% |
| 2 | 3.570 | 91 | 99 | 120 | rBV | 2117453 | 3568686 | 17.56% | 5.330% |
| 3 | 5.393 | 403 | 409 | 428 | rBV | 1920455 | 3113236 | 15.32% | 4.650% |
| 4 | 6.987 | 673 | 680 | 703 | rBV | 1799295 | 3255966 | 16.02% | 4.863% |
| 5 | 7.805 | 803 | 819 | 828 | rBV | 684493 | 1117511 | 5.50% | 1.669% |
| 6 | 8.963 | 1009 | 1016 | 1036 | rBV | 1216802 | 2168208 | 10.67% | 3.238% |
| 7 | 10.604 | 1287 | 1295 | 1310 | rBV | 890635 | 1581231 | 7.78% | 2.362% |
| 8 | 13.069 | 1707 | 1714 | 1729 | rBV | 3612090 | 5385745 | 26.51% | 8.044% |
| 9 | 14.445 | 1938 | 1948 | 1963 | rBV | 1177920 | 1869424 | 9.20% | 2.792% |
| 10 | 15.945 | 2196 | 2203 | 2216 | rBV | 2140489 | 3204614 | 15.77% | 4.786% |
| 11 | 17.204 | 2411 | 2417 | 2422 | rBV | 1263802 | 1832949 | 9.02% | 2.738% |
| 12 | 18.104 | 2563 | 2570 | 2584 | rBV2 | 985553 | 1668621 | 8.21% | 2.492% |
| 13 | 18.928 | 2706 | 2710 | 2720 | rBV | 2212386 | 3514040 | 17.29% | 5.249% |
| 14 | 19.222 | 2754 | 2760 | 2773 | rBV | 393596 | 700493 | 3.45% | 1.046% |
| 15 | 19.339 | 2775 | 2780 | 2796 | rBV | 1858273 | 2810056 | 13.83% | 4.197% |
| 16 | 19.575 | 2816 | 2820 | 2829 | rVB | 302031 | 462300 | 2.28% | 0.690% |
| 17 | 19.769 | 2848 | 2853 | 2861 | rVB | 4045953 | 4938317 | 24.30% | 7.376% |
| 18 | 21.016 | 3062 | 3065 | 3073 | rVB3 | 274698 | 442192 | 2.18% | 0.660% |
| 19 | 21.298 | 3108 | 3113 | 3118 | rBV | 1540966 | 2342437 | 11.53% | 3.499% |
| 20 | 21.422 | 3128 | 3134 | 3157 | rBV | 13343038 | 20318362 | 100.00% | 30.348% |
| 21 | 23.704 | 3516 | 3522 | 3529 | rVB2 | 1229859 | 2393008 | 11.78% | 3.574% |

Sum of corrected areas: 66951831

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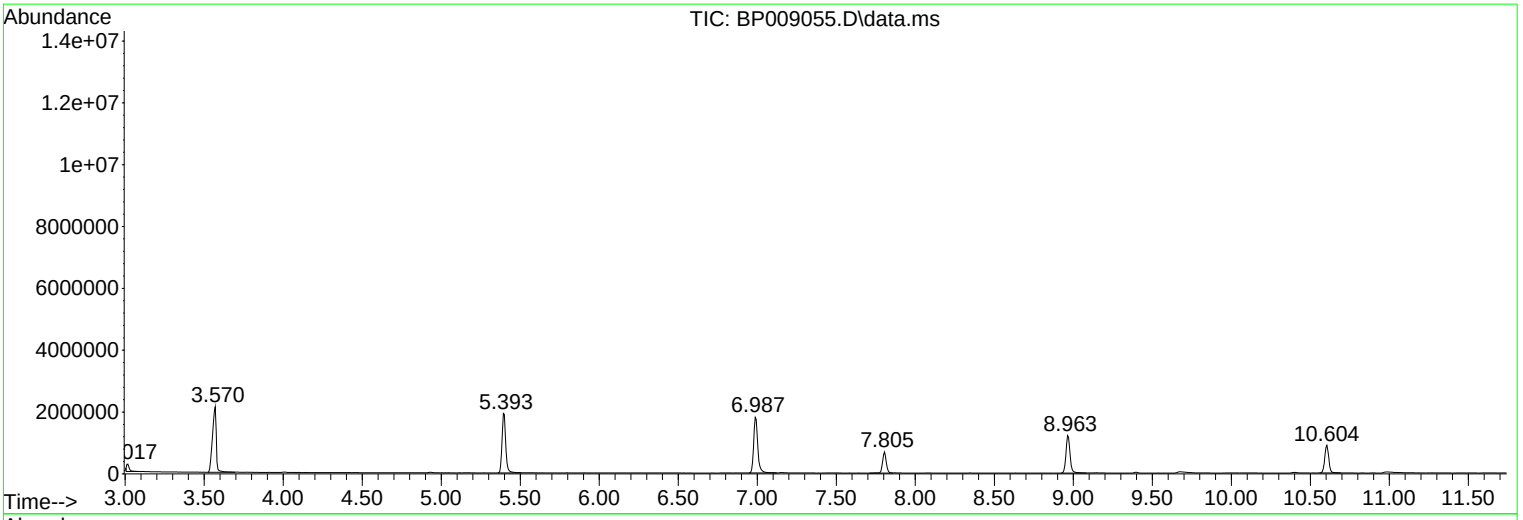
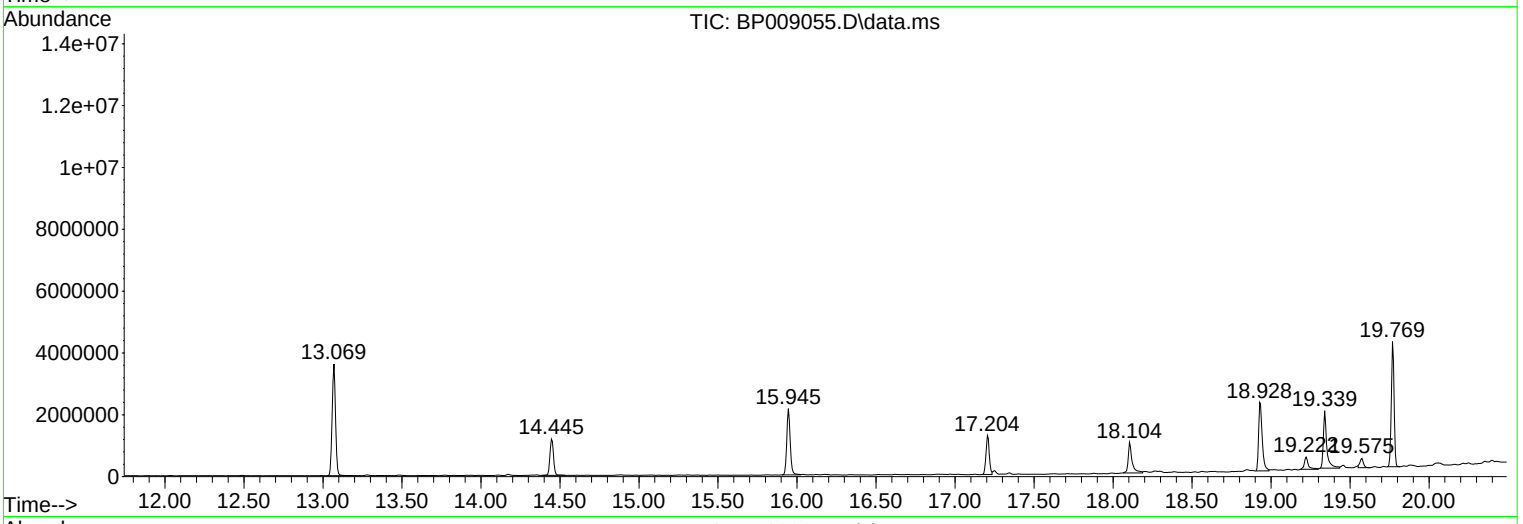
Misc :
ALS Vial : 5 Sample Multiplier: 1

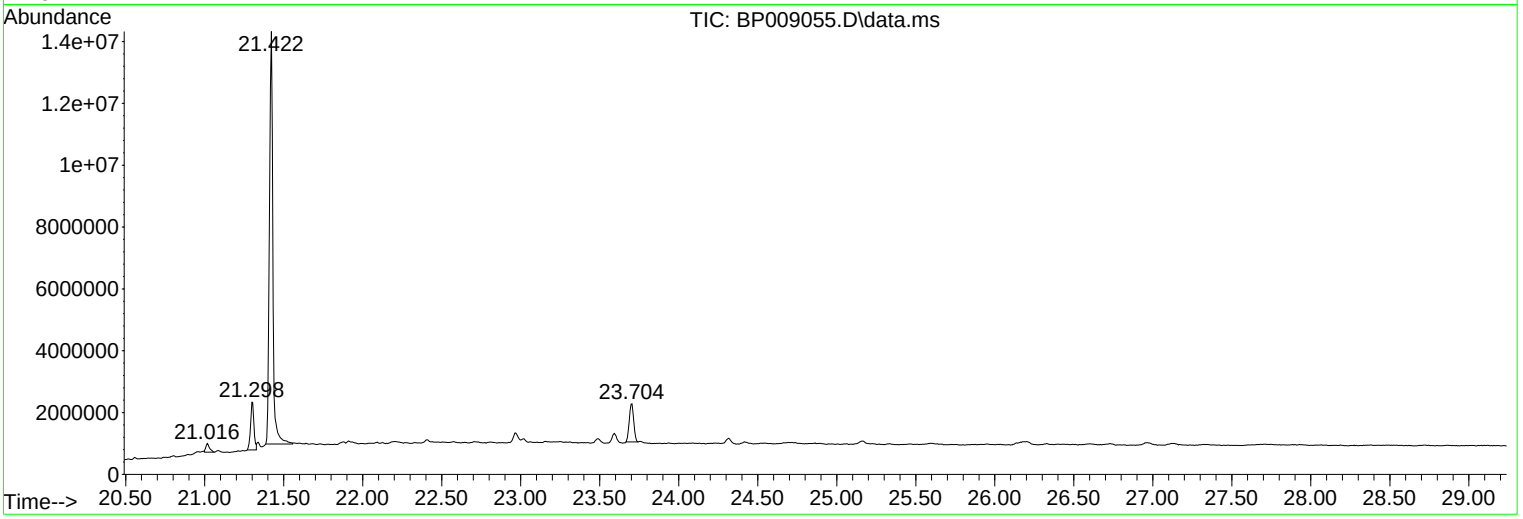
**Instrument :**
BNA_P
**ClientSampleId :**
RO-341

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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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**Instrument :**
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

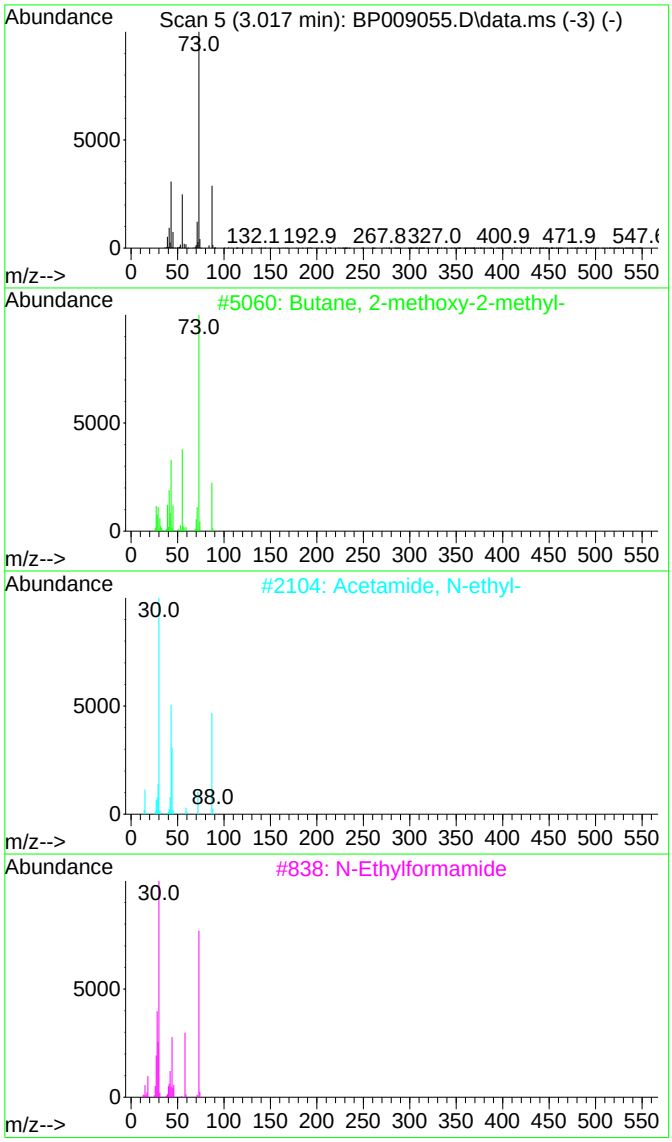
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

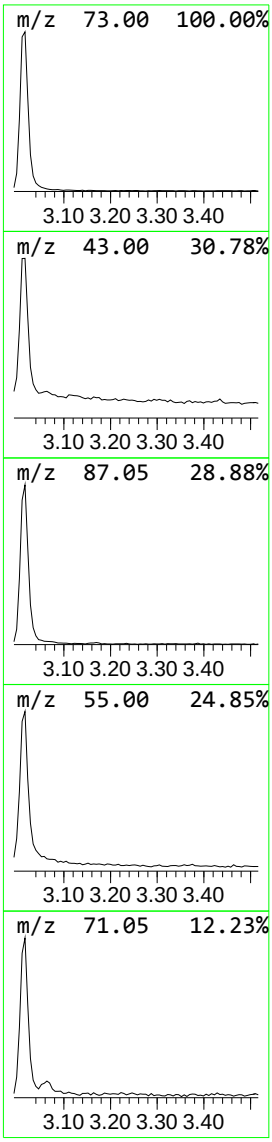
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.017 | 4.73 ng | 264435 | 1,4-Dichlorobenzene-d4 | 7.805 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 10 |
| 3 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 5 | Acetamide, N-(2-hydroxy-3-penten... | 143 | C7H13NO2 | 093393-95-4 | 9 |



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Data File : BP009055.D
Acq On : 08 Feb 2022 13:17
Operator : CG/JU
Sample : N1362-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RO-341

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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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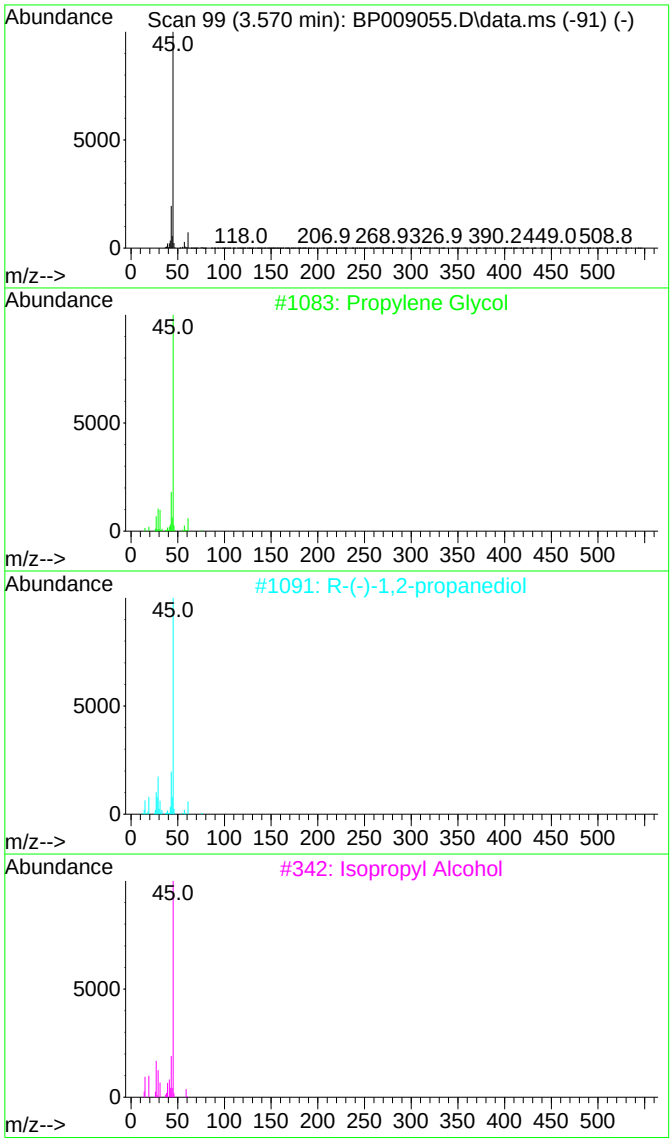
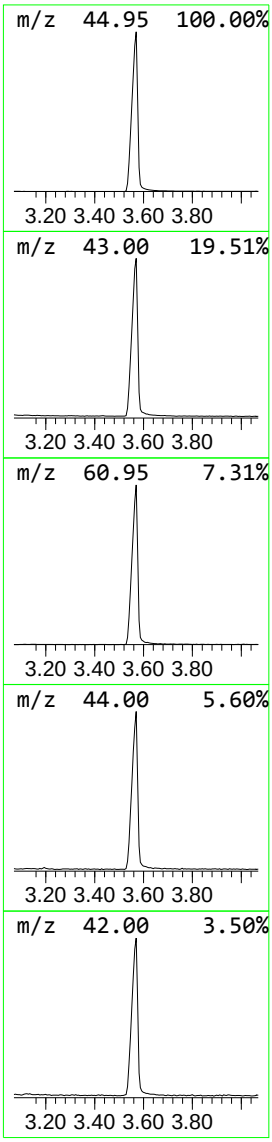
Peak Number 2 Propylene Glycol Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.570 | 63.87 ng | 3568690 | 1,4-Dichlorobenzene-d4 | 7.805 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propylene Glycol | 76 | C3H8O2 | 000057-55-6 | 90 |
| 2 | R-(-)-1,2-propanediol | 76 | C3H8O2 | 004254-14-2 | 78 |
| 3 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 56 |
| 4 | Propanoic acid, 2-hydroxy-, meth... | 104 | C4H8O3 | 000547-64-8 | 40 |
| 5 | 2-Butanol | 74 | C4H10O | 000078-92-2 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009055.D
Acq On : 08 Feb 2022 13:17
Operator : CG/JU
Sample : N1362-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RO-341

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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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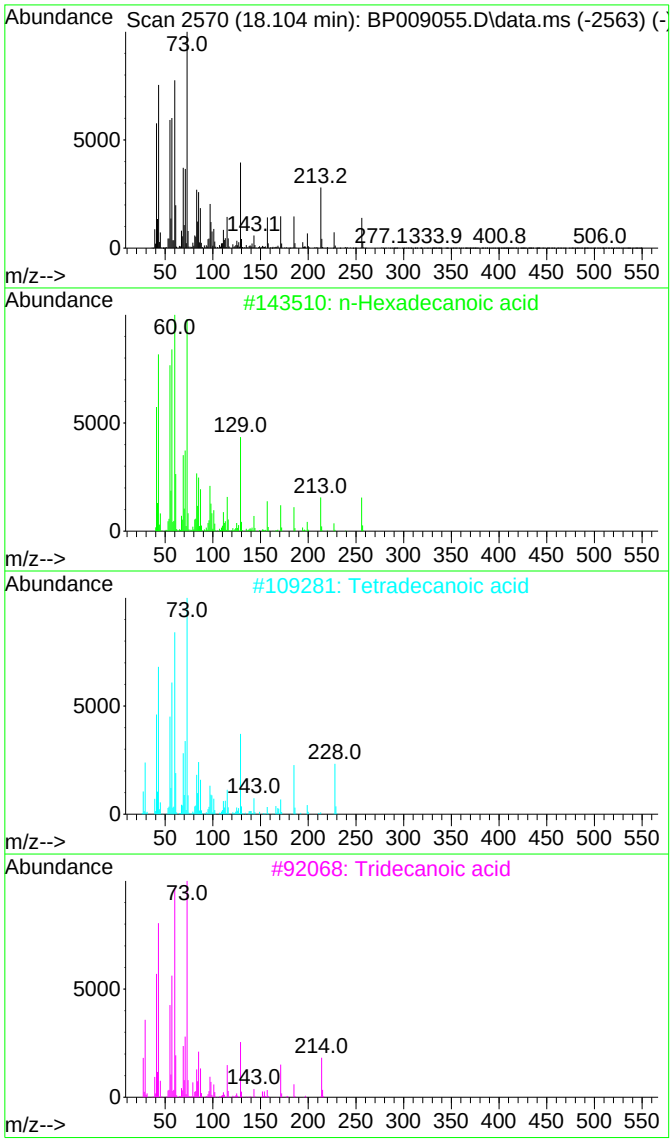
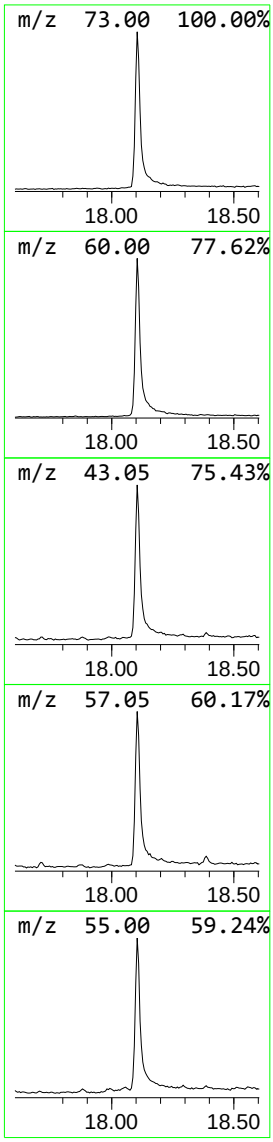
Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.104 | 18.21 ng | 1668620 | Phenanthrene-d10 | 17.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 94 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP020822\
Data File : BP009055.D
Acq On : 08 Feb 2022 13:17
Operator : CG/JU
Sample : N1362-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RO-341

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

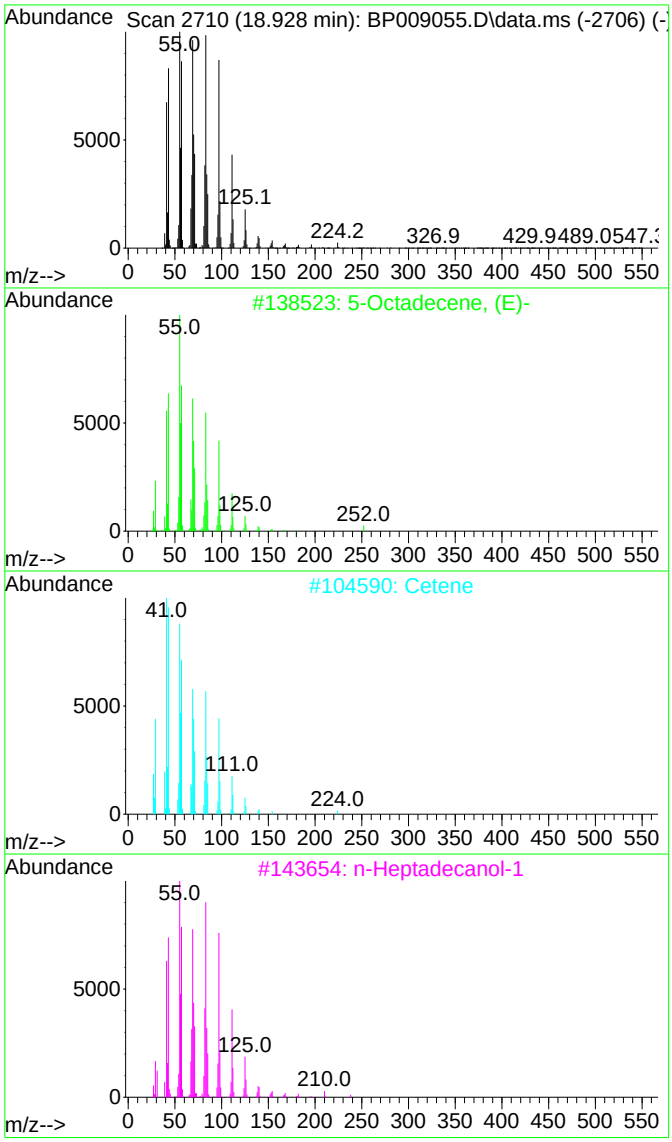
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

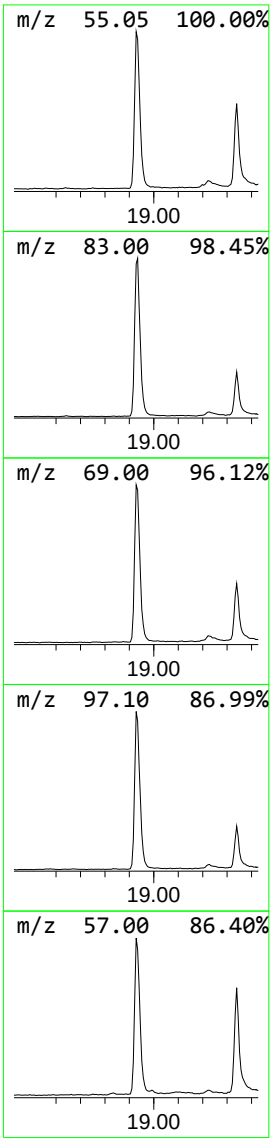
**********

Peak Number 4 5-Octadecene, (E)- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.928 | 38.34 ng | 3514040 | Phenanthrene-d10 | 17.204 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 99 |
| 2 | Cetene | 224 | C16H32 | 000629-73-2 | 96 |
| 3 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 95 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 95 |
| 5 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 94 |



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Acq On : 08 Feb 2022 13:17
Operator : CG/JU
Sample : N1362-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RO-341

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

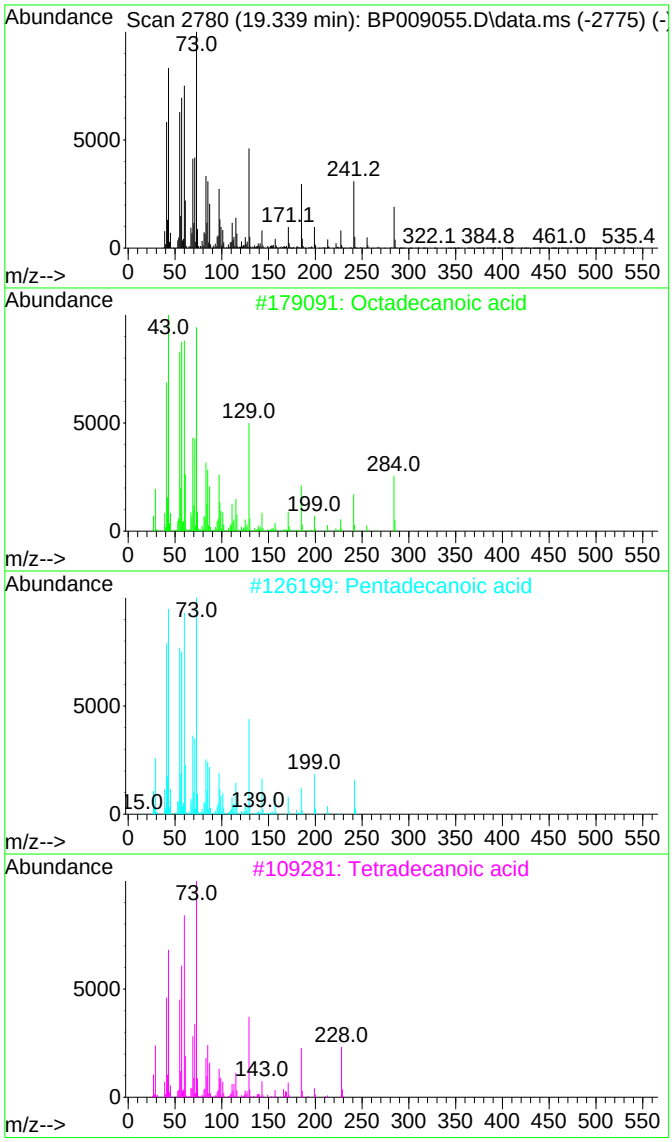
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

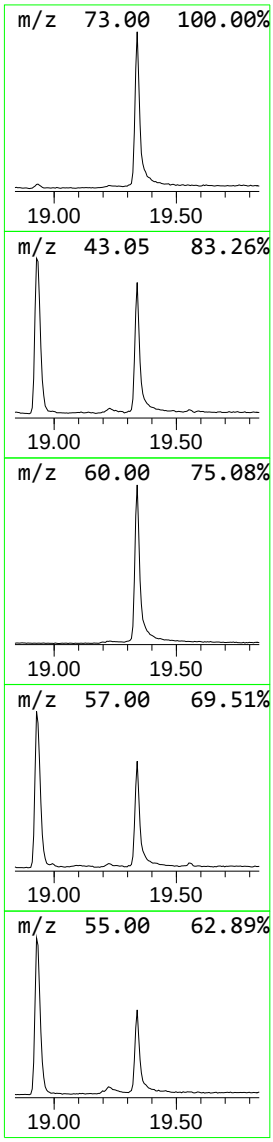
**********

Peak Number 5 Octadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.339 | 23.99 ng | 2810060 | Chrysene-d12 | 21.304 |

| 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 | 90 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 74 |
| 4 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 64 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 64 |



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Sample : N1362-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
RO-341

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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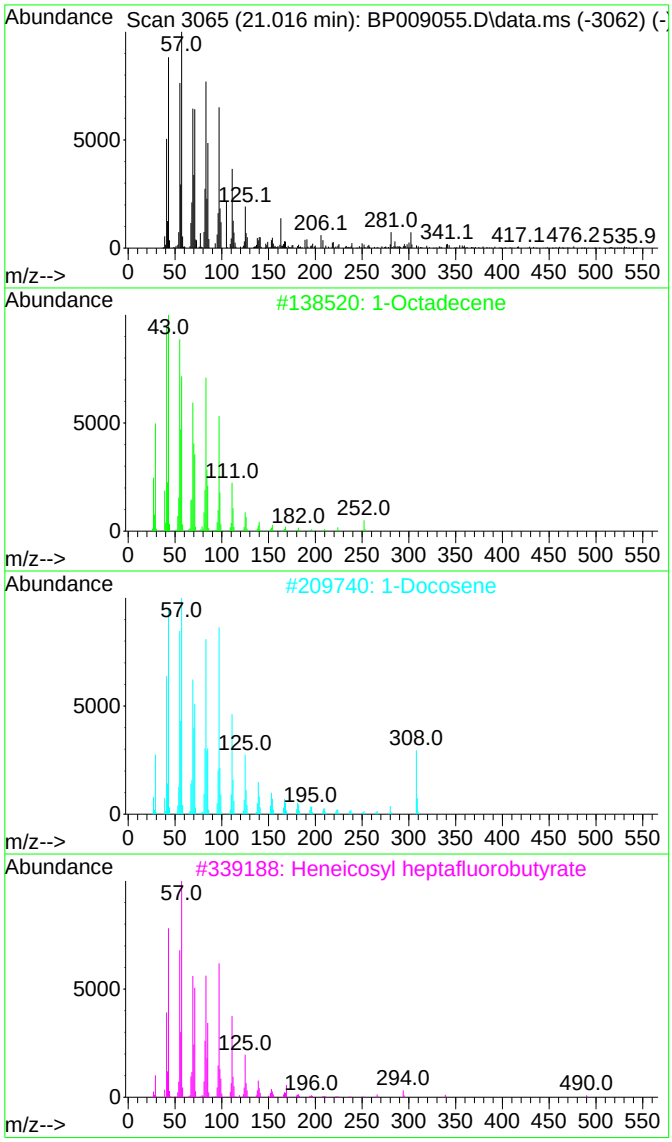
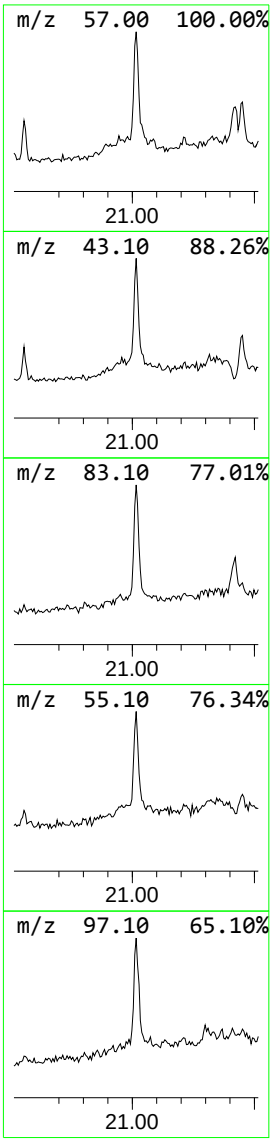
**********

Peak Number 6 1-Octadecene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.016 | 3.78 ng | 442192 | Chrysene-d12 | 21.304 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 95 |
| 2 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 94 |
| 3 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 94 |
| 4 | 1-Eicosene | 280 | C20H40 | 003452-07-1 | 93 |
| 5 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 93 |



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Sample : N1362-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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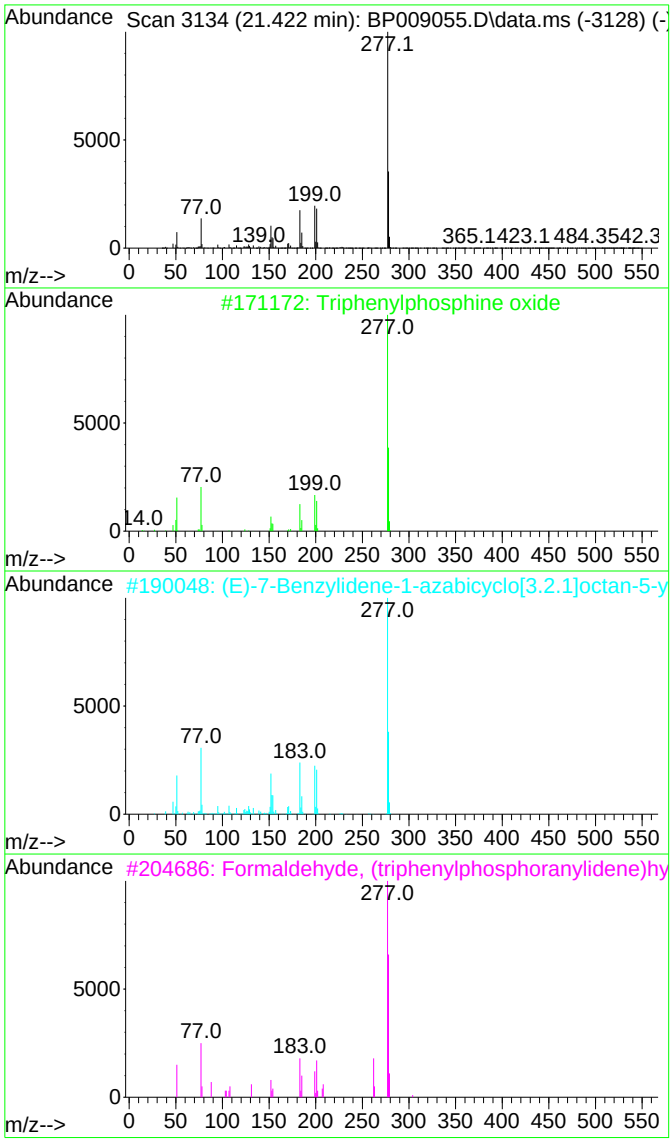
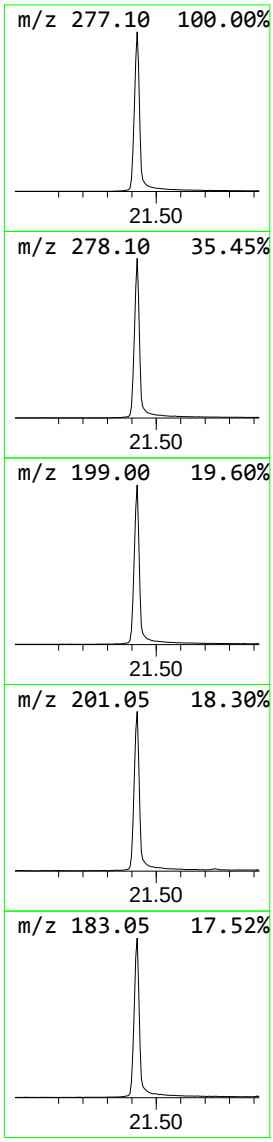
**********

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.422 | 173.48 ng | 20318400 | Chrysene-d12 | 21.304 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 96 |
| 2 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 91 |
| 3 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 37 |
| 4 | 5-Methyl-8-phenylfuro[3',2':5,6]... | 277 | C16H11N3O2 | 1000460-07-9 | 28 |
| 5 | Thiophene-3-carbonitrile, 4-(4-m... | 277 | C13H11NO2S2 | 1000268-75-0 | 9 |



Tentatively Identified Compound (LSC) summary

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 3.017 | 4.7 | ng | 264435 | 1 | 7.805 | 1117510 | 20.0 |
| Propylene Glycol | 3.570 | 63.9 | ng | 3568690 | 1 | 7.805 | 1117510 | 20.0 |
| n-Hexadecanoic ... | 18.104 | 18.2 | ng | 1668620 | 4 | 17.204 | 1832950 | 20.0 |
| 5-Octadecene, (E)- | 18.928 | 38.3 | ng | 3514040 | 4 | 17.204 | 1832950 | 20.0 |
| Octadecanoic acid | 19.339 | 24.0 | ng | 2810060 | 5 | 21.304 | 2342440 | 20.0 |
| 1-Octadecene | 21.016 | 3.8 | ng | 442192 | 5 | 21.304 | 2342440 | 20.0 |
| Triphenylphosph... | 21.422 | 173.5 | ng | 20318400 | 5 | 21.304 | 2342440 | 20.0 |