LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092322\
Data File : BP011786.D
Acq On : 23 Sep 2022 17:01
Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

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-BP092122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011786.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.052 | 7 | 11 | 32 | rVB | 4208669 | 5361041 | 16.49% | 3.697% |
| 2 | 5.016 | 339 | 345 | 353 | rVB | 963266 | 1437977 | 4.42% | 0.992% |
| 3 | 5.475 | 417 | 423 | 436 | rBV | 7490626 | 11130585 | 34.24% | 7.675% |
| 4 | 7.081 | 688 | 696 | 714 | rBV | 7270333 | 11992050 | 36.89% | 8.269% |
| 5 | 7.916 | 831 | 838 | 847 | rBV | 1714241 | 2701292 | 8.31% | 1.863% |
| 6 | 9.081 | 1029 | 1036 | 1051 | rBV | 4514573 | 7623191 | 23.45% | 5.257% |
| 7 | 10.728 | 1309 | 1316 | 1329 | rBV | 2254013 | 3827627 | 11.78% | 2.639% |
| 8 | 13.187 | 1726 | 1734 | 1749 | rBV | 10099317 | 14724200 | 45.30% | 10.153% |
| 9 | 14.563 | 1960 | 1968 | 1982 | rBV | 3208277 | 4659791 | 14.34% | 3.213% |
| 10 | 16.051 | 2214 | 2221 | 2242 | rBV | 6863373 | 9508946 | 29.25% | 6.557% |
| 11 | 17.316 | 2430 | 2436 | 2448 | rVB | 3534783 | 4987092 | 15.34% | 3.439% |
| 12 | 18.204 | 2580 | 2587 | 2609 | rBV | 1066995 | 2185943 | 6.73% | 1.507% |
| 13 | 19.427 | 2791 | 2795 | 2807 | rBV | 503677 | 897236 | 2.76% | 0.619% |
| 14 | 19.874 | 2865 | 2871 | 2882 | rBV | 14797662 | 17489898 | 53.81% | 12.060% |
| 15 | 20.522 | 2977 | 2981 | 2989 | rBV | 203103 | 348819 | 1.07% | 0.241% |
| 16 | 21.110 | 3077 | 3081 | 3090 | rBV4 | 397271 | 824058 | 2.54% | 0.568% |
| 17 | 21.186 | 3090 | 3094 | 3102 | rVV | 422096 | 637557 | 1.96% | 0.440% |
| 18 | 21.398 | 3125 | 3130 | 3138 | rBV | 3803219 | 4875172 | 15.00% | 3.362% |
| 19 | 21.533 | 3146 | 3153 | 3185 | rBV | 18865969 | 32504037 | 100.00% | 22.413% |
| 20 | 21.845 | 3202 | 3206 | 3213 | rVB2 | 510206 | 850730 | 2.62% | 0.587% |
| 21 | 22.539 | 3319 | 3324 | 3331 | rVB | 445021 | 913363 | 2.81% | 0.630% |
| 22 | 23.739 | 3525 | 3528 | 3535 | rVB | 395751 | 665296 | 2.05% | 0.459% |
| 23 | 23.851 | 3540 | 3547 | 3557 | rVB2 | 2279161 | 4874563 | 15.00% | 3.361% |

Sum of corrected areas: 145020464

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ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
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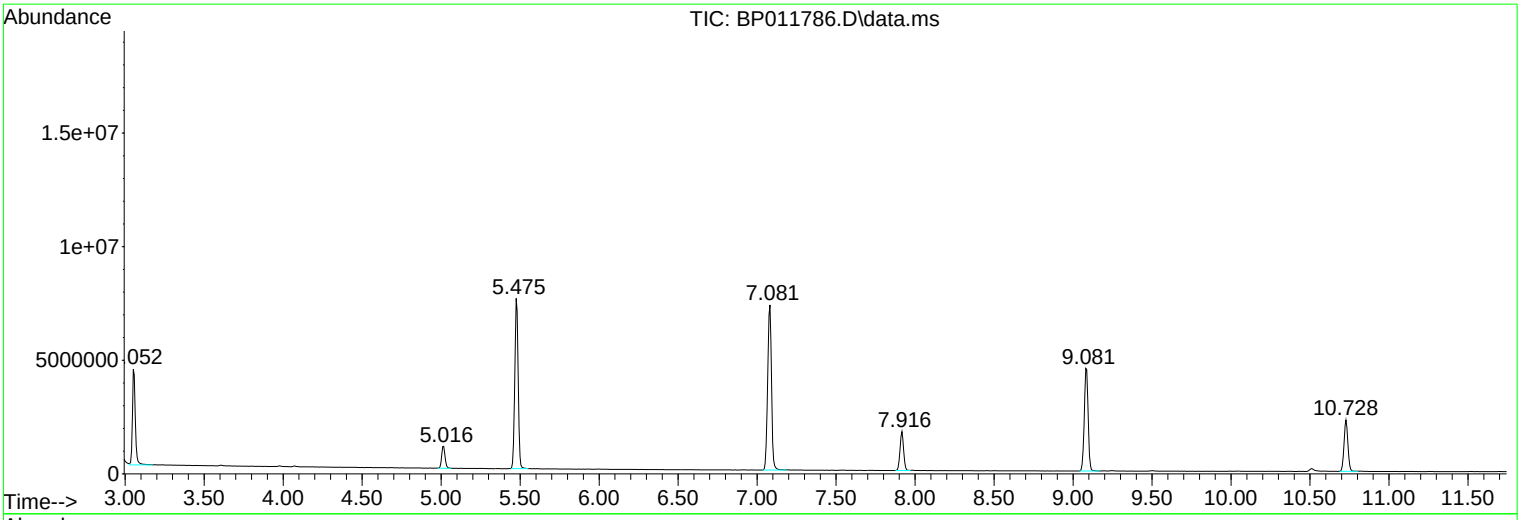
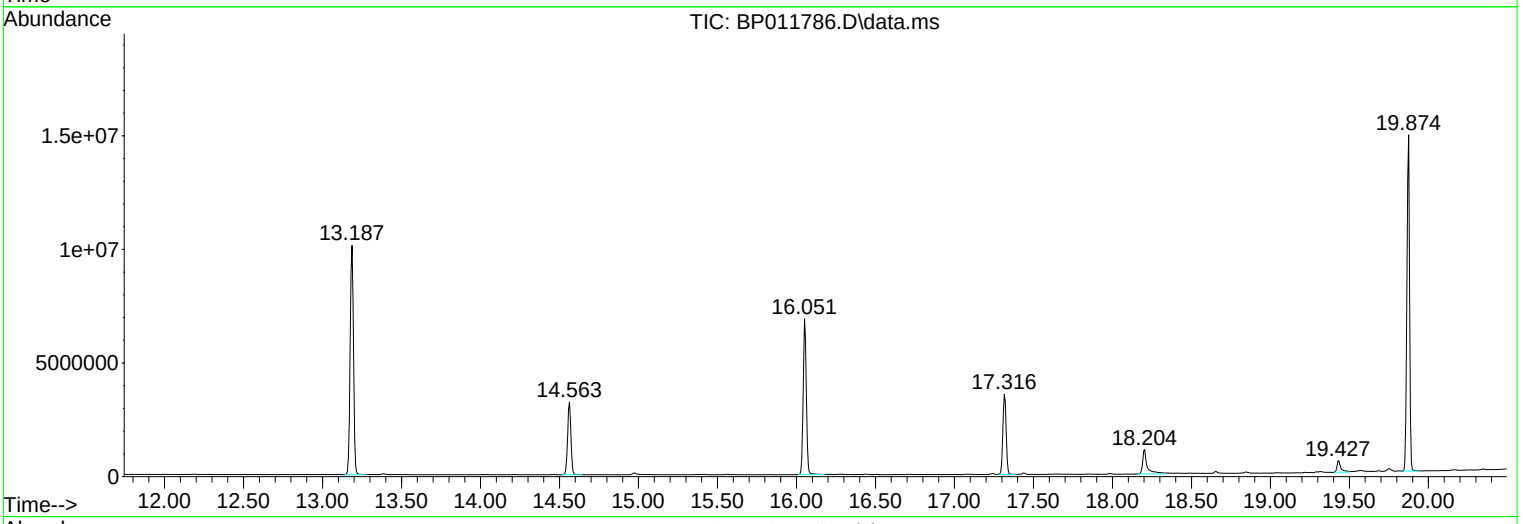
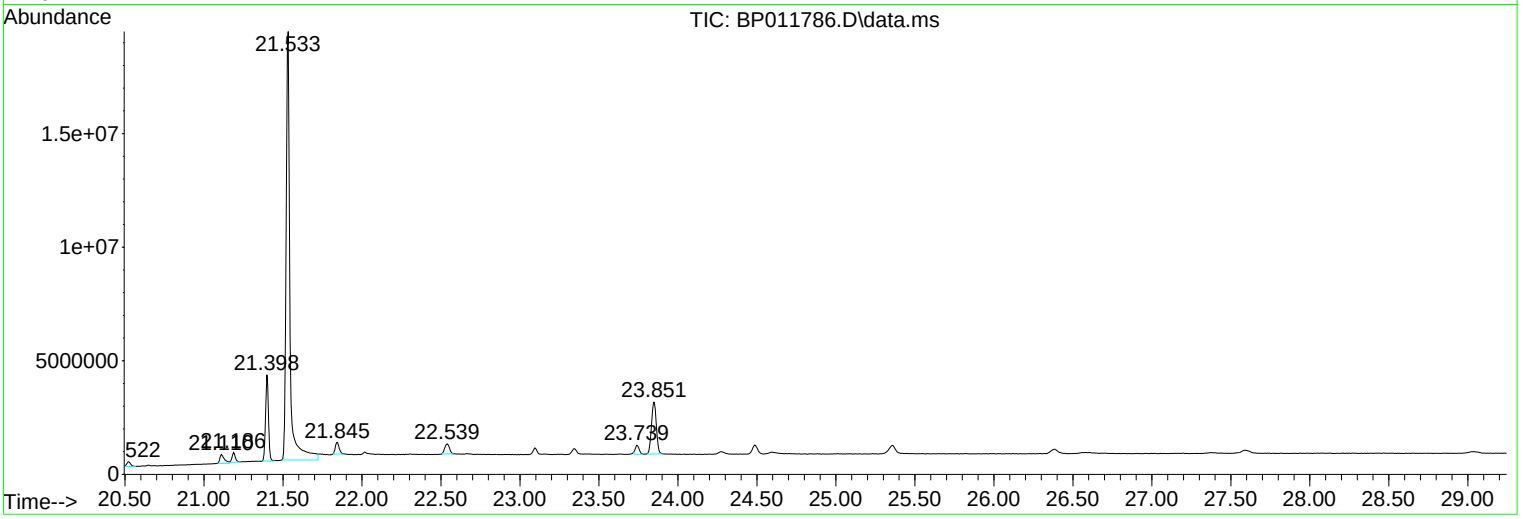
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

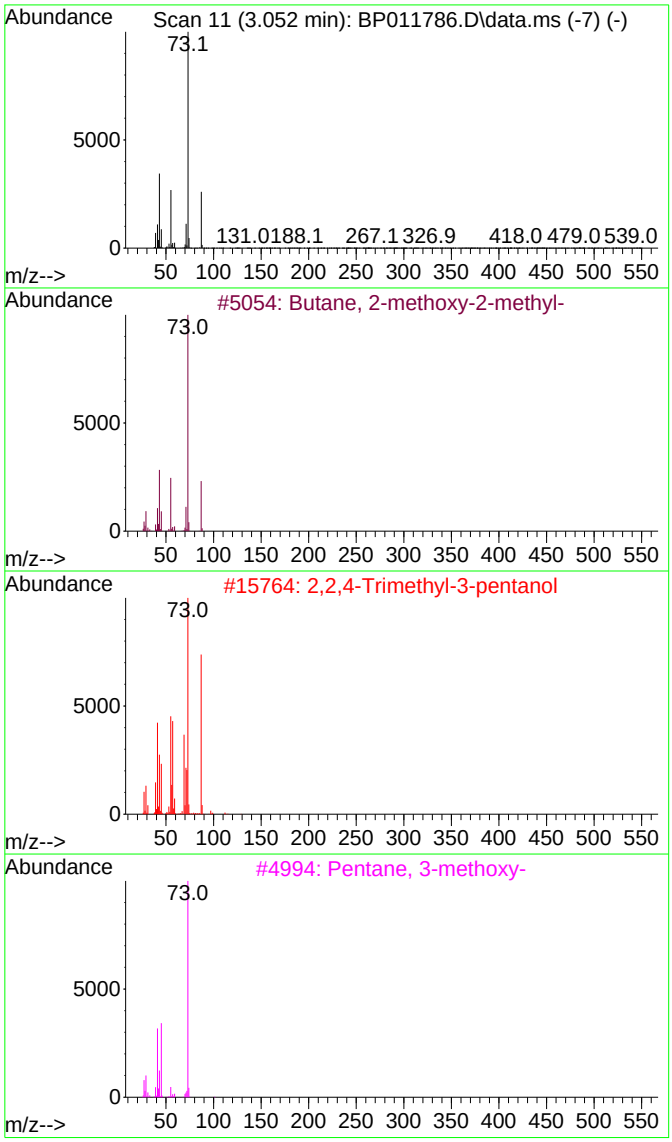
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

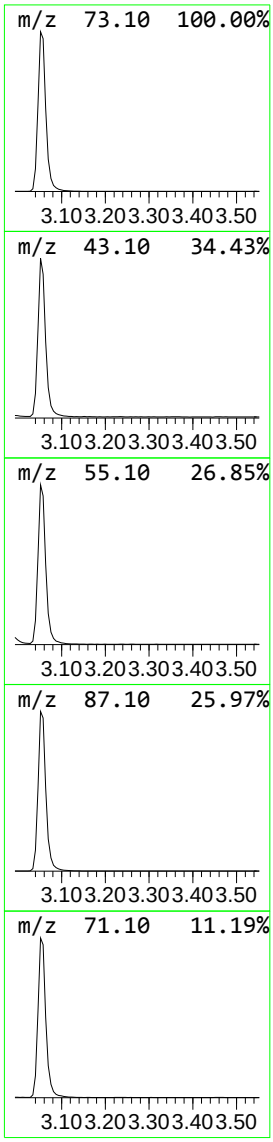
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.052 | 39.69 ng | 5361040 | 1,4-Dichlorobenzene-d4 | 7.916 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 9 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |



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Data File : BP011786.D
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Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

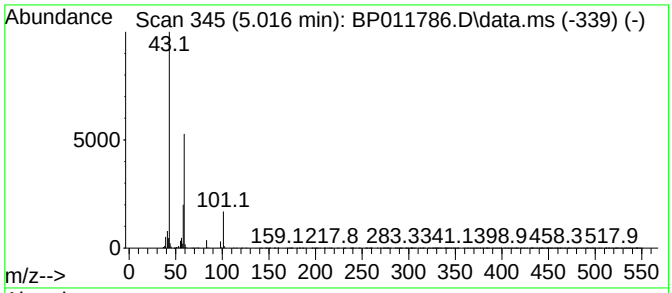
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

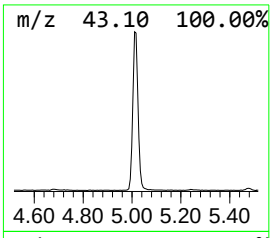
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

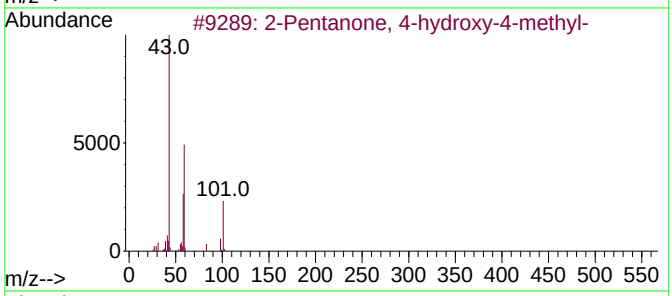
**********
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

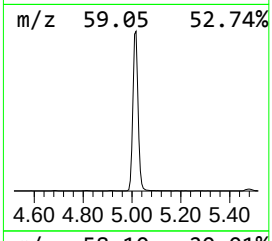
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.016 | 10.65 ng | 1437980 | 1,4-Dichlorobenzene-d4 | 7.916 |

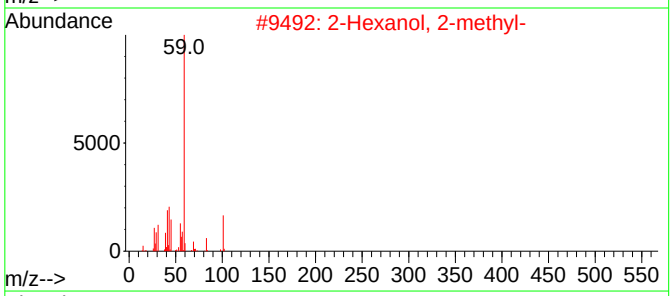
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 83 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 12 |

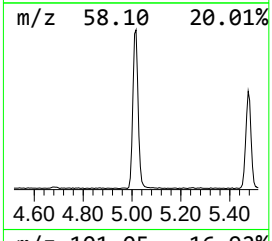


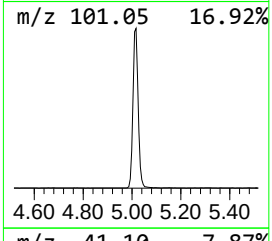



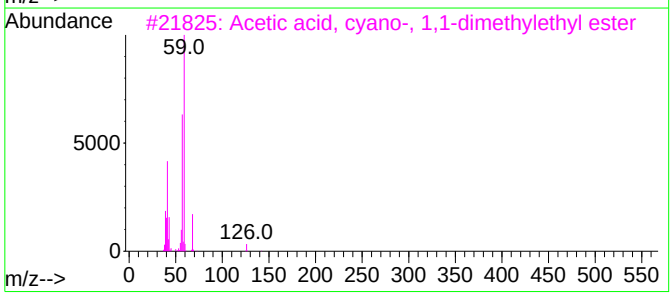



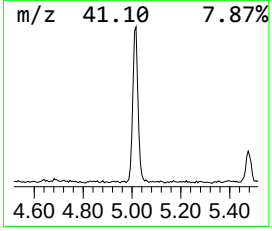



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Acq On : 23 Sep 2022 17:01
Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

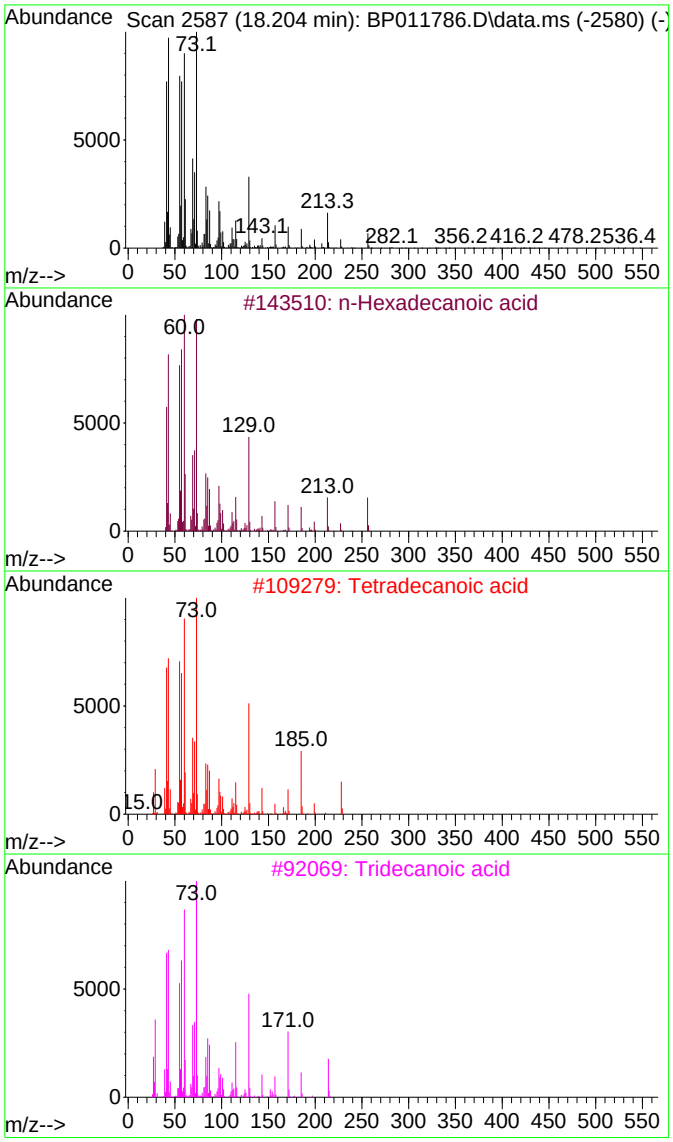
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

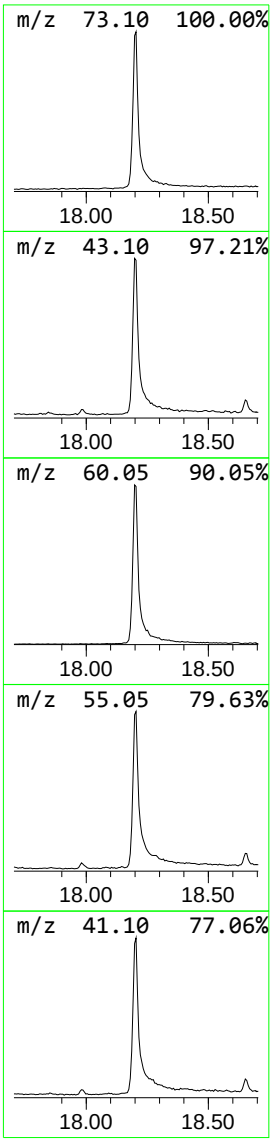
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.204 | 8.77 ng | 2185940 | Phenanthrene-d10 | 17.316 |

| 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 | 90 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 89 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 5 | Isopropyl palmitate | 298 | C19H38O2 | 000142-91-6 | 47 |



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Data File : BP011786.D
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Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

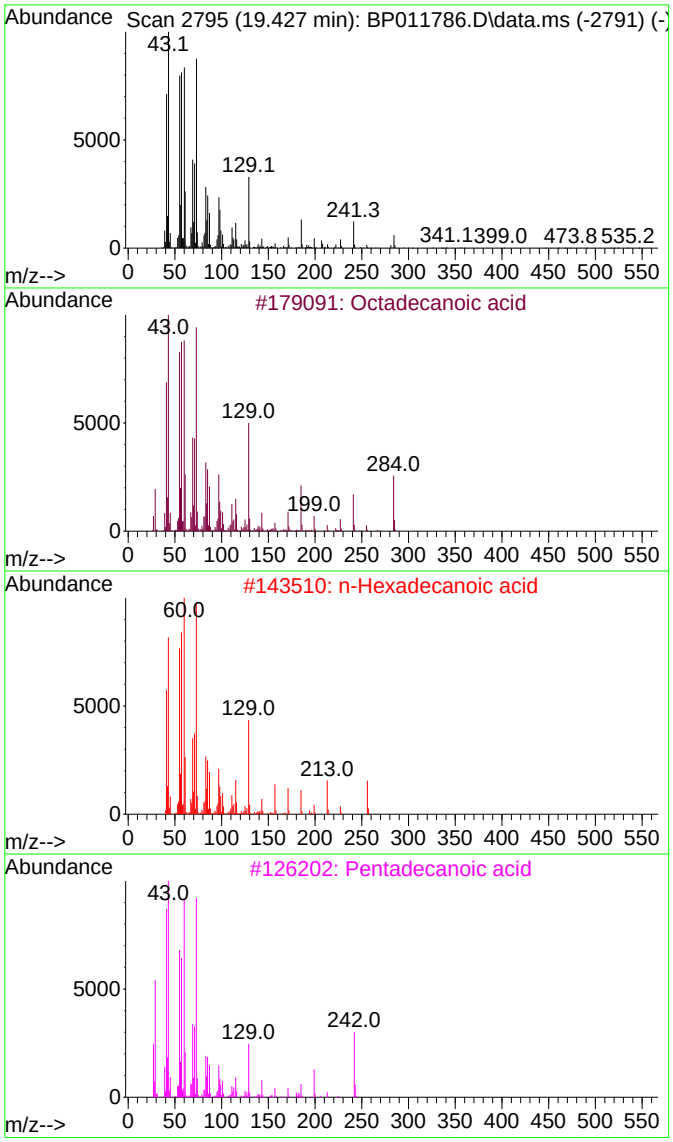
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

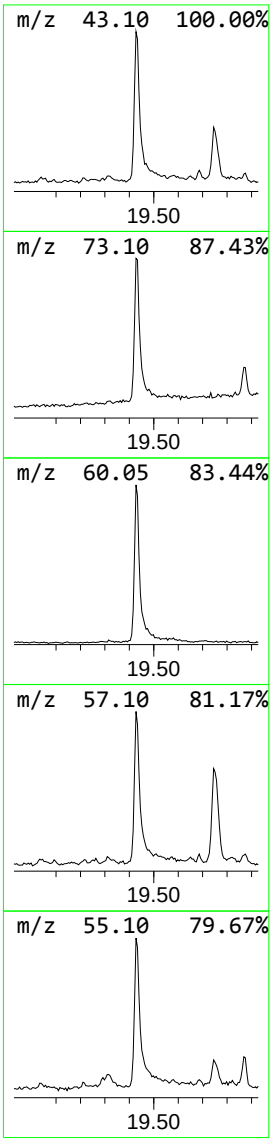
**********

Peak Number 4 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.427 | 3.68 ng | 897236 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 86 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 80 |
| 4 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 78 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 74 |



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Data File : BP011786.D
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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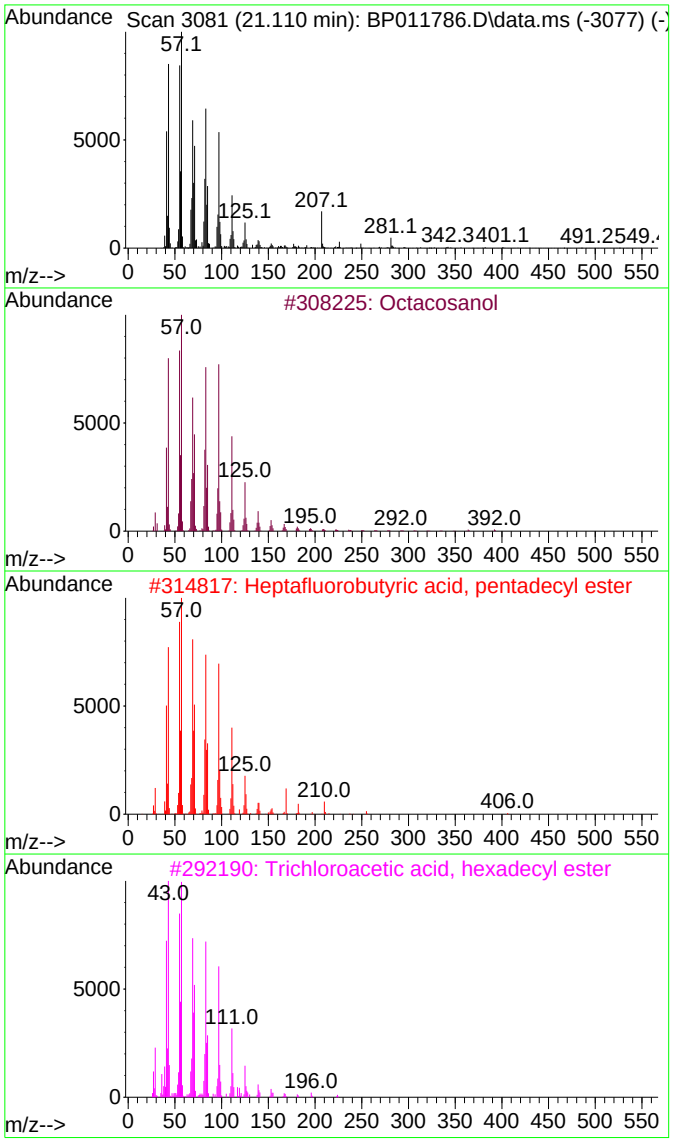
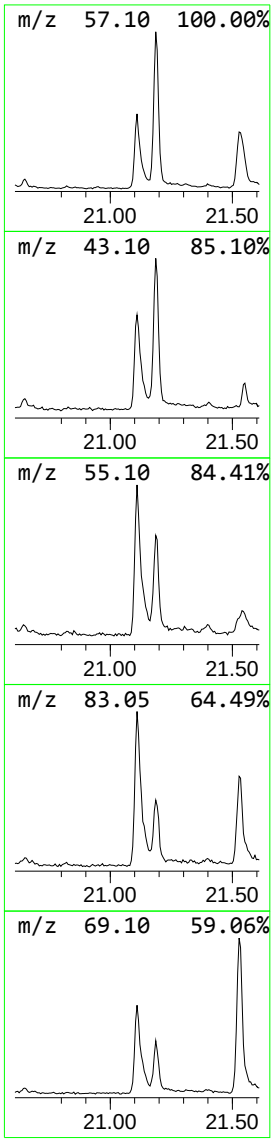
**********

Peak Number 5 Octacosanol Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.110 | 3.38 ng | 824058 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosanol | 410 | C28H58O | 000557-61-9 | 93 |
| 2 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 90 |
| 4 | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 90 |
| 5 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 90 |



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Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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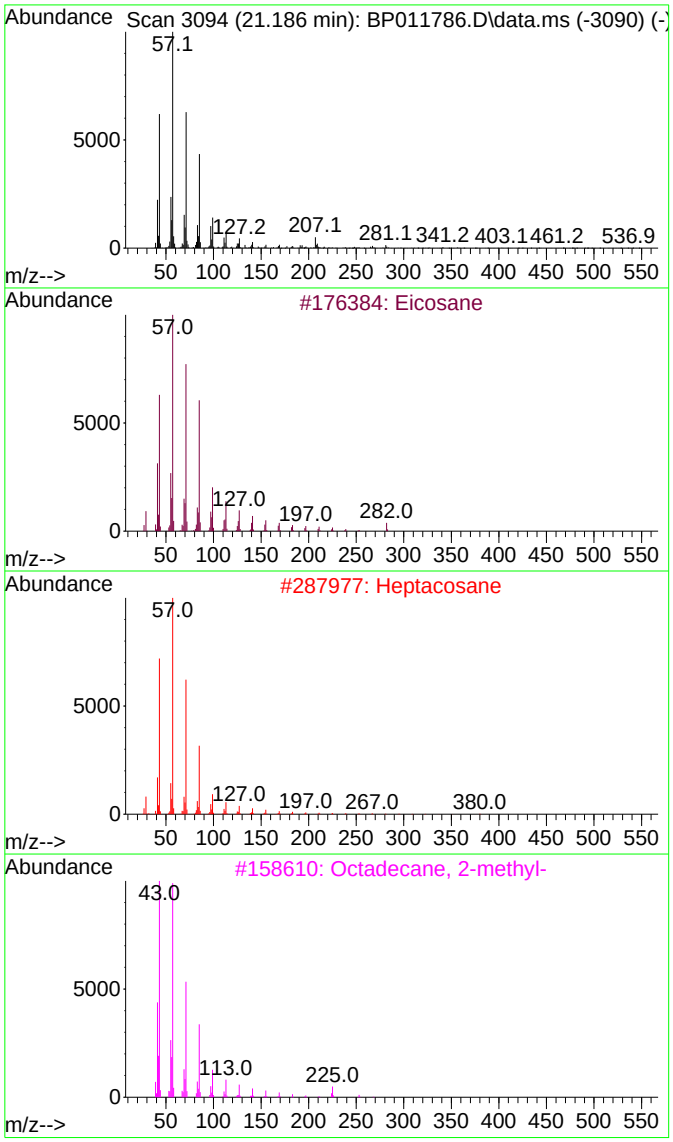
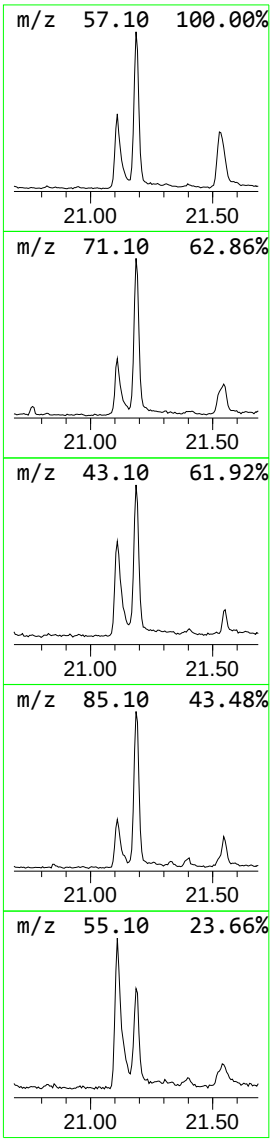
**********

Peak Number 6 Eicosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.186 | 2.62 ng | 637557 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 87 |
| 3 | Octadecane, 2-methyl- | 268 | C19H40 | 001560-88-9 | 87 |
| 4 | 1-Iodo-2-methylundecane | 296 | C12H25I | 073105-67-6 | 87 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |



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Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

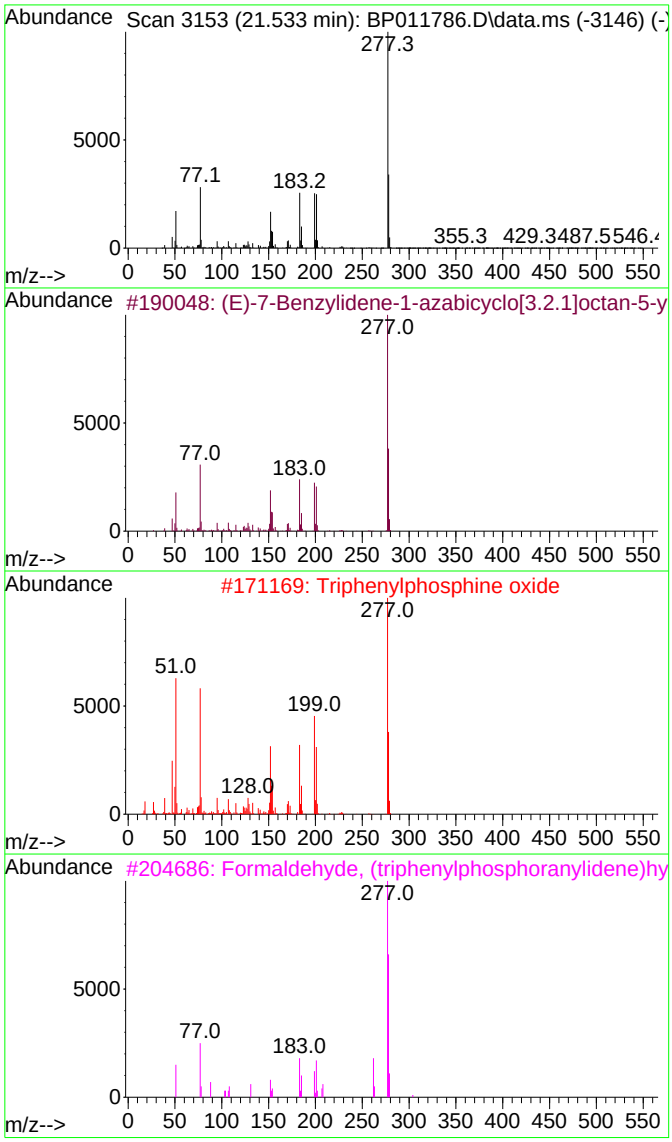
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

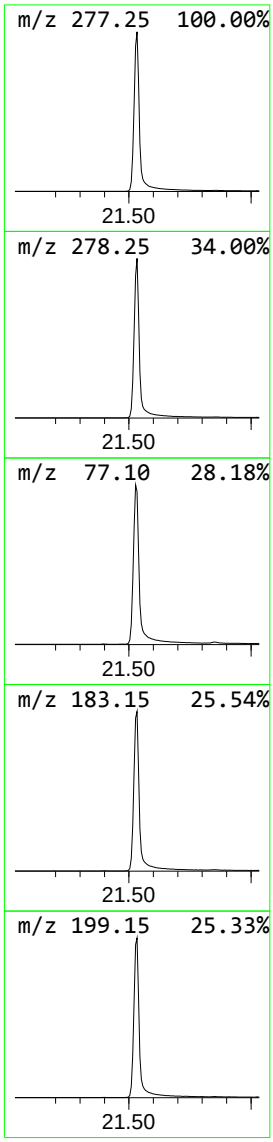
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 (E)-7-Benzylidene-1-azabicy... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.533 | 133.35 ng | 32504000 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 91 |
| 2 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 90 |
| 3 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 64 |
| 4 | Vanadium, cycloheptatrienyl-(pen... | 277 | C17H22V | 1000155-20-5 | 43 |
| 5 | Cobalt,(.eta.<5>-2,4-cyclopentad... | 277 | C16H15BCo | 036682-12-9 | 32 |



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Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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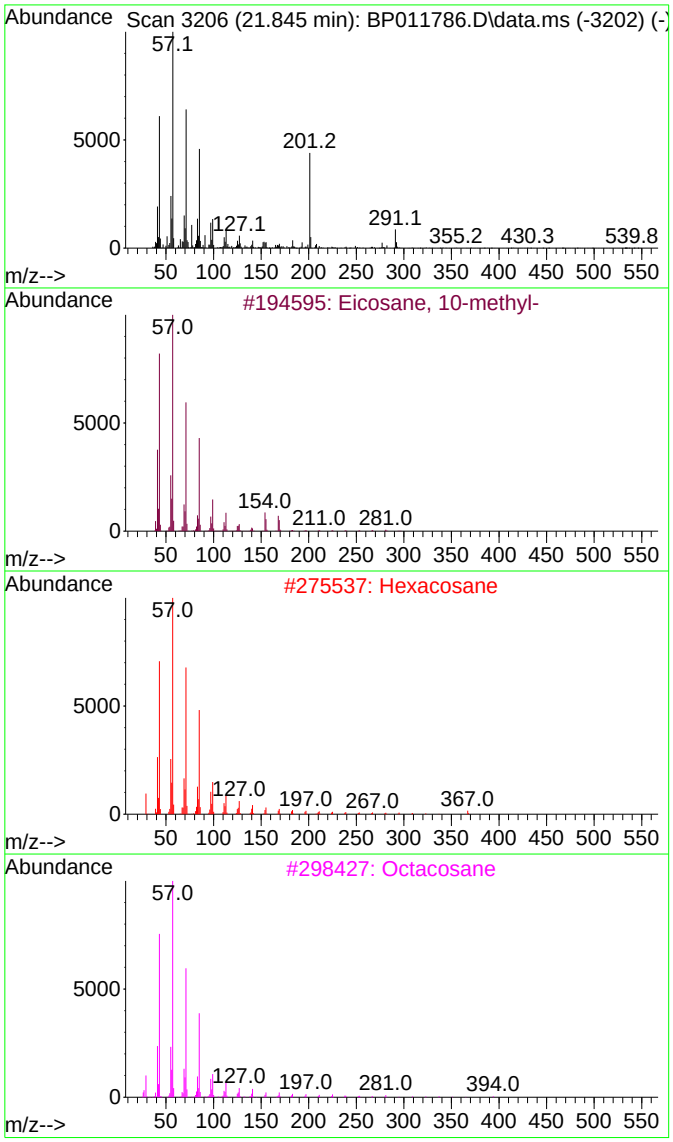
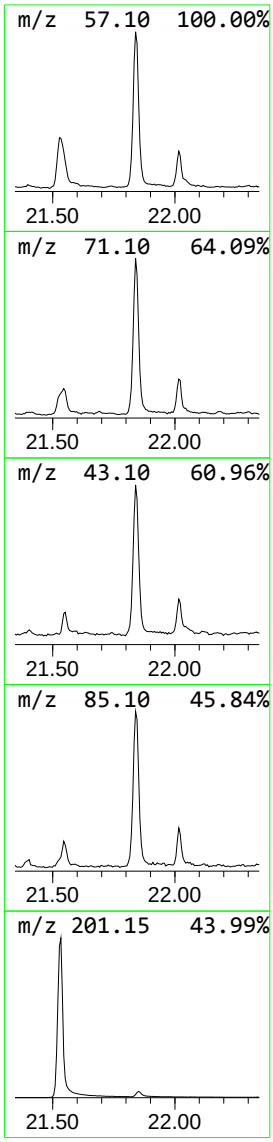
Peak Number 8 Eicosane, 10-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.845 | 3.49 ng | 850730 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 83 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 70 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 70 |
| 4 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 62 |
| 5 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 62 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092322\
Data File : BP011786.D
Acq On : 23 Sep 2022 17:01
Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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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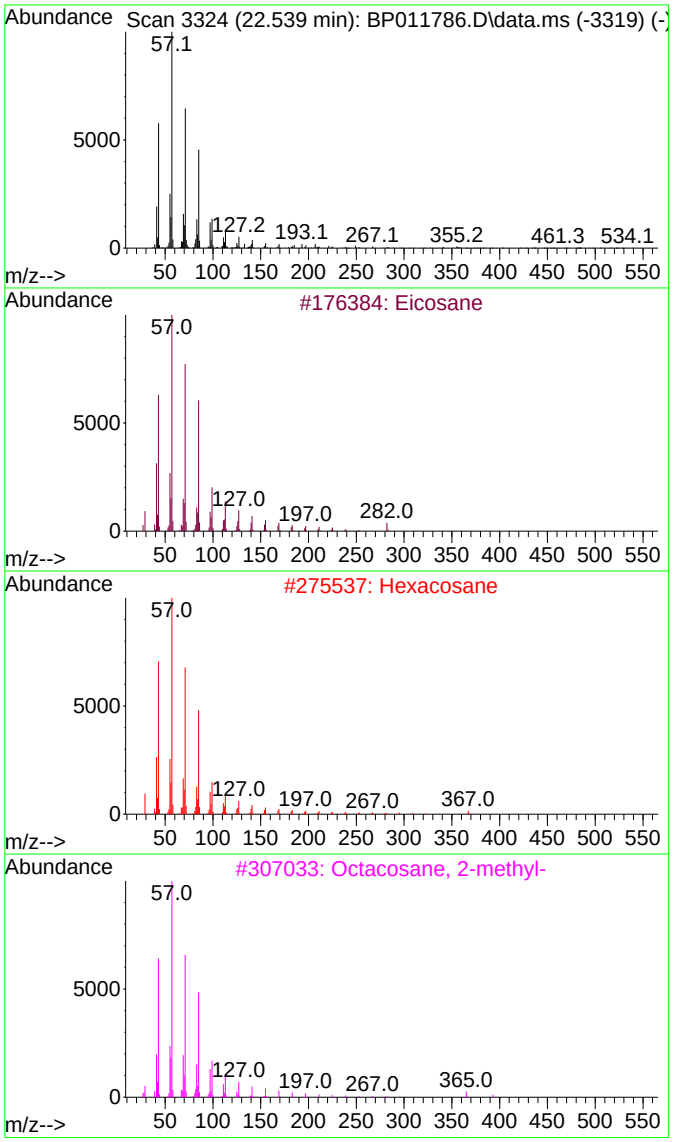
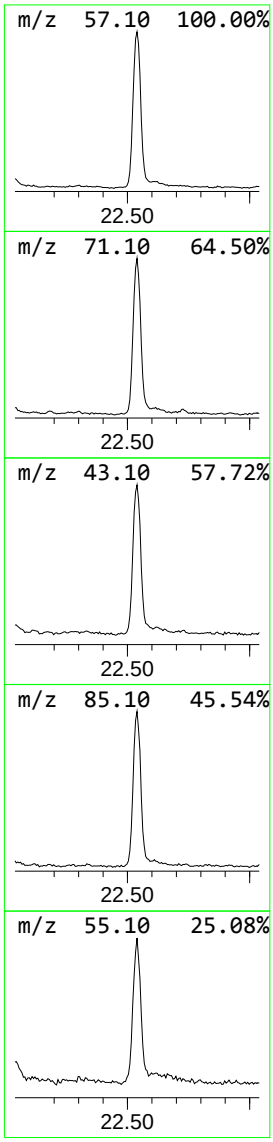
Peak Number 9 Hexacosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.539 | 3.75 ng | 913363 | Chrysene-d12 | 21.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 3 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092322\
Data File : BP011786.D
Acq On : 23 Sep 2022 17:01
Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.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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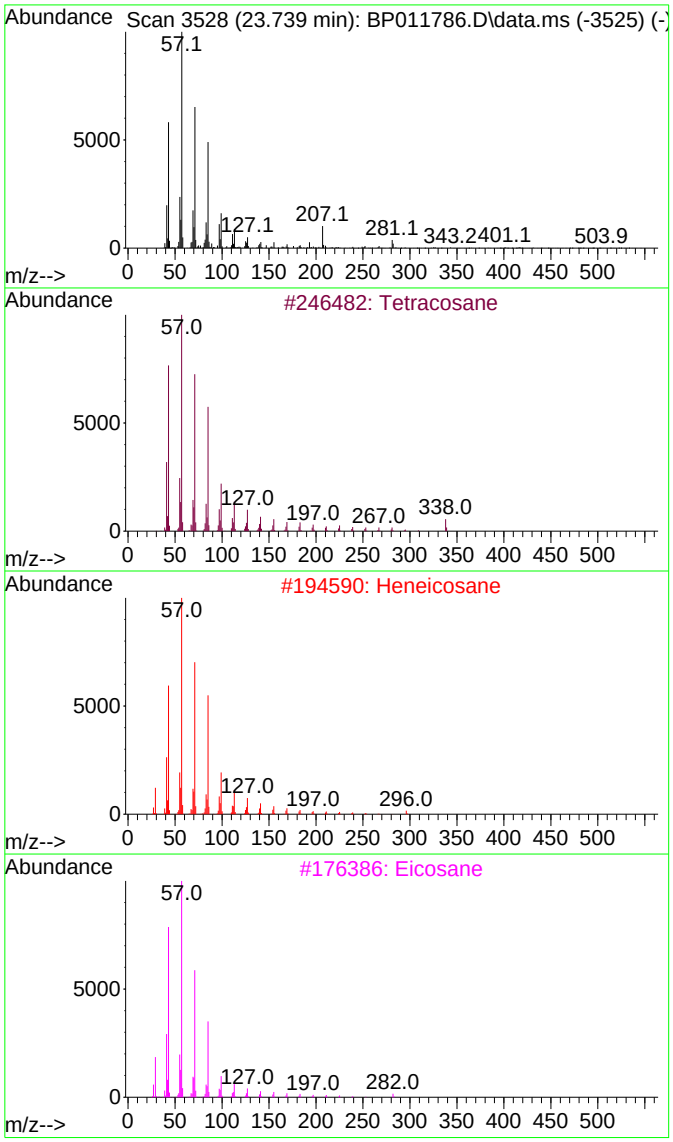
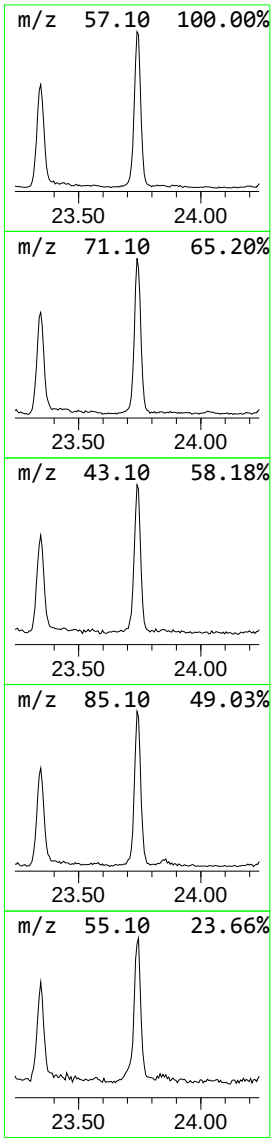
Peak Number 10 Tetracosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.739 | 2.73 ng | 665296 | Perylene-d12 | 23.851 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 93 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 93 |
| 3 | Eicosane | 282 | C20H42 | 000112-95-8 | 90 |
| 4 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 83 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092322\
Data File : BP011786.D
Acq On : 23 Sep 2022 17:01
Operator : CG/JU
Sample : N4780-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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... | 3.052 | 39.7 | ng | 5361040 | 1 | 7.916 | 2701290 | 20.0 |
| 2-Pentanone, 4-... | 5.016 | 10.7 | ng | 1437980 | 1 | 7.916 | 2701290 | 20.0 |
| n-Hexadecanoic ... | 18.204 | 8.8 | ng | 2185940 | 4 | 17.316 | 4987090 | 20.0 |
| Octadecanoic acid | 19.427 | 3.7 | ng | 897236 | 5 | 21.398 | 4875170 | 20.0 |
| Octacosanol | 21.110 | 3.4 | ng | 824058 | 5 | 21.398 | 4875170 | 20.0 |
| Eicosane | 21.186 | 2.6 | ng | 637557 | 5 | 21.398 | 4875170 | 20.0 |
| (E)-7-Benzylide... | 21.533 | 133.3 | ng | 32504000 | 5 | 21.398 | 4875170 | 20.0 |
| Eicosane, 10-me... | 21.845 | 3.5 | ng | 850730 | 5 | 21.398 | 4875170 | 20.0 |
| Hexacosane | 22.539 | 3.8 | ng | 913363 | 5 | 21.398 | 4875170 | 20.0 |
| Tetracosane | 23.739 | 2.7 | ng | 665296 | 6 | 23.851 | 4874560 | 20.0 |