LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

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-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007303.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.446 | 393 | 401 | 413 | rBV | 3642552 | 5419584 | 70.07% | 6.559% |
| 2 | 7.046 | 664 | 673 | 686 | rBV | 3205228 | 5206556 | 67.32% | 6.302% |
| 3 | 7.858 | 804 | 811 | 818 | rBV | 702600 | 1089990 | 14.09% | 1.319% |
| 4 | 9.028 | 1002 | 1010 | 1025 | rBV | 1977219 | 3423292 | 44.26% | 4.143% |
| 5 | 10.446 | 1246 | 1251 | 1260 | rBV | 147108 | 261641 | 3.38% | 0.317% |
| 6 | 10.663 | 1280 | 1288 | 1294 | rBV | 816469 | 1426140 | 18.44% | 1.726% |
| 7 | 13.122 | 1699 | 1706 | 1721 | rBV | 4404102 | 6608696 | 85.45% | 7.999% |
| 8 | 14.222 | 1889 | 1893 | 1900 | rVB | 83066 | 123148 | 1.59% | 0.149% |
| 9 | 14.498 | 1934 | 1940 | 1948 | rVB | 1163820 | 1697371 | 21.95% | 2.054% |
| 10 | 14.922 | 2009 | 2012 | 2019 | rVB | 73121 | 101924 | 1.32% | 0.123% |
| 11 | 15.763 | 2150 | 2155 | 2164 | rBV | 72858 | 190442 | 2.46% | 0.230% |
| 12 | 15.992 | 2188 | 2194 | 2207 | rVB | 3469017 | 4946507 | 63.96% | 5.987% |
| 13 | 16.287 | 2240 | 2244 | 2252 | rVB2 | 79408 | 140116 | 1.81% | 0.170% |
| 14 | 16.551 | 2285 | 2289 | 2295 | rVB3 | 58066 | 85962 | 1.11% | 0.104% |
| 15 | 16.651 | 2301 | 2306 | 2322 | rVB2 | 306389 | 645186 | 8.34% | 0.781% |
| 16 | 17.251 | 2403 | 2408 | 2412 | rBV | 1340489 | 1867364 | 24.14% | 2.260% |
| 17 | 17.292 | 2412 | 2415 | 2421 | rVB | 377213 | 526506 | 6.81% | 0.637% |
| 18 | 17.386 | 2422 | 2431 | 2443 | rBV3 | 452292 | 1583461 | 20.47% | 1.916% |
| 19 | 17.486 | 2444 | 2448 | 2455 | rBV | 90893 | 219515 | 2.84% | 0.266% |
| 20 | 18.145 | 2552 | 2560 | 2570 | rBV2 | 1200808 | 2181103 | 28.20% | 2.640% |
| 21 | 18.304 | 2583 | 2587 | 2592 | rBV2 | 141765 | 273800 | 3.54% | 0.331% |
| 22 | 18.416 | 2601 | 2606 | 2609 | rBV | 453039 | 662850 | 8.57% | 0.802% |
| 23 | 18.457 | 2609 | 2613 | 2625 | rVB | 696293 | 1065961 | 13.78% | 1.290% |
| 24 | 18.645 | 2634 | 2645 | 2655 | rVB2 | 731439 | 2427601 | 31.39% | 2.938% |
| 25 | 18.775 | 2657 | 2667 | 2678 | rVV2 | 809461 | 3309094 | 42.78% | 4.005% |
| 26 | 18.881 | 2678 | 2685 | 2697 | rVB | 3102145 | 6746502 | 87.23% | 8.165% |
| 27 | 19.010 | 2703 | 2707 | 2709 | rBV | 109712 | 170264 | 2.20% | 0.206% |
| 28 | 19.045 | 2710 | 2713 | 2720 | rVB | 231874 | 438125 | 5.66% | 0.530% |
| 29 | 19.233 | 2740 | 2745 | 2746 | rBV | 213225 | 294261 | 3.80% | 0.356% |
| 30 | 19.263 | 2746 | 2750 | 2756 | rVB | 1081799 | 1436147 | 18.57% | 1.738% |
| 31 | 19.375 | 2765 | 2769 | 2773 | rBV | 379920 | 522401 | 6.75% | 0.632% |
| 32 | 19.586 | 2802 | 2805 | 2806 | rBV | 145962 | 154842 | 2.00% | 0.187% |
| 33 | 19.616 | 2806 | 2810 | 2818 | rVB | 944289 | 1357836 | 17.56% | 1.643% |
| 34 | 19.763 | 2830 | 2835 | 2839 | rBV | 519632 | 908046 | 11.74% | 1.099% |
| 35 | 19.816 | 2839 | 2844 | 2849 | rVB | 6414011 | 7734291 | 100.00% | 9.361% |
| 36 | 20.257 | 2916 | 2919 | 2923 | rVB | 136768 | 165048 | 2.13% | 0.200% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

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-BP092121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 20.539 | 2962 | 2967 | 2973 | rBV2 | 738126 | 1418200 | 18.34% | 1.716% |
| 38 | 21.045 | 3050 | 3053 | 3057 | rBV2 | 295462 | 330320 | 4.27% | 0.400% |
| 39 | 21.210 | 3076 | 3081 | 3086 | rVB | 812773 | 1297006 | 16.77% | 1.570% |
| 40 | 21.339 | 3097 | 3103 | 3107 | rBV2 | 2593904 | 4319197 | 55.84% | 5.228% |
| 41 | 21.375 | 3107 | 3109 | 3119 | rVB | 615486 | 834442 | 10.79% | 1.010% |
| 42 | 21.845 | 3184 | 3189 | 3195 | rBV | 878661 | 1539611 | 19.91% | 1.863% |
| 43 | 22.557 | 3305 | 3310 | 3318 | rVB | 742529 | 1432168 | 18.52% | 1.733% |
| 44 | 23.016 | 3383 | 3388 | 3393 | rBV | 467012 | 1096017 | 14.17% | 1.327% |
| 45 | 23.345 | 3439 | 3444 | 3453 | rVB | 683839 | 1493148 | 19.31% | 1.807% |
| 46 | 23.639 | 3490 | 3494 | 3504 | rVB | 591981 | 1177150 | 15.22% | 1.425% |
| 47 | 23.751 | 3507 | 3513 | 3519 | rVV2 | 1159271 | 2274426 | 29.41% | 2.753% |

Sum of corrected areas: 82623258

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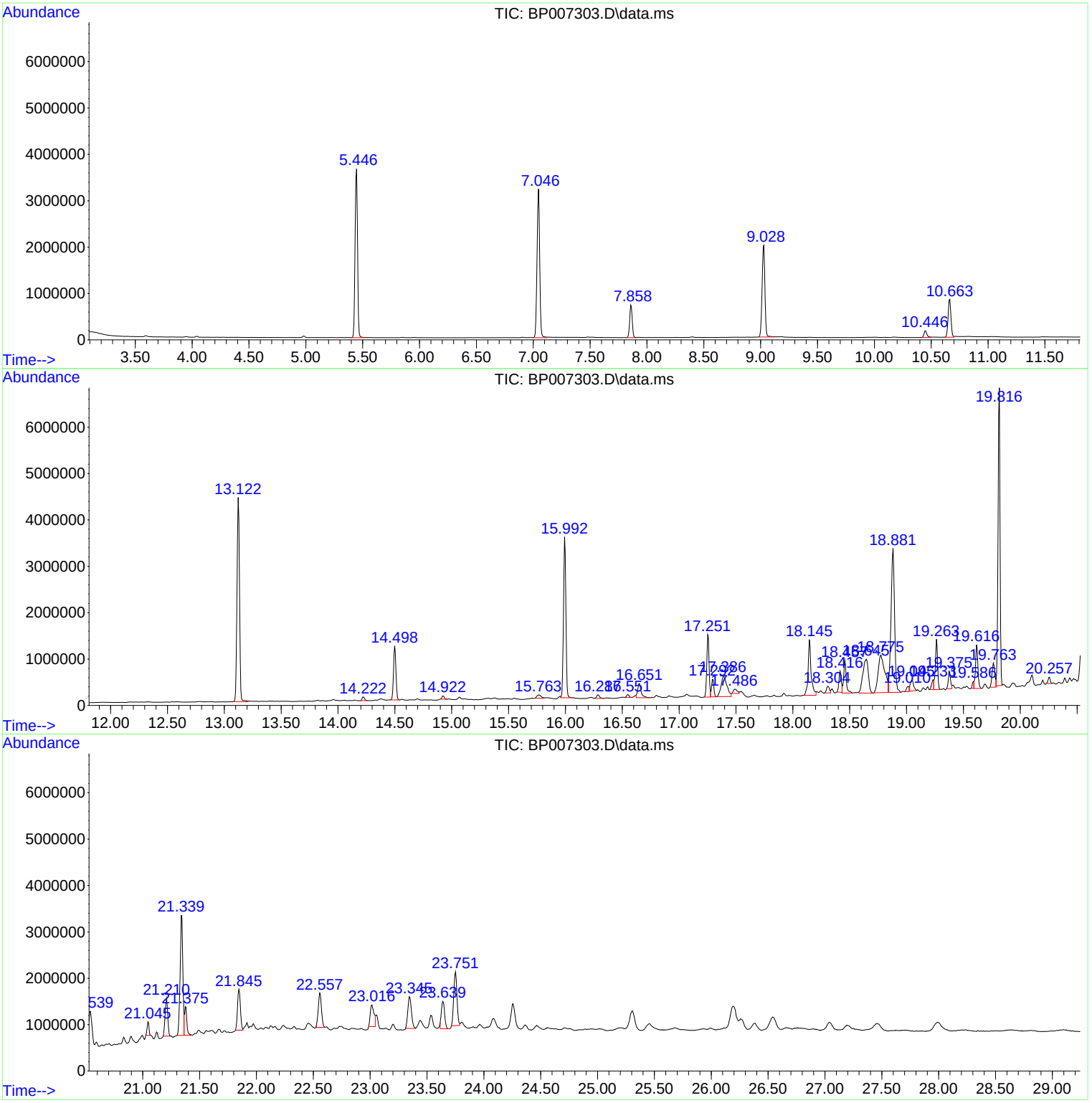
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

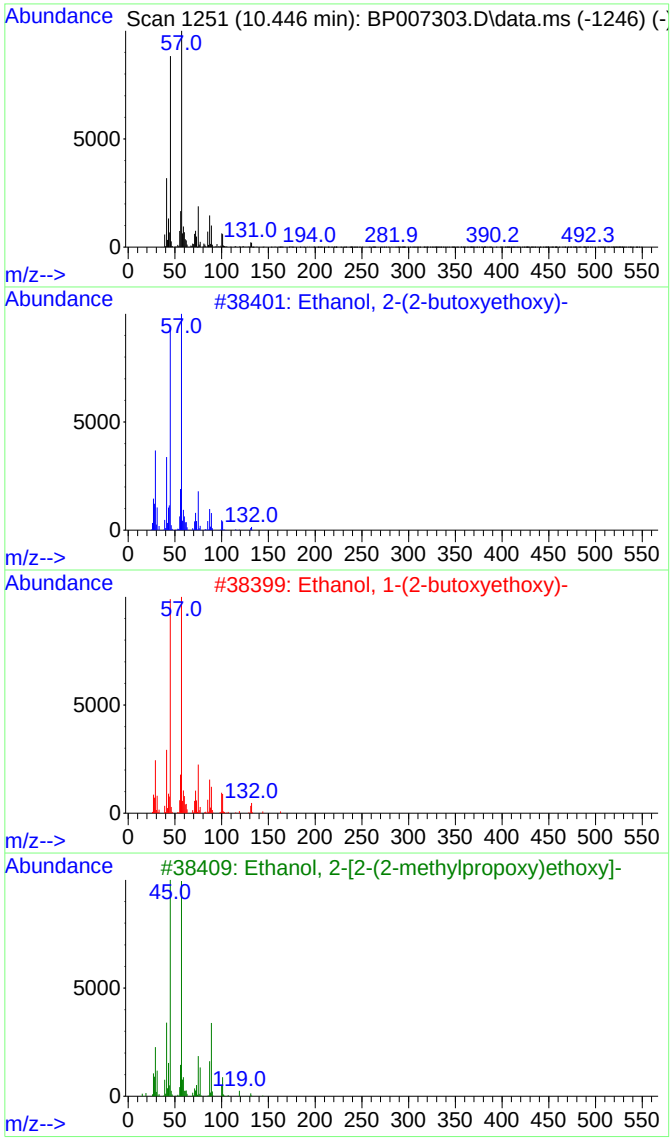
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

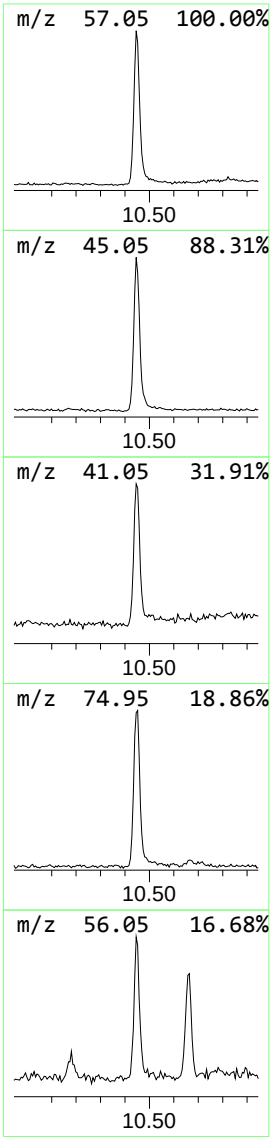
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.446 | 3.67 ng | 261641 | 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 | 90 |
| 3 | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 72 |
| 4 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 64 |
| 5 | Di-sec-Butyl ether | 130 | C8H18O | 006863-58-7 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

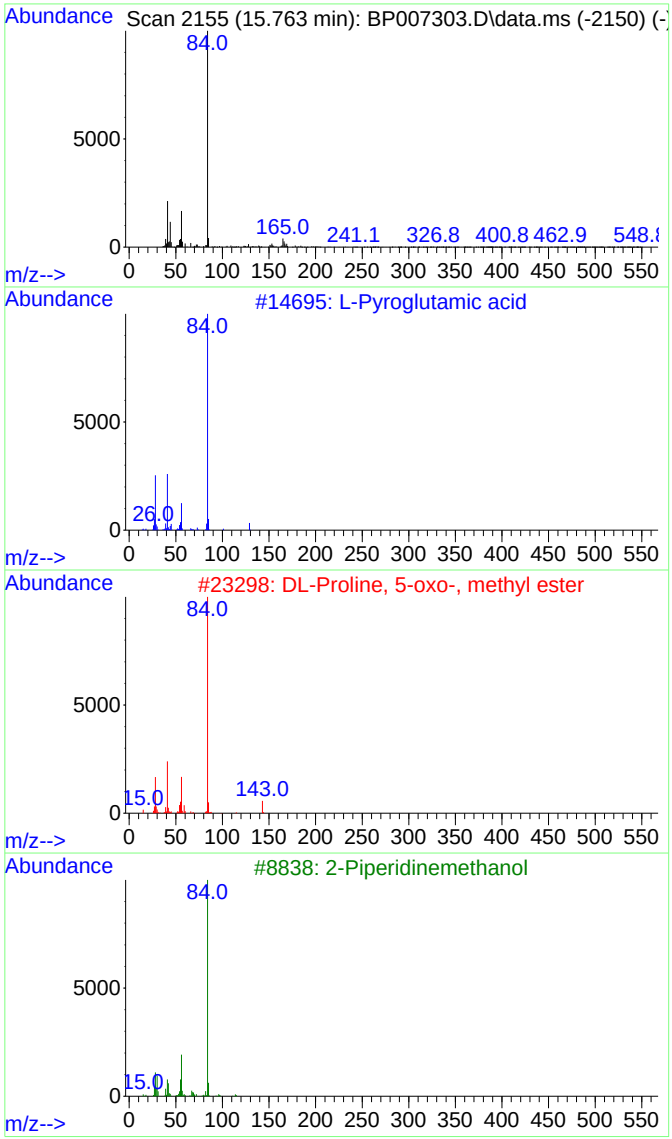
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

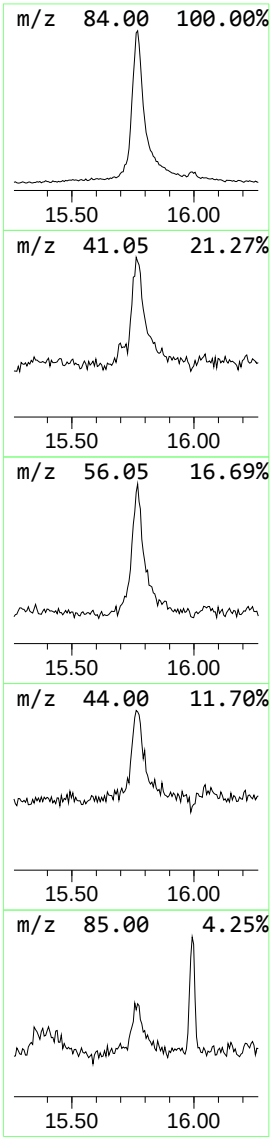
**********

Peak Number 2 L-Pyroglutamic acid Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.763 | 2.24 ng | 190442 | Acenaphthene-d10 | 14.498 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | L-Pyroglutamic acid | 129 | C5H7NO3 | 000098-79-3 | 64 |
| 2 | DL-Proline, 5-oxo-, methyl ester | 143 | C6H9NO3 | 054571-66-3 | 59 |
| 3 | 2-Piperidinemethanol | 115 | C6H13NO | 003433-37-2 | 59 |
| 4 | L-Glutamine | 146 | C5H10N2O3 | 000056-85-9 | 59 |
| 5 | Piperidine, 2-(tetrahydro-2-fura... | 155 | C9H17NO | 1000305-66-0 | 59 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

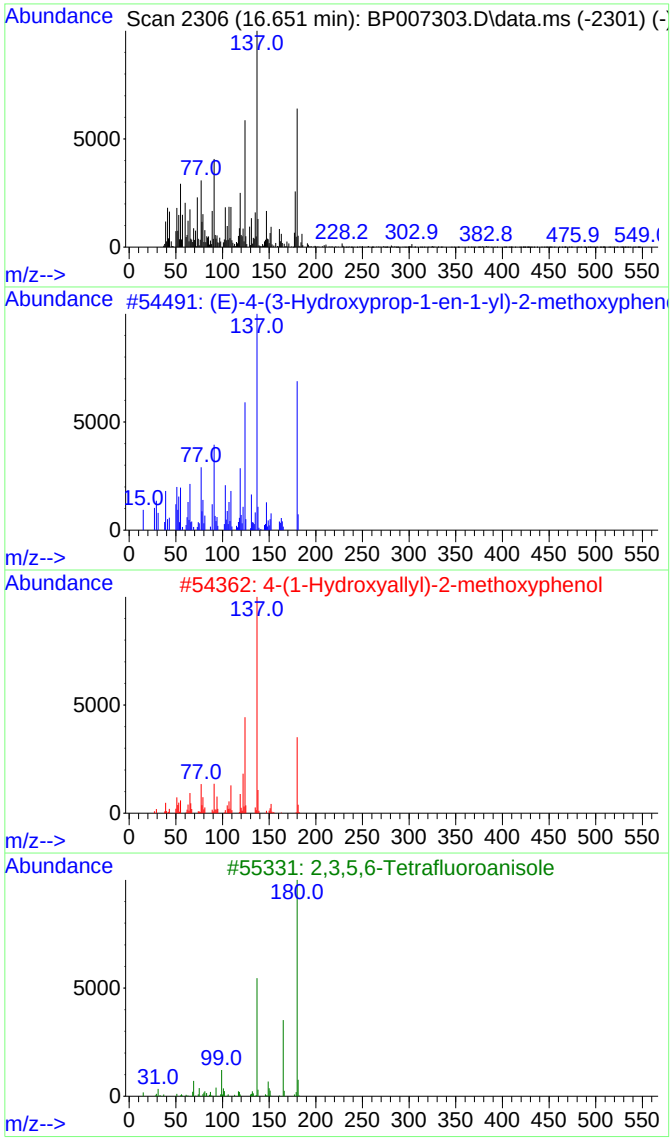
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

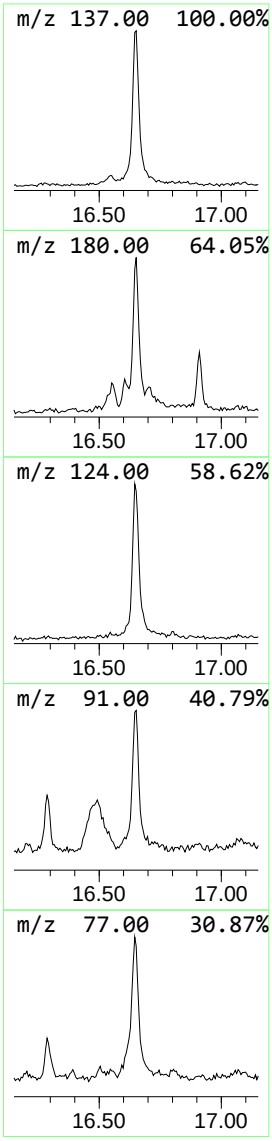
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.651 | 6.91 ng | 645186 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-4-(3-Hydroxyprop-1-en-1-yl)-... | 180 | C10H12O3 | 032811-40-8 | 98 |
| 2 | 4-(1-Hydroxyallyl)-2-methoxyphenol | 180 | C10H12O3 | 112465-50-6 | 62 |
| 3 | 2,3,5,6-Tetrafluoroanisole | 180 | C7H4F4O | 002324-98-3 | 38 |
| 4 | (-)-R-Phenethanamine, 1-methyl-N... | 271 | C17H21NO2 | 1000127-90-4 | 35 |
| 5 | 6-Methylnicotinic acid | 137 | C7H7NO2 | 003222-47-7 | 27 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

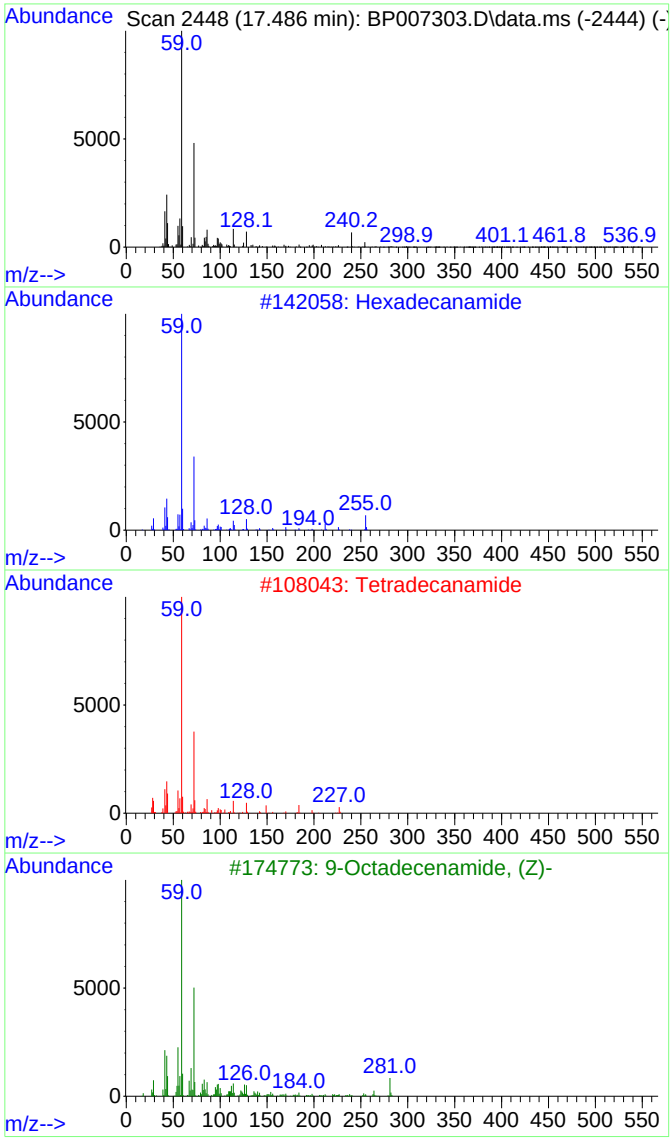
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

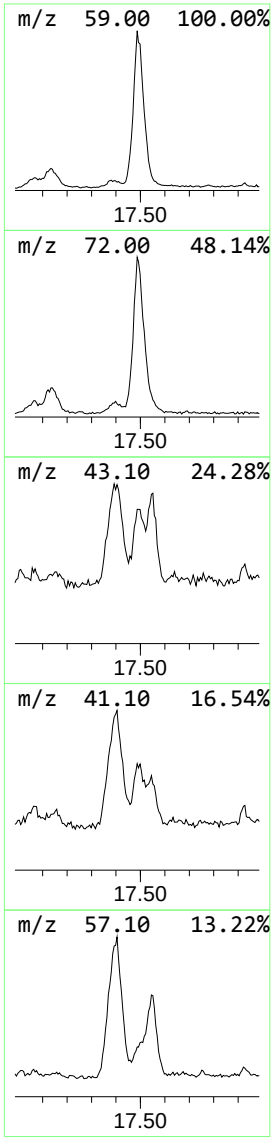
**********

Peak Number 5 Hexadecanamide Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.486 | 2.35 ng | 219515 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanamide | 255 | C16H33NO | 000629-54-9 | 86 |
| 2 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 78 |
| 3 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 72 |
| 4 | Dodecanamide | 199 | C12H25NO | 001120-16-7 | 68 |
| 5 | Pentanamide, 4-methyl- | 115 | C6H13NO | 001119-29-5 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

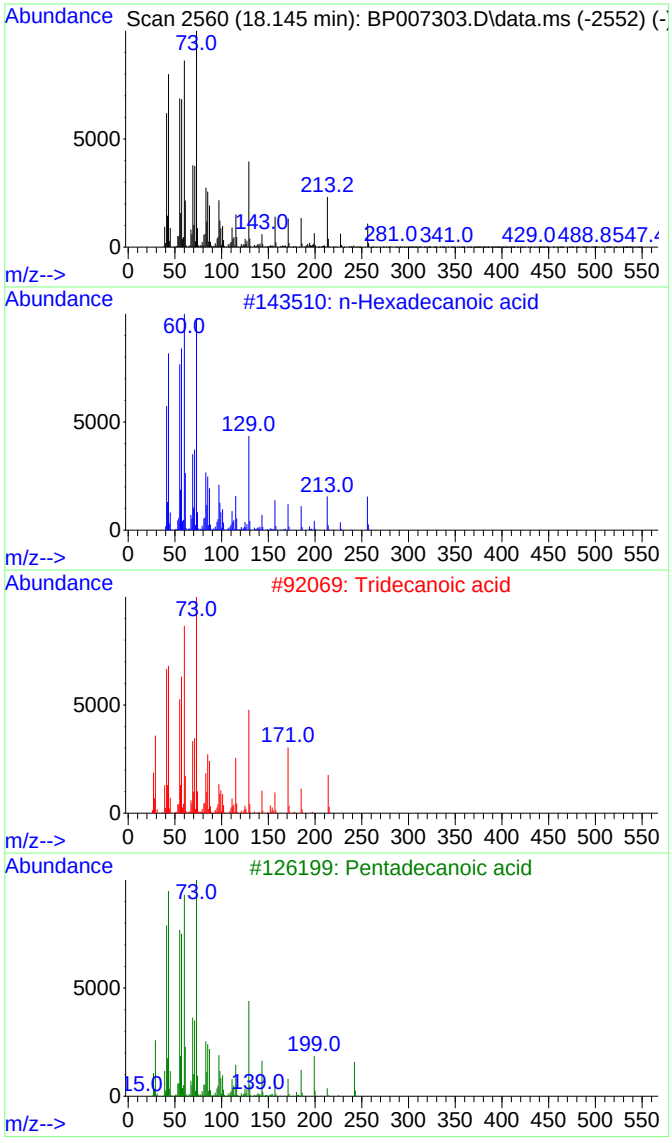
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

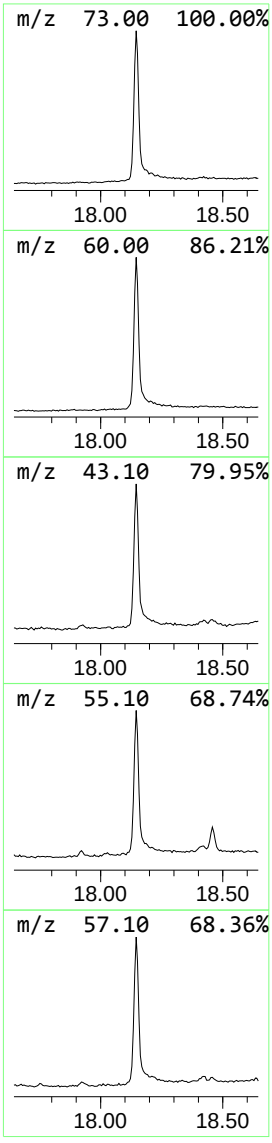
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.145 | 23.36 ng | 2181100 | 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 | 95 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

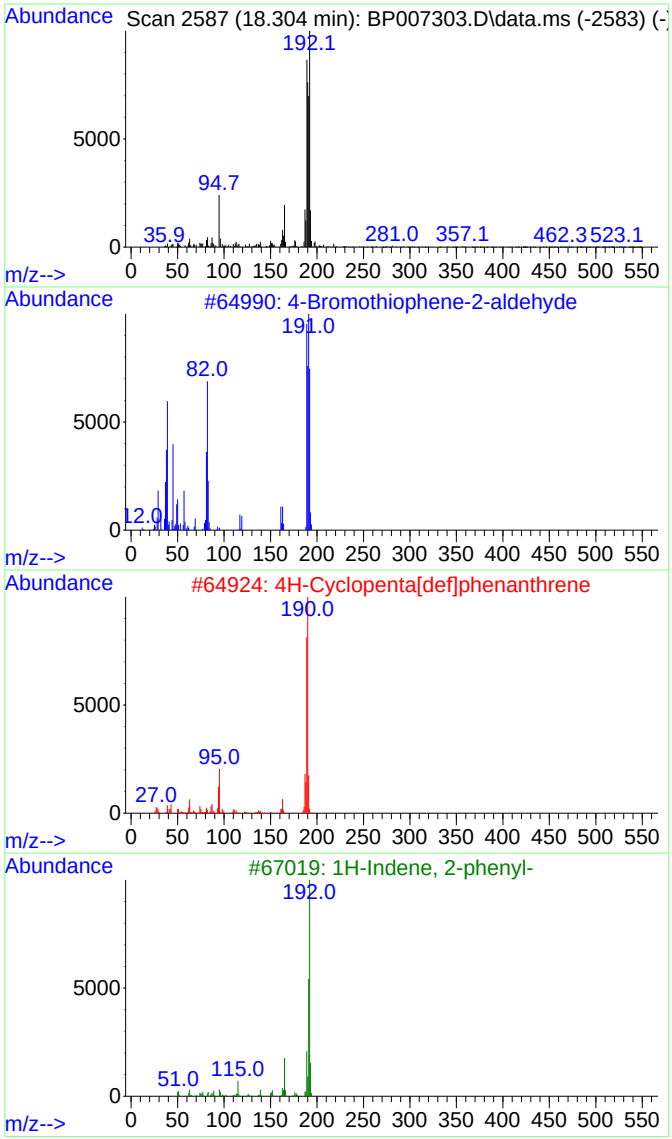
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

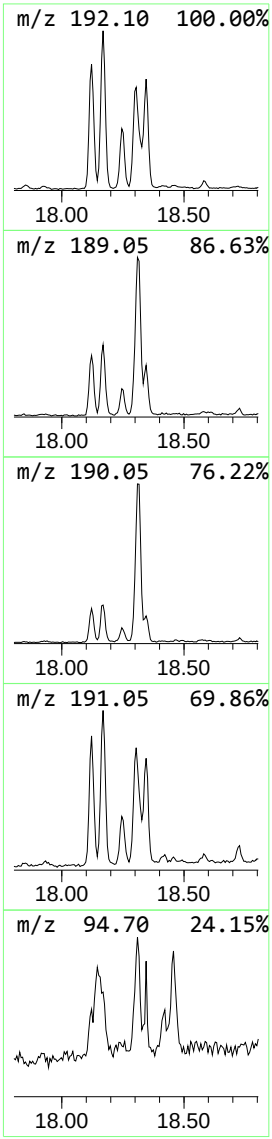
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 4-Bromothiophene-2-aldehyde Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.304 | 2.93 ng | 273800 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Bromothiophene-2-aldehyde | 190 | C5H3BrOS | 018791-75-8 | 58 |
| 2 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 49 |
| 3 | 1H-Indene, 2-phenyl- | 192 | C15H12 | 004505-48-0 | 46 |
| 4 | Phenanthrene, 1-methyl- | 192 | C15H12 | 000832-69-9 | 46 |
| 5 | Anthracene, 1-methyl- | 192 | C15H12 | 000610-48-0 | 46 |



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Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

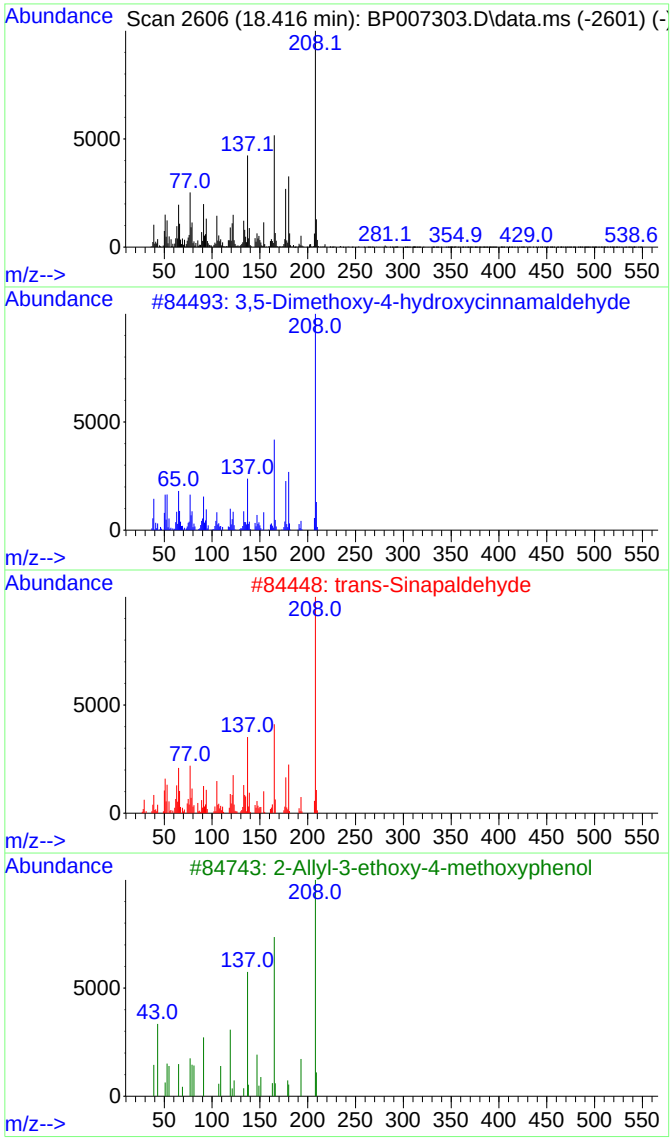
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

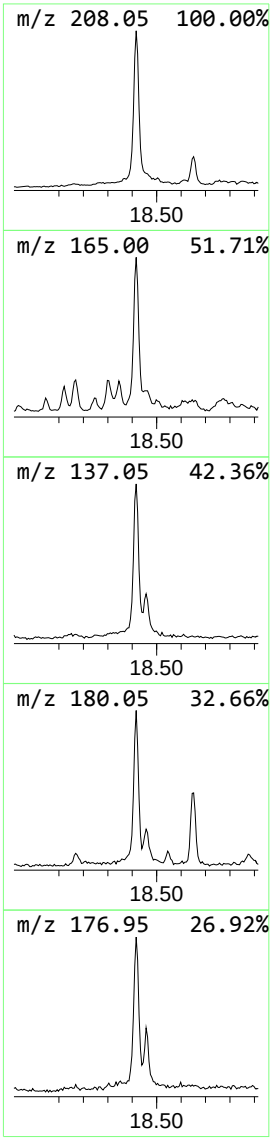
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.416 | 7.10 ng | 662850 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,5-Dimethoxy-4-hydroxycinnamald... | 208 | C11H12O4 | 087345-53-7 | 98 |
| 2 | trans-Sinapaldehyde | 208 | C11H12O4 | 004206-58-0 | 93 |
| 3 | 2-Allyl-3-ethoxy-4-methoxyphenol | 208 | C12H16O3 | 1000122-70-6 | 58 |
| 4 | 1,2-Dimethoxy-4-(3-methoxy-1-pro... | 208 | C12H16O3 | 1000313-35-0 | 50 |
| 5 | Acetic acid, (5-formyl-2-methoxy... | 208 | C11H12O4 | 099865-67-5 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

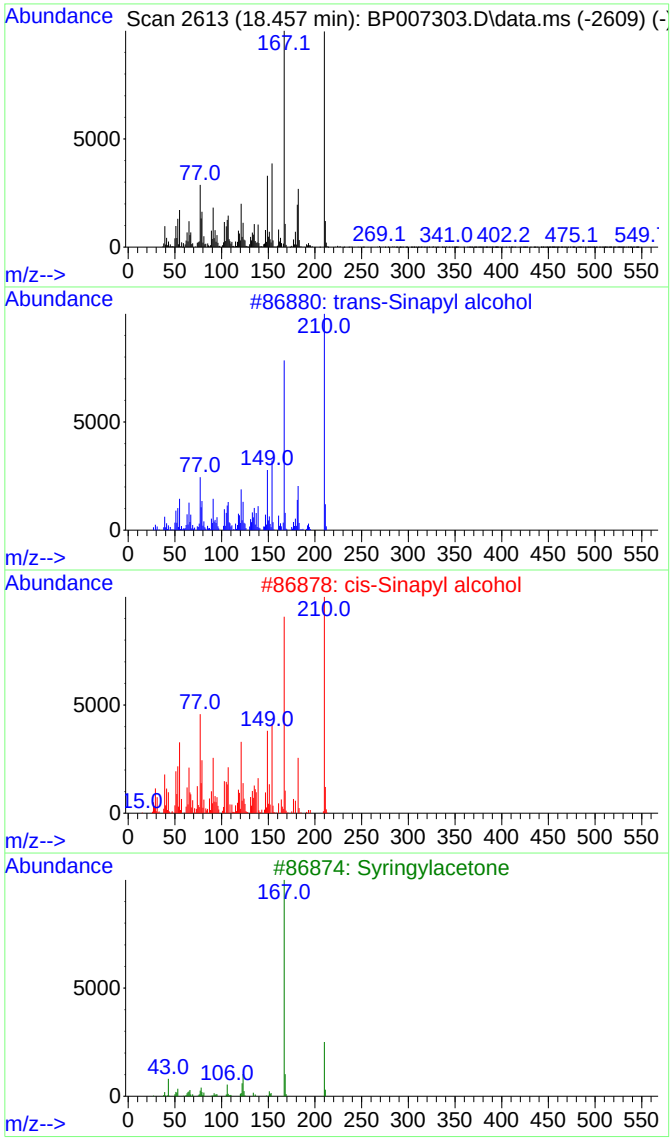
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

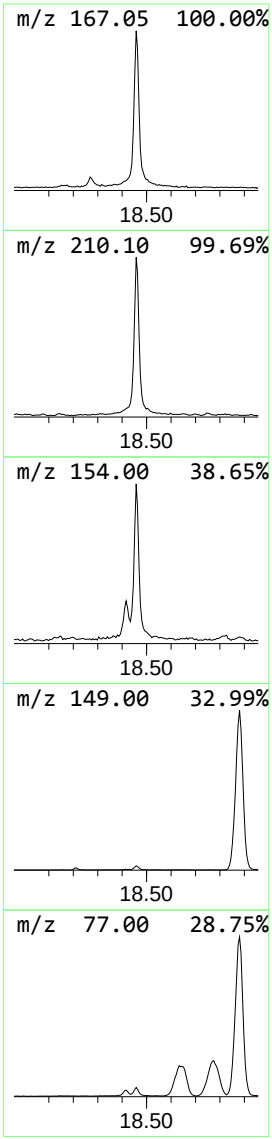
**********

Peak Number 9 trans-Sinapyl alcohol Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.457 | 11.42 ng | 1065960 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | trans-Sinapyl alcohol | 210 | C11H14O4 | 020675-96-1 | 96 |
| 2 | cis-Sinapyl alcohol | 210 | C11H14O4 | 104330-63-4 | 90 |
| 3 | Syringylacetone | 210 | C11H14O4 | 019037-58-2 | 60 |
| 4 | 2-methyl-3-(phenylethynyl)cycloh... | 210 | C15H14O | 1010466-55-6 | 47 |
| 5 | 1-Hydroxy-6-methylphenazine | 210 | C13H10N2O | 014031-08-4 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

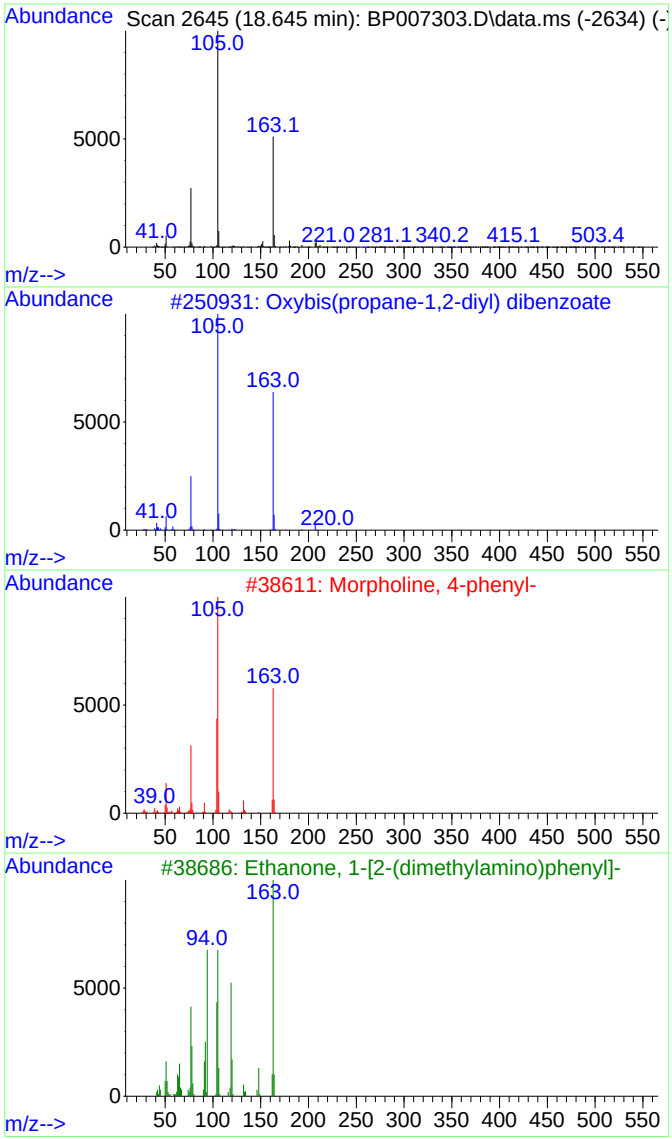
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

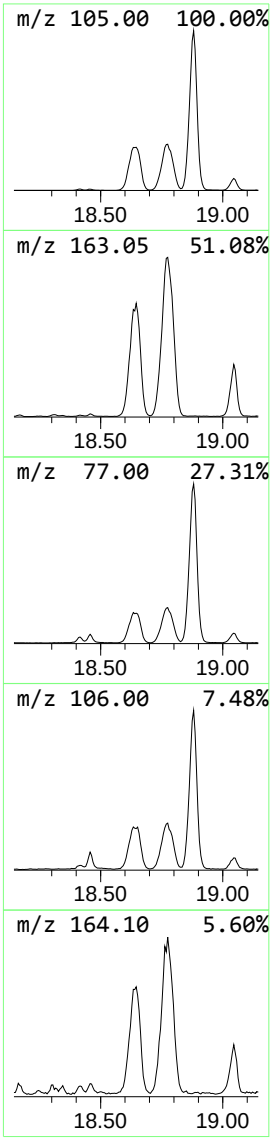
**********

Peak Number 10 unknown18.645 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.645 | 26.00 ng | 2427600 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxybis(propane-1,2-diyl) dibenzoate | 342 | C20H22O5 | 000094-03-1 | 78 |
| 2 | Morpholine, 4-phenyl- | 163 | C10H13NO | 000092-53-5 | 72 |
| 3 | Ethanone, 1-[2-(dimethylamino)ph... | 163 | C10H13NO | 010336-55-7 | 56 |
| 4 | Glyoxylamide, N-phenyl- | 163 | C9H9NO2 | 032331-52-5 | 47 |
| 5 | (3-Phenyloxiran-2-yl)methyl benz... | 254 | C16H14O3 | 1000366-96-1 | 33 |



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Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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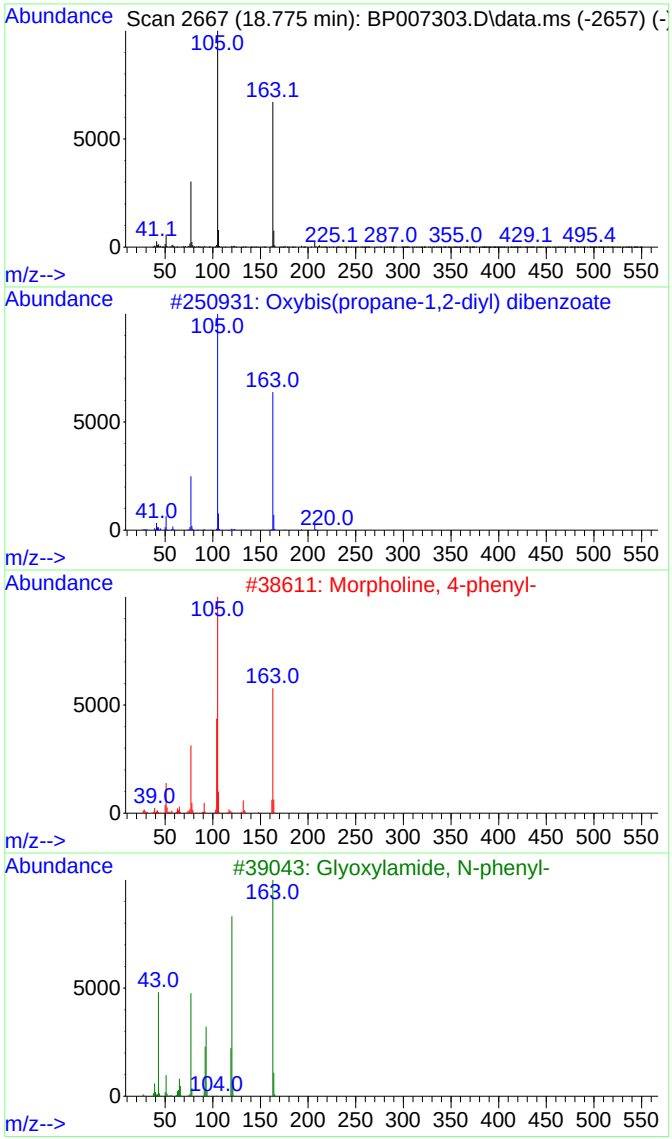
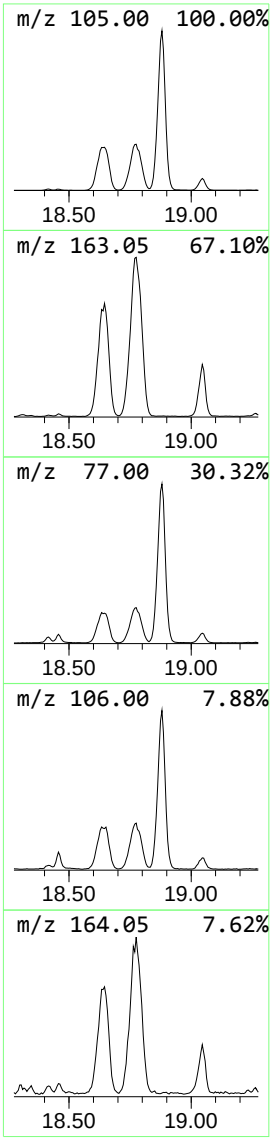
Peak Number 11 Oxybis(propane-1,2-diyl) di... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.775 | 35.44 ng | 3309090 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxybis(propane-1,2-diyl) dibenzoate | 342 | C20H22O5 | 000094-03-1 | 90 |
| 2 | Morpholine, 4-phenyl- | 163 | C10H13NO | 000092-53-5 | 72 |
| 3 | Glyoxylamide, N-phenyl- | 163 | C9H9NO2 | 032331-52-5 | 47 |
| 4 | .delta.2-1,3,4-Oxadiazolin-5-one... | 163 | C7H5N3O2 | 002845-82-1 | 38 |
| 5 | Benzoic acid, 2-benzyloxy-3-brom... | 348 | C17H17BrO3 | 1000191-33-3 | 36 |



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Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

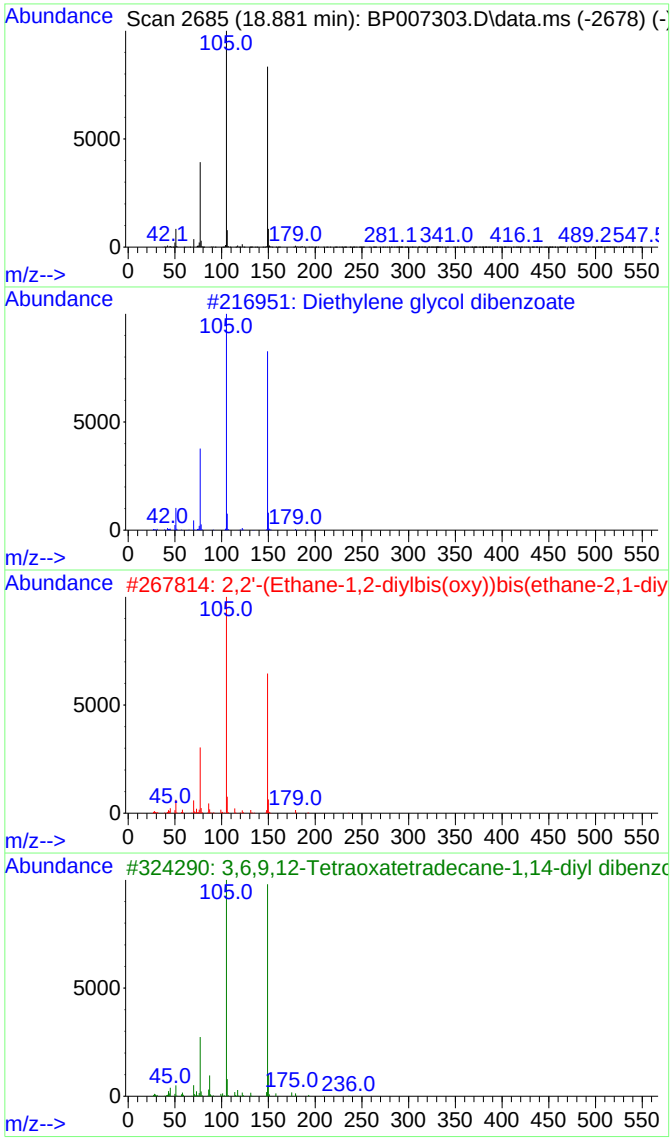
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

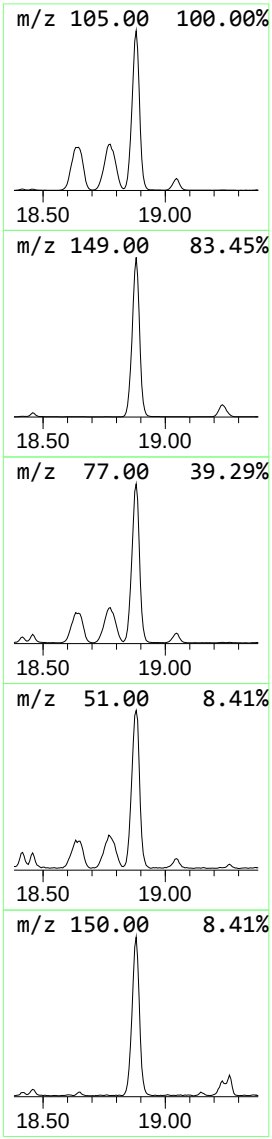
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 12 Diethylene glycol dibenzoate Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.881 | 72.26 ng | 6746500 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Diethylene glycol dibenzoate | 314 | C18H18O5 | 000120-55-8 | 91 |
| 2 | 2,2'-(Ethane-1,2-diylbis(oxy))bi... | 358 | C20H22O6 | 1000366-99-4 | 83 |
| 3 | 3,6,9,12-Tetraoxatetradecane-1,1... | 446 | C24H30O8 | 1000366-97-0 | 78 |
| 4 | Phenyl(2-phenyl-1,3-dioxolan-2-y... | 270 | C17H18O3 | 1000507-07-6 | 72 |
| 5 | Benzoic acid, 2-(3-nitrophenyl)e... | 271 | C15H13NO4 | 1000368-22-4 | 72 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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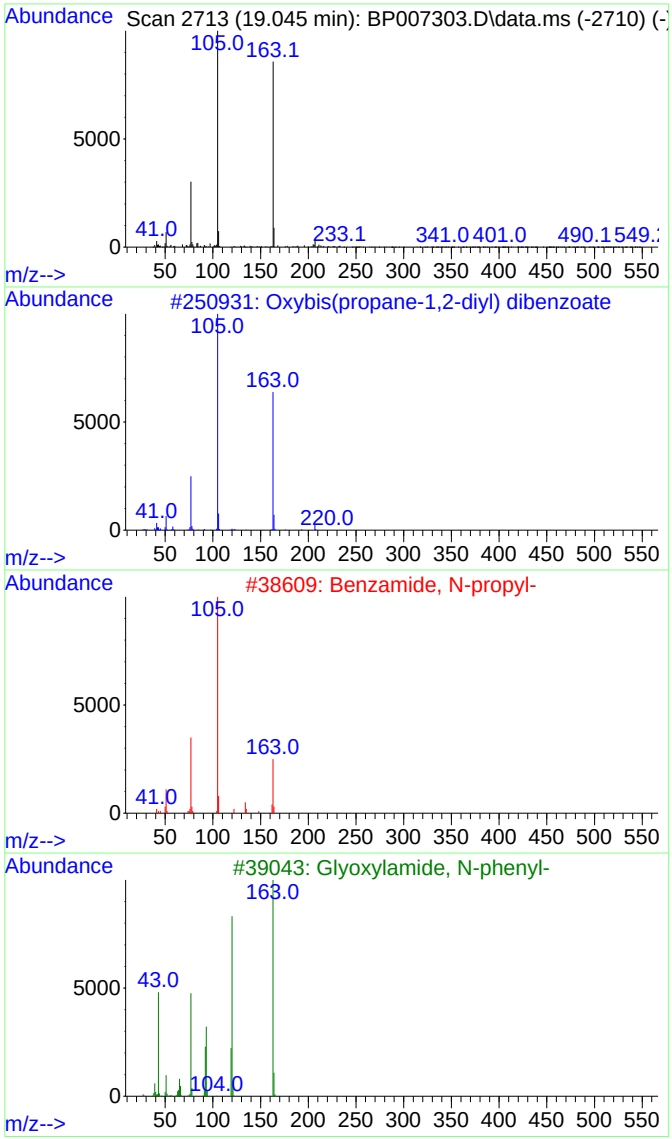
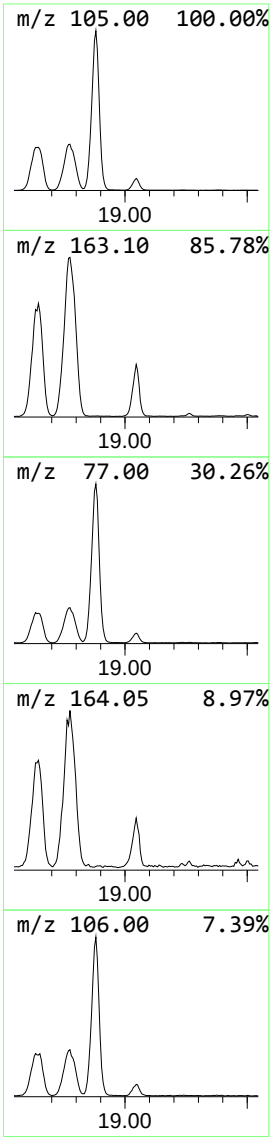
Peak Number 13 Benzamide, N-propyl- Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.045 | 4.69 ng | 438125 | Phenanthrene-d10 | 17.251 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxybis(propane-1,2-diyl) dibenzoate | 342 | C20H22O5 | 000094-03-1 | 78 |
| 2 | Benzamide, N-propyl- | 163 | C10H13NO | 010546-70-0 | 64 |
| 3 | Glyoxylamide, N-phenyl- | 163 | C9H9NO2 | 032331-52-5 | 53 |
| 4 | 3,5-Dimethylphenyl isothiocyanate | 163 | C9H9NS | 040046-30-8 | 50 |
| 5 | .delta.2-1,3,4-Oxadiazolin-5-one... | 163 | C7H5N3O2 | 002845-82-1 | 47 |



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Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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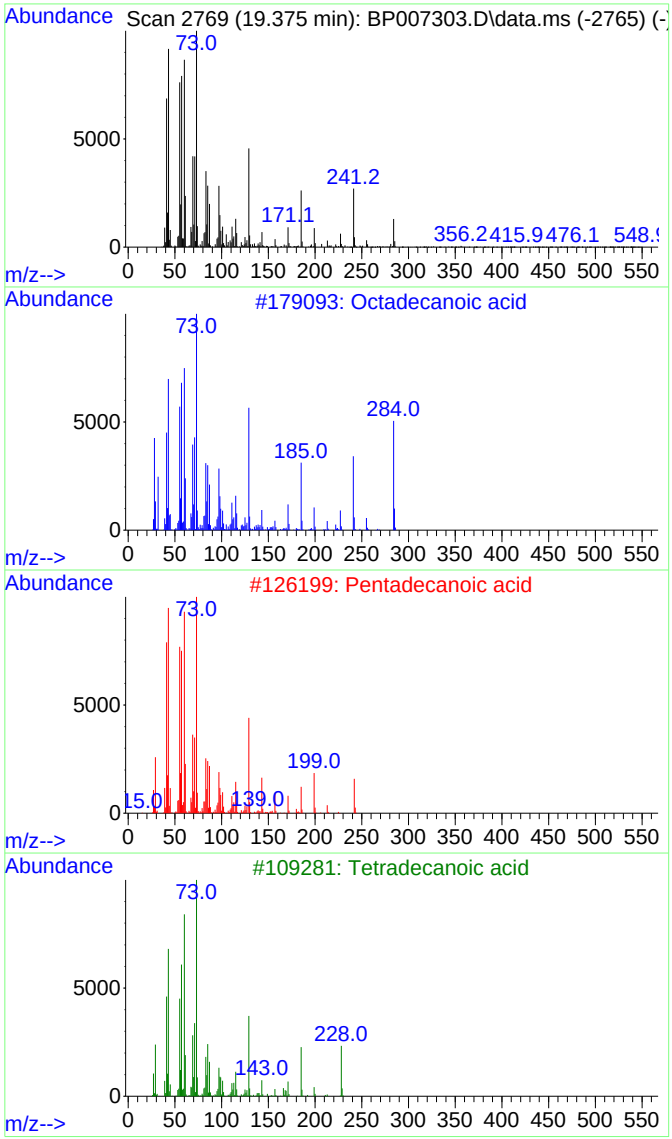
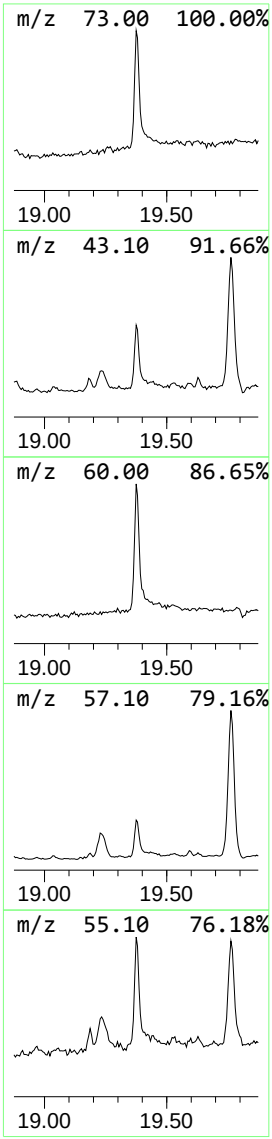
Peak Number 14 Octadecanoic acid Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.375 | 2.42 ng | 522401 | Chrysene-d12 | 21.345 |

| 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 | 83 |
| 4 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 74 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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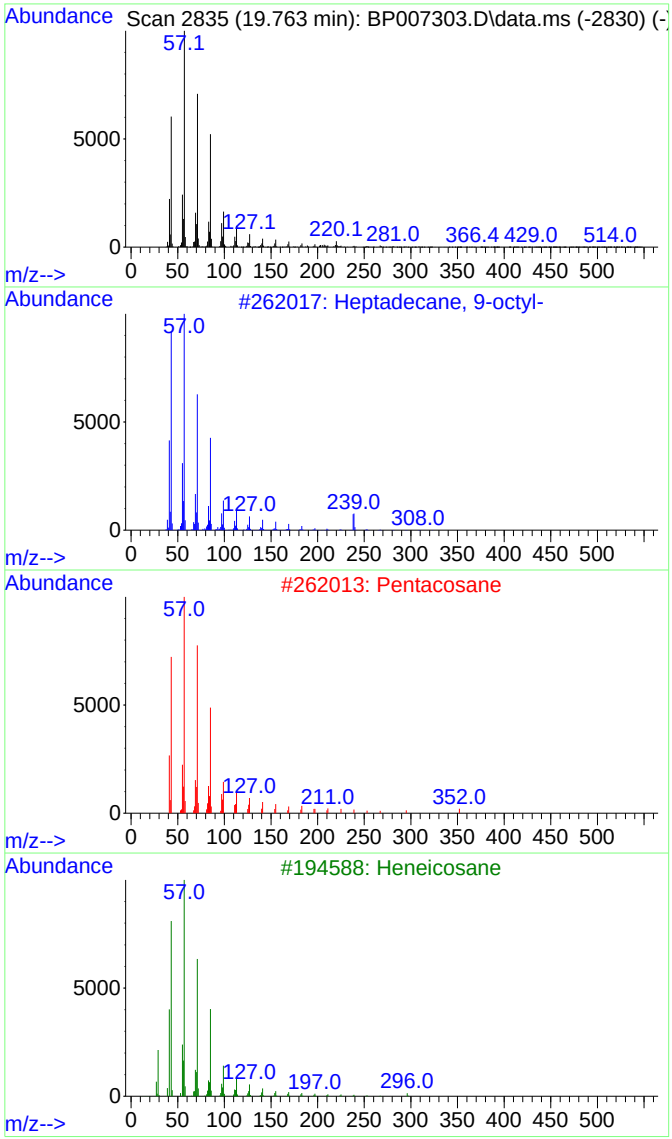
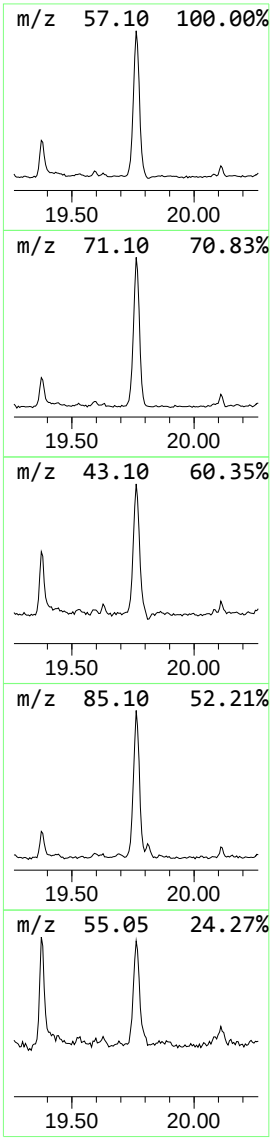
Peak Number 15 Heptadecane, 9-octyl- Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.763 | 4.20 ng | 908046 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 2 | Pentacosane | 352 | C25H52 | 000629-99-2 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Eicosane, 1-iodo- | 408 | C20H41I | 1000406-31-8 | 91 |
| 5 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 87 |



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Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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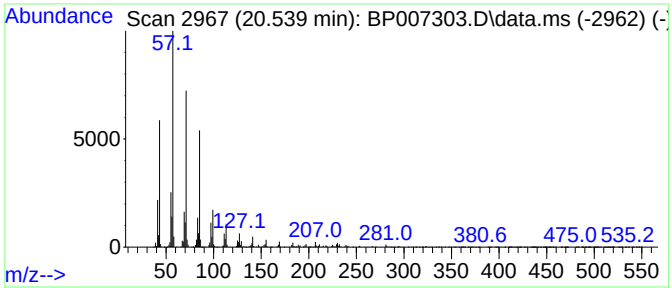
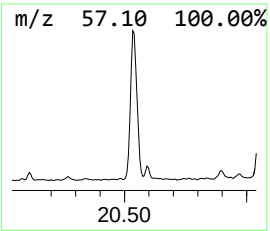
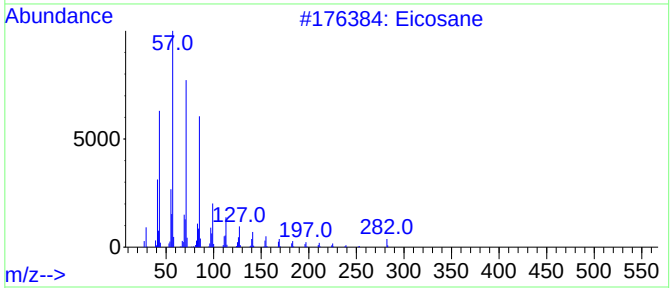
Peak Number 16 Eicosane Concentration Rank 12

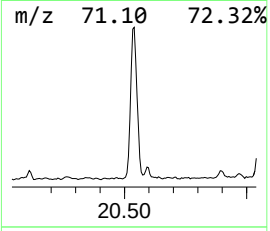
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.539 | 6.57 ng | 1418200 | Chrysene-d12 | 21.345 |

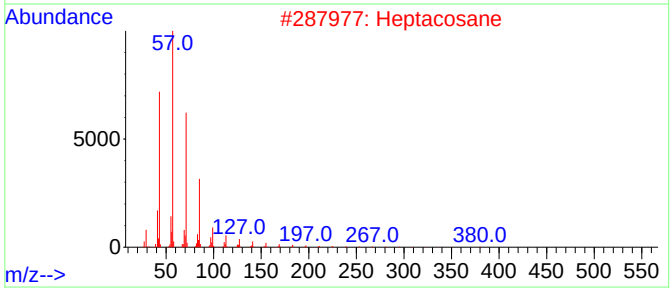
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 98 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 95 |
| 3 | Heptadecane, 9-hexyl- | 324 | C23H48 | 055124-79-3 | 94 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 94 |
| 5 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 93 |

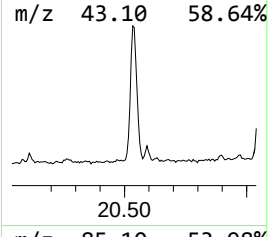


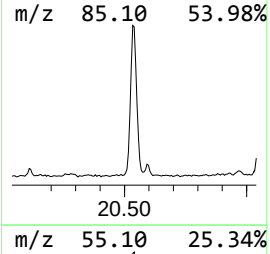



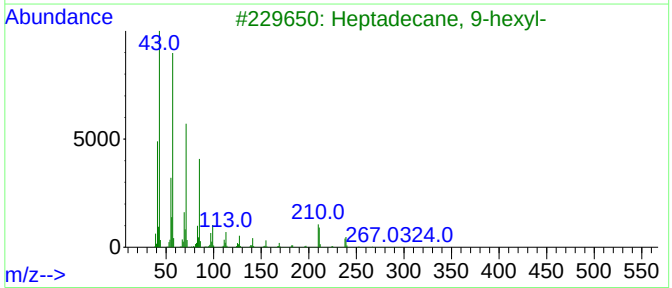



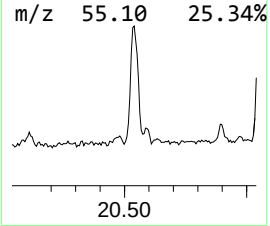



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Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

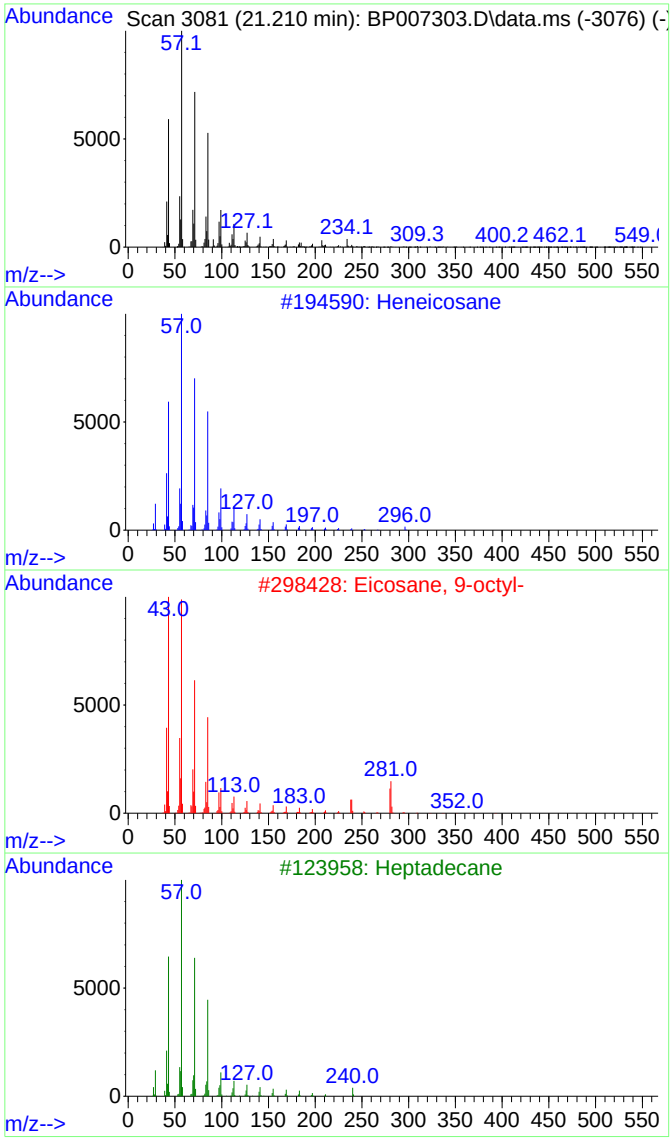
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

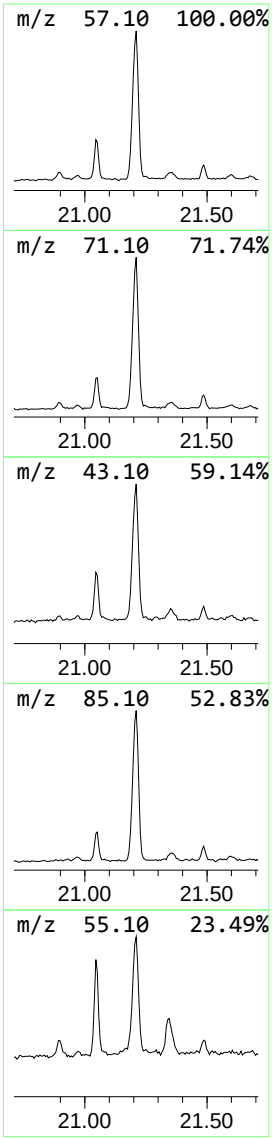
**********

Peak Number 17 Heneicosane Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.210 | 6.01 ng | 1297010 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 97 |
| 2 | Eicosane, 9-octyl- | 394 | C28H58 | 013475-77-9 | 94 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 93 |
| 4 | Docosane, 7-hexyl- | 394 | C28H58 | 055373-86-9 | 93 |
| 5 | Pentadecane, 8-hexyl- | 296 | C21H44 | 013475-75-7 | 93 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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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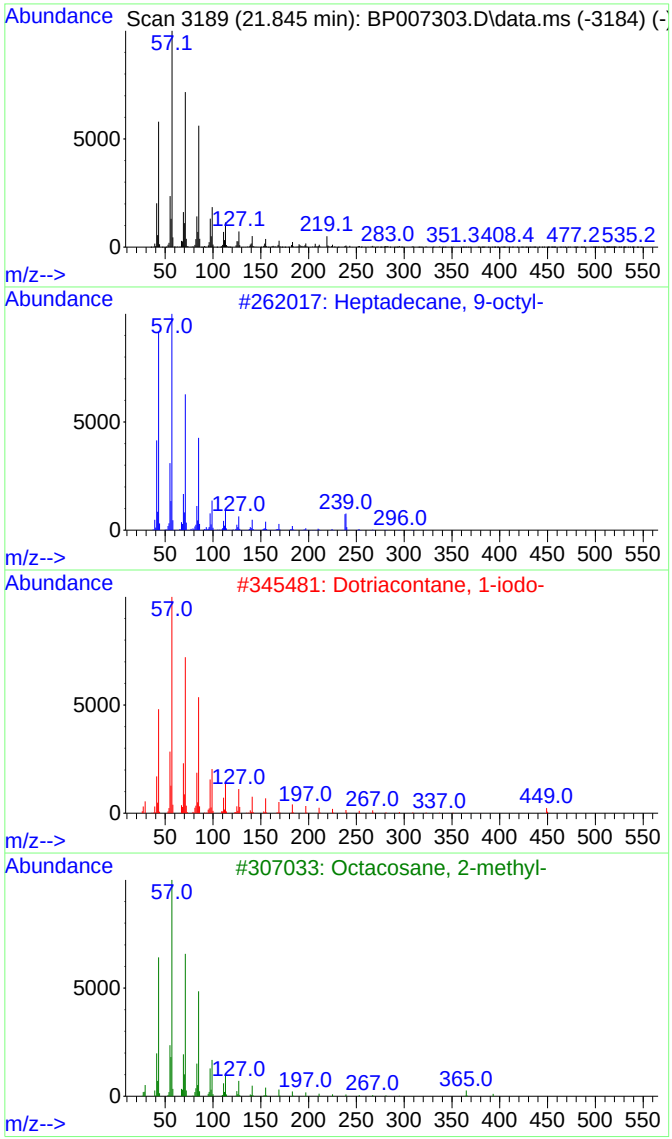
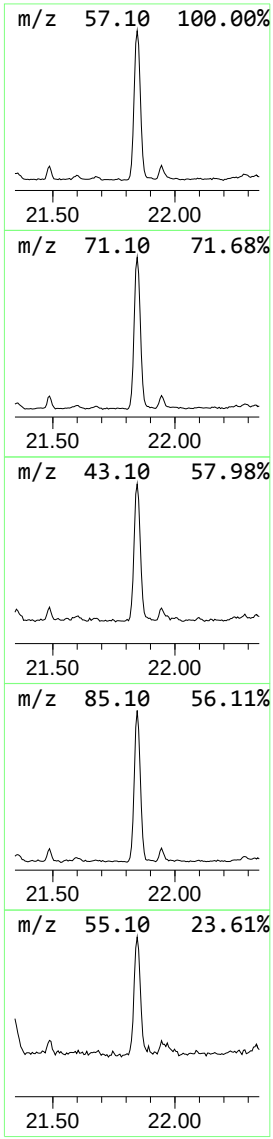
Peak Number 18 Dotriacontane, 1-iodo- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.845 | 7.13 ng | 1539610 | Chrysene-d12 | 21.345 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 2 | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 91 |
| 3 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |



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Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

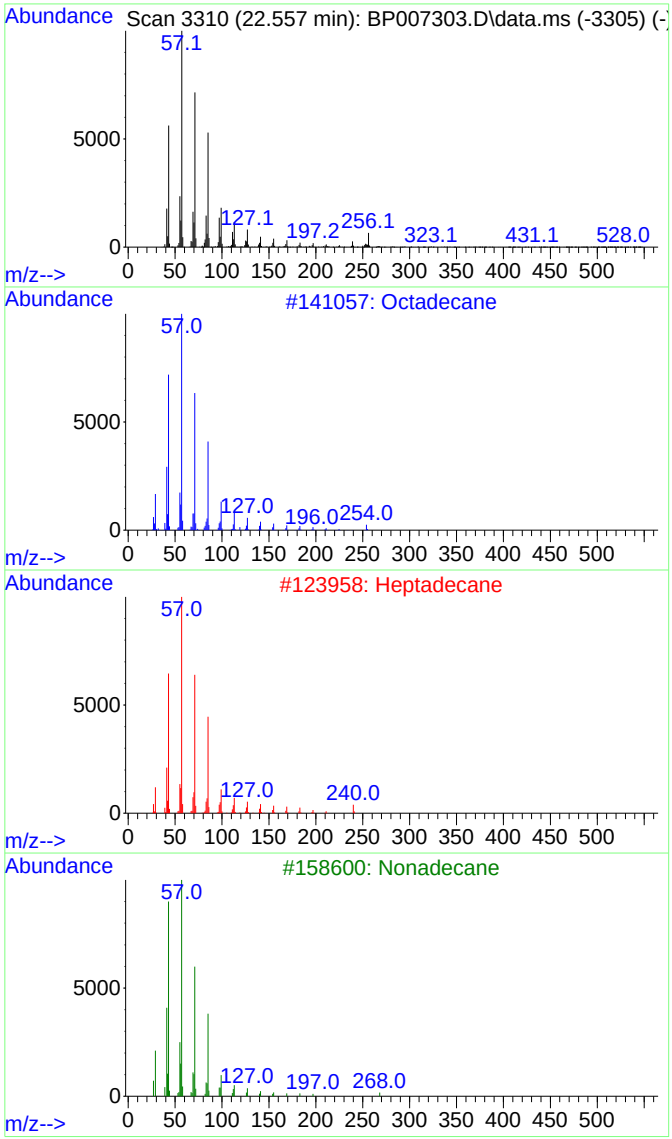
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

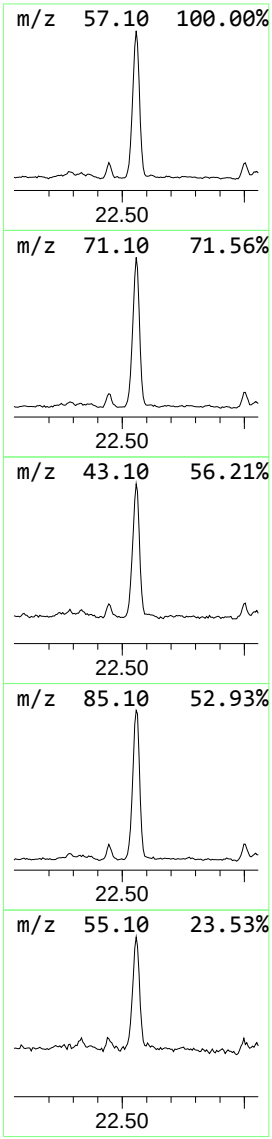
**********

Peak Number 19 Octadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.557 | 12.59 ng | 1432170 | Perylene-d12 | 23.751 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane | 254 | C18H38 | 000593-45-3 | 95 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 94 |
| 3 | Nonadecane | 268 | C19H40 | 000629-92-5 | 94 |
| 4 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 91 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

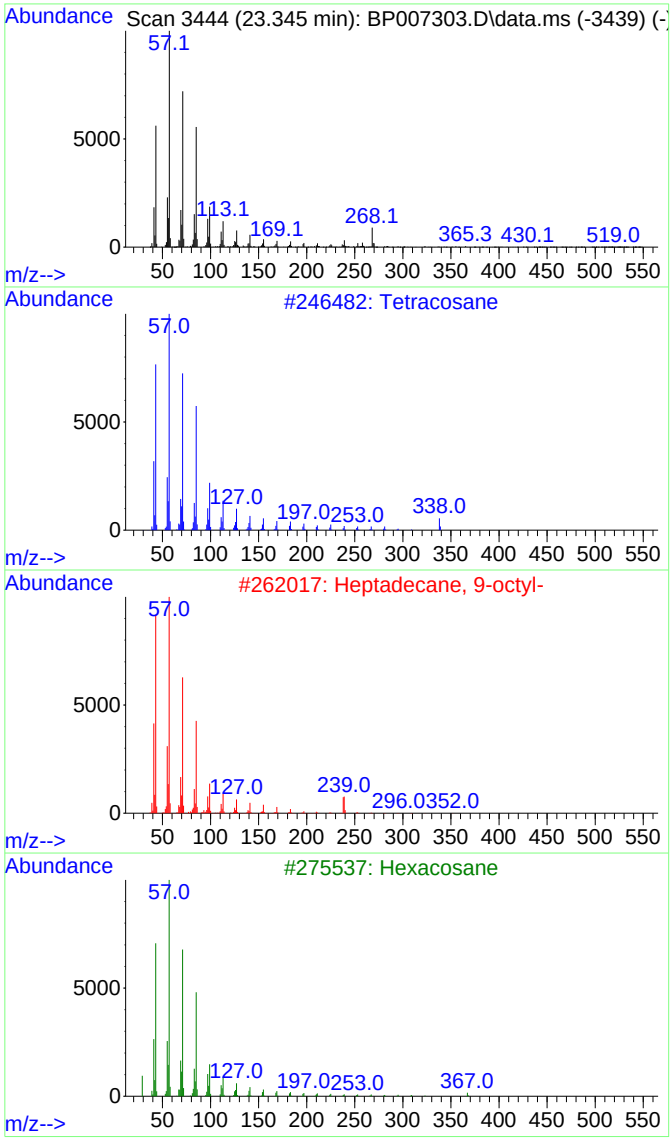
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

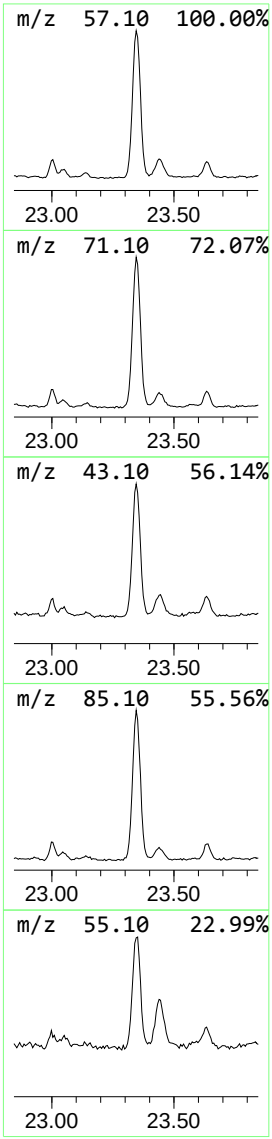
**********

Peak Number 20 Tetracosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.345 | 13.13 ng | 1493150 | Perylene-d12 | 23.751 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 98 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 94 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 93 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 90 |
| 5 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100421\
Data File : BP007303.D
Acq On : 04 Oct 2021 14:05
Operator : CG/JU
Sample : M4035-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 286

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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 |
| Ethanol, 2-(2-b... | 10.446 | 3.7 | ng | 261641 | 2 | 10.663 | 1426140 | 20.0 |
| L-Pyroglutamic ... | 15.763 | 2.2 | ng | 190442 | 3 | 14.498 | 1697370 | 20.0 |
| (E)-4-(3-Hydrox... | 16.651 | 6.9 | ng | 645186 | 4 | 17.251 | 1867360 | 20.0 |
| Hexadecanamide | 17.486 | 2.4 | ng | 219515 | 4 | 17.251 | 1867360 | 20.0 |
| n-Hexadecanoic ... | 18.145 | 23.4 | ng | 2181100 | 4 | 17.251 | 1867360 | 20.0 |
| 4-Bromothiophen... | 18.304 | 2.9 | ng | 273800 | 4 | 17.251 | 1867360 | 20.0 |
| 3,5-Dimethoxy-4... | 18.416 | 7.1 | ng | 662850 | 4 | 17.251 | 1867360 | 20.0 |
| trans-Sinapyl a... | 18.457 | 11.4 | ng | 1065960 | 4 | 17.251 | 1867360 | 20.0 |
| unknown18.645 | 18.645 | 26.0 | ng | 2427600 | 4 | 17.251 | 1867360 | 20.0 |
| Oxybis(propane-... | 18.775 | 35.4 | ng | 3309090 | 4 | 17.251 | 1867360 | 20.0 |
| Diethylene glyc... | 18.881 | 72.3 | ng | 6746500 | 4 | 17.251 | 1867360 | 20.0 |
| Benzamide, N-pr... | 19.045 | 4.7 | ng | 438125 | 4 | 17.251 | 1867360 | 20.0 |
| Octadecanoic acid | 19.375 | 2.4 | ng | 522401 | 5 | 21.345 | 4319200 | 20.0 |
| Heptadecane, 9-... | 19.763 | 4.2 | ng | 908046 | 5 | 21.345 | 4319200 | 20.0 |
| Eicosane | 20.539 | 6.6 | ng | 1418200 | 5 | 21.345 | 4319200 | 20.0 |
| Heneicosane | 21.210 | 6.0 | ng | 1297010 | 5 | 21.345 | 4319200 | 20.0 |
| Dotriacontane, ... | 21.845 | 7.1 | ng | 1539610 | 5 | 21.345 | 4319200 | 20.0 |
| Octadecane | 22.557 | 12.6 | ng | 1432170 | 6 | 23.751 | 2274430 | 20.0 |
| Tetracosane | 23.345 | 13.1 | ng | 1493150 | 6 | 23.751 | 2274430 | 20.0 |