LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

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-BP042921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005414.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.228 | 357 | 364 | 373 | rBV | 543056 | 749980 | 25.99% | 5.059% |
| 2 | 6.816 | 627 | 634 | 646 | rBV | 479643 | 751305 | 26.04% | 5.068% |
| 3 | 7.622 | 763 | 771 | 778 | rBV | 99094 | 152282 | 5.28% | 1.027% |
| 4 | 8.787 | 961 | 969 | 980 | rBV | 297697 | 481975 | 16.70% | 3.251% |
| 5 | 10.410 | 1235 | 1245 | 1252 | rBV | 113116 | 196990 | 6.83% | 1.329% |
| 6 | 12.904 | 1661 | 1669 | 1678 | rBV | 853779 | 1201918 | 41.65% | 8.108% |
| 7 | 14.292 | 1900 | 1905 | 1923 | rVB | 260262 | 539893 | 18.71% | 3.642% |
| 8 | 14.734 | 1975 | 1980 | 1991 | rVB2 | 42304 | 84678 | 2.93% | 0.571% |
| 9 | 15.128 | 2043 | 2047 | 2055 | rVB | 41095 | 66380 | 2.30% | 0.448% |
| 10 | 15.798 | 2152 | 2161 | 2168 | rVB | 997667 | 1397203 | 48.42% | 9.425% |
| 11 | 16.098 | 2209 | 2212 | 2219 | rVB6 | 23037 | 36411 | 1.26% | 0.246% |
| 12 | 16.463 | 2269 | 2274 | 2282 | rVB3 | 79146 | 137827 | 4.78% | 0.930% |
| 13 | 17.057 | 2369 | 2375 | 2380 | rBV | 301899 | 420525 | 14.57% | 2.837% |
| 14 | 17.733 | 2486 | 2490 | 2495 | rBV5 | 38179 | 52147 | 1.81% | 0.352% |
| 15 | 17.969 | 2522 | 2530 | 2538 | rBV | 726798 | 1061755 | 36.80% | 7.162% |
| 16 | 18.239 | 2571 | 2576 | 2580 | rBV2 | 140262 | 205726 | 7.13% | 1.388% |
| 17 | 18.286 | 2580 | 2584 | 2594 | rVB | 193619 | 304277 | 10.55% | 2.053% |
| 18 | 18.486 | 2615 | 2618 | 2626 | rVB3 | 30212 | 46472 | 1.61% | 0.313% |
| 19 | 18.704 | 2649 | 2655 | 2665 | rVB2 | 50742 | 150178 | 5.20% | 1.013% |
| 20 | 18.822 | 2667 | 2675 | 2682 | rBV2 | 80785 | 225081 | 7.80% | 1.518% |
| 21 | 18.904 | 2683 | 2689 | 2700 | rVV | 217522 | 468454 | 16.24% | 3.160% |
| 22 | 19.086 | 2713 | 2720 | 2728 | rVB4 | 55968 | 113151 | 3.92% | 0.763% |
| 23 | 19.204 | 2735 | 2740 | 2757 | rVB | 340913 | 470704 | 16.31% | 3.175% |
| 24 | 19.439 | 2777 | 2780 | 2789 | rVB | 35134 | 59326 | 2.06% | 0.400% |
| 25 | 19.639 | 2808 | 2814 | 2824 | rBV | 2497456 | 2885443 | 100.00% | 19.464% |
| 26 | 19.957 | 2865 | 2868 | 2873 | rVB | 106984 | 121239 | 4.20% | 0.818% |
| 27 | 20.263 | 2916 | 2920 | 2923 | rBV3 | 58400 | 70458 | 2.44% | 0.475% |
| 28 | 20.310 | 2923 | 2928 | 2930 | rBV5 | 42013 | 69627 | 2.41% | 0.470% |
| 29 | 20.422 | 2944 | 2947 | 2951 | rVB5 | 34216 | 40669 | 1.41% | 0.274% |
| 30 | 20.874 | 3021 | 3024 | 3032 | rVB2 | 202663 | 307009 | 10.64% | 2.071% |
| 31 | 20.945 | 3032 | 3036 | 3045 | rBV2 | 253686 | 386588 | 13.40% | 2.608% |
| 32 | 21.163 | 3068 | 3073 | 3077 | rBV | 515282 | 628333 | 21.78% | 4.238% |
| 33 | 21.551 | 3136 | 3139 | 3144 | rVB2 | 52197 | 69974 | 2.43% | 0.472% |
| 34 | 21.733 | 3168 | 3170 | 3172 | rBV2 | 48431 | 54021 | 1.87% | 0.364% |
| 35 | 23.415 | 3450 | 3456 | 3465 | rVB | 355391 | 673632 | 23.35% | 4.544% |
| 36 | 24.710 | 3672 | 3676 | 3680 | rBV6 | 63723 | 143021 | 4.96% | 0.965% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

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-BP042921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

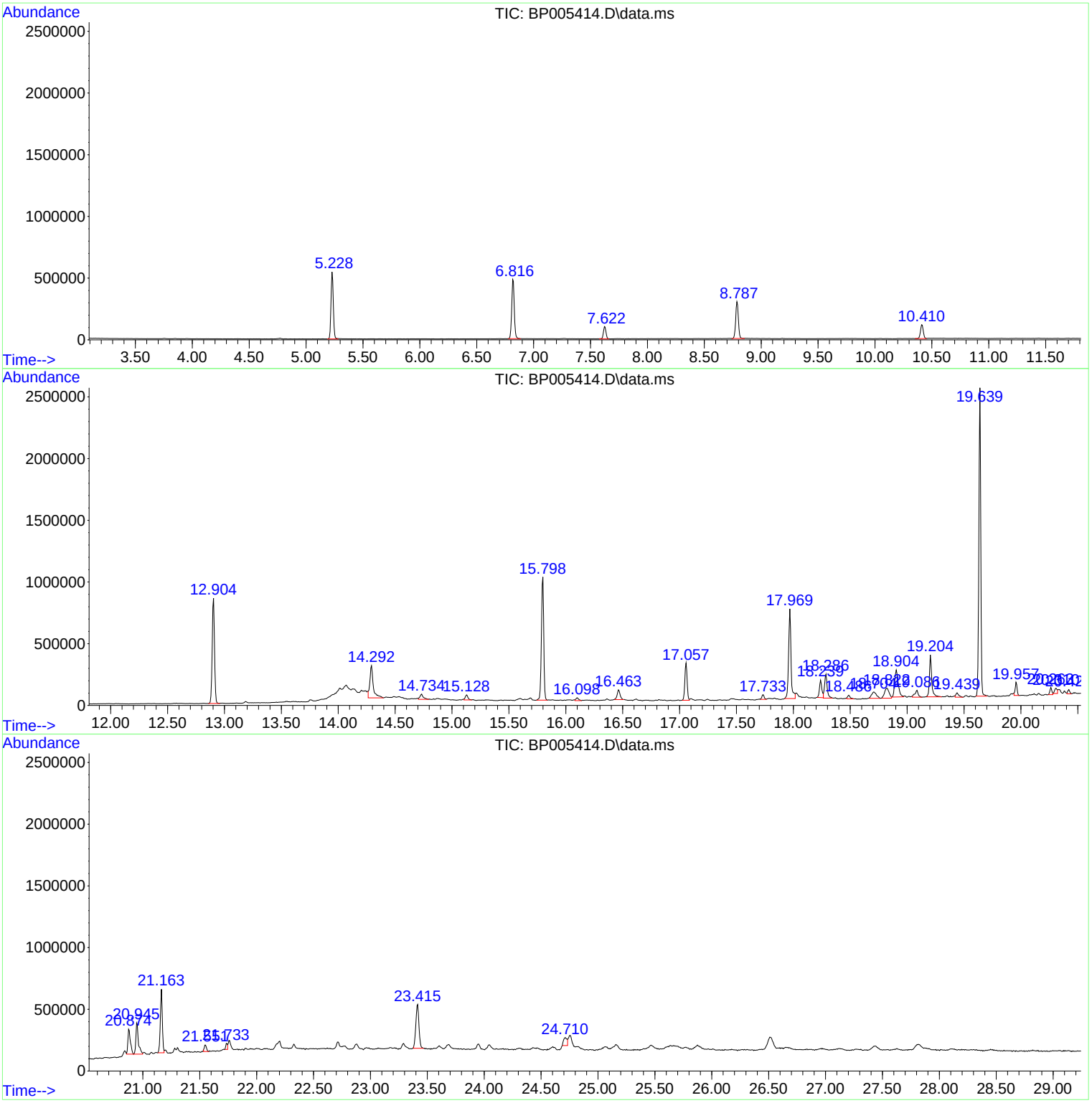
Sum of corrected areas: 14824652

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

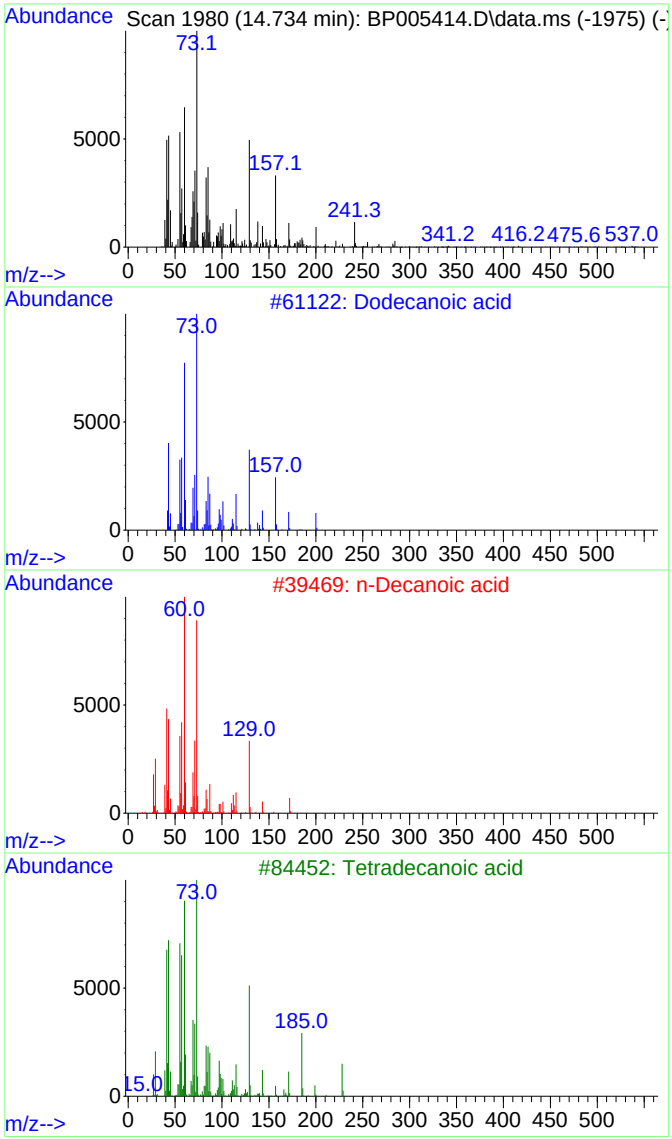
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

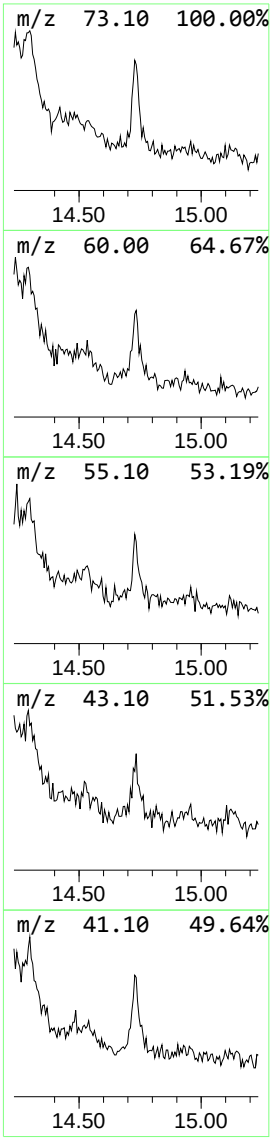
**********

Peak Number 1 Dodecanoic acid Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.734 | 3.14 ng | 84678 | Acenaphthene-d10 | 14.292 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 83 |
| 2 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 60 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 50 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 43 |
| 5 | 12-Bromododecanoic acid | 278 | C12H23BrO2 | 073367-80-3 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

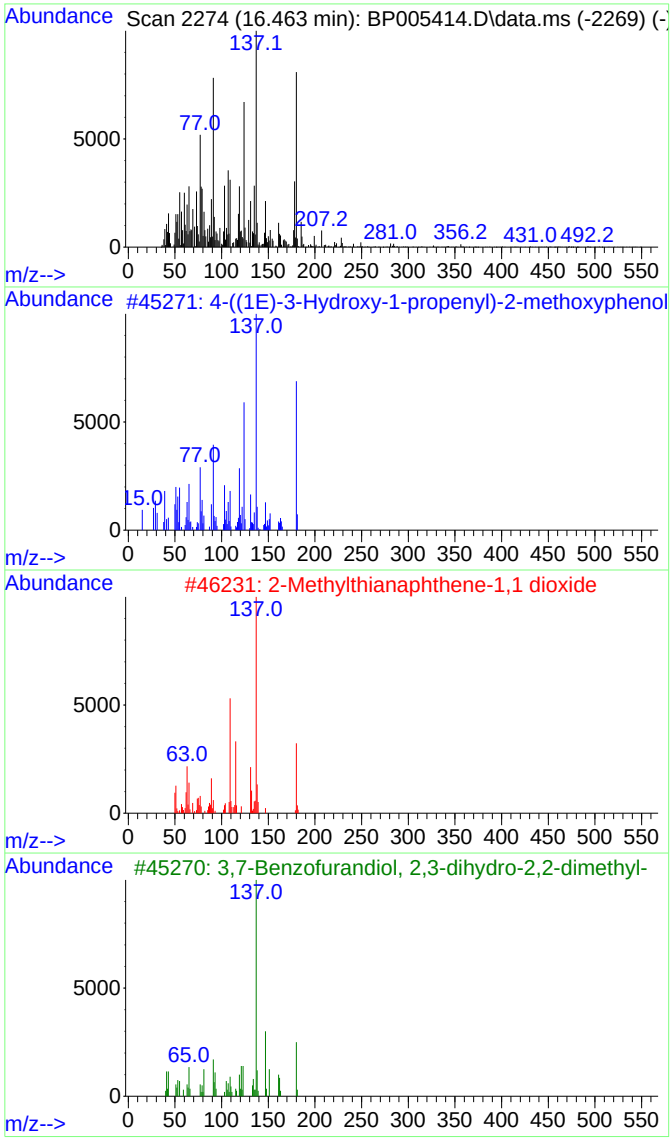
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

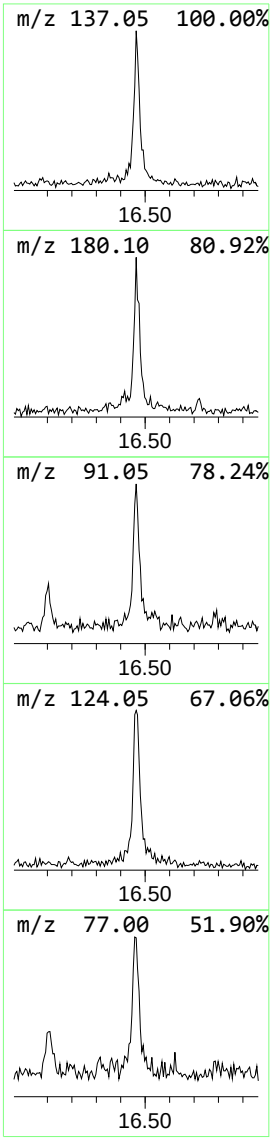
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 4-((1E)-3-Hydroxy-1-propeny... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.463 | 6.55 ng | 137827 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-((1E)-3-Hydroxy-1-propenyl)-2-... | 180 | C10H12O3 | 1000297-95-5 | 81 |
| 2 | 2-Methylthianaphthene-1,1 dioxide | 180 | C9H8O2S | 006224-55-1 | 53 |
| 3 | 3,7-Benzofurandiol, 2,3-dihydro-... | 180 | C10H12O3 | 017781-15-6 | 49 |
| 4 | Benzaldehyde, 2-hydroxy-, oxime | 137 | C7H7NO2 | 000094-67-7 | 47 |
| 5 | Ethanone, 2-chloro-1-(3,4-dihydr... | 186 | C8H7ClO3 | 000099-40-1 | 35 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

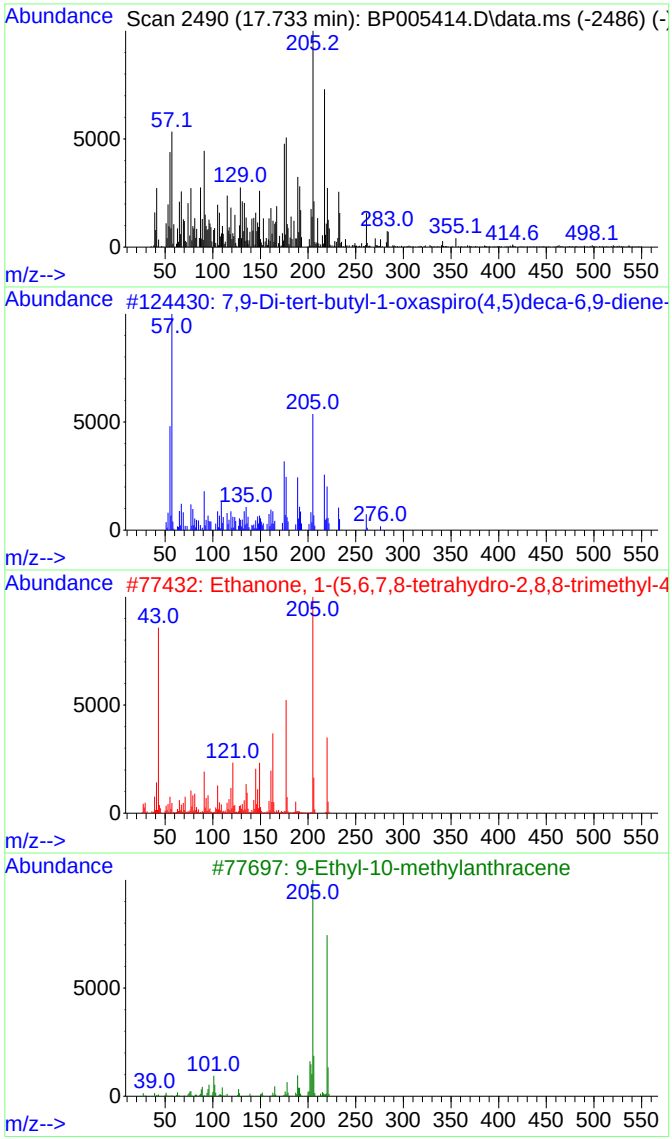
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

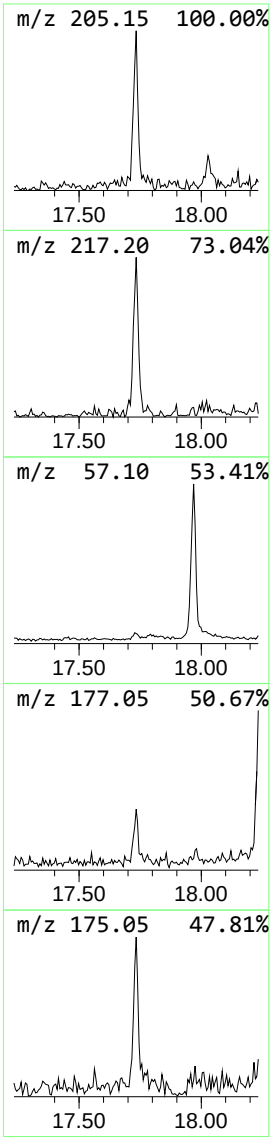
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.733 | 2.48 ng | 52147 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7,9-Di-tert-butyl-1-oxaspiro(4,5... | 276 | C17H24O3 | 082304-66-3 | 93 |
| 2 | Ethanone, 1-(5,6,7,8-tetrahydro-... | 220 | C14H20O2 | 071596-88-8 | 87 |
| 3 | 9-Ethyl-10-methylanthracene | 220 | C17H16 | 019713-49-6 | 42 |
| 4 | Thiophene, 2-(4-nitrophenyl)- | 205 | C10H7NO2S | 059156-21-7 | 41 |
| 5 | 4,6-di-tert-Butyl-m-cresol | 220 | C15H24O | 000497-39-2 | 41 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

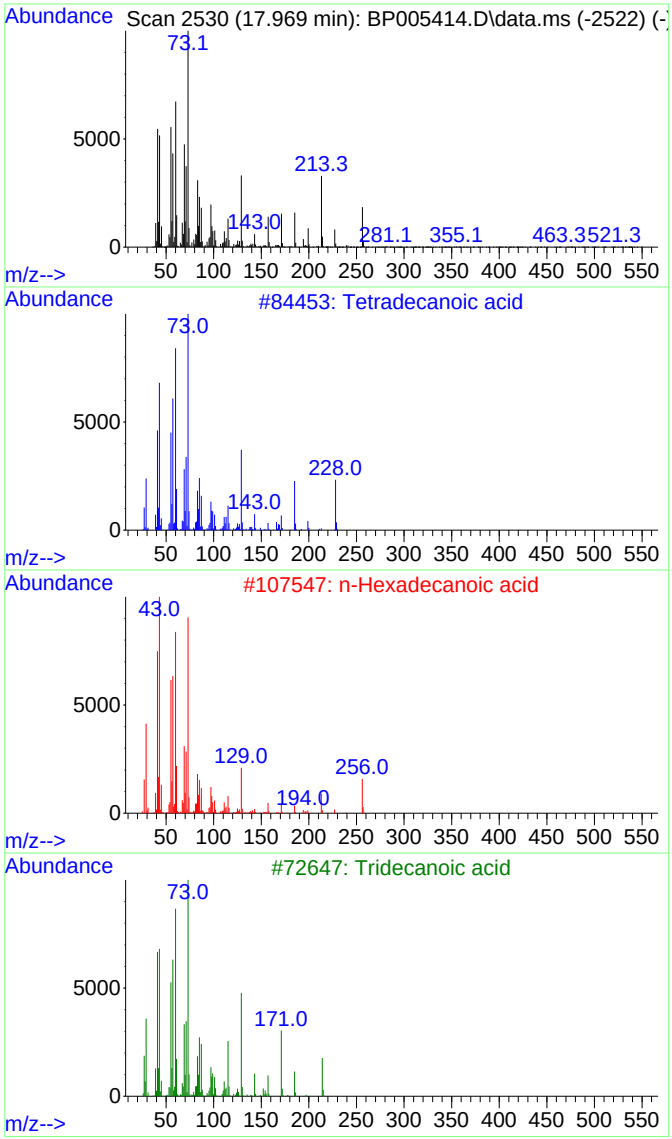
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

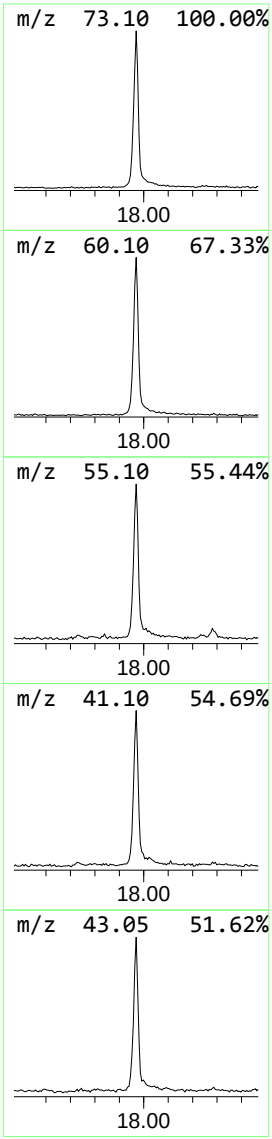
**********

Peak Number 4 Tetradecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.969 | 50.50 ng | 1061760 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 93 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 55 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 52 |
| 5 | N-Acetylisoxazolidine | 115 | C5H9NO2 | 115615-36-6 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

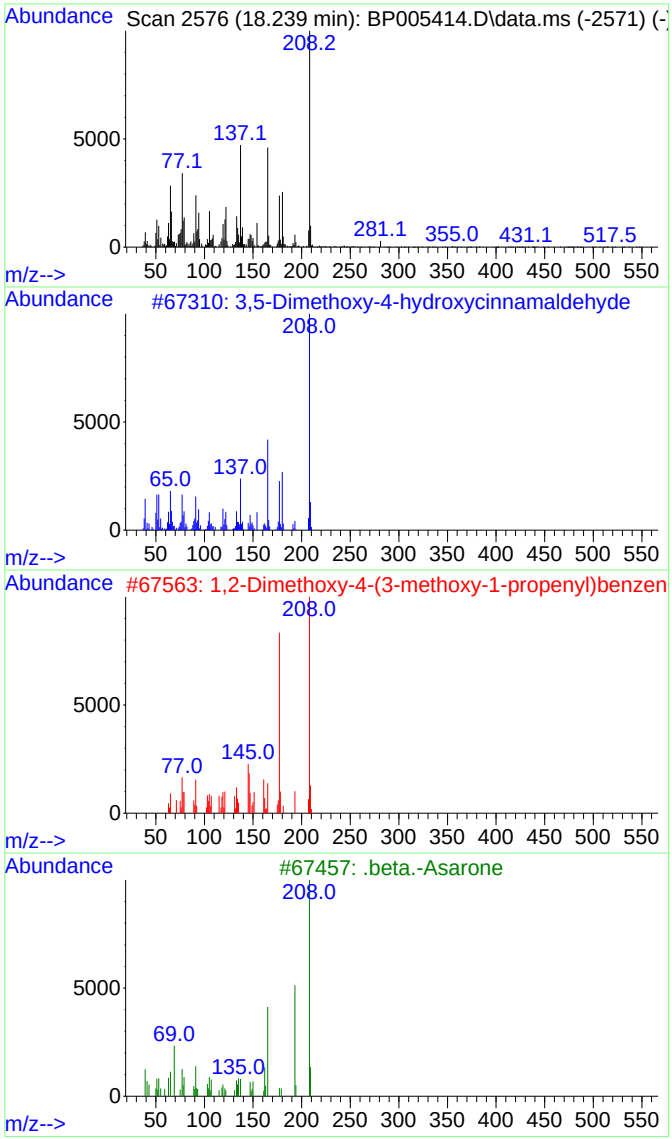
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

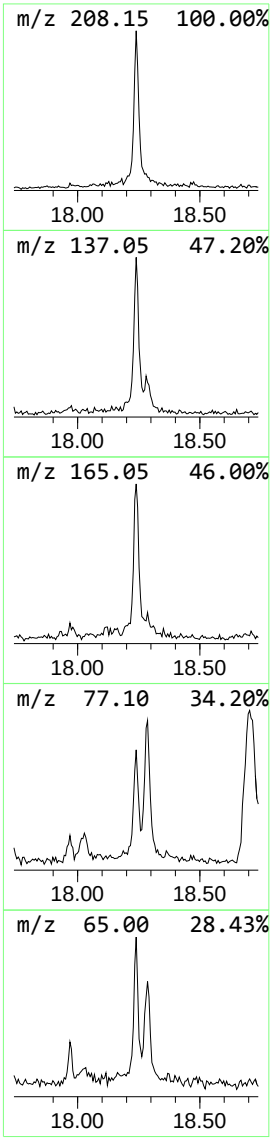
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.239 | 9.78 ng | 205726 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,5-Dimethoxy-4-hydroxycinnamald... | 208 | C11H12O4 | 087345-53-7 | 89 |
| 2 | 1,2-Dimethoxy-4-(3-methoxy-1-pro... | 208 | C12H16O3 | 1000313-35-0 | 46 |
| 3 | .beta.-Asarone | 208 | C12H16O3 | 005273-86-9 | 43 |
| 4 | trans-2,5-Dimethoxycinnamic acid | 208 | C11H12O4 | 038489-74-6 | 35 |
| 5 | Imidazo[5,4-e][1,4]diazepine-4,7... | 208 | C9H12N4O2 | 144105-22-6 | 32 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

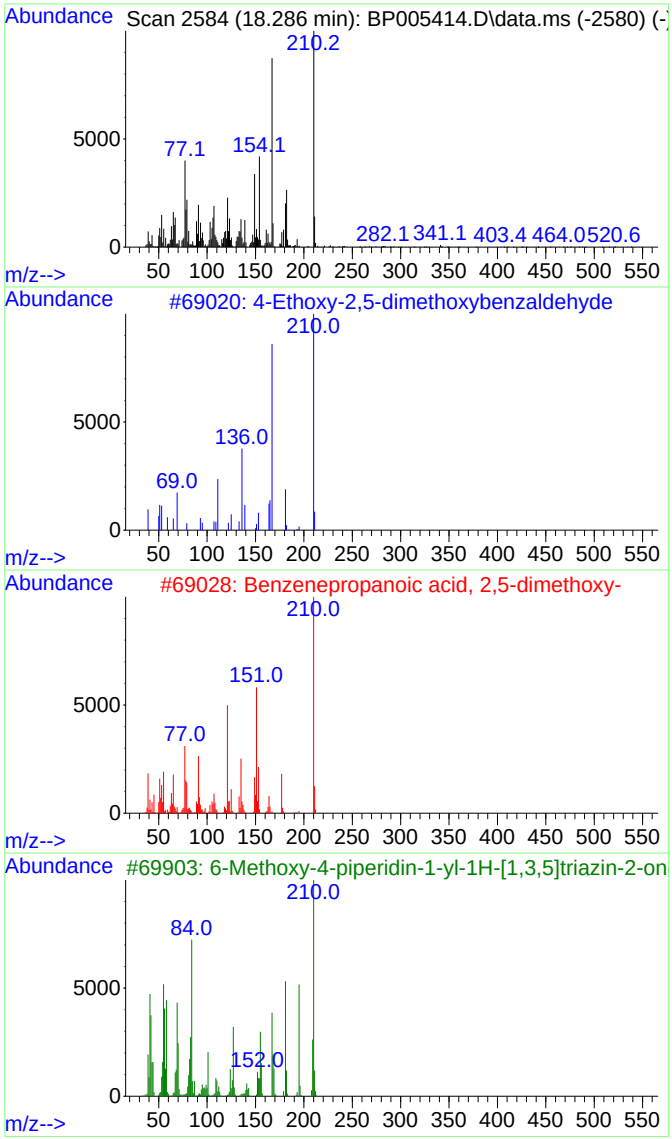
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

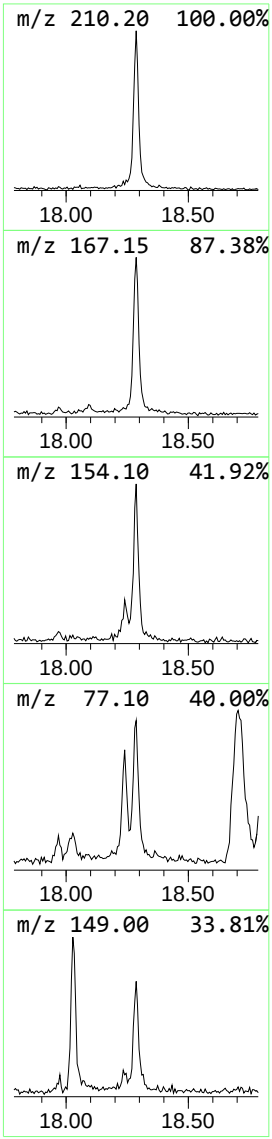
**********

Peak Number 6 unknown18.286 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.286 | 14.47 ng | 304277 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Ethoxy-2,5-dimethoxybenzaldehyde | 210 | C11H14O4 | 1000121-30-2 | 49 |
| 2 | Benzenepropanoic acid, 2,5-dimet... | 210 | C11H14O4 | 010538-49-5 | 38 |
| 3 | 6-Methoxy-4-piperidin-1-yl-1H-[1... | 210 | C9H14N4O2 | 1000300-24-3 | 30 |
| 4 | Phenol, 2,6-dimethyl-4-nitro- | 167 | C8H9NO3 | 002423-71-4 | 30 |
| 5 | Phenol, 2-(2-imidazo[1,2-a]pyrid... | 210 | C13H10N2O | 057636-32-5 | 30 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

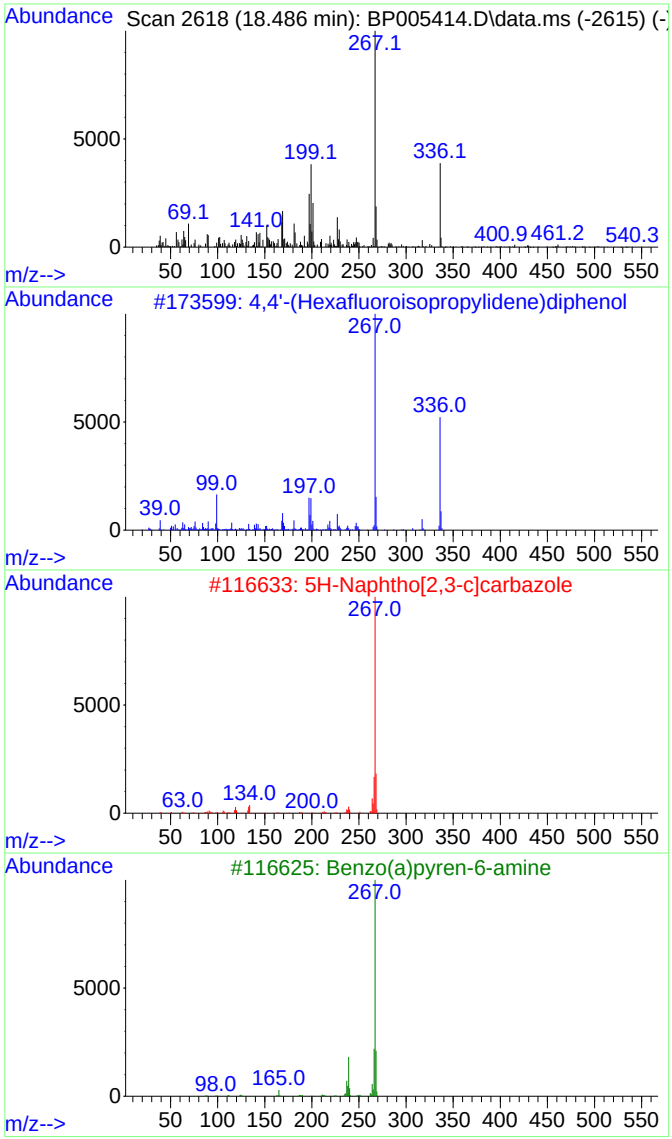
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

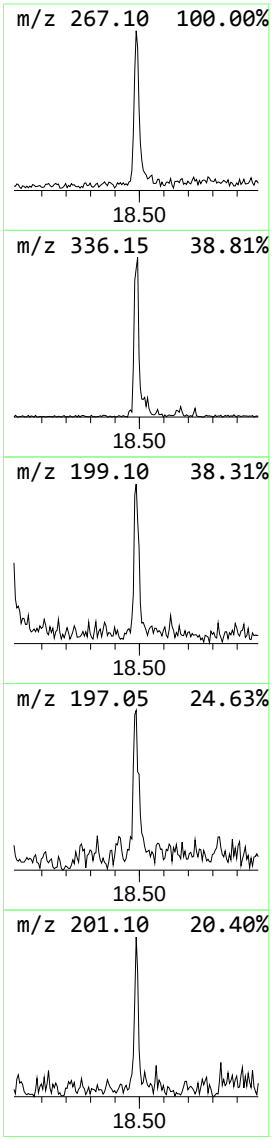
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 4,4'-(Hexafluoroisopropylid... Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.486 | 2.21 ng | 46472 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4,4'-(Hexafluoroisopropylidene)d... | 336 | C15H10F6O2 | 001478-61-1 | 70 |
| 2 | 5H-Naphtho[2,3-c]carbazole | 267 | C20H13N | 000198-96-9 | 30 |
| 3 | Benzo(a)pyren-6-amine | 267 | C20H13N | 007428-83-3 | 27 |
| 4 | Naphthalene, 1-chloro-2,6-dimeth... | 267 | C12H10ClNO4 | 025314-98-1 | 27 |
| 5 | 13H-Dibenzo[a,i]carbazole | 267 | C20H13N | 000239-64-5 | 27 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

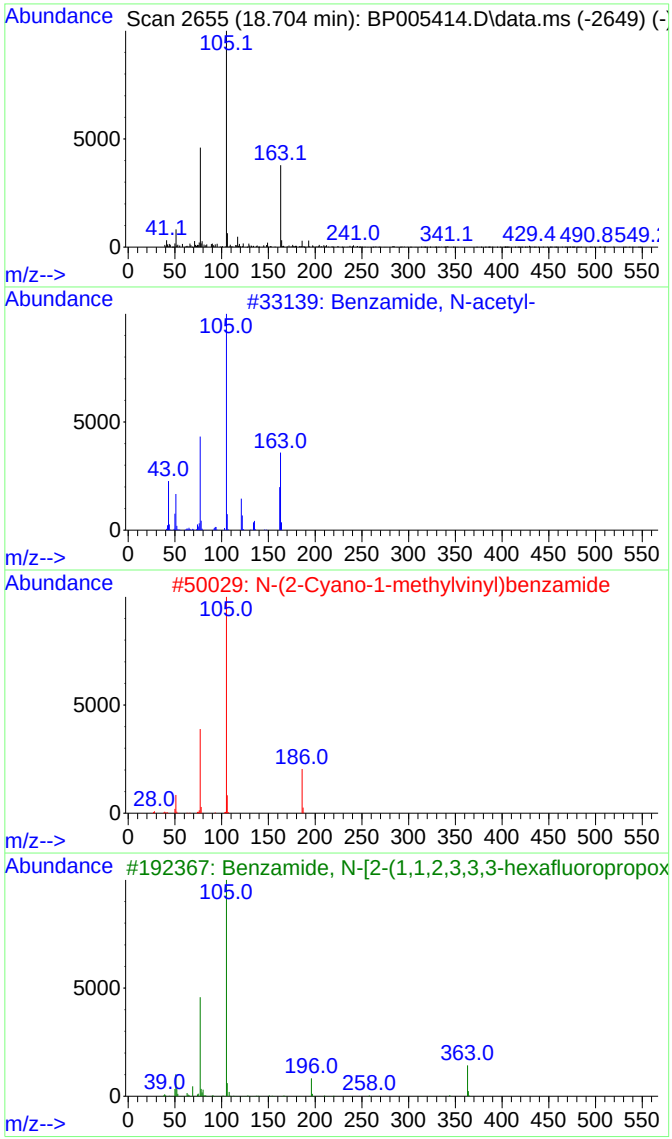
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

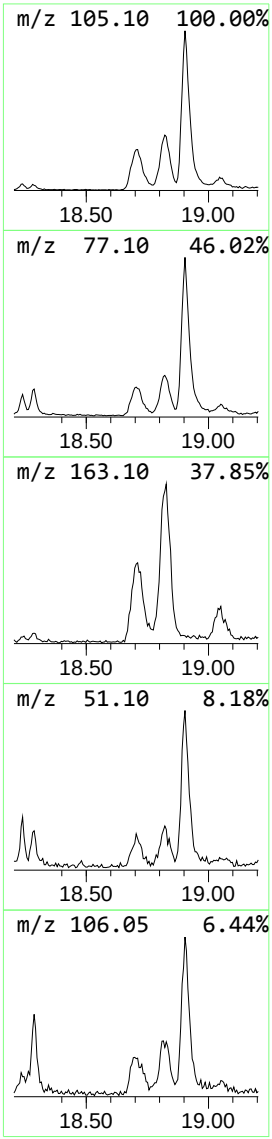
**********

Peak Number 8 Benzamide, N-acetyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.704 | 7.14 ng | 150178 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzamide, N-acetyl- | 163 | C9H9NO2 | 001575-95-7 | 64 |
| 2 | N-(2-Cyano-1-methylvinyl)benzamide | 186 | C11H10N2O | 027036-88-0 | 50 |
| 3 | Benzamide, N-[2-(1,1,2,3,3,3-hex... | 363 | C16H11F6NO2 | 1000258-54-5 | 47 |
| 4 | Benzamide, N-benzoyl-N-(2-triflu... | 369 | C21H14F3NO2 | 1000262-58-9 | 47 |
| 5 | Pyrimidine-4-carboxylic acid, 2-... | 379 | C20H17N3O3S | 1000266-50-6 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

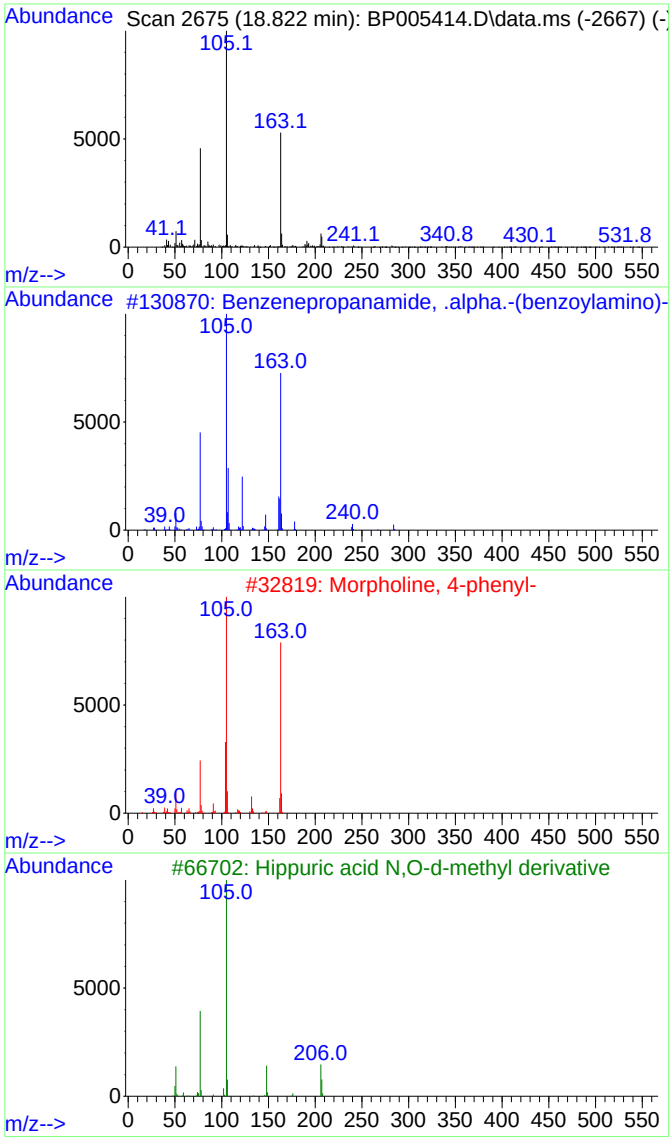
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

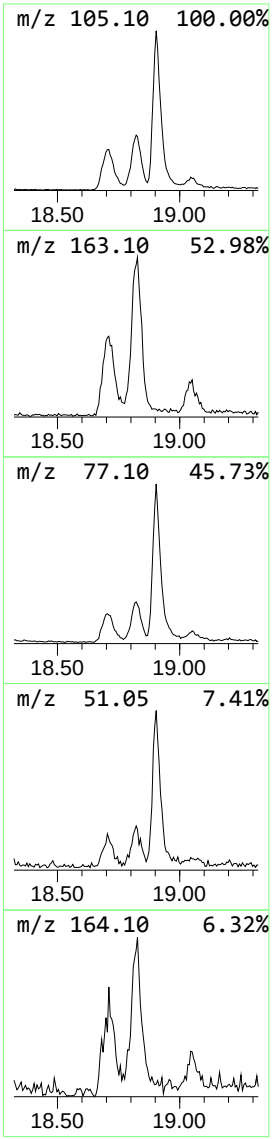
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 9 Benzenepropanamide, .alpha.... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.822 | 10.70 ng | 225081 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenepropanamide, .alpha.-(ben... | 284 | C16H16N2O3 | 058690-81-6 | 56 |
| 2 | Morpholine, 4-phenyl- | 163 | C10H13NO | 000092-53-5 | 43 |
| 3 | Hippuric acid N,O-d-methyl deriv... | 207 | C11H13NO3 | 071533-21-6 | 37 |
| 4 | 2,3,4,5-Tetrafluorobenzyl alcoho... | 236 | C11H12F4O | 1000375-29-5 | 30 |
| 5 | Decyl methyl phthalate | 320 | C19H28O4 | 256481-38-6 | 22 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

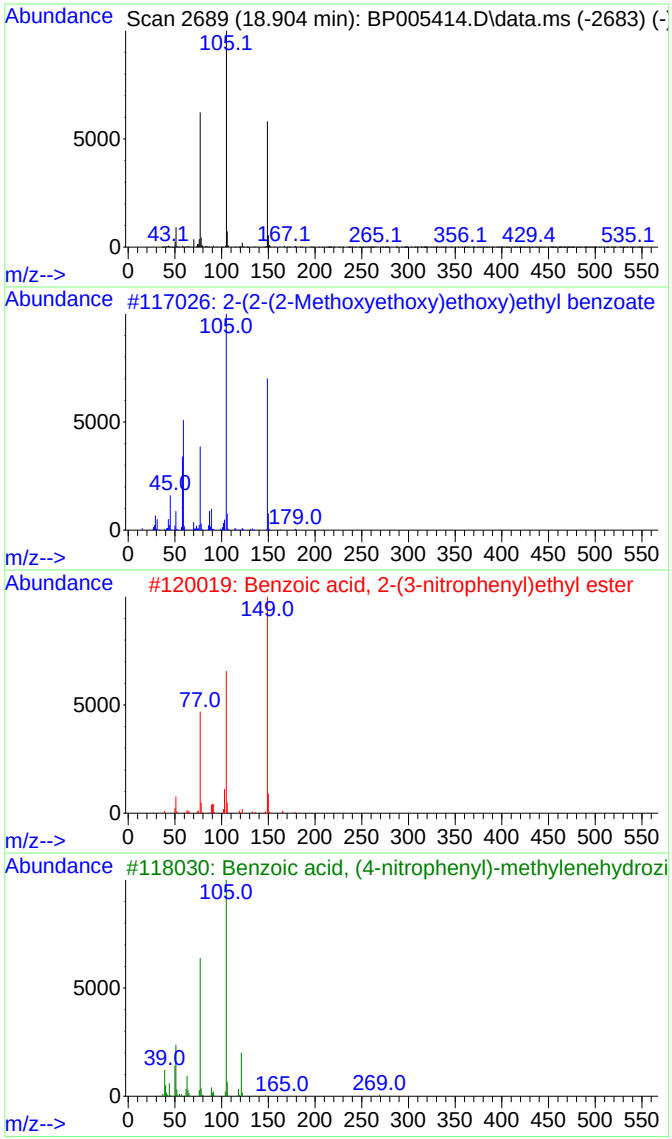
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

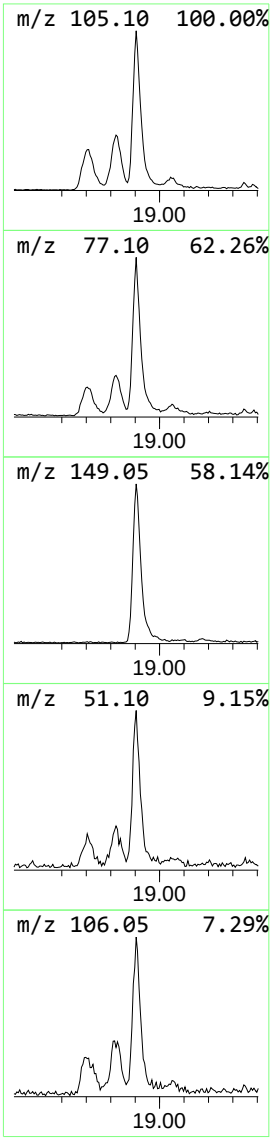
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 2-(2-(2-Methoxyethoxy)ethox... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.904 | 22.28 ng | 468454 | Phenanthrene-d10 | 17.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-(2-(2-Methoxyethoxy)ethoxy)eth... | 268 | C14H20O5 | 1000366-99-1 | 50 |
| 2 | Benzoic acid, 2-(3-nitrophenyl)e... | 271 | C15H13NO4 | 1000368-22-4 | 50 |
| 3 | Benzoic acid, (4-nitrophenyl)-me... | 269 | C14H11N3O3 | 028123-77-5 | 47 |
| 4 | Phenacyl thiocyanate | 177 | C9H7NOS | 005399-30-4 | 47 |
| 5 | Benzoyl bromide | 184 | C7H5BrO | 000618-32-6 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

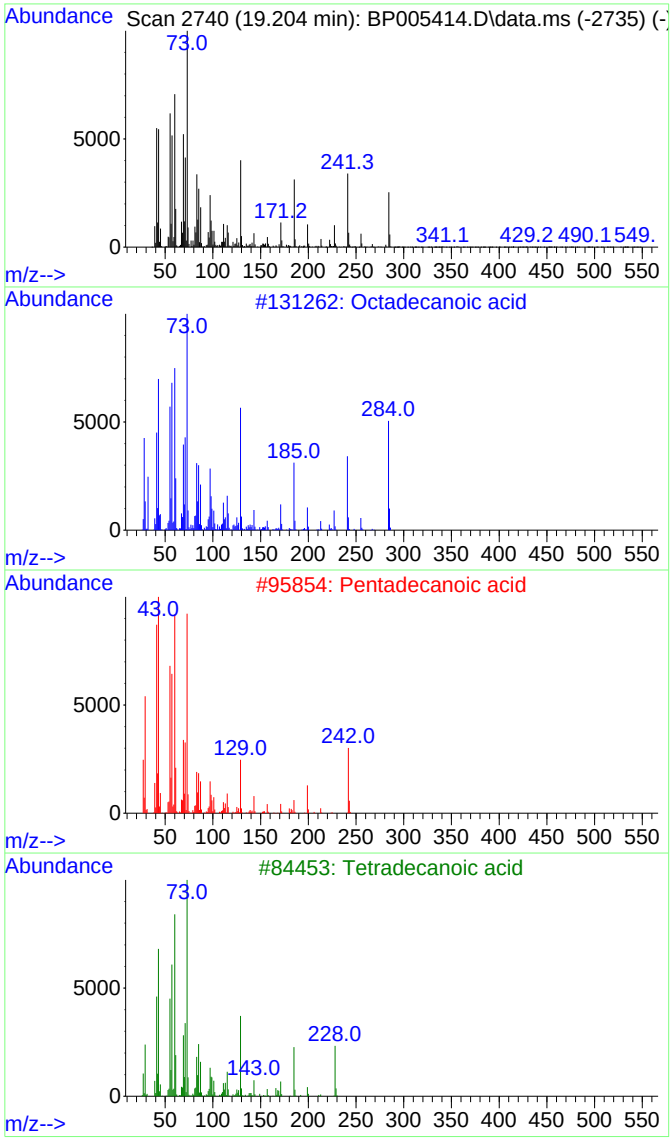
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

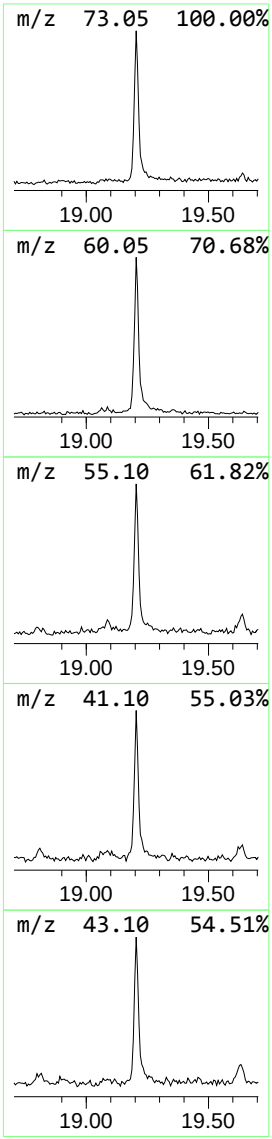
**********

Peak Number 12 Octadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.204 | 14.98 ng | 470704 | Chrysene-d12 | 21.163 |

| 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 | 86 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 55 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 53 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

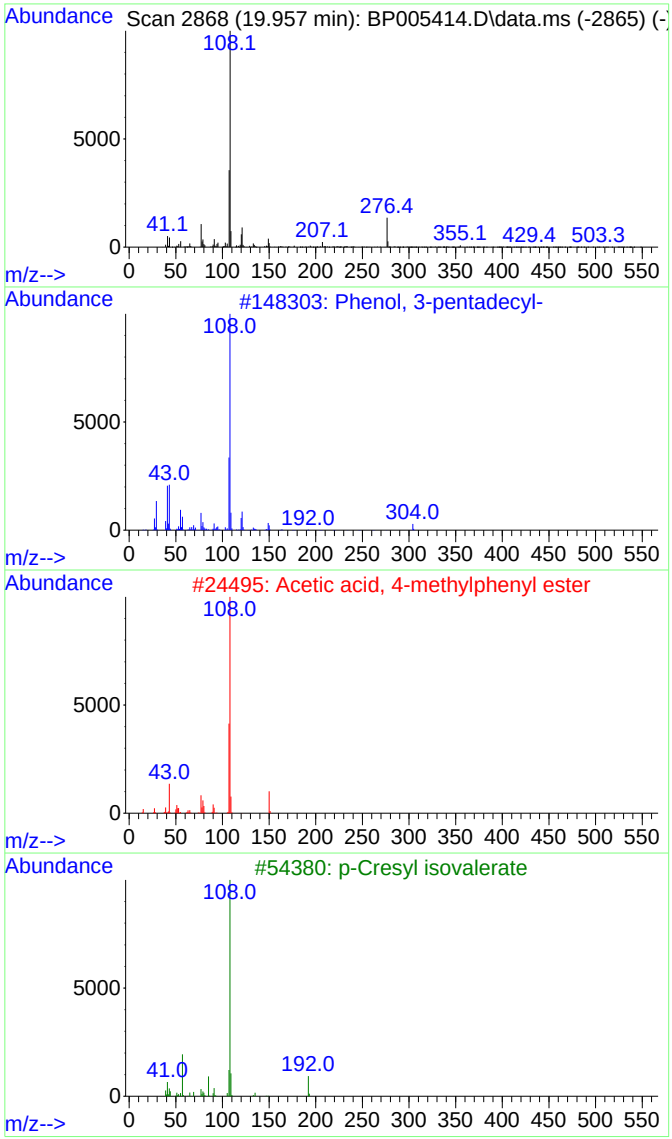
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

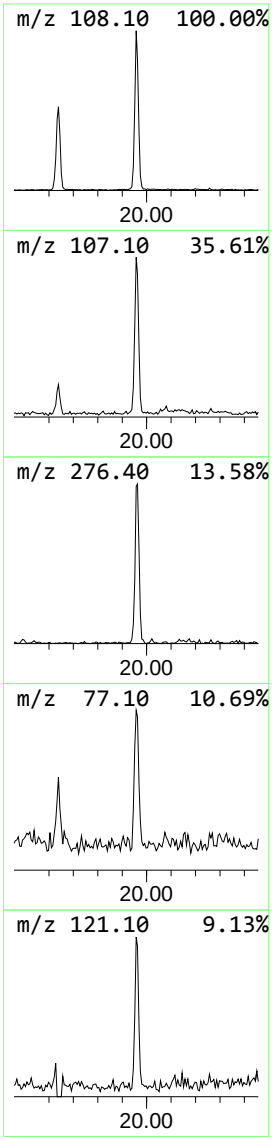
**********

Peak Number 13 Phenol, 3-pentadecyl- Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.957 | 3.86 ng | 121239 | Chrysene-d12 | 21.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 3-pentadecyl- | 304 | C21H36O | 000501-24-6 | 86 |
| 2 | Acetic acid, 4-methylphenyl ester | 150 | C9H10O2 | 000140-39-6 | 59 |
| 3 | p-Cresyl isovalerate | 192 | C12H16O2 | 055066-56-3 | 47 |
| 4 | Valeric acid, 3-methylphenyl ester | 192 | C12H16O2 | 1000307-98-3 | 47 |
| 5 | Carbamic acid, methyl-, 3-methyl... | 165 | C9H11NO2 | 001129-41-5 | 45 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

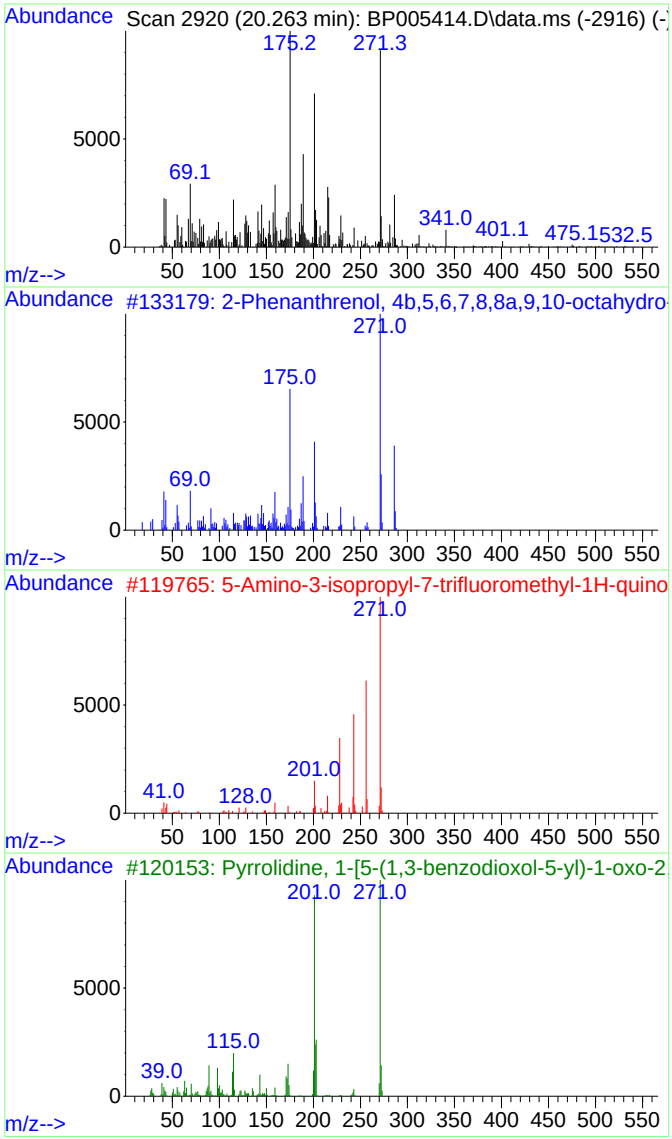
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

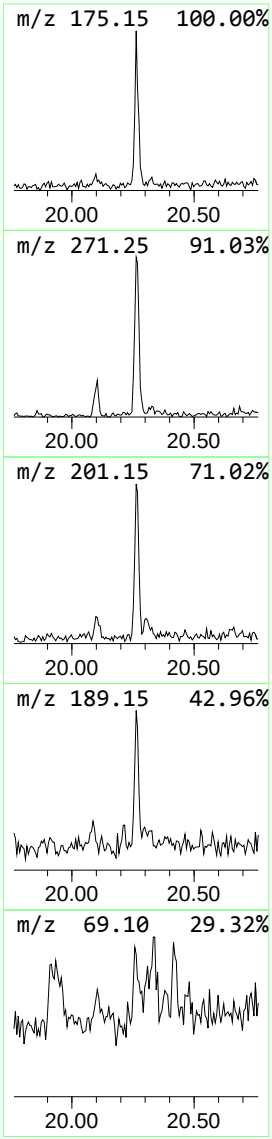
**********

Peak Number 14 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.263 | 2.24 ng | 70458 | Chrysene-d12 | 21.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Phenanthrenol, 4b,5,6,7,8,8a,9... | 286 | C20H30O | 000511-15-9 | 90 |
| 2 | 5-Amino-3-isopropyl-7-trifluorom... | 271 | C12H12F3N3O | 1000318-49-1 | 27 |
| 3 | Pyrrolidine, 1-[5-(1,3-benzodiox... | 271 | C16H17NO3 | 025924-78-1 | 27 |
| 4 | Crinan-1-ol, 2,3-didehydro-,(1.a... | 271 | C16H17NO3 | 1000111-31-3 | 22 |
| 5 | (+)-4-Methoxy-6-ketomorphinan | 271 | C17H21NO2 | 1000129-08-5 | 18 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

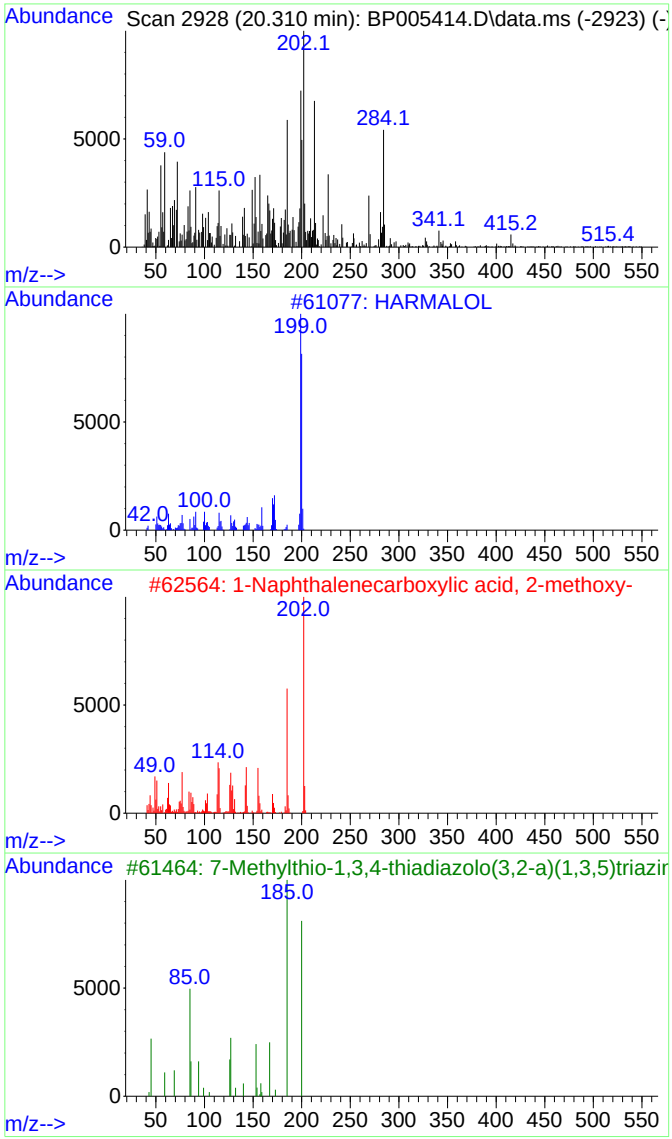
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

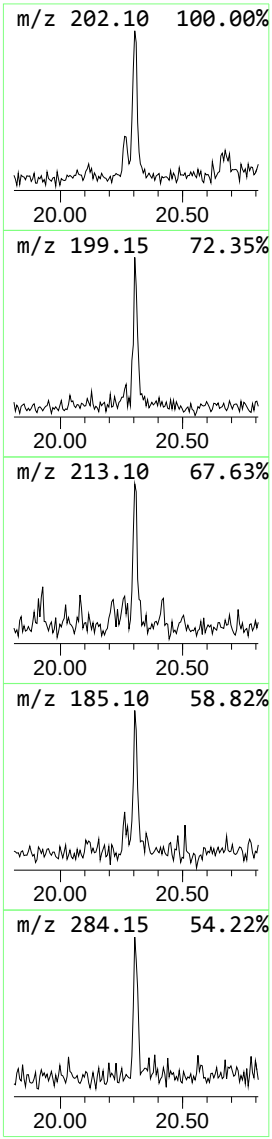
**********

Peak Number 15 unknown20.310 Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.310 | 2.22 ng | 69627 | Chrysene-d12 | 21.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | HARMALOL | 200 | C12H12N2O | 1000357-12-4 | 25 |
| 2 | 1-Naphthalenecarboxylic acid, 2-... | 202 | C12H10O3 | 000947-62-6 | 18 |
| 3 | 7-Methylthio-1,3,4-thiadiazolo(3... | 200 | C5H4N4OS2 | 058326-43-5 | 15 |
| 4 | 4-Hydroxyamino-6-phenylpyrimidin... | 202 | C10H10N4O | 1000111-25-2 | 15 |
| 5 | 4-Chloro-3-ethyl-1,3-benzothiazo... | 213 | C9H8ClNOS | 1000331-84-8 | 15 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

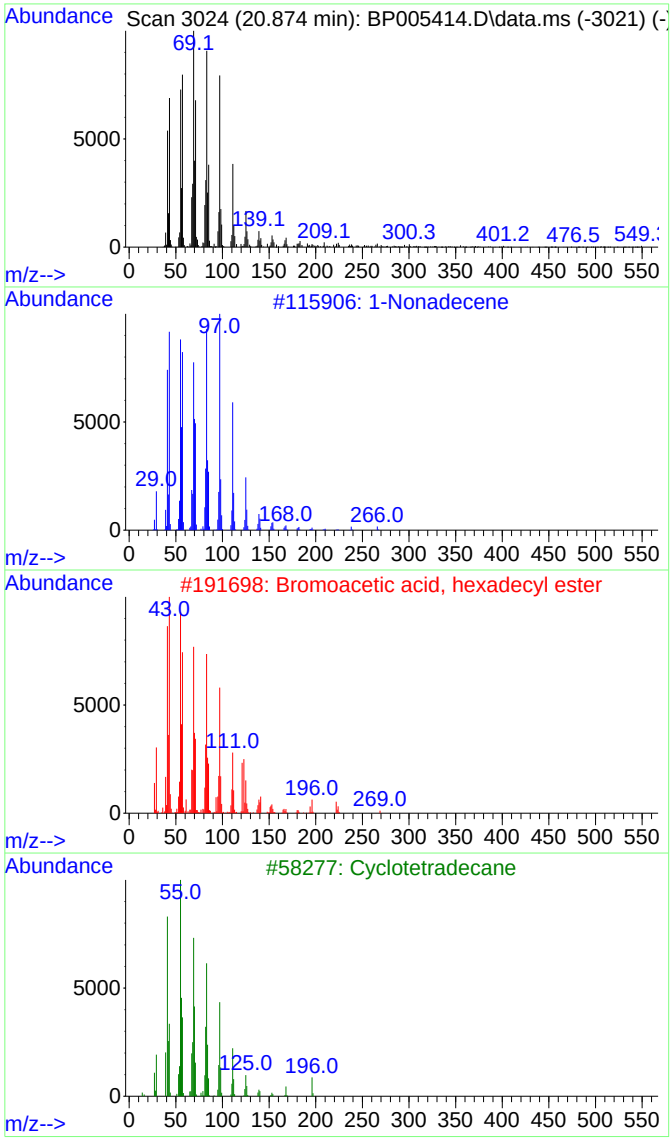
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

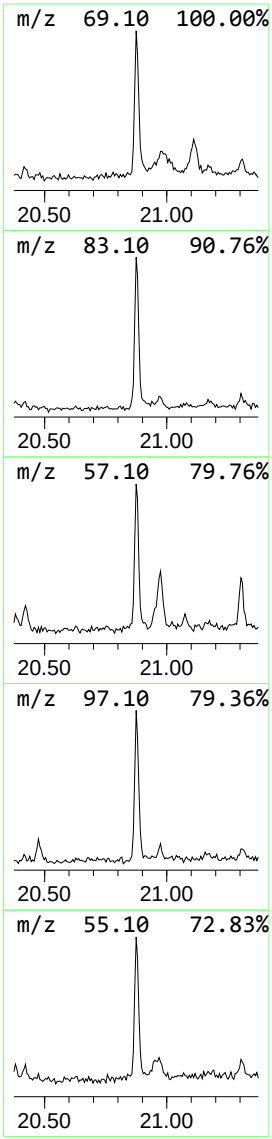
**********

Peak Number 16 1-Nonadecene Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.874 | 9.77 ng | 307009 | Chrysene-d12 | 21.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 95 |
| 2 | Bromoacetic acid, hexadecyl ester | 362 | C18H35BrO2 | 005454-48-8 | 90 |
| 3 | Cyclotetradecane | 196 | C14H28 | 000295-17-0 | 86 |
| 4 | 1-Hexacosanol | 382 | C26H54O | 000506-52-5 | 81 |
| 5 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 70 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

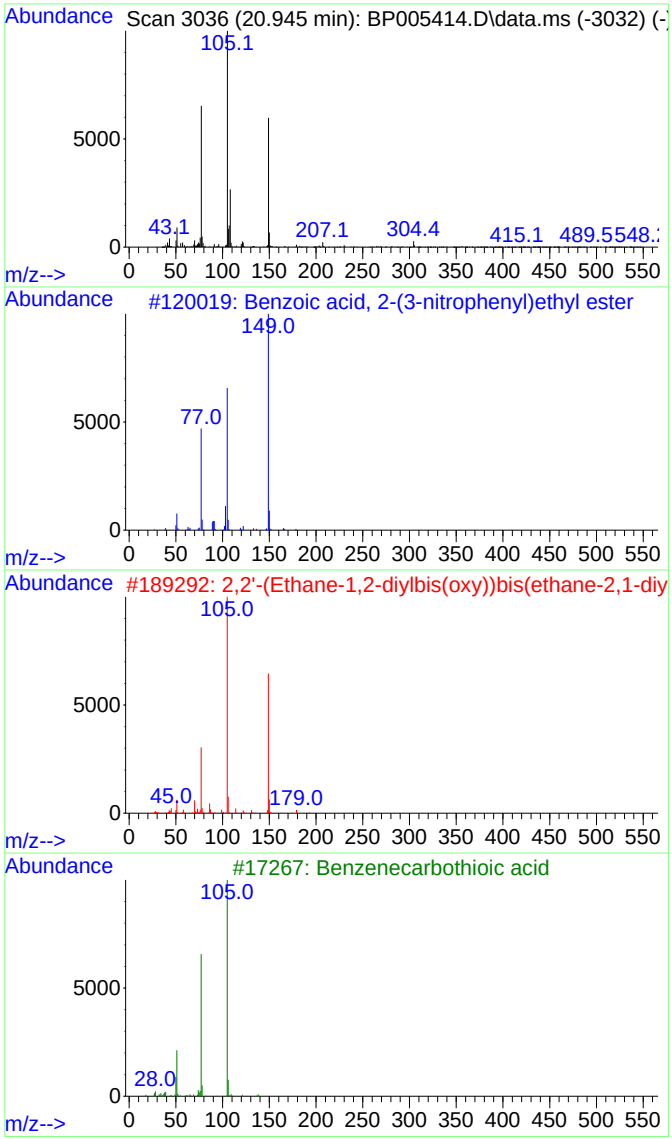
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

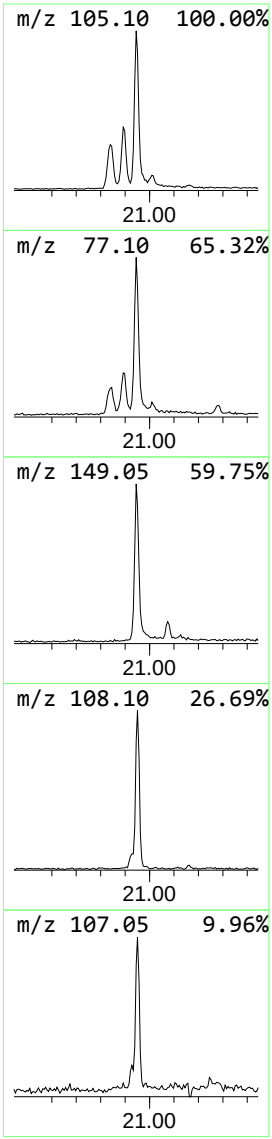
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 17 Benzoic acid, 2-(3-nitrophe... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.945 | 12.31 ng | 386588 | Chrysene-d12 | 21.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, 2-(3-nitrophenyl)e... | 271 | C15H13NO4 | 1000368-22-4 | 59 |
| 2 | 2,2'-(Ethane-1,2-diylbis(oxy))bi... | 358 | C20H22O6 | 1000366-99-4 | 50 |
| 3 | Benzenecarbothioic acid | 138 | C7H6OS | 000098-91-9 | 38 |
| 4 | Diethylene glycol dibenzoate | 314 | C18H18O5 | 000120-55-8 | 38 |
| 5 | 1,2-Propanedione, 1-phenyl- | 148 | C9H8O2 | 000579-07-7 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

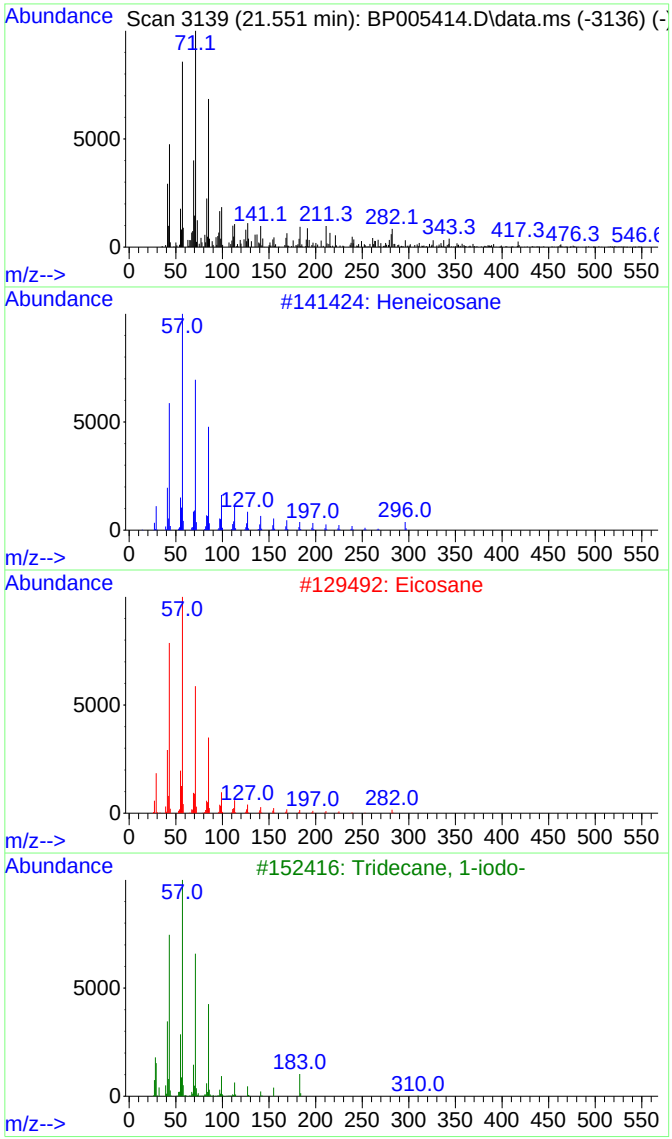
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

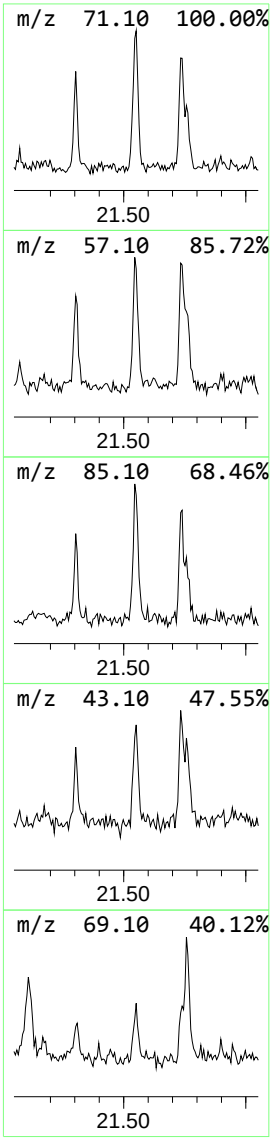
**********

Peak Number 18 Heneicosane Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.551 | 2.23 ng | 69974 | Chrysene-d12 | 21.163 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 83 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 83 |
| 3 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 80 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 80 |
| 5 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 80 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

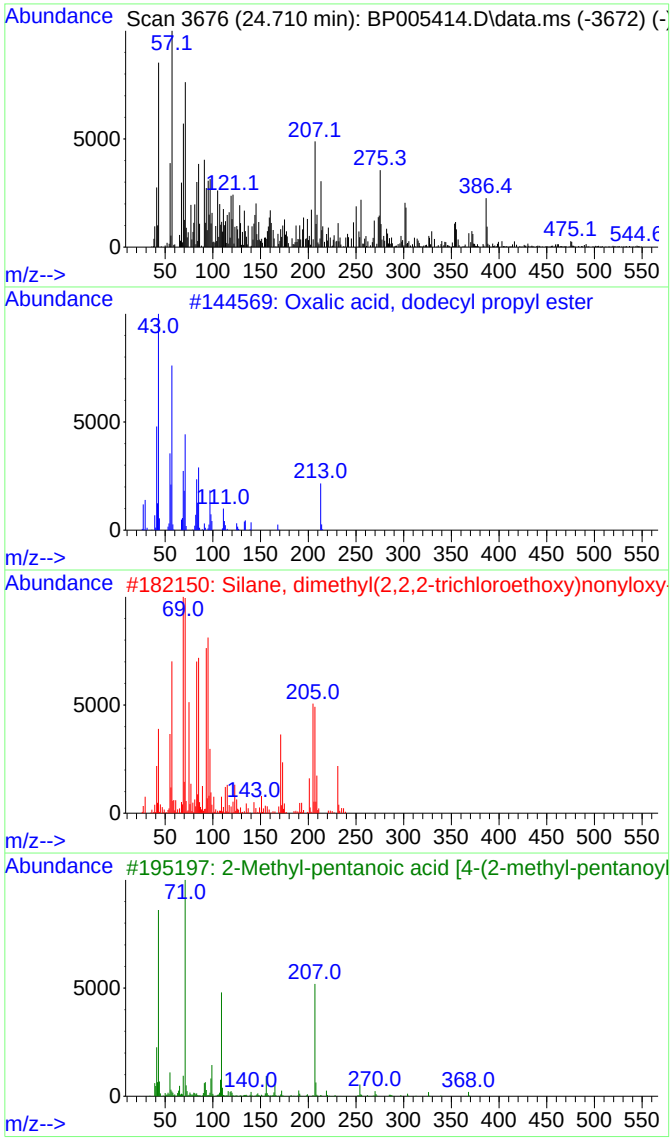
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

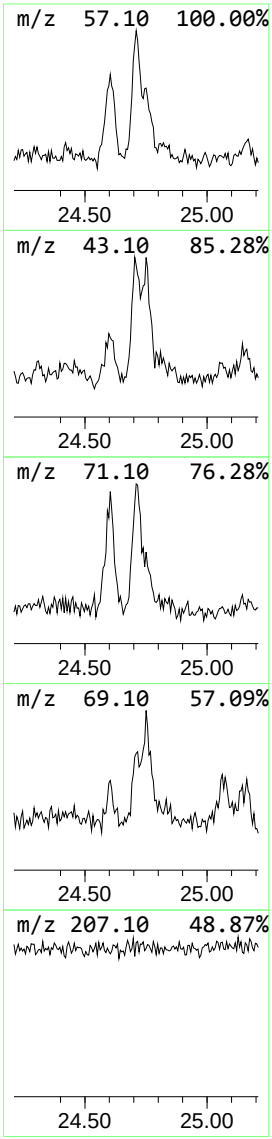
**********

Peak Number 19 unknown24.709 Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.709 | 4.25 ng | 143021 | Perylene-d12 | 23.416 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxalic acid, dodecyl propyl ester | 300 | C17H32O4 | 1000309-26-5 | 38 |
| 2 | Silane, dimethyl(2,2,2-trichloro... | 348 | C13H27Cl3O2Si | 1000347-56-7 | 38 |
| 3 | 2-Methyl-pentanoic acid [4-(2-me... | 368 | C18H28N2O4S | 1000296-31-0 | 35 |
| 4 | Tetratriacontane, 1-bromo- | 556 | C34H69Br | 062108-50-3 | 35 |
| 5 | 4,8,12-trimethyltridecanoic acid... | 438 | C20H33F7O2 | 1000376-66-8 | 27 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005414.D
Acq On : 29 Apr 2021 17:49
Operator : CG/JU
Sample : M2196-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
WALL-D-4075-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Dodecanoic acid | 14.734 | 3.1 | ng | 84678 | 3 | 14.292 | 539893 | 20.0 |
| 4-((1E)-3-Hydro... | 16.463 | 6.5 | ng | 137827 | 4 | 17.057 | 420525 | 20.0 |
| 7,9-Di-tert-but... | 17.733 | 2.5 | ng | 52147 | 4 | 17.057 | 420525 | 20.0 |
| Tetradecanoic acid | 17.969 | 50.5 | ng | 1061760 | 4 | 17.057 | 420525 | 20.0 |
| 3,5-Dimethoxy-4... | 18.239 | 9.8 | ng | 205726 | 4 | 17.057 | 420525 | 20.0 |
| unknown18.286 | 18.286 | 14.5 | ng | 304277 | 4 | 17.057 | 420525 | 20.0 |
| 4,4'-(Hexafluor... | 18.486 | 2.2 | ng | 46472 | 4 | 17.057 | 420525 | 20.0 |
| Benzamide, N-ac... | 18.704 | 7.1 | ng | 150178 | 4 | 17.057 | 420525 | 20.0 |
| Benzenepropanam... | 18.822 | 10.7 | ng | 225081 | 4 | 17.057 | 420525 | 20.0 |
| 2-(2-(2-Methoxy... | 18.904 | 22.3 | ng | 468454 | 4 | 17.057 | 420525 | 20.0 |
| Octadecanoic acid | 19.204 | 15.0 | ng | 470704 | 5 | 21.163 | 628333 | 20.0 |
| Phenol, 3-penta... | 19.957 | 3.9 | ng | 121239 | 5 | 21.163 | 628333 | 20.0 |
| 2-Phenanthrenol... | 20.263 | 2.2 | ng | 70458 | 5 | 21.163 | 628333 | 20.0 |
| unknown20.310 | 20.310 | 2.2 | ng | 69627 | 5 | 21.163 | 628333 | 20.0 |
| 1-Nonadecene | 20.874 | 9.8 | ng | 307009 | 5 | 21.163 | 628333 | 20.0 |
| Benzoic acid, 2... | 20.945 | 12.3 | ng | 386588 | 5 | 21.163 | 628333 | 20.0 |
| Heneicosane | 21.551 | 2.2 | ng | 69974 | 5 | 21.163 | 628333 | 20.0 |
| unknown24.709 | 24.709 | 4.3 | ng | 143021 | 6 | 23.416 | 673632 | 20.0 |