LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005321.D
Acq On : 16 Apr 2021 16:32
Operator : CG/JU
Sample : M1947-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** FS-SB19B(19-20)X

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-BP041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005321.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.264 | 365 | 370 | 379 | rVB | 538796 | 768038 | 41.24% | 8.855% |
| 2 | 6.846 | 635 | 639 | 653 | rVB | 528902 | 861328 | 46.25% | 9.931% |
| 3 | 7.658 | 773 | 777 | 786 | rVB | 119673 | 191557 | 10.29% | 2.209% |
| 4 | 8.822 | 969 | 975 | 985 | rVB | 322107 | 508048 | 27.28% | 5.858% |
| 5 | 10.452 | 1245 | 1252 | 1261 | rBV | 104247 | 166944 | 8.96% | 1.925% |
| 6 | 12.940 | 1668 | 1675 | 1685 | rBV | 726289 | 943380 | 50.65% | 10.877% |
| 7 | 14.328 | 1903 | 1911 | 1922 | rBV2 | 187657 | 263114 | 14.13% | 3.034% |
| 8 | 15.828 | 2160 | 2166 | 2180 | rBV | 481823 | 679955 | 36.51% | 7.840% |
| 9 | 17.092 | 2374 | 2381 | 2386 | rBV | 234050 | 302214 | 16.23% | 3.484% |
| 10 | 17.992 | 2525 | 2534 | 2542 | rBV2 | 53939 | 89416 | 4.80% | 1.031% |
| 11 | 19.116 | 2720 | 2725 | 2732 | rVB | 48905 | 63832 | 3.43% | 0.736% |
| 12 | 19.233 | 2741 | 2745 | 2755 | rBV6 | 16638 | 30039 | 1.61% | 0.346% |
| 13 | 19.469 | 2781 | 2785 | 2795 | rVB | 43182 | 65811 | 3.53% | 0.759% |
| 14 | 19.669 | 2813 | 2819 | 2824 | rBV | 1660146 | 1862483 | 100.00% | 21.474% |
| 15 | 20.345 | 2929 | 2934 | 2941 | rBV2 | 66469 | 93865 | 5.04% | 1.082% |
| 16 | 20.875 | 3019 | 3024 | 3026 | rBV | 45750 | 73768 | 3.96% | 0.851% |
| 17 | 20.910 | 3026 | 3030 | 3037 | rVV2 | 120303 | 277445 | 14.90% | 3.199% |
| 18 | 20.975 | 3037 | 3041 | 3050 | rVB | 253354 | 338152 | 18.16% | 3.899% |
| 19 | 21.192 | 3072 | 3078 | 3082 | rBV | 441298 | 585445 | 31.43% | 6.750% |
| 20 | 21.228 | 3082 | 3084 | 3088 | rVB | 41215 | 45846 | 2.46% | 0.529% |
| 21 | 23.463 | 3458 | 3464 | 3473 | rBV | 253526 | 462719 | 24.84% | 5.335% |

Sum of corrected areas: 8673399

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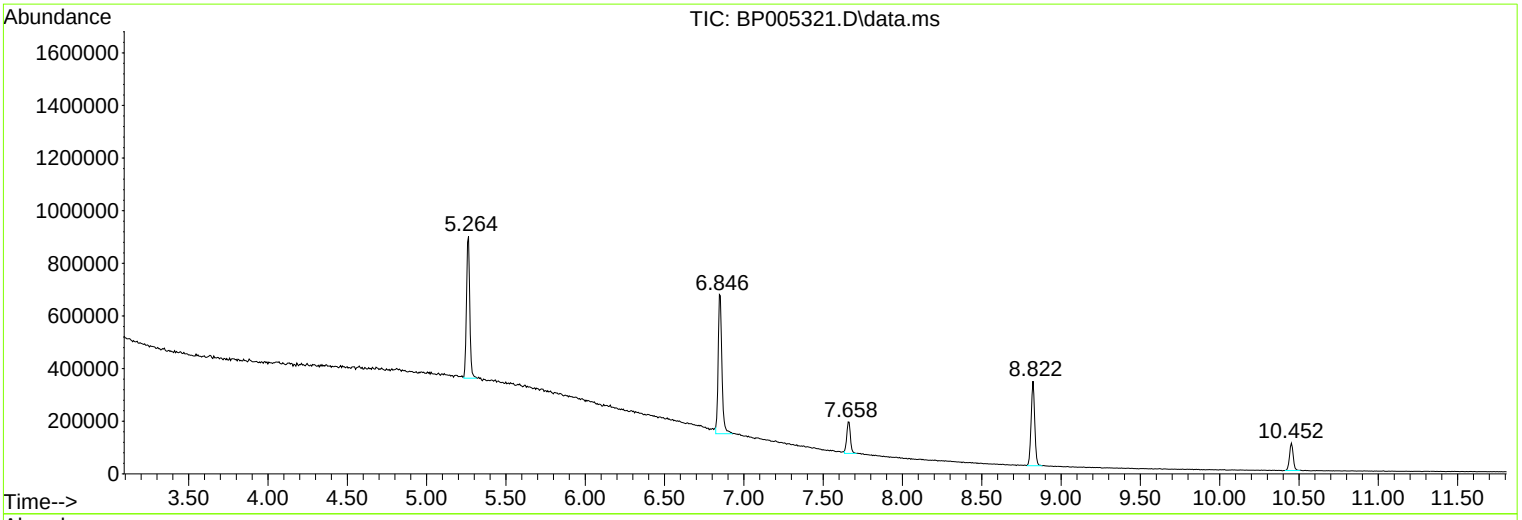
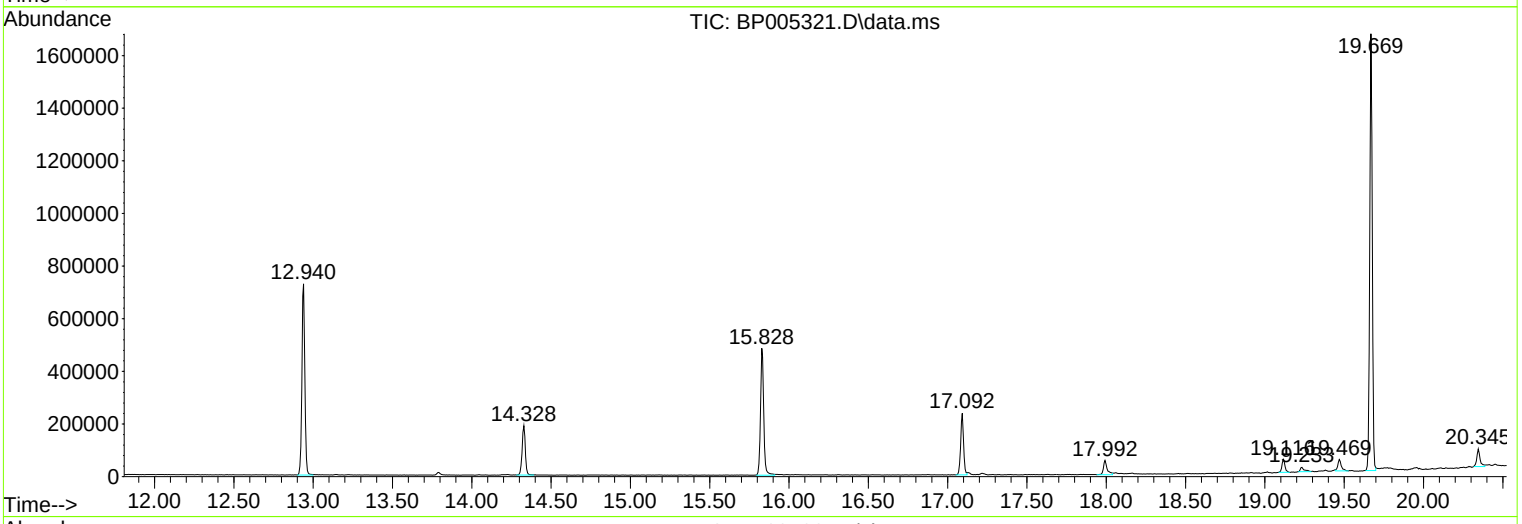
ALS Vial : 13 Sample Multiplier: 1

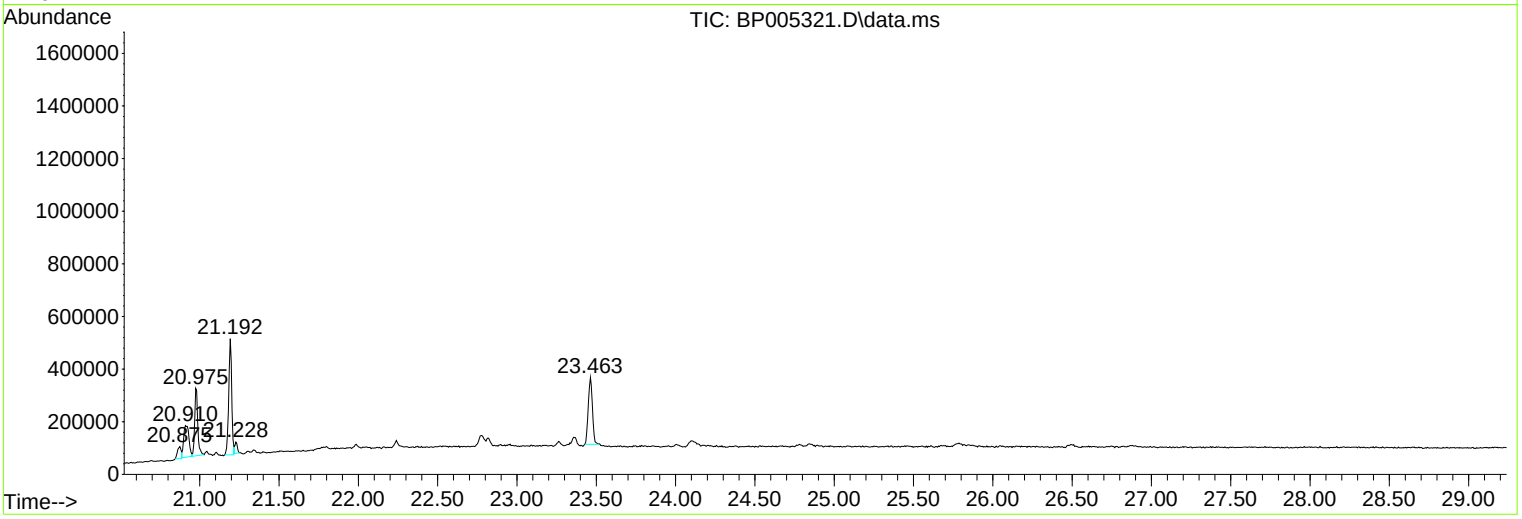
**Instrument :**
BNA_P
**ClientSampleId :**
FS-SB19B(19-20)X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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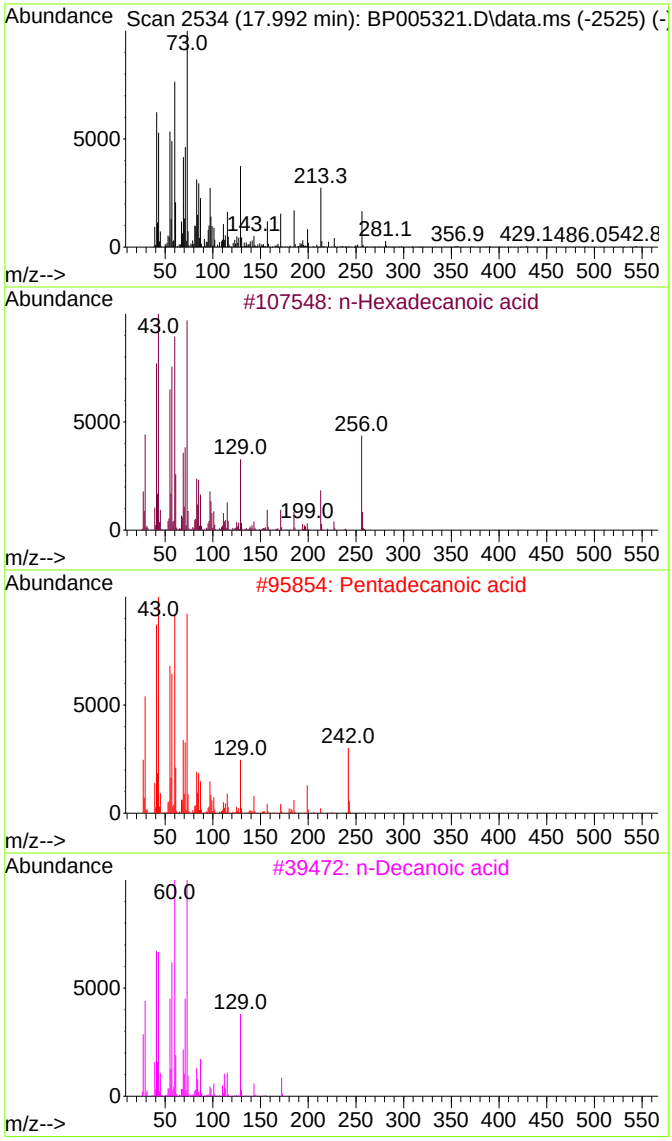
TIC Integration Parameters: LSCINT.P

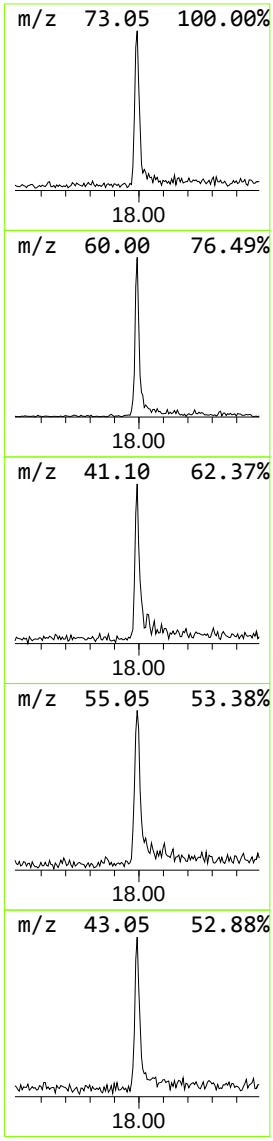
**********

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.992 | 5.92 ng | 89416 | Phenanthrene-d10 | 17.092 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 96 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 78 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 76 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 74 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 72 |



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Data File : BP005321.D
Acq On : 16 Apr 2021 16:32
Operator : CG/JU
Sample : M1947-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
FS-SB19B(19-20)X

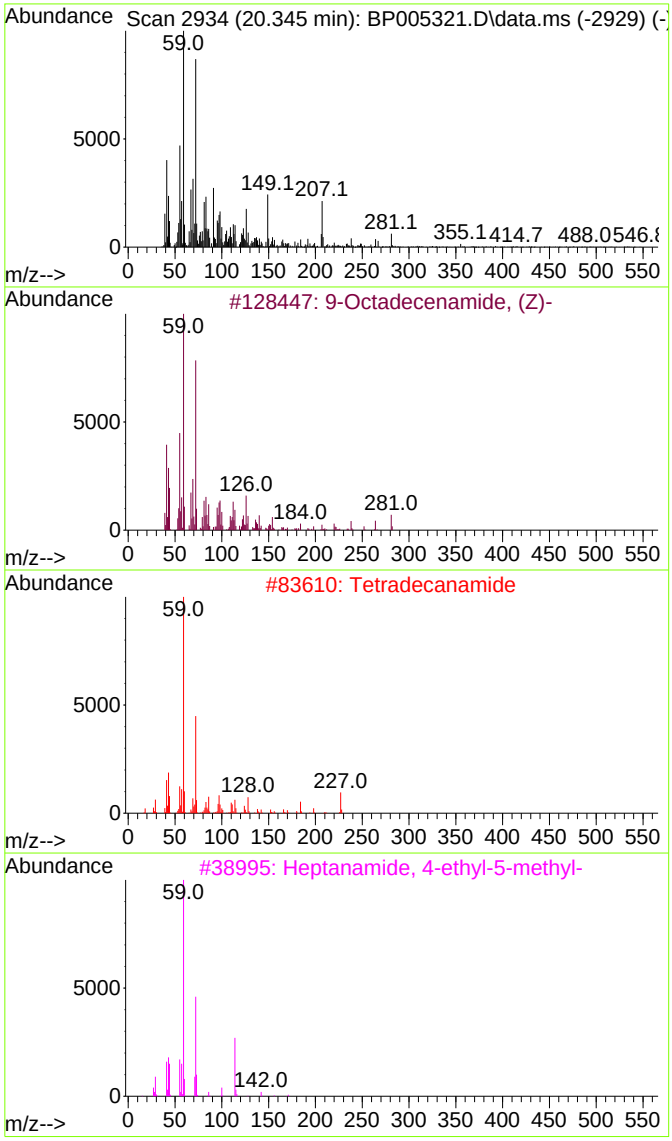
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

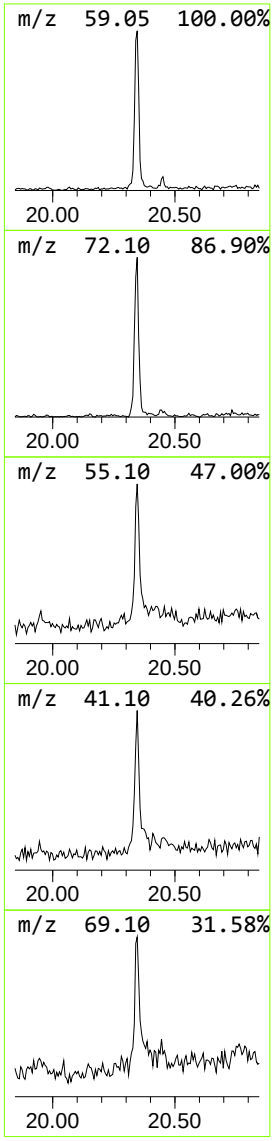
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 9-Octadecenamide, (Z)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.345 | 3.21 ng | 93865 | Chrysene-d12 | 21.192 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 81 |
| 2 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 43 |
| 3 | Heptanamide, 4-ethyl-5-methyl- | 171 | C10H21NO | 054789-40-1 | 43 |
| 4 | Hexadecanamide | 255 | C16H33NO | 000629-54-9 | 35 |
| 5 | Dodecanamide | 199 | C12H25NO | 001120-16-7 | 35 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041621\
Data File : BP005321.D
Acq On : 16 Apr 2021 16:32
Operator : CG/JU
Sample : M1947-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
FS-SB19B(19-20)X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

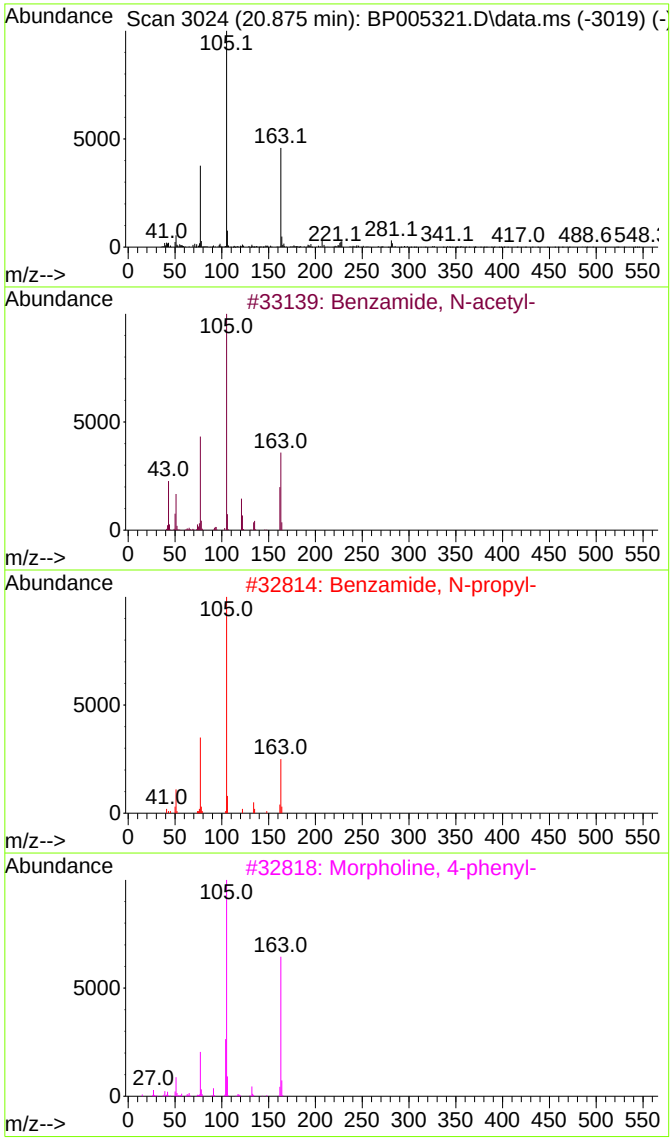
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

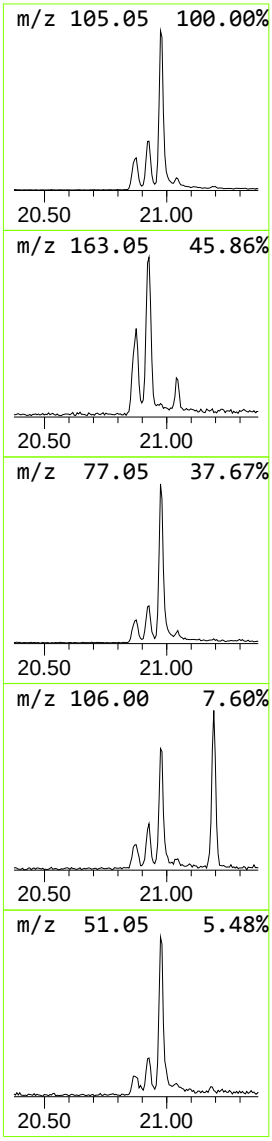
**********

Peak Number 3 Benzamide, N-acetyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.875 | 2.52 ng | 73768 | Chrysene-d12 | 21.192 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzamide, N-acetyl- | 163 | C9H9NO2 | 001575-95-7 | 72 |
| 2 | Benzamide, N-propyl- | 163 | C10H13NO | 010546-70-0 | 72 |
| 3 | Morpholine, 4-phenyl- | 163 | C10H13NO | 000092-53-5 | 50 |
| 4 | Benzoic acid, 2-benzyloxy-3-brom... | 348 | C17H17BrO3 | 1000191-33-3 | 25 |
| 5 | 1-(.beta.-d-2,3-O-Dibenzoylfuran... | 470 | C23H19FN2O8 | 1000286-48-4 | 16 |



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Sample : M1947-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
FS-SB19B(19-20)X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
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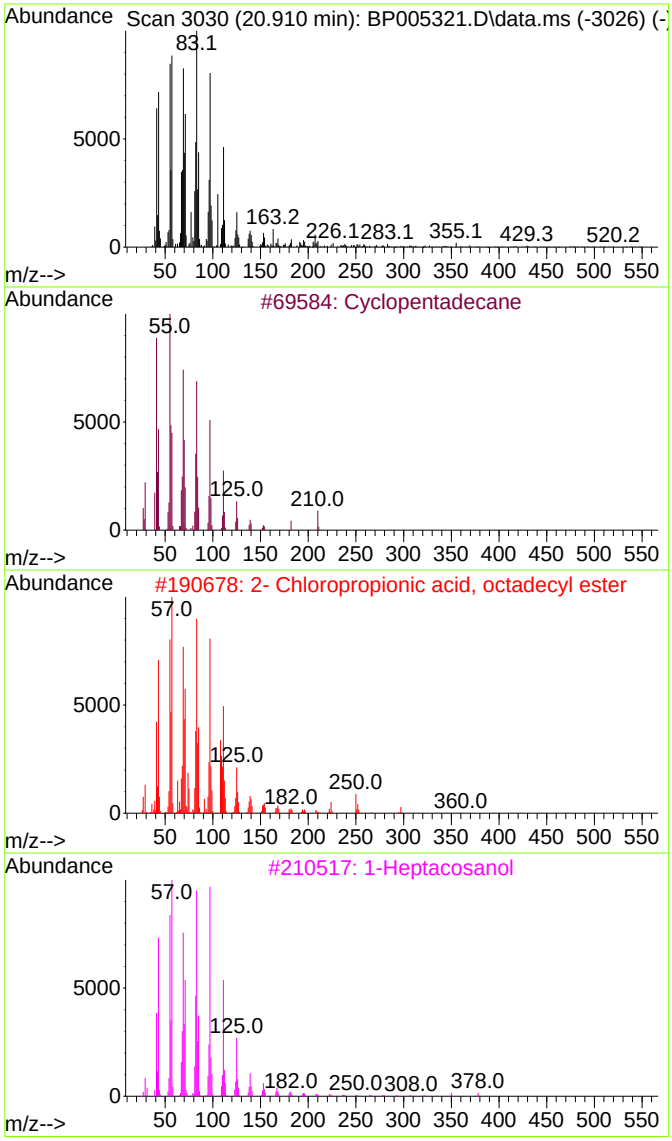
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

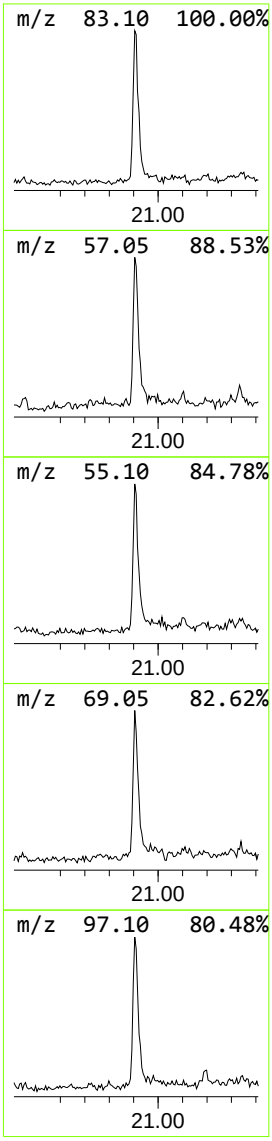
**********

Peak Number 4 Cyclopentadecane Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.910 | 9.48 ng | 277445 | Chrysene-d12 | 21.192 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 95 |
| 2 | 2- Chloropropionic acid, octadec... | 360 | C21H41ClO2 | 088104-31-8 | 93 |
| 3 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 91 |
| 4 | 1-Hexacosanol | 382 | C26H54O | 000506-52-5 | 91 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91 |



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Sample : M1947-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
FS-SB19B(19-20)X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041521.M
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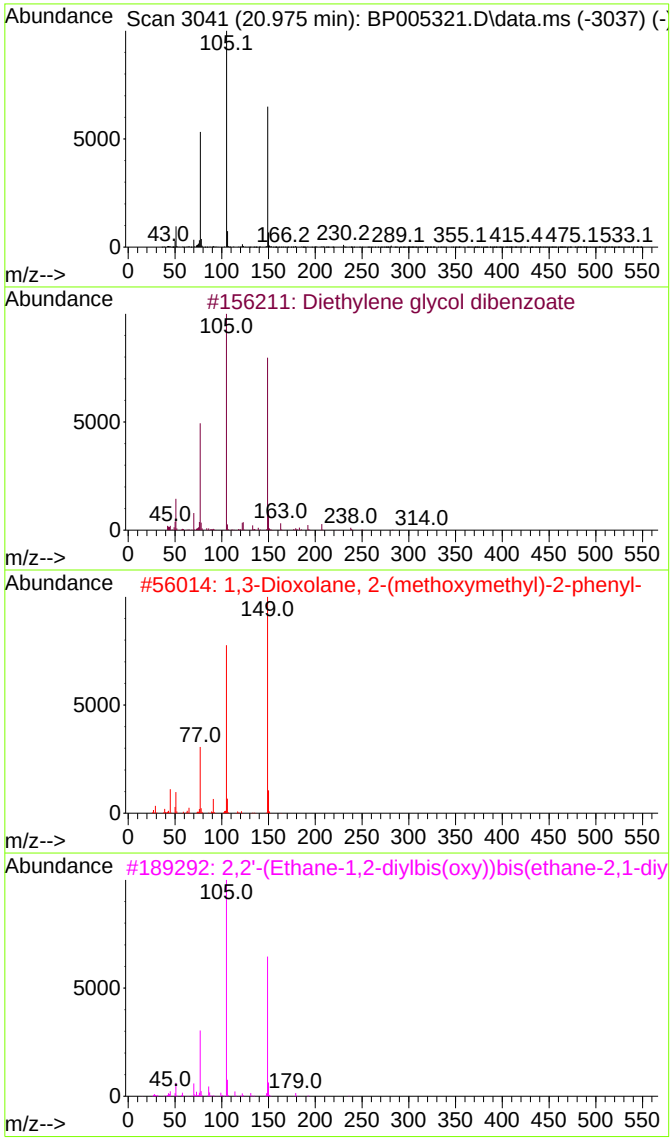
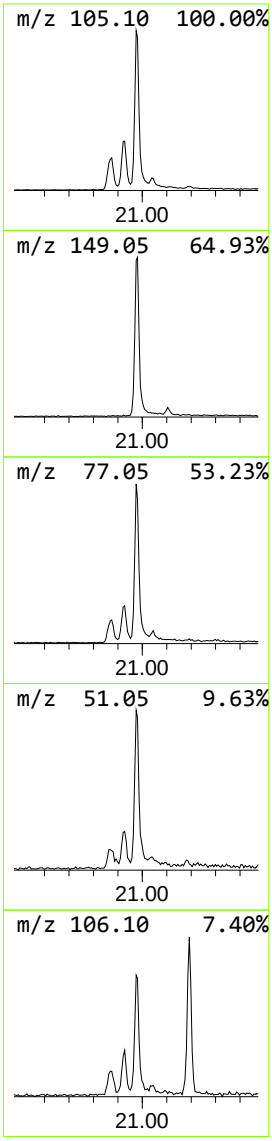
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.975 | 11.55 ng | 338152 | Chrysene-d12 | 21.192 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Diethylene glycol dibenzoate | 314 | C18H18O5 | 000120-55-8 | 78 |
| 2 | 1,3-Dioxolane, 2-(methoxymethyl)... | 194 | C11H14O3 | 1000156-71-2 | 64 |
| 3 | 2,2'-(Ethane-1,2-diylbis(oxy))bi... | 358 | C20H22O6 | 1000366-99-4 | 64 |
| 4 | 2,3-Dimethyl-4a,8a-diphenyl-hexa... | 326 | C20H22O4 | 1000297-07-0 | 59 |
| 5 | 4'-Nitrobenzanilide | 242 | C13H10N2O3 | 003393-96-2 | 47 |



Tentatively Identified Compound (LSC) summary

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ALS Vial : 13 Sample Multiplier: 1

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TIC Integration Parameters: LSCINT.P

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| n-Hexadecanoic ... | 17.992 | 5.9 | ng | 89416 | 4 | 17.092 | 302214 | 20.0 |
| 9-Octadecenamid... | 20.345 | 3.2 | ng | 93865 | 5 | 21.192 | 585445 | 20.0 |
| Benzamide, N-ac... | 20.875 | 2.5 | ng | 73768 | 5 | 21.192 | 585445 | 20.0 |
| Cyclopentadecane | 20.910 | 9.5 | ng | 277445 | 5 | 21.192 | 585445 | 20.0 |
| Diethylene glyc... | 20.975 | 11.6 | ng | 338152 | 5 | 21.192 | 585445 | 20.0 |