LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP071720\
Data File : BP002788.D
Acq On : 17 Jul 2020 12:55
Operator : CG/JU
Sample : L3308-23
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 23

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\8270-BP071020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.187 | 384 | 391 | 409 | rBV | 2339458 | 3530388 | 64.81% | 8.993% |
| 2 | 6.763 | 652 | 659 | 676 | rBV | 2258527 | 3775631 | 69.31% | 9.617% |
| 3 | 7.558 | 787 | 794 | 804 | rBV | 864412 | 1348056 | 24.75% | 3.434% |
| 4 | 8.705 | 981 | 989 | 1009 | rBV | 1437711 | 2416962 | 44.37% | 6.157% |
| 5 | 10.328 | 1255 | 1265 | 1283 | rBV | 1120173 | 1957199 | 35.93% | 4.985% |
| 6 | 12.822 | 1681 | 1689 | 1709 | rBV | 3072018 | 4827670 | 88.63% | 12.297% |
| 7 | 13.669 | 1827 | 1833 | 1851 | rVB | 514051 | 800608 | 14.70% | 2.039% |
| 8 | 14.210 | 1917 | 1925 | 1935 | rBV2 | 1640078 | 2509258 | 46.07% | 6.392% |
| 9 | 15.716 | 2169 | 2181 | 2192 | rBV | 2152064 | 3477073 | 63.83% | 8.857% |
| 10 | 16.969 | 2388 | 2394 | 2404 | rBV | 1940927 | 2777205 | 50.98% | 7.074% |
| 11 | 17.092 | 2412 | 2415 | 2420 | rVB2 | 41631 | 58432 | 1.07% | 0.149% |
| 12 | 17.898 | 2548 | 2552 | 2560 | rBV | 81531 | 132735 | 2.44% | 0.338% |
| 13 | 18.628 | 2672 | 2676 | 2680 | rBV | 63716 | 83943 | 1.54% | 0.214% |
| 14 | 19.063 | 2745 | 2750 | 2756 | rVB3 | 43050 | 64824 | 1.19% | 0.165% |
| 15 | 19.557 | 2829 | 2834 | 2842 | rBV2 | 4154667 | 5447140 | 100.00% | 13.875% |
| 16 | 20.192 | 2938 | 2942 | 2946 | rBV2 | 154356 | 181112 | 3.32% | 0.461% |
| 17 | 20.233 | 2946 | 2949 | 2955 | rVB5 | 72287 | 89793 | 1.65% | 0.229% |
| 18 | 20.816 | 3044 | 3048 | 3058 | rBV | 570205 | 797186 | 14.63% | 2.031% |
| 19 | 21.080 | 3088 | 3093 | 3098 | rBV | 1703269 | 2120251 | 38.92% | 5.401% |
| 20 | 21.692 | 3192 | 3197 | 3207 | rVB4 | 163880 | 334494 | 6.14% | 0.852% |
| 21 | 22.627 | 3353 | 3356 | 3361 | rVB | 224304 | 303118 | 5.56% | 0.772% |
| 22 | 23.274 | 3460 | 3466 | 3473 | rVB | 1008200 | 1824025 | 33.49% | 4.646% |
| 23 | 23.910 | 3569 | 3574 | 3583 | rVB | 184727 | 401489 | 7.37% | 1.023% |

Sum of corrected areas: 39258592

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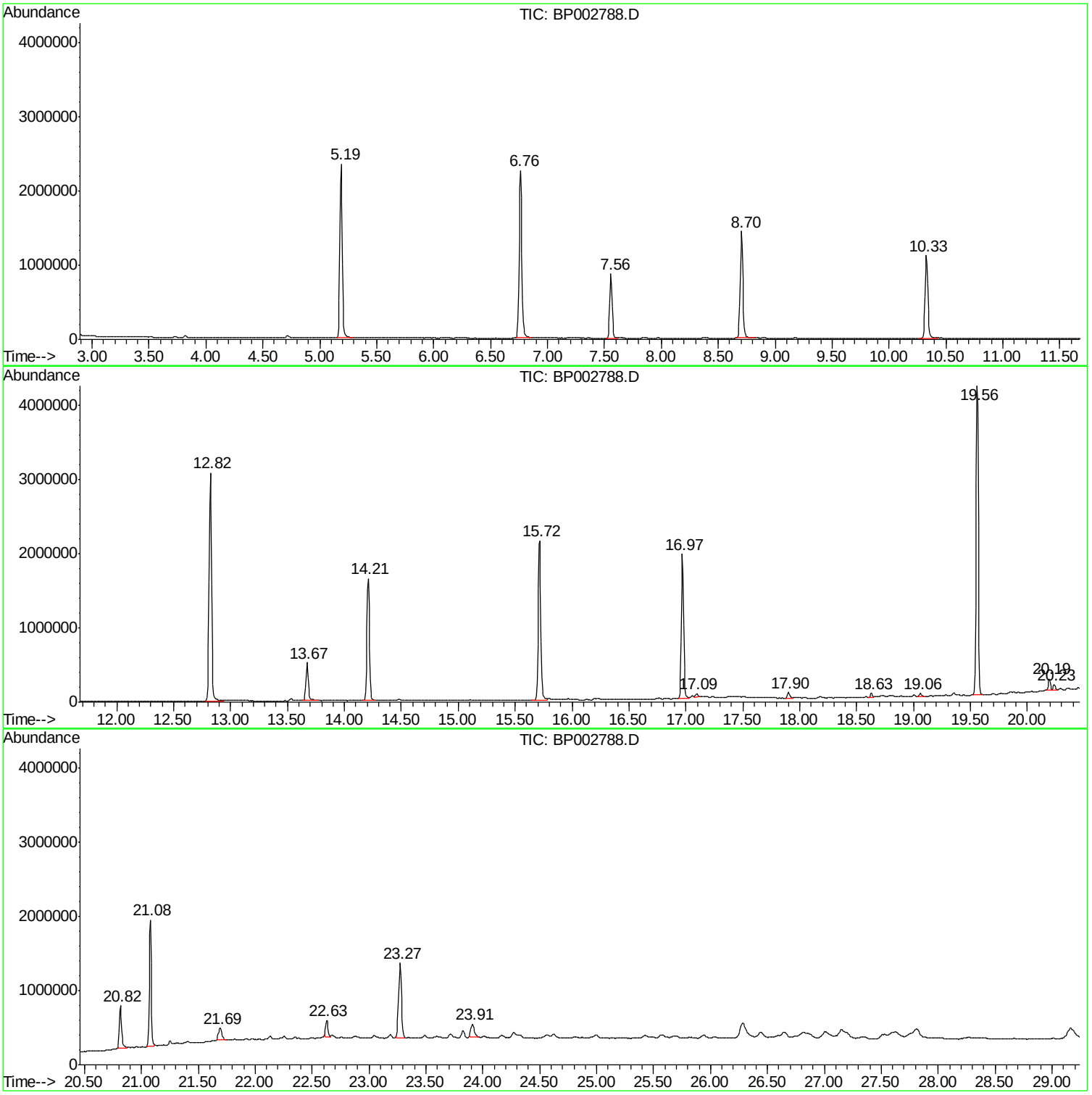
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
23

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP071720\
Data File : BP002788.D
Acq On : 17 Jul 2020 12:55
Operator : CG/JU
Sample : L3308-23
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 23

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

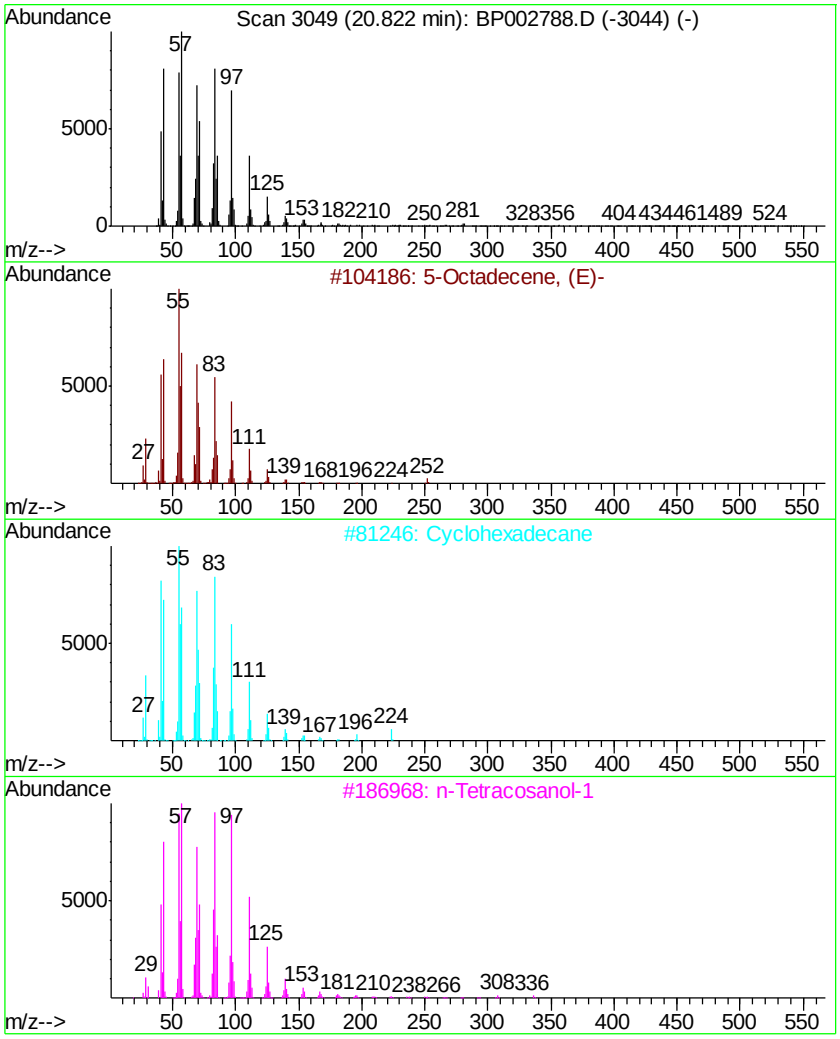
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

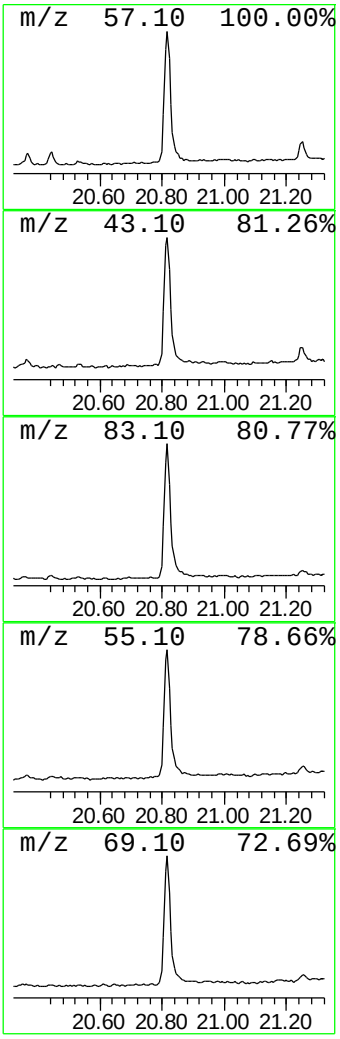
**********

Peak Number 1 5-Octadecene, (E)- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.82 | 7.52 ng | 797186 | Chrysene-d12 | 21.08 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 94 |
| 2 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 94 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 4 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 94 |
| 5 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |



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Sample : L3308-23
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 23

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

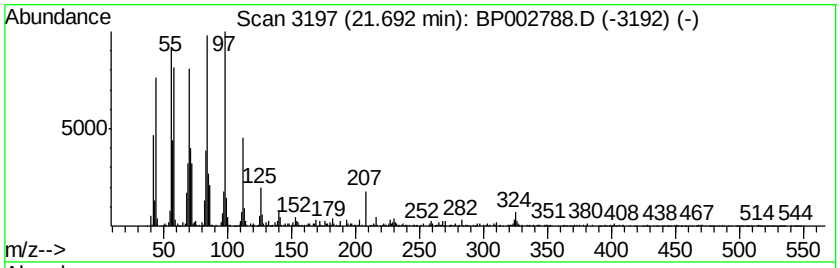
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

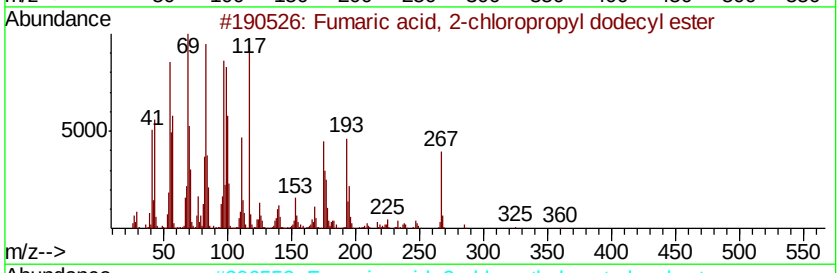
**********

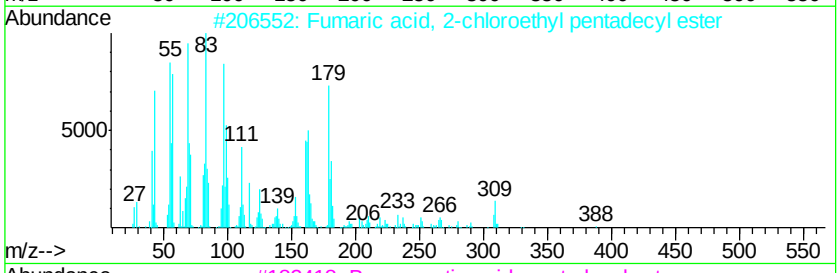
Peak Number 2 Fumaric acid, 2-chloropropy... Concentration Rank 4

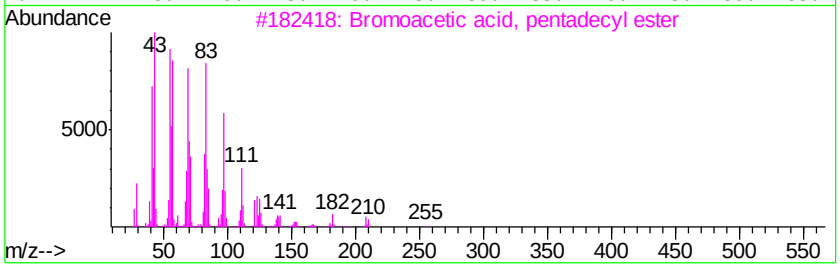
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.69 | 3.16 ng | 334494 | Chrysene-d12 | 21.08 |

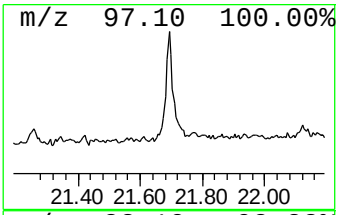
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Fumaric acid, 2-chloropropyl dod... | 360 | C19H33ClO4 | 1000348-57-0 | 96 |
| 2 | Fumaric acid, 2-chloroethyl pent... | 388 | C21H37ClO4 | 1000330-62-1 | 94 |
| 3 | Bromoacetic acid, pentadecyl ester | 348 | C17H33BrO2 | 131143-01-6 | 76 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 74 |
| 5 | 1-Octadecanol | 270 | C18H38O | 000112-92-5 | 70 |

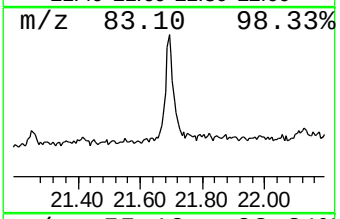


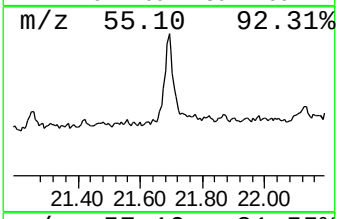



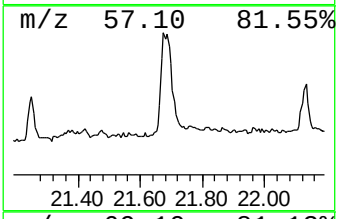



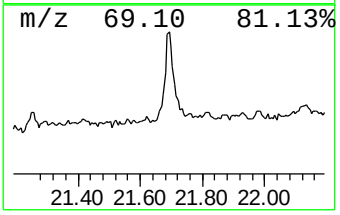



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**Instrument :** BNA_P
**ClientSampleId :** 23

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

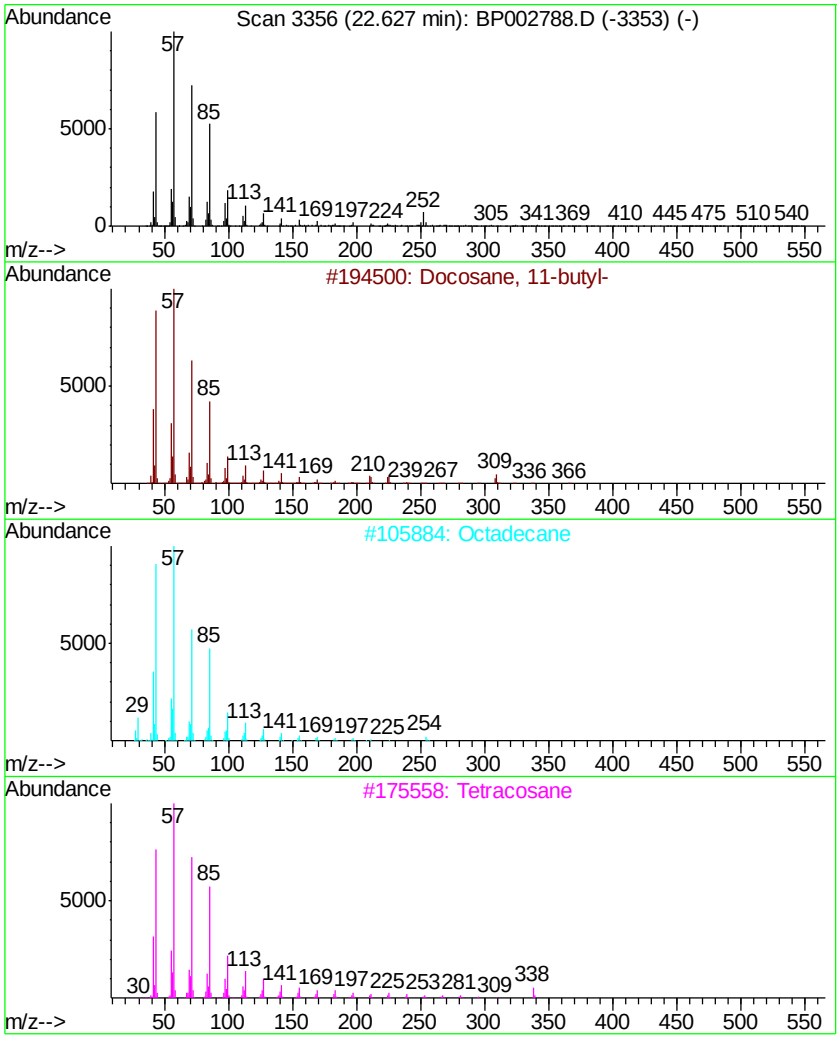
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

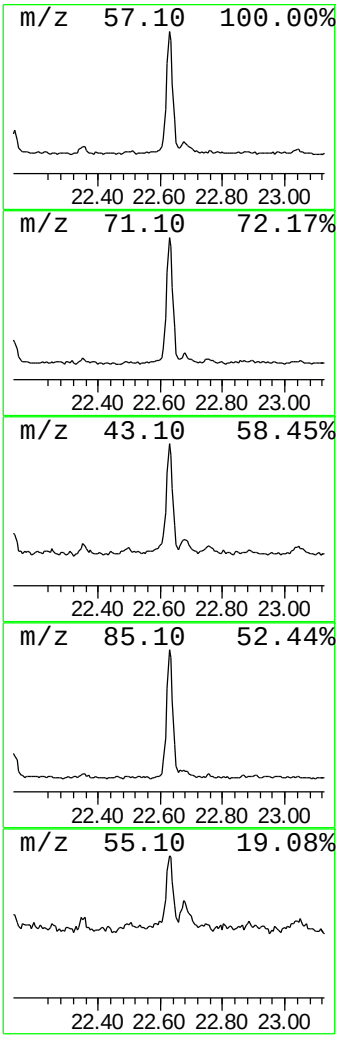
**********

Peak Number 3 Docosane, 11-butyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.63 | 3.32 ng | 303118 | Perylene-d12 | 23.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 93 |
| 2 | Octadecane | 254 | C18H38 | 000593-45-3 | 93 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 93 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 5 | Octadecane, 5,14-dibutyl- | 366 | C26H54 | 055282-13-8 | 89 |



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Misc :
ALS Vial : 5 Sample Multiplier: 1

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**ClientSampleId :** 23

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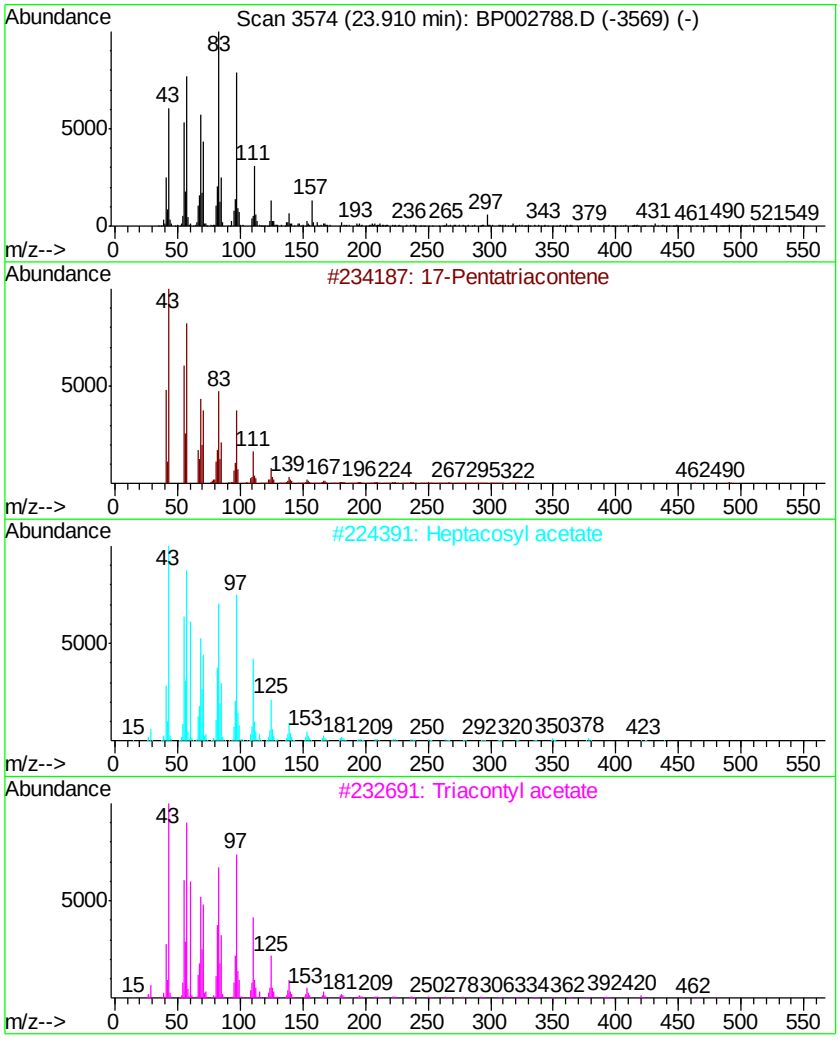
TIC Integration Parameters: LSCINT.P

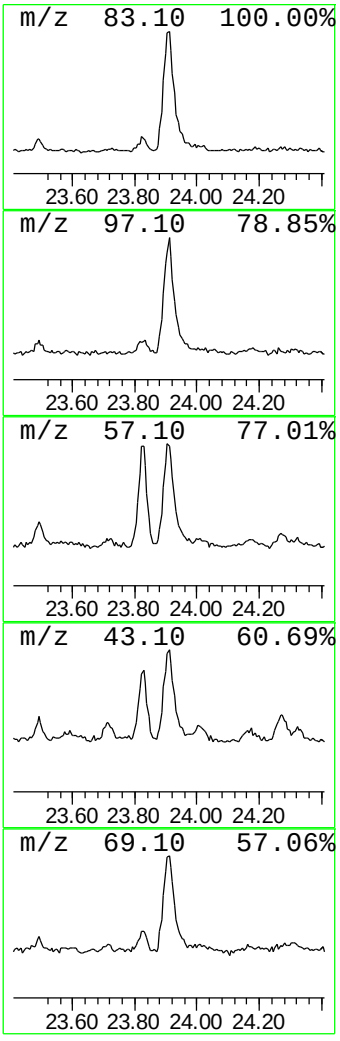
**********

Peak Number 4 17-Pentatriacontene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.91 | 4.40 ng | 401489 | Perylene-d12 | 23.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 70 |
| 2 | Heptacosyl acetate | 438 | C29H58O2 | 1000351-78-2 | 64 |
| 3 | Triacontyl acetate | 480 | C32H64O2 | 041755-58-2 | 60 |
| 4 | Octacosyl acetate | 452 | C30H60O2 | 018206-97-8 | 52 |
| 5 | 1-Hexacosanol | 382 | C26H54O | 000506-52-5 | 47 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP071720\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_P
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP071020.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 |
| 5-Octadecene, (E)- | 20.82 | 7.5 | ng | 797186 | 5 | 21.08 | 2120250 | 20.0 |
| Fumaric acid, 2-c... | 21.69 | 3.2 | ng | 334494 | 5 | 21.08 | 2120250 | 20.0 |
| Docosane, 11-butyl- | 22.63 | 3.3 | ng | 303118 | 6 | 23.27 | 1824030 | 20.0 |
| 17-Pentatriacontene | 23.91 | 4.4 | ng | 401489 | 6 | 23.27 | 1824030 | 20.0 |