LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099559.D
Acq On : 16 Oct 2017 22:17
Operator : SJ/JU
Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 | 5.069 | 504 | 507 | 523 | rBV | 386480 | 551596 | 18.88% | 2.365% |
| 2 | 5.475 | 571 | 576 | 592 | rBV | 2163479 | 2310487 | 79.09% | 9.905% |
| 3 | 6.481 | 742 | 747 | 761 | rBV | 2098130 | 2569047 | 87.94% | 11.014% |
| 4 | 6.616 | 766 | 770 | 773 | rBV | 2551959 | 2438311 | 83.47% | 10.453% |
| 5 | 6.845 | 805 | 809 | 816 | rBV | 638781 | 580935 | 19.89% | 2.491% |
| 6 | 6.998 | 831 | 835 | 839 | rBV | 2209278 | 1996851 | 68.36% | 8.561% |
| 7 | 7.410 | 900 | 905 | 908 | rBV | 1584195 | 1546249 | 52.93% | 6.629% |
| 8 | 8.122 | 1023 | 1026 | 1039 | rBV | 863889 | 799479 | 27.37% | 3.428% |
| 9 | 8.681 | 1118 | 1121 | 1130 | rBB | 35750 | 32275 | 1.10% | 0.138% |
| 10 | 9.198 | 1204 | 1209 | 1213 | rBV | 2895561 | 2921261 | 100.00% | 12.524% |
| 11 | 9.592 | 1272 | 1276 | 1285 | rVB | 630115 | 490564 | 16.79% | 2.103% |
| 12 | 9.881 | 1321 | 1325 | 1329 | rBV | 1035109 | 853477 | 29.22% | 3.659% |
| 13 | 10.592 | 1443 | 1446 | 1451 | rVB | 97433 | 77276 | 2.65% | 0.331% |
| 14 | 10.675 | 1455 | 1460 | 1463 | rBV | 1205856 | 1200604 | 41.10% | 5.147% |
| 15 | 11.369 | 1574 | 1578 | 1581 | rBV | 927757 | 767323 | 26.27% | 3.290% |
| 16 | 11.880 | 1661 | 1665 | 1667 | rBV2 | 33870 | 38903 | 1.33% | 0.167% |
| 17 | 12.951 | 1843 | 1847 | 1851 | rBV | 2141313 | 2123981 | 72.71% | 9.106% |
| 18 | 13.422 | 1923 | 1927 | 1930 | rVB | 44425 | 41741 | 1.43% | 0.179% |
| 19 | 13.833 | 1993 | 1997 | 2008 | rBV | 120415 | 158368 | 5.42% | 0.679% |
| 20 | 14.010 | 2024 | 2027 | 2031 | rBV | 579515 | 564199 | 19.31% | 2.419% |
| 21 | 14.457 | 2100 | 2103 | 2110 | rBV4 | 21338 | 39021 | 1.34% | 0.167% |
| 22 | 14.833 | 2164 | 2167 | 2171 | rVB | 214670 | 200160 | 6.85% | 0.858% |
| 23 | 15.092 | 2208 | 2211 | 2214 | rVB | 42161 | 40621 | 1.39% | 0.174% |
| 24 | 15.486 | 2271 | 2278 | 2286 | rBV | 470890 | 616662 | 21.11% | 2.644% |
| 25 | 15.898 | 2343 | 2348 | 2353 | rVB2 | 56461 | 82537 | 2.83% | 0.354% |
| 26 | 16.398 | 2428 | 2433 | 2439 | rBV2 | 38251 | 70707 | 2.42% | 0.303% |
| 27 | 16.980 | 2526 | 2532 | 2539 | rVB3 | 38066 | 81439 | 2.79% | 0.349% |
| 28 | 17.668 | 2644 | 2649 | 2661 | rVB3 | 26699 | 69529 | 2.38% | 0.298% |
| 29 | 18.492 | 2783 | 2789 | 2803 | rVB9 | 16935 | 61759 | 2.11% | 0.265% |

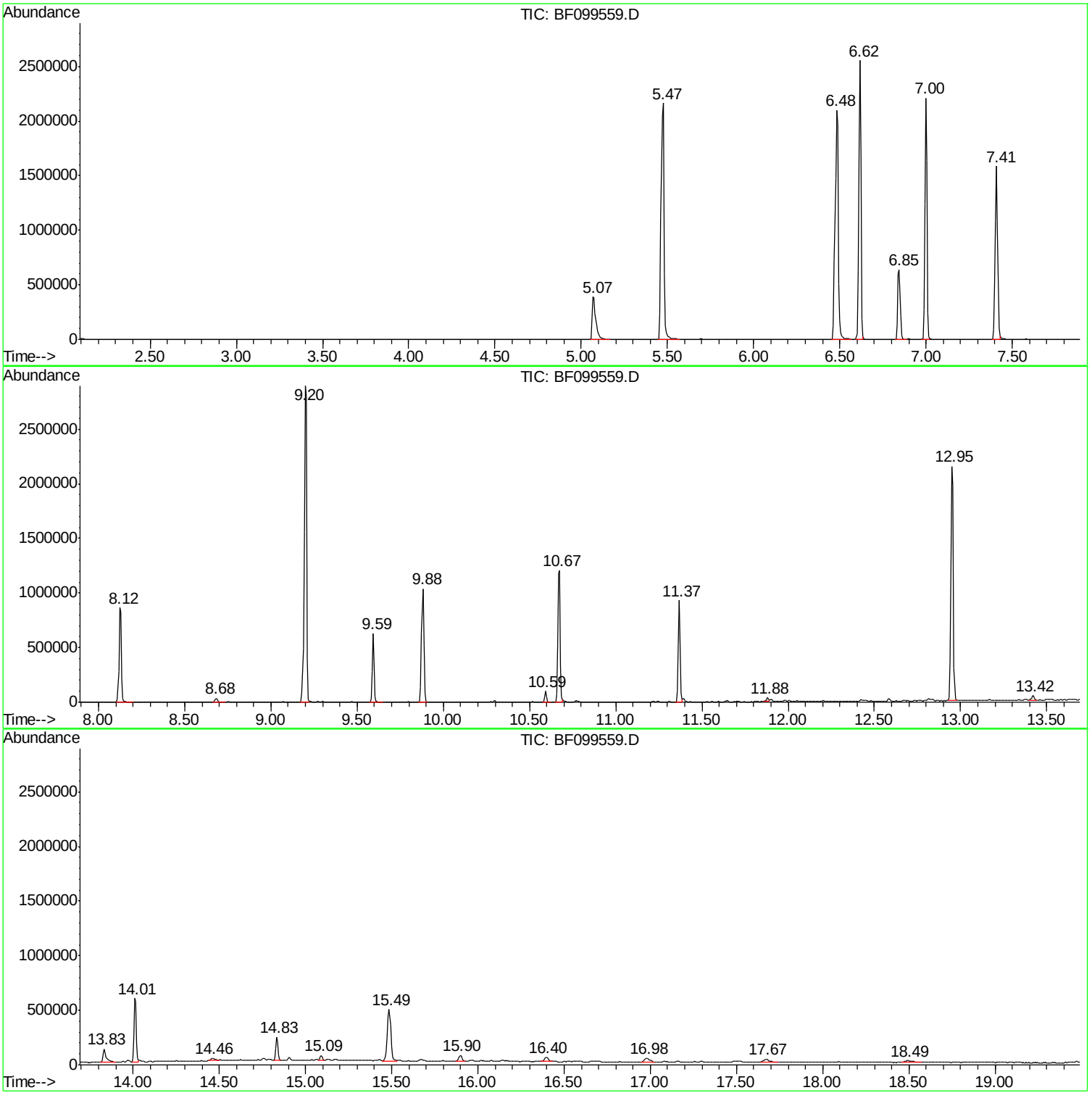
Sum of corrected areas: 23325362

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099559.D
Acq On : 16 Oct 2017 22:17
Operator : SJ/JU
Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Data File : BF099559.D
Acq On : 16 Oct 2017 22:17
Operator : SJ/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

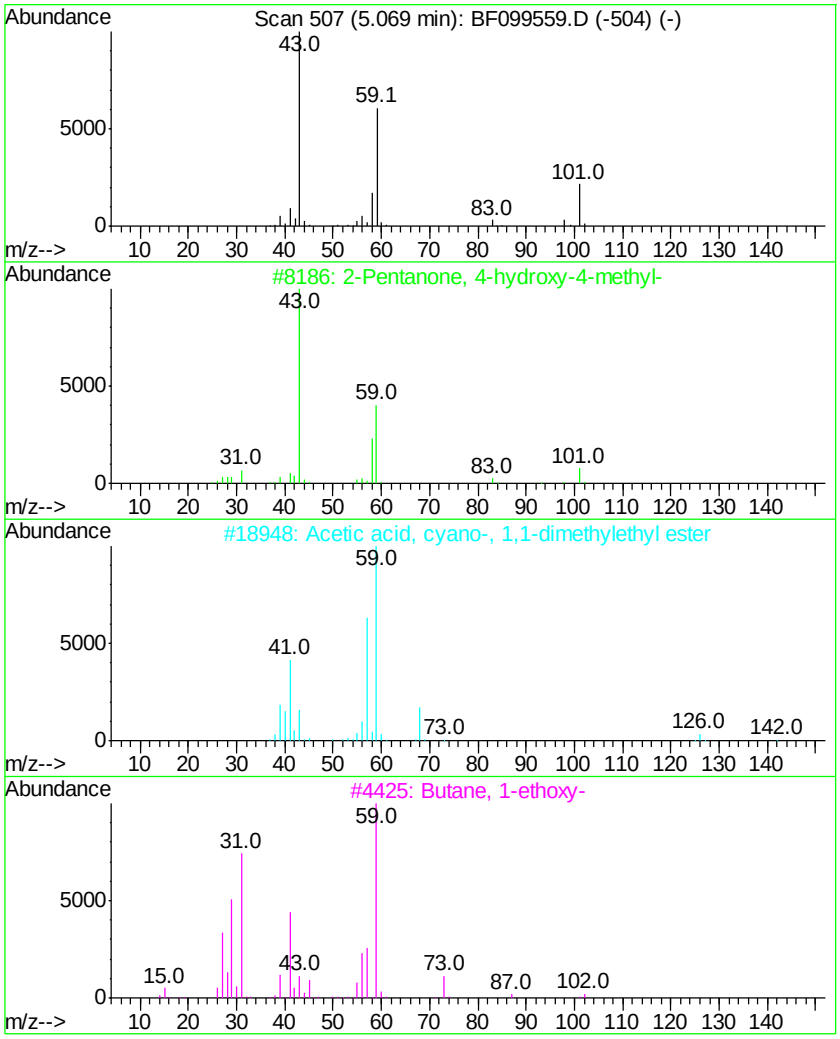
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

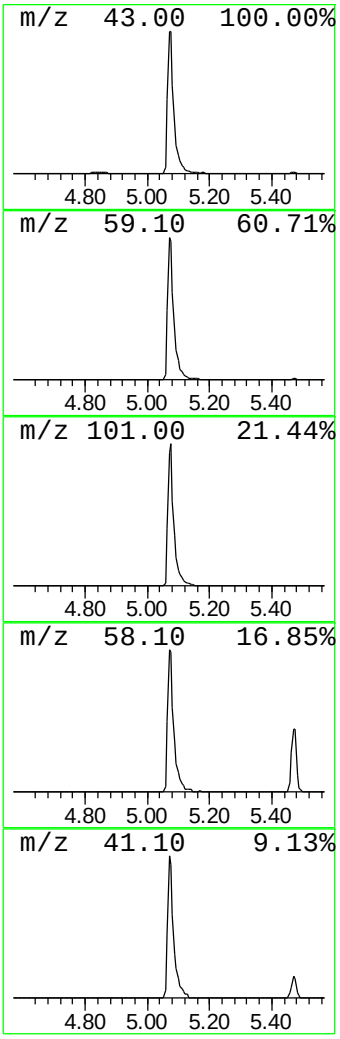
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.07 | 18.99 ng | 551596 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



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Data File : BF099559.D
Acq On : 16 Oct 2017 22:17
Operator : SJ/JU
Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

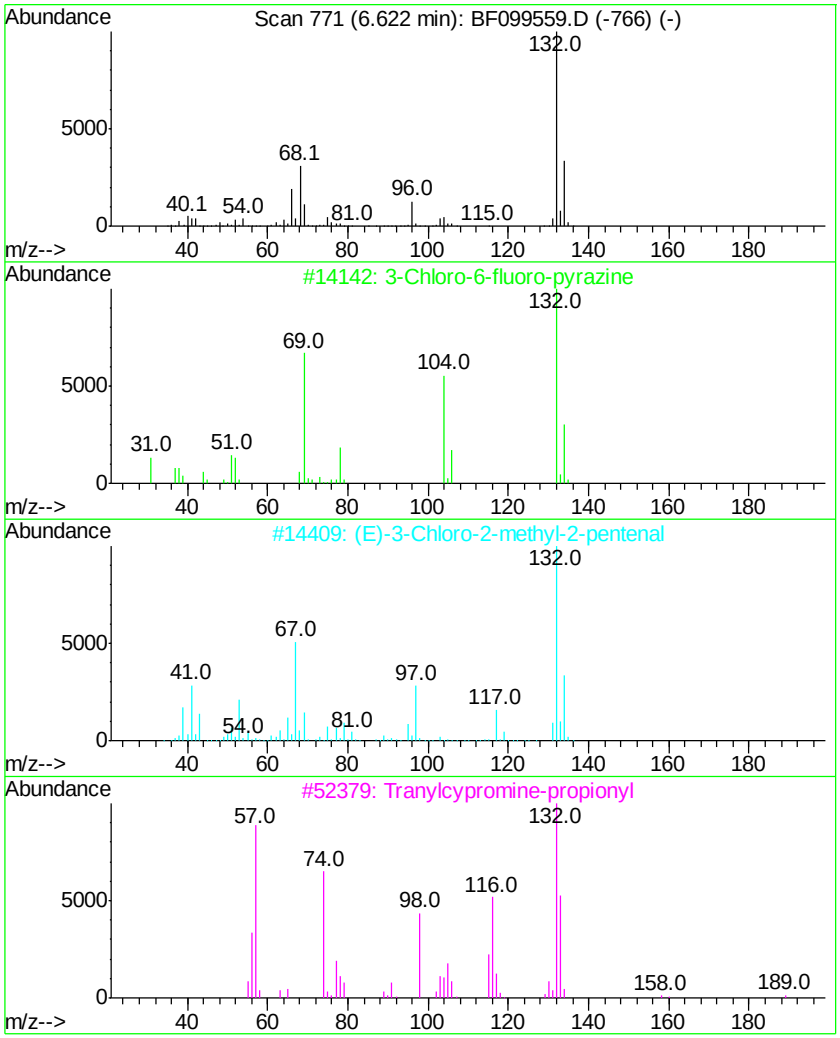
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

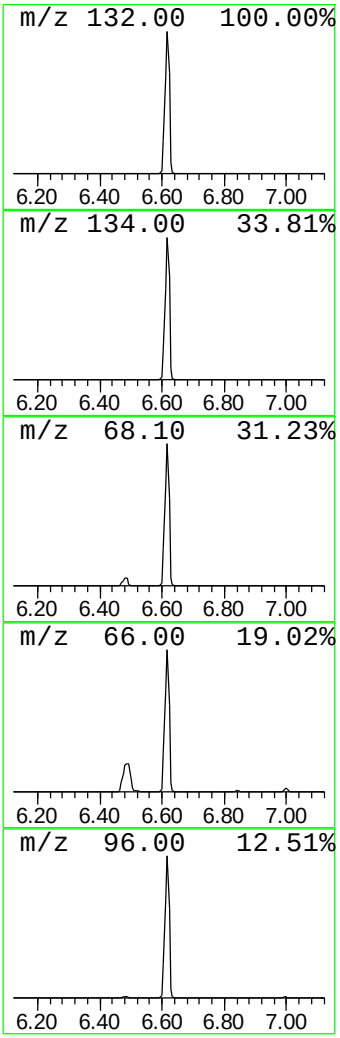
**********

Peak Number 2 unknown6.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 83.94 ng | 2438310 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 35 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | 1H-Indazole, 7-methyl- | 132 | C8H8N2 | 1000316-00-7 | 10 |



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Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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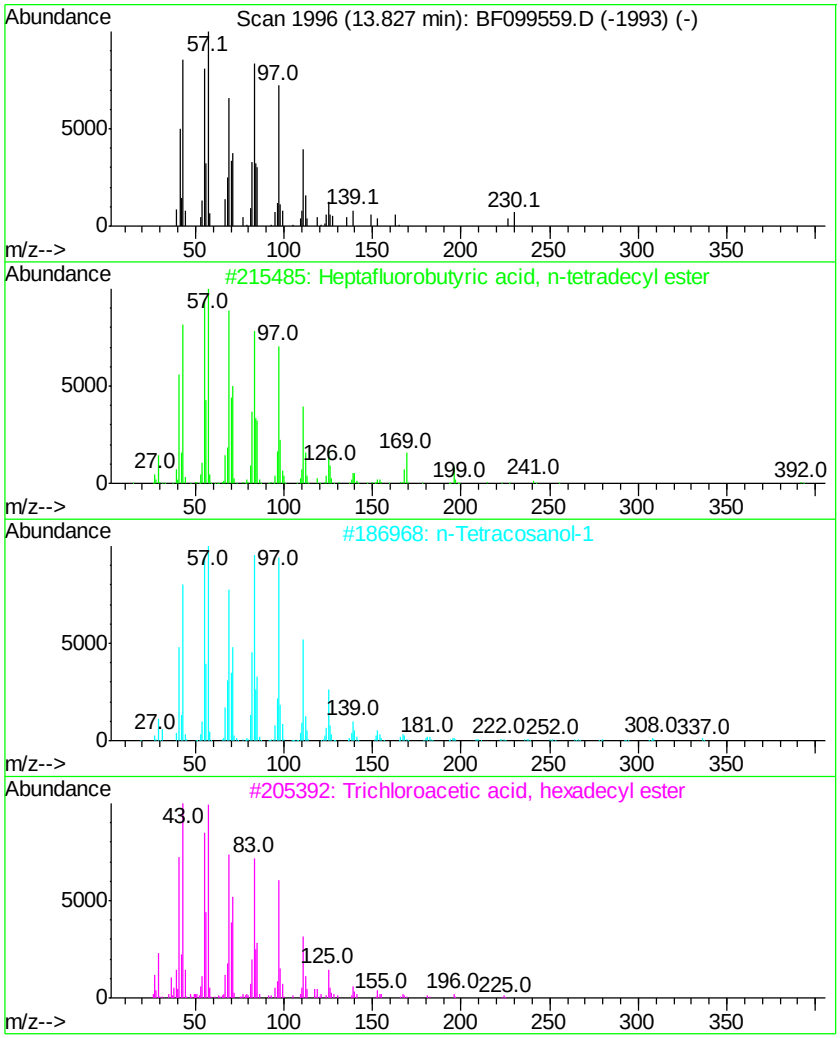
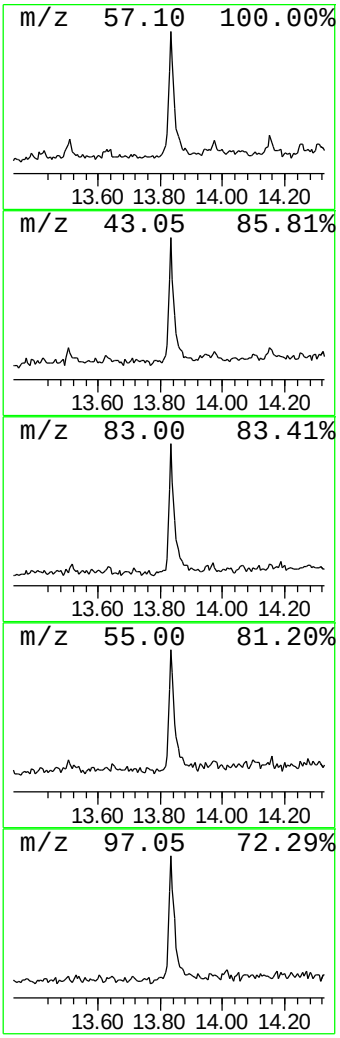
Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.83 | 5.61 ng | 158368 | Chrysene-d12 | 14.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 95 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 4 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |
| 5 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |



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Acq On : 16 Oct 2017 22:17
Operator : SJ/JU
Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

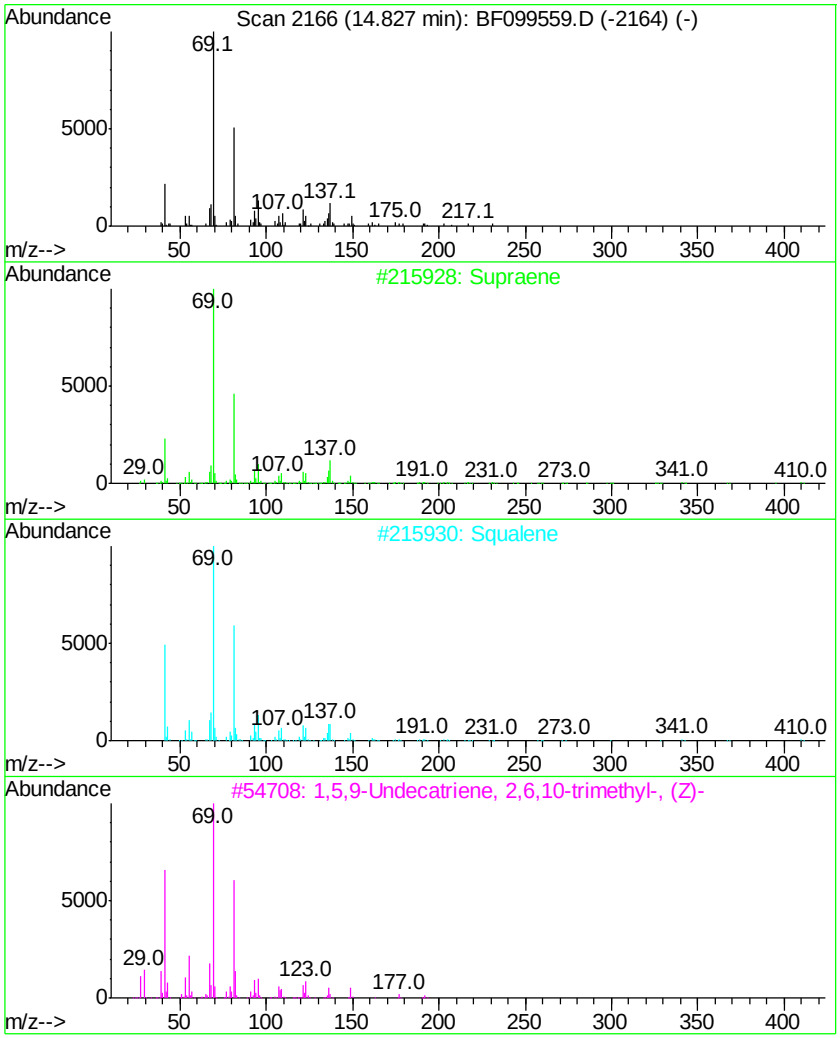
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

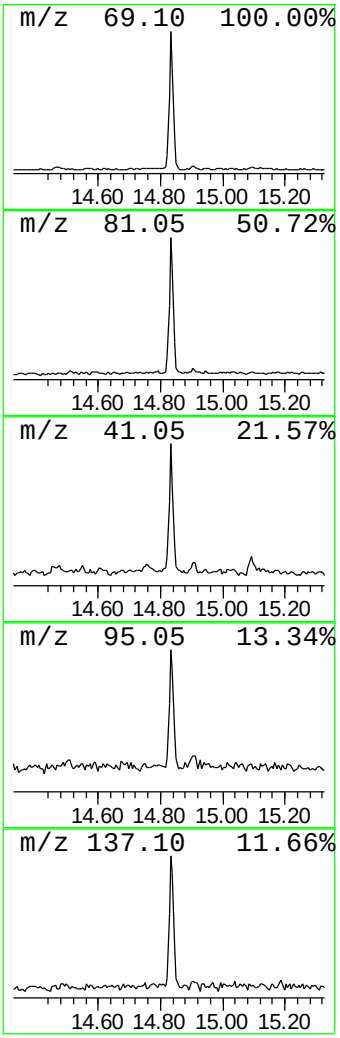
**********

Peak Number 5 Supraene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.83 | 6.49 ng | 200160 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 91 |
| 2 | Squalene | 410 | C30H50 | 000111-02-4 | 91 |
| 3 | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24 | 062951-96-6 | 86 |
| 4 | 1,5,9-Decatriene, 2,3,5,8-tetram... | 192 | C14H24 | 230646-72-7 | 72 |
| 5 | 1,5-Heptadiene, 3,3,6-trimethyl- | 138 | C10H18 | 035387-63-4 | 58 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
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Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

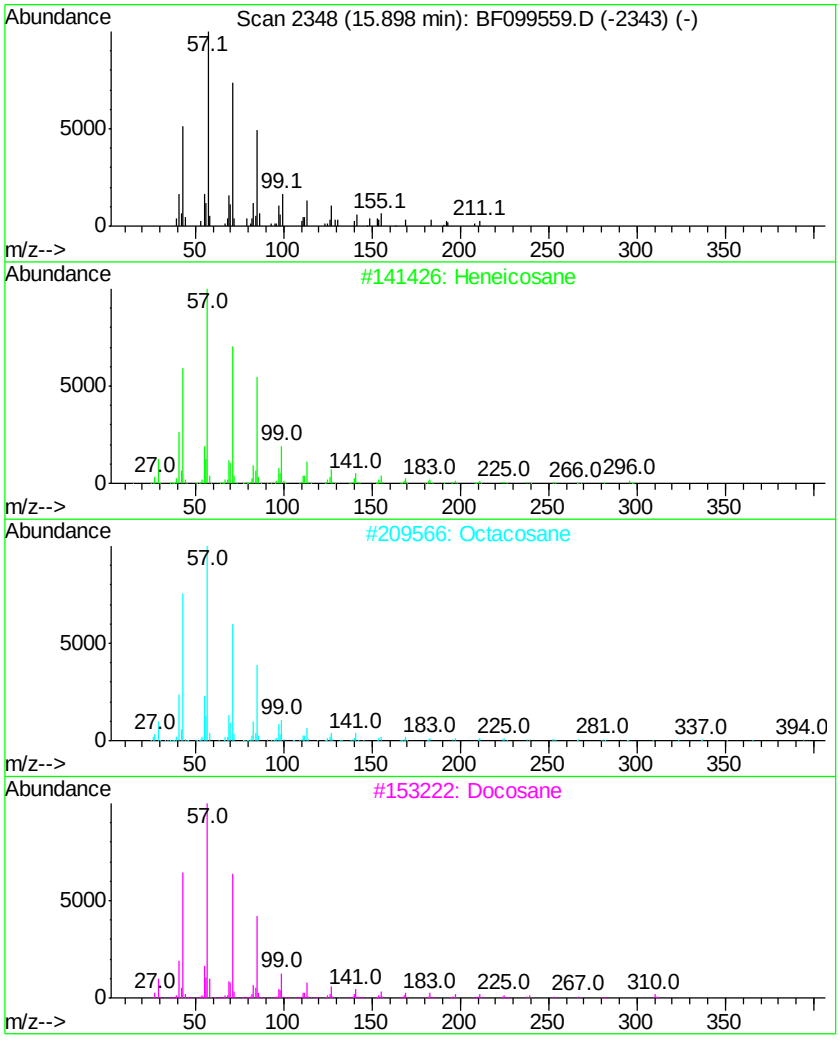
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

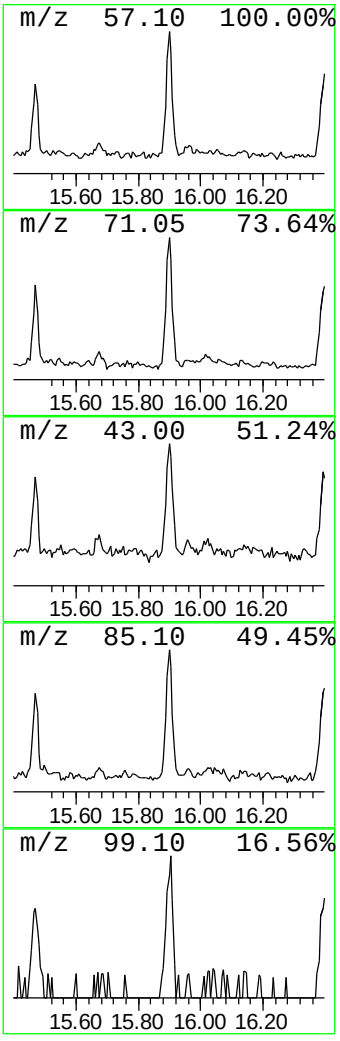
**********

Peak Number 6 Heneicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.90 | 2.68 ng | 82537 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Docosane | 310 | C22H46 | 000629-97-0 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Triacontane | 422 | C30H62 | 000638-68-6 | 91 |



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Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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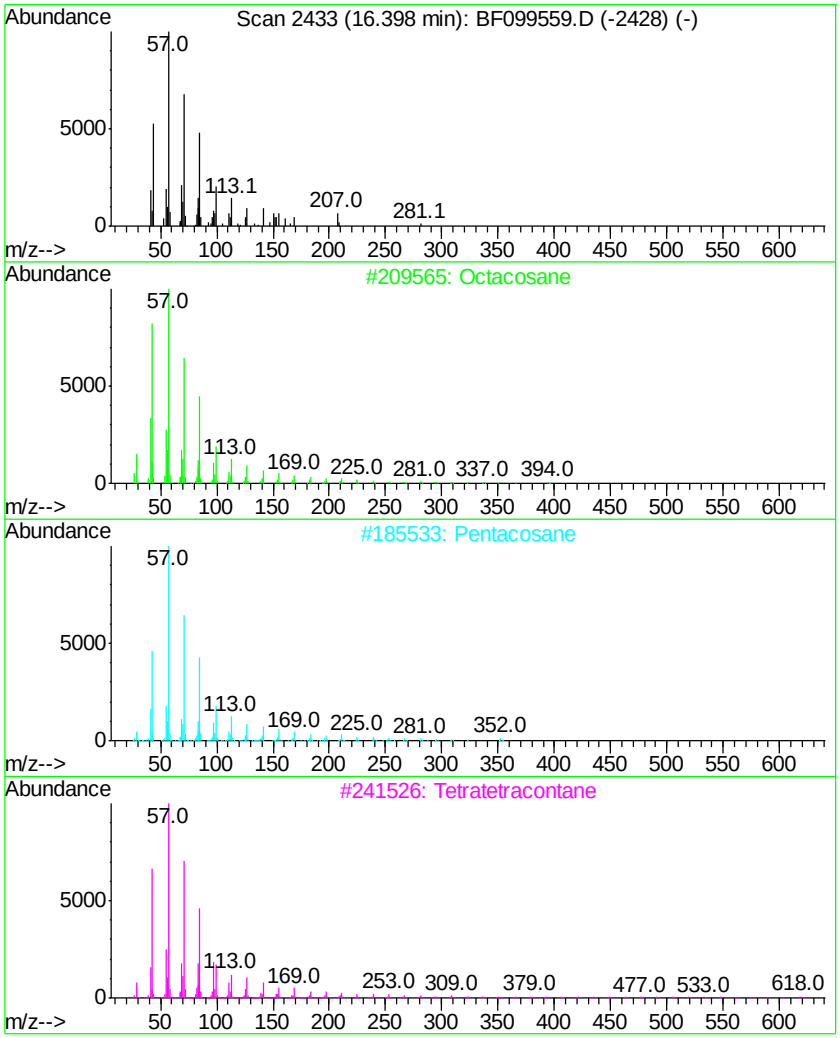
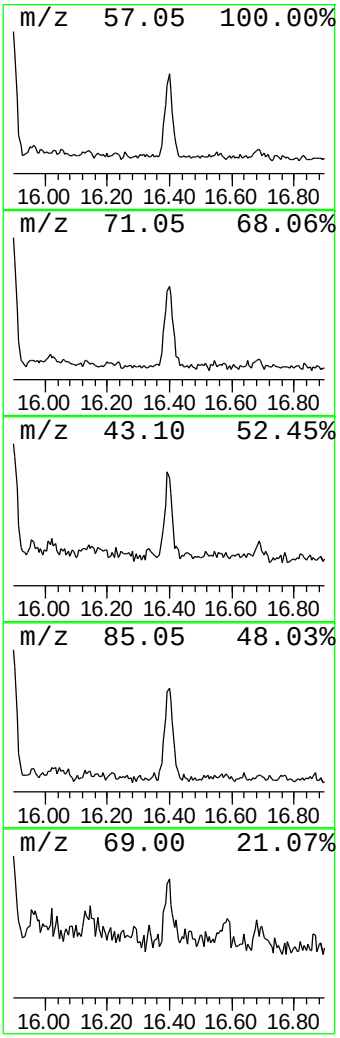
Peak Number 7 Octacosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.40 | 2.29 ng | 70707 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Pentacosane | 352 | C25H52 | 000629-99-2 | 91 |
| 3 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 91 |
| 4 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 5 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |



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Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

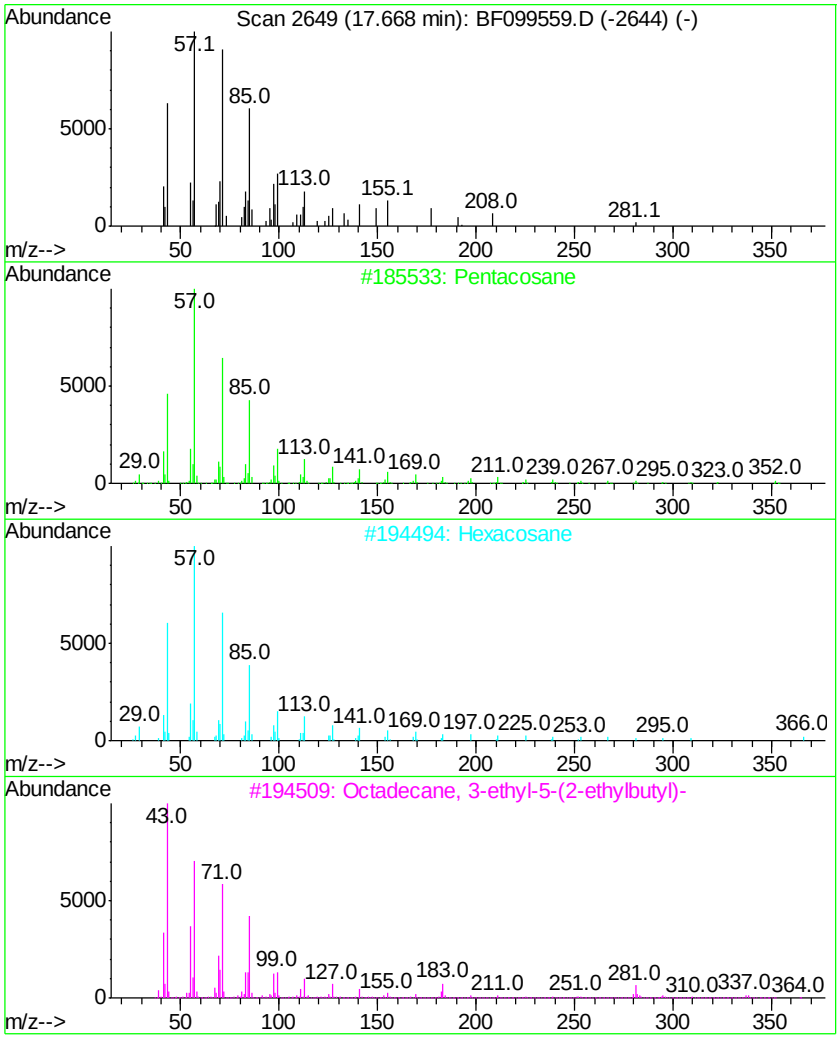
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

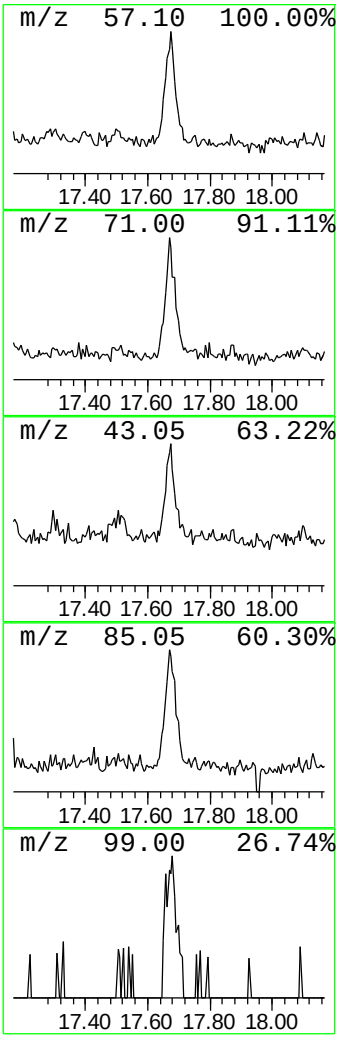
**********

Peak Number 9 Pentacosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.67 | 2.26 ng | 69529 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentacosane | 352 | C25H52 | 000629-99-2 | 72 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 72 |
| 3 | Octadecane, 3-ethyl-5-(2-ethylbu... | 366 | C26H54 | 055282-12-7 | 72 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 53 |
| 5 | Nonane, 1-iodo- | 254 | C9H19I | 004282-42-2 | 50 |



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Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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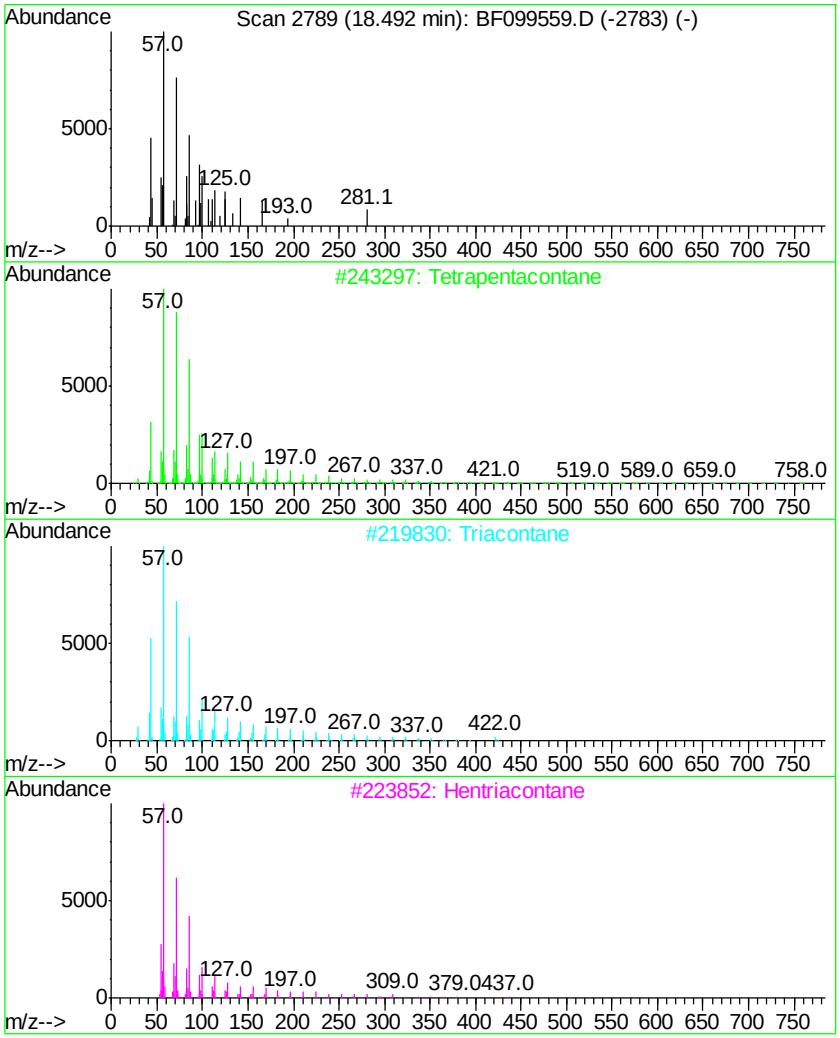
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

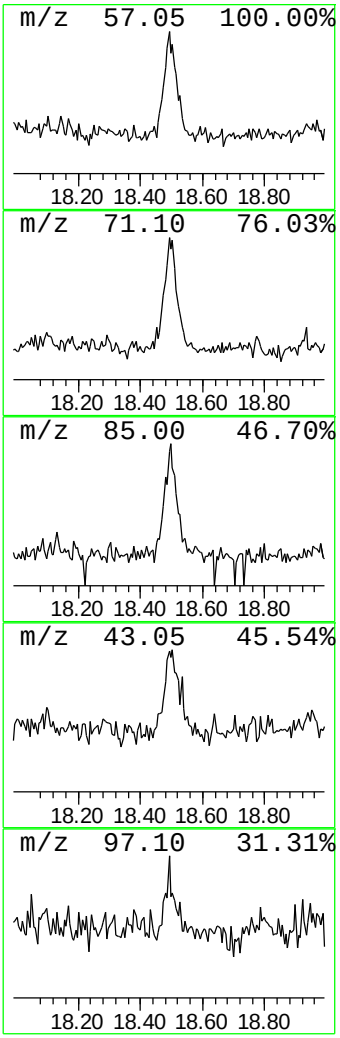
**********

Peak Number 10 Tetrapentacontane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.49 | 2.00 ng | 61759 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetrapentacontane | 759 | C54H110 | 005856-66-6 | 64 |
| 2 | Triacontane | 422 | C30H62 | 000638-68-6 | 64 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 64 |
| 4 | Tetratriacontane | 479 | C34H70 | 014167-59-0 | 64 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 59 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099559.D
Acq On : 16 Oct 2017 22:17
Operator : SJ/JU
Sample : I5782-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S4(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 |
| 2-Pentanone, 4-hy... | 5.07 | 19.0 | ng | 551596 | 1 | 6.85 | 580935 | 20.0 |
| unknown6.62 | 6.62 | 83.9 | ng | 2438310 | 1 | 6.85 | 580935 | 20.0 |
| Heptafluorobutyri... | 13.83 | 5.6 | ng | 158368 | 5 | 14.01 | 564199 | 20.0 |
| Supraene | 14.83 | 6.5 | ng | 200160 | 6 | 15.49 | 616662 | 20.0 |
| Heneicosane | 15.90 | 2.7 | ng | 82537 | 6 | 15.49 | 616662 | 20.0 |
| Octacosane | 16.40 | 2.3 | ng | 70707 | 6 | 15.49 | 616662 | 20.0 |
| Pentacosane | 17.67 | 2.3 | ng | 69529 | 6 | 15.49 | 616662 | 20.0 |
| Tetrapentacontane | 18.49 | 2.0 | ng | 61759 | 6 | 15.49 | 616662 | 20.0 |