LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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 | 4.575 | 454 | 457 | 473 | rBV | 162739 | 309999 | 10.20% | 1.194% |
| 2 | 5.039 | 532 | 536 | 560 | rBV | 2561447 | 2923702 | 96.18% | 11.257% |
| 3 | 6.116 | 715 | 719 | 732 | rBV | 2699233 | 3039692 | 100.00% | 11.704% |
| 4 | 6.216 | 732 | 736 | 743 | rVB | 2626337 | 2693164 | 88.60% | 10.369% |
| 5 | 6.445 | 771 | 775 | 785 | rVB | 744428 | 709443 | 23.34% | 2.732% |
| 6 | 6.598 | 797 | 801 | 812 | rBV | 2086184 | 1918829 | 63.13% | 7.388% |
| 7 | 7.016 | 868 | 872 | 875 | rBV | 2064536 | 1906625 | 62.72% | 7.341% |
| 8 | 7.157 | 894 | 896 | 908 | rVB2 | 21097 | 33925 | 1.12% | 0.131% |
| 9 | 7.728 | 989 | 993 | 1006 | rBV | 1130688 | 1050734 | 34.57% | 4.046% |
| 10 | 8.804 | 1171 | 1176 | 1179 | rBV | 2709327 | 2709557 | 89.14% | 10.432% |
| 11 | 9.198 | 1240 | 1243 | 1248 | rBV | 483912 | 404170 | 13.30% | 1.556% |
| 12 | 9.422 | 1278 | 1281 | 1284 | rBV | 41320 | 35772 | 1.18% | 0.138% |
| 13 | 9.463 | 1284 | 1288 | 1292 | rBV | 1178991 | 1068093 | 35.14% | 4.112% |
| 14 | 9.922 | 1363 | 1366 | 1369 | rVB | 70341 | 62310 | 2.05% | 0.240% |
| 15 | 10.139 | 1398 | 1403 | 1405 | rBV2 | 24939 | 31924 | 1.05% | 0.123% |
| 16 | 10.251 | 1418 | 1422 | 1429 | rBV | 1581406 | 1589077 | 52.28% | 6.118% |
| 17 | 10.386 | 1442 | 1445 | 1452 | rBV | 92207 | 105799 | 3.48% | 0.407% |
| 18 | 10.833 | 1516 | 1521 | 1524 | rBV2 | 60071 | 52726 | 1.73% | 0.203% |
| 19 | 10.933 | 1535 | 1538 | 1541 | rBV | 1034695 | 955590 | 31.44% | 3.679% |
| 20 | 10.957 | 1541 | 1542 | 1547 | rVB | 55222 | 41315 | 1.36% | 0.159% |
| 21 | 11.492 | 1630 | 1633 | 1640 | rBV2 | 170749 | 181280 | 5.96% | 0.698% |
| 22 | 12.139 | 1740 | 1743 | 1747 | rBV | 78181 | 70314 | 2.31% | 0.271% |
| 23 | 12.274 | 1762 | 1766 | 1773 | rBV3 | 51184 | 76709 | 2.52% | 0.295% |
| 24 | 12.363 | 1777 | 1781 | 1788 | rVB | 89157 | 93771 | 3.08% | 0.361% |
| 25 | 12.521 | 1803 | 1808 | 1811 | rBV | 1874643 | 1880800 | 61.87% | 7.242% |
| 26 | 12.762 | 1843 | 1849 | 1853 | rBV4 | 21430 | 33523 | 1.10% | 0.129% |
| 27 | 13.439 | 1958 | 1964 | 1973 | rBV2 | 149700 | 251507 | 8.27% | 0.968% |
| 28 | 13.557 | 1980 | 1984 | 1994 | rVB | 802207 | 808288 | 26.59% | 3.112% |
| 29 | 14.074 | 2069 | 2072 | 2077 | rVB2 | 41558 | 55598 | 1.83% | 0.214% |
| 30 | 14.409 | 2125 | 2129 | 2132 | rBV | 97288 | 104617 | 3.44% | 0.403% |
| 31 | 14.898 | 2208 | 2212 | 2217 | rBV | 510692 | 605495 | 19.92% | 2.331% |
| 32 | 17.168 | 2591 | 2598 | 2609 | rVB | 44774 | 168033 | 5.53% | 0.647% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

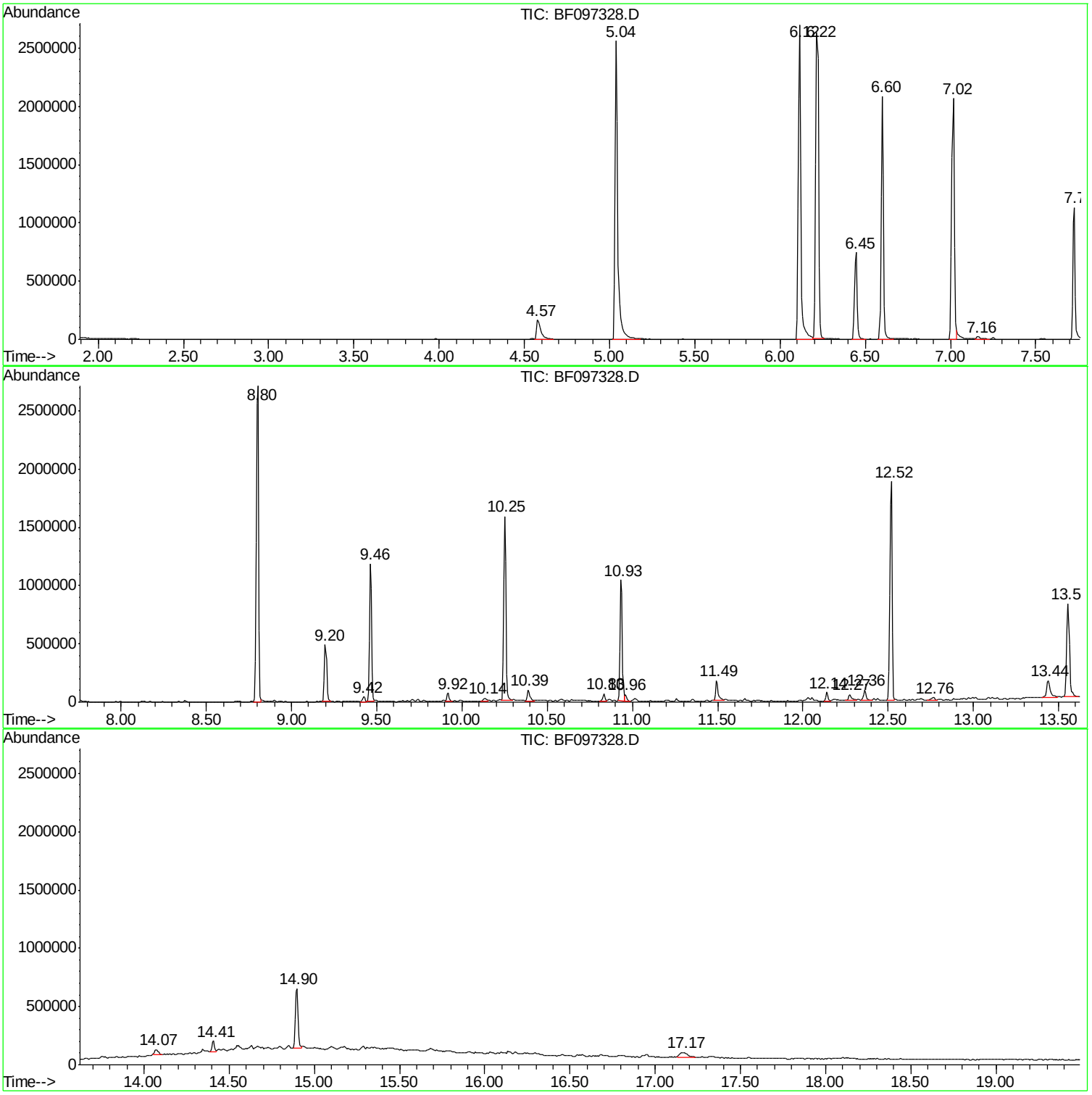
Sum of corrected areas: 25972381

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

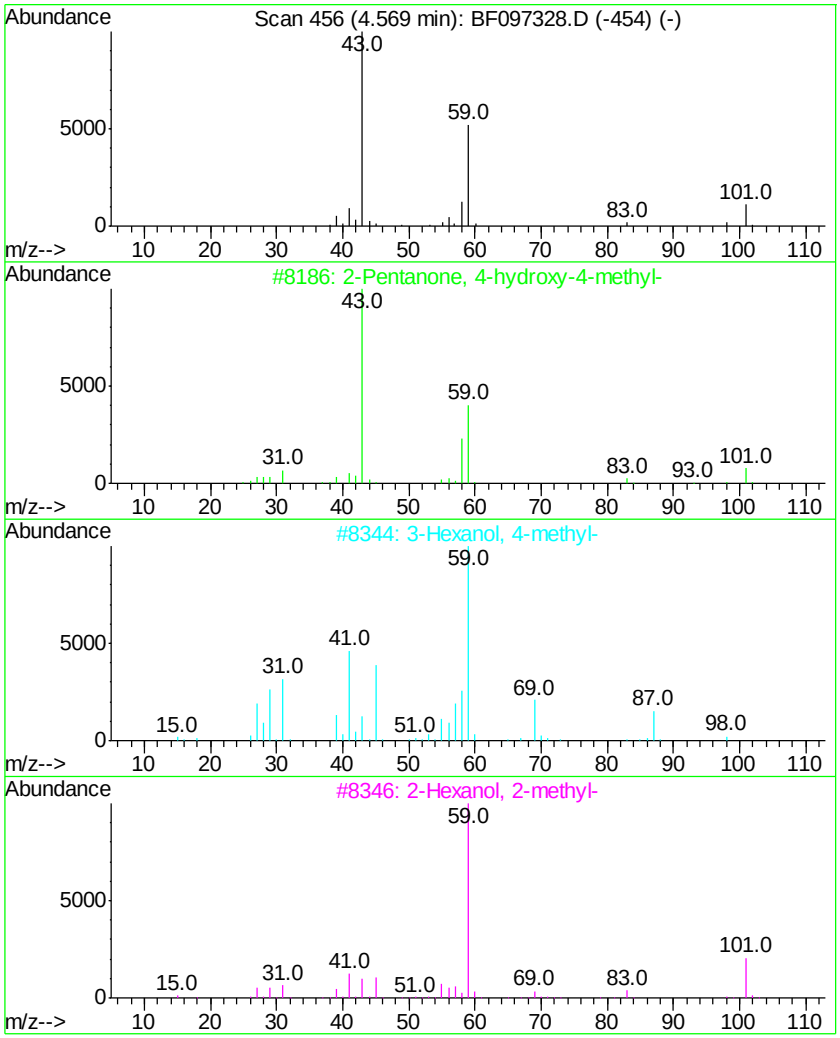
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

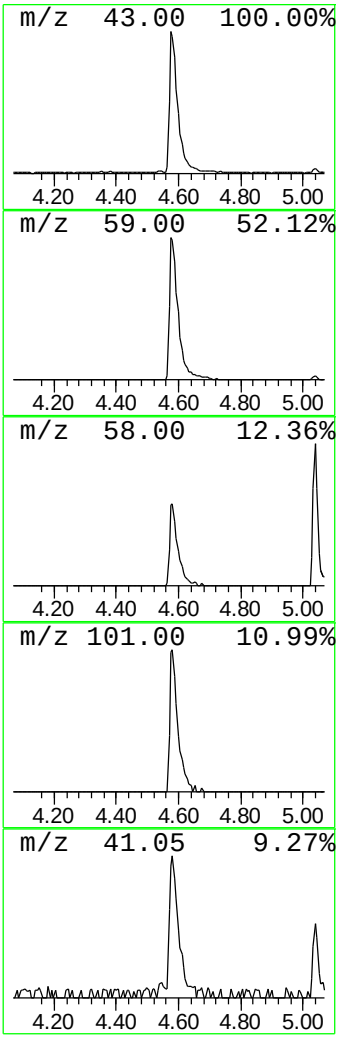
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.57 | 8.74 ng | 309999 | 1,4-Dichlorobenzene-d4 | 6.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

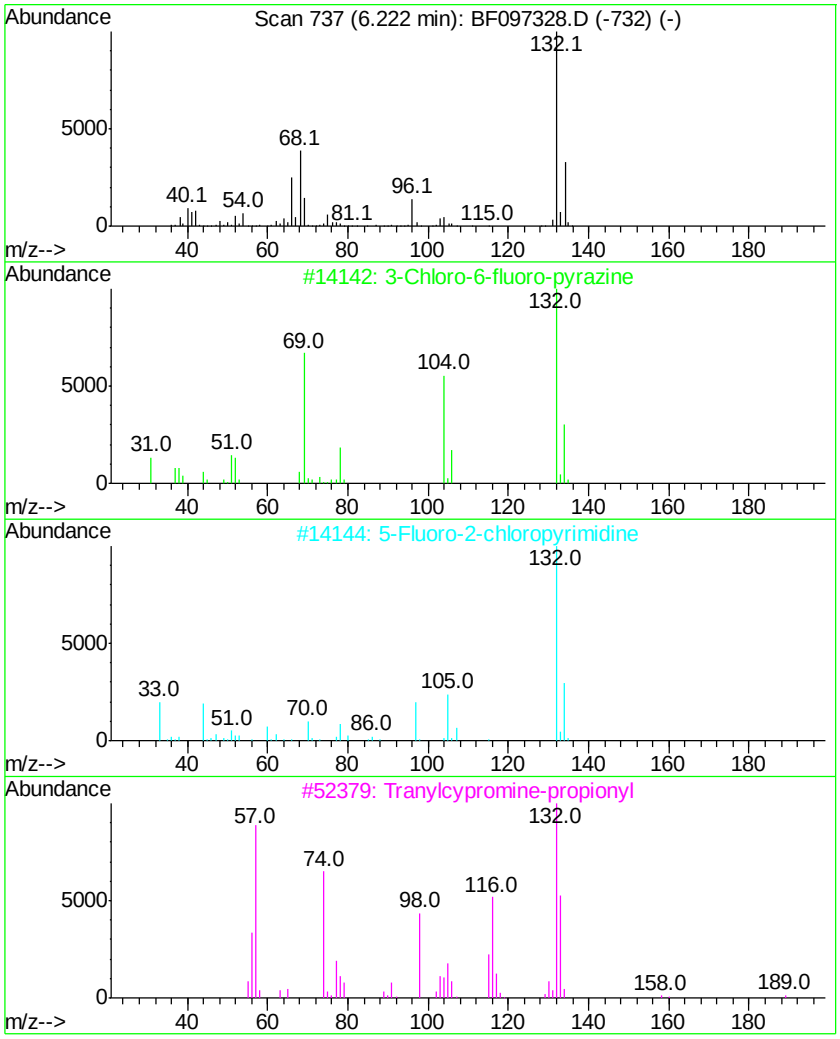
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

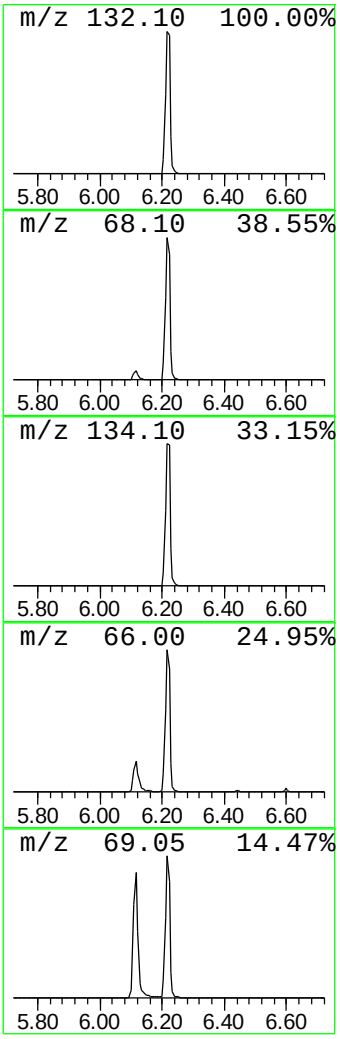
**********

Peak Number 2 unknown6.22 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.22 | 75.92 ng | 2693160 | 1,4-Dichlorobenzene-d4 | 6.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

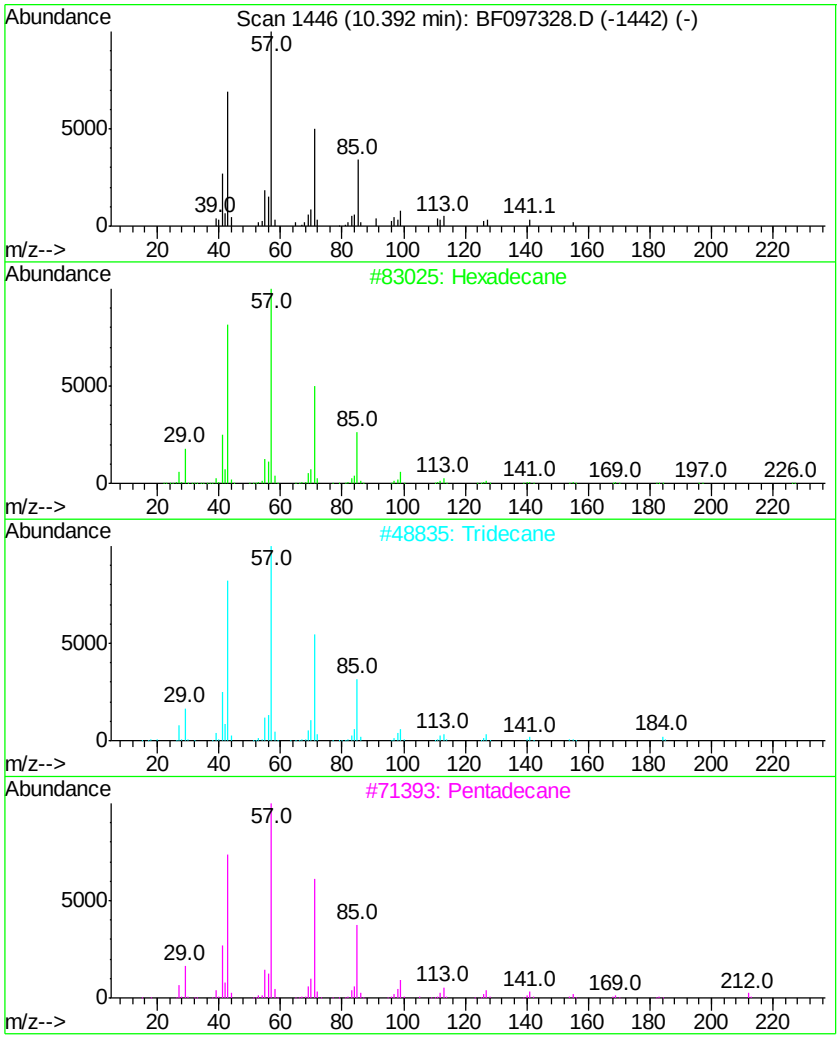
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

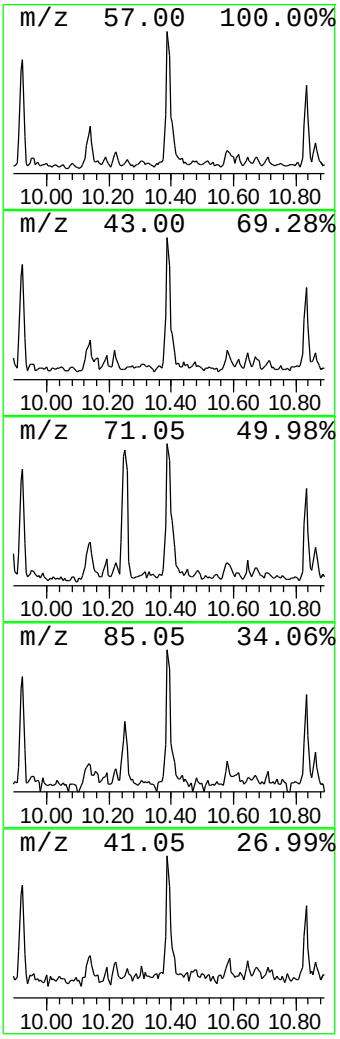
**********

Peak Number 4 Hexadecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.39 | 2.21 ng | 105799 | Phenanthrene-d10 | 10.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 2 | Tridecane | 184 | C13H28 | 000629-50-5 | 83 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 83 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 78 |
| 5 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 59 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

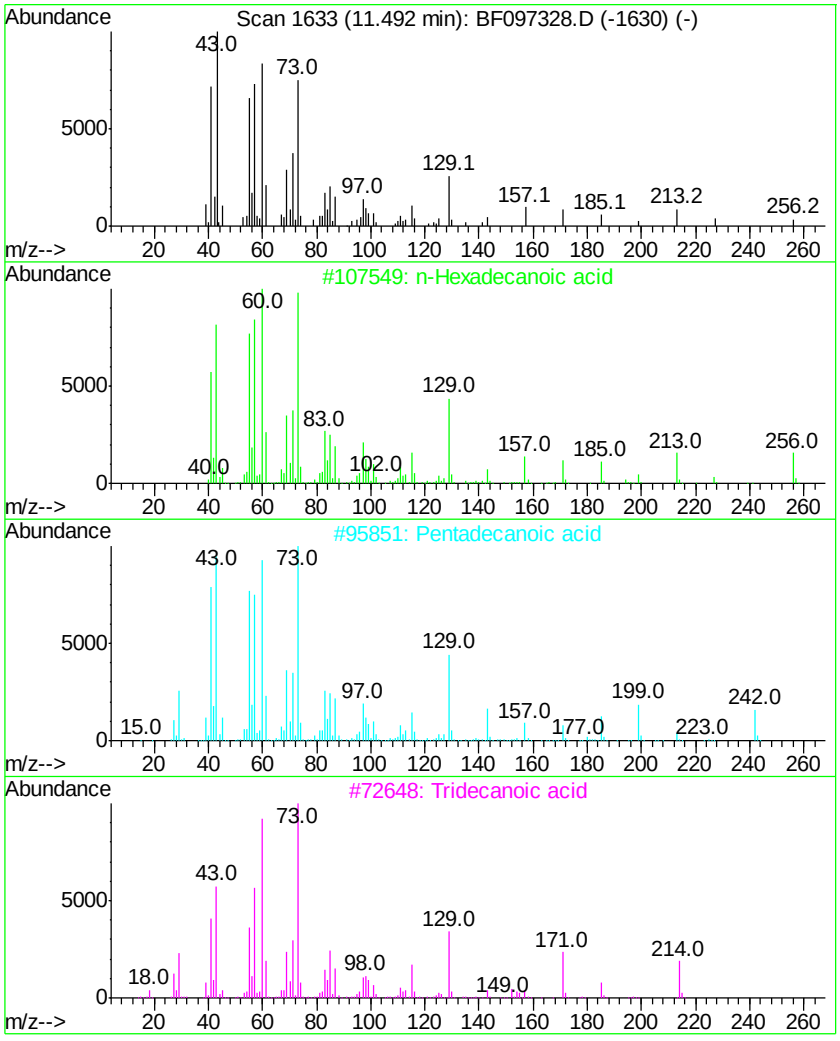
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

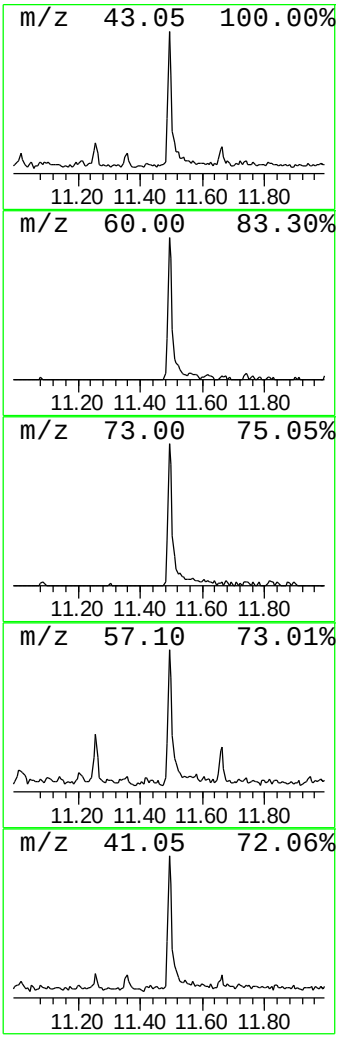
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.49 | 3.79 ng | 181280 | Phenanthrene-d10 | 10.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 78 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 78 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

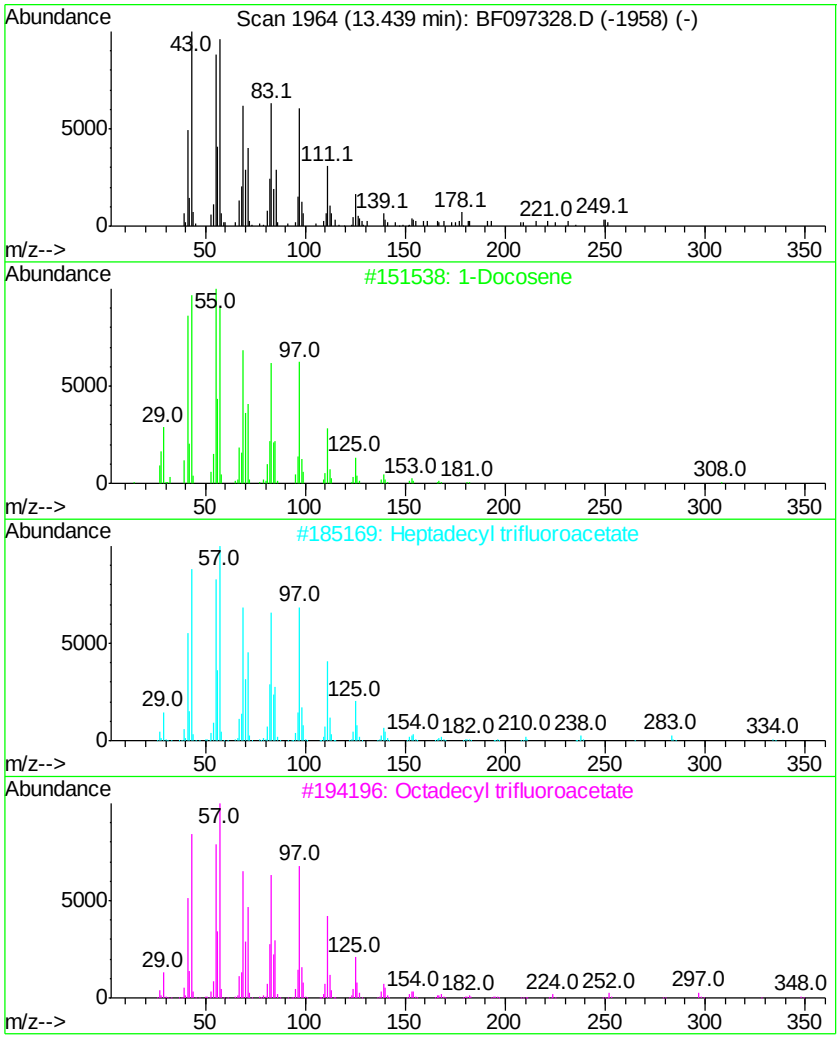
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

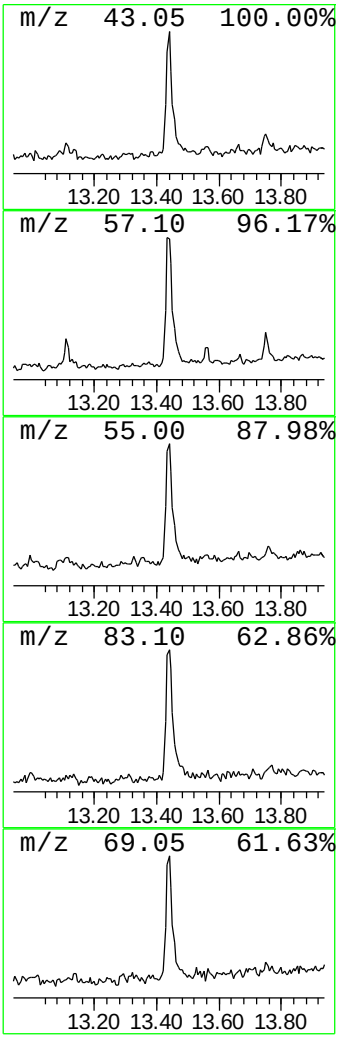
**********

Peak Number 7 1-Docosene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.44 | 6.22 ng | 251507 | Chrysene-d12 | 13.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 94 |
| 2 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 94 |
| 3 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 91 |
| 4 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 91 |
| 5 | Pentafluoropropionic acid, hexad... | 388 | C19H33F5O2 | 006222-07-7 | 91 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

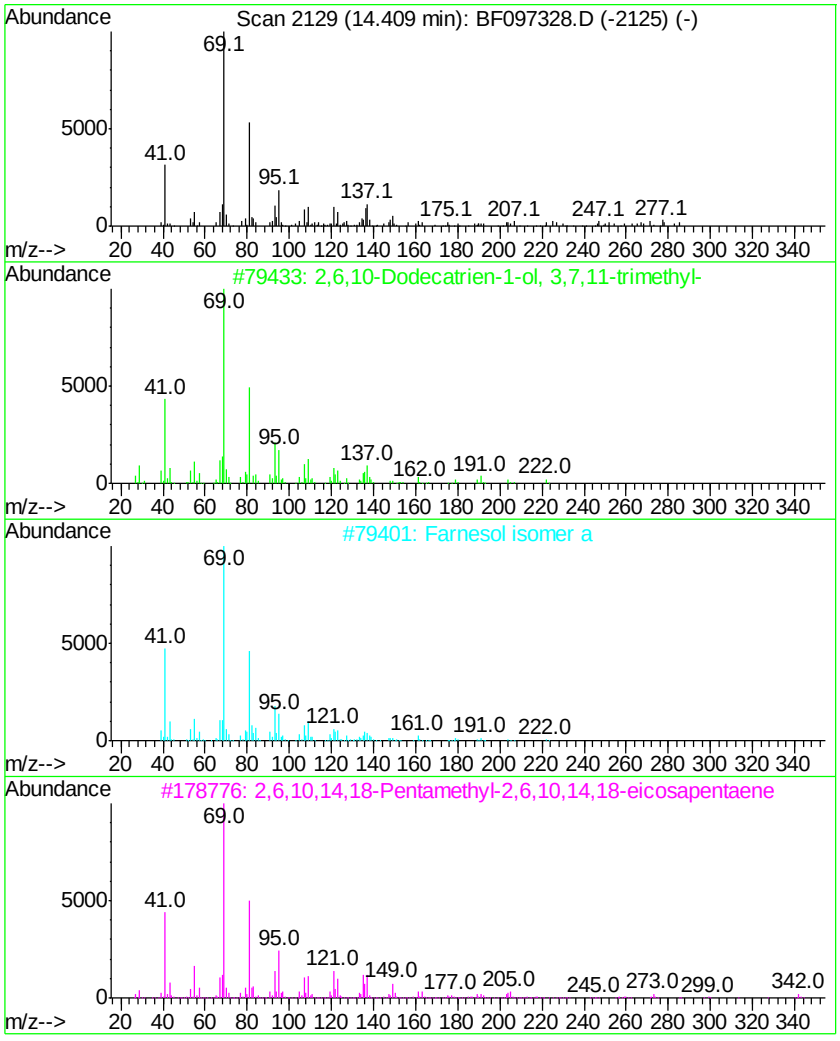
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

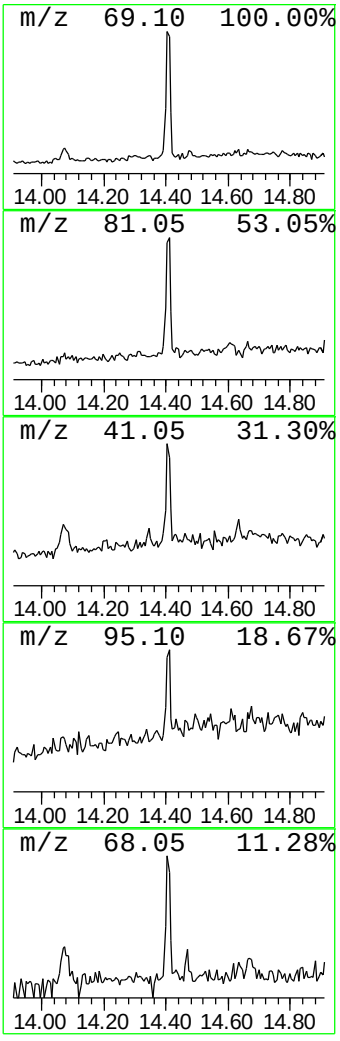
**********

Peak Number 8 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.41 | 3.46 ng | 104617 | Perylene-d12 | 14.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 004602-84-0 | 93 |
| 2 | Farnesol isomer a | 222 | C15H26O | 1000108-92-4 | 90 |
| 3 | 2,6,10,14,18-Pentamethyl-2,6,10,... | 342 | C25H42 | 075581-03-2 | 87 |
| 4 | Squalene | 410 | C30H50 | 000111-02-4 | 86 |
| 5 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 83 |



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Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

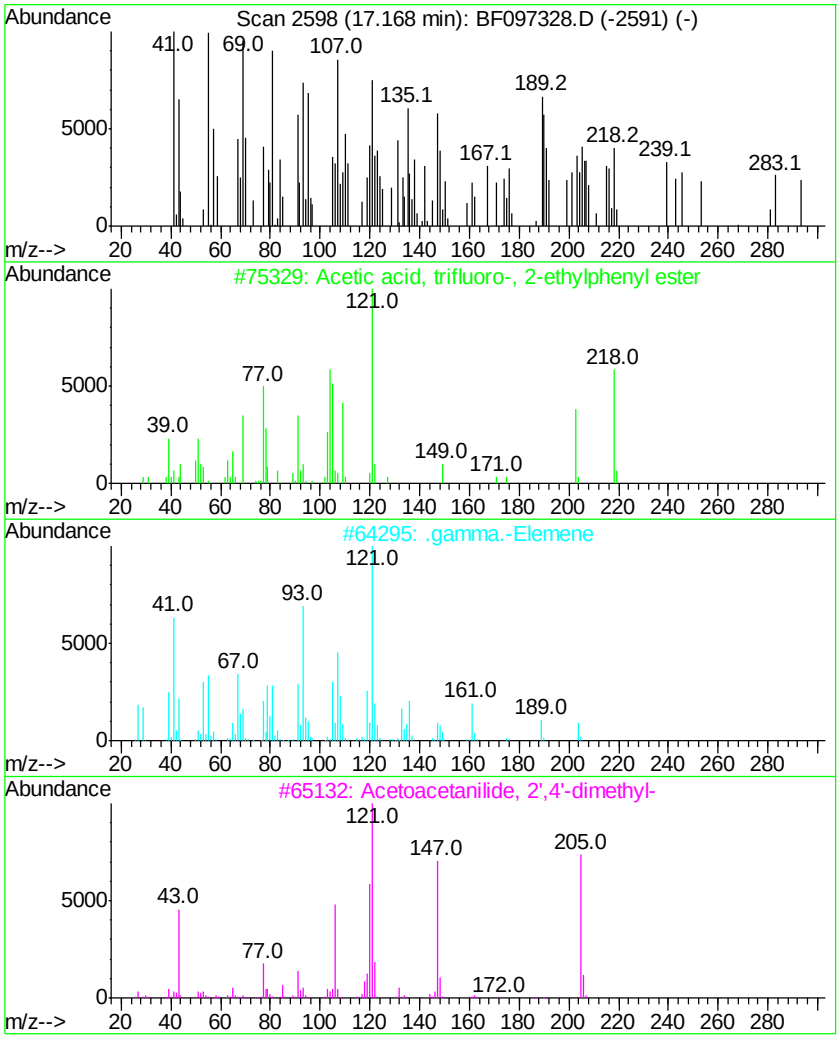
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

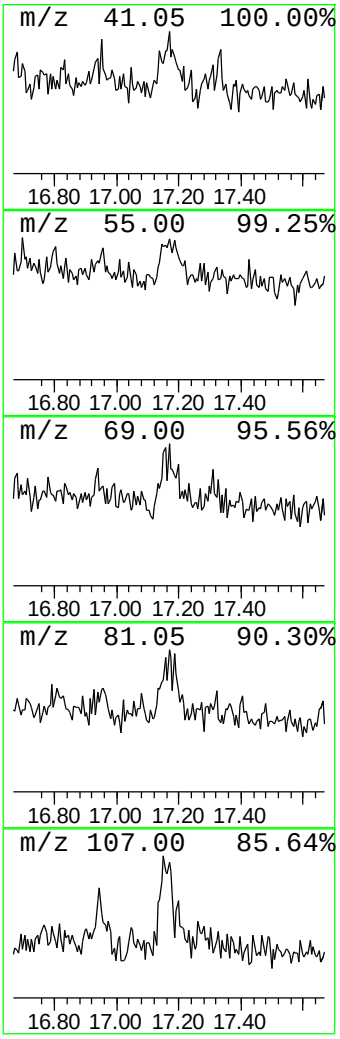
**********

Peak Number 9 unknown17.17 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.17 | 5.55 ng | 168033 | Perylene-d12 | 14.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetic acid, trifluoro-, 2-ethyl... | 218 | C10H9F3O2 | 031083-13-3 | 38 |
| 2 | .gamma.-Elemene | 204 | C15H24 | 029873-99-2 | 25 |
| 3 | Acetoacetanilide, 2',4'-dimethyl- | 205 | C12H15NO2 | 000097-36-9 | 25 |
| 4 | Aromandendrene | 204 | C15H24 | 000489-39-4 | 25 |
| 5 | Indeno[2,1-a]indene, hexadecahydro- | 218 | C16H26 | 056292-67-2 | 20 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080317\
Data File : BF097328.D
Acq On : 3 Aug 2017 20:35
Operator : SJ/JU
Sample : I4559-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-GF-02-008-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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... | 4.57 | 8.7 | ng | 309999 | 1 | 6.45 | 709443 | 20.0 |
| unknown6.22 | 6.22 | 75.9 | ng | 2693160 | 1 | 6.45 | 709443 | 20.0 |
| Hexadecane | 10.39 | 2.2 | ng | 105799 | 4 | 10.93 | 955590 | 20.0 |
| n-Hexadecanoic acid | 11.49 | 3.8 | ng | 181280 | 4 | 10.93 | 955590 | 20.0 |
| 1-Docosene | 13.44 | 6.2 | ng | 251507 | 5 | 13.56 | 808288 | 20.0 |
| 2,6,10-Dodecatrie... | 14.41 | 3.5 | ng | 104617 | 6 | 14.90 | 605495 | 20.0 |
| unknown17.17 | 17.17 | 5.5 | ng | 168033 | 6 | 14.90 | 605495 | 20.0 |