LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

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-BF121417.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 | 5.034 | 497 | 501 | 519 | rBV | 160096 | 305225 | 7.27% | 0.844% |
| 2 | 5.422 | 563 | 567 | 597 | rBV | 3277312 | 4103985 | 97.77% | 11.354% |
| 3 | 6.439 | 736 | 740 | 758 | rBV | 3341297 | 4197433 | 100.00% | 11.612% |
| 4 | 6.569 | 758 | 762 | 779 | rVB | 3737378 | 3771304 | 89.85% | 10.434% |
| 5 | 6.792 | 797 | 800 | 809 | rBV | 863064 | 858155 | 20.44% | 2.374% |
| 6 | 6.951 | 823 | 827 | 844 | rBV | 2810588 | 2836507 | 67.58% | 7.847% |
| 7 | 7.363 | 893 | 897 | 909 | rBV | 2258756 | 2651563 | 63.17% | 7.336% |
| 8 | 8.075 | 1015 | 1018 | 1038 | rVB | 1111758 | 1140034 | 27.16% | 3.154% |
| 9 | 8.633 | 1110 | 1113 | 1125 | rBV | 243684 | 244371 | 5.82% | 0.676% |
| 10 | 9.151 | 1196 | 1201 | 1204 | rBV | 3505687 | 3308651 | 78.83% | 9.154% |
| 11 | 9.545 | 1265 | 1268 | 1274 | rBV | 552711 | 495277 | 11.80% | 1.370% |
| 12 | 9.833 | 1313 | 1317 | 1328 | rVB | 1217303 | 1225026 | 29.19% | 3.389% |
| 13 | 10.545 | 1434 | 1438 | 1443 | rBV | 966993 | 800998 | 19.08% | 2.216% |
| 14 | 10.627 | 1448 | 1452 | 1465 | rBV | 2191006 | 2245427 | 53.50% | 6.212% |
| 15 | 10.721 | 1465 | 1468 | 1473 | rVB | 32938 | 44134 | 1.05% | 0.122% |
| 16 | 11.321 | 1566 | 1570 | 1578 | rBV | 1391595 | 1263925 | 30.11% | 3.497% |
| 17 | 12.621 | 1786 | 1791 | 1795 | rBV2 | 39257 | 59428 | 1.42% | 0.164% |
| 18 | 12.904 | 1835 | 1839 | 1842 | rBV | 2920559 | 2699483 | 64.31% | 7.468% |
| 19 | 13.786 | 1985 | 1989 | 1996 | rBV | 144423 | 191967 | 4.57% | 0.531% |
| 20 | 13.968 | 2016 | 2020 | 2030 | rBV | 826087 | 813982 | 19.39% | 2.252% |
| 21 | 14.415 | 2091 | 2096 | 2103 | rBV2 | 89468 | 156132 | 3.72% | 0.432% |
| 22 | 14.774 | 2153 | 2157 | 2165 | rVB | 119517 | 131637 | 3.14% | 0.364% |
| 23 | 15.027 | 2197 | 2200 | 2204 | rBV | 47694 | 50699 | 1.21% | 0.140% |
| 24 | 15.433 | 2264 | 2269 | 2281 | rVB | 486096 | 687161 | 16.37% | 1.901% |
| 25 | 17.709 | 2648 | 2656 | 2665 | rBV10 | 35650 | 113851 | 2.71% | 0.315% |
| 26 | 18.915 | 2854 | 2861 | 2870 | rBV10 | 56872 | 154335 | 3.68% | 0.427% |
| 27 | 19.421 | 2935 | 2947 | 2956 | rBV3 | 503253 | 1595326 | 38.01% | 4.414% |

Sum of corrected areas: 36146016

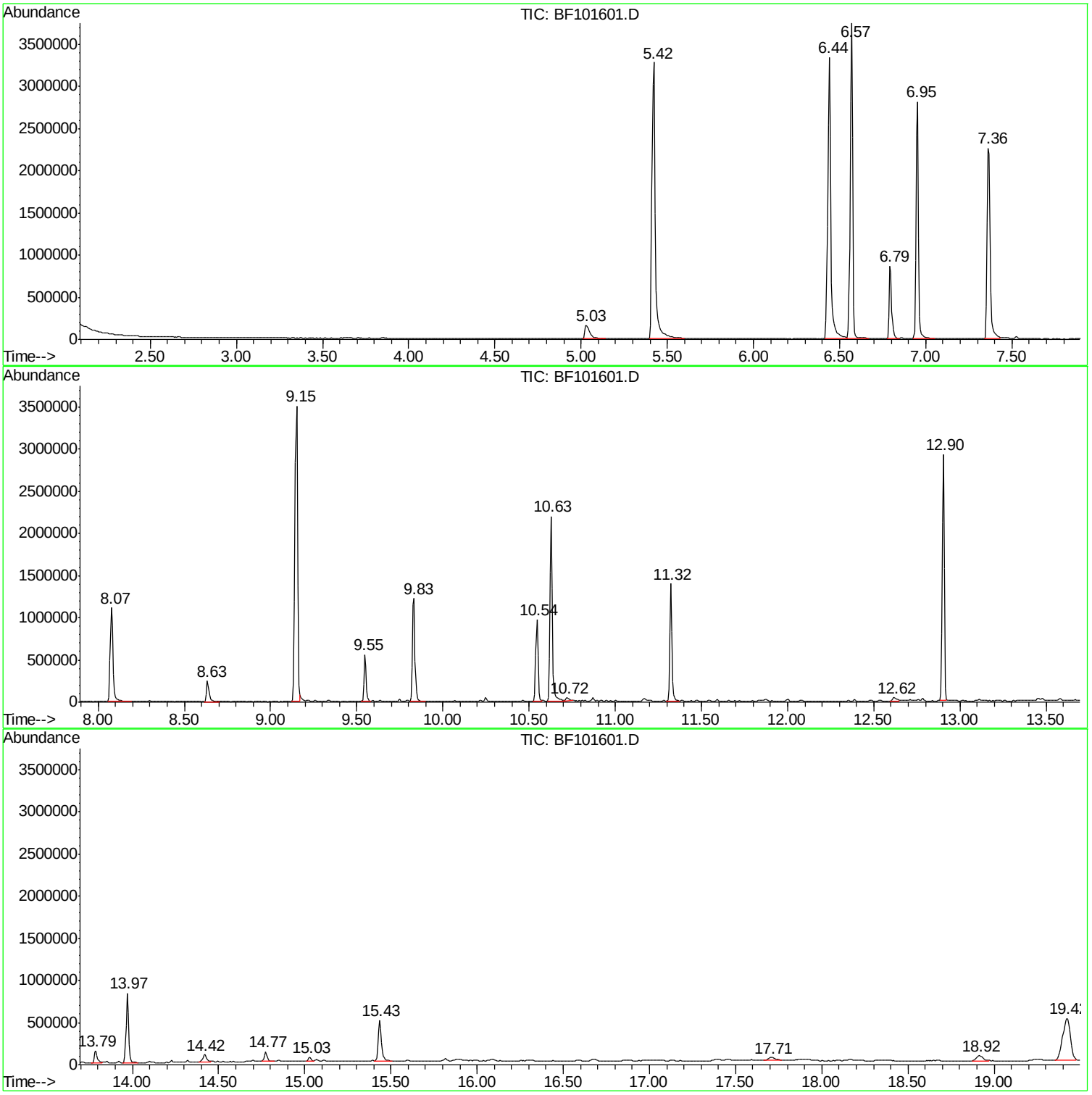
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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

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Data File : BF101601.D
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Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

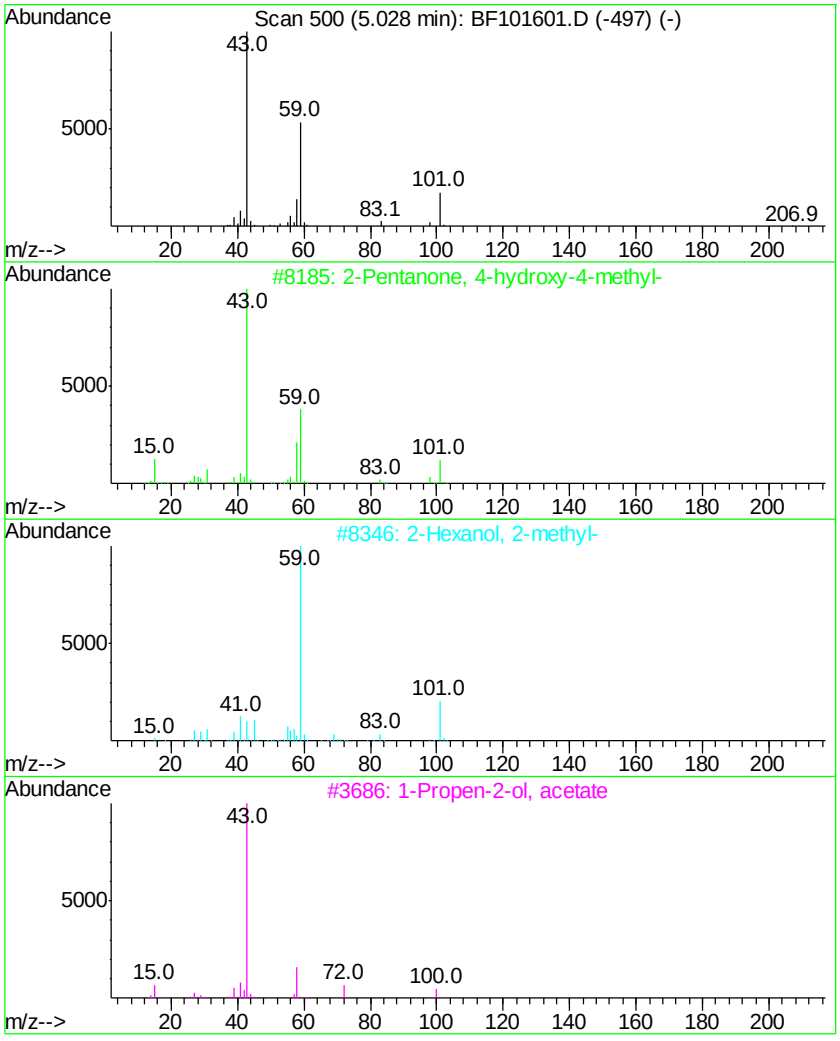
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

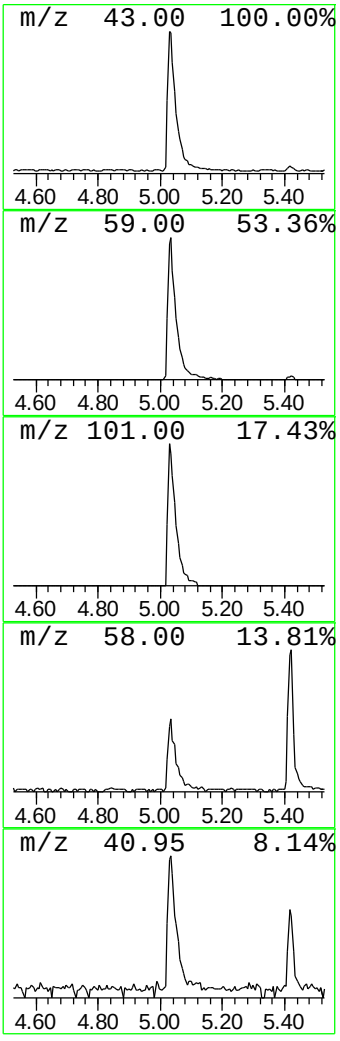
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.03 | 7.11 ng | 305225 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 9 |



Library Search Compound Report

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Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

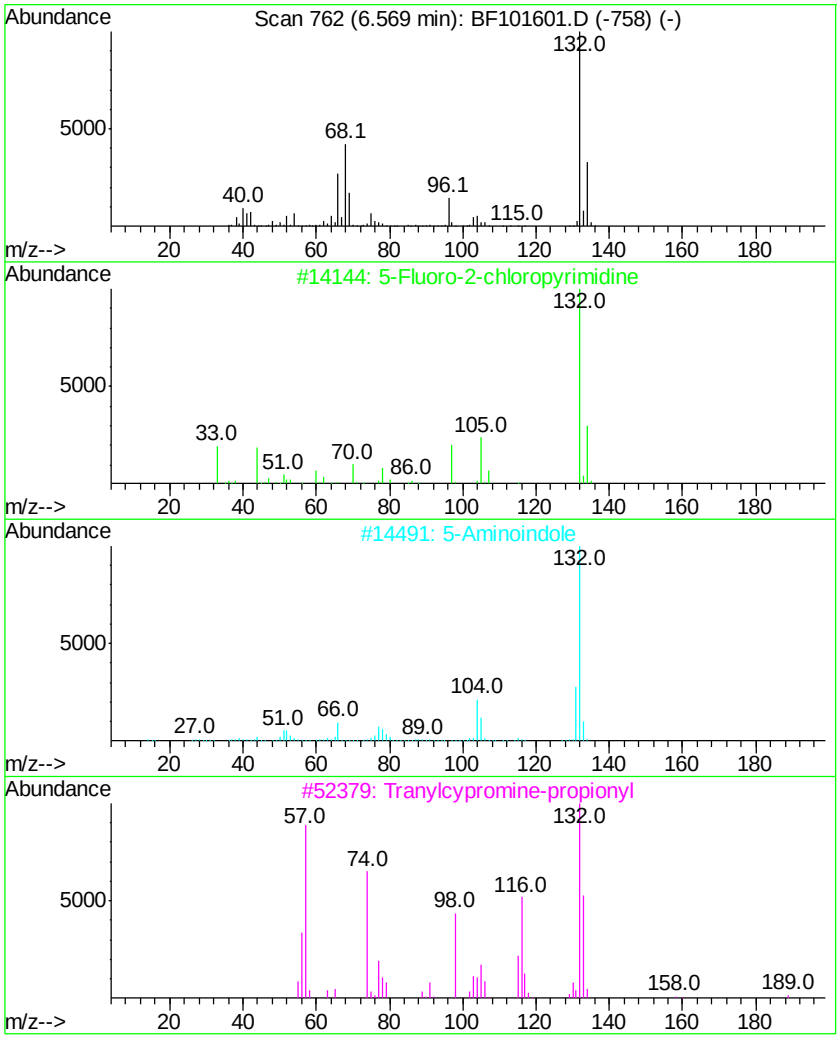
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

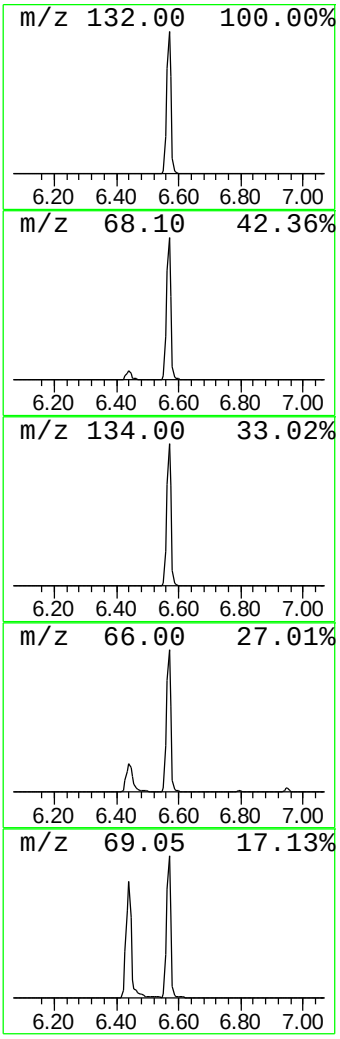
**********

Peak Number 2 unknown6.57 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.57 | 87.89 ng | 3771300 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

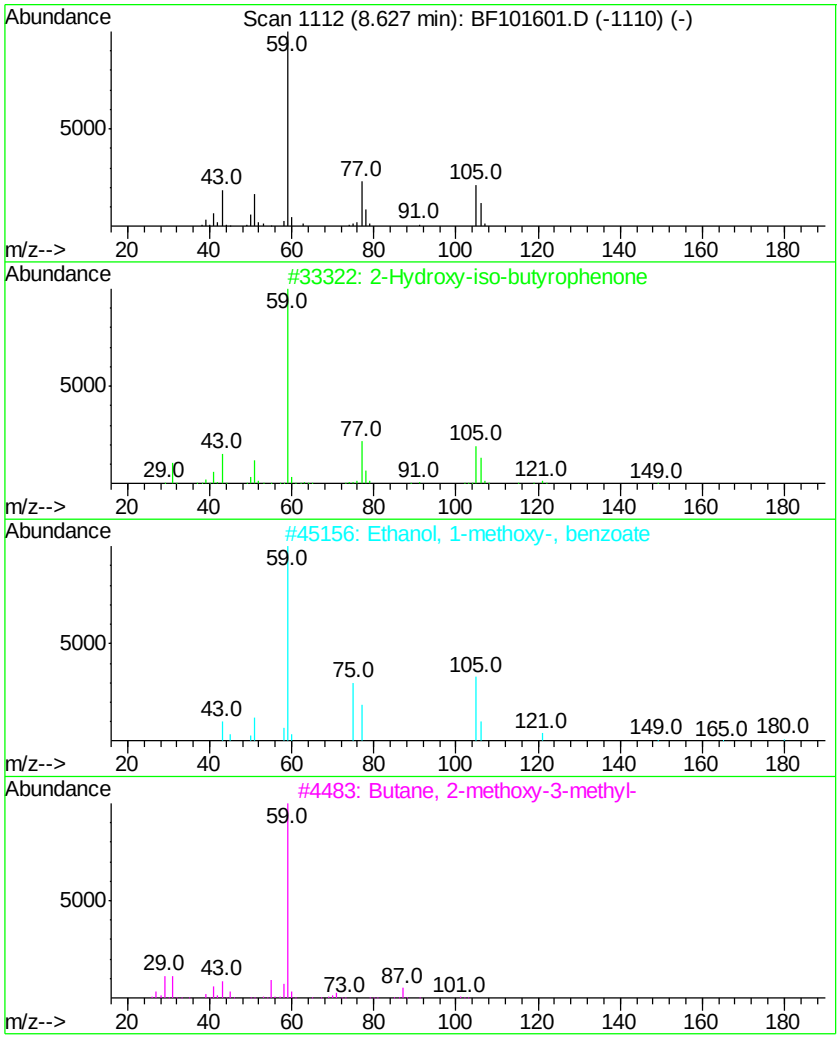
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

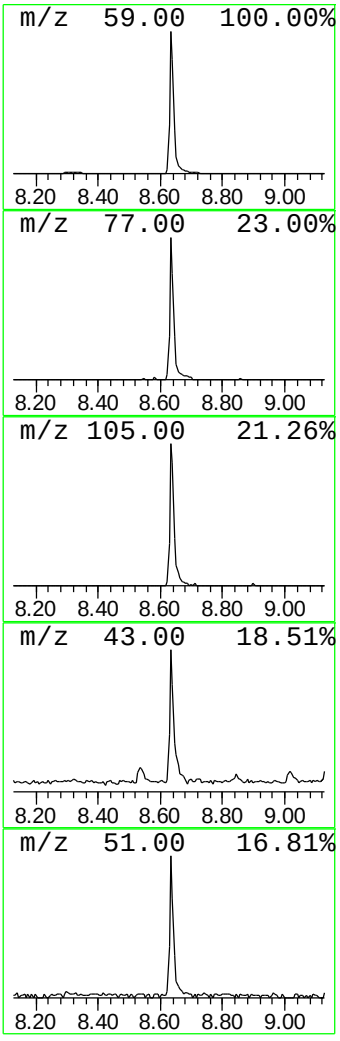
**********

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.63 | 4.29 ng | 244371 | Naphthalene-d8 | 8.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hydroxy-iso-butyrophenone | 164 | C10H12O2 | 007473-98-5 | 90 |
| 2 | Ethanol, 1-methoxy-, benzoate | 180 | C10H12O3 | 051835-44-0 | 72 |
| 3 | Butane, 2-methoxy-3-methyl- | 102 | C6H14O | 062016-49-3 | 32 |
| 4 | Hexanamide | 115 | C6H13NO | 000628-02-4 | 9 |
| 5 | Propanoic acid, 2-hydroxy-2-meth... | 132 | C6H12O3 | 000080-55-7 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

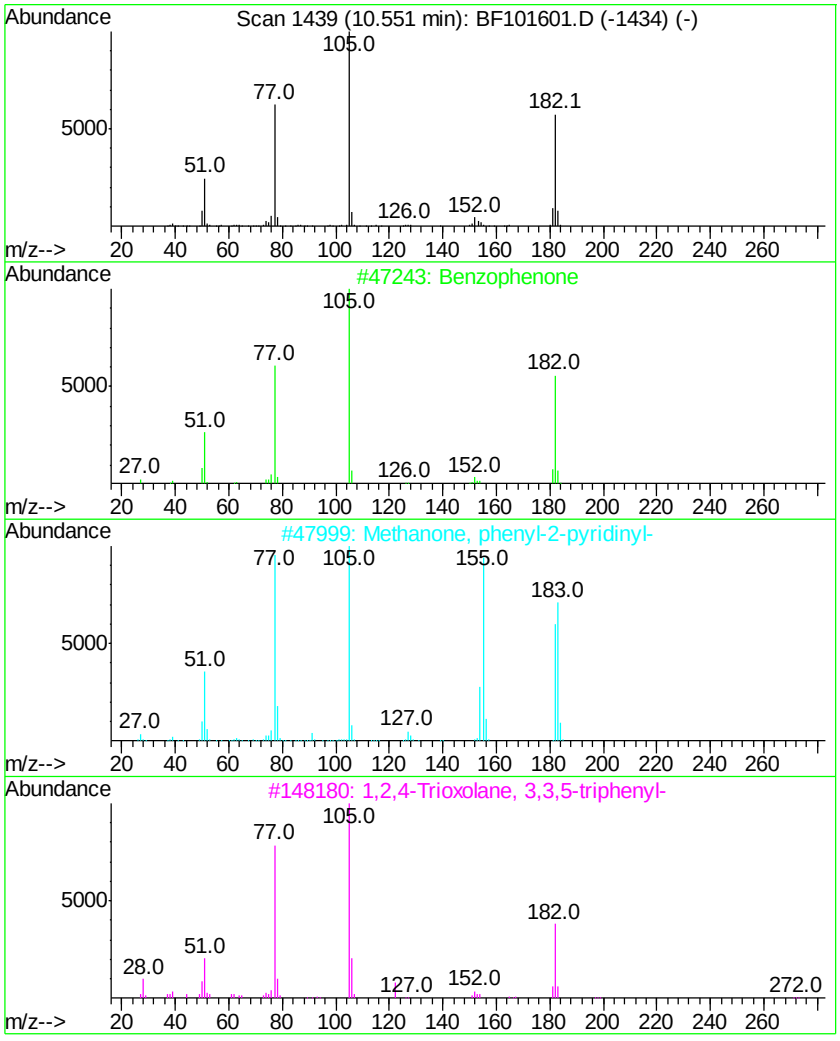
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

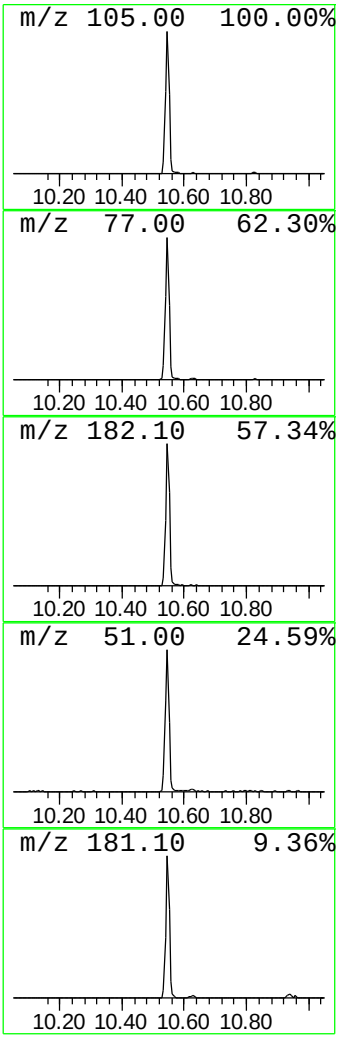
**********

Peak Number 5 Benzophenone Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.55 | 13.08 ng | 800998 | Acenaphthene-d10 | 9.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Methanone, phenyl-2-pyridinyl- | 183 | C12H9NO | 000091-02-1 | 72 |
| 3 | 1,2,4-Trioxolane, 3,3,5-triphenyl- | 304 | C20H16O3 | 023246-12-0 | 72 |
| 4 | Azobenzene | 182 | C12H10N2 | 000103-33-3 | 64 |
| 5 | Phenyl 4-pyridyl ketone | 183 | C12H9NO | 014548-46-0 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

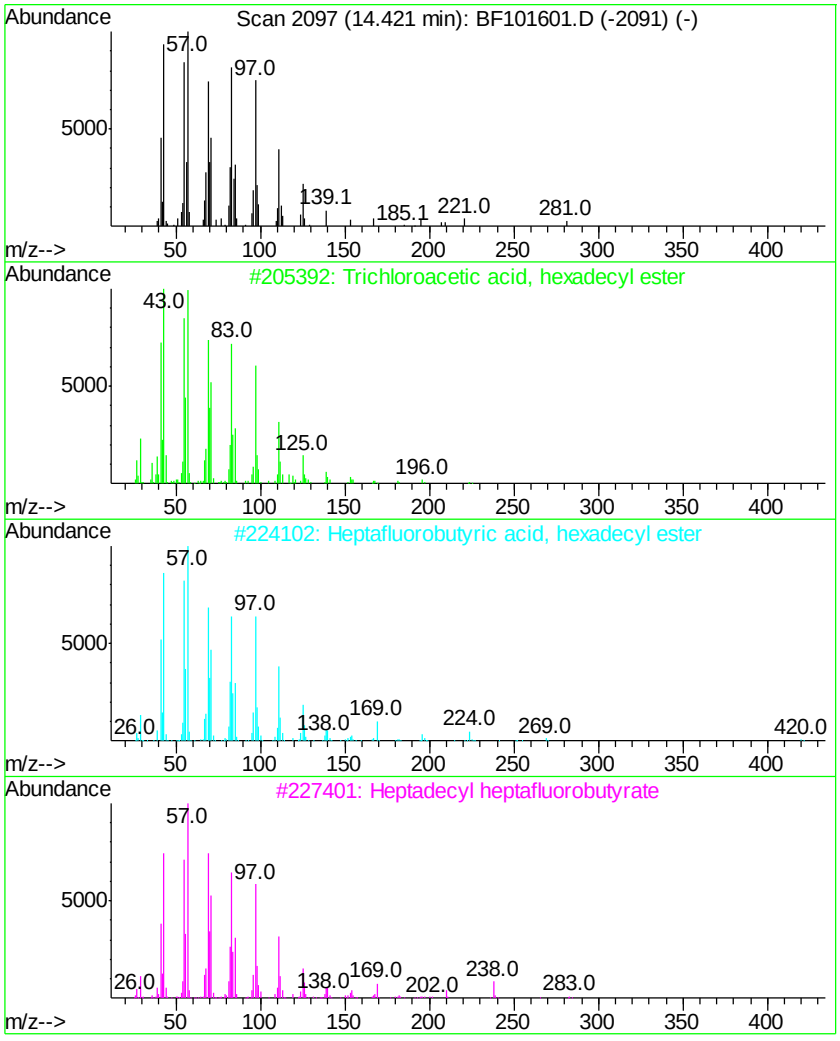
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

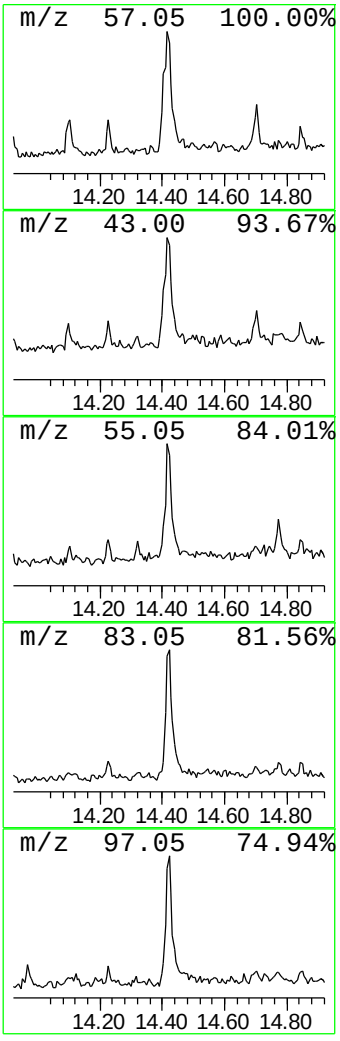
**********

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.42 | 3.84 ng | 156132 | Chrysene-d12 | 13.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 95 |
| 2 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 94 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 4 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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TIC Library : C:\DATABASE\NIST11.L
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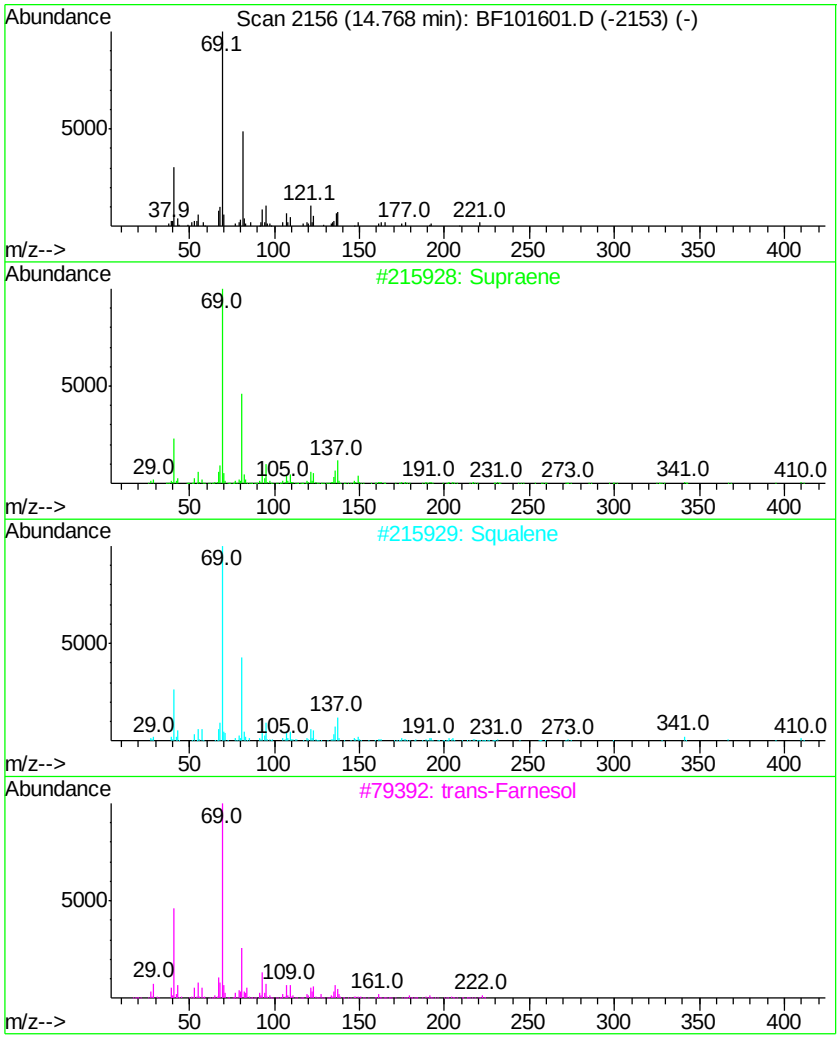
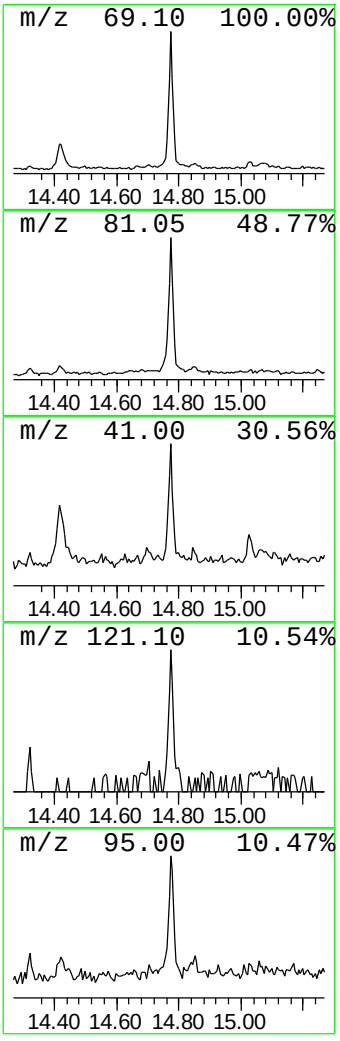
**********

Peak Number 8 Supraene Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.77 | 3.83 ng | 131637 | Perylene-d12 | 15.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Supraene | 410 | C30H50 | 007683-64-9 | 90 |
| 2 | Squalene | 410 | C30H50 | 000111-02-4 | 87 |
| 3 | trans-Farnesol | 222 | C15H26O | 000106-28-5 | 72 |
| 4 | 1,5-Heptadiene, 3,4-dimethyl- | 124 | C9H16 | 1000061-77-9 | 53 |
| 5 | 2,6-Octadiene, 4-methyl- | 124 | C9H16 | 074498-94-5 | 53 |



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Sample : I6961-02
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**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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TIC Library : C:\DATABASE\NIST11.L
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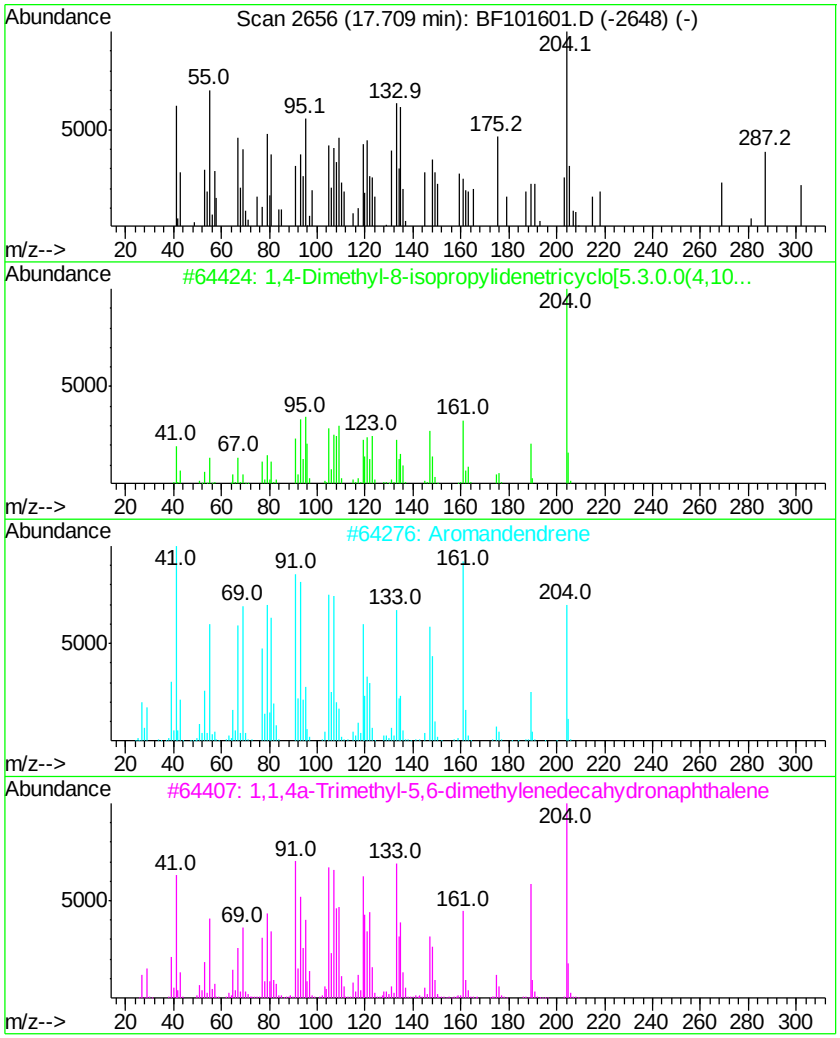
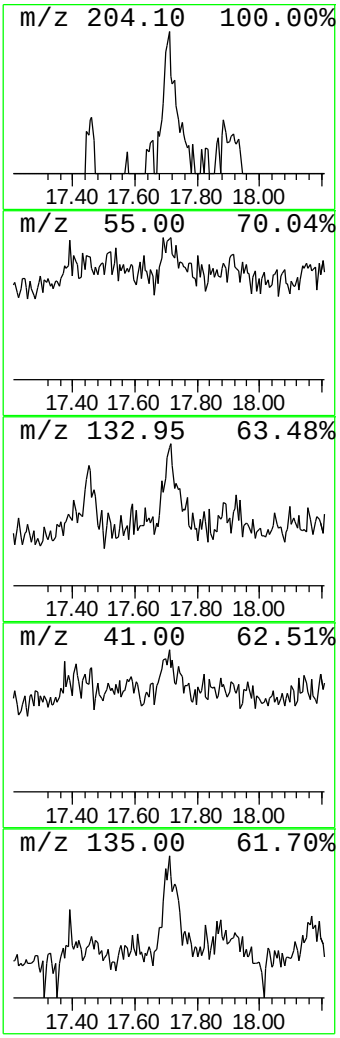
**********

Peak Number 9 unknown17.71 Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.71 | 3.31 ng | 113851 | Perylene-d12 | 15.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Dimethyl-8-isopropylidenetri... | 204 | C15H24 | 1000140-07-7 | 46 |
| 2 | Aromandendrene | 204 | C15H24 | 000489-39-4 | 45 |
| 3 | 1,1,4a-Trimethyl-5,6-dimethylene... | 204 | C15H24 | 1000193-60-8 | 45 |
| 4 | 2H-Cyclopentacyclooctene, 4,5,6,... | 204 | C15H24 | 1000221-85-8 | 43 |
| 5 | Naphthalene, 1,2,3,5,6,7,8,8a-oc... | 204 | C15H24 | 004630-07-3 | 38 |



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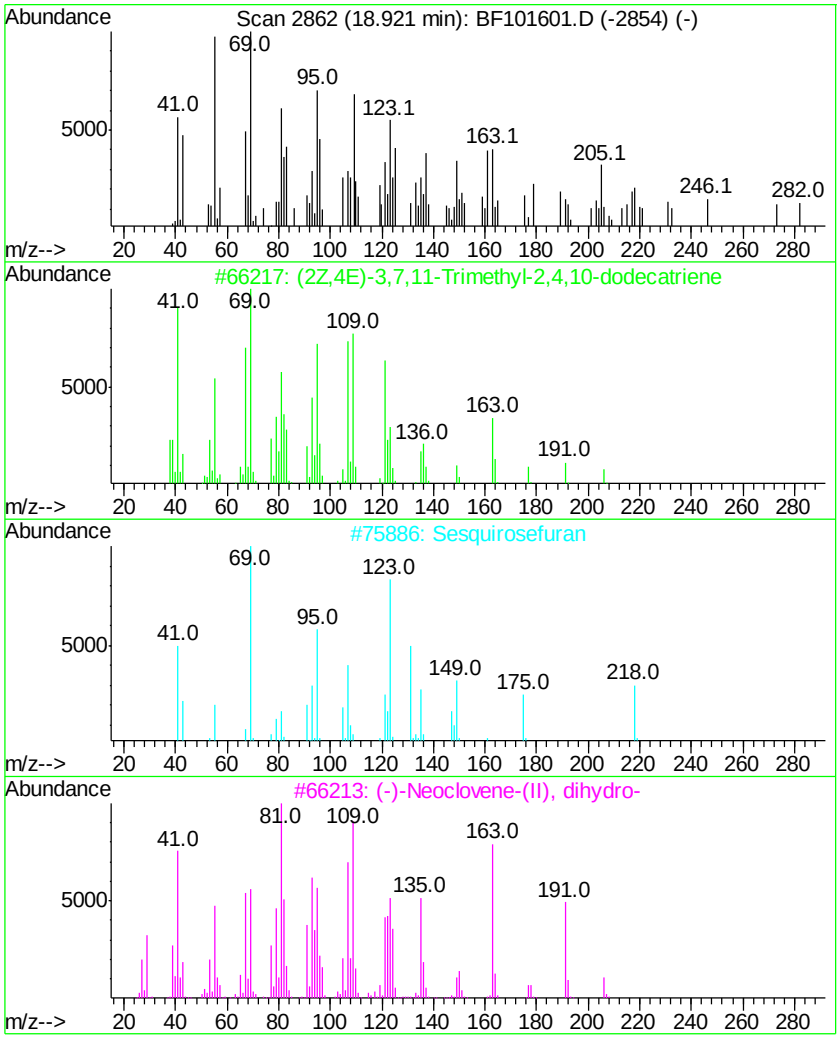
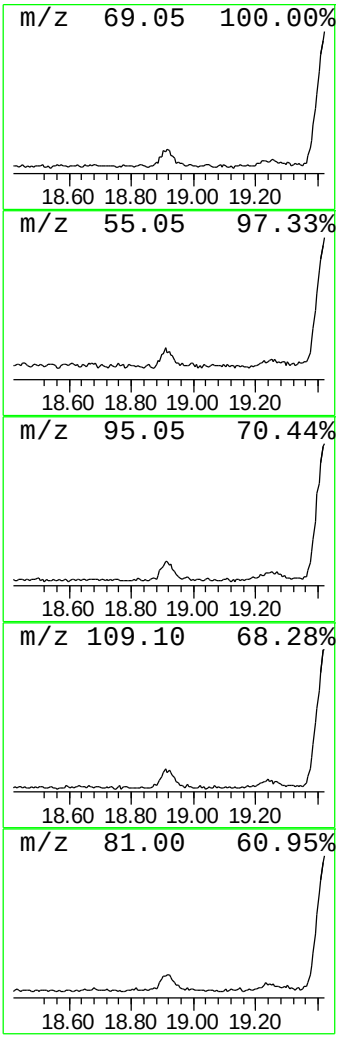
**********

Peak Number 10 (2Z,4E)-3,7,11-Trimethyl-2,... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.92 | 4.49 ng | 154335 | Perylene-d12 | 15.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (2Z,4E)-3,7,11-Trimethyl-2,4,10-... | 206 | C15H26 | 172549-29-0 | 60 |
| 2 | Sesquirosefuran | 218 | C15H22O | 039007-93-7 | 51 |
| 3 | (-)-Neoclovene-(II), dihydro- | 206 | C15H26 | 1000152-83-6 | 47 |
| 4 | Bicyclo[2.2.1]heptane, 2,2,3-tri... | 138 | C10H18 | 020536-40-7 | 38 |
| 5 | Cyclohexane, 1,1,2-trimethyl-3,5... | 206 | C15H26 | 062337-97-7 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

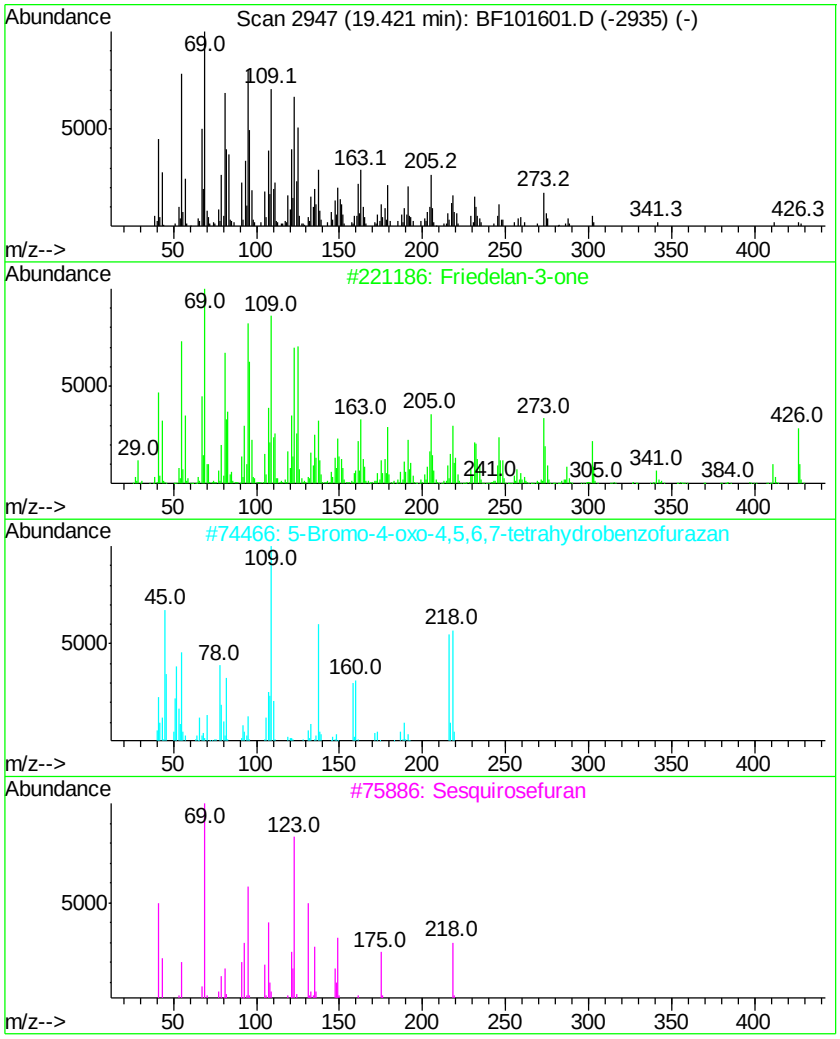
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

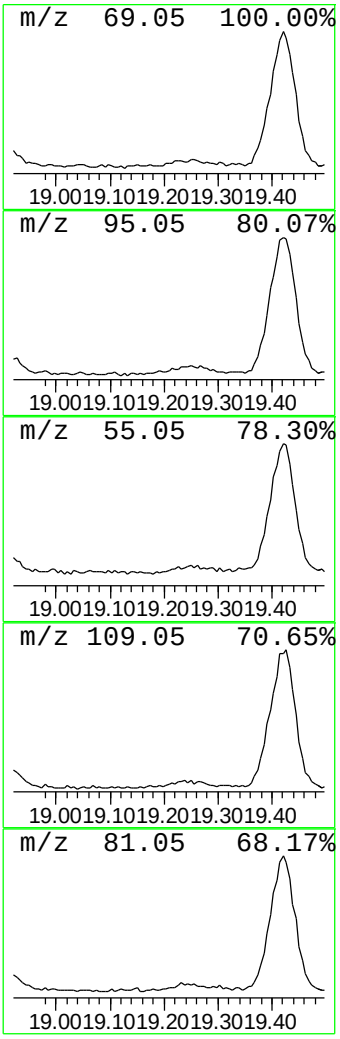
**********

Peak Number 11 Friedelan-3-one Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.42 | 46.43 ng | 1595330 | Perylene-d12 | 15.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Friedelan-3-one | 426 | C30H50O | 000559-74-0 | 95 |
| 2 | 5-Bromo-4-oxo-4,5,6,7-tetrahydro... | 216 | C6H5BrN2O2 | 300574-36-1 | 90 |
| 3 | Sesquirosefuran | 218 | C15H22O | 039007-93-7 | 64 |
| 4 | Methyl Camphorsulfonates | 246 | C11H18O4S | 046471-67-4 | 60 |
| 5 | 2,2,6-Trimethyl-1-(2-methyl-cycl... | 218 | C15H22O | 1000188-72-8 | 55 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122117\
Data File : BF101601.D
Acq On : 21 Dec 2017 12:40
Operator : SJ/JU
Sample : I6961-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** EPE-108-1(20-22)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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... | 5.03 | 7.1 | ng | 305225 | 1 | 6.79 | 858155 | 20.0 |
| unknown6.57 | 6.57 | 87.9 | ng | 3771300 | 1 | 6.79 | 858155 | 20.0 |
| 2-Hydroxy-iso-but... | 8.63 | 4.3 | ng | 244371 | 2 | 8.07 | 1140030 | 20.0 |
| Benzophenone | 10.55 | 13.1 | ng | 800998 | 3 | 9.83 | 1225030 | 20.0 |
| Trichloroacetic a... | 14.42 | 3.8 | ng | 156132 | 5 | 13.97 | 813982 | 20.0 |
| Supraene | 14.77 | 3.8 | ng | 131637 | 6 | 15.43 | 687161 | 20.0 |
| unknown17.71 | 17.71 | 3.3 | ng | 113851 | 6 | 15.43 | 687161 | 20.0 |
| (2Z,4E)-3,7,11-Tr... | 18.92 | 4.5 | ng | 154335 | 6 | 15.43 | 687161 | 20.0 |
| Friedelan-3-one | 19.42 | 46.4 | ng | 1595330 | 6 | 15.43 | 687161 | 20.0 |