LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

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-BF011415.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 | 1.327 | 20 | 21 | 26 | rBV | 36413 | 63387 | 7.10% | 0.846% |
| 2 | 1.407 | 26 | 28 | 47 | rVB | 289123 | 652956 | 73.19% | 8.714% |
| 3 | 3.830 | 238 | 240 | 248 | rBV | 14821 | 36026 | 4.04% | 0.481% |
| 4 | 4.802 | 322 | 325 | 337 | rVB | 115235 | 249888 | 28.01% | 3.335% |
| 5 | 5.076 | 345 | 349 | 353 | rBV | 4725 | 10076 | 1.13% | 0.134% |
| 6 | 7.179 | 531 | 533 | 537 | rBV | 78661 | 134072 | 15.03% | 1.789% |
| 7 | 7.259 | 537 | 540 | 547 | rVV | 327800 | 553398 | 62.03% | 7.386% |
| 8 | 7.762 | 581 | 584 | 588 | rVB | 102956 | 159257 | 17.85% | 2.125% |
| 9 | 8.082 | 609 | 612 | 619 | rVB | 349772 | 584583 | 65.52% | 7.802% |
| 10 | 8.768 | 669 | 672 | 676 | rBV | 6463 | 12090 | 1.36% | 0.161% |
| 11 | 9.065 | 695 | 698 | 707 | rBV | 286959 | 442616 | 49.61% | 5.907% |
| 12 | 10.676 | 835 | 839 | 842 | rBV | 148489 | 225524 | 25.28% | 3.010% |
| 13 | 11.945 | 945 | 950 | 953 | rBV | 9838 | 16194 | 1.82% | 0.216% |
| 14 | 12.379 | 986 | 988 | 990 | rBV | 6506 | 10569 | 1.18% | 0.141% |
| 15 | 12.528 | 999 | 1001 | 1005 | rBV | 14677 | 29015 | 3.25% | 0.387% |
| 16 | 13.065 | 1045 | 1048 | 1052 | rBV2 | 6834 | 9719 | 1.09% | 0.130% |
| 17 | 13.328 | 1068 | 1071 | 1075 | rBV | 540129 | 892162 | 100.00% | 11.907% |
| 18 | 13.762 | 1105 | 1109 | 1112 | rBV | 154540 | 243612 | 27.31% | 3.251% |
| 19 | 14.563 | 1176 | 1179 | 1182 | rBV | 47979 | 68323 | 7.66% | 0.912% |
| 20 | 14.803 | 1197 | 1200 | 1205 | rVB2 | 155060 | 246384 | 27.62% | 3.288% |
| 21 | 15.054 | 1219 | 1222 | 1226 | rVB | 25848 | 39402 | 4.42% | 0.526% |
| 22 | 15.168 | 1229 | 1232 | 1233 | rVV | 13817 | 22681 | 2.54% | 0.303% |
| 23 | 15.203 | 1233 | 1235 | 1239 | rVB | 12002 | 18866 | 2.11% | 0.252% |
| 24 | 15.294 | 1239 | 1243 | 1247 | rBV | 18172 | 28794 | 3.23% | 0.384% |
| 25 | 16.048 | 1304 | 1309 | 1312 | rBV2 | 9027 | 15010 | 1.68% | 0.200% |
| 26 | 16.140 | 1315 | 1317 | 1320 | rVB2 | 19221 | 25776 | 2.89% | 0.344% |
| 27 | 16.311 | 1328 | 1332 | 1335 | rBV | 170054 | 299315 | 33.55% | 3.995% |
| 28 | 16.460 | 1343 | 1345 | 1348 | rBV2 | 6271 | 9169 | 1.03% | 0.122% |
| 29 | 16.517 | 1348 | 1350 | 1353 | rBV | 314644 | 485381 | 54.41% | 6.478% |
| 30 | 16.677 | 1362 | 1364 | 1369 | rBV2 | 9094 | 15093 | 1.69% | 0.201% |
| 31 | 16.837 | 1376 | 1378 | 1384 | rBV3 | 4807 | 8992 | 1.01% | 0.120% |
| 32 | 17.077 | 1396 | 1399 | 1405 | rVB | 6434 | 9598 | 1.08% | 0.128% |
| 33 | 17.534 | 1437 | 1439 | 1444 | rVB | 10227 | 12103 | 1.36% | 0.162% |
| 34 | 17.637 | 1445 | 1448 | 1450 | rBV | 213052 | 253935 | 28.46% | 3.389% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

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-BF011415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 18.323 | 1506 | 1508 | 1510 | rBV | 24224 | 24828 | 2.78% | 0.331% |
| 36 | 18.449 | 1516 | 1519 | 1522 | rBV | 7708 | 9177 | 1.03% | 0.122% |
| 37 | 18.551 | 1526 | 1528 | 1531 | rVB | 12930 | 11566 | 1.30% | 0.154% |
| 38 | 18.631 | 1533 | 1535 | 1538 | rBV | 100813 | 112117 | 12.57% | 1.496% |
| 39 | 19.786 | 1633 | 1636 | 1638 | rVB | 13564 | 12764 | 1.43% | 0.170% |
| 40 | 19.877 | 1641 | 1644 | 1647 | rBV | 715813 | 818037 | 91.69% | 10.917% |
| 41 | 20.540 | 1700 | 1702 | 1705 | rVB | 22275 | 25752 | 2.89% | 0.344% |
| 42 | 20.689 | 1712 | 1715 | 1716 | rBV | 7897 | 10884 | 1.22% | 0.145% |
| 43 | 21.157 | 1754 | 1756 | 1759 | rBV | 252681 | 278313 | 31.20% | 3.714% |
| 44 | 21.306 | 1765 | 1769 | 1772 | rVB2 | 6472 | 10057 | 1.13% | 0.134% |
| 45 | 22.963 | 1911 | 1914 | 1917 | rBV | 188705 | 255930 | 28.69% | 3.416% |
| 46 | 24.118 | 2011 | 2015 | 2018 | rVB3 | 5257 | 10404 | 1.17% | 0.139% |
| 47 | 24.552 | 2050 | 2053 | 2057 | rBV5 | 2988 | 9952 | 1.12% | 0.133% |
| 48 | 24.998 | 2091 | 2092 | 2097 | rBV4 | 3646 | 9010 | 1.01% | 0.120% |
| 49 | 25.181 | 2104 | 2108 | 2111 | rBV6 | 3024 | 10218 | 1.15% | 0.136% |

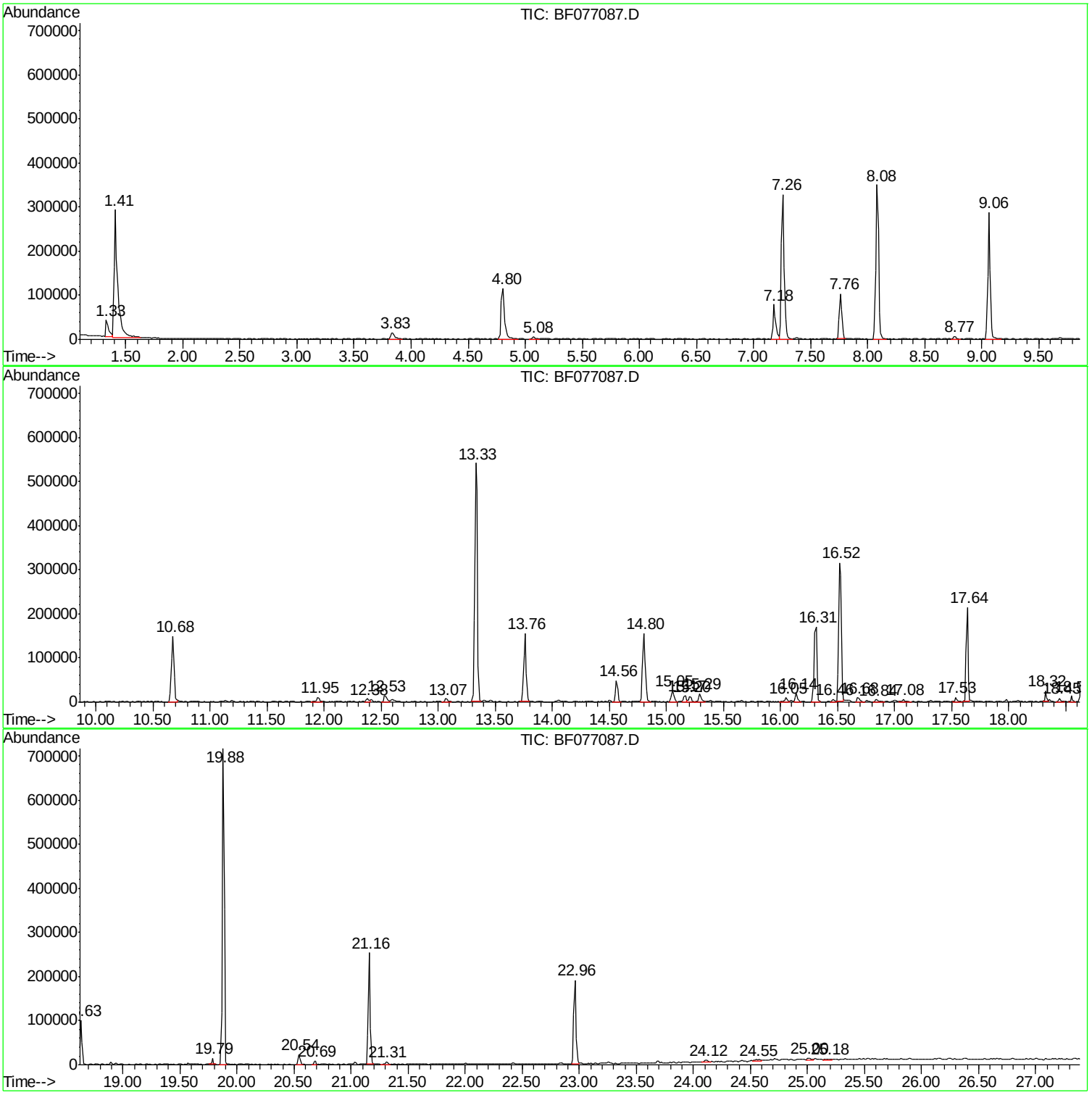
Sum of corrected areas: 7492975

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

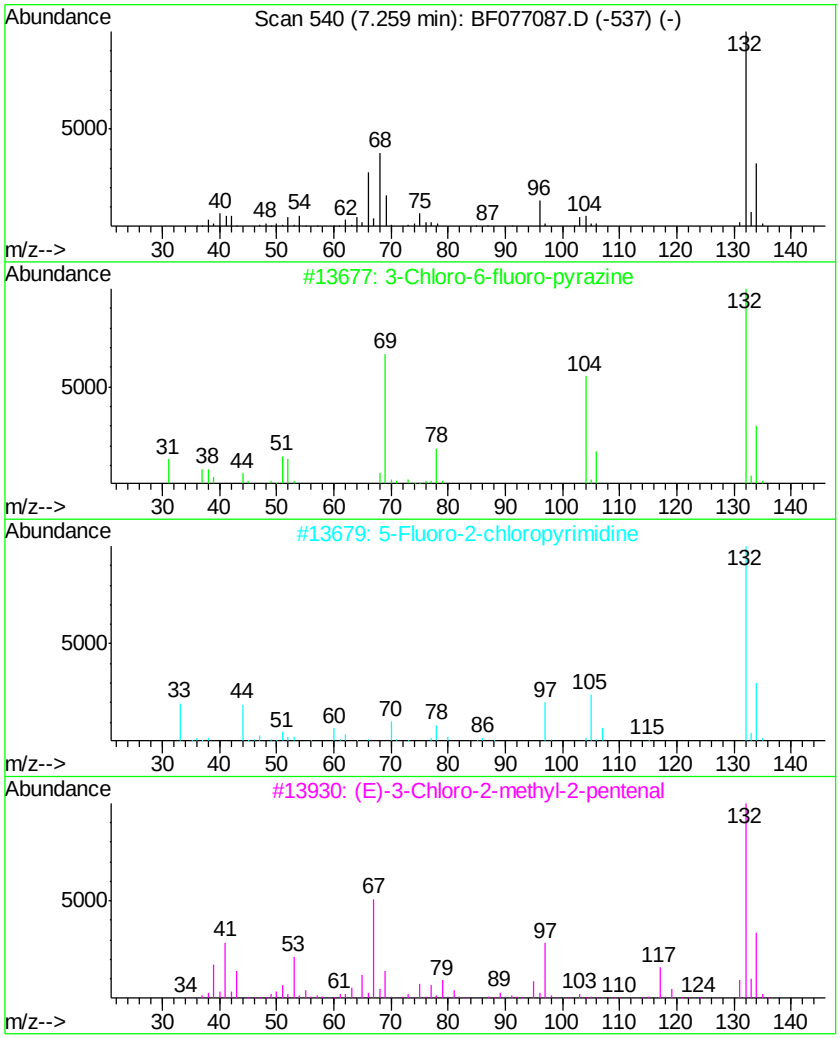
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

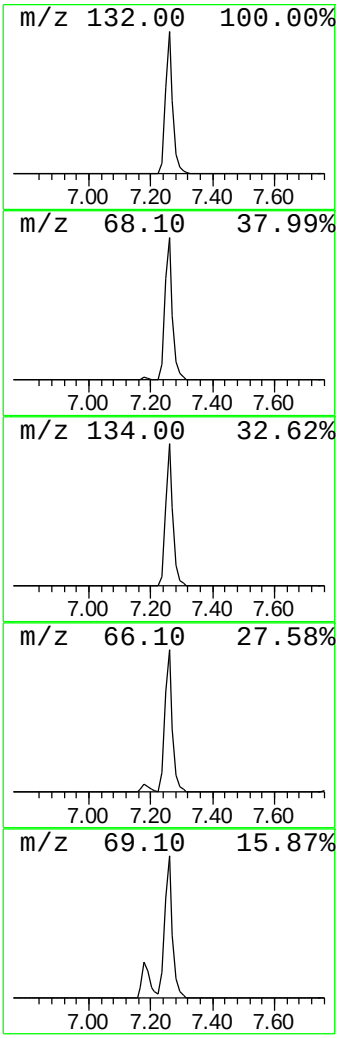
**********

Peak Number 4 unknown7.26 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.26 | 69.50 ng | 553398 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 25 |
| 3 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 25 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 5 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 12 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

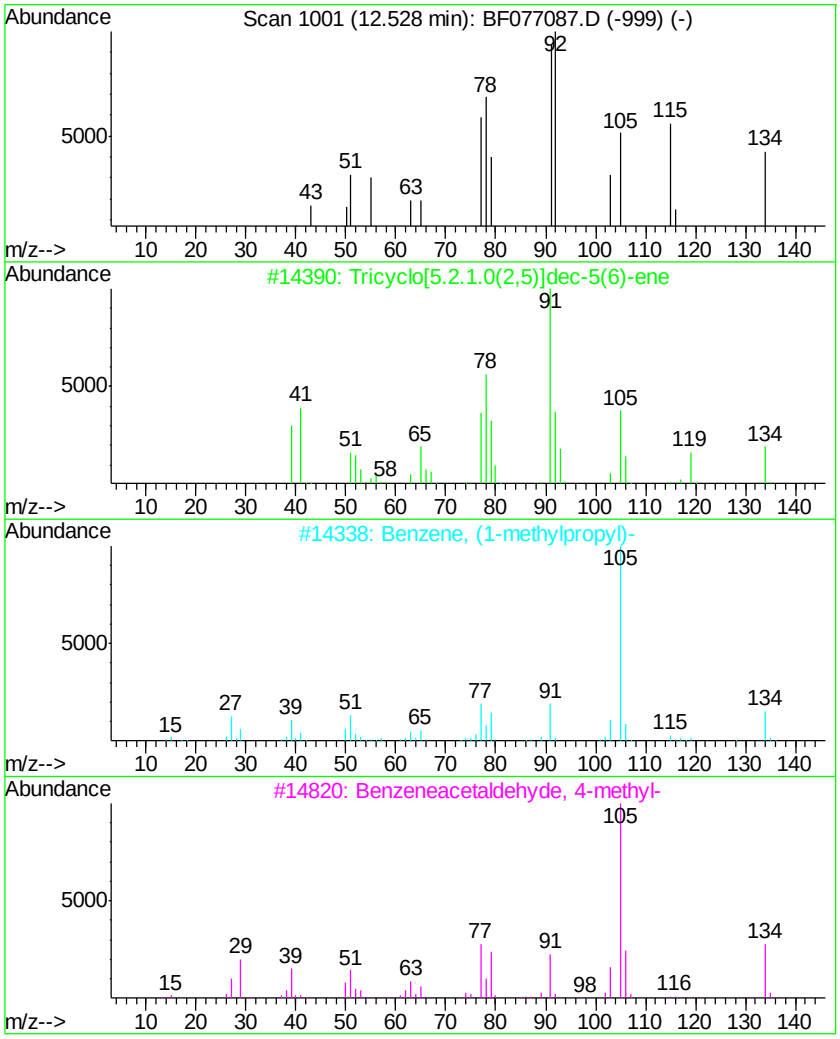
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

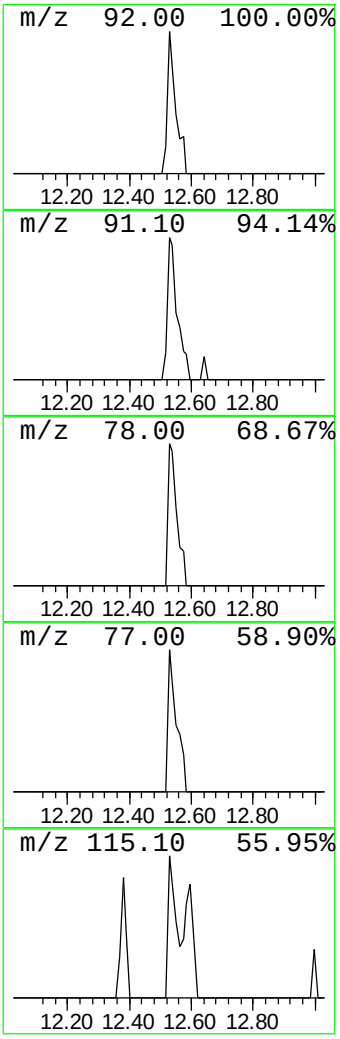
**********

Peak Number 6 unknown12.53 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.53 | 2.57 ng | 29015 | Naphthalene-d8 | 10.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tricyclo[5.2.1.0(2,5)]dec-5(6)-ene | 134 | C10H14 | 1000223-17-6 | 37 |
| 2 | Benzene, (1-methylpropyl)- | 134 | C10H14 | 000135-98-8 | 35 |
| 3 | Benzeneacetaldehyde, 4-methyl- | 134 | C9H10O | 000104-09-6 | 35 |
| 4 | Propene, 3-phenyl-3-ol- | 134 | C9H10O | 025975-32-0 | 25 |
| 5 | Bicyclo[4.2.0]oct-1-ene, 7-endo-... | 134 | C10H14 | 1000142-18-3 | 23 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

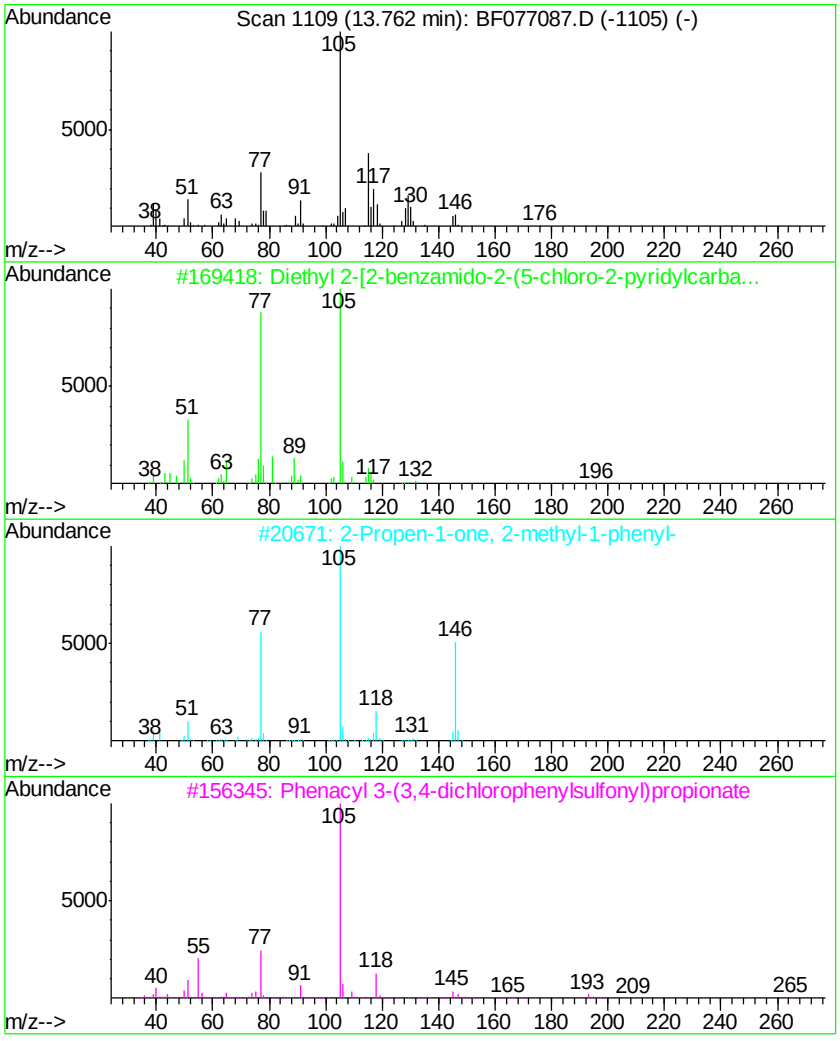
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

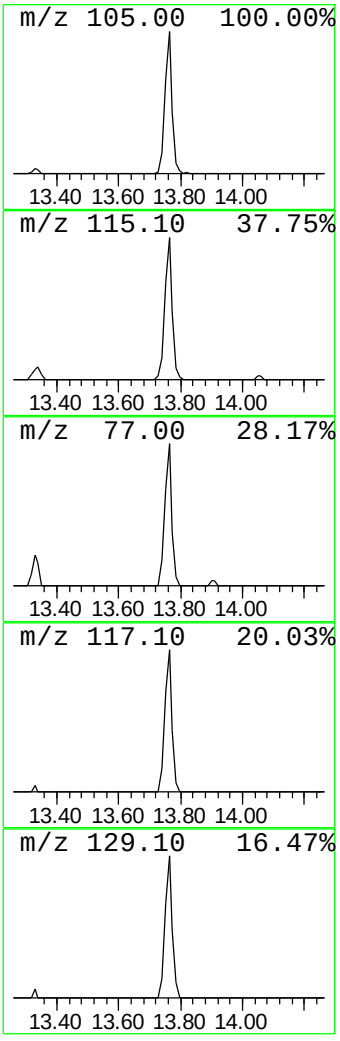
**********

Peak Number 7 unknown13.76 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.76 | 19.78 ng | 243612 | Acenaphthene-d10 | 14.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Diethyl 2-[2-benzamido-2-(5-chlo... | 513 | C25H25ClN3O5P | 300381-21-9 | 38 |
| 2 | 2-Propen-1-one, 2-methyl-1-phenyl- | 146 | C10H10O | 000769-60-8 | 27 |
| 3 | Phenacyl 3-(3,4-dichlorophenylsu... | 400 | C17H14Cl2O5S | 1000225-01-1 | 22 |
| 4 | .+/-.-2-Phenylbutyrophenone | 224 | C16H16O | 077542-11-1 | 14 |
| 5 | p-Chlorophenyl (2-(benzoyloxy)et... | 319 | C16H14ClNO4 | 094207-34-8 | 12 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

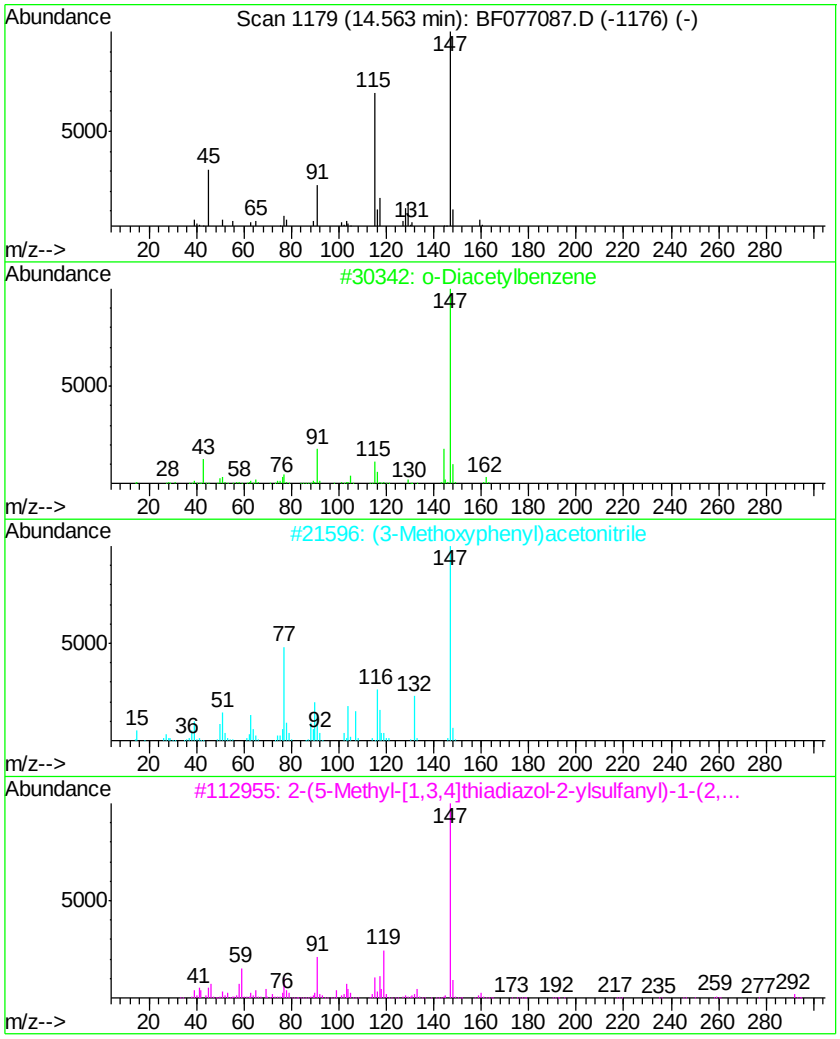
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

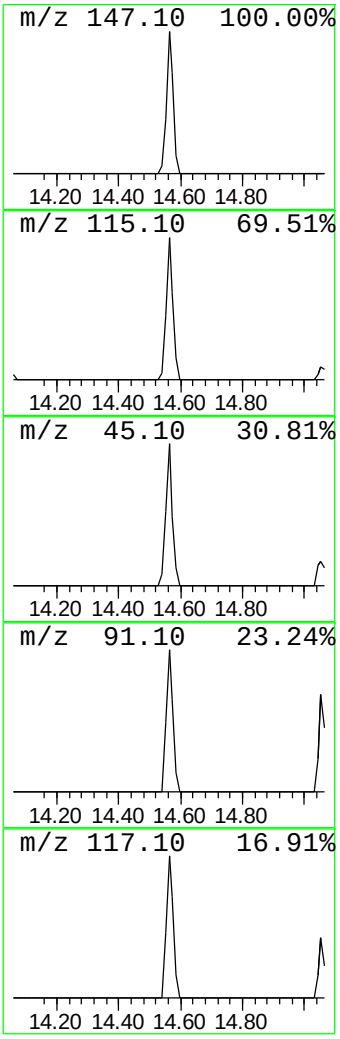
**********

Peak Number 8 unknown14.56 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.56 | 5.55 ng | 68323 | Acenaphthene-d10 | 14.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | o-Diacetylbenzene | 162 | C10H10O2 | 000704-00-7 | 37 |
| 2 | (3-Methoxyphenyl)acetonitrile | 147 | C9H9NO | 019924-43-7 | 32 |
| 3 | 2-(5-Methyl-[1,3,4]thiadiazol-2-... | 292 | C14H16N2OS2 | 1000296-87-8 | 32 |
| 4 | Benzo[b]furan-5-carboxylic acid,... | 274 | C15H11ClO3 | 1000268-06-4 | 25 |
| 5 | 4-Dimethyl(trimethylsilyl)silylo... | 330 | C18H42OSi2 | 1000245-68-5 | 23 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

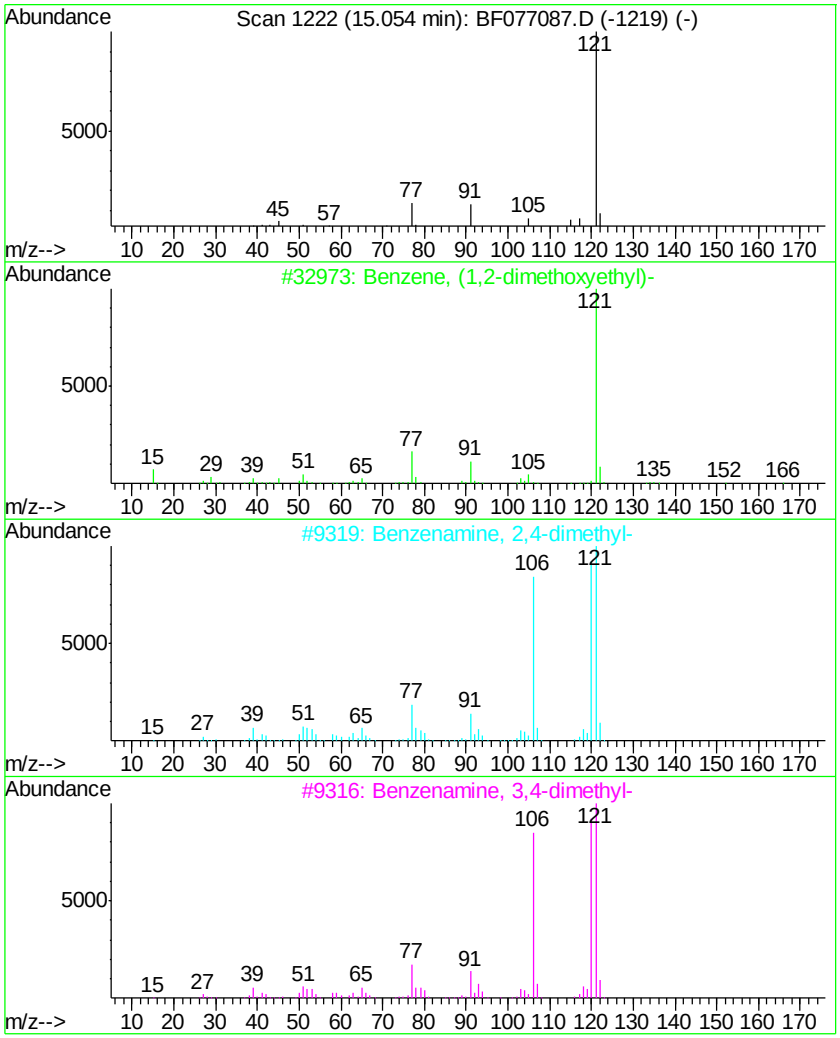
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

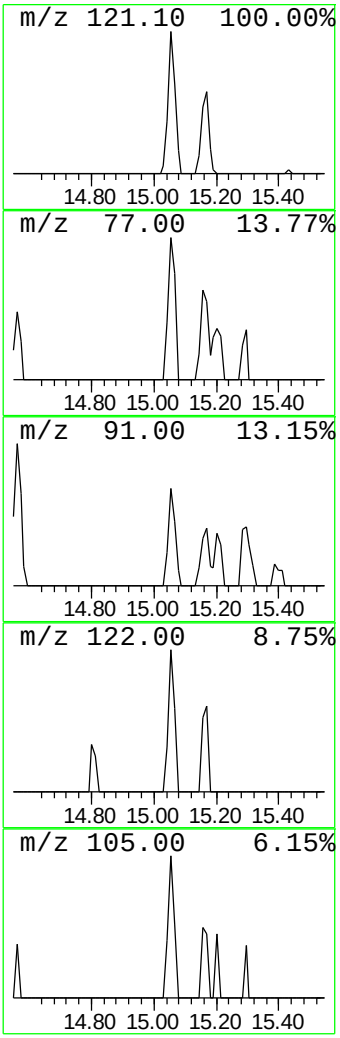
**********

Peak Number 9 Benzene, (1,2-dimethoxyethyl)- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.05 | 3.20 ng | 39402 | Acenaphthene-d10 | 14.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, (1,2-dimethoxyethyl)- | 166 | C10H14O2 | 004013-37-0 | 56 |
| 2 | Benzenamine, 2,4-dimethyl- | 121 | C8H11N | 000095-68-1 | 50 |
| 3 | Benzenamine, 3,4-dimethyl- | 121 | C8H11N | 000095-64-7 | 50 |
| 4 | Benzenamine, 3,5-dimethyl- | 121 | C8H11N | 000108-69-0 | 50 |
| 5 | R(-)-2-Methoxy-2-phenylacetic acid | 166 | C9H10O3 | 1000132-09-7 | 43 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

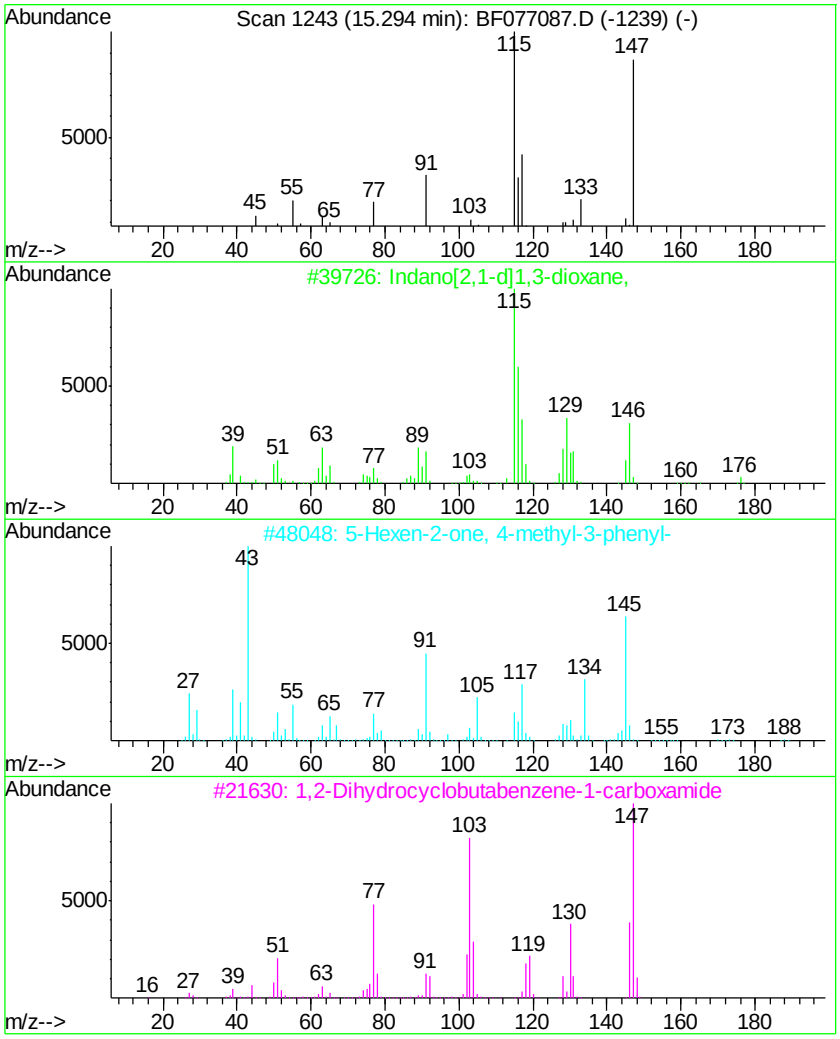
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

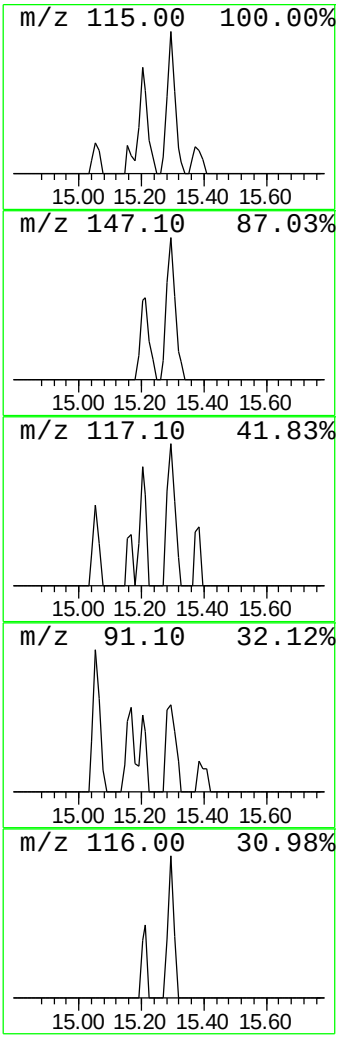
**********

Peak Number 10 unknown15.29 Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.29 | 2.34 ng | 28794 | Acenaphthene-d10 | 14.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Indano[2,1-d]1,3-dioxane, | 176 | C11H12O2 | 102688-70-0 | 23 |
| 2 | 5-Hexen-2-one, 4-methyl-3-phenyl- | 188 | C13H16O | 040931-43-9 | 22 |
| 3 | 1,2-Dihydrocyclobutabenzene-1-ca... | 147 | C9H9NO | 052199-49-2 | 22 |
| 4 | Benzene, 1-ethynyl-4-nitro- | 147 | C8H5NO2 | 000937-31-5 | 12 |
| 5 | Isoquinoline, 5,6,7,8-tetrahydro... | 147 | C10H13N | 037009-20-4 | 12 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

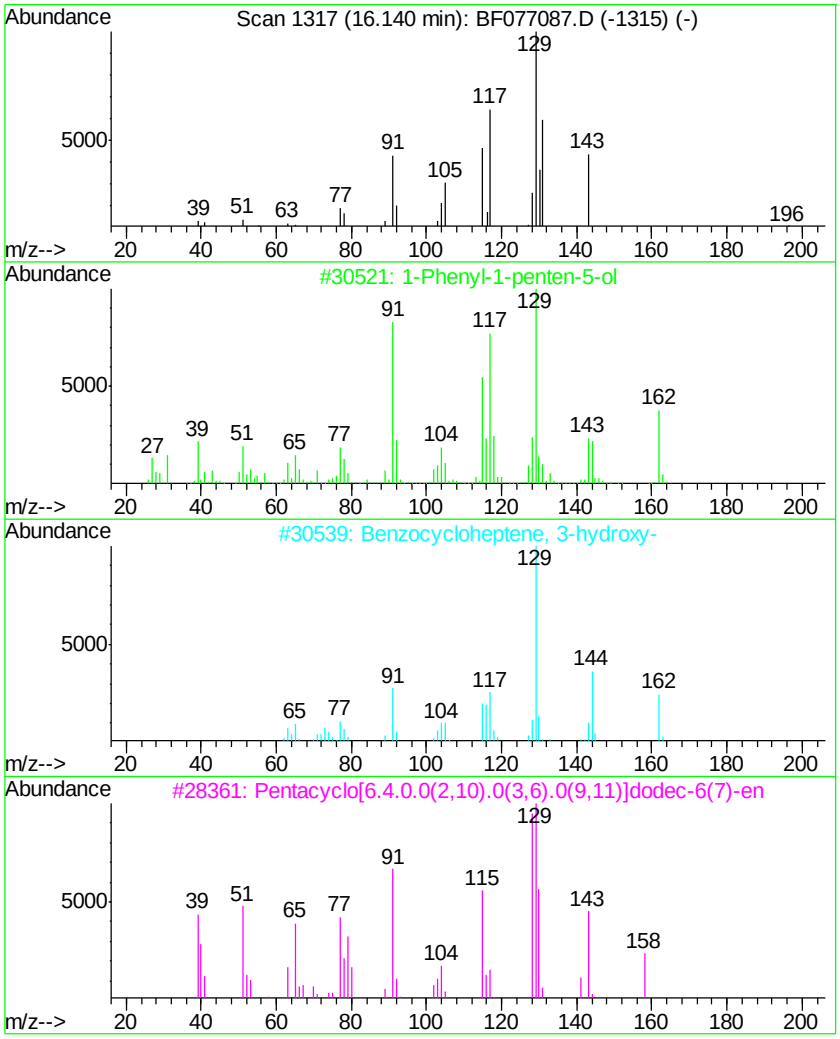
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

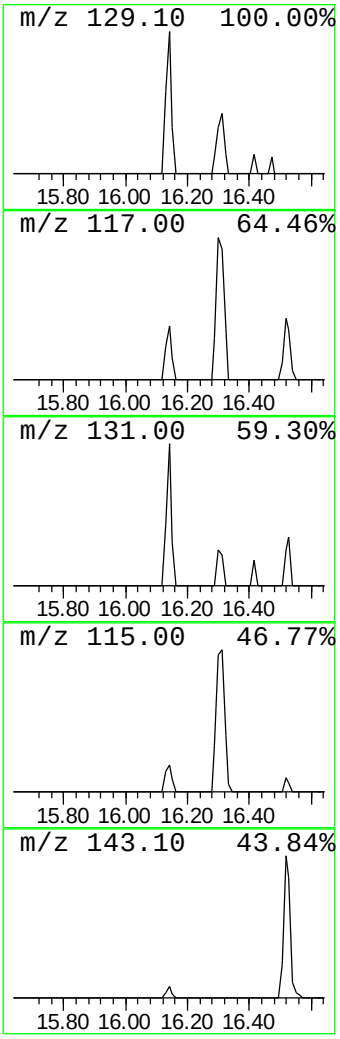
**********

Peak Number 11 1-Phenyl-1-penten-5-ol Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.14 | 2.09 ng | 25776 | Acenaphthene-d10 | 14.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Phenyl-1-penten-5-ol | 162 | C11H14O | 037464-86-1 | 50 |
| 2 | Benzocycloheptene, 3-hydroxy- | 162 | C11H14O | 005200-96-4 | 38 |
| 3 | Pentacyclo[6.4.0.0(2,10).0(3,6).... | 158 | C12H14 | 1000223-17-5 | 38 |
| 4 | 1-Hydroxymethyl-1,2,3,4-tetrahyd... | 178 | C11H14O2 | 343332-31-0 | 37 |
| 5 | 6-Azatetracyclo[6.5.0.0(1,7).0(4... | 187 | C12H13NO | 056689-39-5 | 25 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

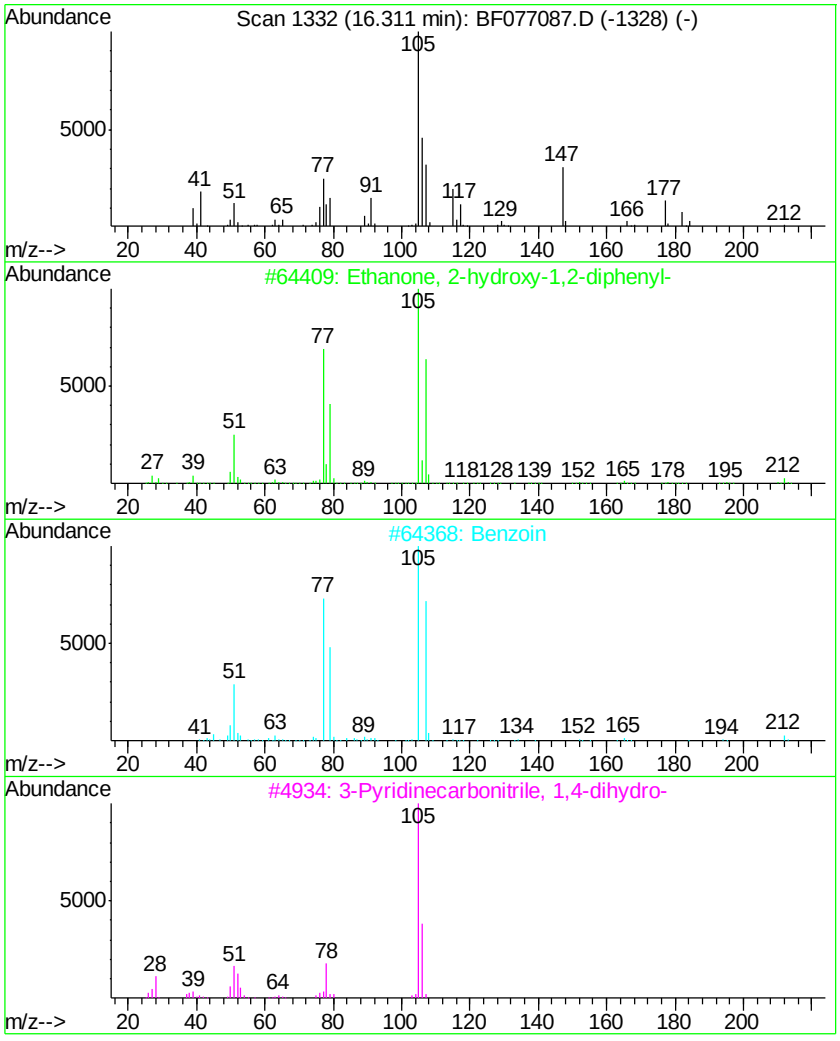
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

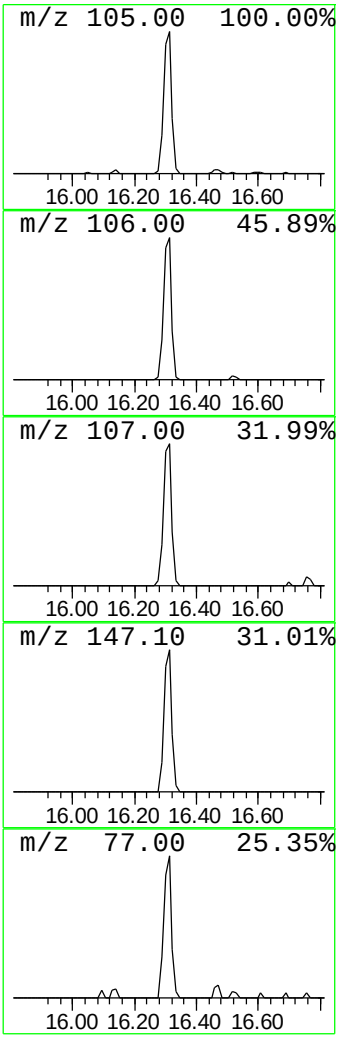
**********

Peak Number 12 unknown16.31 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.31 | 23.57 ng | 299315 | Phenanthrene-d10 | 17.64 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanone, 2-hydroxy-1,2-diphenyl- | 212 | C14H12O2 | 000119-53-9 | 25 |
| 2 | Benzoin | 212 | C14H12O2 | 000579-44-2 | 25 |
| 3 | 3-Pyridinecarbonitrile, 1,4-dihy... | 106 | C6H6N2 | 023974-91-6 | 22 |
| 4 | Benzamide, N-butyl- | 177 | C11H15NO | 002782-40-3 | 22 |
| 5 | Diethyl 2-[2-benzamido-2-(5-chlo... | 513 | C25H25ClN3O5P | 300381-21-9 | 12 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
Data File : BF077087.D
Acq On : 27 Jan 2015 16:27
Operator : TP/IZ
Sample : G1139-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown7.26 | 7.26 | 69.5 | ng | 553398 | 1 | 7.76 | 159257 | 20.0 |
| unknown12.53 | 12.53 | 2.6 | ng | 29015 | 2 | 10.68 | 225524 | 20.0 |
| unknown13.76 | 13.76 | 19.8 | ng | 243612 | 3 | 14.80 | 246384 | 20.0 |
| unknown14.56 | 14.56 | 5.5 | ng | 68323 | 3 | 14.80 | 246384 | 20.0 |
| Benzene, (1,2-dim... | 15.05 | 3.2 | ng | 39402 | 3 | 14.80 | 246384 | 20.0 |
| unknown15.29 | 15.29 | 2.3 | ng | 28794 | 3 | 14.80 | 246384 | 20.0 |
| 1-Phenyl-1-penten... | 16.14 | 2.1 | ng | 25776 | 3 | 14.80 | 246384 | 20.0 |
| unknown16.31 | 16.31 | 23.6 | ng | 299315 | 4 | 17.64 | 253935 | 20.0 |