LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

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_G\Methods\8270-BG122116.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 | 5.270 | 409 | 414 | 423 | rVB | 147581 | 258514 | 4.44% | 0.992% |
| 2 | 5.751 | 490 | 496 | 506 | rBV | 505068 | 885329 | 15.19% | 3.399% |
| 3 | 7.373 | 765 | 772 | 783 | rBV | 323584 | 649277 | 11.14% | 2.492% |
| 4 | 7.743 | 828 | 835 | 846 | rBV | 871015 | 1568875 | 26.93% | 6.022% |
| 5 | 8.213 | 906 | 915 | 922 | rBV | 201630 | 355330 | 6.10% | 1.364% |
| 6 | 8.536 | 960 | 970 | 979 | rBV | 754577 | 1348466 | 23.14% | 5.176% |
| 7 | 9.394 | 1109 | 1116 | 1130 | rBV | 653636 | 1283754 | 22.03% | 4.928% |
| 8 | 11.039 | 1388 | 1396 | 1404 | rBV | 253085 | 493854 | 8.48% | 1.896% |
| 9 | 13.460 | 1800 | 1808 | 1815 | rBV | 1834245 | 2947702 | 50.59% | 11.315% |
| 10 | 14.277 | 1942 | 1947 | 1953 | rVB | 92026 | 137748 | 2.36% | 0.529% |
| 11 | 14.835 | 2032 | 2042 | 2048 | rBV | 465989 | 791415 | 13.58% | 3.038% |
| 12 | 16.327 | 2289 | 2296 | 2305 | rVV | 1970173 | 3033202 | 52.06% | 11.644% |
| 13 | 16.539 | 2327 | 2332 | 2339 | rVB | 108367 | 161539 | 2.77% | 0.620% |
| 14 | 16.633 | 2341 | 2348 | 2352 | rBV | 202517 | 295233 | 5.07% | 1.133% |
| 15 | 16.686 | 2352 | 2357 | 2364 | rVV4 | 176791 | 381883 | 6.55% | 1.466% |
| 16 | 16.750 | 2364 | 2368 | 2372 | rVV | 212815 | 298801 | 5.13% | 1.147% |
| 17 | 16.797 | 2372 | 2376 | 2381 | rVB | 125312 | 168859 | 2.90% | 0.648% |
| 18 | 16.897 | 2391 | 2393 | 2397 | rVB | 73725 | 86383 | 1.48% | 0.332% |
| 19 | 16.956 | 2397 | 2403 | 2409 | rVB3 | 201104 | 395982 | 6.80% | 1.520% |
| 20 | 17.020 | 2409 | 2414 | 2417 | rBV | 195256 | 288878 | 4.96% | 1.109% |
| 21 | 17.091 | 2422 | 2426 | 2433 | rVB2 | 136865 | 224135 | 3.85% | 0.860% |
| 22 | 17.584 | 2503 | 2510 | 2517 | rBV | 619114 | 984811 | 16.90% | 3.780% |
| 23 | 18.419 | 2648 | 2652 | 2656 | rVB6 | 48653 | 59740 | 1.03% | 0.229% |
| 24 | 20.164 | 2943 | 2949 | 2955 | rVB | 4461307 | 5826535 | 100.00% | 22.366% |
| 25 | 21.456 | 3163 | 3169 | 3176 | rBV | 50835 | 139995 | 2.40% | 0.537% |
| 26 | 21.874 | 3234 | 3240 | 3249 | rVB | 859188 | 1484164 | 25.47% | 5.697% |
| 27 | 25.281 | 3809 | 3820 | 3833 | rBV | 471591 | 1499879 | 25.74% | 5.758% |

Sum of corrected areas: 26050283

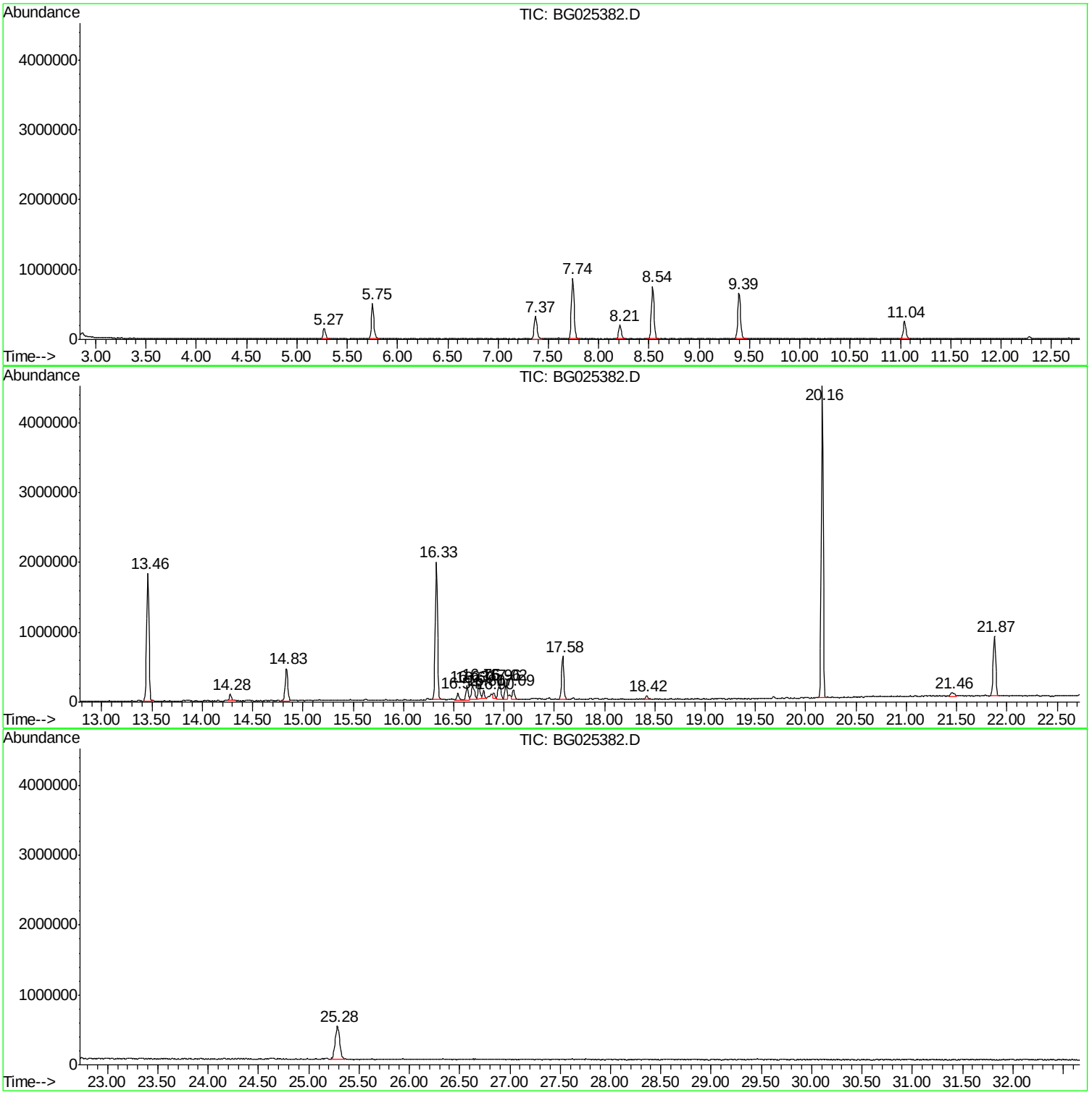
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

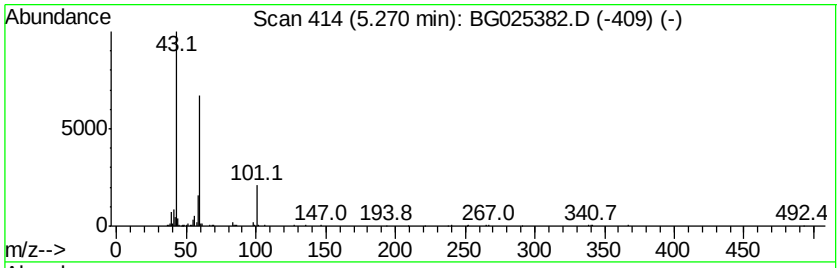
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

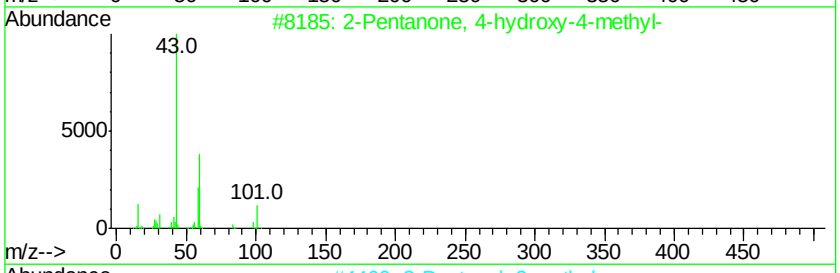
**********

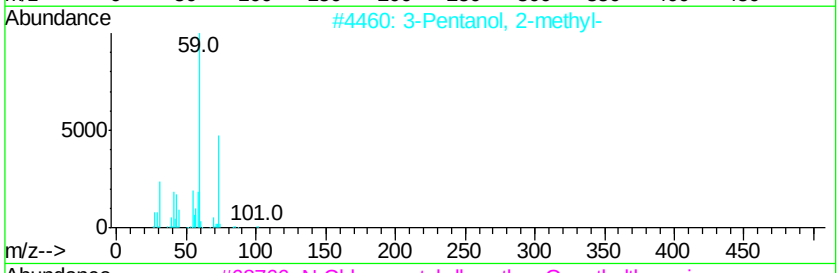
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

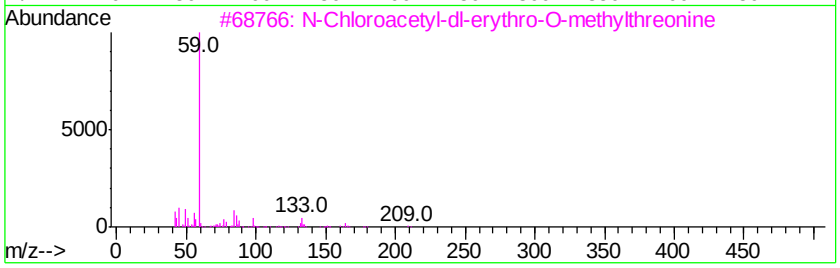
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.27 | 14.55 ng | 258514 | 1,4-Dichlorobenzene-d4 | 8.21 |

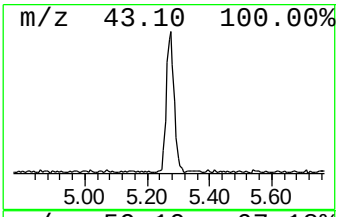
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | 3-Pentanol, 2-methyl- | 102 | C6H14O | 000565-67-3 | 17 |
| 3 | N-Chloroacetyl-dl-erythro-O-meth... | 209 | C7H12ClNO4 | 1000214-48-1 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Guanidine | 59 | CH5N3 | 000113-00-8 | 9 |

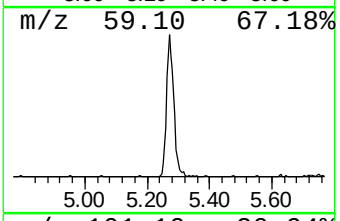


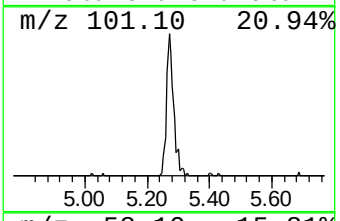



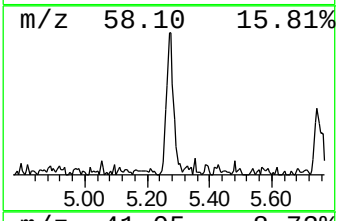



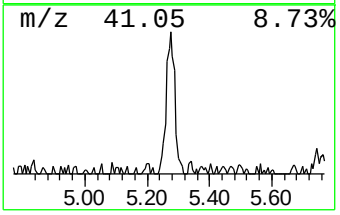



Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

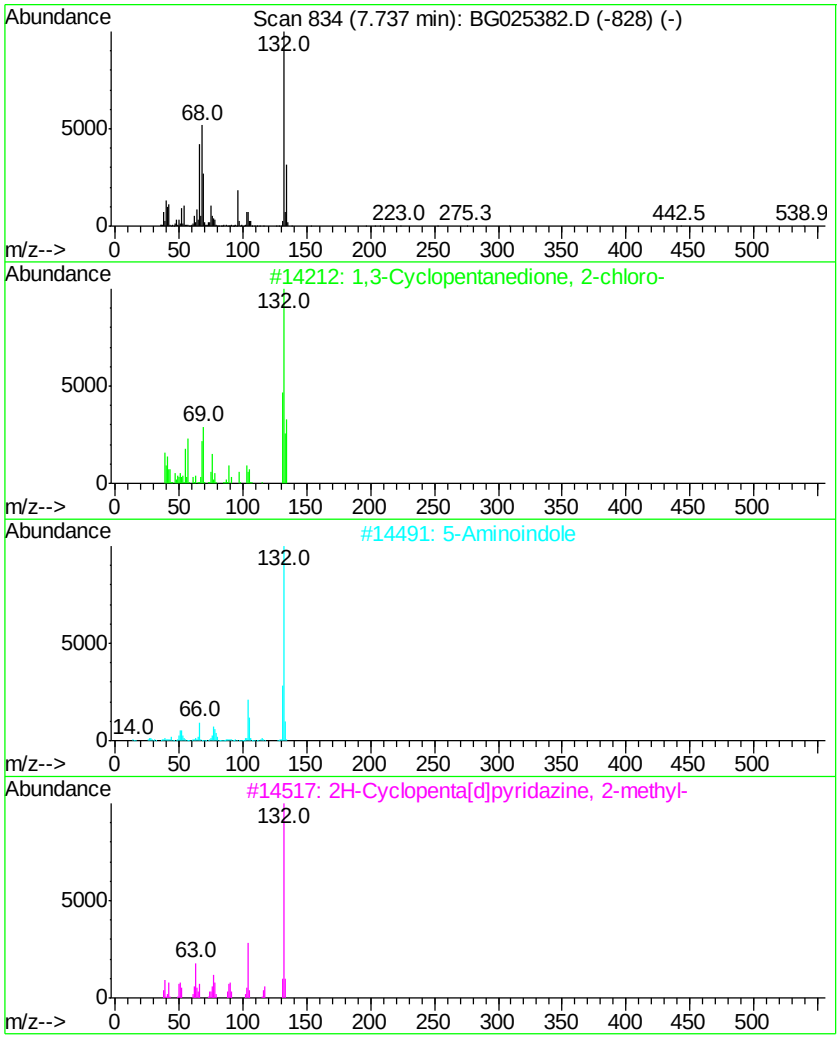
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

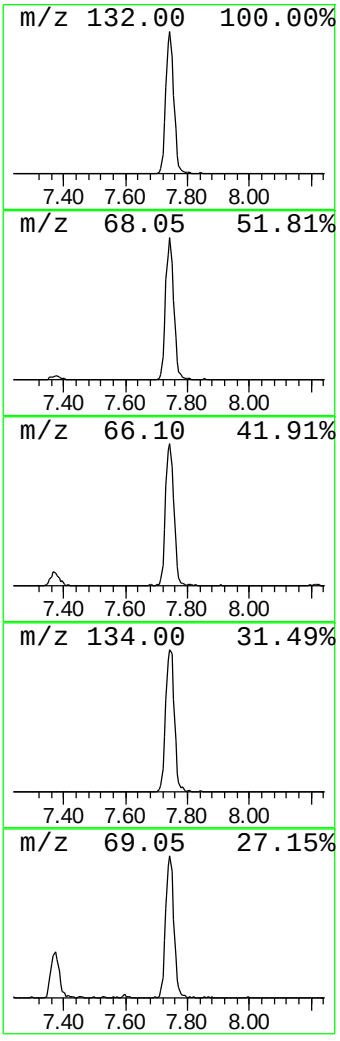
**********

Peak Number 2 unknown7.74 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.74 | 88.31 ng | 1568880 | 1,4-Dichlorobenzene-d4 | 8.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 16 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 14 |
| 3 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 14 |
| 4 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 14 |
| 5 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 14 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

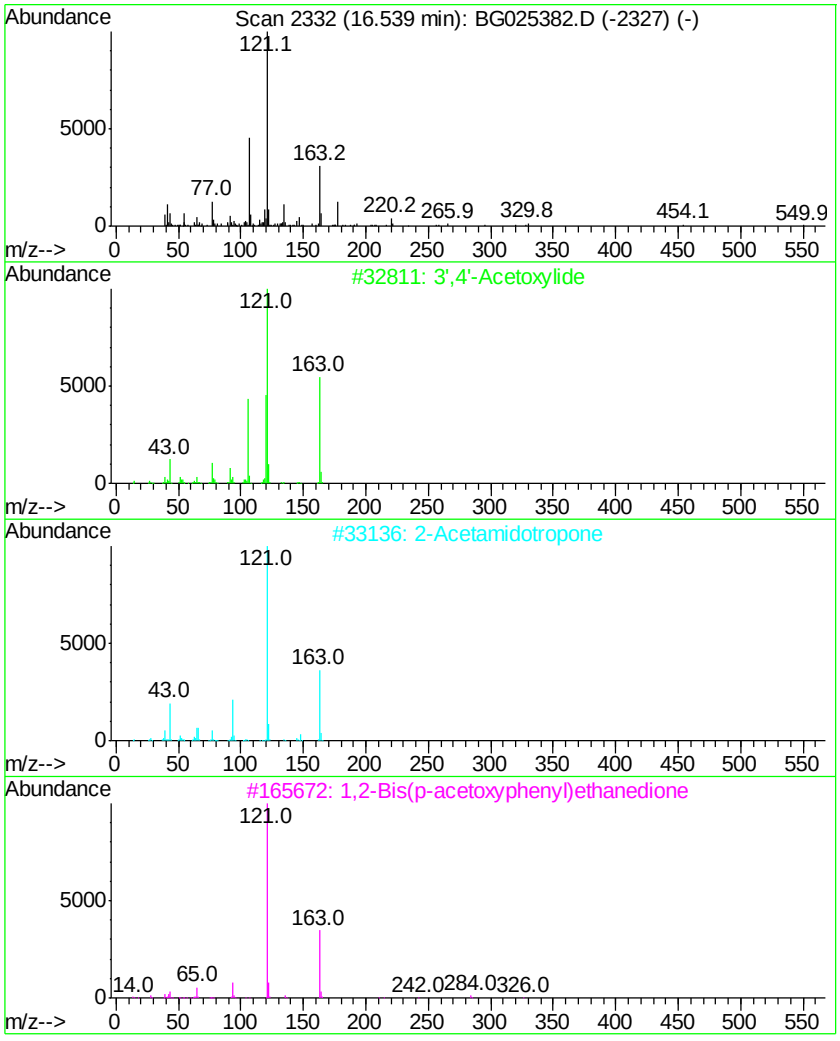
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

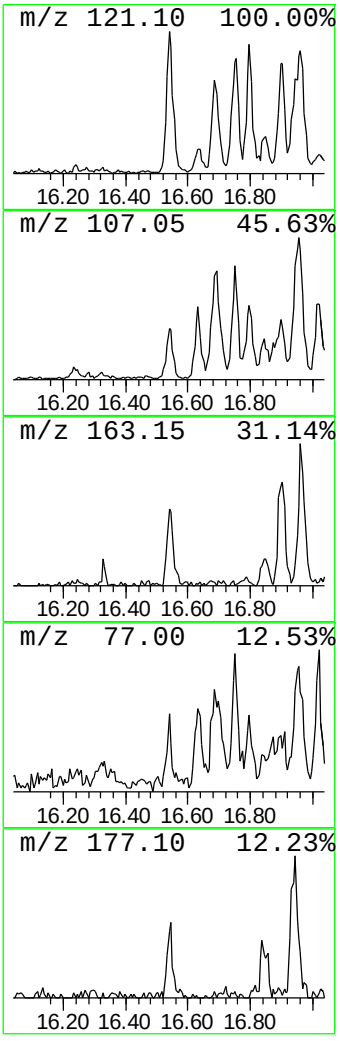
**********

Peak Number 4 unknown16.54 Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.54 | 3.28 ng | 161539 | Phenanthrene-d10 | 17.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3',4'-Acetoxylide | 163 | C10H13NO | 002198-54-1 | 46 |
| 2 | 2-Acetamidotropone | 163 | C9H9NO2 | 006422-12-4 | 43 |
| 3 | 1,2-Bis(p-acetoxyphenyl)ethanedione | 326 | C18H14O6 | 093655-79-9 | 43 |
| 4 | Benzenamine, 3,5-dimethyl- | 121 | C8H11N | 000108-69-0 | 38 |
| 5 | 2H-1,2,3,4-Tetrazol-5-amine, N-[... | 205 | C9H11N5O | 1000337-56-1 | 38 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

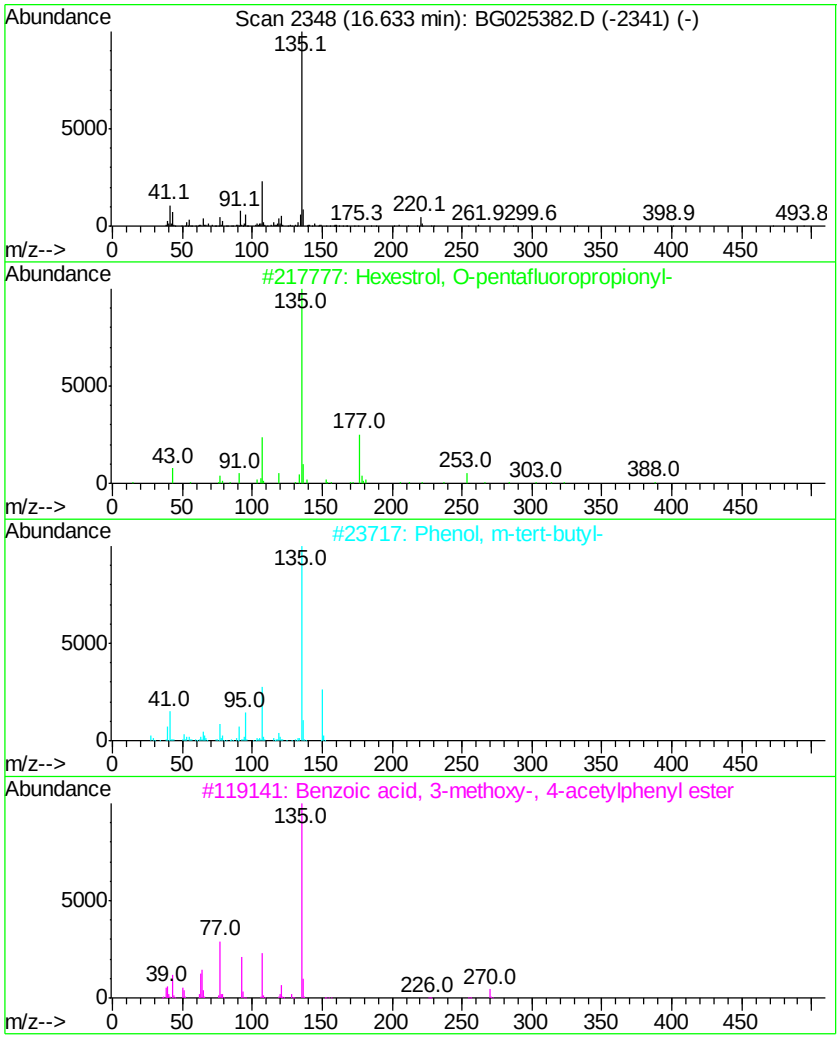
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

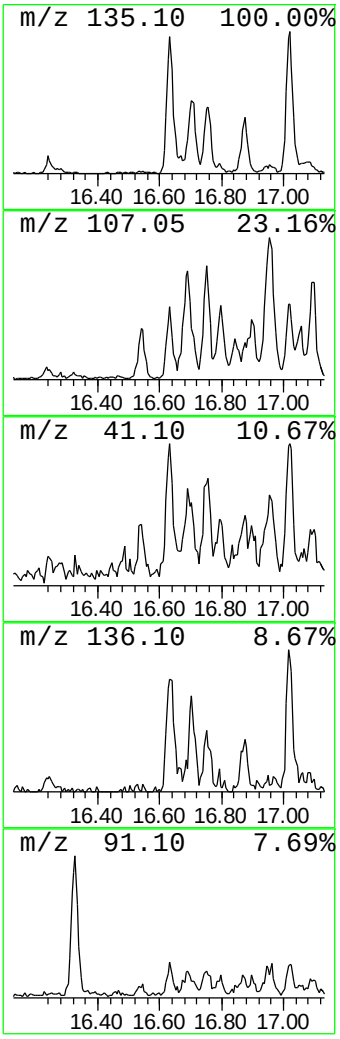
**********

Peak Number 5 Hexestrol, O-pentafluoropro... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.63 | 6.00 ng | 295233 | Phenanthrene-d10 | 17.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexestrol, O-pentafluoropropionyl- | 416 | C21H21F5O3 | 1000365-43-4 | 72 |
| 2 | Phenol, m-tert-butyl- | 150 | C10H14O | 000585-34-2 | 72 |
| 3 | Benzoic acid, 3-methoxy-, 4-acet... | 270 | C16H14O4 | 306763-70-2 | 64 |
| 4 | Phenol, 4-(1,1-dimethylpropyl)- | 164 | C11H16O | 000080-46-6 | 64 |
| 5 | ((1,2-Diethylethylene)bis(p-phen... | 354 | C22H26O4 | 004547-76-6 | 64 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

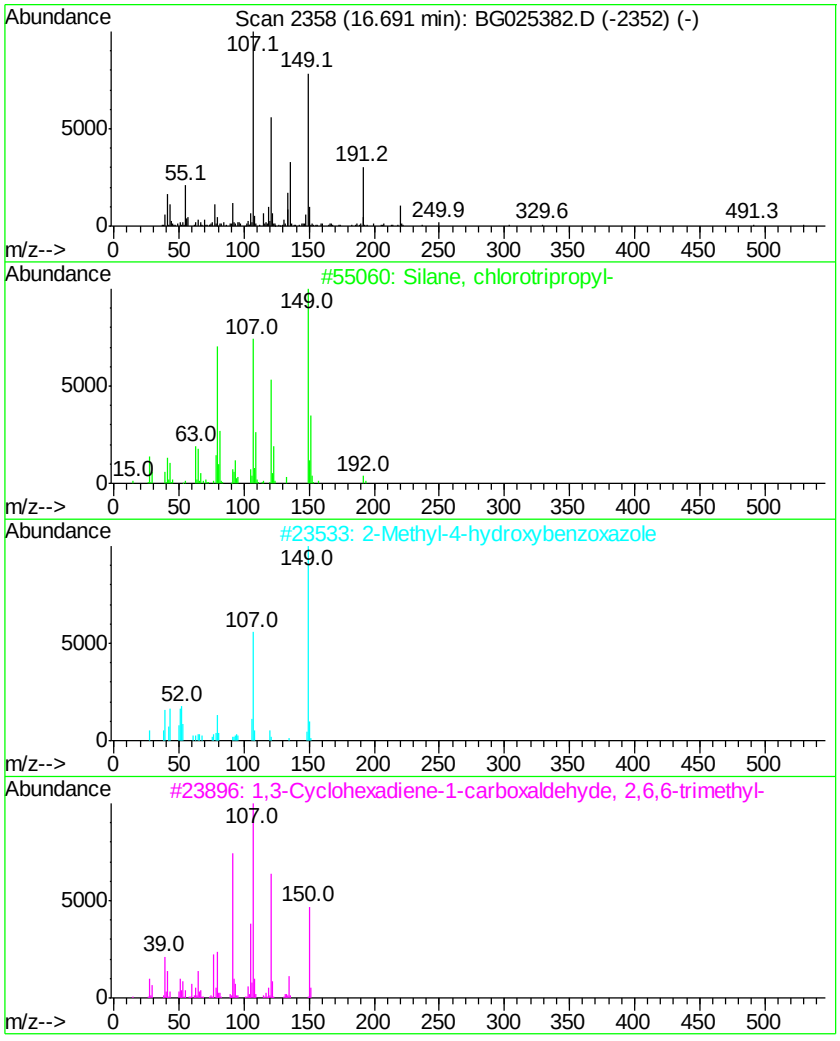
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

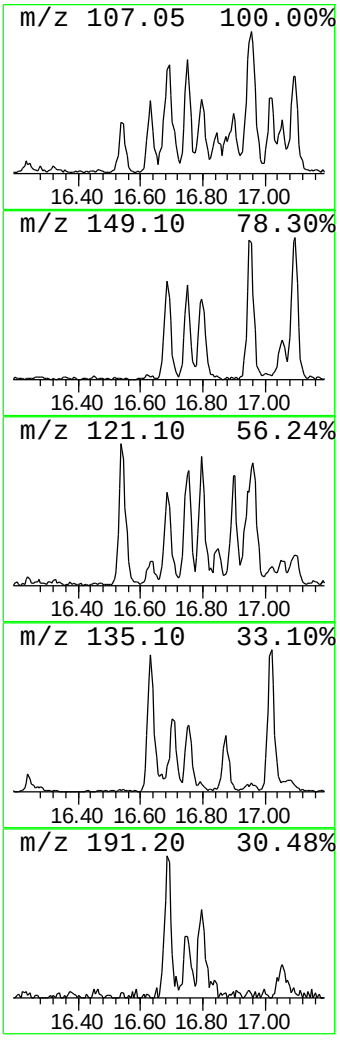
**********

Peak Number 6 Silane, chlorotripropyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.69 | 7.76 ng | 381883 | Phenanthrene-d10 | 17.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Silane, chlorotripropyl- | 192 | C9H21ClSi | 000995-25-5 | 64 |
| 2 | 2-Methyl-4-hydroxybenzoxazole | 149 | C8H7NO2 | 051110-60-2 | 43 |
| 3 | 1,3-Cyclohexadiene-1-carboxaldeh... | 150 | C10H14O | 000116-26-7 | 38 |
| 4 | Butanamide, N-(2-methylphenyl)-3... | 191 | C11H13NO2 | 000093-68-5 | 38 |
| 5 | Benzene, 1-ethoxy-4-ethyl- | 150 | C10H14O | 001585-06-4 | 38 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

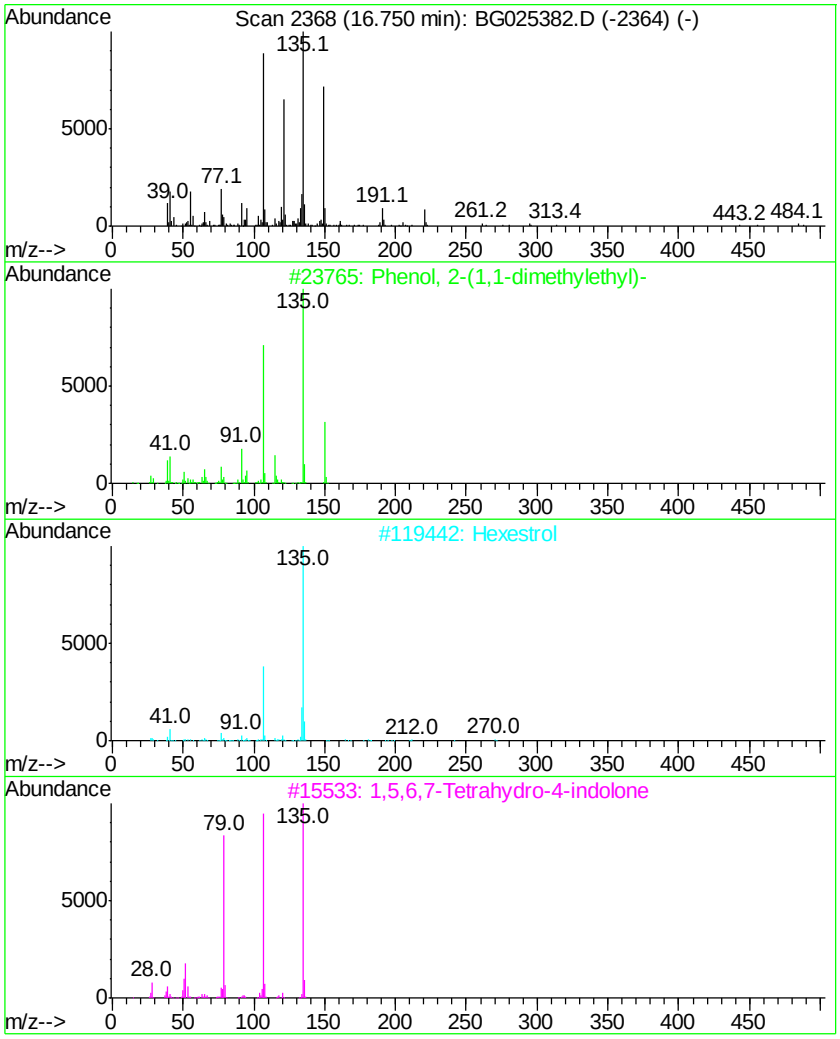
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

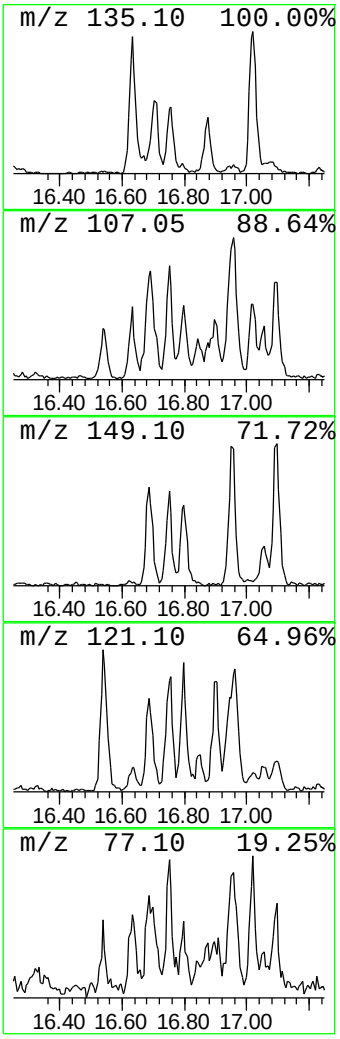
**********

Peak Number 7 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.75 | 6.07 ng | 298801 | Phenanthrene-d10 | 17.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 2-(1,1-dimethylethyl)- | 150 | C10H14O | 000088-18-6 | 70 |
| 2 | Hexestrol | 270 | C18H22O2 | 005635-50-7 | 53 |
| 3 | 1,5,6,7-Tetrahydro-4-indolone | 135 | C8H9NO | 013754-86-4 | 50 |
| 4 | Oxiranecarboxylic acid, 3-phenyl... | 192 | C11H12O3 | 002272-55-1 | 43 |
| 5 | Acetamide, N-methyl-N-phenyl- | 149 | C9H11NO | 000579-10-2 | 43 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

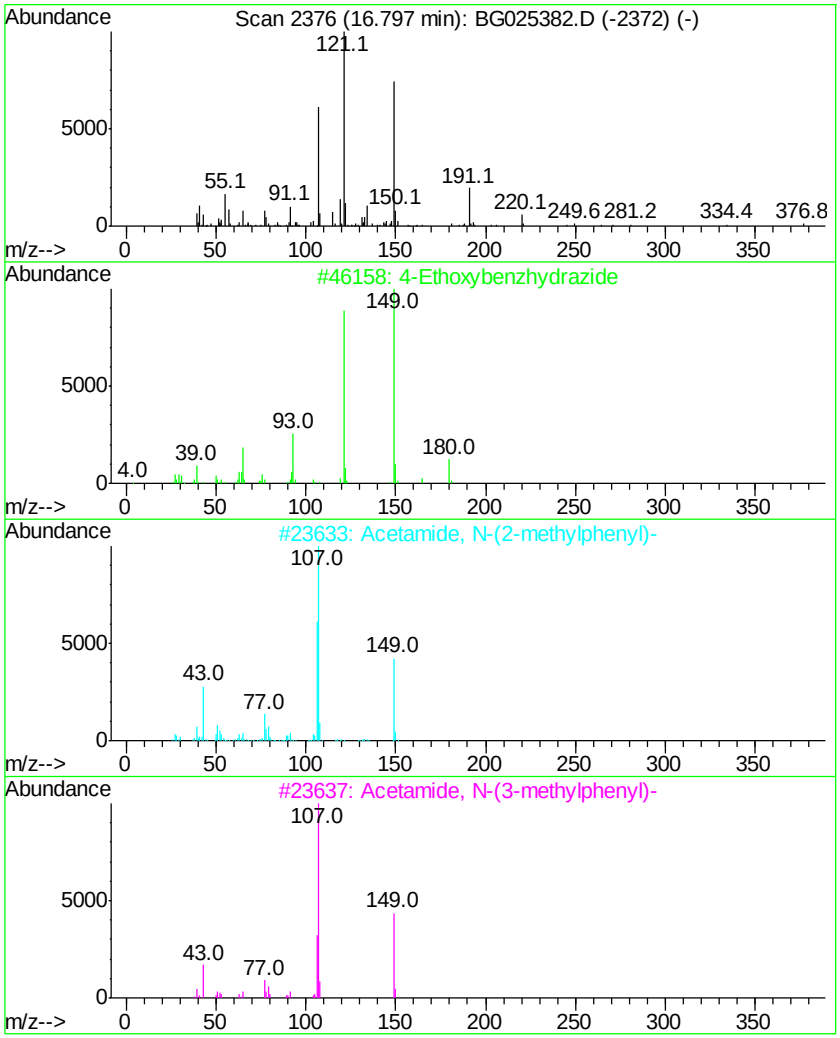
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

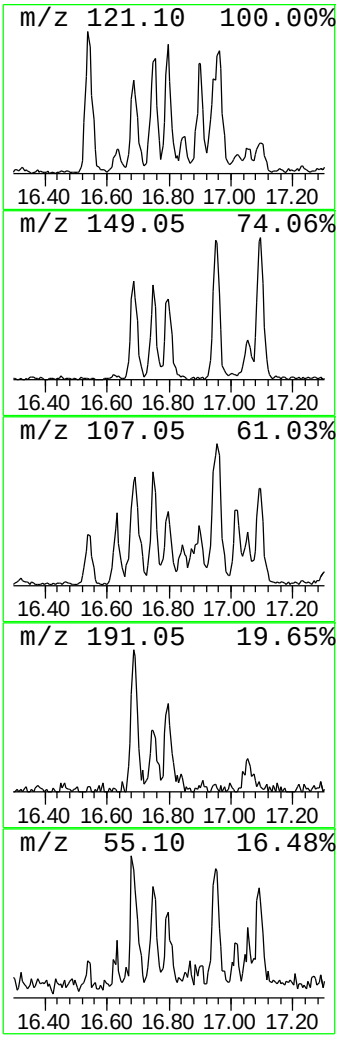
**********

Peak Number 8 4-Ethoxybenzhydrazide Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.80 | 3.43 ng | 168859 | Phenanthrene-d10 | 17.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Ethoxybenzhydrazide | 180 | C9H12N2O2 | 058586-81-5 | 50 |
| 2 | Acetamide, N-(2-methylphenyl)- | 149 | C9H11NO | 000120-66-1 | 38 |
| 3 | Acetamide, N-(3-methylphenyl)- | 149 | C9H11NO | 000537-92-8 | 35 |
| 4 | Isoxazole, 4,5-dihydro-5-[(4-met... | 191 | C11H13NO2 | 1000362-14-0 | 30 |
| 5 | Tricyclo[3.3.1.1(3,7)]decanone, ... | 276 | C10H13IO | 056781-85-2 | 27 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

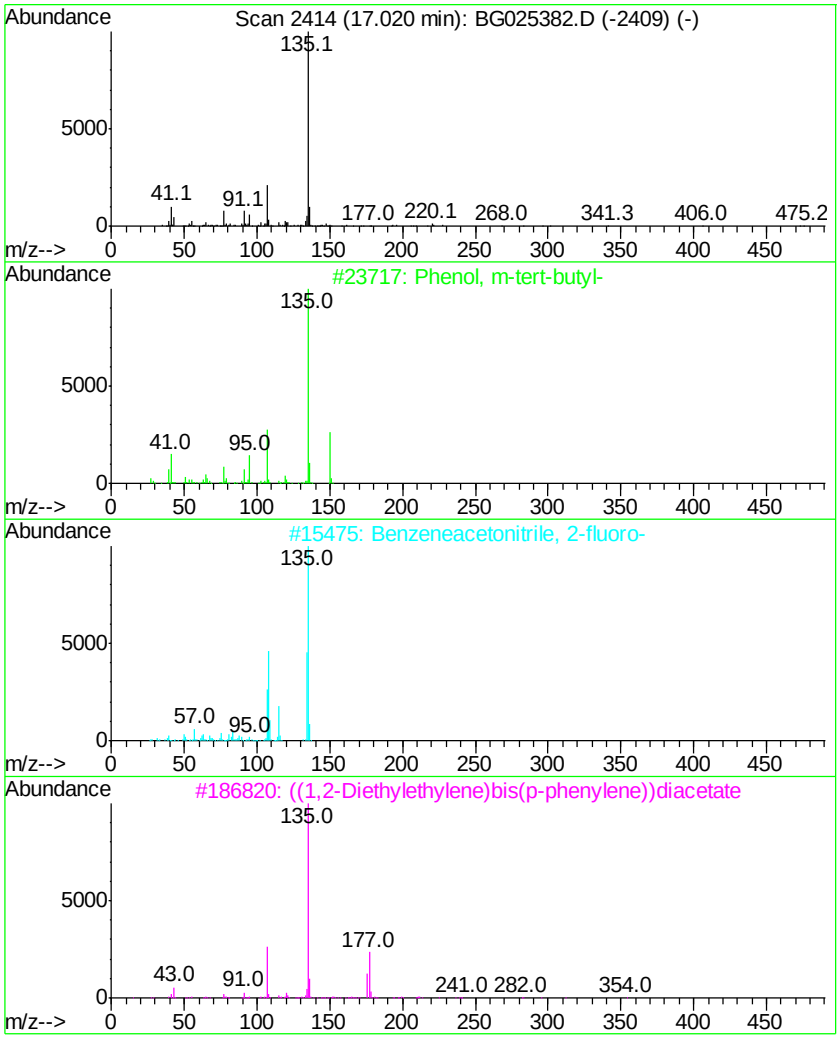
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

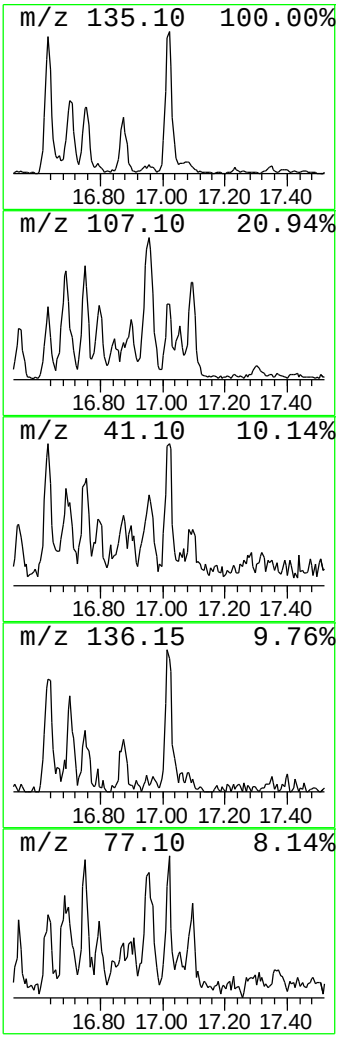
**********

Peak Number 10 Phenol, m-tert-butyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.02 | 5.87 ng | 288878 | Phenanthrene-d10 | 17.58 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, m-tert-butyl- | 150 | C10H14O | 000585-34-2 | 72 |
| 2 | Benzeneacetonitrile, 2-fluoro- | 135 | C8H6FN | 000326-62-5 | 72 |
| 3 | ((1,2-Diethylethylene)bis(p-phen... | 354 | C22H26O4 | 004547-76-6 | 72 |
| 4 | Benzeneacetonitrile, 3-fluoro- | 135 | C8H6FN | 000501-00-8 | 72 |
| 5 | Phenol, 4-(1,1,3,3-tetramethylbu... | 206 | C14H22O | 000140-66-9 | 64 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

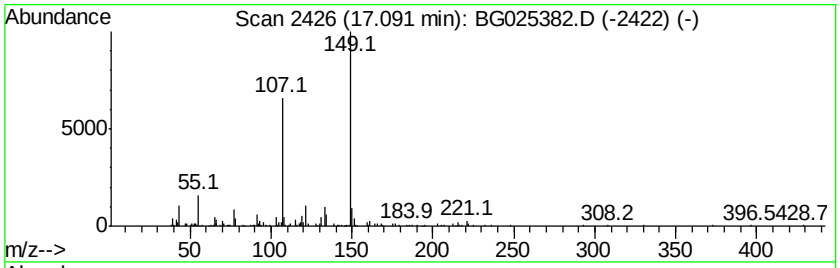
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

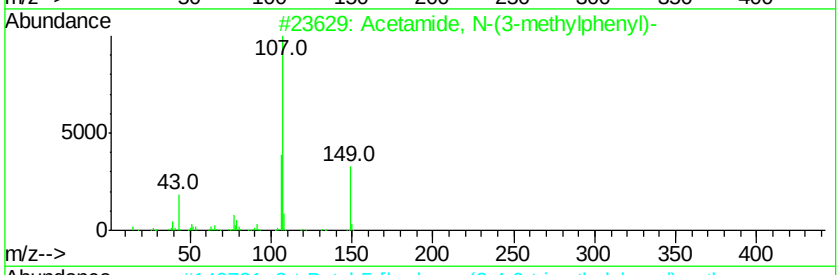
**********

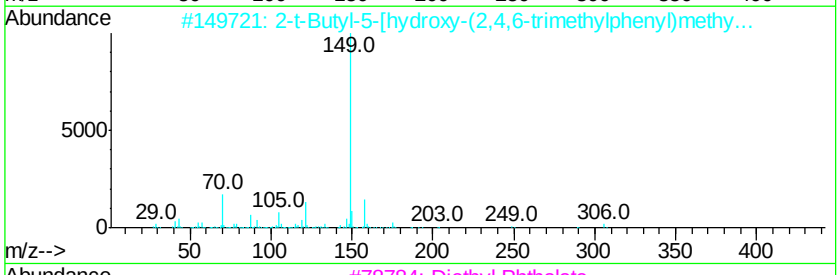
Peak Number 11 Acetamide, N-(3-methylphenyl)- Concentration Rank 9

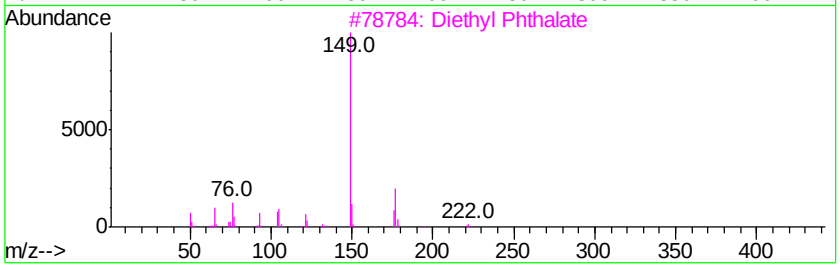
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.09 | 4.55 ng | 224135 | Phenanthrene-d10 | 17.58 |

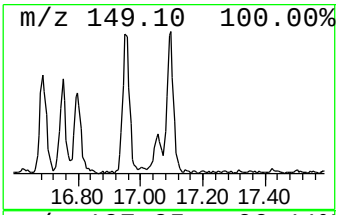
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetamide, N-(3-methylphenyl)- | 149 | C9H11NO | 000537-92-8 | 64 |
| 2 | 2-t-Butyl-5-[hydroxy-(2,4,6-trim... | 306 | C18H26O4 | 092572-63-9 | 47 |
| 3 | Diethyl Phthalate | 222 | C12H14O4 | 000084-66-2 | 47 |
| 4 | 6-Amino-1-methylpurine | 149 | C6H7N5 | 005142-22-3 | 47 |
| 5 | Phthalic acid, cyclohexyl 4-form... | 352 | C21H20O5 | 1000315-73-5 | 47 |

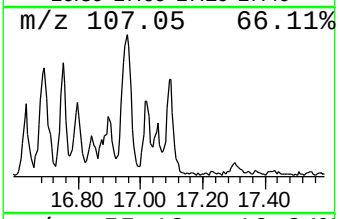


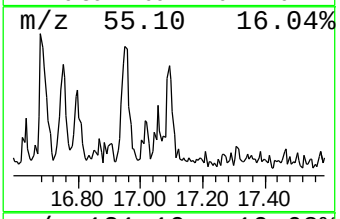



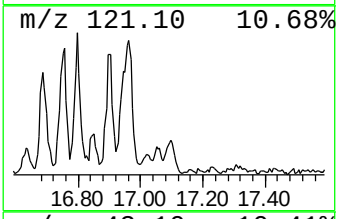



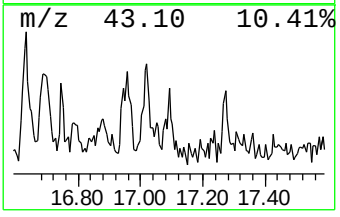



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG122216\
Data File : BG025382.D
Acq On : 22 Dec 2016 10:11
Operator : UM/SJ
Sample : H6166-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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... | 5.27 | 14.6 | ng | 258514 | 1 | 8.21 | 355330 | 20.0 |
| unknown7.74 | 7.74 | 88.3 | ng | 1568880 | 1 | 8.21 | 355330 | 20.0 |
| unknown16.54 | 16.54 | 3.3 | ng | 161539 | 4 | 17.58 | 984811 | 20.0 |
| Hexestrol, O-pent... | 16.63 | 6.0 | ng | 295233 | 4 | 17.58 | 984811 | 20.0 |
| Silane, chlorotri... | 16.69 | 7.8 | ng | 381883 | 4 | 17.58 | 984811 | 20.0 |
| Phenol, 2-(1,1-di... | 16.75 | 6.1 | ng | 298801 | 4 | 17.58 | 984811 | 20.0 |
| 4-Ethoxybenzhydra... | 16.80 | 3.4 | ng | 168859 | 4 | 17.58 | 984811 | 20.0 |
| Phenol, m-tert-bu... | 17.02 | 5.9 | ng | 288878 | 4 | 17.58 | 984811 | 20.0 |
| Acetamide, N-(3-m... | 17.09 | 4.5 | ng | 224135 | 4 | 17.58 | 984811 | 20.0 |