LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128608.D
Acq On : 31 May 2022 22:03
Operator : CG\JU
Sample : N2951-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128608.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.510 | 544 | 548 | 561 | rBV | 1964111 | 2219027 | 78.90% | 12.570% |
| 2 | 6.534 | 718 | 722 | 730 | rBV | 1843394 | 2238154 | 79.58% | 12.678% |
| 3 | 6.845 | 771 | 775 | 778 | rBV | 794805 | 666996 | 23.71% | 3.778% |
| 4 | 7.410 | 865 | 871 | 874 | rBV | 1573599 | 1511498 | 53.74% | 8.562% |
| 5 | 8.128 | 989 | 993 | 996 | rBV | 971965 | 839272 | 29.84% | 4.754% |
| 6 | 9.204 | 1171 | 1176 | 1179 | rBV | 3348177 | 2812550 | 100.00% | 15.932% |
| 7 | 9.880 | 1287 | 1291 | 1295 | rBV | 1019187 | 900812 | 32.03% | 5.103% |
| 8 | 10.680 | 1423 | 1427 | 1430 | rBV | 1588773 | 1360816 | 48.38% | 7.708% |
| 9 | 10.786 | 1442 | 1445 | 1456 | rVB9 | 15986 | 36157 | 1.29% | 0.205% |
| 10 | 11.369 | 1541 | 1544 | 1548 | rBV | 882642 | 783236 | 27.85% | 4.437% |
| 11 | 11.904 | 1632 | 1635 | 1643 | rBV3 | 66674 | 119554 | 4.25% | 0.677% |
| 12 | 12.574 | 1746 | 1749 | 1755 | rVB | 165030 | 209039 | 7.43% | 1.184% |
| 13 | 12.963 | 1810 | 1815 | 1818 | rBV | 2168738 | 1985554 | 70.60% | 11.247% |
| 14 | 13.351 | 1877 | 1881 | 1886 | rVB3 | 114339 | 151454 | 5.38% | 0.858% |
| 15 | 13.592 | 1918 | 1922 | 1929 | rVB | 78894 | 104879 | 3.73% | 0.594% |
| 16 | 13.898 | 1971 | 1974 | 1980 | rBV7 | 30919 | 45114 | 1.60% | 0.256% |
| 17 | 14.015 | 1990 | 1994 | 1997 | rVB | 602007 | 566285 | 20.13% | 3.208% |
| 18 | 14.057 | 1998 | 2001 | 2006 | rVB2 | 91987 | 119056 | 4.23% | 0.674% |
| 19 | 14.115 | 2007 | 2011 | 2015 | rVB | 170681 | 175071 | 6.22% | 0.992% |
| 20 | 14.721 | 2110 | 2114 | 2118 | rBV3 | 69518 | 98062 | 3.49% | 0.555% |
| 21 | 15.486 | 2240 | 2244 | 2249 | rBV | 392509 | 503569 | 17.90% | 2.852% |
| 22 | 17.303 | 2550 | 2553 | 2559 | rVB3 | 119310 | 207806 | 7.39% | 1.177% |

Sum of corrected areas: 17653961

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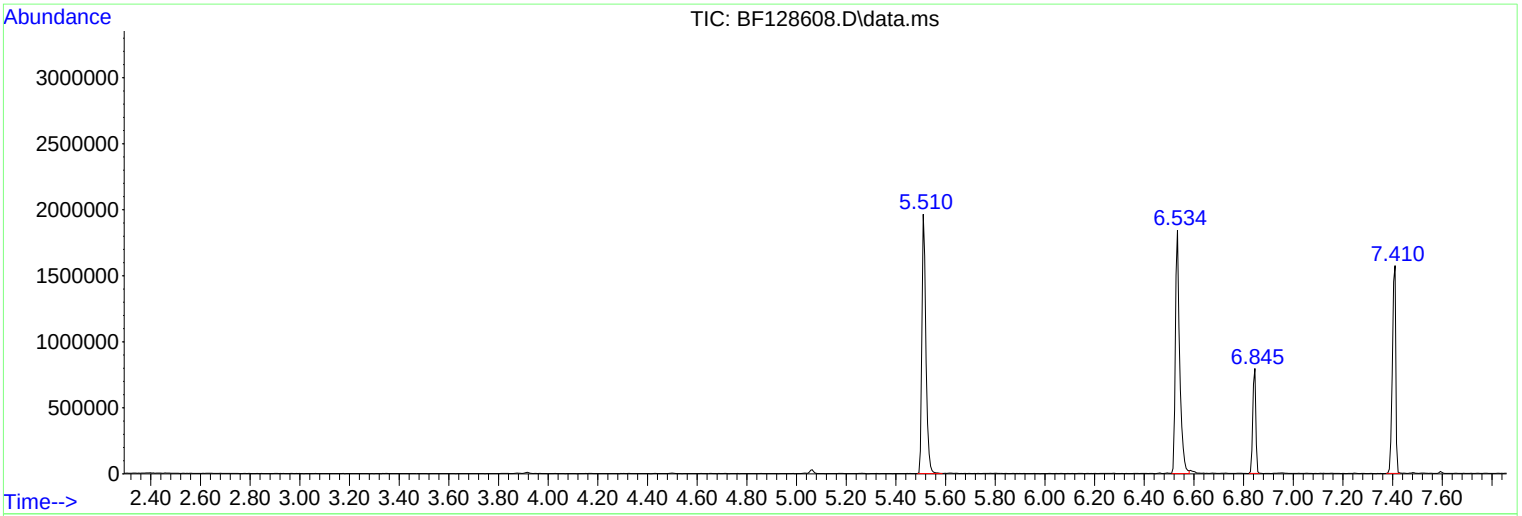
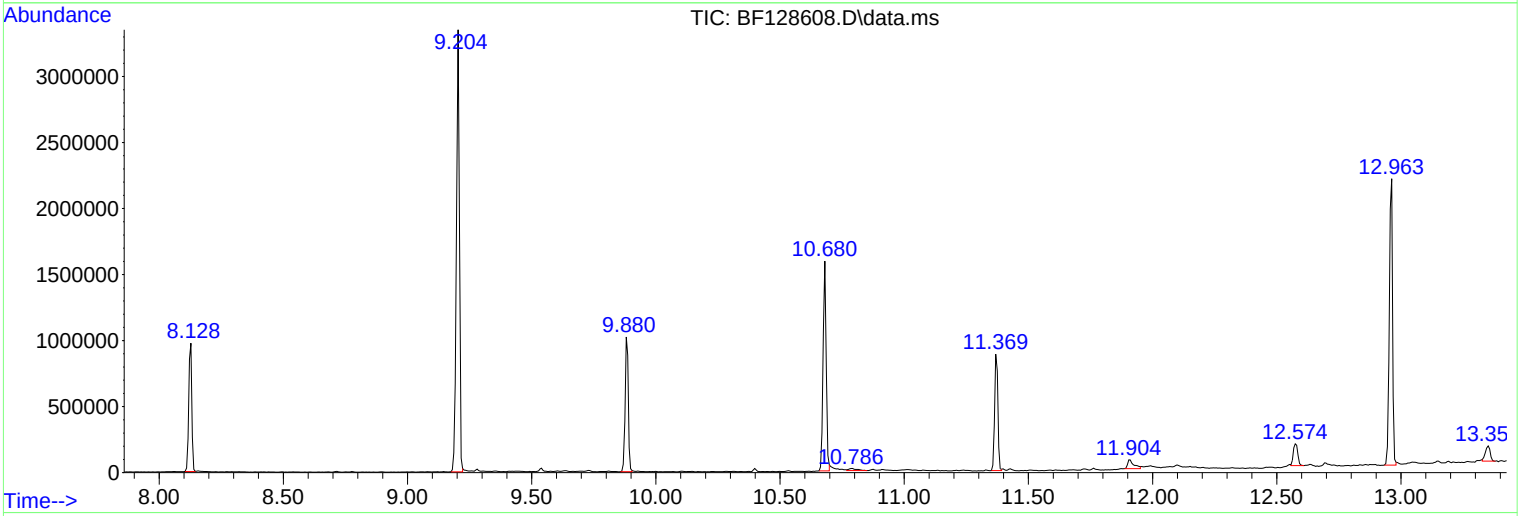
Misc :
ALS Vial : 17 Sample Multiplier: 1

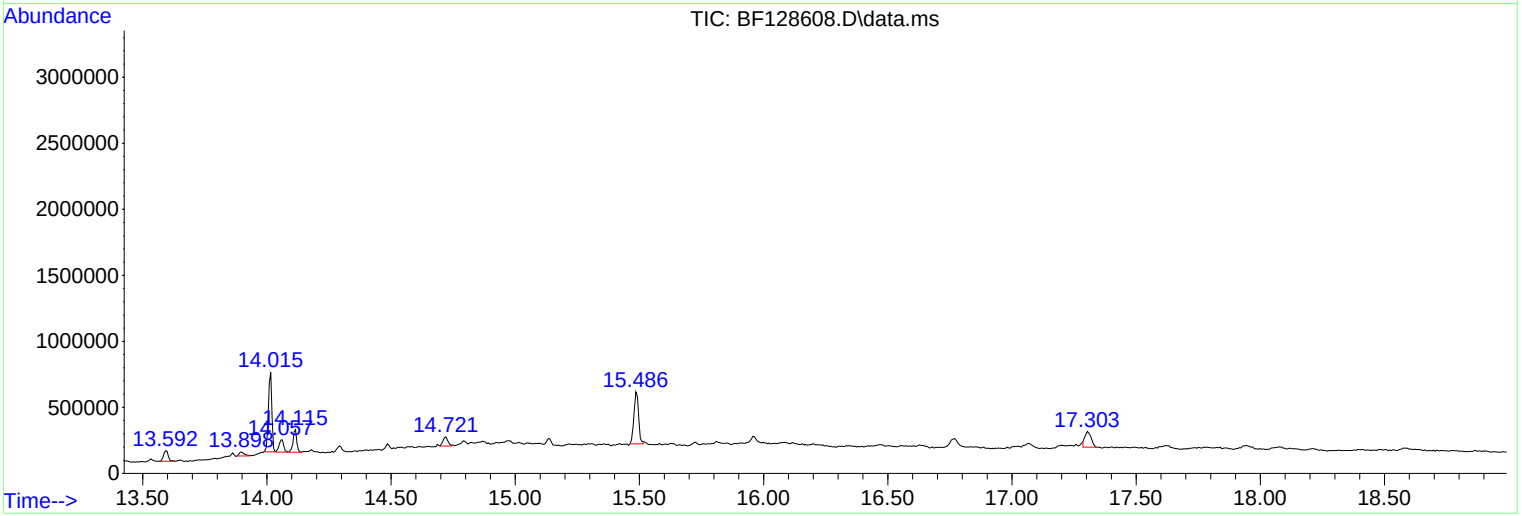
**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Sample : N2951-25
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ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

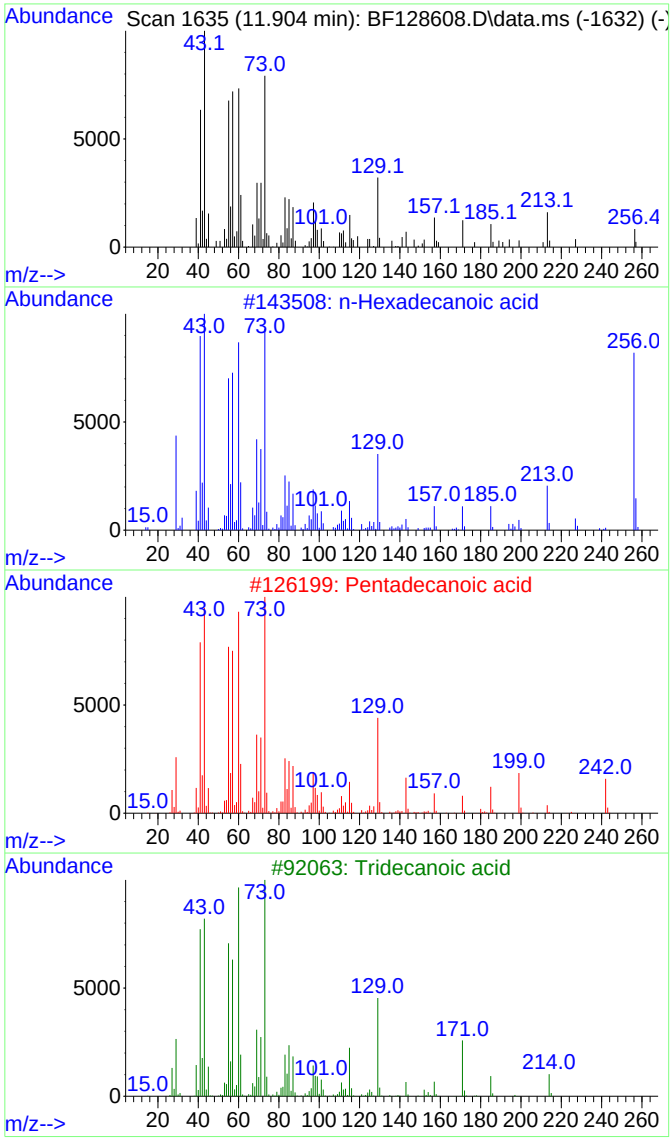
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

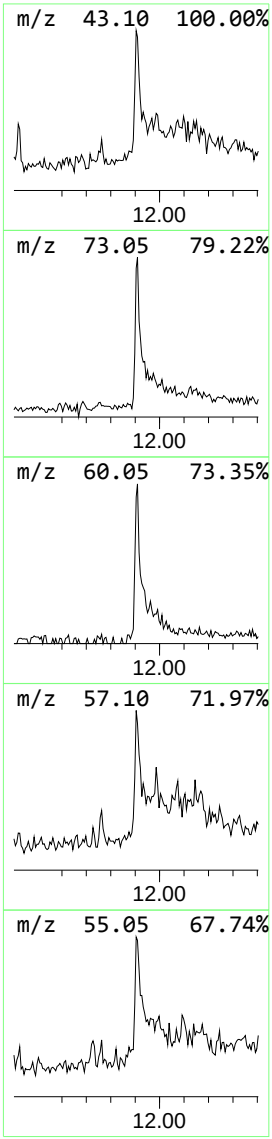
**********

Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.904 | 3.05 ng | 119554 | Phenanthrene-d10 | 11.369 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 81 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 59 |



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Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

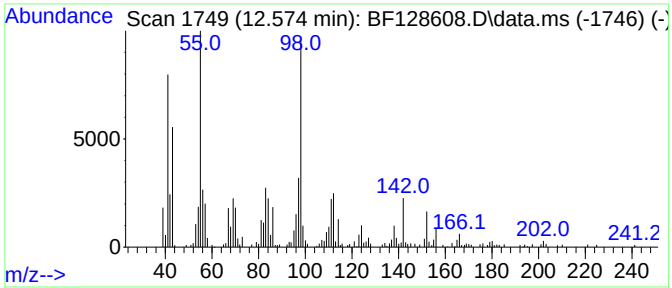
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

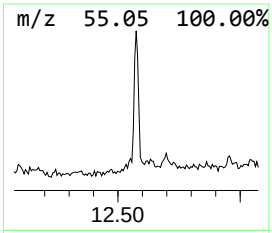
**********

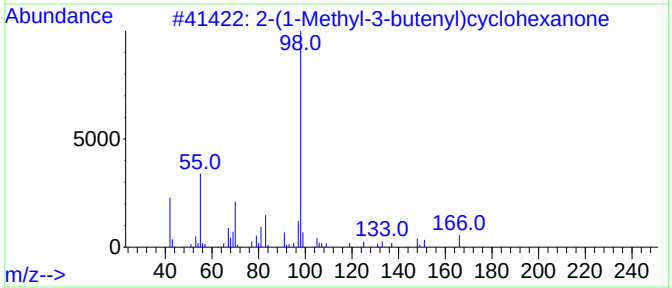
Peak Number 2 unknown12.574 Concentration Rank 4

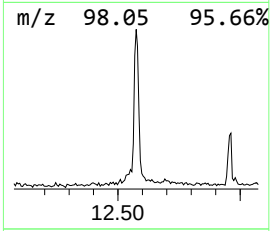
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.574 | 5.34 ng | 209039 | Phenanthrene-d10 | 11.369 |

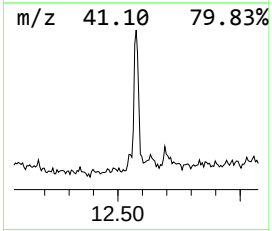
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-(1-Methyl-3-butenyl)cyclohexanone | 166 | C11H18O | 1000424-67-7 | 38 |
| 2 | n-Heptylamine, N-acetyl-1-cyano- | 182 | C10H18N2O | 1000227-03-9 | 38 |
| 3 | Propionamide, 3-(1-piperidyl)- | 156 | C8H16N2O | 004269-30-1 | 38 |
| 4 | 8-Methyl-2-(2-piperidin-1-ylethy... | 311 | C18H21N3S | 1000311-60-9 | 35 |
| 5 | 3-Piperidin-1-yl-propionic acid,... | 171 | C8H17N3O | 1000302-98-0 | 35 |

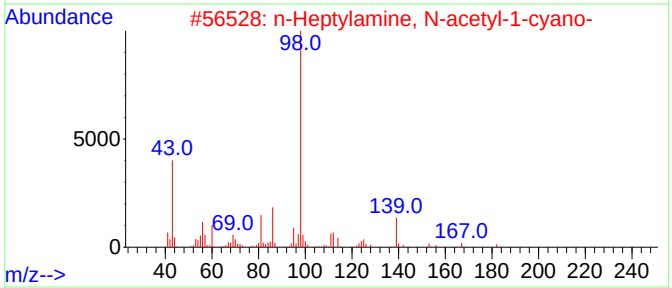


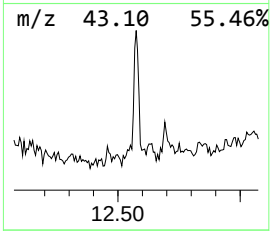



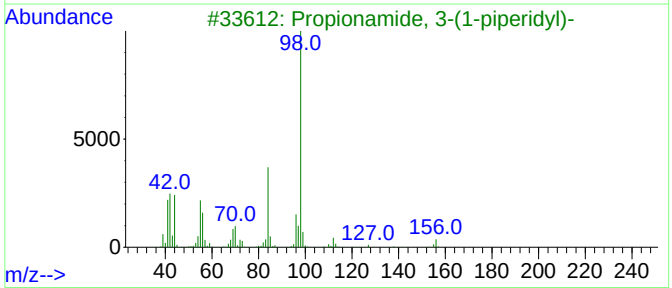



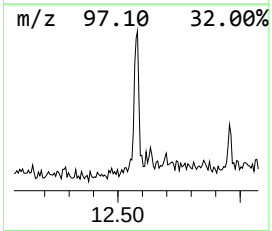



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Data File : BF128608.D
Acq On : 31 May 2022 22:03
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Sample : N2951-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

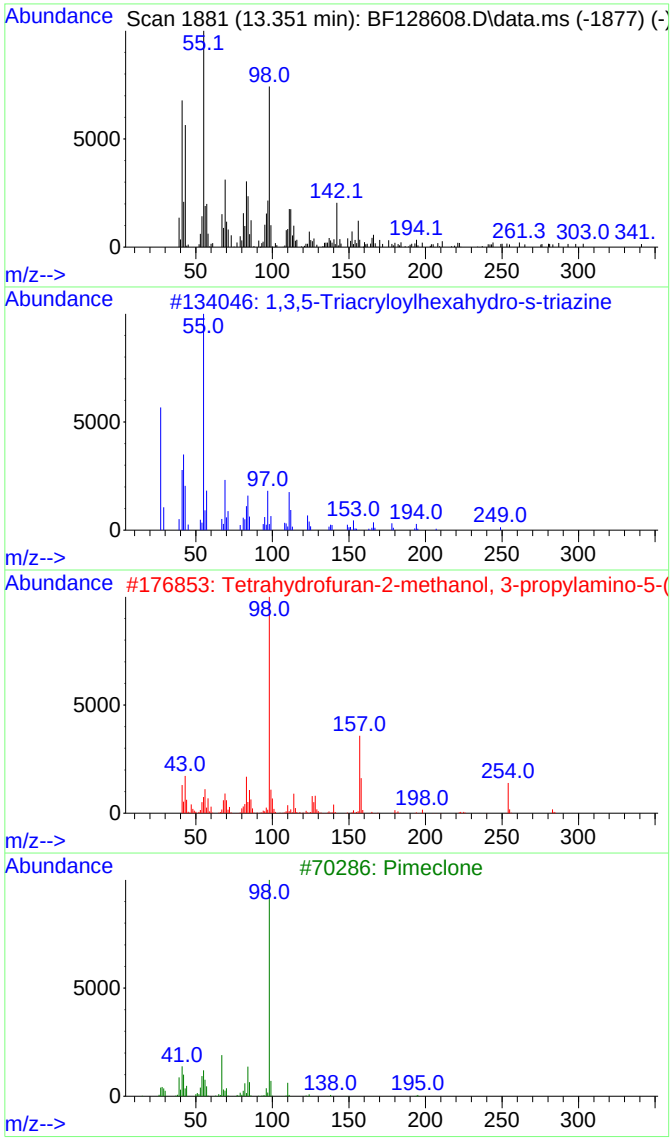
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

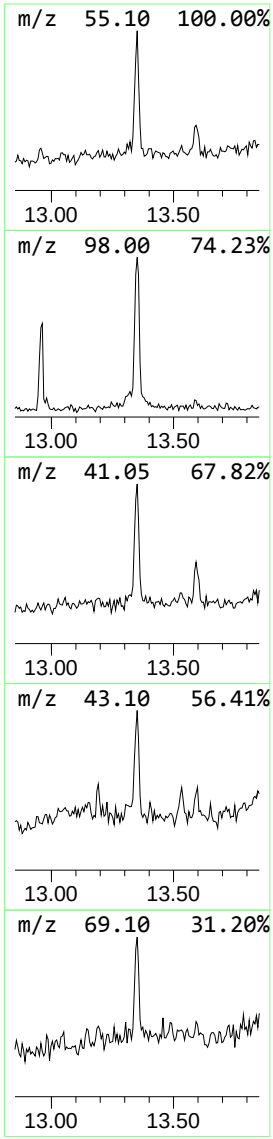
**********

Peak Number 3 unknown13.351 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.351 | 5.35 ng | 151454 | Chrysene-d12 | 14.015 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3,5-Triacryloylhexahydro-s-tri... | 249 | C12H15N3O3 | 000959-52-4 | 48 |
| 2 | Tetrahydrofuran-2-methanol, 3-pr... | 283 | C13H21N3O4 | 1000116-79-8 | 43 |
| 3 | Pimeclone | 195 | C12H21NO | 000534-84-9 | 43 |
| 4 | 1-Cyclopenten-3-one, 1-(ethoxyca... | 170 | C8H10O4 | 1010164-70-4 | 43 |
| 5 | 1H-Imidazole-2-methanol | 98 | C4H6N2O | 003724-26-3 | 38 |



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Sample : N2951-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

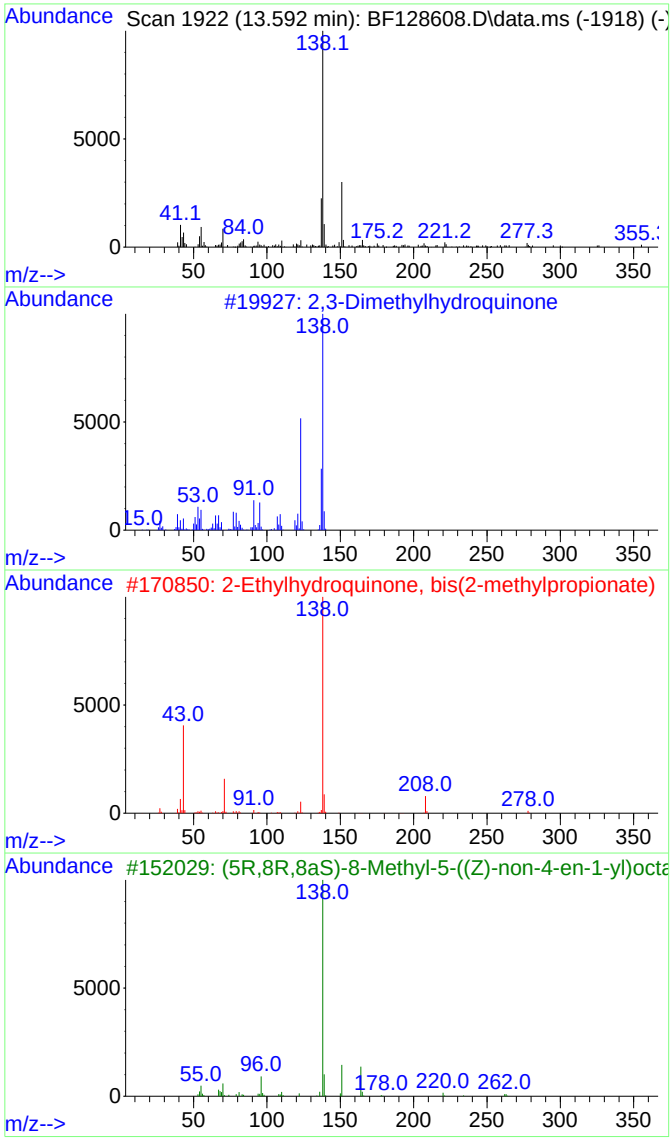
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

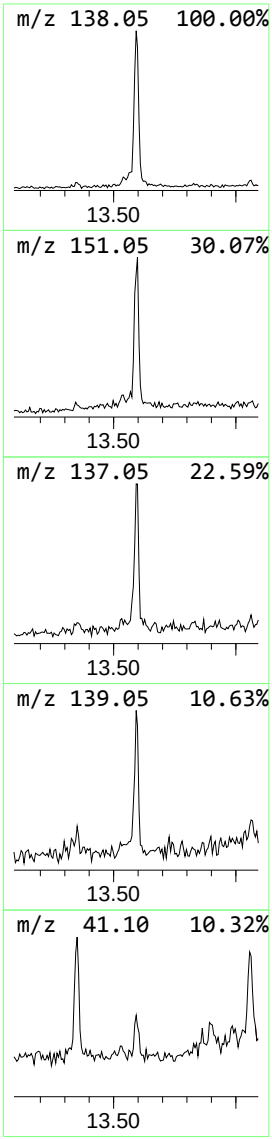
**********

Peak Number 4 2,3-Dimethylhydroquinone Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.592 | 3.70 ng | 104879 | Chrysene-d12 | 14.015 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,3-Dimethylhydroquinone | 138 | C8H10O2 | 000608-43-5 | 59 |
| 2 | 2-Ethylhydroquinone, bis(2-methy... | 278 | C16H22O4 | 1000463-14-5 | 50 |
| 3 | (5R,8R,8aS)-8-Methyl-5-((Z)-non-... | 263 | C18H33N | 1000367-14-0 | 50 |
| 4 | Succinic acid, dec-2-yl 2-methox... | 378 | C22H34O5 | 1000390-96-5 | 50 |
| 5 | Gephyrotoxin 207a | 207 | C14H25N | 141724-48-3 | 49 |



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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
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TIC Integration Parameters: LSCINT.P

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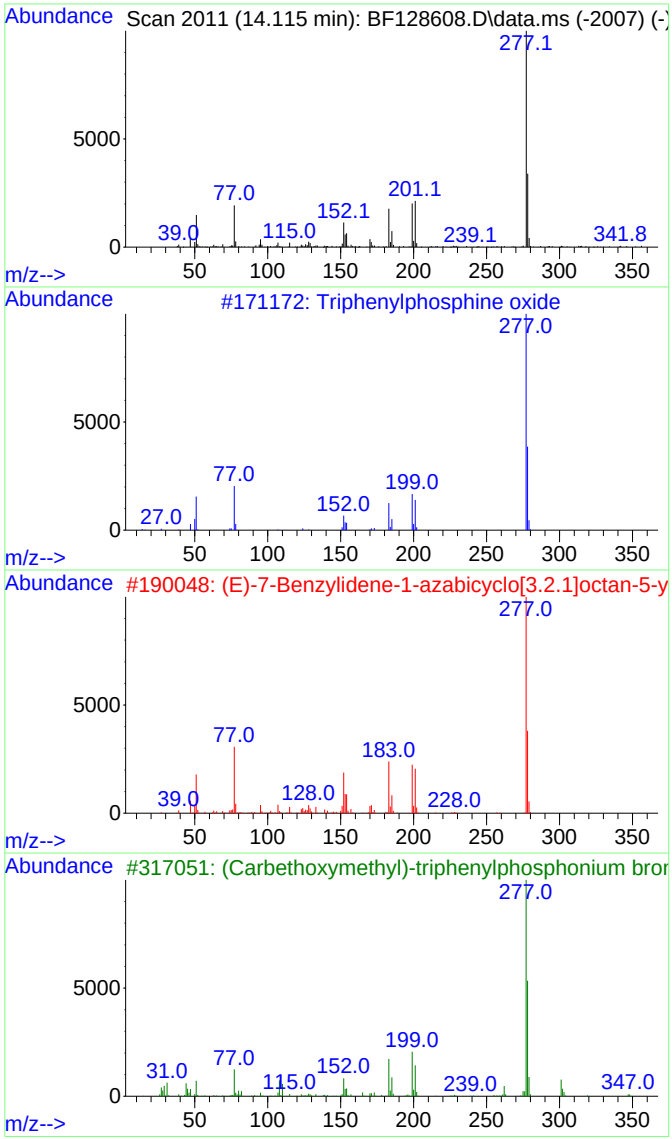
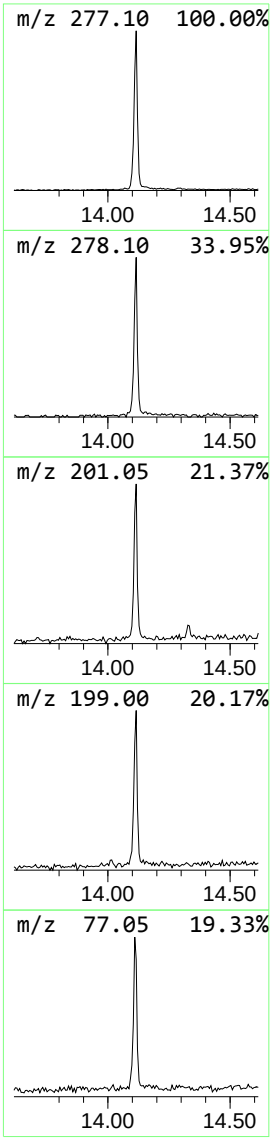
Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.116 | 6.18 ng | 175071 | Chrysene-d12 | 14.015 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 98 |
| 2 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 91 |
| 3 | (Carbethoxymethyl)-triphenylphos... | 428 | C22H22BrO2P | 001530-45-6 | 38 |
| 4 | Cobalt,(.eta.<5>-2,4-cyclopentad... | 277 | C16H15BCo | 036682-12-9 | 35 |
| 5 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 33 |



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Operator : CG\JU
Sample : N2951-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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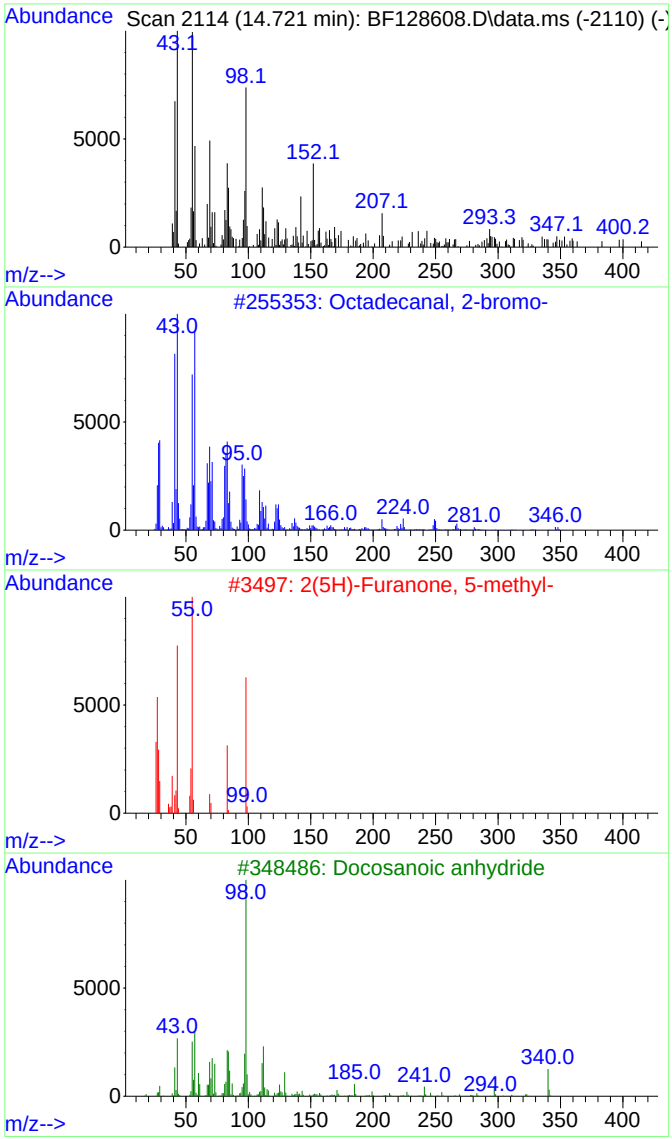
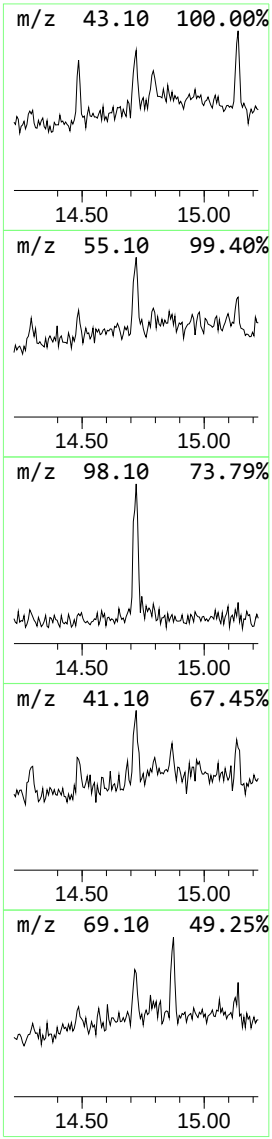
Peak Number 6 Octadecanal, 2-bromo- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.721 | 3.46 ng | 98062 | Chrysene-d12 | 14.015 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanal, 2-bromo- | 346 | C18H35BrO | 056599-95-2 | 51 |
| 2 | 2(5H)-Furanone, 5-methyl- | 98 | C5H6O2 | 000591-11-7 | 38 |
| 3 | Docosanoic anhydride | 663 | C44H86O3 | 055726-23-3 | 38 |
| 4 | 3-(5-Amino-2H-1,2,4-triazol-3-yl... | 142 | C5H10N4O | 018595-97-6 | 38 |
| 5 | N,N'-Dimethyl-5-pyrrolidinone-3-... | 156 | C7H12N2O2 | 089851-99-0 | 38 |



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Sample : N2951-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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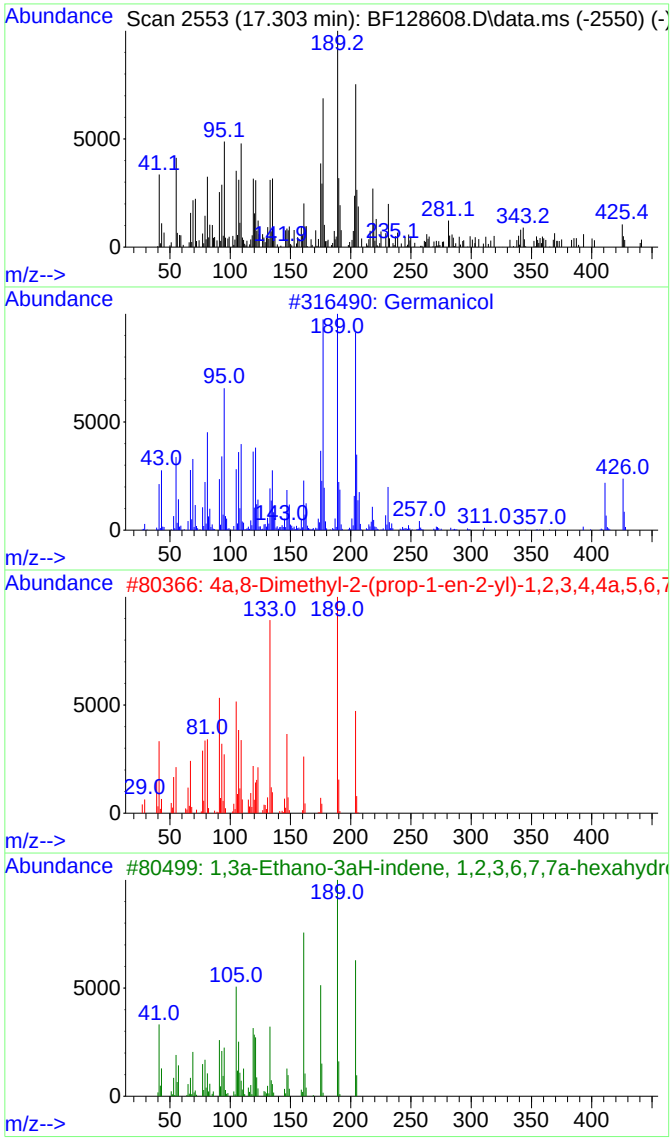
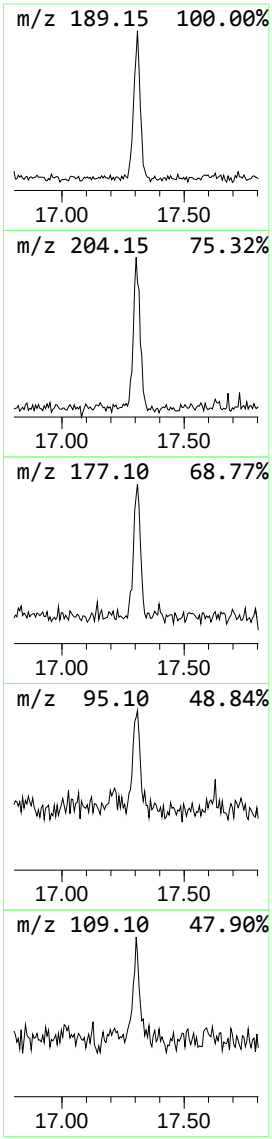
Peak Number 7 Germanicol Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.304 | 8.25 ng | 207806 | Perylene-d12 | 15.486 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Germanicol | 426 | C30H50O | 000465-02-1 | 80 |
| 2 | 4a,8-Dimethyl-2-(prop-1-en-2-yl)... | 204 | C15H24 | 103827-22-1 | 55 |
| 3 | 1,3a-Ethano-3aH-indene, 1,2,3,6,... | 204 | C15H24 | 004545-68-0 | 43 |
| 4 | Naphthalene, 1,2,3,4,4a,5,6,8a-o... | 204 | C15H24 | 000473-13-2 | 38 |
| 5 | 2,3-Dimethoxy-5-aminocinnamonitrile | 204 | C11H12N2O2 | 1000214-46-5 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF053122\
Data File : BF128608.D
Acq On : 31 May 2022 22:03
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Sample : N2951-25
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
P036-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| n-Hexadecanoic ... | 11.904 | 3.0 | ng | 119554 | 4 | 11.369 | 783236 | 20.0 |
| unknown12.574 | 12.574 | 5.3 | ng | 209039 | 4 | 11.369 | 783236 | 20.0 |
| unknown13.351 | 13.351 | 5.3 | ng | 151454 | 5 | 14.015 | 566285 | 20.0 |
| 2,3-Dimethylhyd... | 13.592 | 3.7 | ng | 104879 | 5 | 14.015 | 566285 | 20.0 |
| Triphenylphosph... | 14.116 | 6.2 | ng | 175071 | 5 | 14.015 | 566285 | 20.0 |
| Octadecanal, 2-... | 14.721 | 3.5 | ng | 98062 | 5 | 14.015 | 566285 | 20.0 |
| Germanicol | 17.304 | 8.3 | ng | 207806 | 6 | 15.486 | 503569 | 20.0 |