LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-04-052621

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124105.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.157 | 4 | 12 | 19 | rVB | 513643 | 682513 | 54.27% | 6.269% |
| 2 | 2.269 | 25 | 31 | 35 | rBV2 | 14918 | 19156 | 1.52% | 0.176% |
| 3 | 5.104 | 510 | 513 | 517 | rVB | 24492 | 26990 | 2.15% | 0.248% |
| 4 | 5.504 | 576 | 581 | 584 | rBV | 1135022 | 1101083 | 87.56% | 10.113% |
| 5 | 6.510 | 746 | 752 | 755 | rBV | 1092770 | 1080502 | 85.92% | 9.924% |
| 6 | 6.704 | 782 | 785 | 794 | rBB | 30900 | 29825 | 2.37% | 0.274% |
| 7 | 6.875 | 811 | 814 | 818 | rBV | 352878 | 285068 | 22.67% | 2.618% |
| 8 | 7.439 | 905 | 910 | 913 | rBV | 868778 | 745682 | 59.30% | 6.849% |
| 9 | 8.157 | 1029 | 1032 | 1036 | rBV | 352564 | 314221 | 24.99% | 2.886% |
| 10 | 9.233 | 1211 | 1215 | 1218 | rBV | 1442765 | 1257520 | 100.00% | 11.550% |
| 11 | 9.351 | 1231 | 1235 | 1237 | rBV | 31490 | 29151 | 2.32% | 0.268% |
| 12 | 9.628 | 1279 | 1282 | 1286 | rVB | 47286 | 43383 | 3.45% | 0.398% |
| 13 | 9.775 | 1304 | 1307 | 1311 | rVB2 | 26633 | 20014 | 1.59% | 0.184% |
| 14 | 9.916 | 1327 | 1331 | 1334 | rBV | 449884 | 329255 | 26.18% | 3.024% |
| 15 | 10.704 | 1461 | 1465 | 1468 | rBV | 851394 | 699604 | 55.63% | 6.426% |
| 16 | 10.827 | 1482 | 1486 | 1489 | rBV5 | 10641 | 15576 | 1.24% | 0.143% |
| 17 | 11.404 | 1580 | 1584 | 1586 | rBV | 324276 | 298561 | 23.74% | 2.742% |
| 18 | 11.422 | 1586 | 1587 | 1590 | rVV | 52853 | 36115 | 2.87% | 0.332% |
| 19 | 11.474 | 1593 | 1596 | 1599 | rVB | 22447 | 19116 | 1.52% | 0.176% |
| 20 | 11.927 | 1670 | 1673 | 1677 | rVB2 | 64892 | 54877 | 4.36% | 0.504% |
| 21 | 12.016 | 1685 | 1688 | 1690 | rBV3 | 21244 | 23045 | 1.83% | 0.212% |
| 22 | 12.457 | 1759 | 1763 | 1764 | rBV3 | 18774 | 18987 | 1.51% | 0.174% |
| 23 | 12.492 | 1764 | 1769 | 1774 | rVV6 | 23442 | 42194 | 3.36% | 0.388% |
| 24 | 12.616 | 1786 | 1790 | 1795 | rBV | 203659 | 172110 | 13.69% | 1.581% |
| 25 | 12.710 | 1802 | 1806 | 1809 | rBV2 | 27417 | 27668 | 2.20% | 0.254% |
| 26 | 12.774 | 1814 | 1817 | 1820 | rVV5 | 14567 | 24030 | 1.91% | 0.221% |
| 27 | 12.845 | 1823 | 1829 | 1836 | rVV | 186398 | 208411 | 16.57% | 1.914% |
| 28 | 12.992 | 1850 | 1854 | 1857 | rBV | 1219140 | 1146645 | 91.18% | 10.531% |
| 29 | 13.151 | 1879 | 1881 | 1882 | rBV2 | 16767 | 14882 | 1.18% | 0.137% |
| 30 | 13.174 | 1882 | 1885 | 1888 | rVB3 | 44610 | 41833 | 3.33% | 0.384% |
| 31 | 13.216 | 1888 | 1892 | 1894 | rBV3 | 23998 | 32433 | 2.58% | 0.298% |
| 32 | 13.239 | 1894 | 1896 | 1899 | rVB | 35756 | 32452 | 2.58% | 0.298% |
| 33 | 13.274 | 1899 | 1902 | 1906 | rBV5 | 31311 | 43421 | 3.45% | 0.399% |
| 34 | 13.368 | 1916 | 1918 | 1921 | rVB3 | 18381 | 13941 | 1.11% | 0.128% |
| 35 | 13.398 | 1921 | 1923 | 1924 | rBV2 | 14743 | 14585 | 1.16% | 0.134% |
| 36 | 13.792 | 1988 | 1990 | 1993 | rVB4 | 23398 | 21916 | 1.74% | 0.201% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
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Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-04-052621

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 13.821 | 1993 | 1995 | 1997 | rVB3 | 21917 | 16467 | 1.31% | 0.151% |
| 38 | 13.845 | 1997 | 1999 | 2002 | rBV3 | 22962 | 20273 | 1.61% | 0.186% |
| 39 | 13.892 | 2004 | 2007 | 2016 | rVB3 | 119591 | 233311 | 18.55% | 2.143% |
| 40 | 14.045 | 2027 | 2033 | 2035 | rBV2 | 405086 | 494363 | 39.31% | 4.541% |
| 41 | 14.068 | 2035 | 2037 | 2040 | rVB | 127667 | 100277 | 7.97% | 0.921% |
| 42 | 14.151 | 2048 | 2051 | 2055 | rBV6 | 24891 | 37179 | 2.96% | 0.341% |
| 43 | 14.186 | 2055 | 2057 | 2060 | rBV4 | 23518 | 28190 | 2.24% | 0.259% |
| 44 | 15.098 | 2208 | 2212 | 2215 | rBV | 139288 | 224527 | 17.85% | 2.062% |
| 45 | 15.404 | 2261 | 2264 | 2268 | rVB | 67838 | 82588 | 6.57% | 0.759% |
| 46 | 15.468 | 2271 | 2275 | 2281 | rBV | 139158 | 206311 | 16.41% | 1.895% |
| 47 | 15.533 | 2282 | 2286 | 2289 | rBV2 | 204917 | 242594 | 19.29% | 2.228% |
| 48 | 16.704 | 2480 | 2485 | 2488 | rBV7 | 34640 | 59833 | 4.76% | 0.550% |
| 49 | 17.027 | 2536 | 2540 | 2547 | rVB3 | 56846 | 107599 | 8.56% | 0.988% |
| 50 | 17.480 | 2613 | 2617 | 2622 | rVB2 | 36297 | 67492 | 5.37% | 0.620% |

Sum of corrected areas: 10887769

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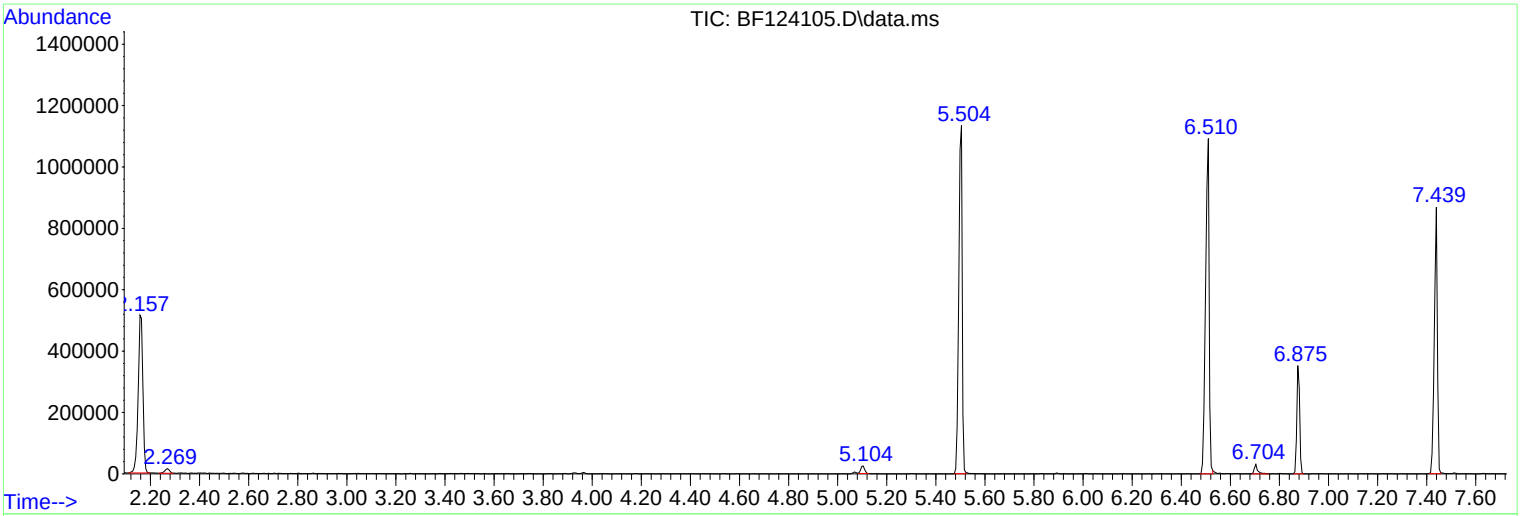
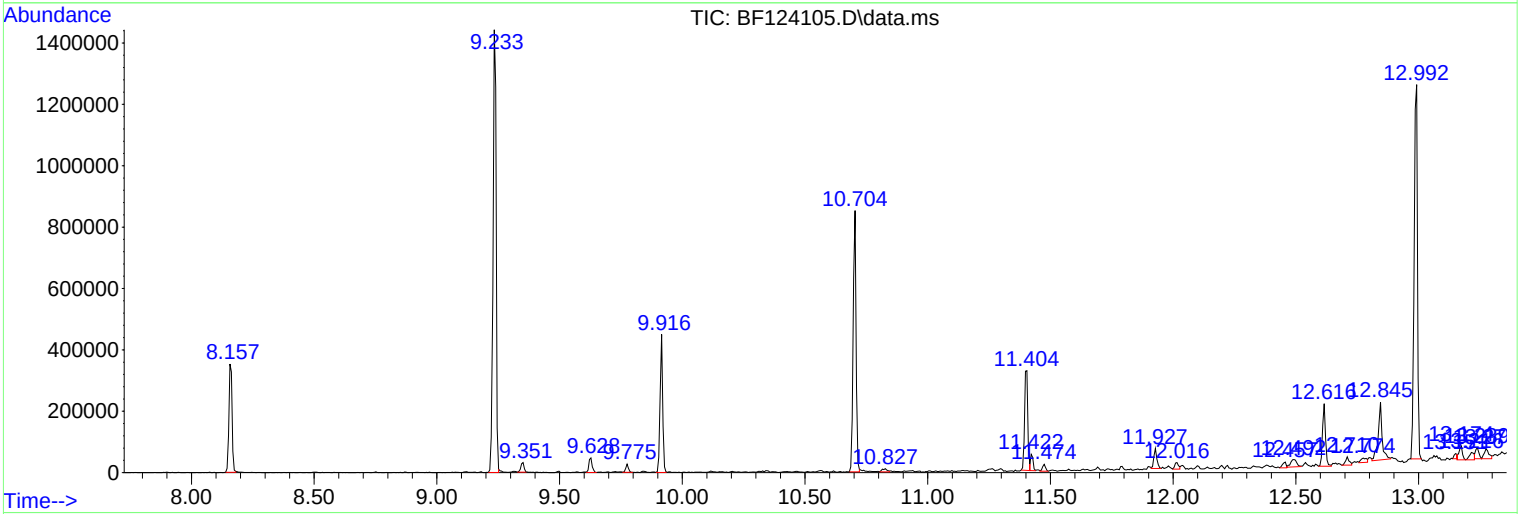
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

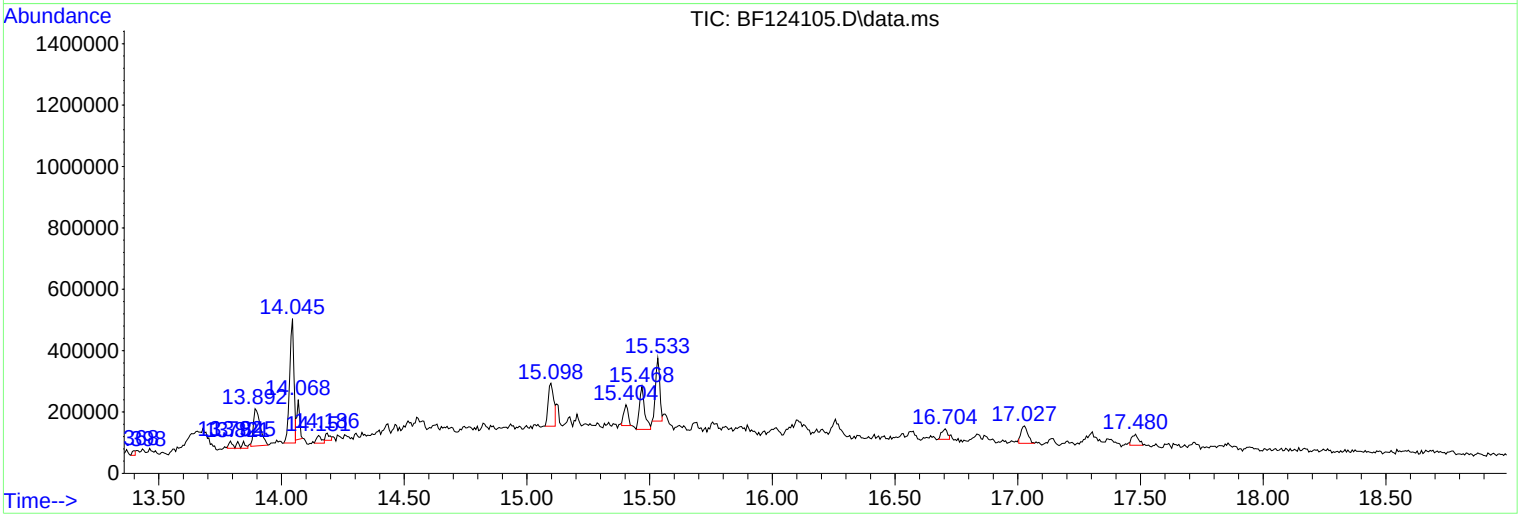
**Instrument :**
BNA_F
**ClientSampleId :**
SU-04-052621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SU-04-052621

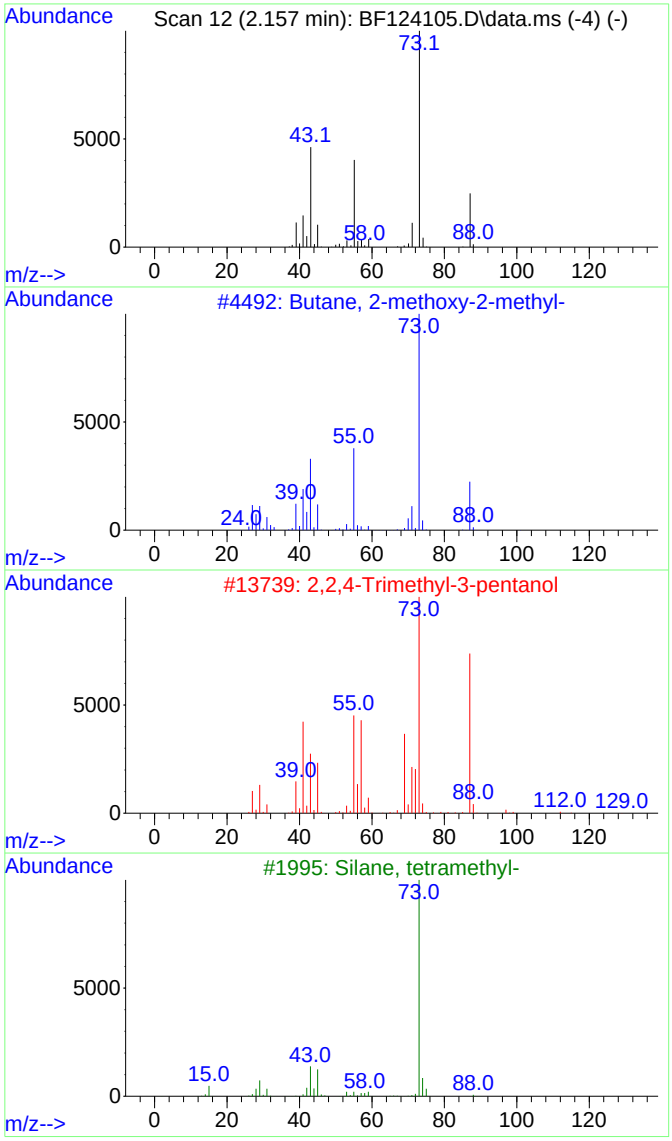
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

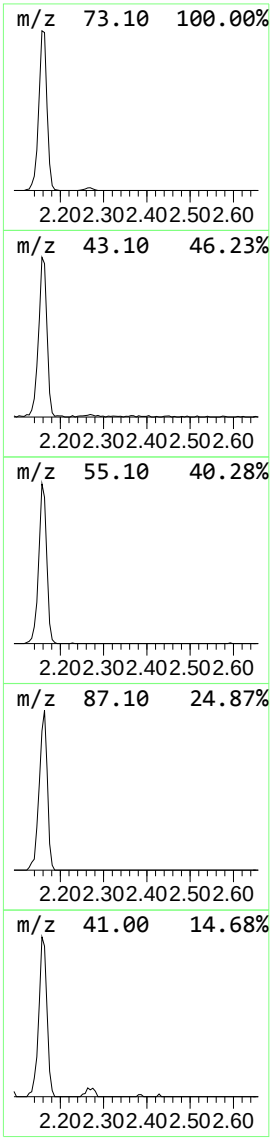
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.157 | 47.88 ng | 682513 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 72 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 38 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SU-04-052621

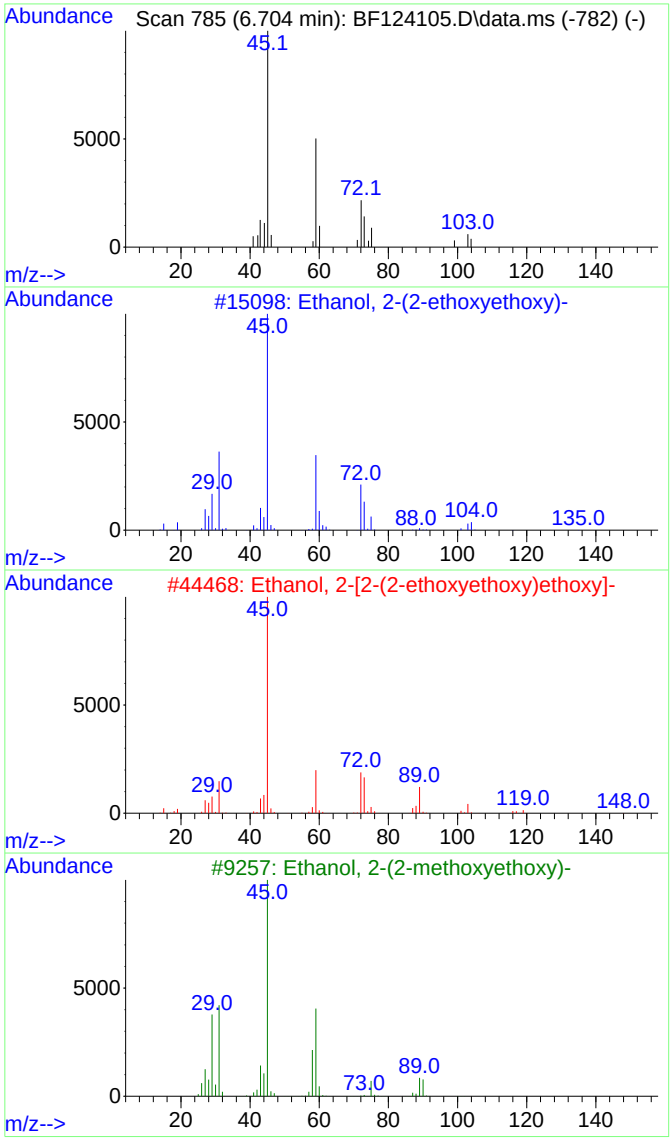
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

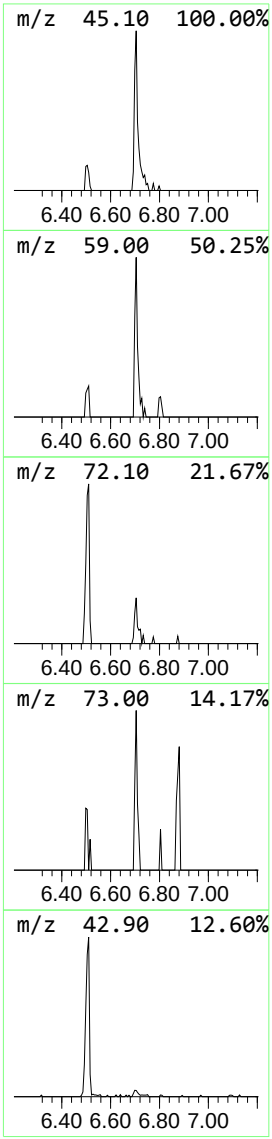
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.704 | 2.09 ng | 29825 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-ethoxyethoxy)- | 134 | C6H14O3 | 000111-90-0 | 72 |
| 2 | Ethanol, 2-[2-(2-ethoxyethoxy)et... | 178 | C8H18O4 | 000112-50-5 | 38 |
| 3 | Ethanol, 2-(2-methoxyethoxy)- | 120 | C5H12O3 | 000111-77-3 | 38 |
| 4 | Diethyl carbitol | 162 | C8H18O3 | 000112-36-7 | 38 |
| 5 | 2-Propanol, 1-(1-methylethoxy)- | 118 | C6H14O2 | 003944-36-3 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SU-04-052621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

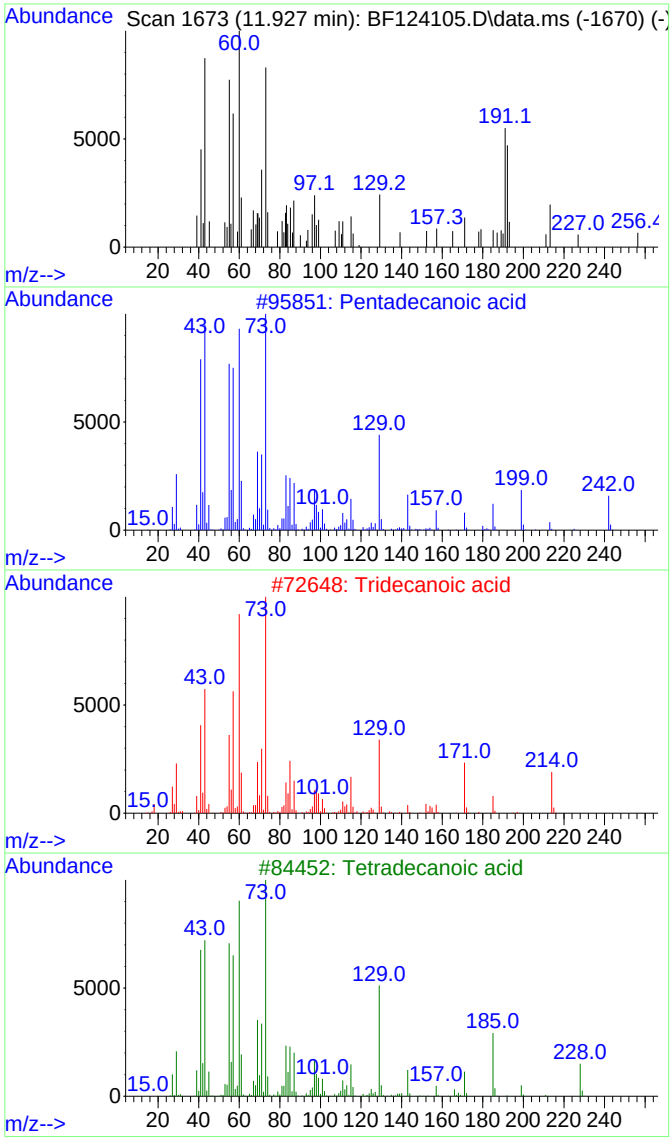
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

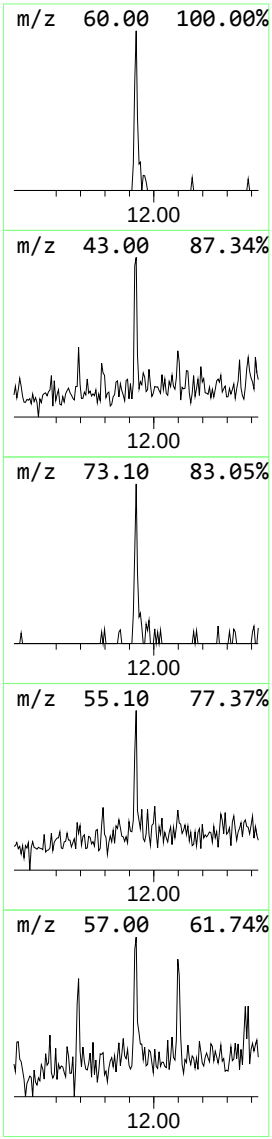
**********

Peak Number 3 unknown11.927 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.927 | 3.68 ng | 54877 | Phenanthrene-d10 | 11.404 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 46 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 43 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 43 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 38 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SU-04-052621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

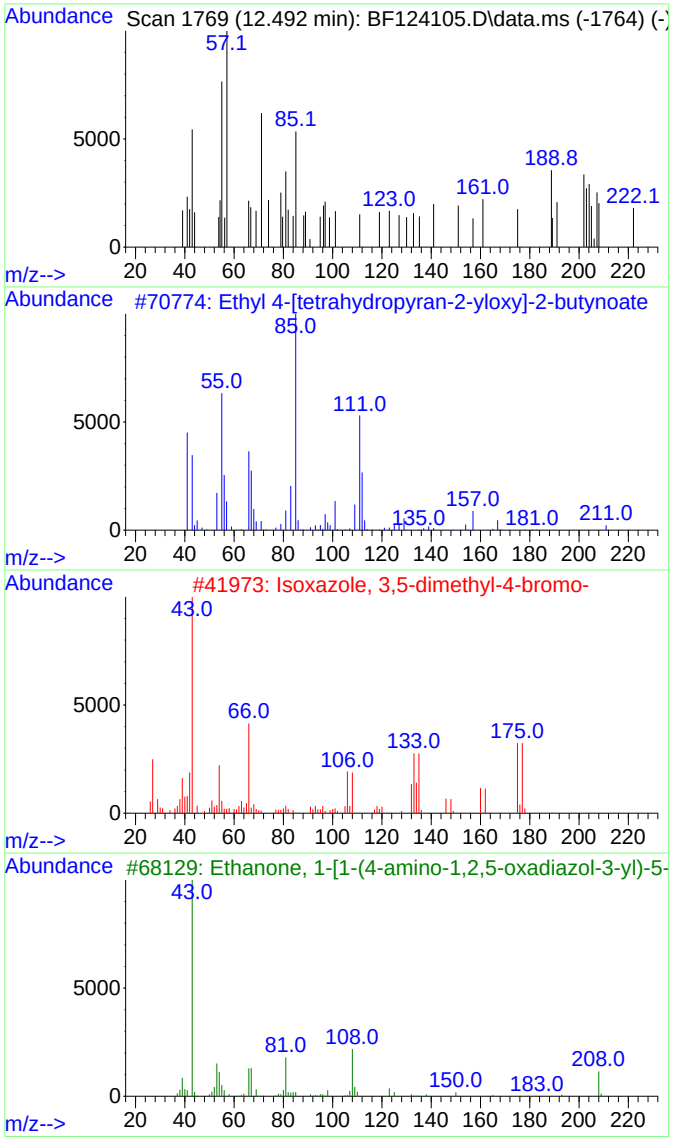
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

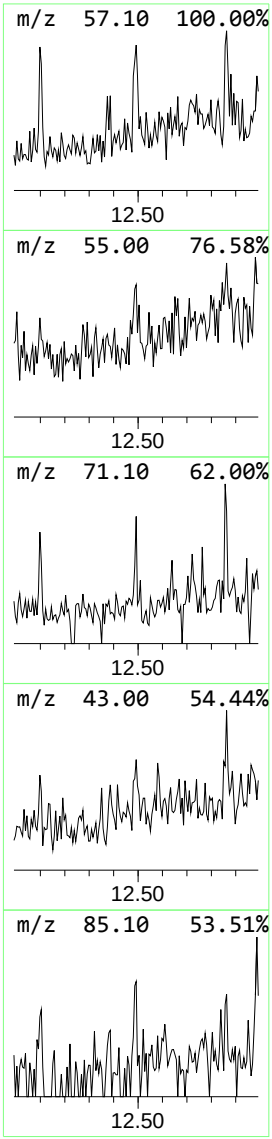
**********

Peak Number 4 unknown12.492 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.492 | 2.83 ng | 42194 | Phenanthrene-d10 | 11.404 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethyl 4-[tetrahydropyran-2-yloxy... | 212 | C11H16O4 | 031555-03-0 | 16 |
| 2 | Isoxazole, 3,5-dimethyl-4-bromo- | 175 | C5H6BrNO | 010558-25-5 | 11 |
| 3 | Ethanone, 1-[1-(4-amino-1,2,5-ox... | 208 | C7H8N6O2 | 313952-93-1 | 10 |
| 4 | 4-(6,6-Dimethyl-2-methylene-cycl... | 204 | C14H20O | 1000192-39-8 | 9 |
| 5 | (+-)-cis-3,4-Dimethyl-2-phenylte... | 207 | C12H17NS | 092772-63-9 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
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Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
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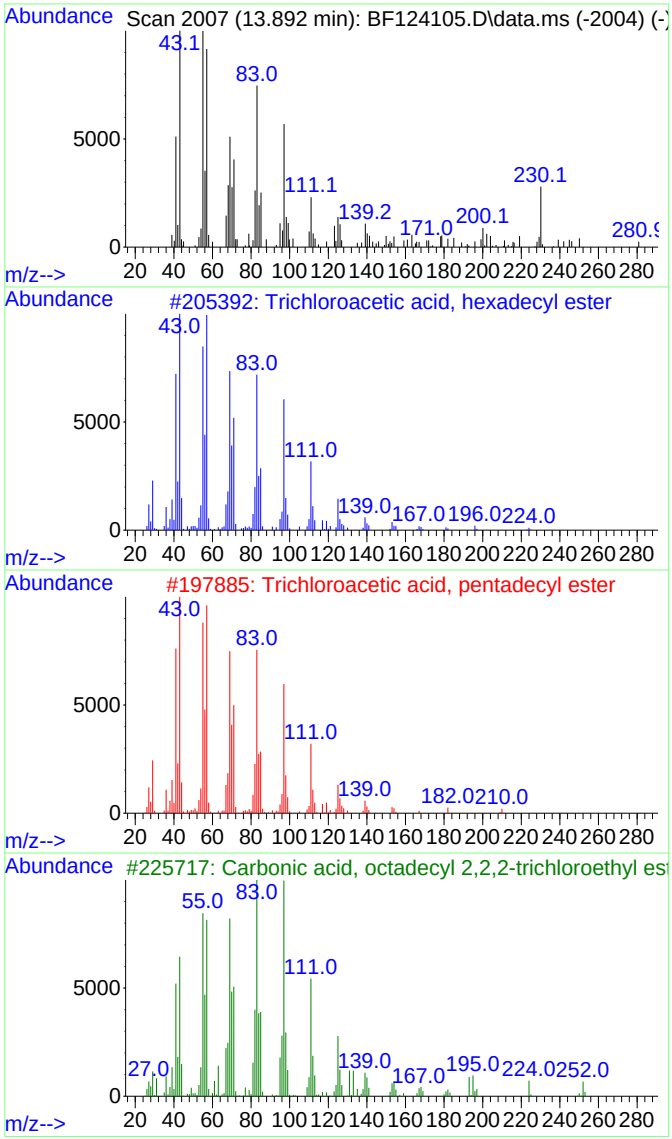
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

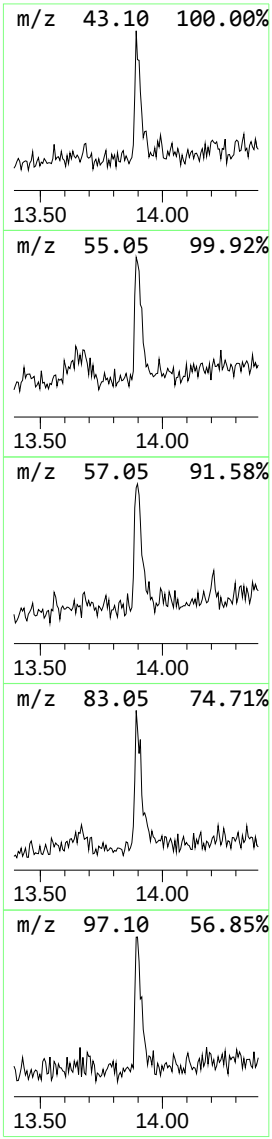
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.892 | 9.44 ng | 233311 | Chrysene-d12 | 14.045 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 83 |
| 2 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 83 |
| 3 | Carbonic acid, octadecyl 2,2,2-t... | 444 | C21H39Cl3O3 | 1000314-56-3 | 83 |
| 4 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 80 |
| 5 | Octacosanol | 410 | C28H58O | 000557-61-9 | 80 |



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Data File : BF124105.D
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Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SU-04-052621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

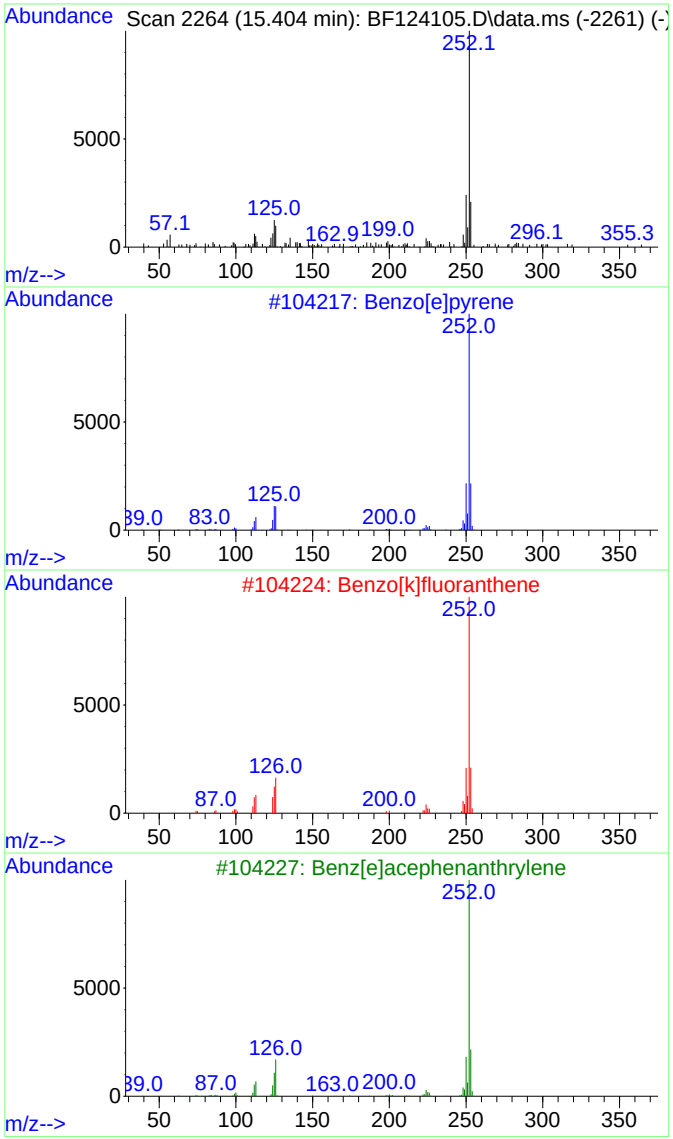
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

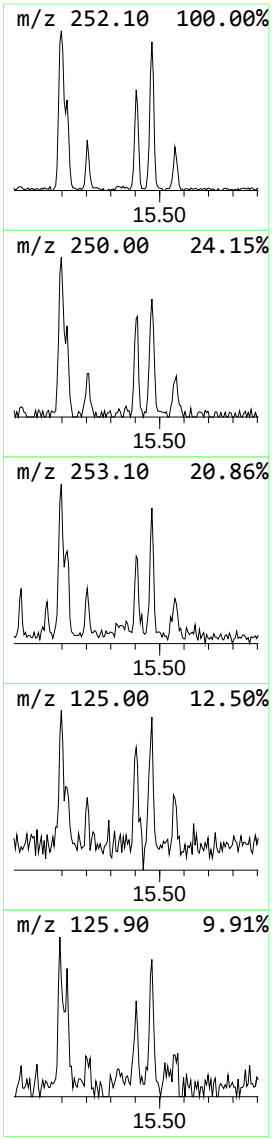
**********

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.404 | 6.81 ng | 82588 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 91 |
| 2 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 81 |
| 3 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 76 |
| 4 | Benzo[j]fluoranthene | 252 | C20H12 | 000205-82-3 | 74 |
| 5 | Perylene | 252 | C20H12 | 000198-55-0 | 74 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SU-04-052621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

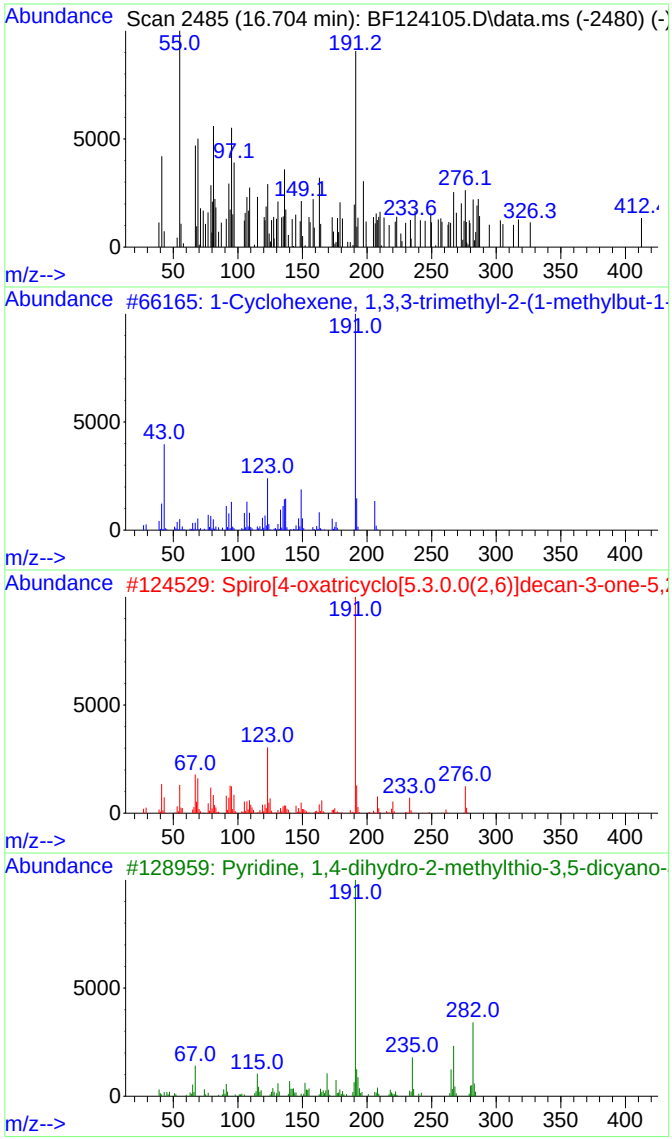
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

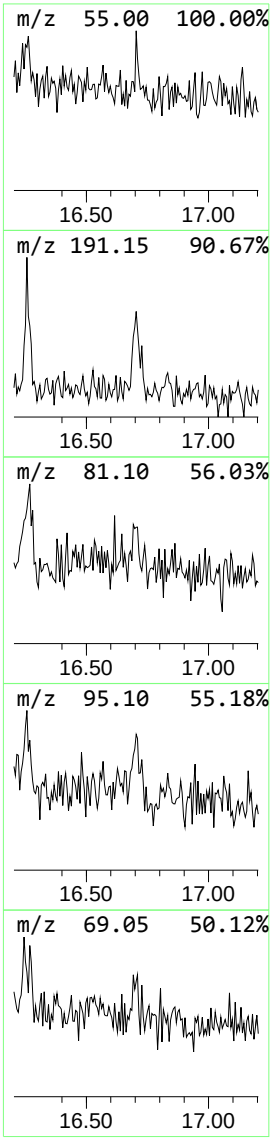
**********

Peak Number 7 unknown16.704 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.704 | 4.93 ng | 59833 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Cyclohexene, 1,3,3-trimethyl-2... | 206 | C14H22O | 1000197-08-4 | 38 |
| 2 | Spiro[4-oxatricyclo[5.3.0.0(2,6)... | 276 | C18H28O2 | 1000156-82-9 | 22 |
| 3 | Pyridine, 1,4-dihydro-2-methylth... | 282 | C15H14N4S | 202405-67-2 | 22 |
| 4 | 2-Fluoro-6-trifluoromethylbenzoi... | 418 | C23H34F4O2 | 1000338-54-0 | 22 |
| 5 | Isophthalic acid, neopentyl prop... | 278 | C16H22O4 | 1000343-85-9 | 18 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052721\
Data File : BF124105.D
Acq On : 27 May 2021 22:09
Operator : JU/CG
Sample : M2531-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-04-052621

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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 |
| Butane, 2-metho... | 2.157 | 47.9 | ng | 682513 | 1 | 6.875 | 285068 | 20.0 |
| Ethanol, 2-(2-e... | 6.704 | 2.1 | ng | 29825 | 1 | 6.875 | 285068 | 20.0 |
| unknown11.927 | 11.927 | 3.7 | ng | 54877 | 4 | 11.404 | 298561 | 20.0 |
| unknown12.492 | 12.492 | 2.8 | ng | 42194 | 4 | 11.404 | 298561 | 20.0 |
| Trichloroacetic... | 13.892 | 9.4 | ng | 233311 | 5 | 14.045 | 494363 | 20.0 |
| Benzo[e]pyrene | 15.404 | 6.8 | ng | 82588 | 6 | 15.533 | 242594 | 20.0 |
| unknown16.704 | 16.704 | 4.9 | ng | 59833 | 6 | 15.533 | 242594 | 20.0 |