LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

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-BF111319.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 | 2.210 | 14 | 21 | 28 | rVB | 733601 | 939488 | 20.57% | 2.189% |
| 2 | 3.669 | 264 | 269 | 284 | rBV | 56585 | 83536 | 1.83% | 0.195% |
| 3 | 4.528 | 406 | 415 | 418 | rBV | 3303787 | 3990264 | 87.36% | 9.297% |
| 4 | 5.139 | 509 | 519 | 522 | rBV | 2072287 | 2669072 | 58.43% | 6.219% |
| 5 | 5.522 | 580 | 584 | 588 | rBV | 840207 | 694524 | 15.21% | 1.618% |
| 6 | 6.533 | 751 | 756 | 769 | rBV | 2796185 | 2995297 | 65.58% | 6.979% |
| 7 | 6.681 | 777 | 781 | 784 | rBV | 1991818 | 1846854 | 40.43% | 4.303% |
| 8 | 6.916 | 817 | 821 | 824 | rBV | 1490037 | 1246545 | 27.29% | 2.904% |
| 9 | 7.069 | 843 | 847 | 851 | rBV | 3406534 | 3196210 | 69.97% | 7.447% |
| 10 | 7.233 | 871 | 875 | 878 | rBV | 92323 | 81372 | 1.78% | 0.190% |
| 11 | 7.475 | 911 | 916 | 919 | rBV | 2745731 | 2548260 | 55.79% | 5.938% |
| 12 | 8.204 | 1035 | 1040 | 1043 | rBV | 1904555 | 1708888 | 37.41% | 3.982% |
| 13 | 9.280 | 1218 | 1223 | 1226 | rBV | 5325554 | 4567661 | 100.00% | 10.643% |
| 14 | 9.674 | 1286 | 1290 | 1293 | rBV | 283372 | 243207 | 5.32% | 0.567% |
| 15 | 9.963 | 1335 | 1339 | 1343 | rBV | 2288183 | 1922100 | 42.08% | 4.479% |
| 16 | 10.751 | 1467 | 1473 | 1477 | rBV | 199539 | 170073 | 3.72% | 0.396% |
| 17 | 10.857 | 1487 | 1491 | 1494 | rBV | 118666 | 119008 | 2.61% | 0.277% |
| 18 | 11.457 | 1589 | 1593 | 1595 | rBV | 2250786 | 1857937 | 40.68% | 4.329% |
| 19 | 11.480 | 1595 | 1597 | 1600 | rVV | 405648 | 308210 | 6.75% | 0.718% |
| 20 | 11.527 | 1600 | 1605 | 1609 | rVB3 | 91553 | 108746 | 2.38% | 0.253% |
| 21 | 11.957 | 1672 | 1678 | 1680 | rBV | 56763 | 58646 | 1.28% | 0.137% |
| 22 | 11.986 | 1680 | 1683 | 1686 | rVB | 78205 | 69761 | 1.53% | 0.163% |
| 23 | 12.074 | 1694 | 1698 | 1700 | rBV | 75142 | 96463 | 2.11% | 0.225% |
| 24 | 12.674 | 1796 | 1800 | 1803 | rBV | 635810 | 554157 | 12.13% | 1.291% |
| 25 | 12.904 | 1833 | 1839 | 1845 | rBV | 567908 | 597361 | 13.08% | 1.392% |
| 26 | 13.045 | 1859 | 1863 | 1870 | rVB | 4245785 | 3971489 | 86.95% | 9.254% |
| 27 | 13.121 | 1871 | 1876 | 1880 | rBV2 | 46732 | 74368 | 1.63% | 0.173% |
| 28 | 13.227 | 1892 | 1894 | 1898 | rVB | 70079 | 70080 | 1.53% | 0.163% |
| 29 | 13.333 | 1908 | 1912 | 1915 | rBV2 | 64767 | 69149 | 1.51% | 0.161% |
| 30 | 13.739 | 1977 | 1981 | 1986 | rVB | 56907 | 64185 | 1.41% | 0.150% |
| 31 | 13.851 | 1995 | 2000 | 2003 | rBV2 | 48412 | 76400 | 1.67% | 0.178% |
| 32 | 13.957 | 2013 | 2018 | 2035 | rVB6 | 119350 | 441898 | 9.67% | 1.030% |
| 33 | 14.104 | 2035 | 2043 | 2046 | rBV2 | 1677390 | 1890244 | 41.38% | 4.404% |
| 34 | 14.127 | 2046 | 2047 | 2053 | rVB | 298031 | 214693 | 4.70% | 0.500% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 14.492 | 2104 | 2109 | 2112 | rVB | 61513 | 70238 | 1.54% | 0.164% |
| 36 | 14.574 | 2119 | 2123 | 2128 | rBV4 | 95440 | 111484 | 2.44% | 0.260% |
| 37 | 14.892 | 2173 | 2177 | 2181 | rVB | 113548 | 119856 | 2.62% | 0.279% |
| 38 | 14.968 | 2187 | 2190 | 2193 | rBV3 | 49087 | 63197 | 1.38% | 0.147% |
| 39 | 15.162 | 2218 | 2223 | 2226 | rBV | 257156 | 407260 | 8.92% | 0.949% |
| 40 | 15.245 | 2233 | 2237 | 2240 | rBV | 122256 | 133415 | 2.92% | 0.311% |
| 41 | 15.474 | 2272 | 2276 | 2283 | rVB | 153037 | 214515 | 4.70% | 0.500% |
| 42 | 15.539 | 2283 | 2287 | 2294 | rBV | 168026 | 215711 | 4.72% | 0.503% |
| 43 | 15.609 | 2294 | 2299 | 2303 | rBV | 1132681 | 1448836 | 31.72% | 3.376% |
| 44 | 15.639 | 2303 | 2304 | 2311 | rVB2 | 159195 | 178928 | 3.92% | 0.417% |
| 45 | 16.103 | 2379 | 2383 | 2389 | rVB | 88378 | 129669 | 2.84% | 0.302% |
| 46 | 16.639 | 2469 | 2474 | 2478 | rBV | 42901 | 74011 | 1.62% | 0.172% |
| 47 | 17.127 | 2552 | 2557 | 2566 | rBV2 | 52764 | 105472 | 2.31% | 0.246% |
| 48 | 17.592 | 2632 | 2636 | 2646 | rVB | 47232 | 99088 | 2.17% | 0.231% |

Sum of corrected areas: 42917826

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
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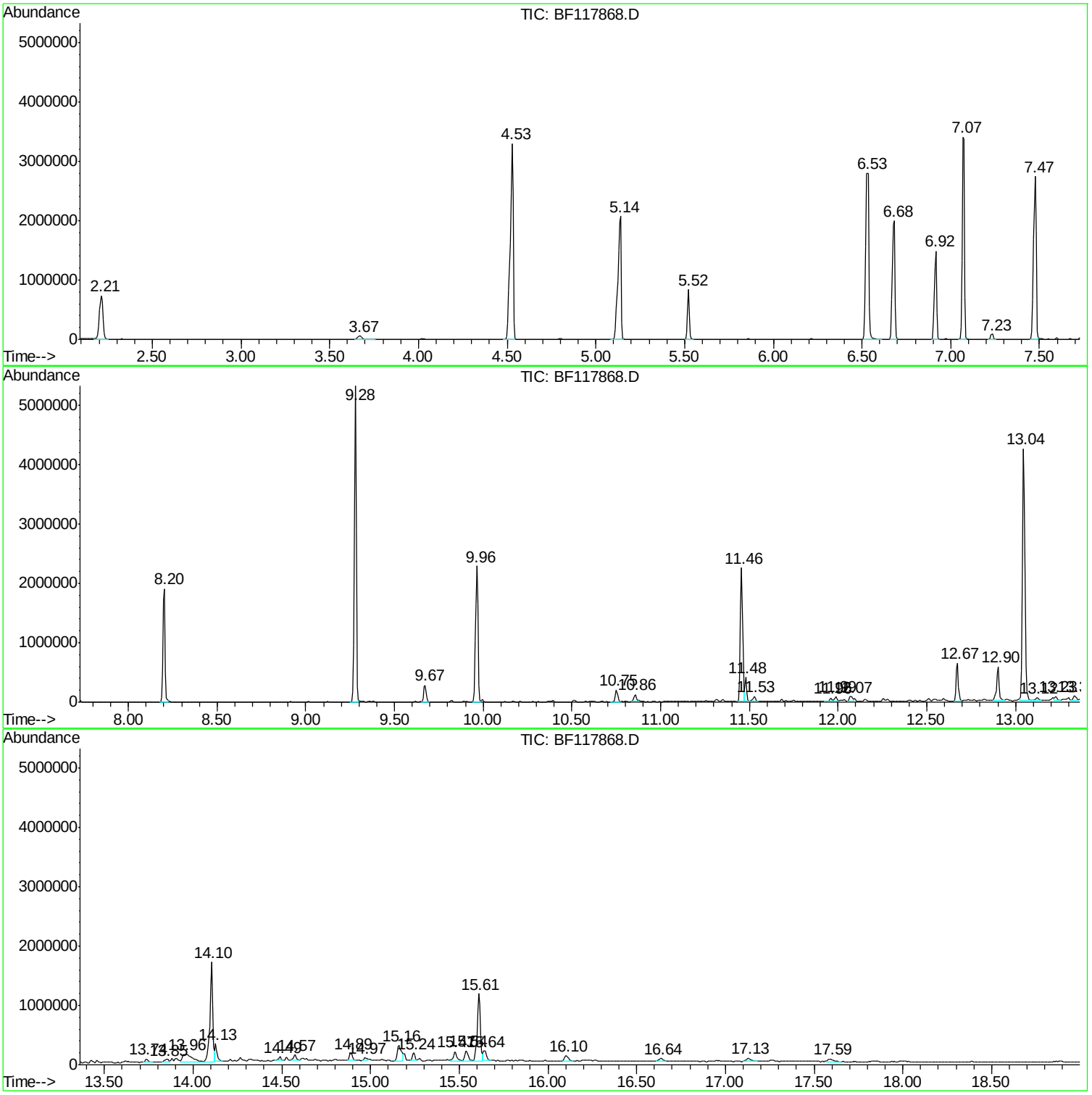
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
14-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

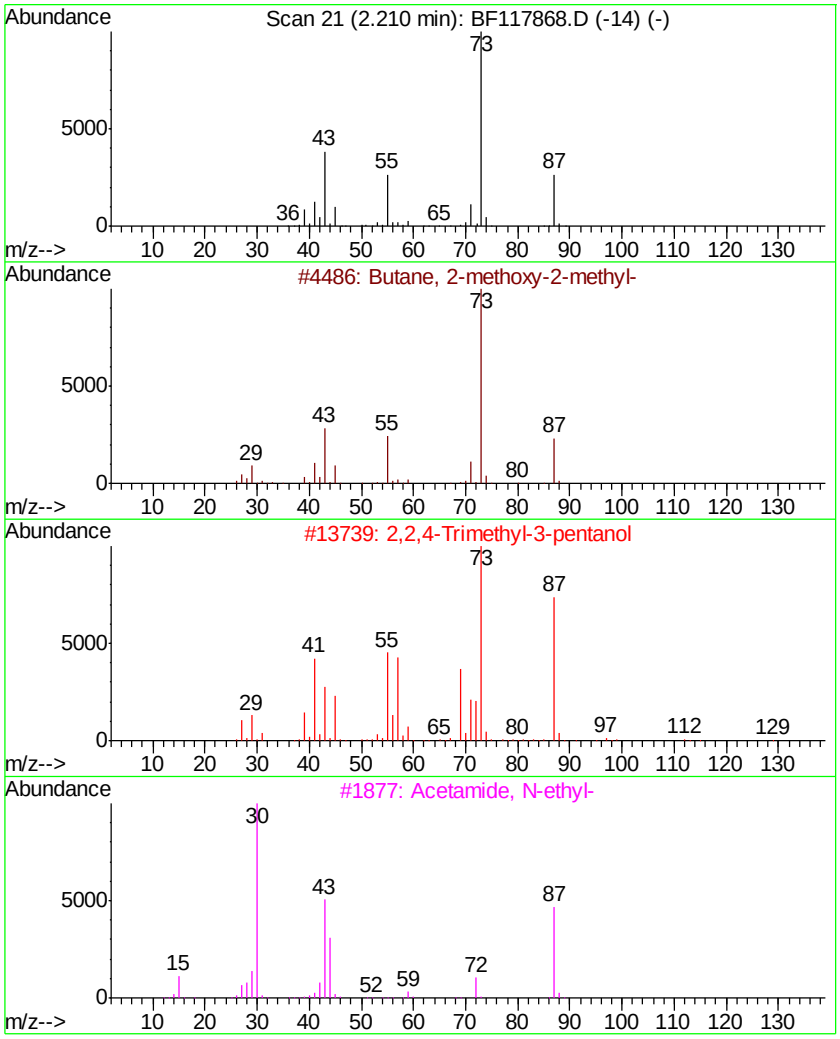
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

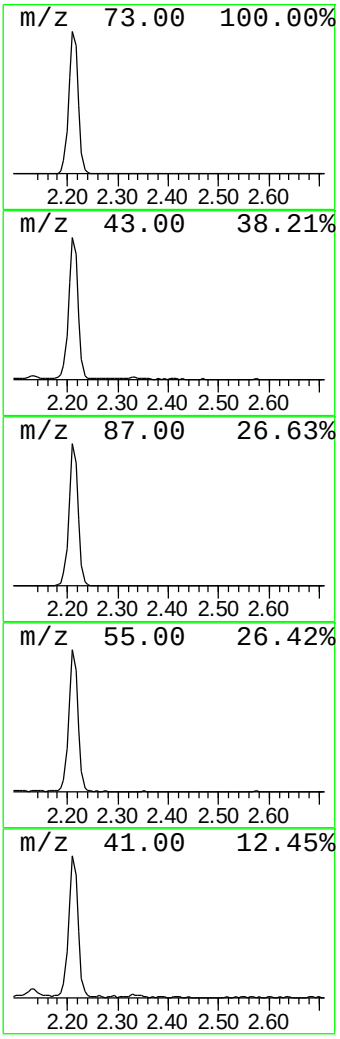
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.21 | 15.07 ng | 939488 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 27 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 5 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 23 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

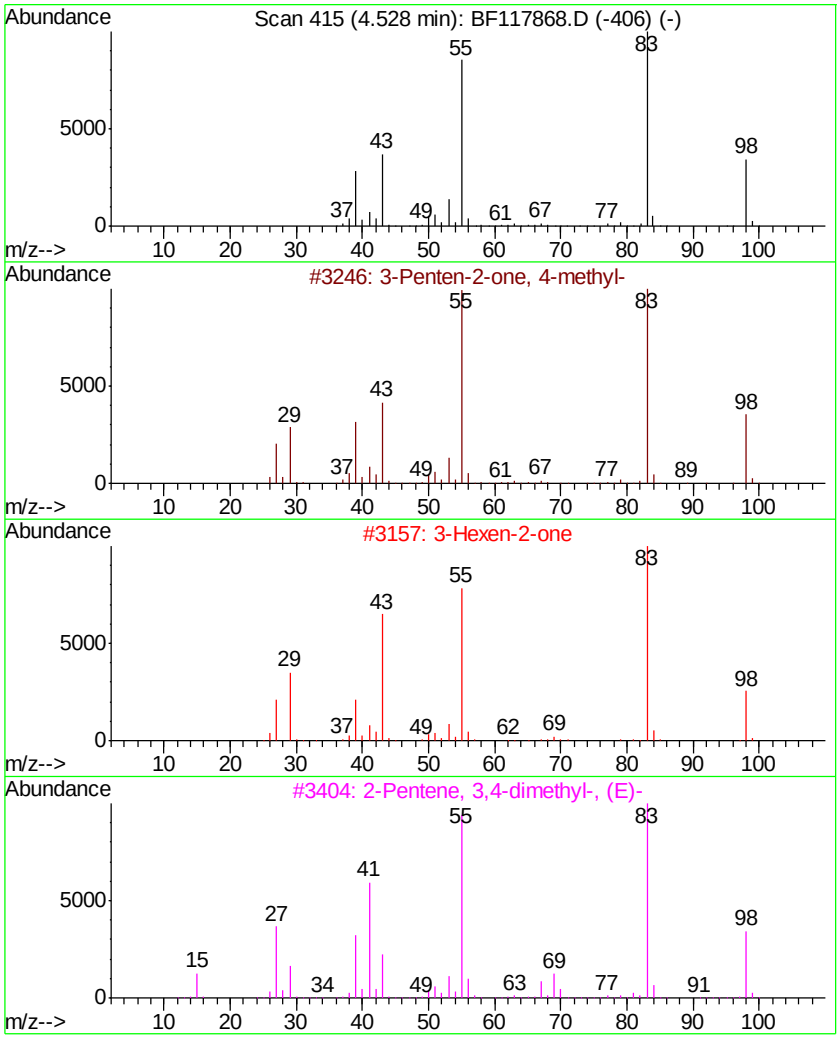
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

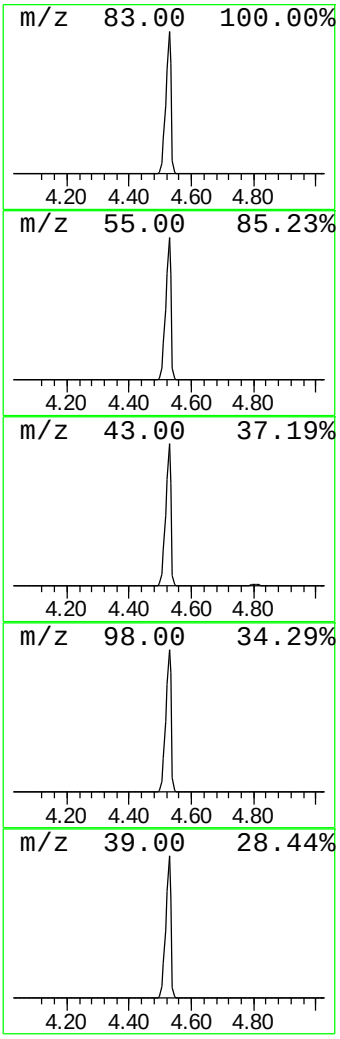
**********

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.53 | 64.02 ng | 3990260 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 95 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 91 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |
| 5 | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14 | 000762-63-0 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

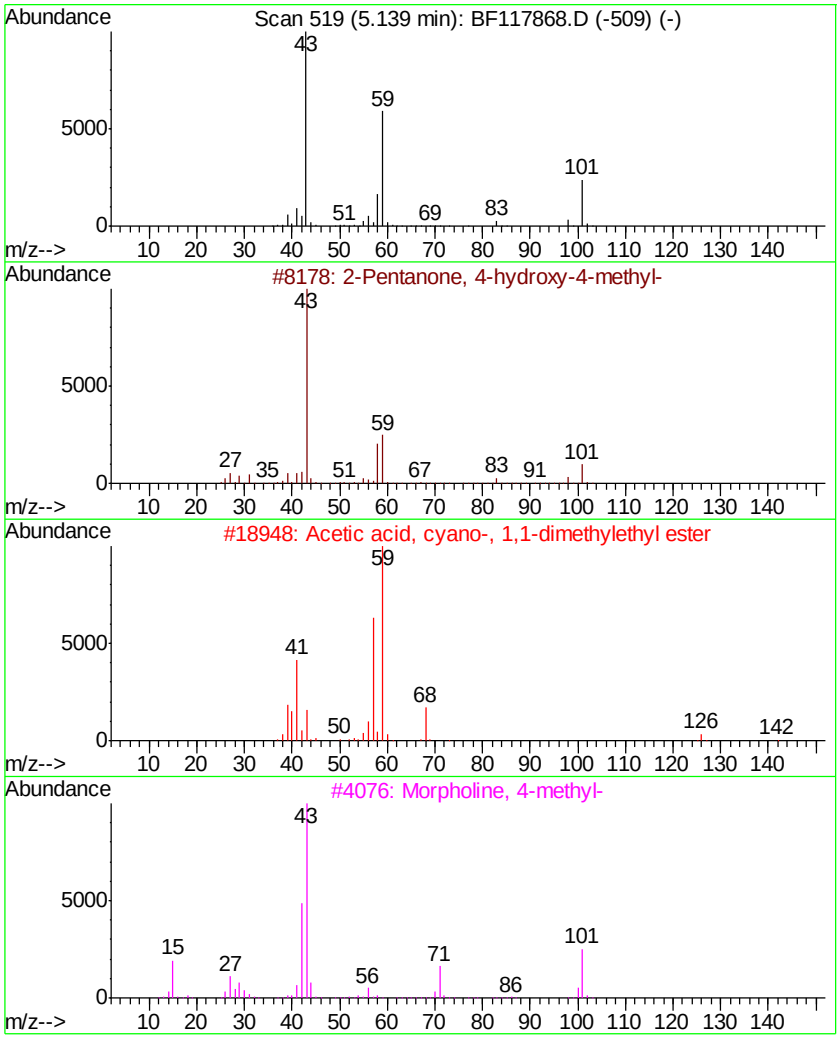
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

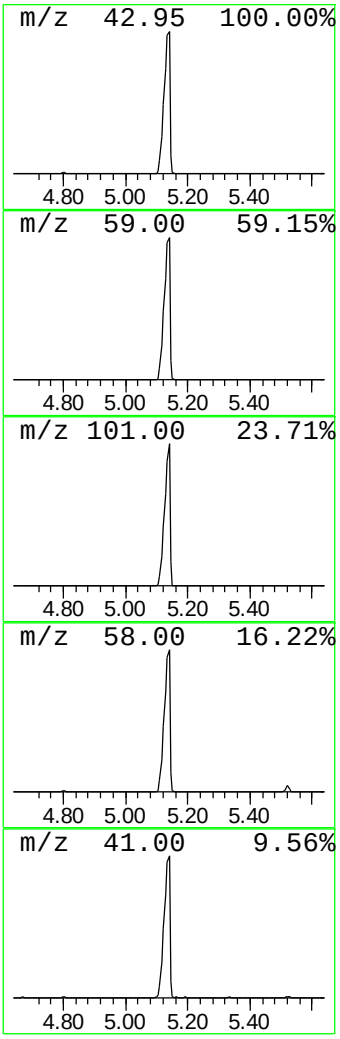
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.14 | 42.82 ng | 2669070 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 5 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

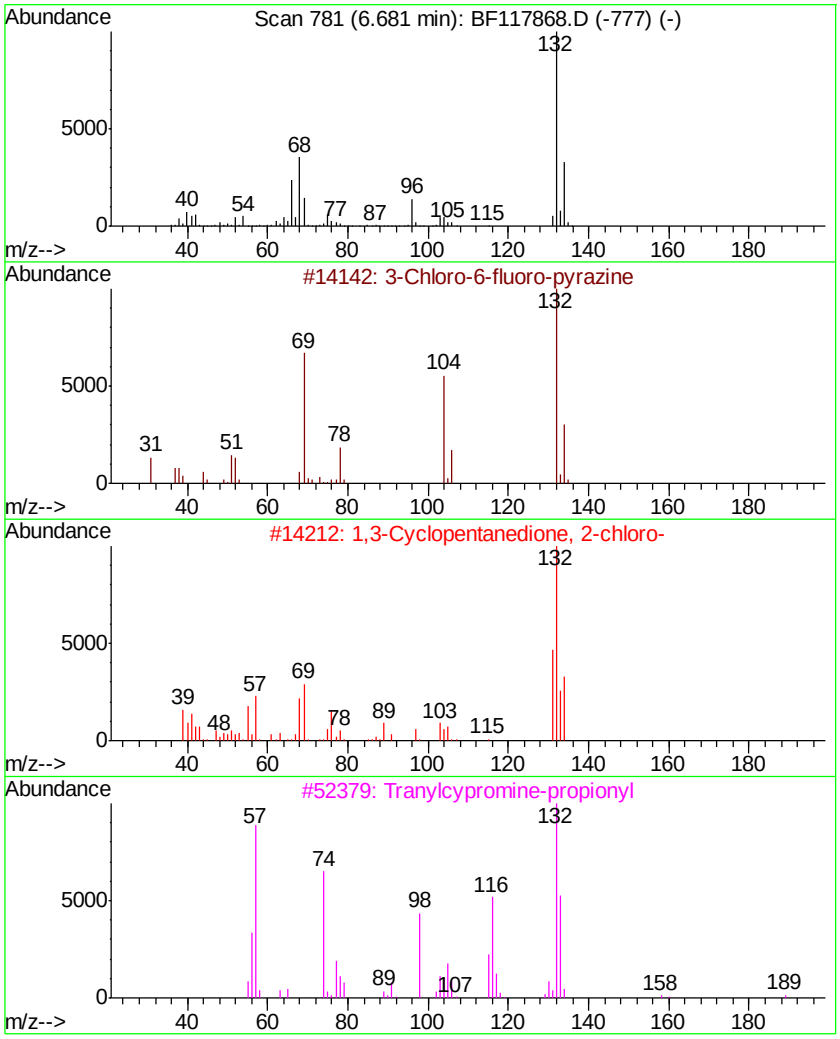
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

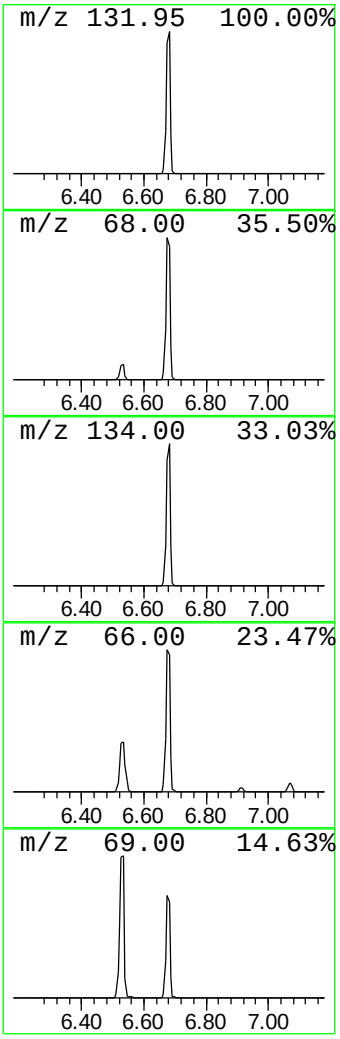
**********

Peak Number 4 unknown6.68 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.68 | 29.63 ng | 1846850 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 23 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
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Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

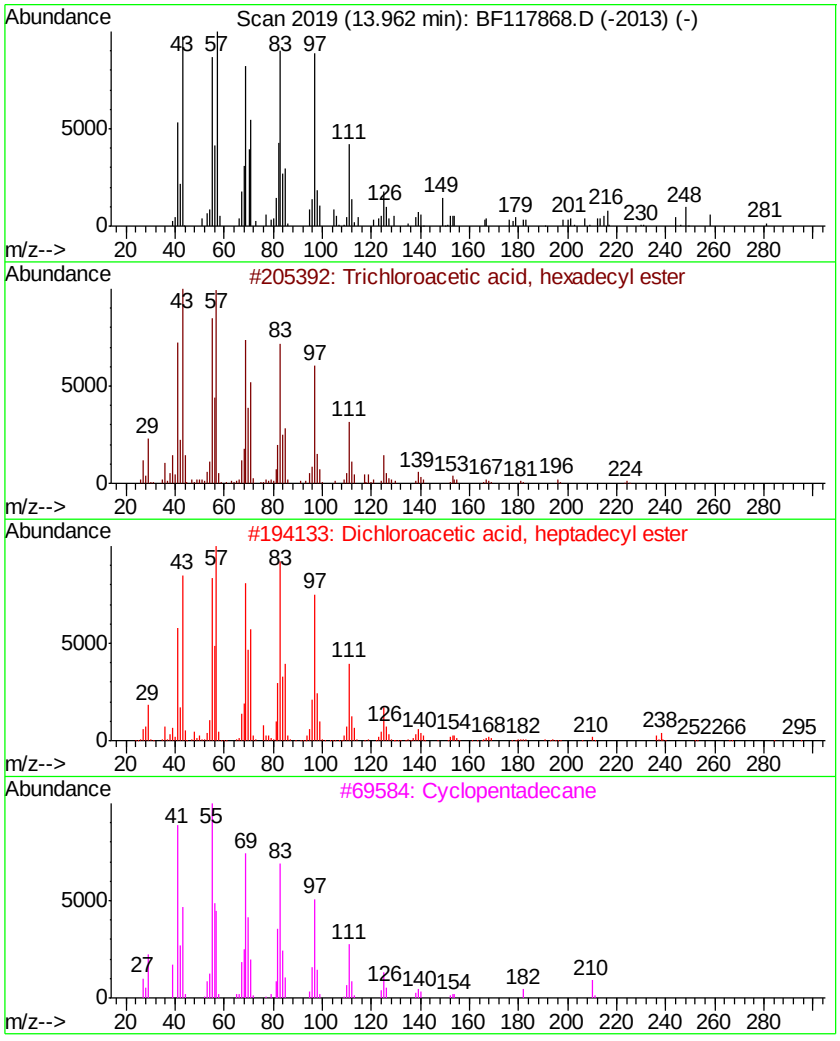
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

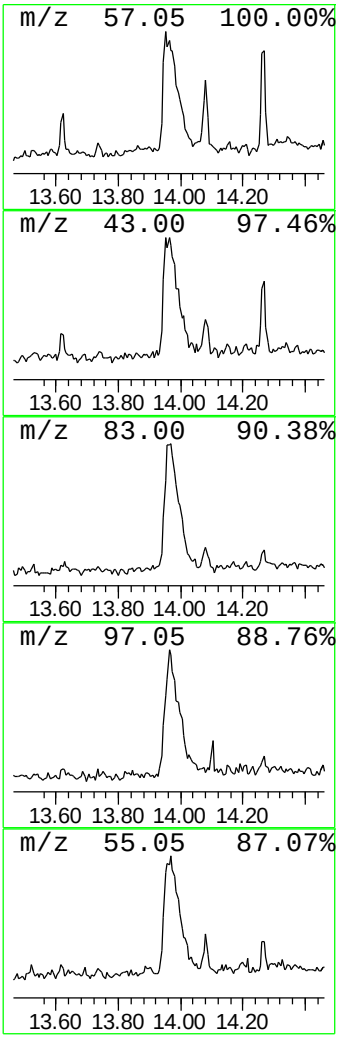
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.96 | 4.68 ng | 441898 | Chrysene-d12 | 14.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 90 |
| 2 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 90 |
| 3 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 89 |
| 4 | 1-Hexacosanol | 382 | C26H54O | 000506-52-5 | 87 |
| 5 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 76 |



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Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

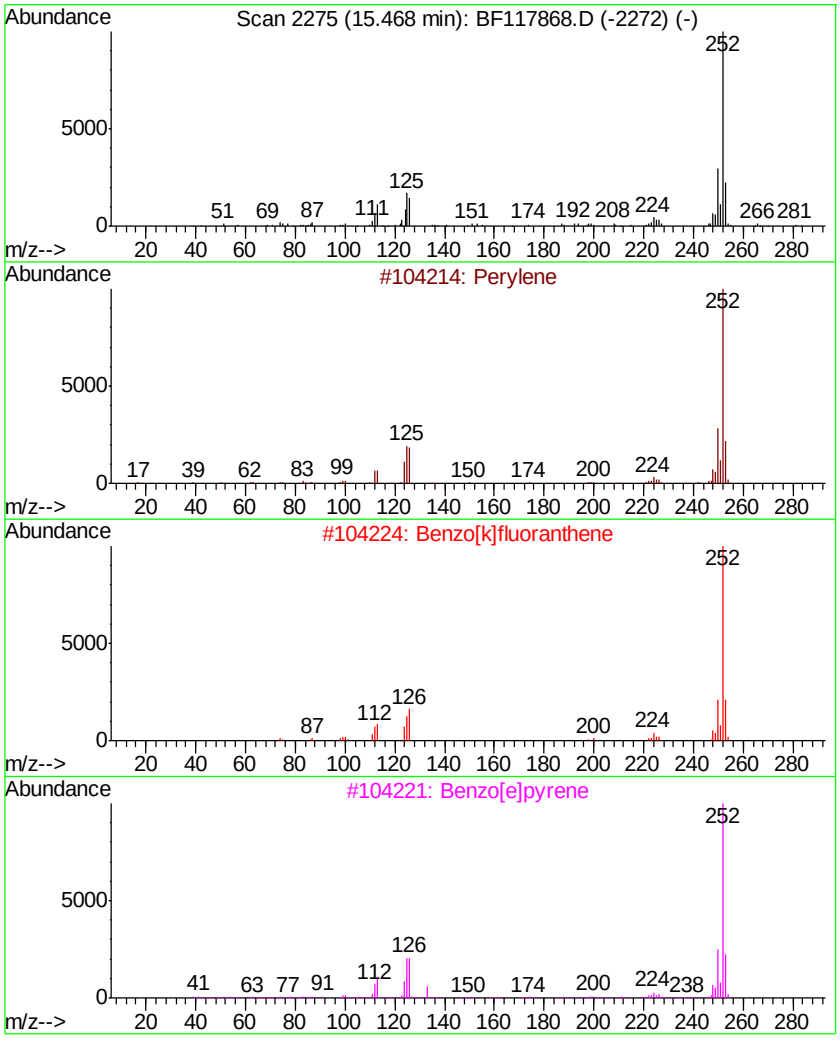
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

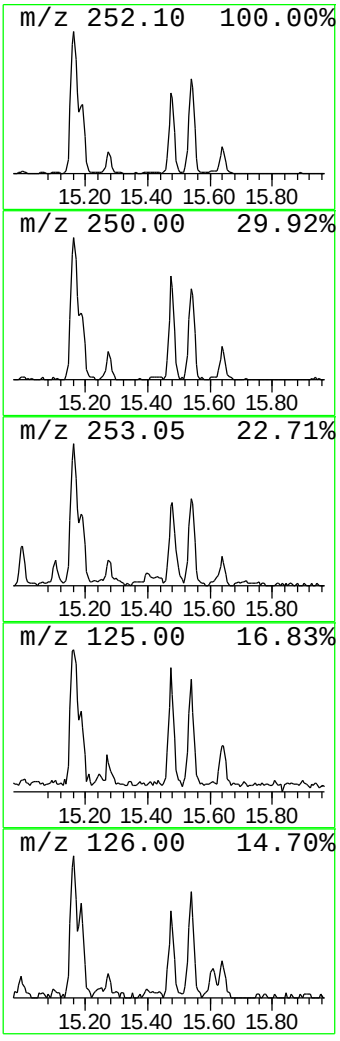
**********

Peak Number 8 Perylene Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.47 | 2.96 ng | 214515 | Perylene-d12 | 15.61 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Perylene | 252 | C20H12 | 000198-55-0 | 99 |
| 2 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 98 |
| 3 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 98 |
| 4 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 96 |
| 5 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
Data File : BF117868.D
Acq On : 19 Nov 2019 19:14
Operator : JU
Sample : K5904-18
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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-methoxy... | 2.21 | 15.1 | ng | 939488 | 1 | 6.92 | 1246550 | 20.0 |
| 3-Penten-2-one, 4... | 4.53 | 64.0 | ng | 3990260 | 1 | 6.92 | 1246550 | 20.0 |
| 2-Pentanone, 4-hy... | 5.14 | 42.8 | ng | 2669070 | 1 | 6.92 | 1246550 | 20.0 |
| unknown6.68 | 6.68 | 29.6 | ng | 1846850 | 1 | 6.92 | 1246550 | 20.0 |
| Trichloroacetic a... | 13.96 | 4.7 | ng | 441898 | 5 | 14.10 | 1890240 | 20.0 |
| Perylene | 15.47 | 3.0 | ng | 214515 | 6 | 15.61 | 1448840 | 20.0 |