LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139118.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.252 | 17 | 27 | 34 | rVB | 945801 | 1543042 | 66.89% | 7.578% |
| 2 | 3.440 | 224 | 229 | 246 | rBV | 27112 | 56352 | 2.44% | 0.277% |
| 3 | 4.016 | 321 | 327 | 333 | rBV | 25774 | 38784 | 1.68% | 0.190% |
| 4 | 5.128 | 506 | 516 | 522 | rBV | 91063 | 146331 | 6.34% | 0.719% |
| 5 | 5.516 | 576 | 582 | 588 | rBV | 1583962 | 2184450 | 94.69% | 10.728% |
| 6 | 6.516 | 745 | 752 | 757 | rBV | 1626768 | 2271368 | 98.46% | 11.154% |
| 7 | 6.722 | 780 | 787 | 797 | rBV | 21463 | 31255 | 1.35% | 0.153% |
| 8 | 6.898 | 811 | 817 | 822 | rBV | 487712 | 608956 | 26.40% | 2.990% |
| 9 | 7.063 | 835 | 845 | 850 | rBV2 | 24326 | 40642 | 1.76% | 0.200% |
| 10 | 7.457 | 905 | 912 | 917 | rBV | 1084184 | 1425130 | 61.78% | 6.999% |
| 11 | 8.175 | 1029 | 1034 | 1042 | rVB | 598452 | 789083 | 34.21% | 3.875% |
| 12 | 8.486 | 1082 | 1087 | 1096 | rBV | 35937 | 47638 | 2.07% | 0.234% |
| 13 | 9.251 | 1211 | 1217 | 1222 | rBV | 1793063 | 2306921 | 100.00% | 11.329% |
| 14 | 9.933 | 1327 | 1333 | 1338 | rBV | 726219 | 895682 | 38.83% | 4.399% |
| 15 | 10.028 | 1341 | 1349 | 1356 | rBV2 | 37393 | 58748 | 2.55% | 0.289% |
| 16 | 10.722 | 1461 | 1467 | 1472 | rBV | 1216685 | 1617692 | 70.12% | 7.944% |
| 17 | 11.416 | 1580 | 1585 | 1594 | rBV2 | 697485 | 1044017 | 45.26% | 5.127% |
| 18 | 11.945 | 1666 | 1675 | 1685 | rBV2 | 210888 | 361607 | 15.67% | 1.776% |
| 19 | 12.027 | 1685 | 1689 | 1692 | rBV | 33166 | 46556 | 2.02% | 0.229% |
| 20 | 12.469 | 1760 | 1764 | 1767 | rBV2 | 21855 | 28792 | 1.25% | 0.141% |
| 21 | 12.627 | 1786 | 1791 | 1797 | rBV | 160661 | 209351 | 9.07% | 1.028% |
| 22 | 12.733 | 1804 | 1809 | 1816 | rBV2 | 104183 | 164649 | 7.14% | 0.809% |
| 23 | 12.857 | 1823 | 1830 | 1844 | rVB2 | 155293 | 329872 | 14.30% | 1.620% |
| 24 | 13.004 | 1847 | 1855 | 1860 | rBV | 1488355 | 1867164 | 80.94% | 9.169% |
| 25 | 13.074 | 1862 | 1867 | 1875 | rBV4 | 18230 | 41022 | 1.78% | 0.201% |
| 26 | 13.186 | 1879 | 1886 | 1890 | rVB | 23809 | 44372 | 1.92% | 0.218% |
| 27 | 13.386 | 1911 | 1920 | 1922 | rBV3 | 35975 | 85550 | 3.71% | 0.420% |
| 28 | 13.686 | 1968 | 1971 | 1978 | rVB | 15205 | 25344 | 1.10% | 0.124% |
| 29 | 13.804 | 1986 | 1991 | 1993 | rBV2 | 16222 | 26605 | 1.15% | 0.131% |
| 30 | 13.904 | 2004 | 2008 | 2015 | rBV3 | 71549 | 130277 | 5.65% | 0.640% |
| 31 | 13.968 | 2016 | 2019 | 2023 | rVB2 | 23649 | 29605 | 1.28% | 0.145% |
| 32 | 14.057 | 2028 | 2034 | 2044 | rVB2 | 473209 | 739785 | 32.07% | 3.633% |
| 33 | 14.539 | 2112 | 2116 | 2122 | rBV5 | 21236 | 47433 | 2.06% | 0.233% |
| 34 | 15.098 | 2206 | 2211 | 2222 | rVB | 57217 | 143076 | 6.20% | 0.703% |
| 35 | 15.198 | 2223 | 2228 | 2237 | rBV2 | 28803 | 51816 | 2.25% | 0.254% |
| 36 | 15.404 | 2259 | 2263 | 2268 | rBV | 28175 | 41461 | 1.80% | 0.204% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 15.468 | 2268 | 2274 | 2279 | rVV | 42491 | 69218 | 3.00% | 0.340% |
| 38 | 15.533 | 2279 | 2285 | 2301 | rVB | 358121 | 561321 | 24.33% | 2.757% |
| 39 | 16.039 | 2366 | 2371 | 2375 | rBV2 | 14869 | 24699 | 1.07% | 0.121% |
| 40 | 16.098 | 2375 | 2381 | 2389 | rVV9 | 13793 | 34856 | 1.51% | 0.171% |
| 41 | 17.004 | 2530 | 2535 | 2545 | rVB2 | 18391 | 43434 | 1.88% | 0.213% |
| 42 | 17.451 | 2605 | 2611 | 2618 | rVB | 14158 | 28477 | 1.23% | 0.140% |
| 43 | 18.221 | 2735 | 2742 | 2753 | rVB8 | 30729 | 80634 | 3.50% | 0.396% |

Sum of corrected areas: 20363067

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
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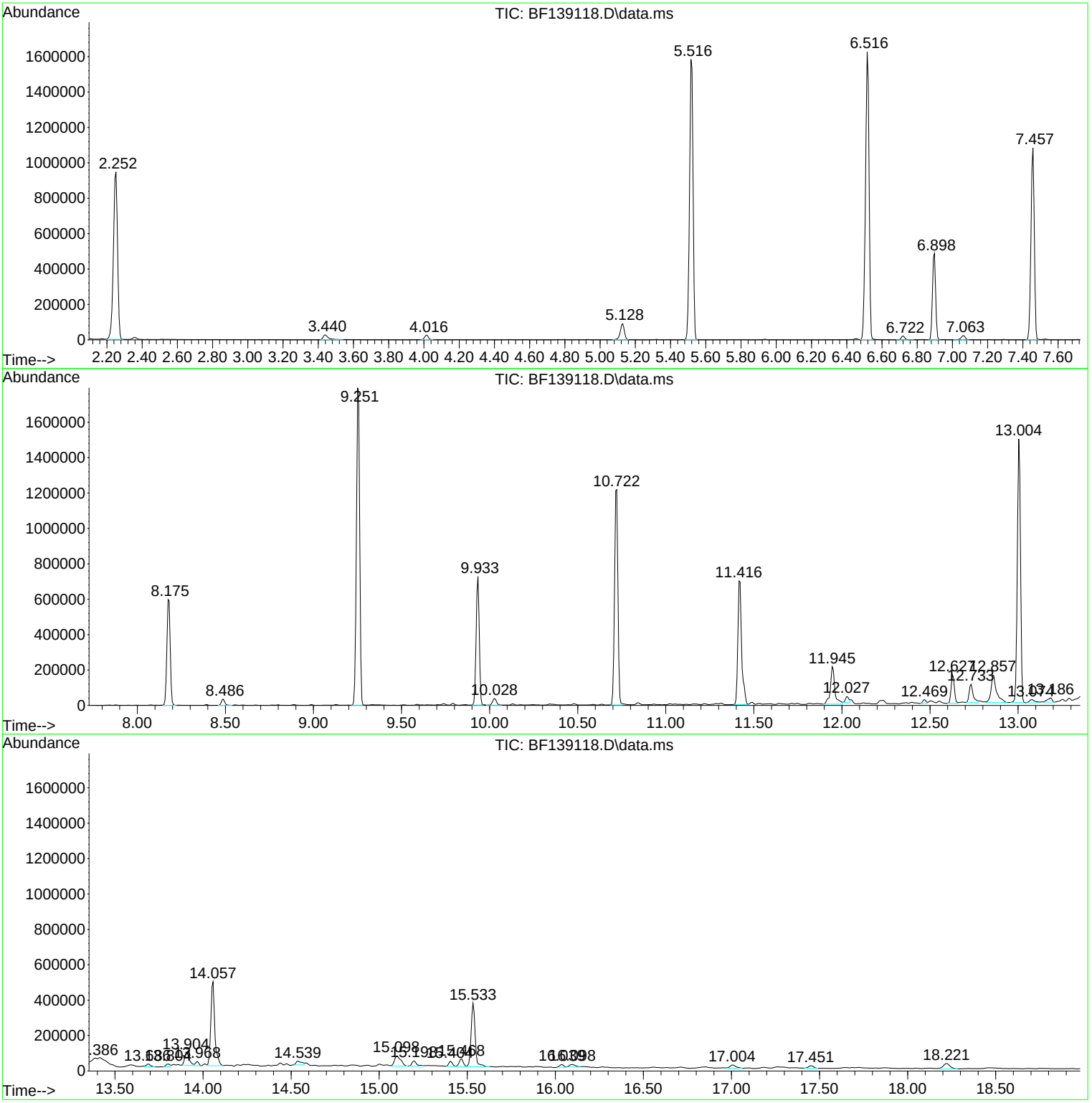
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

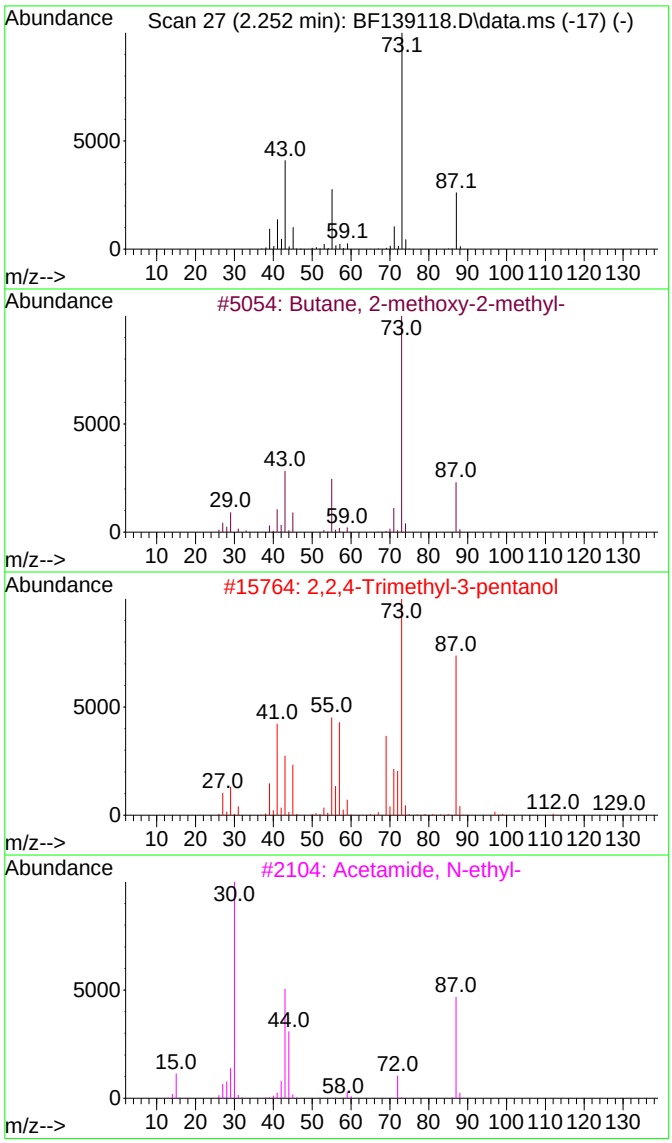
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

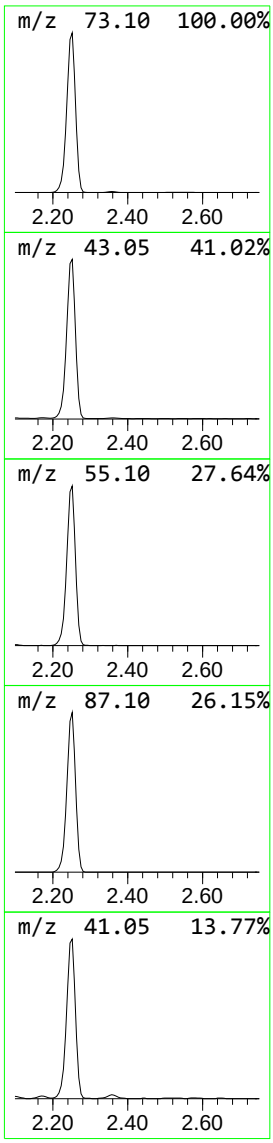
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.252 | 50.68 ng | 1543040 | 1,4-Dichlorobenzene-d4 | 6.898 |

| 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 | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

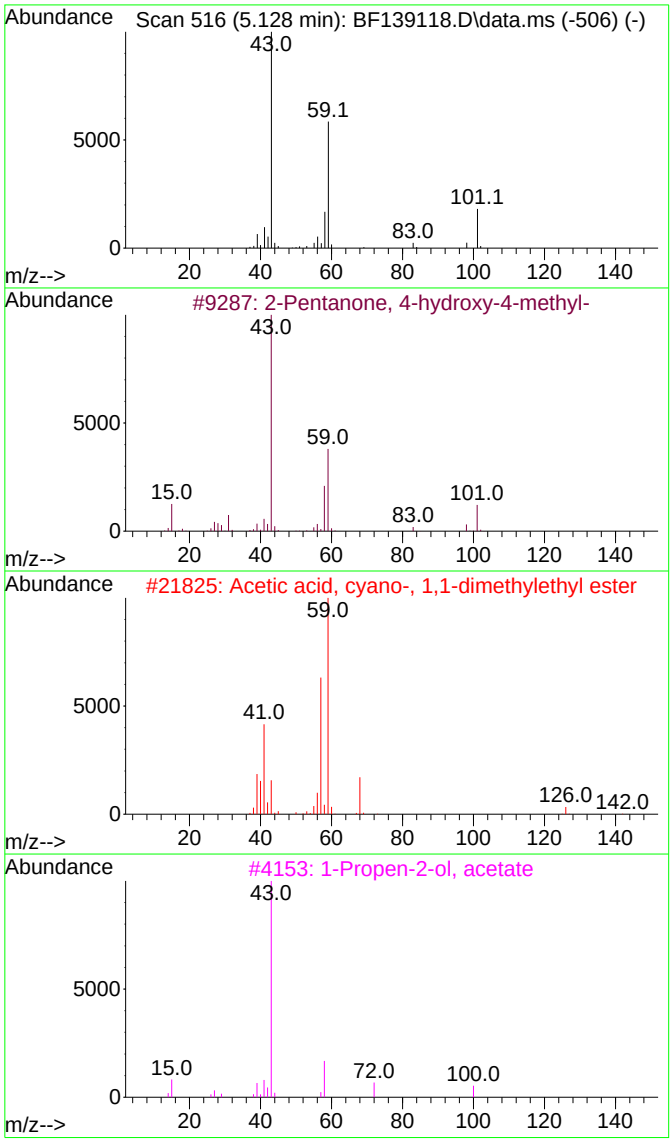
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

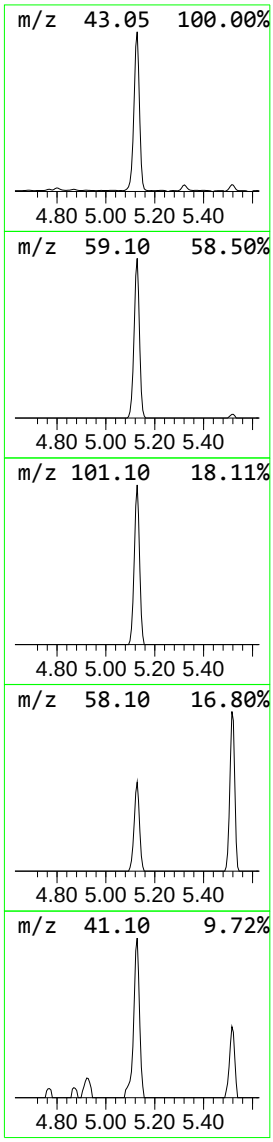
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.128 | 4.81 ng | 146331 | 1,4-Dichlorobenzene-d4 | 6.898 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 12 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

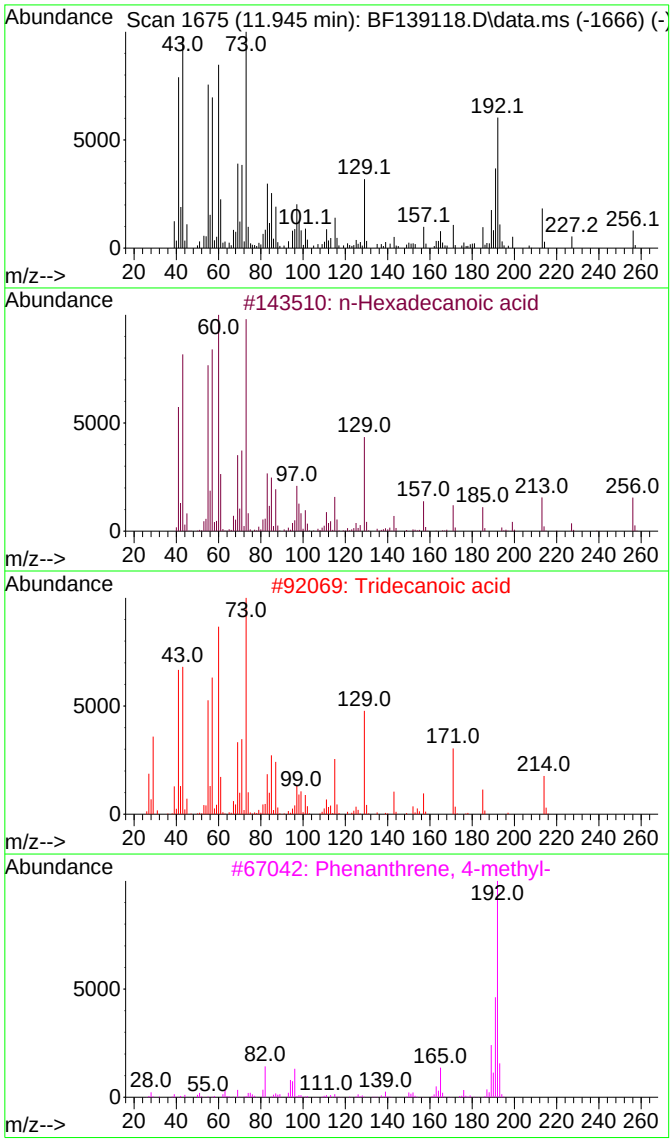
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

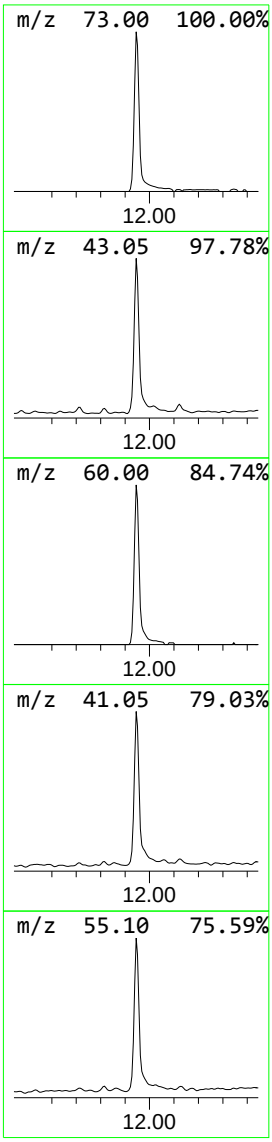
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.945 | 6.93 ng | 361607 | Phenanthrene-d10 | 11.422 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Phenanthrene, 4-methyl- | 192 | C15H12 | 000832-64-4 | 90 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 70 |
| 5 | Anthracene, 2-methyl- | 192 | C15H12 | 000613-12-7 | 68 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

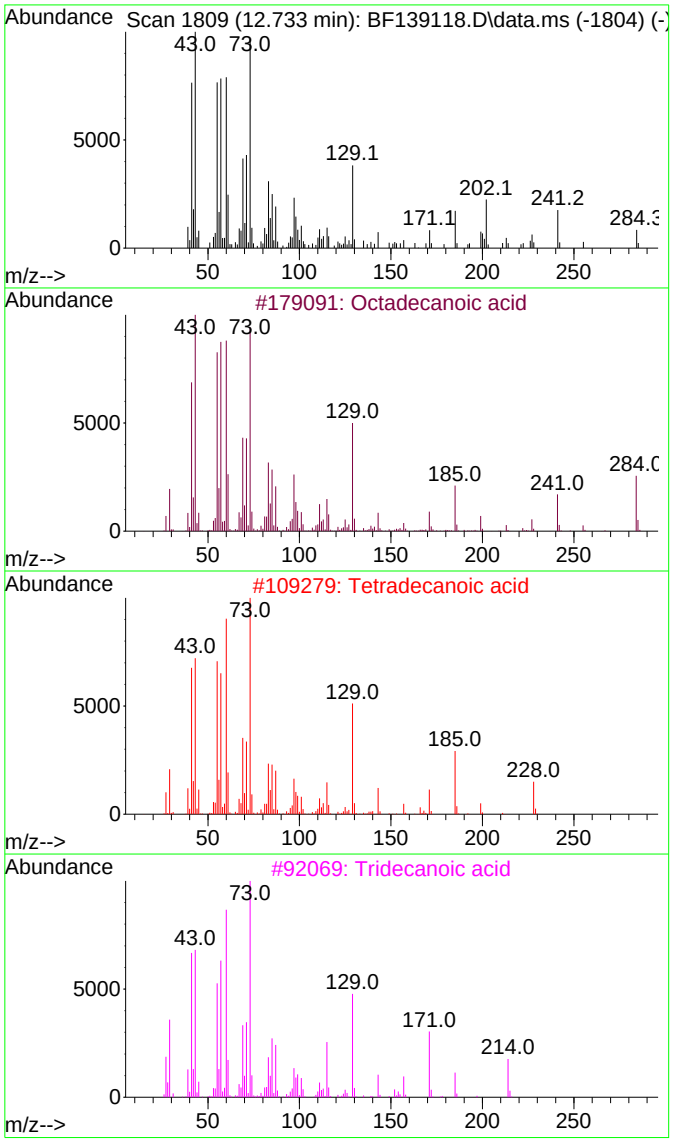
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

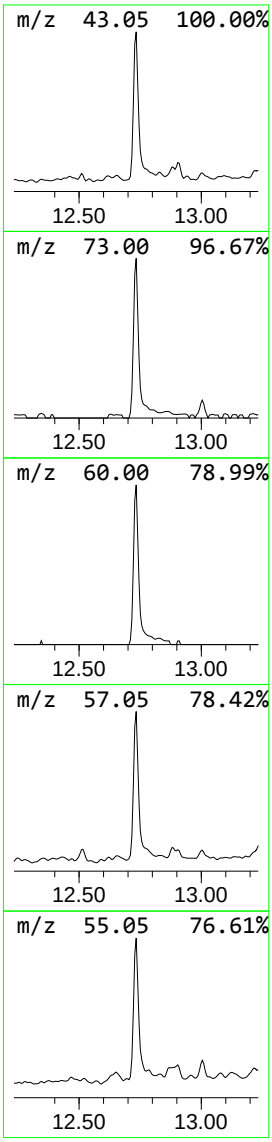
**********

Peak Number 4 Octadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.733 | 3.15 ng | 164649 | Phenanthrene-d10 | 11.422 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 93 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 91 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 5 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87 |



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Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
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**Instrument :**
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

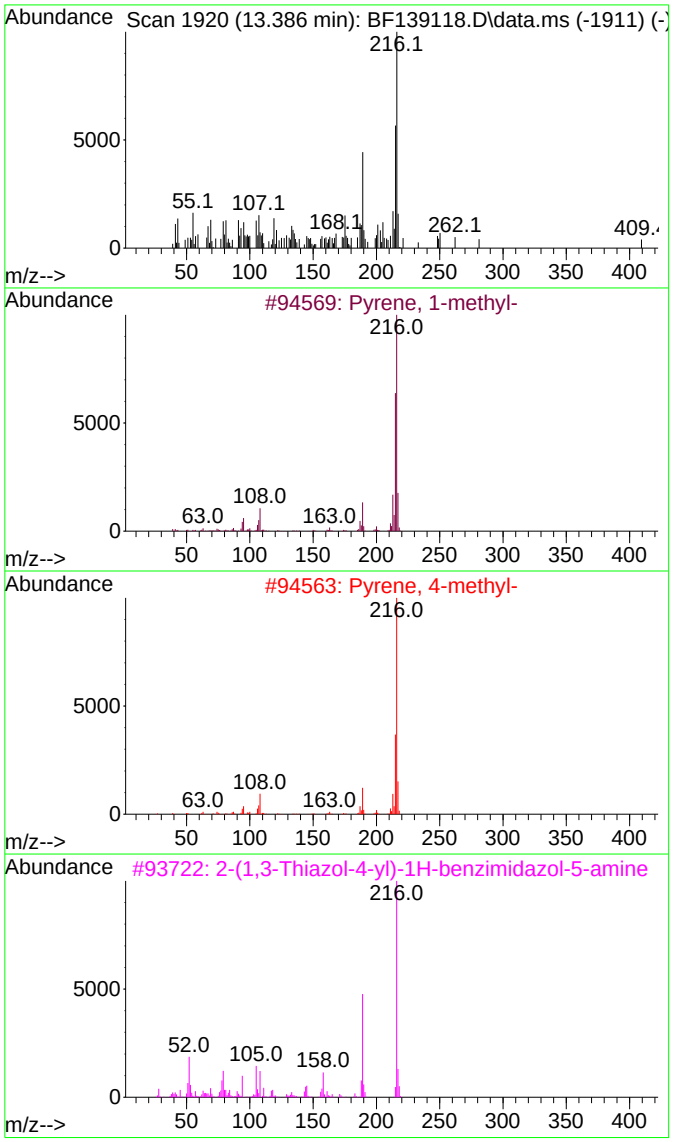
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

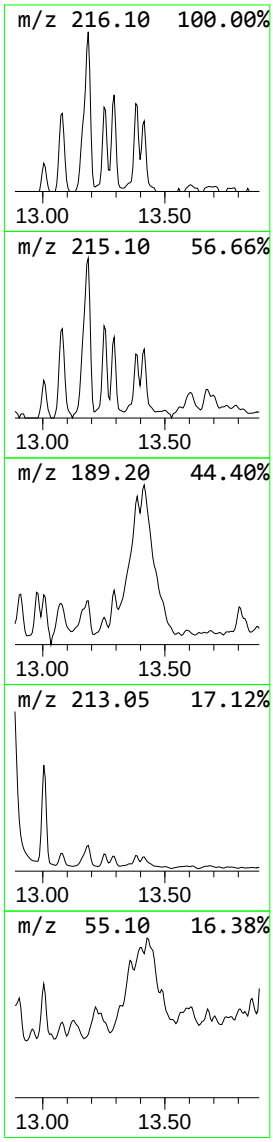
**********

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.386 | 2.31 ng | 85550 | Chrysene-d12 | 14.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pyrene, 1-methyl- | 216 | C17H12 | 002381-21-7 | 91 |
| 2 | Pyrene, 4-methyl- | 216 | C17H12 | 003353-12-6 | 91 |
| 3 | 2-(1,3-Thiazol-4-yl)-1H-benzimid... | 216 | C10H8N4S | 025893-06-5 | 83 |
| 4 | Pyrene, 2-methyl- | 216 | C17H12 | 003442-78-2 | 76 |
| 5 | Benzoic acid, 3-(5-formyl-2-furyl)- | 216 | C12H8O4 | 304884-54-6 | 64 |



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Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

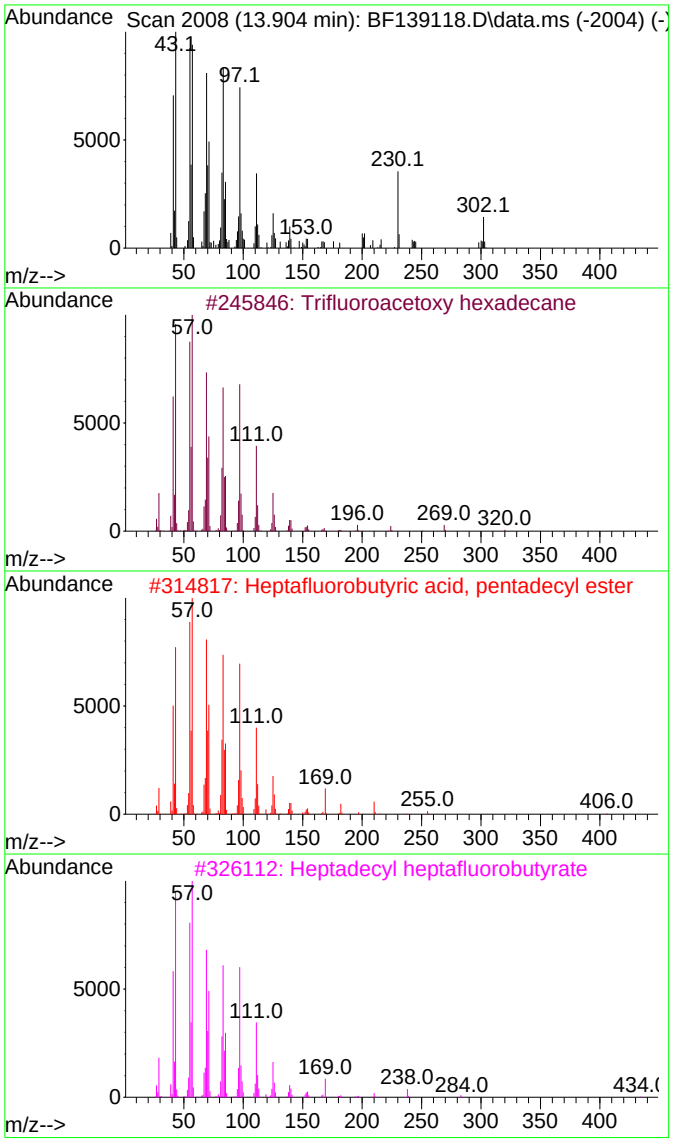
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

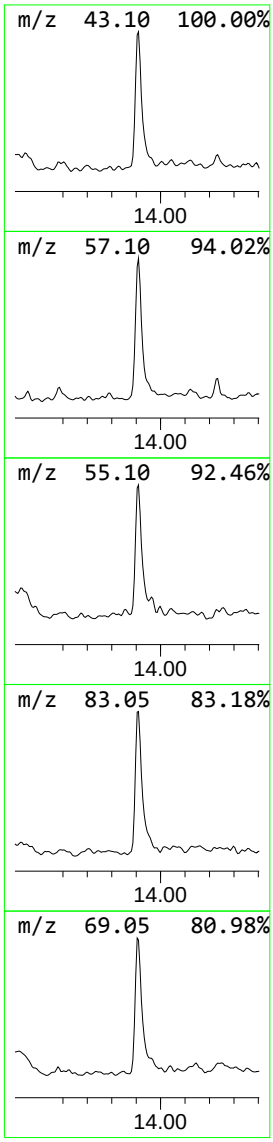
**********

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.904 | 3.52 ng | 130277 | Chrysene-d12 | 14.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 93 |
| 2 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 93 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 93 |
| 4 | 1-Octadecanol | 270 | C18H38O | 000112-92-5 | 93 |
| 5 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 93 |



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Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

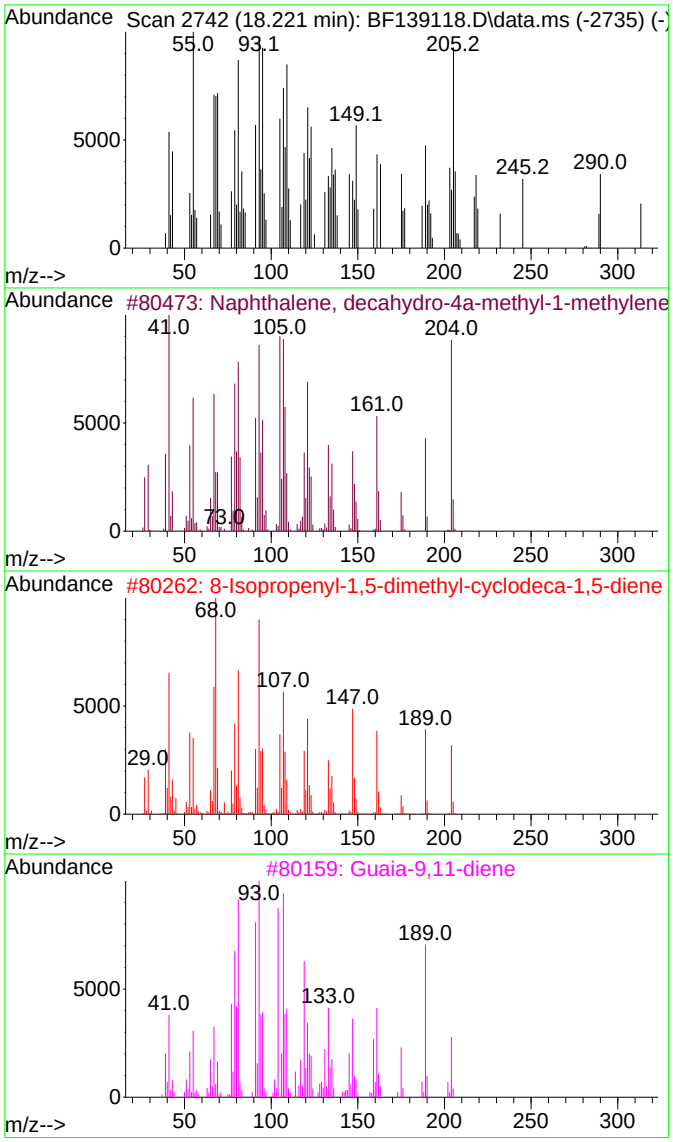
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

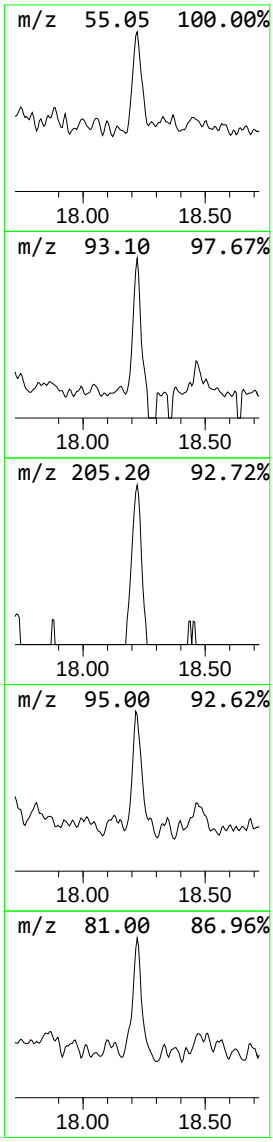
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 Naphthalene, decahydro-4a-m... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.221 | 2.87 ng | 80634 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, decahydro-4a-methyl... | 204 | C15H24 | 017066-67-0 | 74 |
| 2 | 8-Isopropenyl-1,5-dimethyl-cyclo... | 204 | C15H24 | 1000193-62-7 | 55 |
| 3 | Guaia-9,11-diene | 204 | C15H24 | 1000374-19-8 | 51 |
| 4 | 1,5-Cyclodecadiene, 1,5-dimethyl... | 204 | C15H24 | 075023-40-4 | 49 |
| 5 | 1,8-Nonadiene, 2,7-dimethyl-5-(1... | 192 | C14H24 | 068702-20-5 | 43 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139118.D
Acq On : 22 Aug 2024 12:52
Operator : RC/JU
Sample : P3663-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
914-J-SD-0-0.5-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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 |
| Butane, 2-metho... | 2.252 | 50.7 | ng | 1543040 | 1 | 6.898 | 608956 | 20.0 |
| 2-Pentanone, 4-... | 5.128 | 4.8 | ng | 146331 | 1 | 6.898 | 608956 | 20.0 |
| n-Hexadecanoic ... | 11.945 | 6.9 | ng | 361607 | 4 | 11.422 | 1044020 | 20.0 |
| Octadecanoic acid | 12.733 | 3.1 | ng | 164649 | 4 | 11.422 | 1044020 | 20.0 |
| Pyrene, 1-methyl- | 13.386 | 2.3 | ng | 85550 | 5 | 14.057 | 739785 | 20.0 |
| Trifluoroacetox... | 13.904 | 3.5 | ng | 130277 | 5 | 14.057 | 739785 | 20.0 |
| Naphthalene, de... | 18.221 | 2.9 | ng | 80634 | 6 | 15.533 | 561321 | 20.0 |