LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139028.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.122 | 3 | 5 | 15 | rVB | 549490 | 754445 | 78.97% | 8.418% |
| 2 | 2.487 | 55 | 67 | 78 | rBB | 427763 | 739076 | 77.36% | 8.247% |
| 3 | 3.422 | 221 | 226 | 246 | rBV | 4506 | 20011 | 2.09% | 0.223% |
| 4 | 4.557 | 413 | 419 | 427 | rVB | 78850 | 113069 | 11.83% | 1.262% |
| 5 | 5.063 | 500 | 505 | 515 | rBV | 37626 | 59160 | 6.19% | 0.660% |
| 6 | 5.469 | 569 | 574 | 592 | rBV | 649405 | 897906 | 93.98% | 10.019% |
| 7 | 6.481 | 741 | 746 | 774 | rBV | 701330 | 955399 | 100.00% | 10.661% |
| 8 | 6.686 | 777 | 781 | 791 | rVV | 5441 | 10298 | 1.08% | 0.115% |
| 9 | 6.833 | 801 | 806 | 813 | rVB | 195493 | 242251 | 25.36% | 2.703% |
| 10 | 6.981 | 827 | 831 | 836 | rBV | 98162 | 119675 | 12.53% | 1.335% |
| 11 | 7.398 | 895 | 902 | 919 | rBV | 448321 | 605352 | 63.36% | 6.755% |
| 12 | 7.657 | 942 | 946 | 955 | rBV | 12778 | 20111 | 2.10% | 0.224% |
| 13 | 8.116 | 1019 | 1024 | 1036 | rVB | 249605 | 311471 | 32.60% | 3.476% |
| 14 | 8.339 | 1058 | 1062 | 1070 | rVB2 | 8980 | 11917 | 1.25% | 0.133% |
| 15 | 8.433 | 1074 | 1078 | 1089 | rBV | 46031 | 72150 | 7.55% | 0.805% |
| 16 | 9.186 | 1201 | 1206 | 1214 | rBV | 623955 | 767501 | 80.33% | 8.564% |
| 17 | 9.863 | 1317 | 1321 | 1332 | rBV | 270859 | 353320 | 36.98% | 3.942% |
| 18 | 9.957 | 1332 | 1337 | 1344 | rBV2 | 26371 | 47300 | 4.95% | 0.528% |
| 19 | 10.657 | 1451 | 1456 | 1469 | rBV | 388285 | 502813 | 52.63% | 5.611% |
| 20 | 10.769 | 1471 | 1475 | 1479 | rVB2 | 8247 | 10992 | 1.15% | 0.123% |
| 21 | 11.357 | 1564 | 1575 | 1582 | rBV | 260797 | 354791 | 37.14% | 3.959% |
| 22 | 11.463 | 1588 | 1593 | 1598 | rBV3 | 20724 | 34030 | 3.56% | 0.380% |
| 23 | 11.786 | 1643 | 1648 | 1656 | rBV2 | 25069 | 47415 | 4.96% | 0.529% |
| 24 | 11.863 | 1656 | 1661 | 1673 | rVB5 | 29441 | 60962 | 6.38% | 0.680% |
| 25 | 12.933 | 1838 | 1843 | 1848 | rVB | 371847 | 451316 | 47.24% | 5.036% |
| 26 | 13.492 | 1932 | 1938 | 1945 | rBV6 | 5918 | 14076 | 1.47% | 0.157% |
| 27 | 13.739 | 1975 | 1980 | 1986 | rVB | 57176 | 73128 | 7.65% | 0.816% |
| 28 | 13.821 | 1988 | 1994 | 2003 | rBV2 | 35129 | 89684 | 9.39% | 1.001% |
| 29 | 13.886 | 2003 | 2005 | 2014 | rVB3 | 13073 | 18749 | 1.96% | 0.209% |
| 30 | 13.998 | 2019 | 2024 | 2031 | rVB | 142719 | 183497 | 19.21% | 2.048% |
| 31 | 14.439 | 2094 | 2099 | 2102 | rBV2 | 31297 | 54721 | 5.73% | 0.611% |
| 32 | 14.515 | 2110 | 2112 | 2118 | rVB | 14959 | 18430 | 1.93% | 0.206% |
| 33 | 14.815 | 2160 | 2163 | 2171 | rVB | 8219 | 11674 | 1.22% | 0.130% |
| 34 | 14.892 | 2171 | 2176 | 2182 | rVB | 14085 | 18831 | 1.97% | 0.210% |
| 35 | 15.074 | 2202 | 2207 | 2211 | rBV | 51002 | 68447 | 7.16% | 0.764% |
| 36 | 15.133 | 2211 | 2217 | 2218 | rBV4 | 7495 | 12916 | 1.35% | 0.144% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 15.462 | 2267 | 2273 | 2290 | rVB | 121234 | 196520 | 20.57% | 2.193% |
| 38 | 15.651 | 2300 | 2305 | 2313 | rBV | 27035 | 42004 | 4.40% | 0.469% |
| 39 | 15.874 | 2337 | 2343 | 2349 | rBV | 36312 | 59056 | 6.18% | 0.659% |
| 40 | 16.656 | 2470 | 2476 | 2485 | rBV3 | 20126 | 40069 | 4.19% | 0.447% |
| 41 | 17.527 | 2617 | 2624 | 2631 | rVB6 | 31080 | 67507 | 7.07% | 0.753% |
| 42 | 17.662 | 2642 | 2647 | 2659 | rVB3 | 23667 | 53188 | 5.57% | 0.593% |
| 43 | 17.786 | 2661 | 2668 | 2684 | rVV10 | 39211 | 178384 | 18.67% | 1.990% |
| 44 | 17.915 | 2685 | 2690 | 2697 | rVV7 | 19854 | 70145 | 7.34% | 0.783% |
| 45 | 18.003 | 2699 | 2705 | 2723 | rVB10 | 39027 | 128139 | 13.41% | 1.430% |

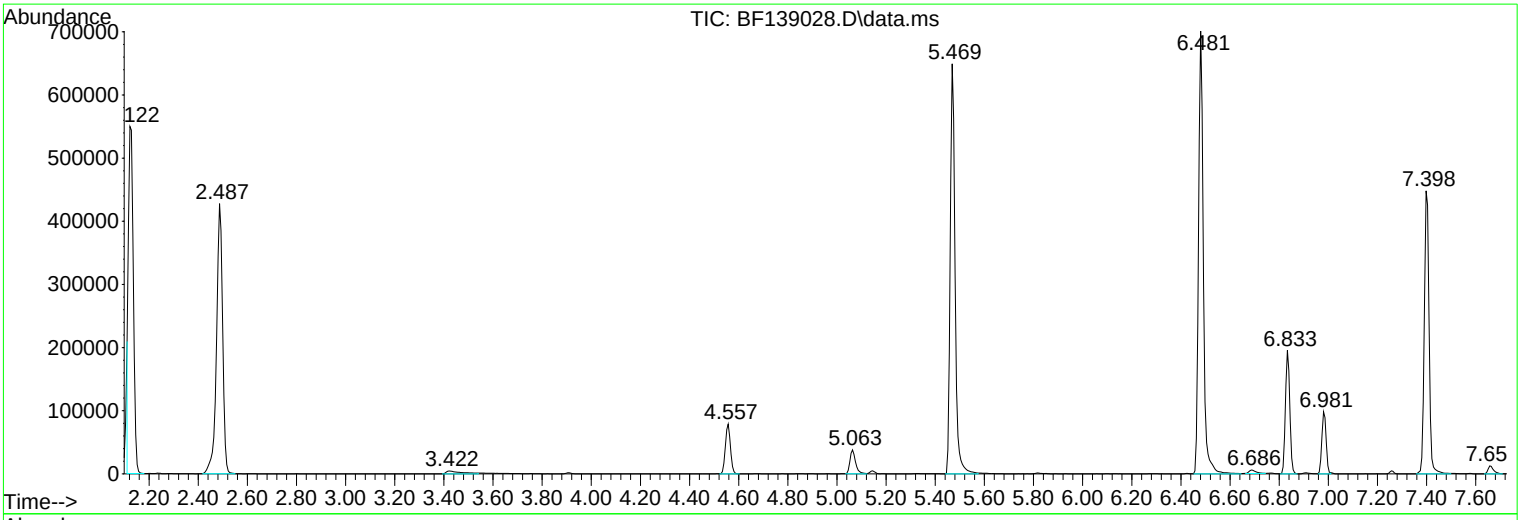
Sum of corrected areas: 8961896

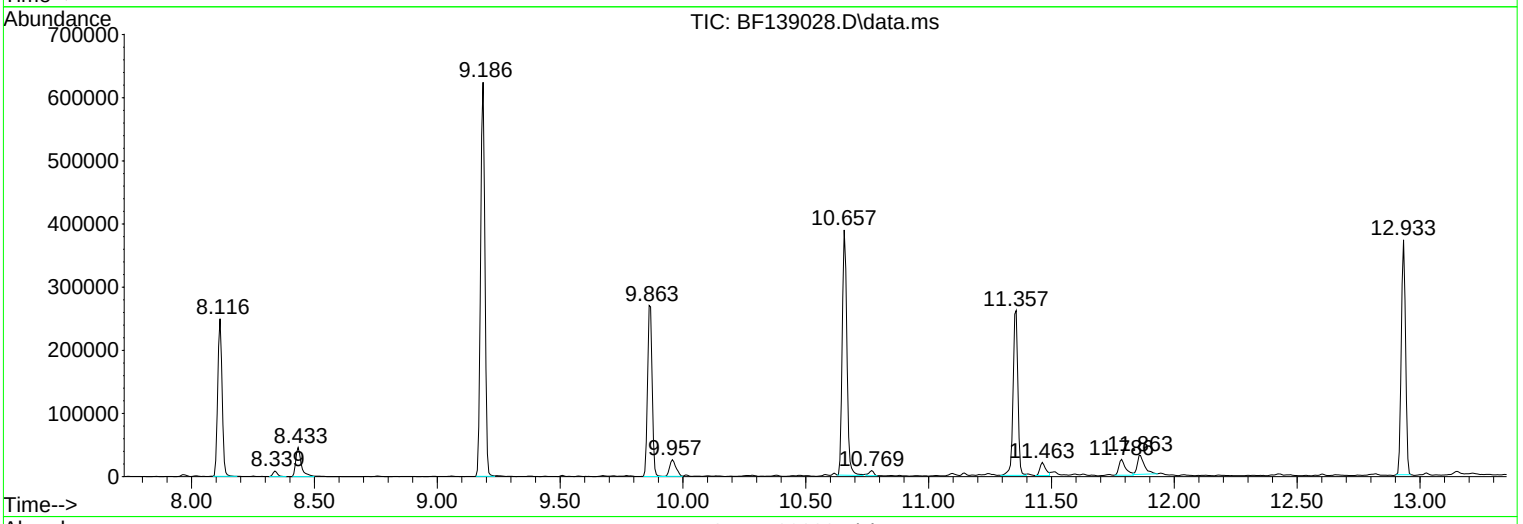
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

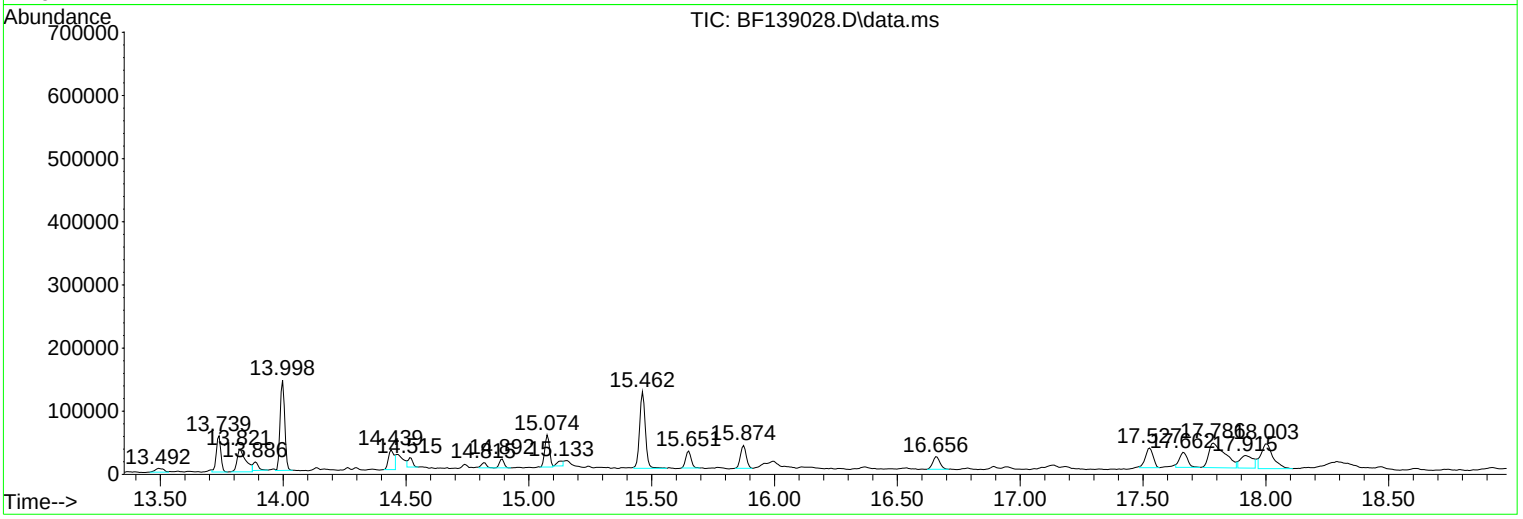
**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

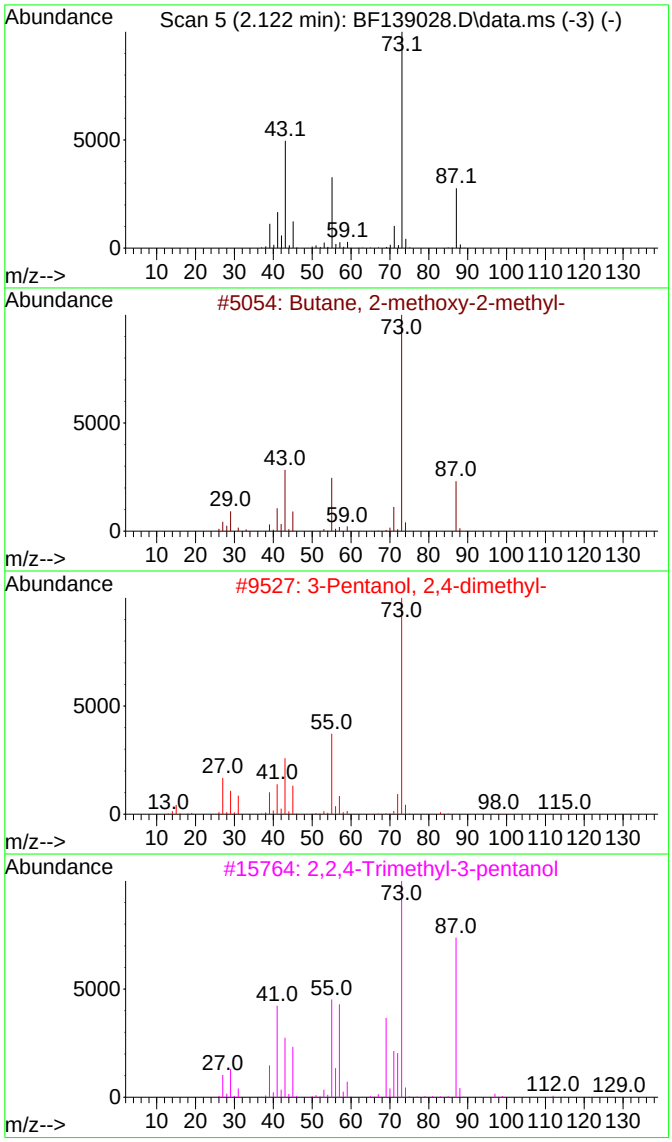
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

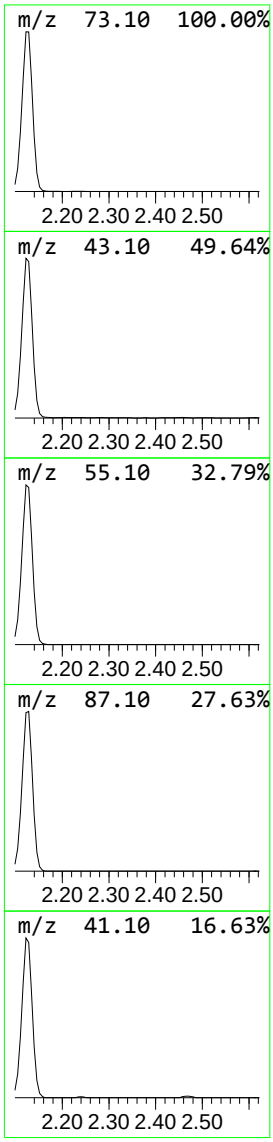
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.122 | 62.29 ng | 754445 | 1,4-Dichlorobenzene-d4 | 6.833 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 43 |
| 3 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 23 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

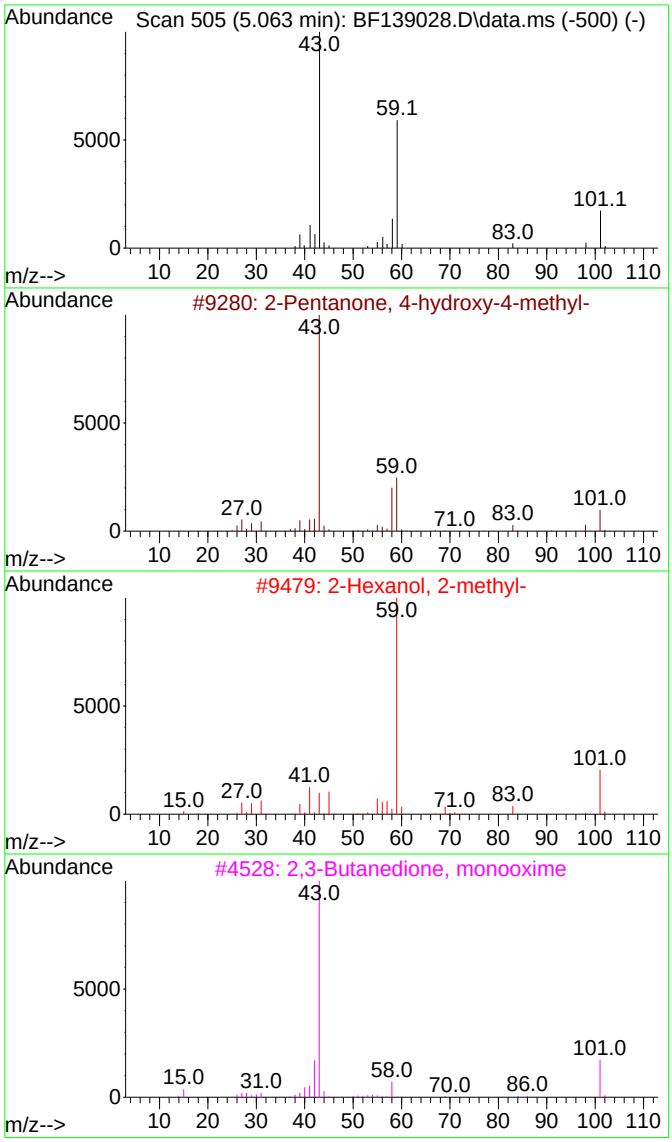
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

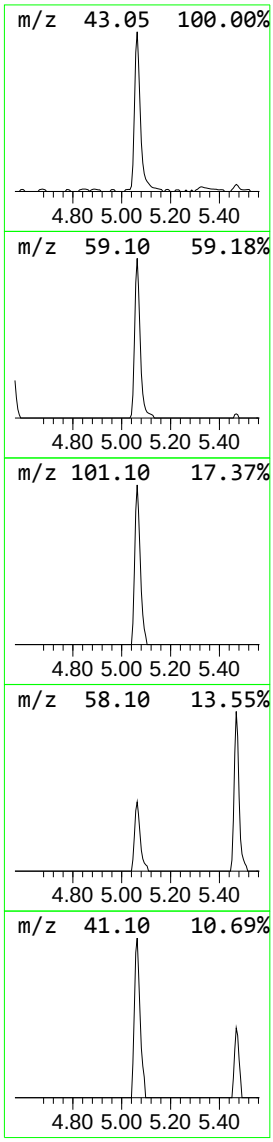
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.063 | 4.88 ng | 59160 | 1,4-Dichlorobenzene-d4 | 6.833 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |
| 5 | 4-Penten-2-one, 4-methyl- | 98 | C6H10O | 003744-02-3 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

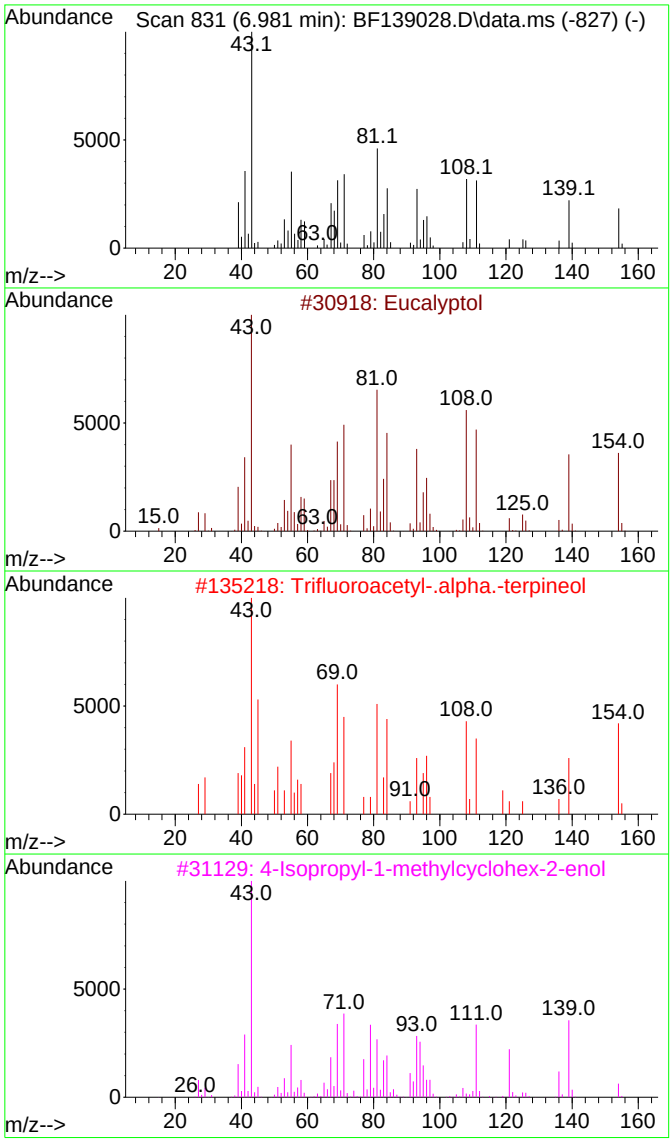
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

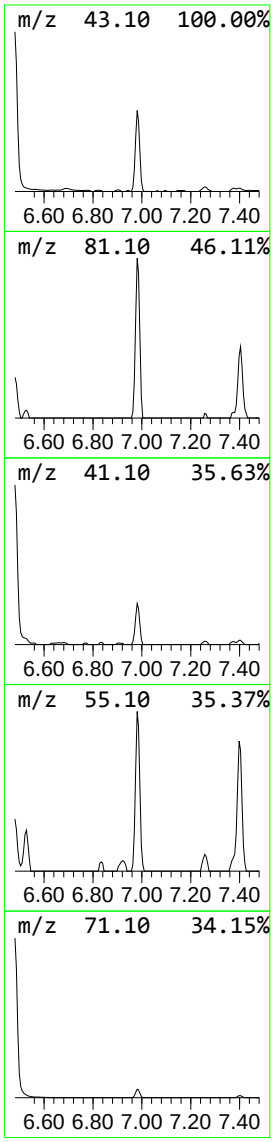
**********

Peak Number 5 Eucalyptol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.981 | 9.88 ng | 119675 | 1,4-Dichlorobenzene-d4 | 6.833 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eucalyptol | 154 | C10H18O | 000470-82-6 | 98 |
| 2 | Trifluoroacetyl-.alpha.-terpineol | 250 | C12H17F3O2 | 1000058-17-6 | 58 |
| 3 | 4-Isopropyl-1-methylcyclohex-2-enol | 154 | C10H18O | 000619-62-5 | 43 |
| 4 | 5-Hepten-2-one, 6-methyl- | 126 | C8H14O | 000110-93-0 | 22 |
| 5 | 2-(3'-Oxo-butyl)-cyclopentanone | 154 | C9H14O2 | 1010143-37-2 | 18 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

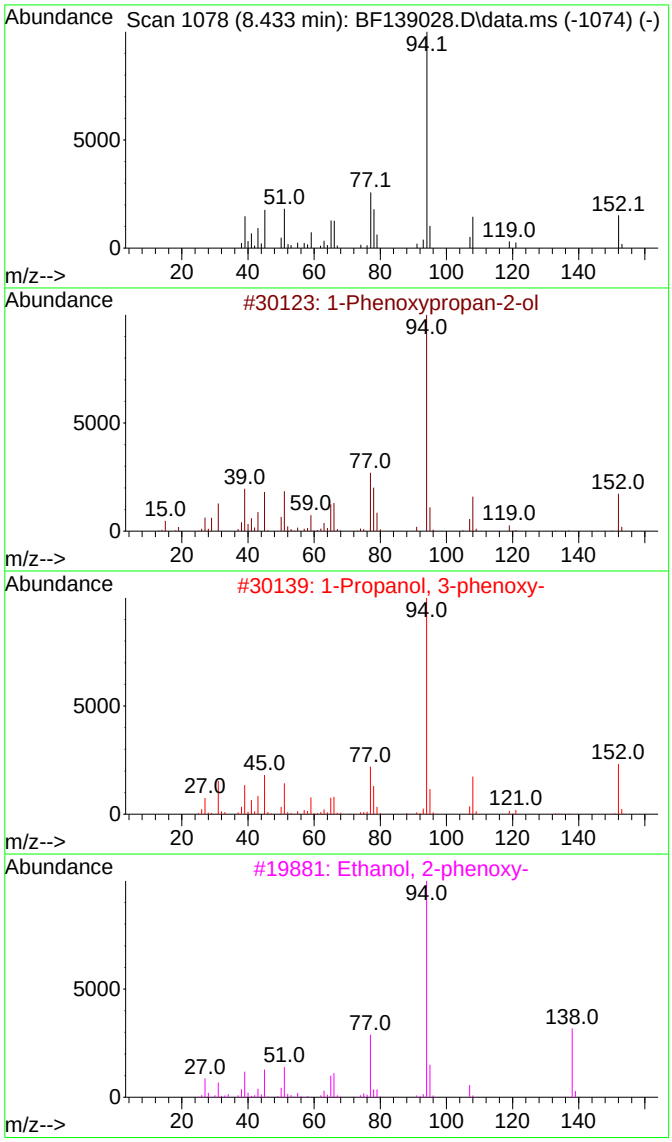
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

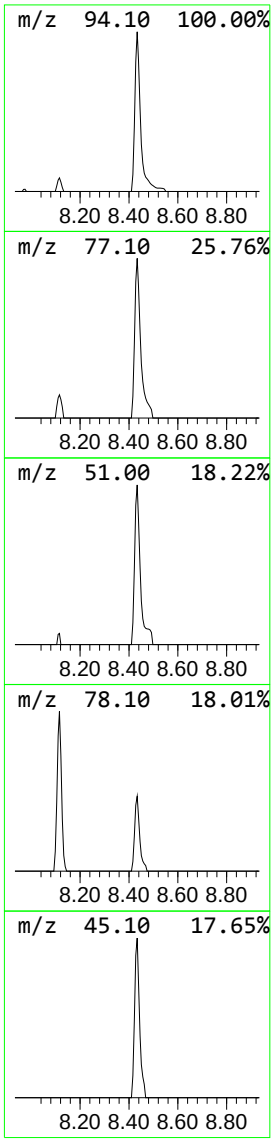
**********

Peak Number 6 1-Phenoxypropan-2-ol Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.433 | 4.63 ng | 72150 | Naphthalene-d8 | 8.116 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Phenoxypropan-2-ol | 152 | C9H12O2 | 000770-35-4 | 96 |
| 2 | 1-Propanol, 3-phenoxy- | 152 | C9H12O2 | 006180-61-6 | 91 |
| 3 | Ethanol, 2-phenoxy- | 138 | C8H10O2 | 000122-99-6 | 64 |
| 4 | 1-Propanol, 2-phenoxy- | 152 | C9H12O2 | 004169-04-4 | 64 |
| 5 | 3-(.alpha.-Hydroxyethyl)-aniline | 137 | C8H11NO | 002454-37-7 | 59 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

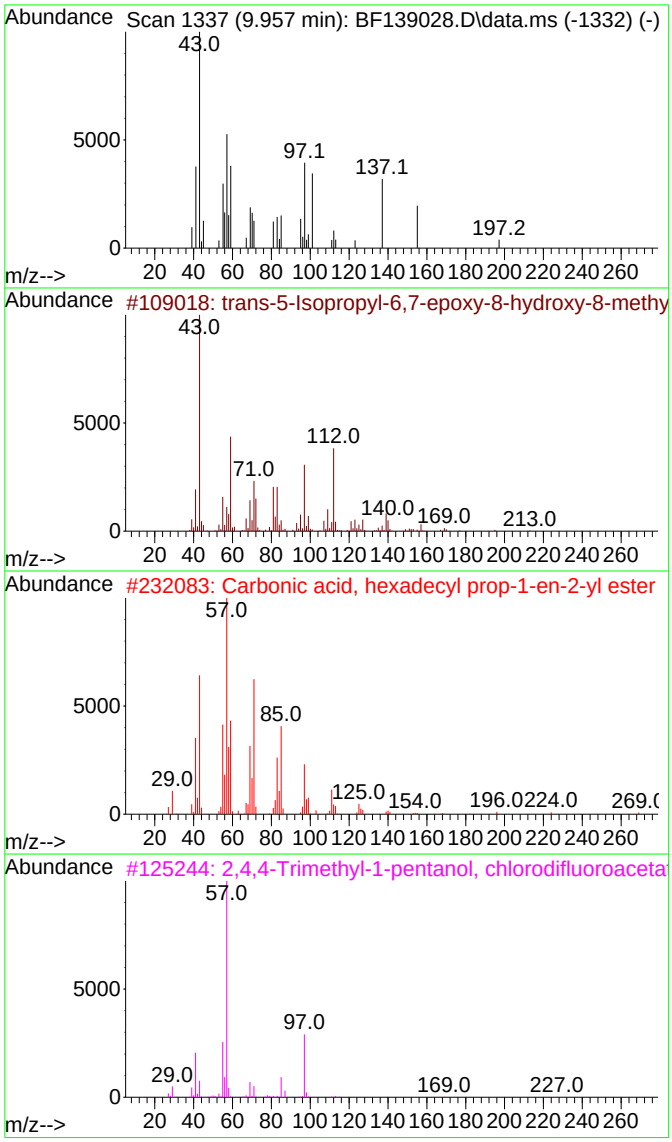
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

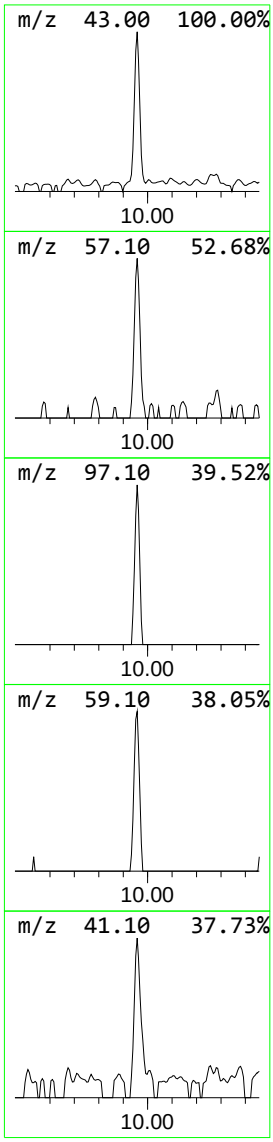
**********

Peak Number 7 unknown9.957 Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.957 | 2.68 ng | 47300 | Acenaphthene-d10 | 9.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | trans-5-Isopropyl-6,7-epoxy-8-hy... | 228 | C13H24O3 | 058002-07-6 | 37 |
| 2 | Carbonic acid, hexadecyl prop-1-... | 326 | C20H38O3 | 1000382-90-3 | 12 |
| 3 | 2,4,4-Trimethyl-1-pentanol, chlo... | 242 | C10H17ClF2O2 | 1000447-27-2 | 10 |
| 4 | Pentadecane, 1-bromo- | 290 | C15H31Br | 000629-72-1 | 10 |
| 5 | Carbonic acid, octadecyl prop-1-... | 354 | C22H42O3 | 1000383-11-5 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

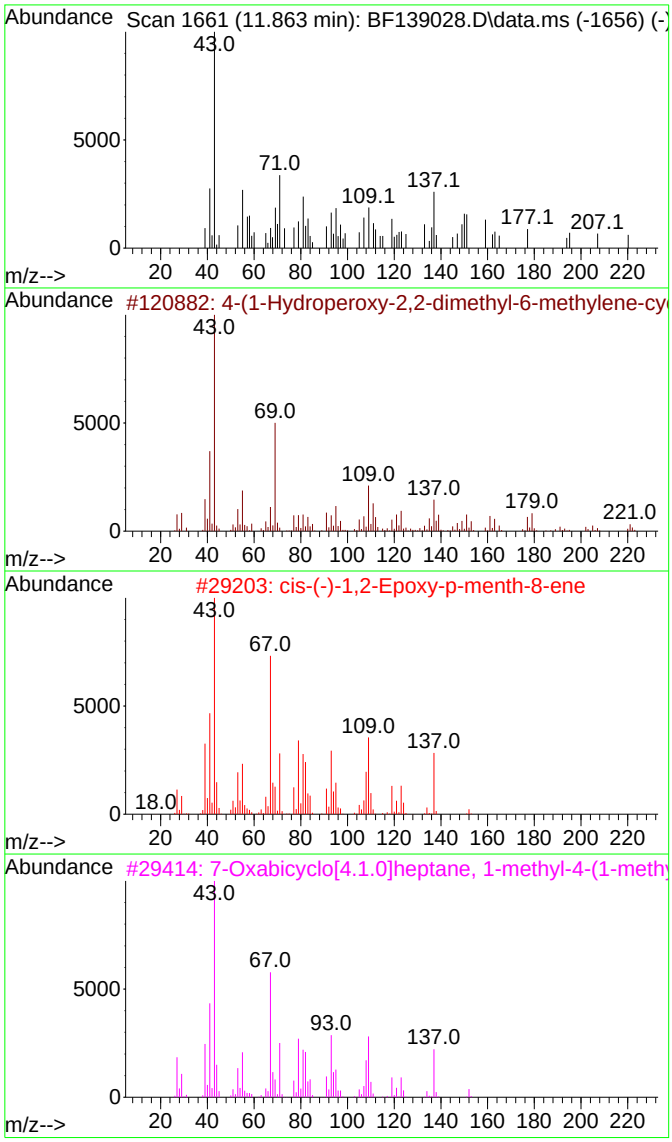
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

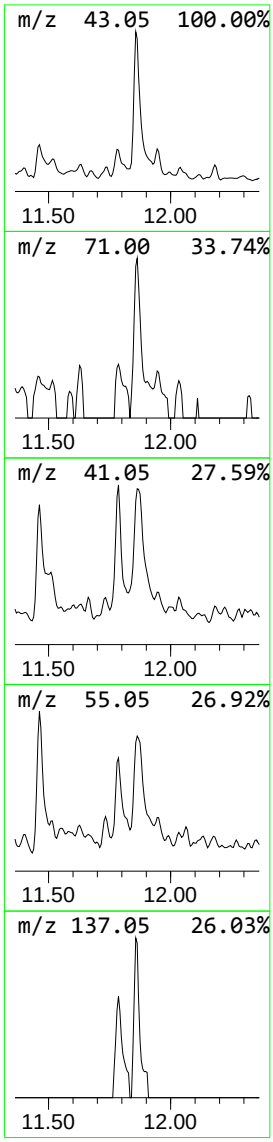
**********

Peak Number 8 unknown11.863 Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.863 | 3.44 ng | 60962 | Phenanthrene-d10 | 11.357 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-(1-Hydroperoxy-2,2-dimethyl-6-... | 238 | C14H22O3 | 125284-20-0 | 16 |
| 2 | cis-(-)-1,2-Epoxy-p-menth-8-ene | 152 | C10H16O | 032543-51-4 | 14 |
| 3 | 7-Oxabicyclo[4.1.0]heptane, 1-me... | 152 | C10H16O | 001195-92-2 | 14 |
| 4 | (1-Cyclopropylimidazol-2-yl)meth... | 137 | C7H11N3 | 1000444-19-0 | 14 |
| 5 | Bicyclo[3.1.1]heptan-3-one, 6,6-... | 194 | C12H18O2 | 1000163-98-0 | 11 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

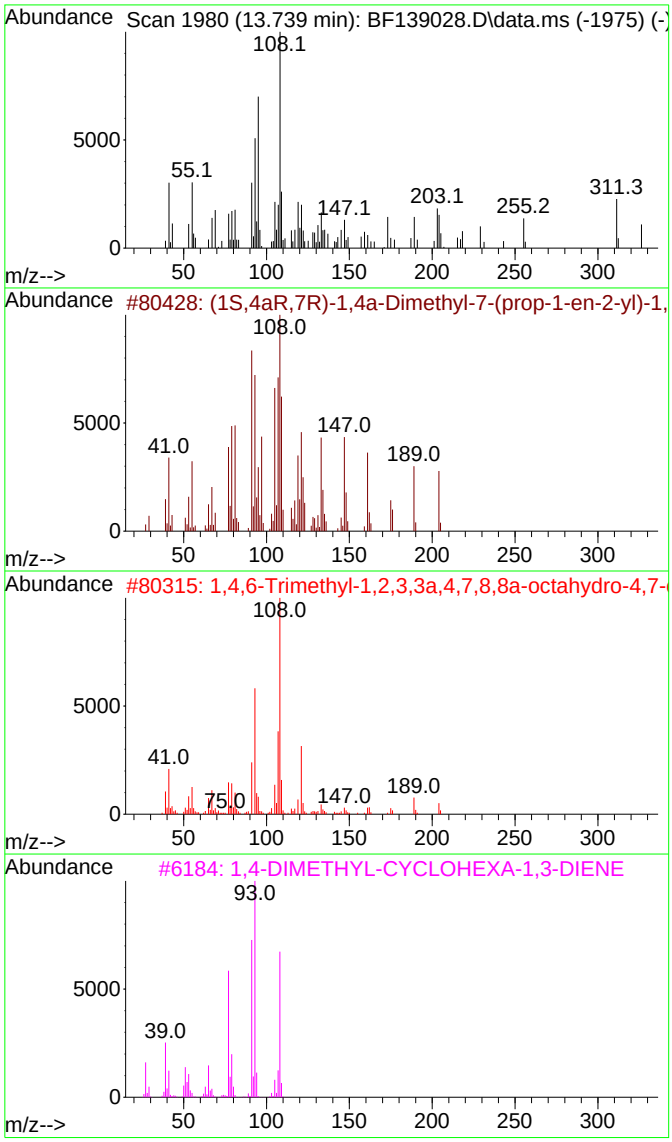
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

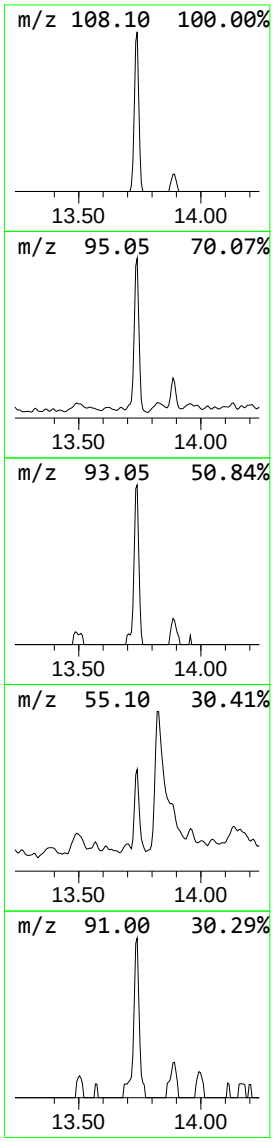
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 9 (1S,4aR,7R)-1,4a-Dimethyl-7... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.739 | 7.97 ng | 73128 | Chrysene-d12 | 13.998 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (1S,4aR,7R)-1,4a-Dimethyl-7-(pro... | 204 | C15H24 | 052026-55-8 | 52 |
| 2 | 1,4,6-Trimethyl-1,2,3,3a,4,7,8,8... | 204 | C15H24 | 065128-08-7 | 43 |
| 3 | 1,4-DIMETHYL-CYCLOHEXA-1,3-DIENE | 108 | C8H12 | 026120-52-5 | 43 |
| 4 | (3S,4aR,5S,8aS)-4a,5-Dimethyl-3-... | 218 | C15H22O | 022489-11-8 | 38 |
| 5 | (4,6-Dimethylpyrimidin-2-yl)(5-m... | 204 | C9H12N6 | 1010317-06-5 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

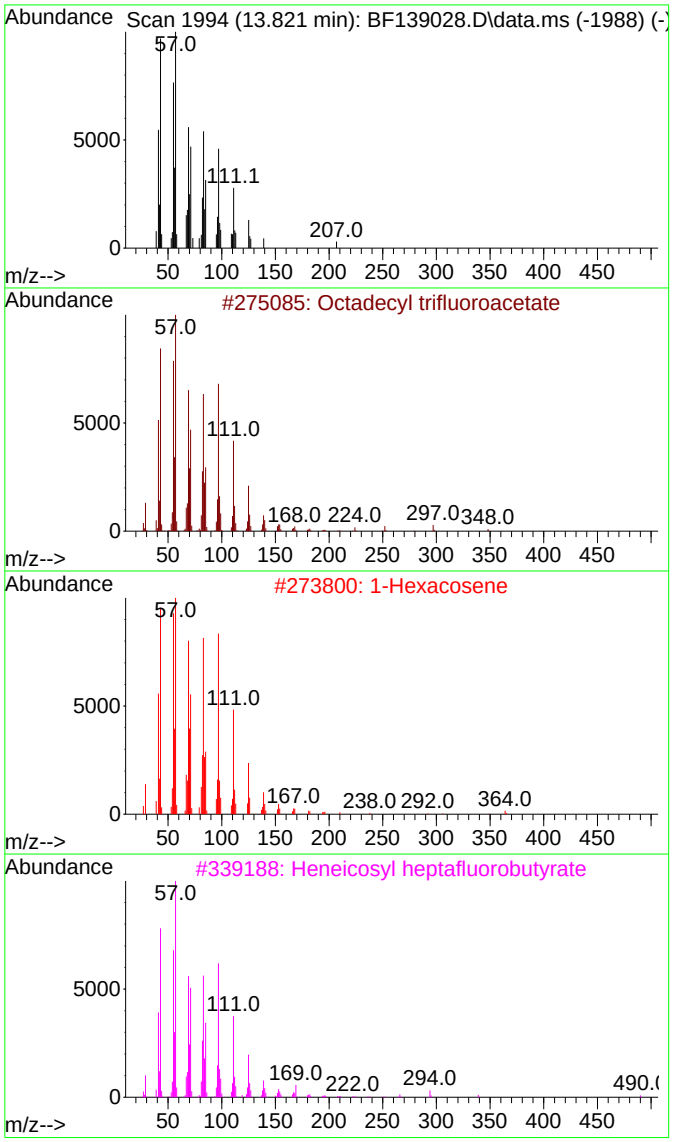
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

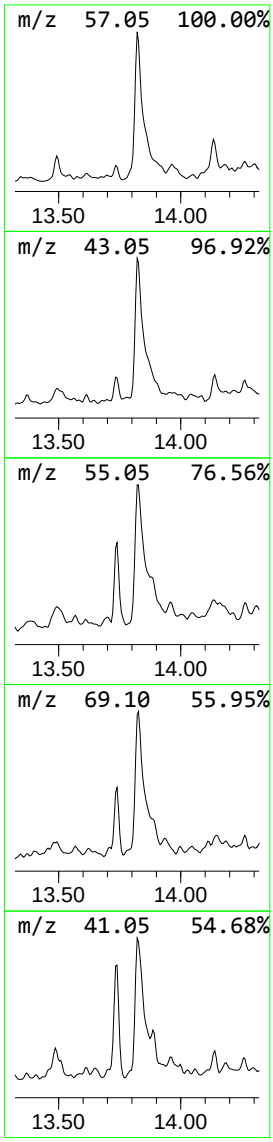
**********

Peak Number 10 Octadecyl trifluoroacetate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.821 | 9.77 ng | 89684 | Chrysene-d12 | 13.998 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 91 |
| 2 | 1-Hexacosene | 364 | C26H52 | 018835-33-1 | 91 |
| 3 | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 91 |
| 4 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 91 |
| 5 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1010351-87-0 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

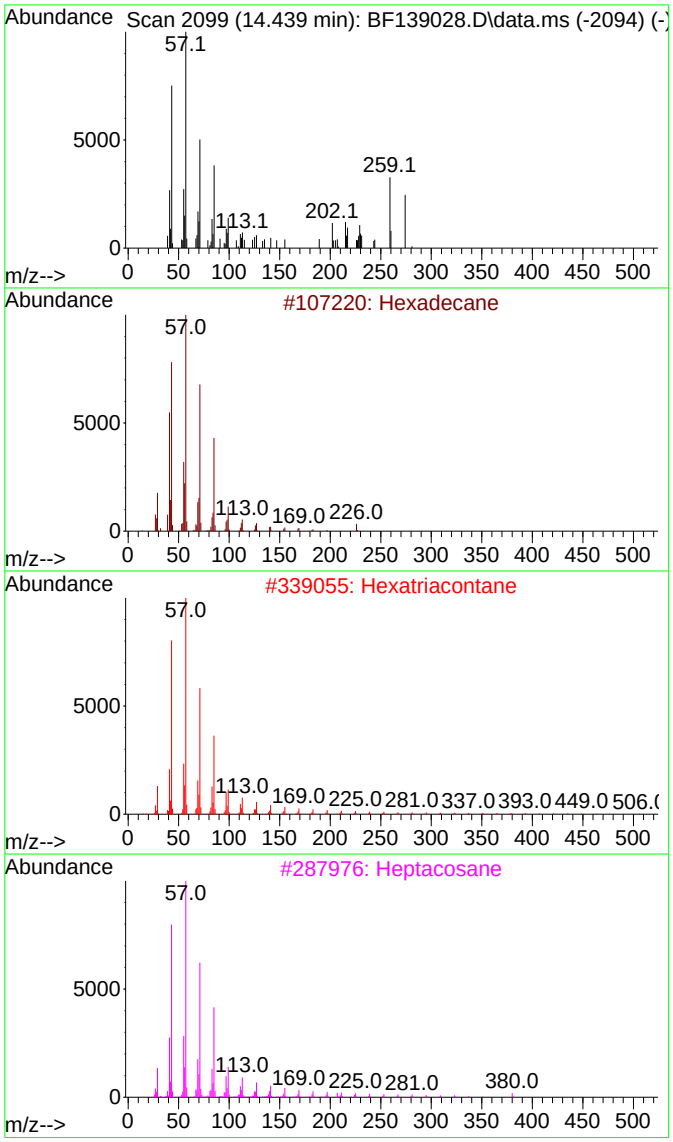
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

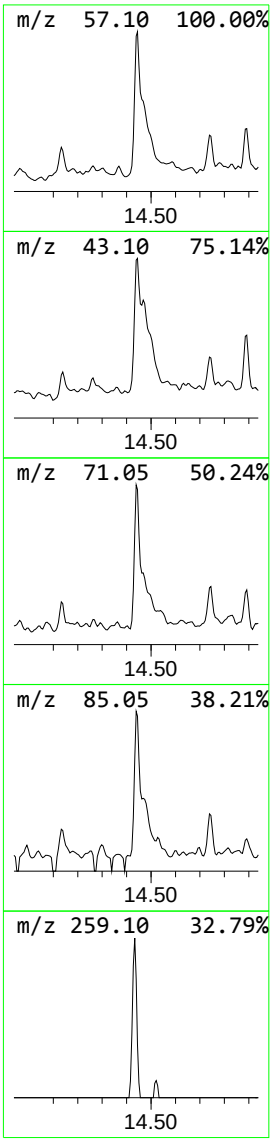
**********

Peak Number 11 Hexadecane Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.439 | 5.96 ng | 54721 | Chrysene-d12 | 13.998 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |
| 2 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 50 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 50 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 50 |
| 5 | Nonadecane | 268 | C19H40 | 000629-92-5 | 50 |



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Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

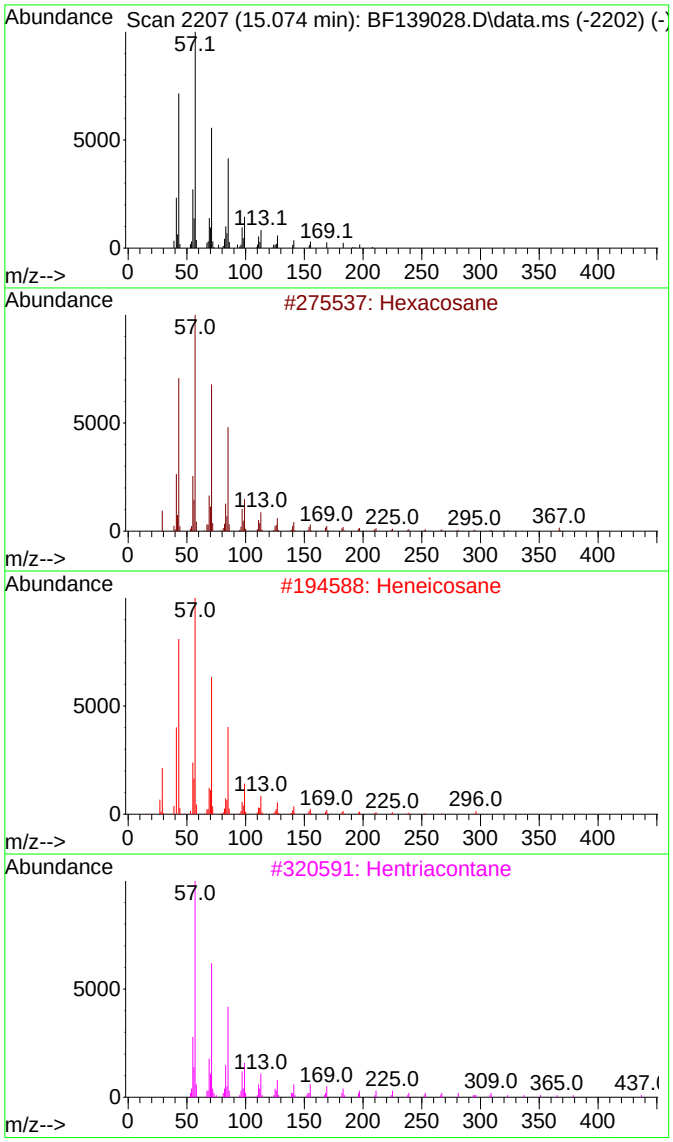
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

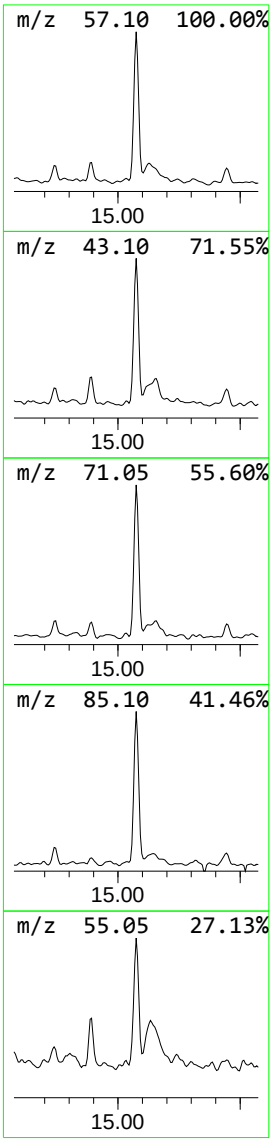
**********

Peak Number 12 Hexacosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.074 | 6.97 ng | 68447 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

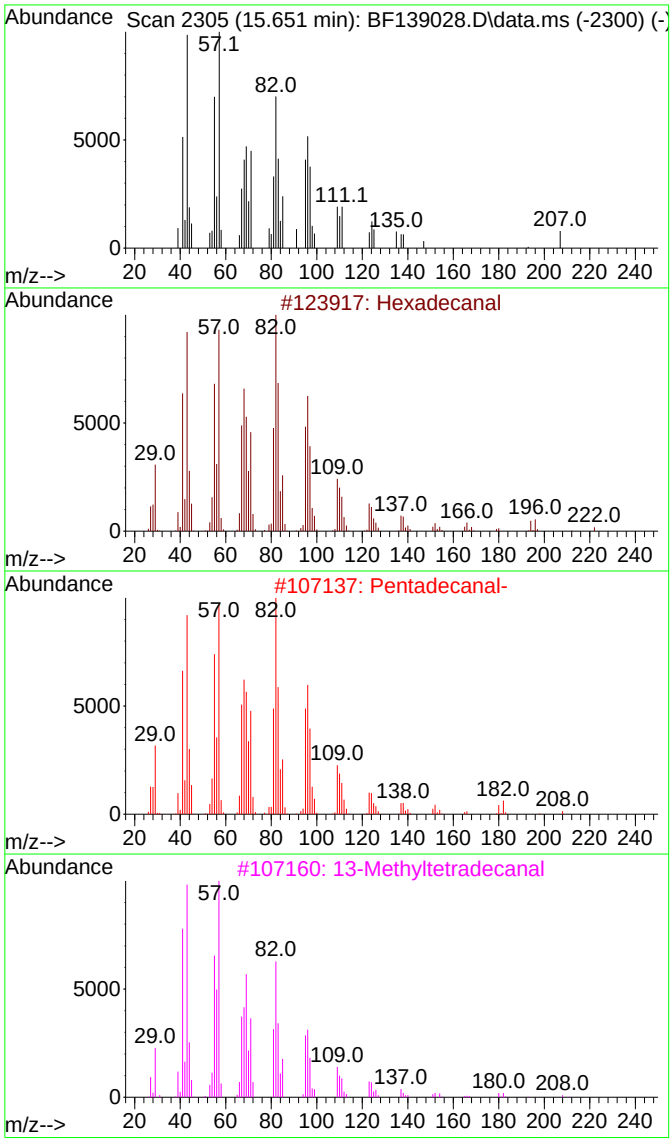
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

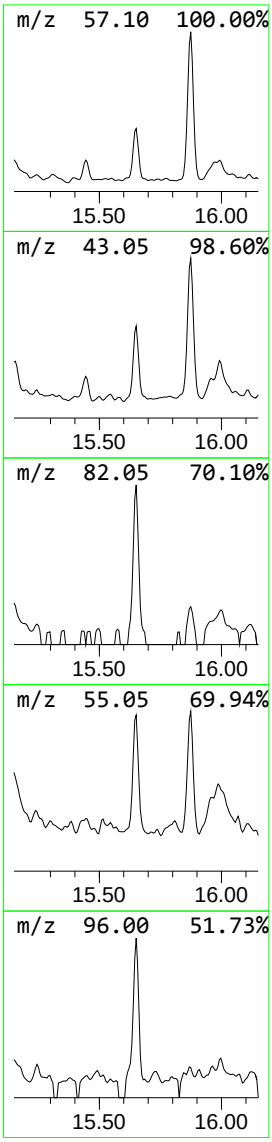
**********

Peak Number 13 Hexadecanal Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.651 | 4.27 ng | 42004 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanal | 240 | C16H32O | 000629-80-1 | 83 |
| 2 | Pentadecanal- | 226 | C15H30O | 002765-11-9 | 83 |
| 3 | 13-Methyltetradecanal | 226 | C15H30O | 075853-51-9 | 80 |
| 4 | 1,19-Eicosadiene | 278 | C20H38 | 014811-95-1 | 58 |
| 5 | Tetradecanal | 212 | C14H28O | 000124-25-4 | 52 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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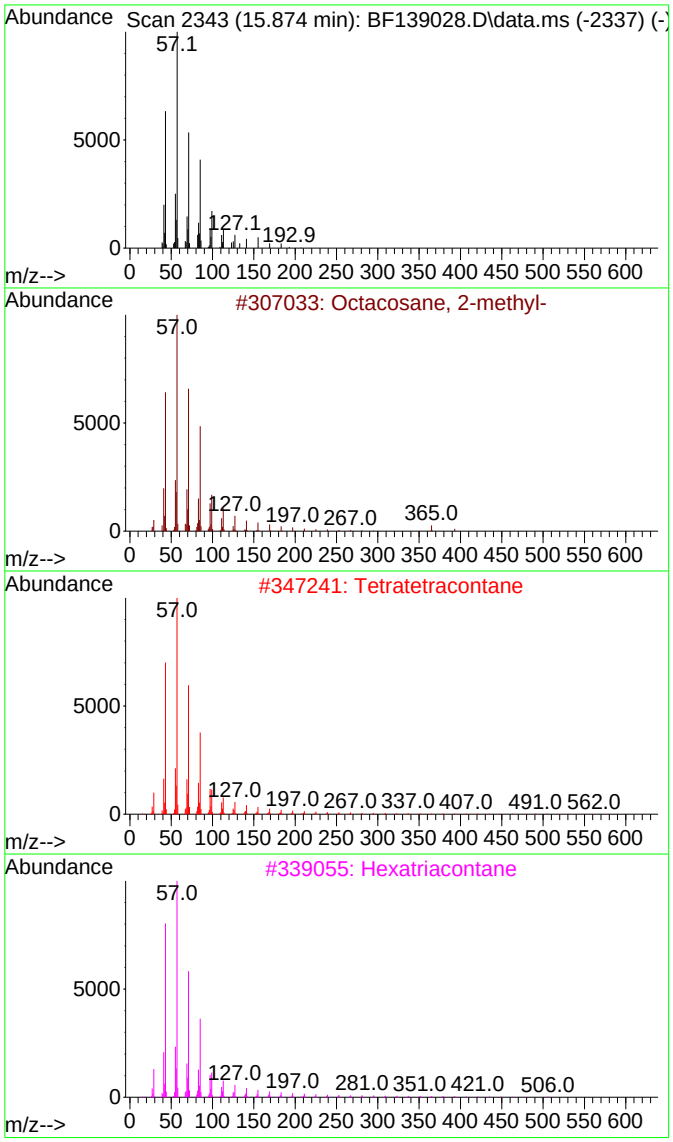
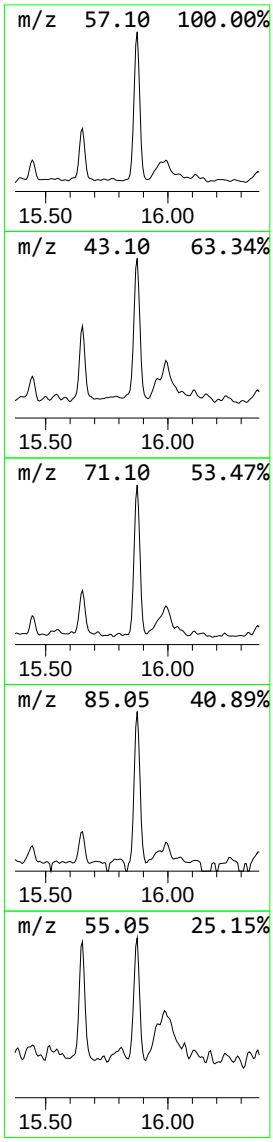
Peak Number 14 Octacosane, 2-methyl- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.874 | 6.01 ng | 59056 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane, 2-methyl- | 408 | C29H60 | 001560-98-1 | 91 |
| 2 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 91 |
| 3 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 91 |
| 4 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
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Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

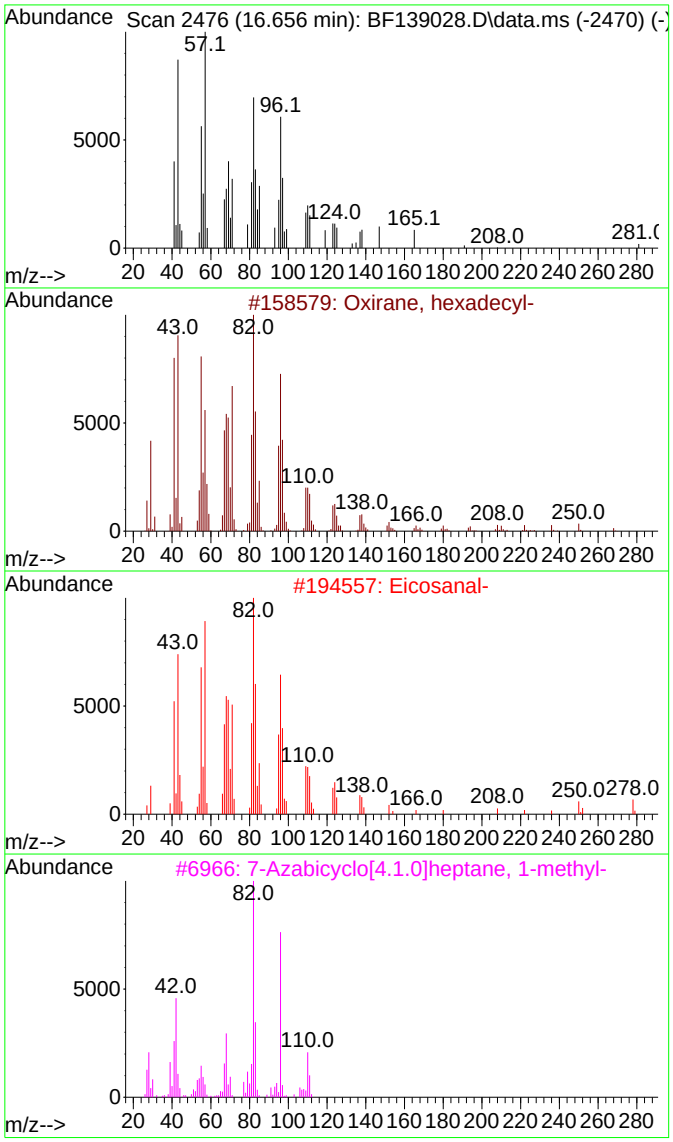
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

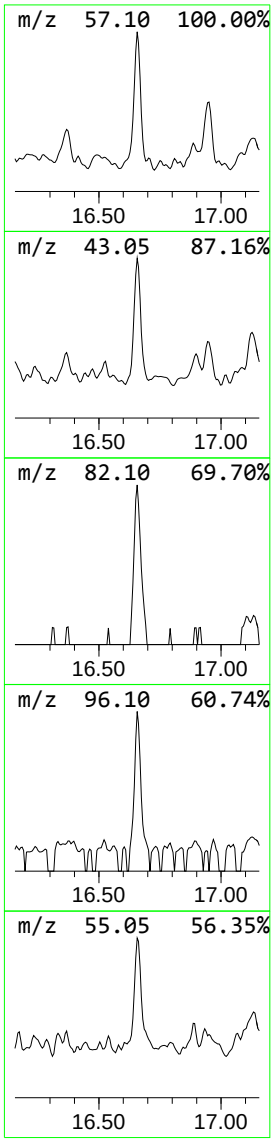
**********

Peak Number 15 Oxirane, hexadecyl- Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.656 | 4.08 ng | 40069 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 72 |
| 2 | Eicosanal- | 296 | C20H40O | 002400-66-0 | 58 |
| 3 | 7-Azabicyclo[4.1.0]heptane, 1-me... | 111 | C7H13N | 025022-25-7 | 43 |
| 4 | 1-Hentetracontanol | 593 | C41H84O | 040710-42-7 | 30 |
| 5 | Oxalic acid, isobutyl tetradecyl... | 342 | C20H38O4 | 1000309-37-9 | 18 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

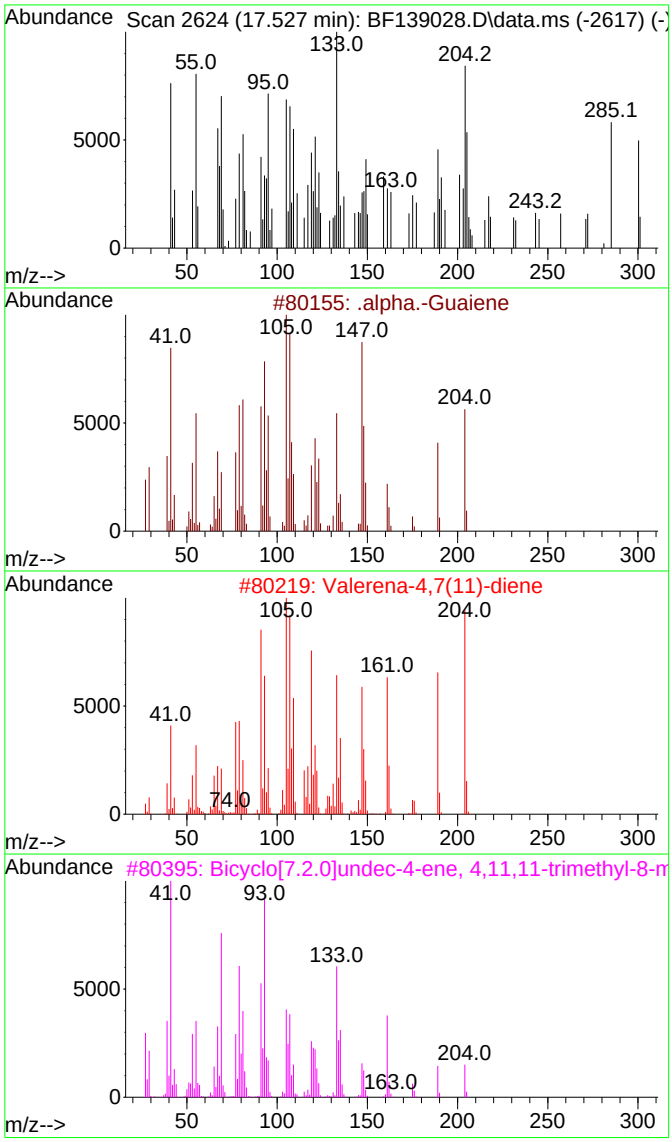
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

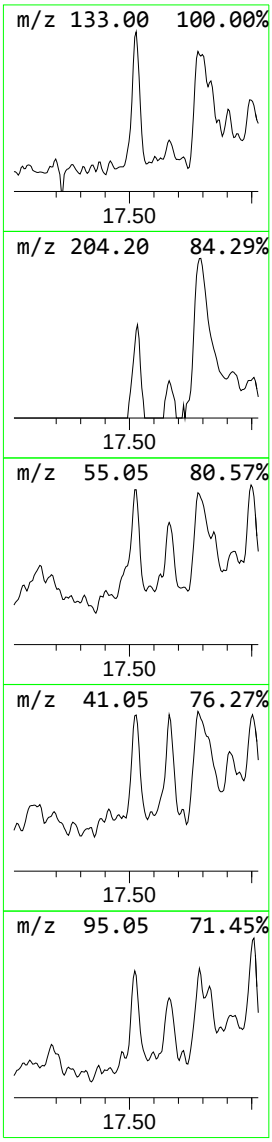
**********

Peak Number 16 .alpha.-Guaiene Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.527 | 6.87 ng | 67507 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .alpha.-Guaiene | 204 | C15H24 | 003691-12-1 | 50 |
| 2 | Valerena-4,7(11)-diene | 204 | C15H24 | 351222-66-7 | 45 |
| 3 | Bicyclo[7.2.0]undec-4-ene, 4,11,... | 204 | C15H24 | 000118-65-0 | 43 |
| 4 | 1H-Cyclopropa[a]naphthalene, 1a,... | 204 | C15H24 | 000489-29-2 | 41 |
| 5 | Naphthalene, decahydro-4a-methyl... | 204 | C15H24 | 017066-67-0 | 38 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

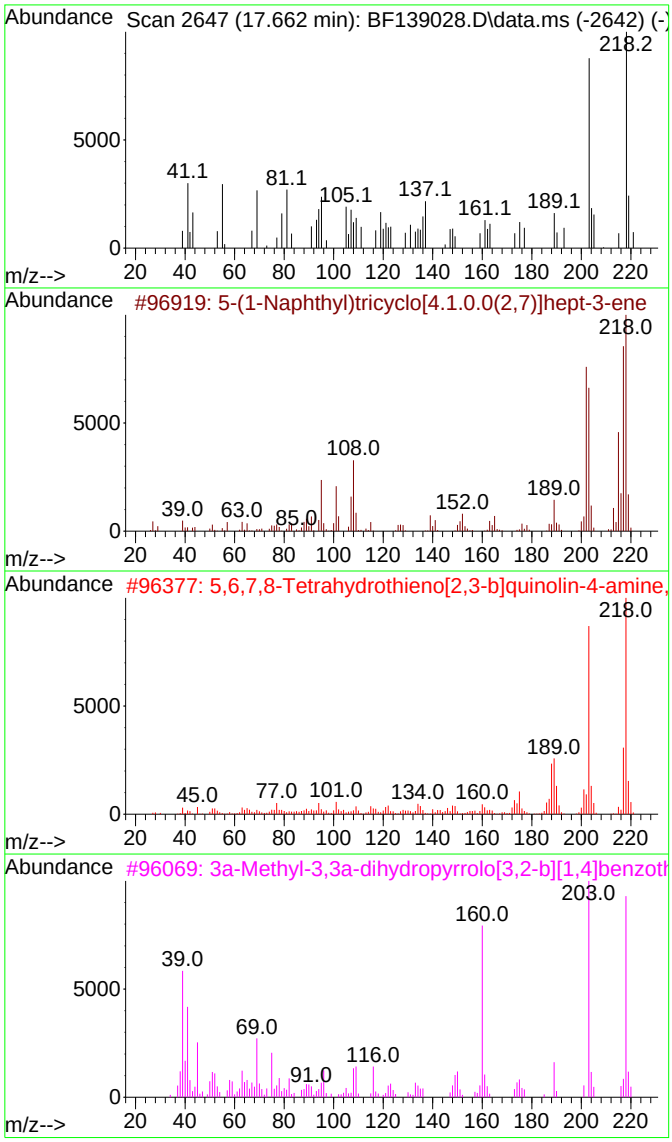
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

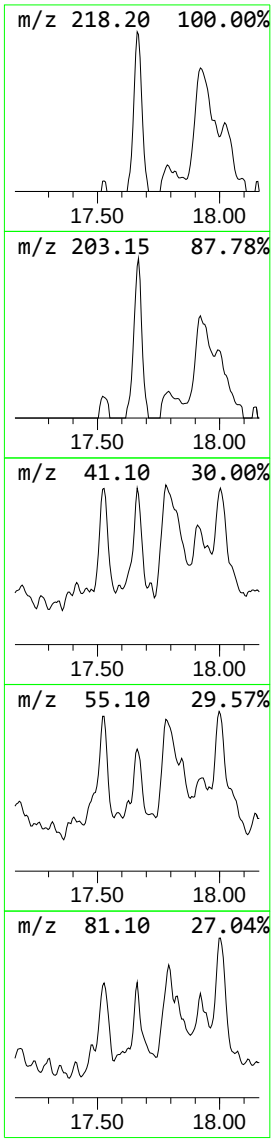
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 17 5-(1-Naphthyl)tricyclo[4.1.... Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.662 | 5.41 ng | 53188 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-(1-Naphthyl)tricyclo[4.1.0.0(2... | 218 | C17H14 | 107729-05-5 | 72 |
| 2 | 5,6,7,8-Tetrahydrothieno[2,3-b]q... | 218 | C12H14N2S | 134315-44-9 | 58 |
| 3 | 3a-Methyl-3,3a-dihydropyrrolo[3,... | 218 | C11H10N2OS | 017163-68-7 | 58 |
| 4 | 4-Allyl-5-pyridin-3-yl-2,4-dihyd... | 218 | C10H10N4S | 1000300-40-5 | 52 |
| 5 | Olean-12-en-3-ol, acetate, (3.be... | 468 | C32H52O2 | 001616-93-9 | 52 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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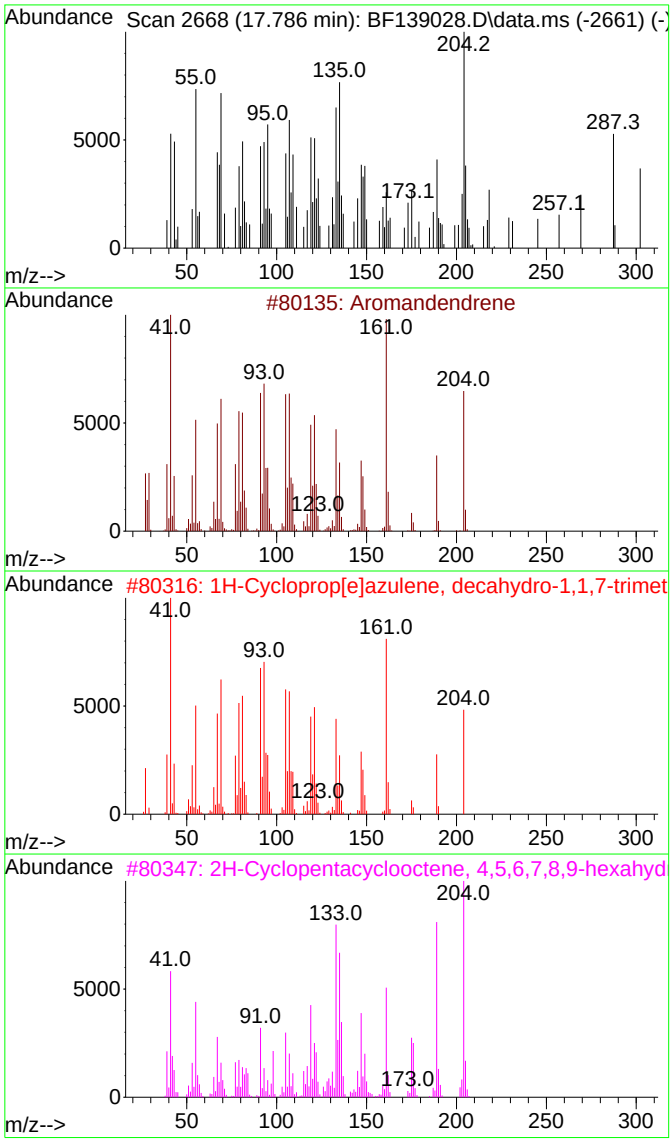
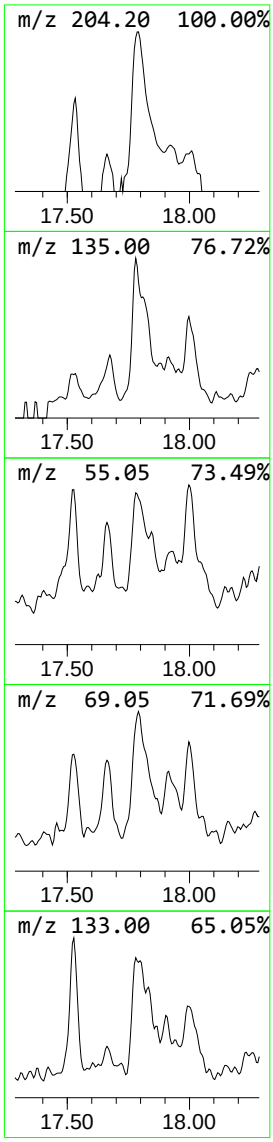
Peak Number 18 Aromandendrene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.786 | 18.15 ng | 178384 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Aromandendrene | 204 | C15H24 | 000489-39-4 | 70 |
| 2 | 1H-Cycloprop[e]azulene, decahydr... | 204 | C15H24 | 072747-25-2 | 60 |
| 3 | 2H-Cyclopentacyclooctene, 4,5,6,... | 204 | C15H24 | 1000221-85-8 | 53 |
| 4 | Azulene, 1,2,3,5,6,7,8,8a-octahy... | 204 | C15H24 | 003691-11-0 | 49 |
| 5 | Aciphyllene | 204 | C15H24 | 087745-31-1 | 42 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

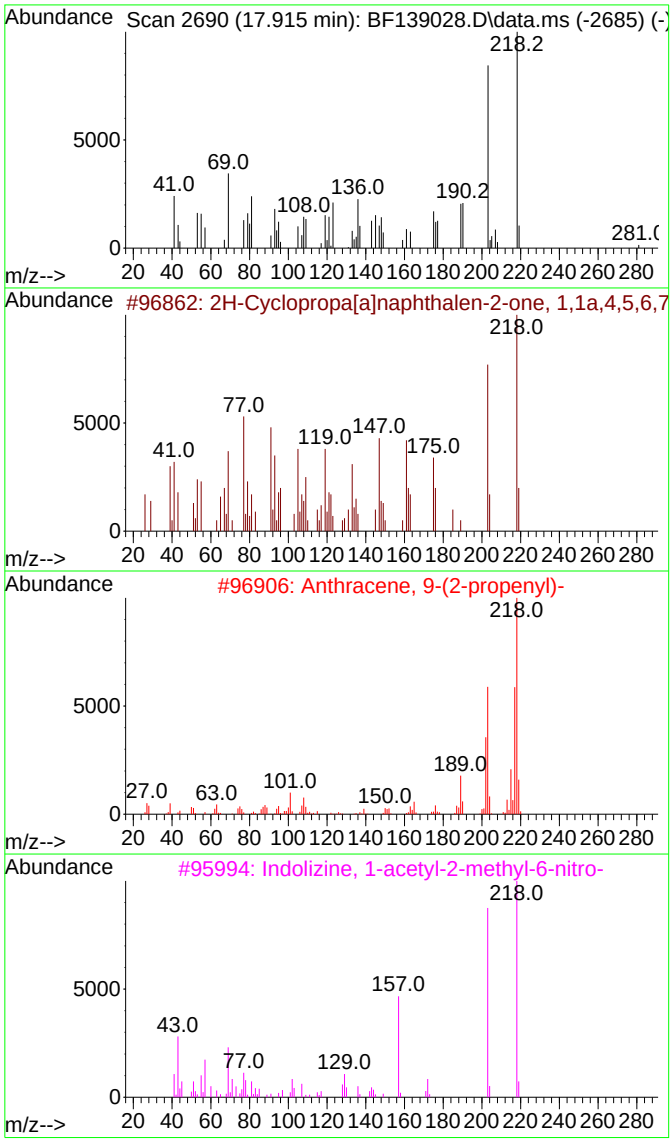
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

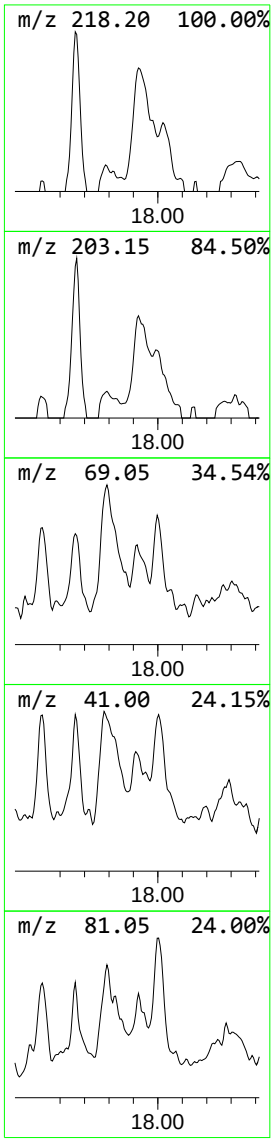
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 19 2H-Cyclopropa[a]naphthalen-... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.915 | 7.14 ng | 70145 | Perylene-d12 | 15.462 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2H-Cyclopropa[a]naphthalen-2-one... | 218 | C15H22O | 006831-17-0 | 50 |
| 2 | Anthracene, 9-(2-propenyl)- | 218 | C17H14 | 023707-65-5 | 50 |
| 3 | Indolizine, 1-acetyl-2-methyl-6-... | 218 | C11H10N2O3 | 1000071-33-1 | 49 |
| 4 | Naphthalene, 1-(4-methylphenyl)- | 218 | C17H14 | 027331-34-6 | 43 |
| 5 | 2,4(1H,3H)-Quinazolinedione, 1,3... | 218 | C12H14N2O2 | 002049-84-5 | 43 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

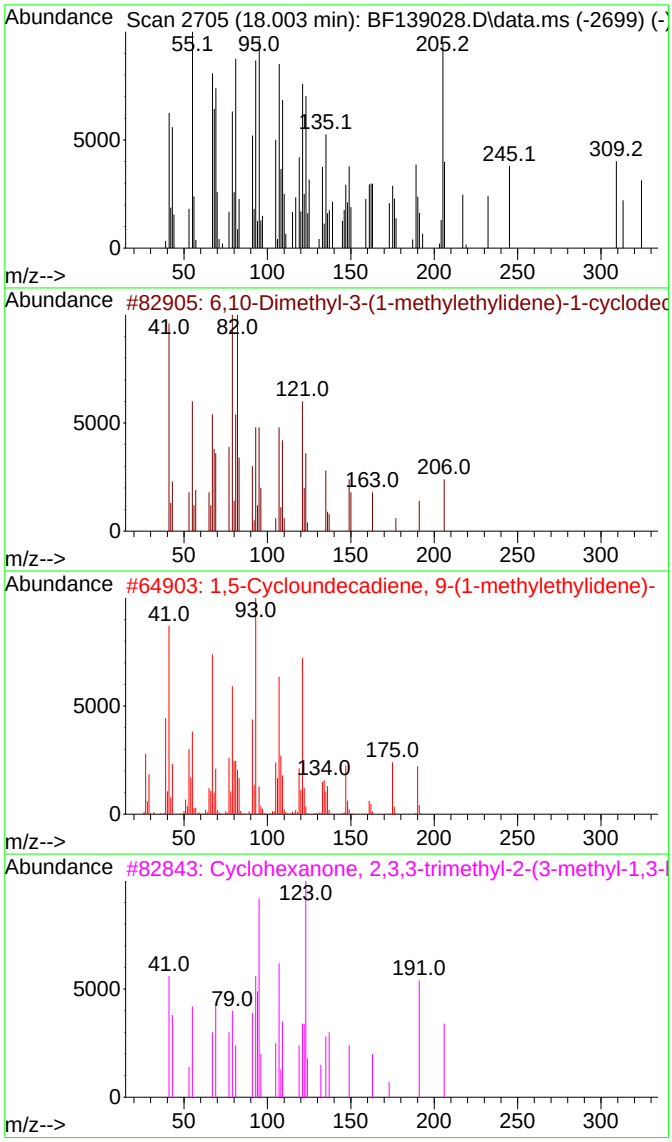
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

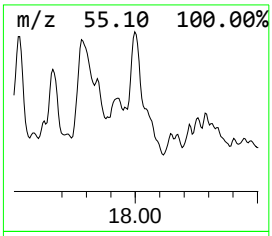
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 20 6,10-Dimethyl-3-(1-methylet... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.003 | 13.04 ng | 128139 | Perylene-d12 | 15.462 |

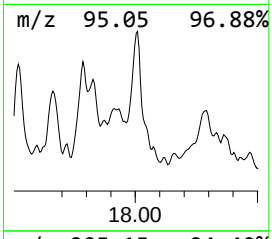
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6,10-Dimethyl-3-(1-methylethylid... | 206 | C15H26 | 069239-71-0 | 66 |
| 2 | 1,5-Cycloundecadiene, 9-(1-methy... | 190 | C14H22 | 062338-55-0 | 47 |
| 3 | Cyclohexanone, 2,3,3-trimethyl-2... | 206 | C14H22O | 069296-90-8 | 42 |
| 4 | 1-(2-Pyridyl)piperazine | 163 | C9H13N3 | 034803-66-2 | 38 |
| 5 | 9-Cedranone | 220 | C15H24O | 1000156-23-2 | 30 |



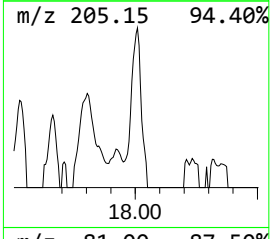


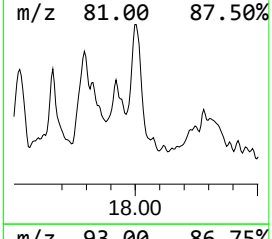






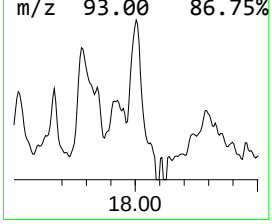










Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139028.D
Acq On : 15 Aug 2024 18:08
Operator : RC/JU
Sample : P3580-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
925-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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... | 2.122 | 62.3 | ng | 754445 | 1 | 6.833 | 242251 | 20.0 |
| 2-Pentanone, 4-... | 5.063 | 4.9 | ng | 59160 | 1 | 6.833 | 242251 | 20.0 |
| Eucalyptol | 6.981 | 9.9 | ng | 119675 | 1 | 6.833 | 242251 | 20.0 |
| 1-Phenoxypropan... | 8.433 | 4.6 | ng | 72150 | 2 | 8.116 | 311471 | 20.0 |
| unknown9.957 | 9.957 | 2.7 | ng | 47300 | 3 | 9.869 | 353320 | 20.0 |
| unknown11.863 | 11.863 | 3.4 | ng | 60962 | 4 | 11.357 | 354791 | 20.0 |
| (1S,4aR,7R)-1,4... | 13.739 | 8.0 | ng | 73128 | 5 | 13.998 | 183497 | 20.0 |
| Octadecyl trifl... | 13.821 | 9.8 | ng | 89684 | 5 | 13.998 | 183497 | 20.0 |
| Hexadecane | 14.439 | 6.0 | ng | 54721 | 5 | 13.998 | 183497 | 20.0 |
| Hexacosane | 15.074 | 7.0 | ng | 68447 | 6 | 15.462 | 196520 | 20.0 |
| Hexadecanal | 15.651 | 4.3 | ng | 42004 | 6 | 15.462 | 196520 | 20.0 |
| Octacosane, 2-m... | 15.874 | 6.0 | ng | 59056 | 6 | 15.462 | 196520 | 20.0 |
| Oxirane, hexade... | 16.656 | 4.1 | ng | 40069 | 6 | 15.462 | 196520 | 20.0 |
| .alpha.-Guaiene | 17.527 | 6.9 | ng | 67507 | 6 | 15.462 | 196520 | 20.0 |
| 5-(1-Naphthyl)t... | 17.662 | 5.4 | ng | 53188 | 6 | 15.462 | 196520 | 20.0 |
| Aromandendrene | 17.786 | 18.1 | ng | 178384 | 6 | 15.462 | 196520 | 20.0 |
| 2H-Cyclopropa[a... | 17.915 | 7.1 | ng | 70145 | 6 | 15.462 | 196520 | 20.0 |
| 6,10-Dimethyl-3... | 18.003 | 13.0 | ng | 128139 | 6 | 15.462 | 196520 | 20.0 |