LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

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_M\Methods\8270-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039060.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.057 | 295 | 301 | 310 | rBV | 1529632 | 2107735 | 26.94% | 3.066% |
| 2 | 5.522 | 373 | 380 | 392 | rBV | 3534025 | 4922943 | 62.92% | 7.160% |
| 3 | 7.128 | 645 | 653 | 666 | rBV | 3429187 | 5153694 | 65.87% | 7.496% |
| 4 | 7.969 | 789 | 796 | 803 | rBV | 981854 | 1498928 | 19.16% | 2.180% |
| 5 | 9.134 | 987 | 994 | 1002 | rBV | 1924706 | 3054677 | 39.04% | 4.443% |
| 6 | 10.781 | 1267 | 1274 | 1283 | rBV | 1224630 | 2013691 | 25.74% | 2.929% |
| 7 | 13.233 | 1684 | 1691 | 1700 | rBV | 3944396 | 5592831 | 71.48% | 8.134% |
| 8 | 14.333 | 1872 | 1878 | 1884 | rBV | 109144 | 188520 | 2.41% | 0.274% |
| 9 | 14.439 | 1890 | 1896 | 1904 | rBV2 | 46944 | 103598 | 1.32% | 0.151% |
| 10 | 14.610 | 1918 | 1925 | 1931 | rBV | 1682708 | 2398471 | 30.65% | 3.488% |
| 11 | 15.963 | 2148 | 2155 | 2166 | rVB | 307980 | 450007 | 5.75% | 0.655% |
| 12 | 16.092 | 2170 | 2177 | 2190 | rBV | 3264696 | 4605258 | 58.86% | 6.698% |
| 13 | 17.351 | 2385 | 2391 | 2395 | rBV | 2011808 | 2827011 | 36.13% | 4.112% |
| 14 | 17.392 | 2395 | 2398 | 2405 | rVV | 490931 | 692645 | 8.85% | 1.007% |
| 15 | 17.486 | 2409 | 2414 | 2419 | rVV | 127772 | 188313 | 2.41% | 0.274% |
| 16 | 18.245 | 2536 | 2543 | 2546 | rBV2 | 472464 | 765943 | 9.79% | 1.114% |
| 17 | 18.274 | 2546 | 2548 | 2554 | rVV | 206875 | 309665 | 3.96% | 0.450% |
| 18 | 18.357 | 2558 | 2562 | 2568 | rVV | 68677 | 125333 | 1.60% | 0.182% |
| 19 | 18.427 | 2568 | 2574 | 2577 | rVV2 | 156138 | 306768 | 3.92% | 0.446% |
| 20 | 18.462 | 2577 | 2580 | 2584 | rVB | 86137 | 112986 | 1.44% | 0.164% |
| 21 | 18.727 | 2621 | 2625 | 2629 | rBV | 80562 | 103144 | 1.32% | 0.150% |
| 22 | 19.145 | 2691 | 2696 | 2700 | rBV | 101285 | 164170 | 2.10% | 0.239% |
| 23 | 19.280 | 2715 | 2719 | 2727 | rBV2 | 68487 | 129359 | 1.65% | 0.188% |
| 24 | 19.404 | 2732 | 2740 | 2747 | rBV | 1708373 | 2351927 | 30.06% | 3.421% |
| 25 | 19.521 | 2755 | 2760 | 2763 | rBV2 | 233871 | 346862 | 4.43% | 0.504% |
| 26 | 19.556 | 2763 | 2766 | 2770 | rVB | 86842 | 117381 | 1.50% | 0.171% |
| 27 | 19.739 | 2792 | 2797 | 2798 | rBV | 219831 | 292395 | 3.74% | 0.425% |
| 28 | 19.768 | 2798 | 2802 | 2810 | rVV | 1463467 | 2003529 | 25.61% | 2.914% |
| 29 | 19.839 | 2811 | 2814 | 2820 | rVB2 | 80631 | 115399 | 1.47% | 0.168% |
| 30 | 19.974 | 2829 | 2837 | 2842 | rBV | 6281002 | 7824100 | 100.00% | 11.380% |
| 31 | 20.092 | 2852 | 2857 | 2863 | rBV4 | 117047 | 296171 | 3.79% | 0.431% |
| 32 | 20.227 | 2876 | 2880 | 2881 | rBV3 | 87615 | 112962 | 1.44% | 0.164% |
| 33 | 20.262 | 2883 | 2886 | 2892 | rVB | 263050 | 359190 | 4.59% | 0.522% |
| 34 | 20.362 | 2899 | 2903 | 2906 | rBV | 150259 | 192483 | 2.46% | 0.280% |
| 35 | 20.421 | 2908 | 2913 | 2917 | rVB2 | 170544 | 271006 | 3.46% | 0.394% |
| 36 | 20.562 | 2934 | 2937 | 2940 | rBV | 86072 | 102630 | 1.31% | 0.149% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

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_M\Methods\8270-BM030823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 20.603 | 2942 | 2944 | 2948 | rVV2 | 83998 | 98281 | 1.26% | 0.143% |
| 38 | 20.662 | 2951 | 2954 | 2958 | rVB2 | 98486 | 111707 | 1.43% | 0.162% |
| 39 | 21.009 | 3009 | 3013 | 3019 | rBV | 139725 | 195766 | 2.50% | 0.285% |
| 40 | 21.174 | 3039 | 3041 | 3045 | rVB | 148316 | 148838 | 1.90% | 0.216% |
| 41 | 21.233 | 3045 | 3051 | 3059 | rBV4 | 540086 | 1101556 | 14.08% | 1.602% |
| 42 | 21.527 | 3094 | 3101 | 3105 | rBV2 | 3018373 | 5377815 | 68.73% | 7.822% |
| 43 | 21.568 | 3105 | 3108 | 3116 | rVB | 1084353 | 1433852 | 18.33% | 2.085% |
| 44 | 23.221 | 3384 | 3389 | 3395 | rBV | 880810 | 2121923 | 27.12% | 3.086% |
| 45 | 23.744 | 3474 | 3478 | 3486 | rVB | 496377 | 944987 | 12.08% | 1.374% |
| 46 | 23.850 | 3491 | 3496 | 3504 | rVB | 741750 | 1452903 | 18.57% | 2.113% |
| 47 | 23.962 | 3509 | 3515 | 3522 | rBV2 | 1746006 | 3565647 | 45.57% | 5.186% |

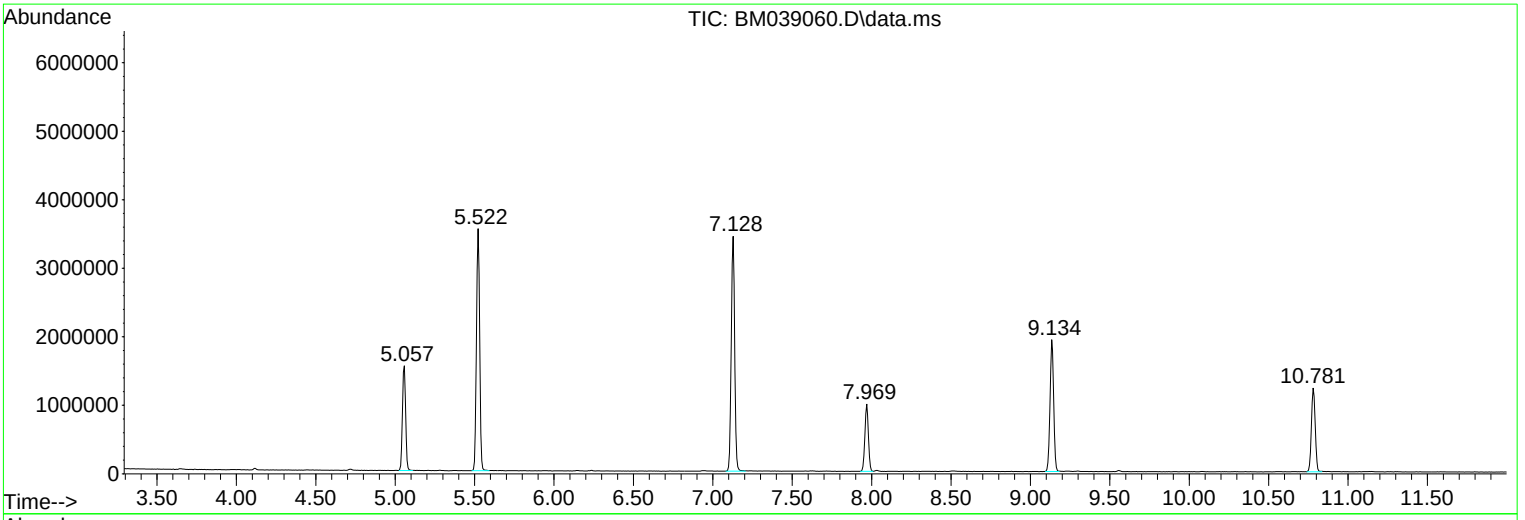
Sum of corrected areas: 68755000

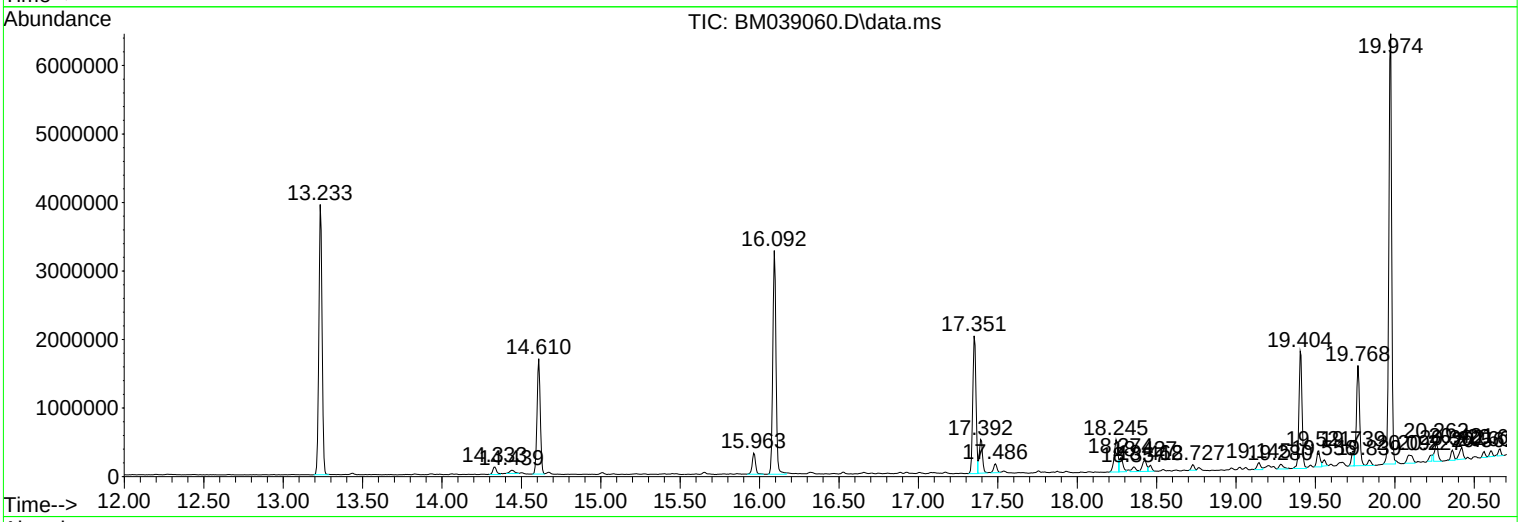
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

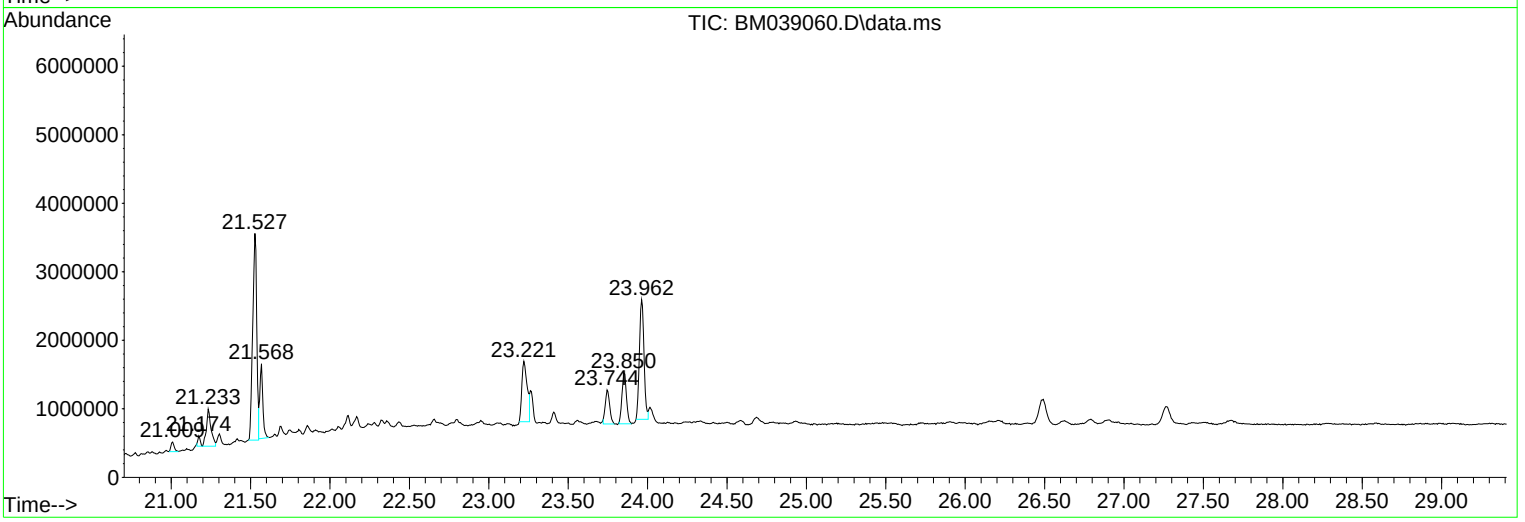
**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

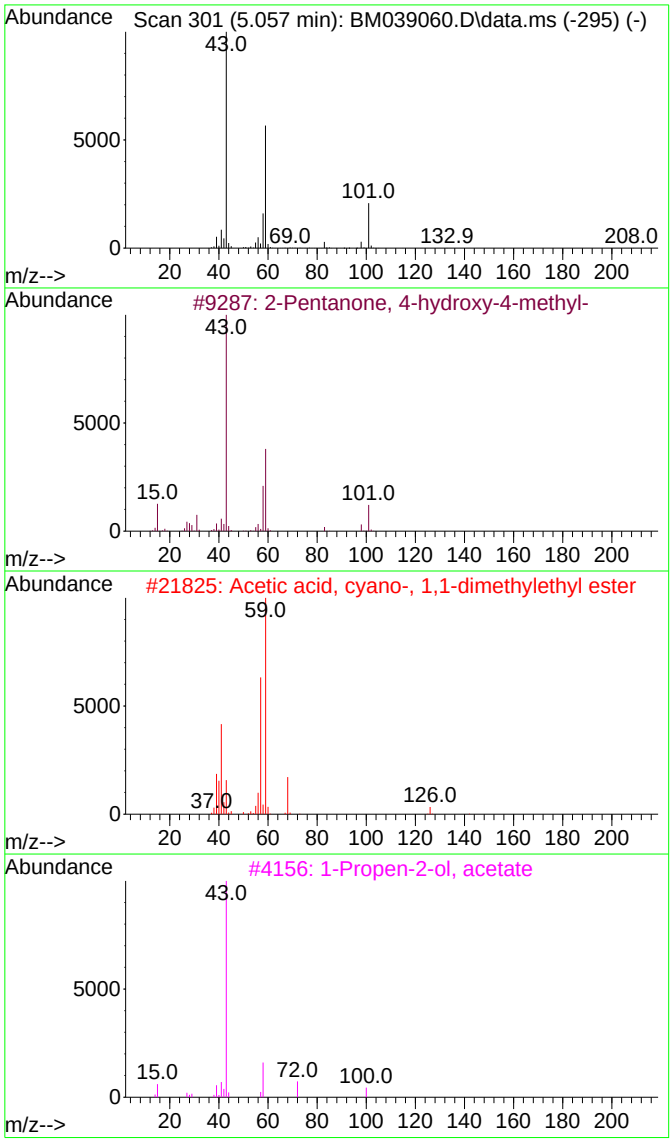
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

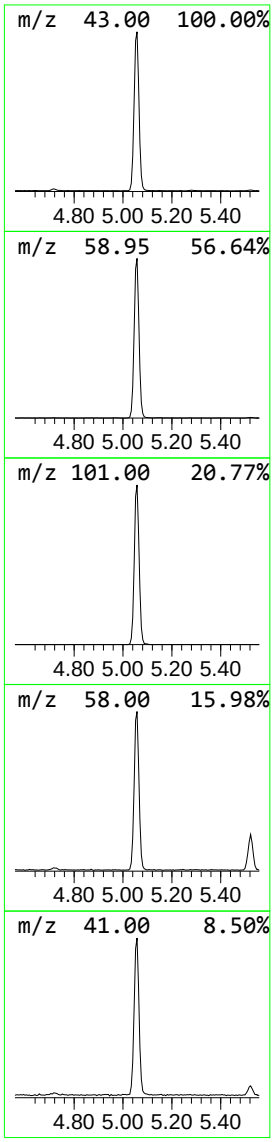
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.057 | 28.12 ng | 2107740 | 1,4-Dichlorobenzene-d4 | 7.969 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

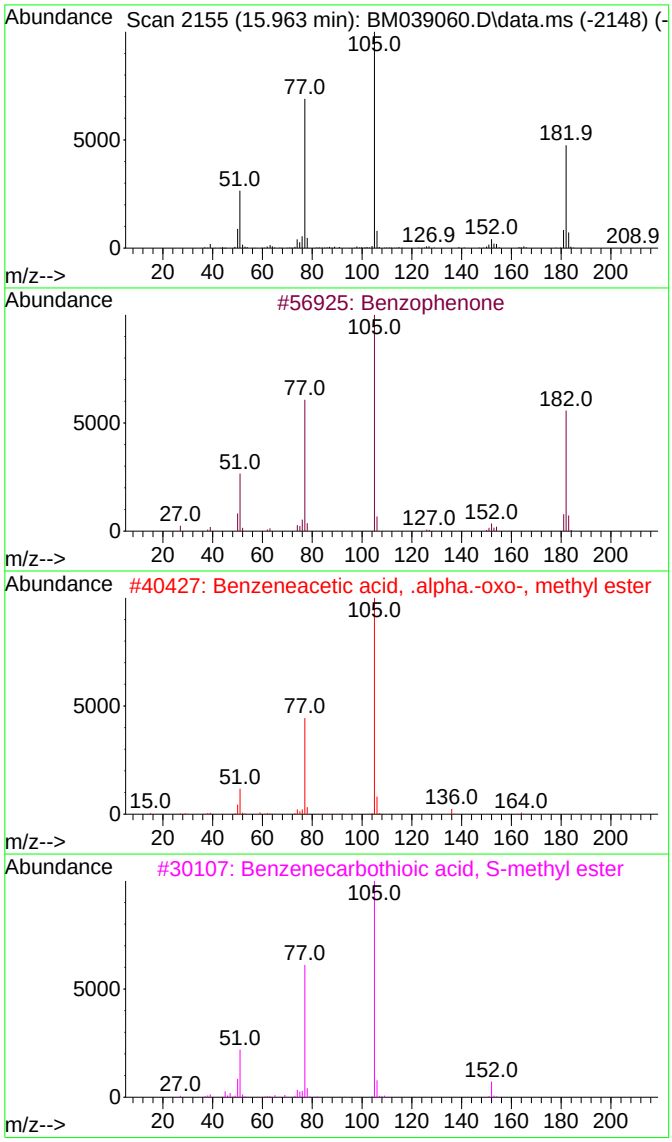
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

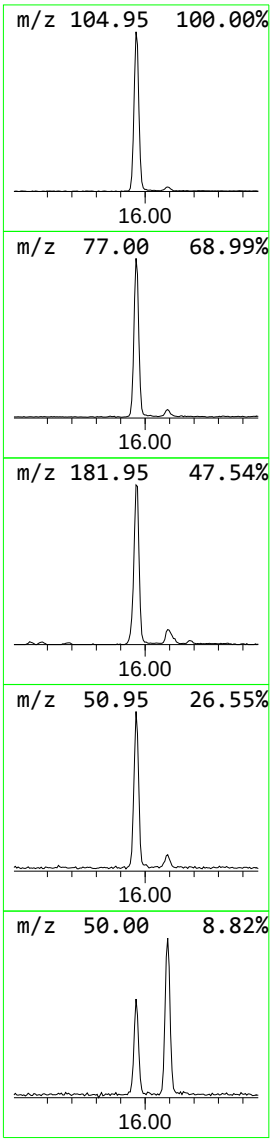
**********

Peak Number 2 Benzophenone Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.963 | 3.75 ng | 450007 | Acenaphthene-d10 | 14.610 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Benzeneacetic acid, .alpha.-oxo-... | 164 | C9H8O3 | 015206-55-0 | 53 |
| 3 | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS | 005925-68-8 | 49 |
| 4 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 49 |
| 5 | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 49 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

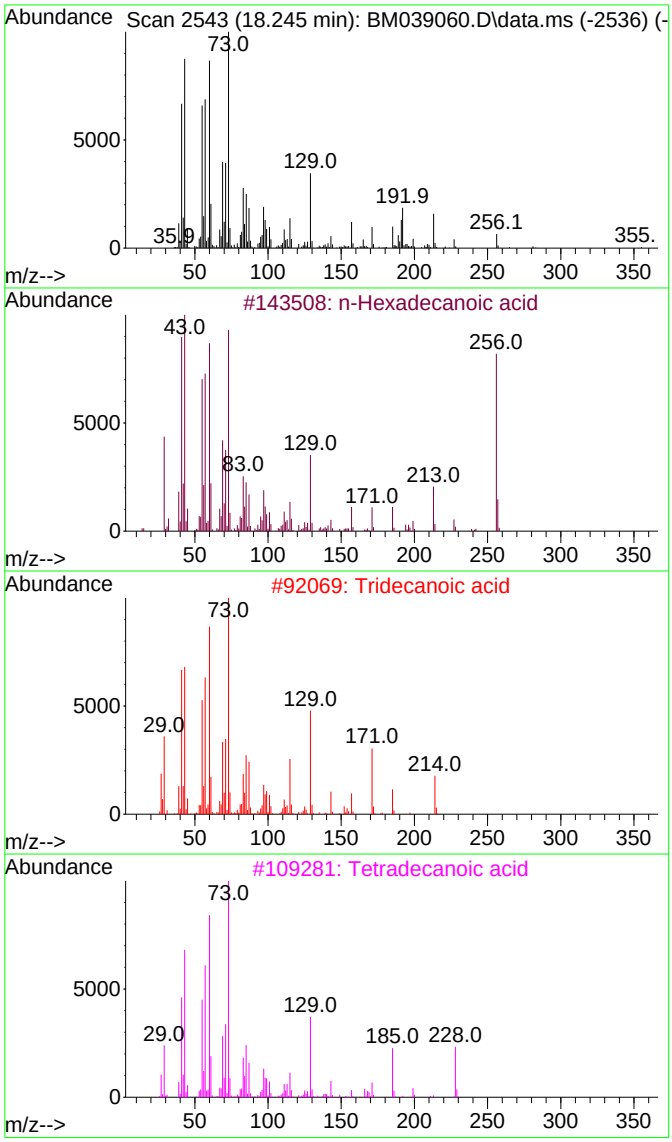
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

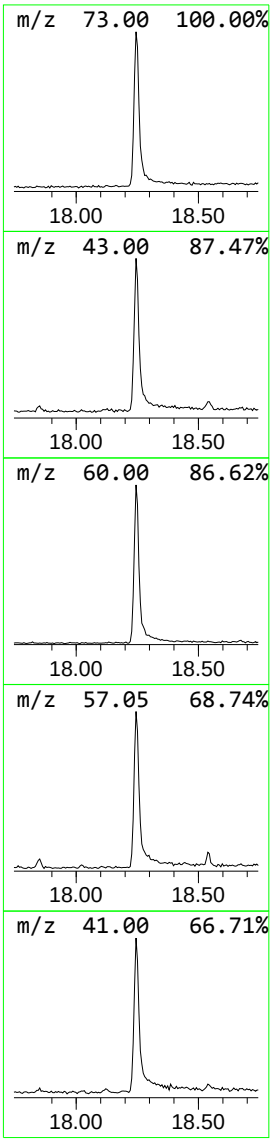
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.245 | 5.42 ng | 765943 | Phenanthrene-d10 | 17.351 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 93 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 5 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 83 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

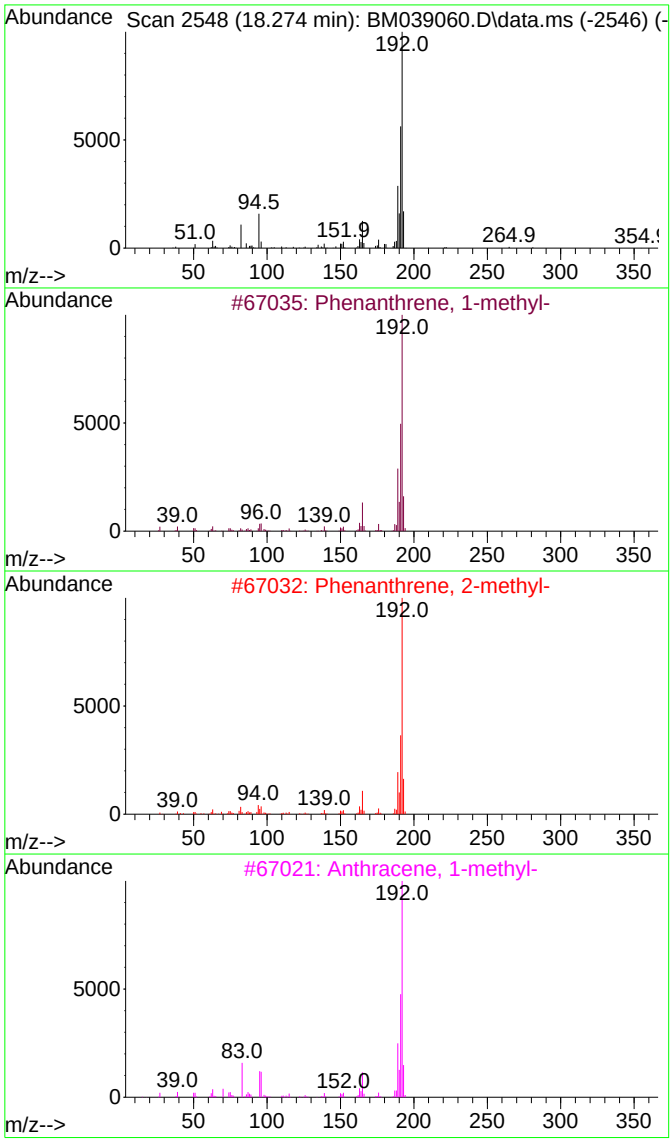
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

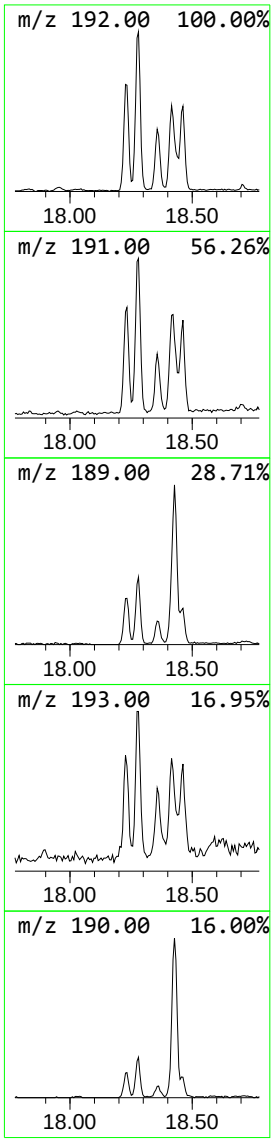
**********

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.274 | 2.19 ng | 309665 | Phenanthrene-d10 | 17.351 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenanthrene, 1-methyl- | 192 | C15H12 | 000832-69-9 | 96 |
| 2 | Phenanthrene, 2-methyl- | 192 | C15H12 | 002531-84-2 | 94 |
| 3 | Anthracene, 1-methyl- | 192 | C15H12 | 000610-48-0 | 91 |
| 4 | Anthracene, 2-methyl- | 192 | C15H12 | 000613-12-7 | 91 |
| 5 | 1H-Cyclopropa[l]phenanthrene,1a,... | 192 | C15H12 | 000949-41-7 | 90 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

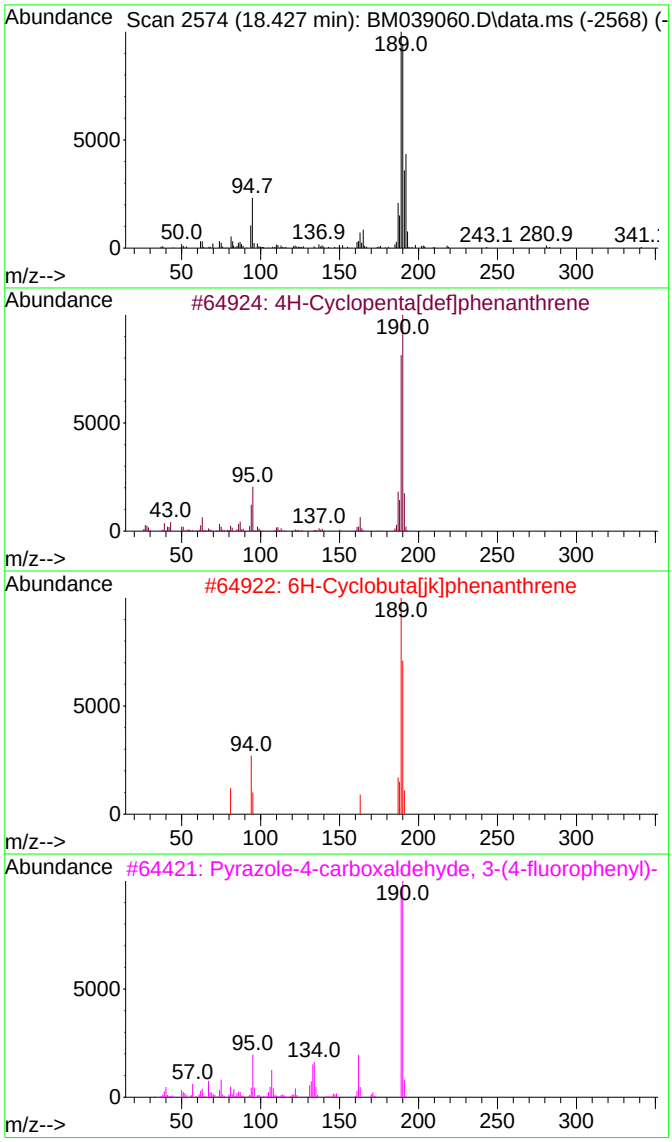
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

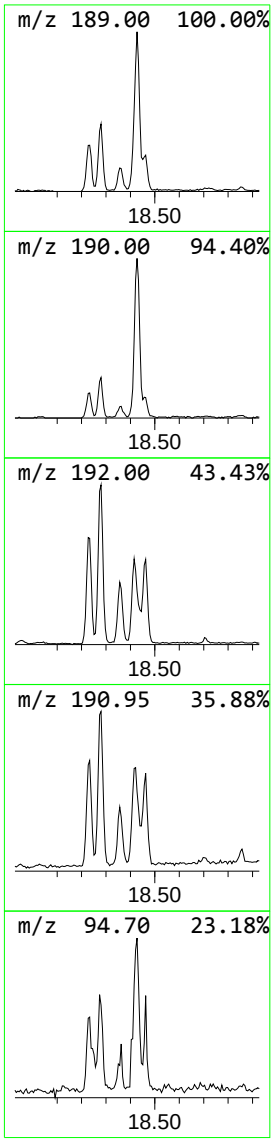
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.427 | 2.17 ng | 306768 | Phenanthrene-d10 | 17.351 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 89 |
| 2 | 6H-Cyclobuta[jk]phenanthrene | 190 | C15H10 | 083469-43-6 | 53 |
| 3 | Pyrazole-4-carboxaldehyde, 3-(4-... | 190 | C10H7FN2O | 306936-57-2 | 50 |
| 4 | Thiophene-3-carboxaldehyde, 5-ch... | 190 | C5H4BClO3S | 036155-87-0 | 50 |
| 5 | Carbonic acid, ethyl 2-formyl-4,... | 262 | C10H8Cl2O4 | 1000331-34-4 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

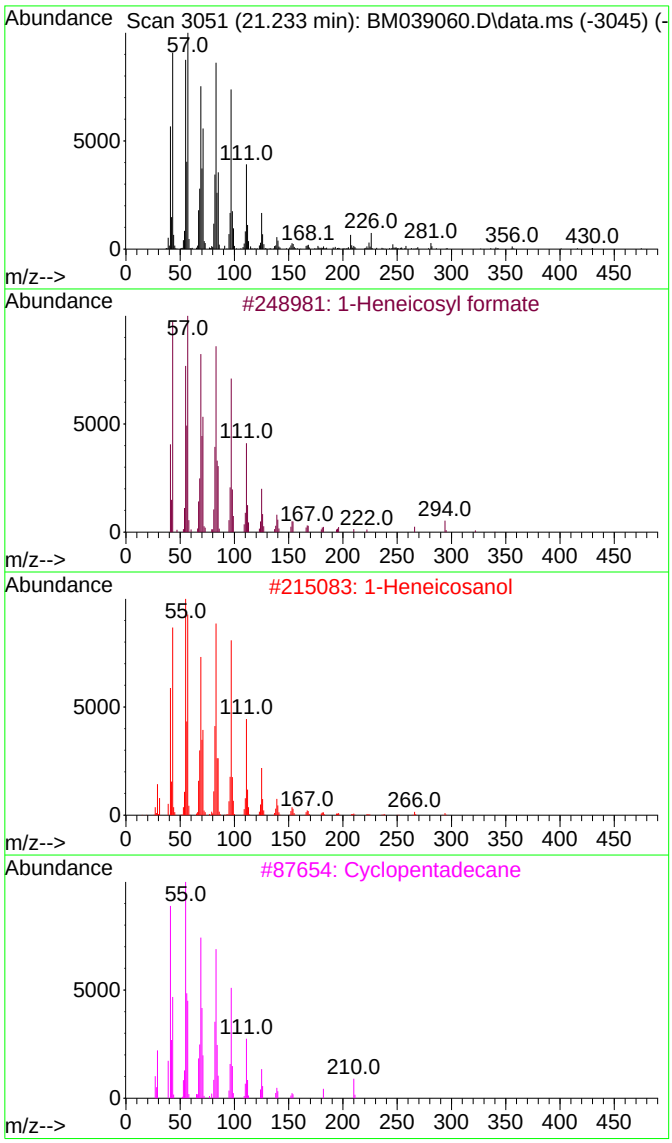
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

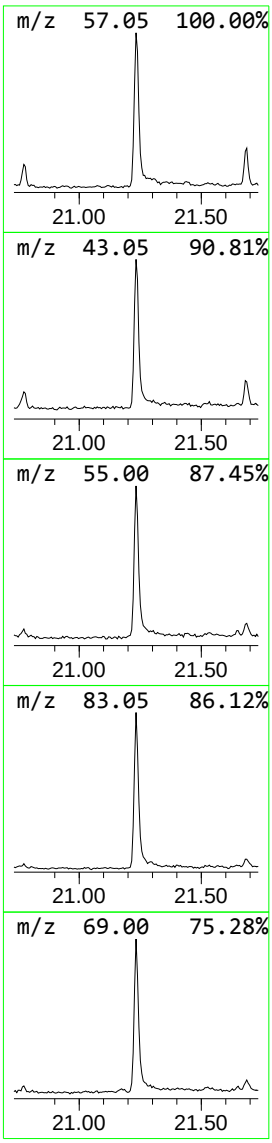
**********

Peak Number 6 1-Heneicosyl formate Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.233 | 4.10 ng | 1101560 | Chrysene-d12 | 21.527 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 95 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 3 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 94 |
| 4 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 94 |
| 5 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 94 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

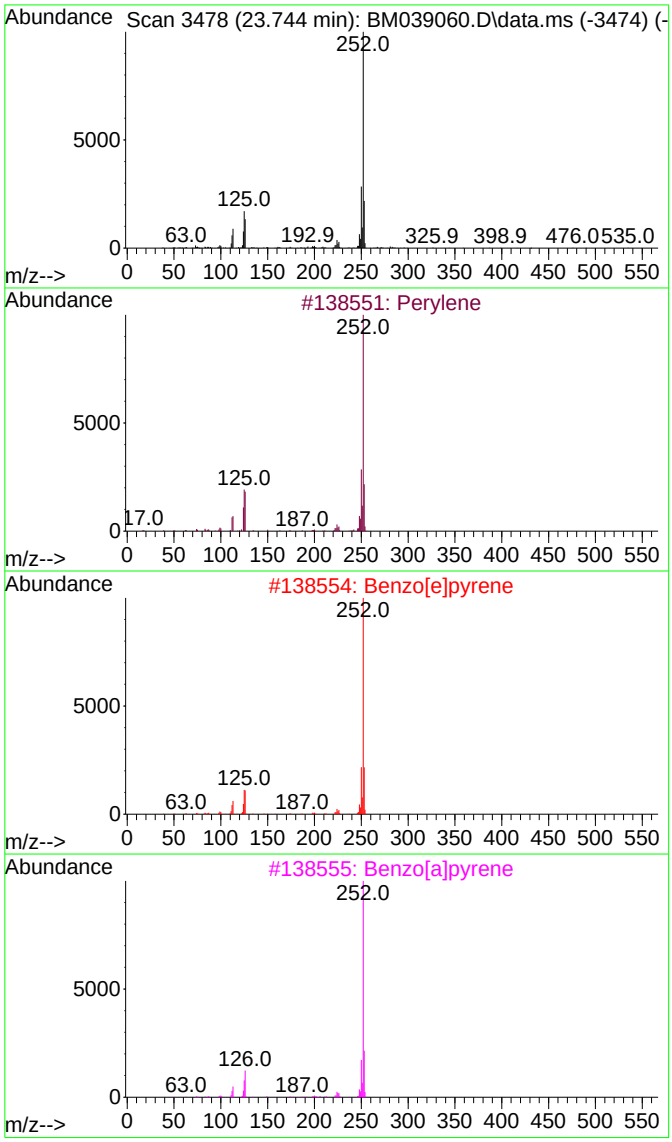
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

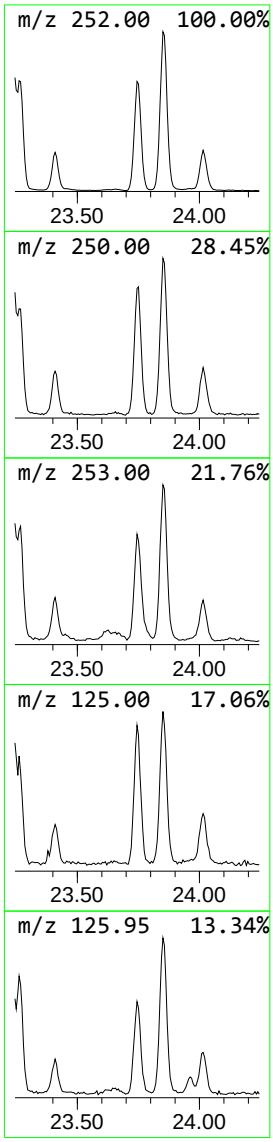
**********

Peak Number 7 Perylene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.744 | 5.30 ng | 944987 | Perylene-d12 | 23.962 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Perylene | 252 | C20H12 | 000198-55-0 | 99 |
| 2 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 98 |
| 3 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 96 |
| 4 | Benzo[j]fluoranthene | 252 | C20H12 | 000205-82-3 | 95 |
| 5 | Benzo[b]fluoranthene | 252 | C20H12 | 000205-99-2 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032023\
Data File : BM039060.D
Acq On : 21 Mar 2023 00:57
Operator : CG/JU
Sample : 01964-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_M
**ClientSampleId :**
MAPLE-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.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 |
| 2-Pentanone, 4-... | 5.057 | 28.1 | ng | 2107740 | 1 | 7.969 | 1498930 | 20.0 |
| Benzophenone | 15.963 | 3.8 | ng | 450007 | 3 | 14.610 | 2398470 | 20.0 |
| n-Hexadecanoic ... | 18.245 | 5.4 | ng | 765943 | 4 | 17.351 | 2827010 | 20.0 |
| Phenanthrene, 1... | 18.274 | 2.2 | ng | 309665 | 4 | 17.351 | 2827010 | 20.0 |
| 4H-Cyclopenta[d... | 18.427 | 2.2 | ng | 306768 | 4 | 17.351 | 2827010 | 20.0 |
| 1-Heneicosyl fo... | 21.233 | 4.1 | ng | 1101560 | 5 | 21.527 | 5377820 | 20.0 |
| Perylene | 23.744 | 5.3 | ng | 944987 | 6 | 23.962 | 3565650 | 20.0 |