LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

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_G\Methods\8270-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061082.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.158 | 24 | 29 | 34 | rVB3 | 14369 | 23453 | 2.77% | 0.317% |
| 2 | 3.681 | 113 | 118 | 121 | rBV2 | 5374 | 8581 | 1.01% | 0.116% |
| 3 | 5.526 | 425 | 432 | 443 | rBV | 219166 | 356902 | 42.20% | 4.819% |
| 4 | 7.106 | 692 | 701 | 714 | rBV | 233077 | 406212 | 48.03% | 5.485% |
| 5 | 7.935 | 833 | 842 | 849 | rBV | 121863 | 201674 | 23.85% | 2.723% |
| 6 | 9.086 | 1030 | 1038 | 1046 | rBV | 156414 | 269625 | 31.88% | 3.641% |
| 7 | 10.732 | 1309 | 1318 | 1324 | rBV | 145325 | 269205 | 31.83% | 3.635% |
| 8 | 13.182 | 1729 | 1735 | 1742 | rBV | 406496 | 612223 | 72.39% | 8.267% |
| 9 | 13.881 | 1849 | 1854 | 1860 | rVB5 | 6057 | 11275 | 1.33% | 0.152% |
| 10 | 14.280 | 1917 | 1922 | 1929 | rBV3 | 7606 | 15018 | 1.78% | 0.203% |
| 11 | 14.562 | 1963 | 1970 | 1977 | rBV | 224675 | 355465 | 42.03% | 4.800% |
| 12 | 14.627 | 1977 | 1981 | 1987 | rVB3 | 15092 | 21252 | 2.51% | 0.287% |
| 13 | 14.956 | 2032 | 2037 | 2043 | rBV2 | 11116 | 19123 | 2.26% | 0.258% |
| 14 | 15.608 | 2143 | 2148 | 2157 | rBV2 | 22835 | 38716 | 4.58% | 0.523% |
| 15 | 16.049 | 2217 | 2223 | 2230 | rBV | 354501 | 542003 | 64.09% | 7.319% |
| 16 | 16.284 | 2258 | 2263 | 2264 | rBV3 | 9938 | 10176 | 1.20% | 0.137% |
| 17 | 16.307 | 2266 | 2267 | 2272 | rVB4 | 10470 | 9862 | 1.17% | 0.133% |
| 18 | 16.613 | 2311 | 2319 | 2324 | rBV9 | 6684 | 15848 | 1.87% | 0.214% |
| 19 | 17.130 | 2402 | 2407 | 2412 | rVB4 | 23416 | 38865 | 4.60% | 0.525% |
| 20 | 17.306 | 2431 | 2437 | 2441 | rBV | 277621 | 434506 | 51.38% | 5.867% |
| 21 | 17.353 | 2441 | 2445 | 2449 | rVB | 158780 | 230496 | 27.26% | 3.113% |
| 22 | 17.441 | 2454 | 2460 | 2465 | rVB | 59718 | 91854 | 10.86% | 1.240% |
| 23 | 17.500 | 2465 | 2470 | 2474 | rBV7 | 10456 | 22343 | 2.64% | 0.302% |
| 24 | 17.712 | 2501 | 2506 | 2510 | rBV | 15398 | 28708 | 3.39% | 0.388% |
| 25 | 18.205 | 2583 | 2590 | 2593 | rBV3 | 78138 | 140383 | 16.60% | 1.896% |
| 26 | 18.317 | 2606 | 2609 | 2613 | rVB4 | 12515 | 13334 | 1.58% | 0.180% |
| 27 | 18.381 | 2615 | 2620 | 2624 | rBV4 | 42649 | 75542 | 8.93% | 1.020% |
| 28 | 18.681 | 2668 | 2671 | 2674 | rBV2 | 17054 | 19087 | 2.26% | 0.258% |
| 29 | 18.934 | 2711 | 2714 | 2717 | rBV4 | 19323 | 18253 | 2.16% | 0.246% |
| 30 | 19.069 | 2733 | 2737 | 2738 | rBV4 | 11498 | 14337 | 1.70% | 0.194% |
| 31 | 19.098 | 2739 | 2742 | 2747 | rVV2 | 29148 | 48483 | 5.73% | 0.655% |
| 32 | 19.239 | 2764 | 2766 | 2773 | rVB8 | 16519 | 20104 | 2.38% | 0.271% |
| 33 | 19.363 | 2782 | 2787 | 2793 | rBV | 261830 | 363839 | 43.02% | 4.913% |
| 34 | 19.421 | 2793 | 2797 | 2802 | rBV | 101624 | 134840 | 15.94% | 1.821% |
| 35 | 19.480 | 2805 | 2807 | 2810 | rVB3 | 20949 | 20610 | 2.44% | 0.278% |
| 36 | 19.727 | 2845 | 2849 | 2857 | rVB | 231169 | 346212 | 40.94% | 4.675% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

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_G\Methods\8270-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 19.880 | 2873 | 2875 | 2876 | rBV2 | 16987 | 14011 | 1.66% | 0.189% |
| 38 | 19.927 | 2878 | 2883 | 2888 | rVV | 657713 | 845694 | 100.00% | 11.420% |
| 39 | 20.220 | 2930 | 2933 | 2936 | rVB | 55707 | 65762 | 7.78% | 0.888% |
| 40 | 20.320 | 2947 | 2950 | 2954 | rVB | 34099 | 40712 | 4.81% | 0.550% |
| 41 | 20.520 | 2980 | 2984 | 2986 | rBV | 33199 | 46917 | 5.55% | 0.634% |
| 42 | 21.566 | 3155 | 3162 | 3167 | rBV2 | 311737 | 696350 | 82.34% | 9.403% |
| 43 | 21.613 | 3167 | 3170 | 3177 | rVB | 130801 | 202515 | 23.95% | 2.735% |
| 44 | 24.686 | 3688 | 3693 | 3701 | rVB | 106907 | 245015 | 28.97% | 3.309% |

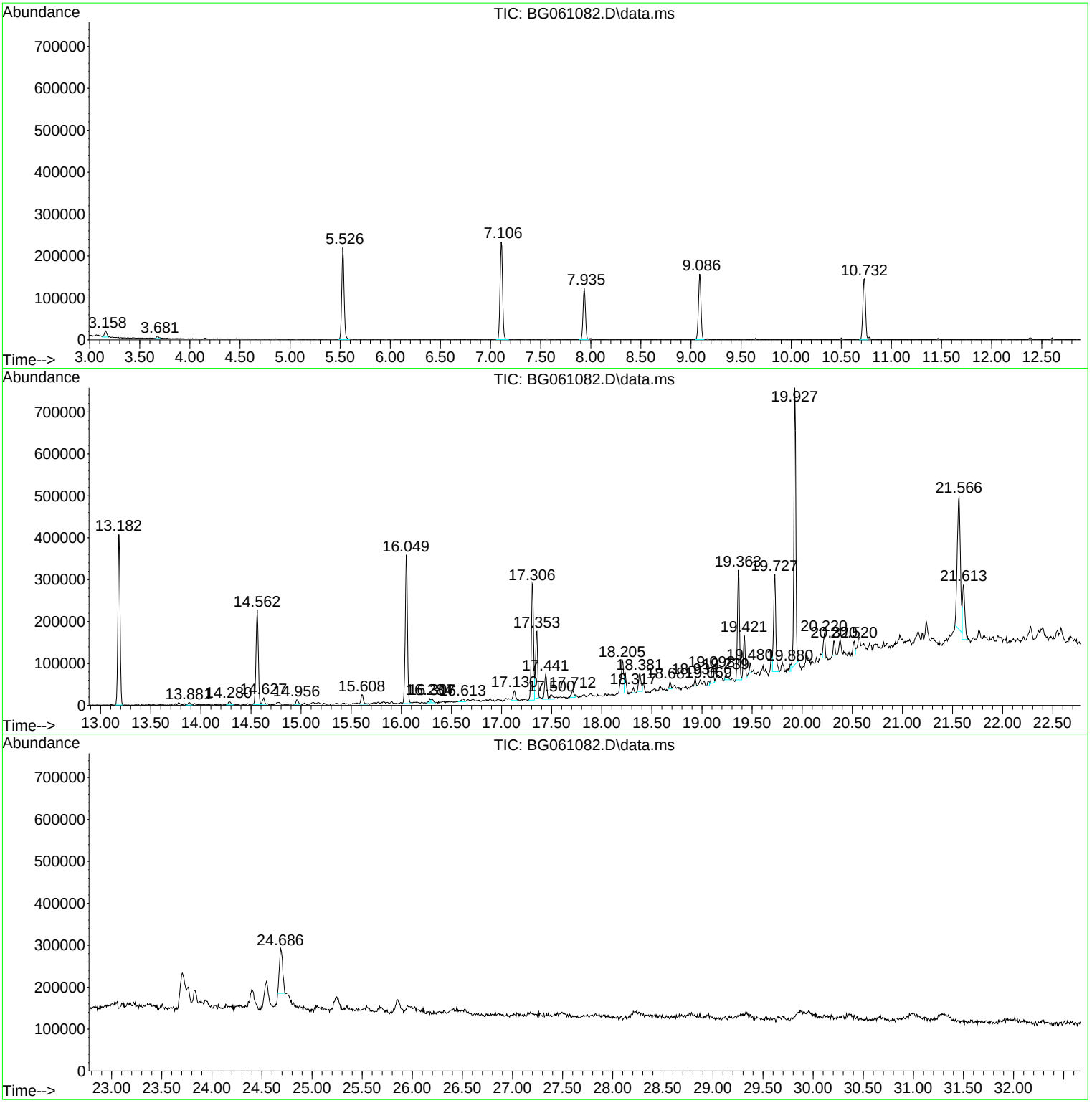
Sum of corrected areas: 7405385

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

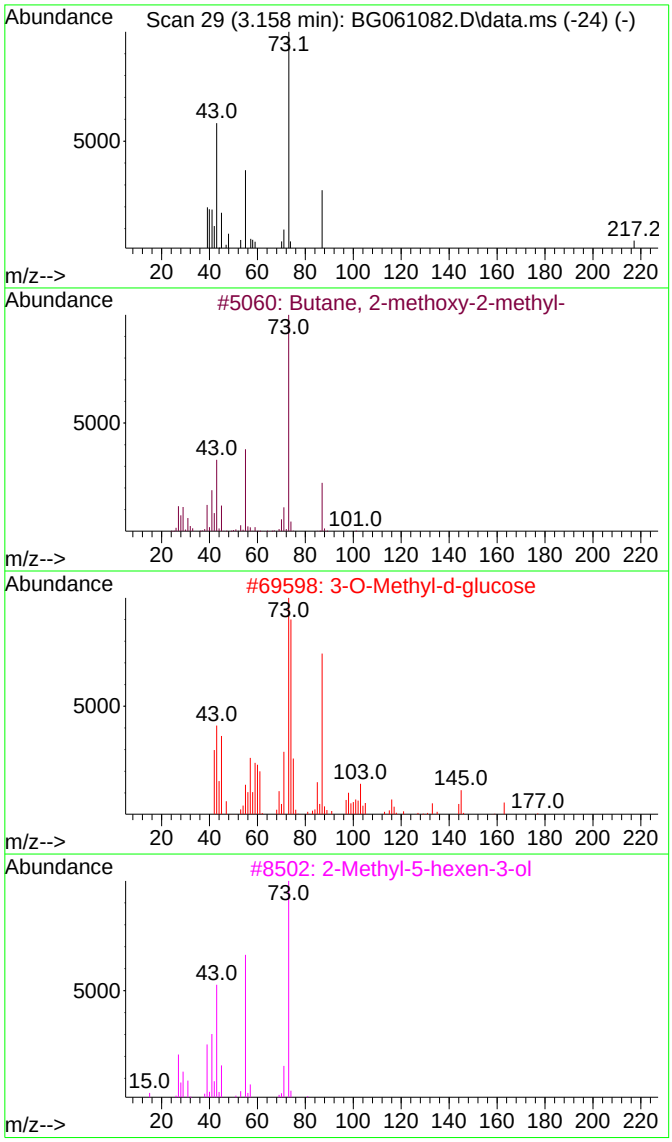
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

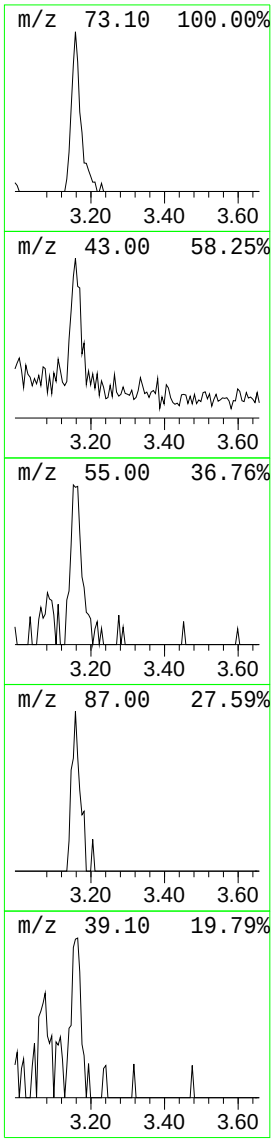
**********

Peak Number 1 unknown3.158 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.158 | 2.33 ng | 23453 | 1,4-Dichlorobenzene-d4 | 7.935 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 42 |
| 2 | 3-O-Methyl-d-glucose | 194 | C7H14O6 | 1000127-25-9 | 38 |
| 3 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 17 |
| 4 | 3-Pentanol, 3-methyl- | 102 | C6H14O | 000077-74-7 | 17 |
| 5 | 3,4-Dimethyl-5-hexen-3-ol | 128 | C8H16O | 001569-45-5 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

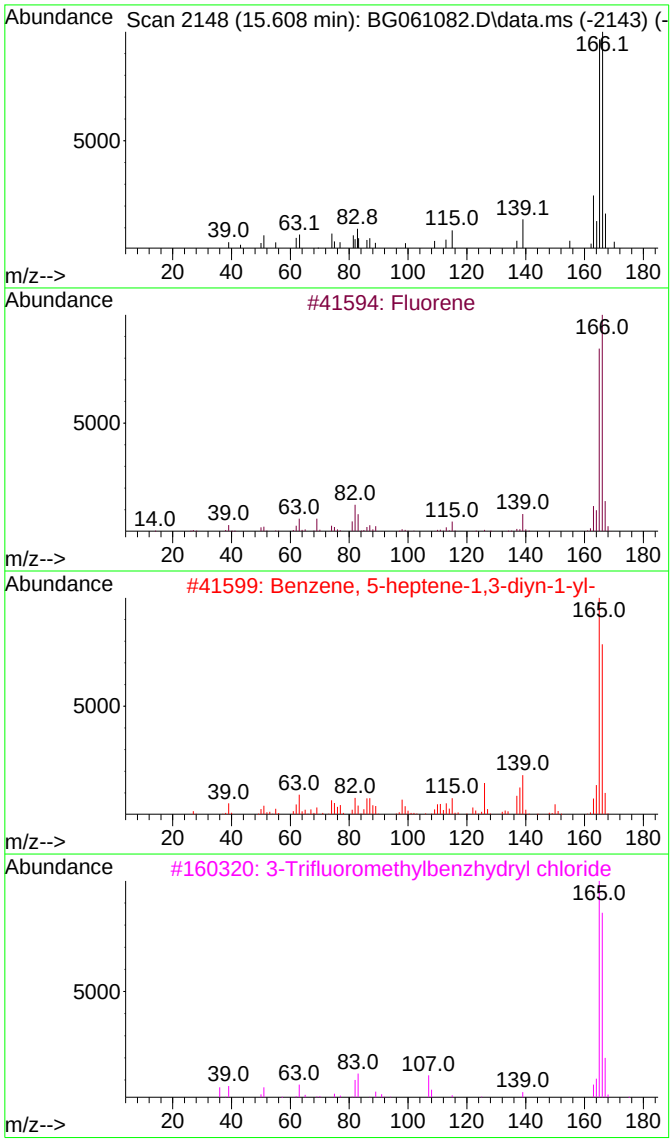
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

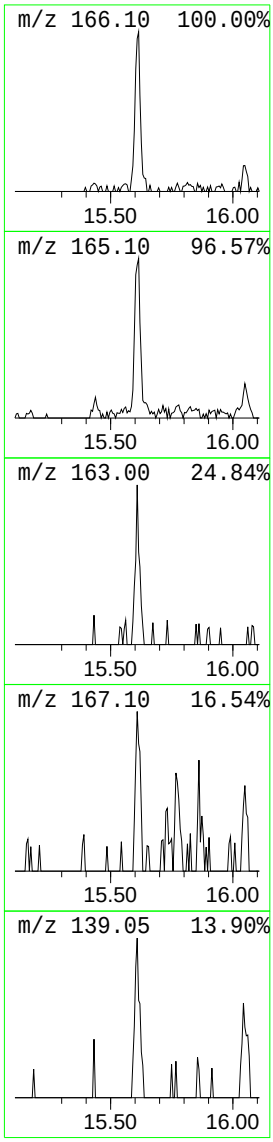
**********

Peak Number 2 Benzene, 5-heptene-1,3-diyn... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.608 | 2.18 ng | 38716 | Acenaphthene-d10 | 14.562 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Fluorene | 166 | C13H10 | 000086-73-7 | 90 |
| 2 | Benzene, 5-heptene-1,3-diyn-1-yl- | 166 | C13H10 | 013678-98-3 | 80 |
| 3 | 3-Trifluoromethylbenzhydryl chlo... | 270 | C14H10ClF3 | 067240-79-3 | 50 |
| 4 | Benzaldehyde, 2,4-dihydroxy-3,6-... | 166 | C9H10O3 | 034883-14-2 | 45 |
| 5 | Benzaldehyde, 4,6-dihydroxy-2,3-... | 166 | C9H10O3 | 002990-31-0 | 36 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

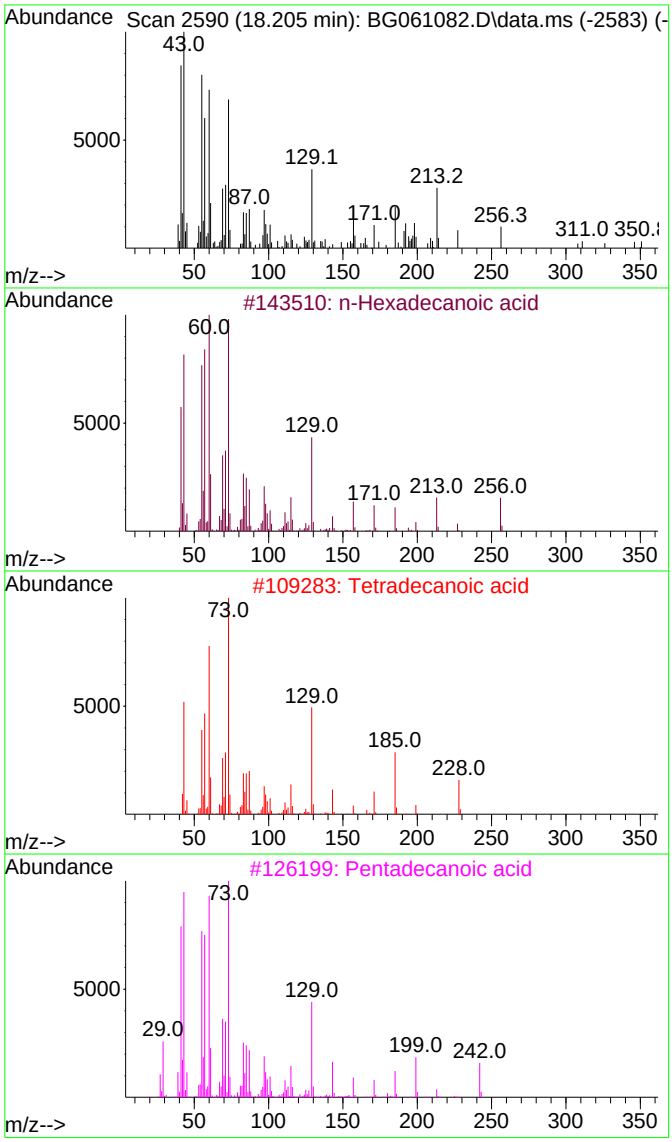
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

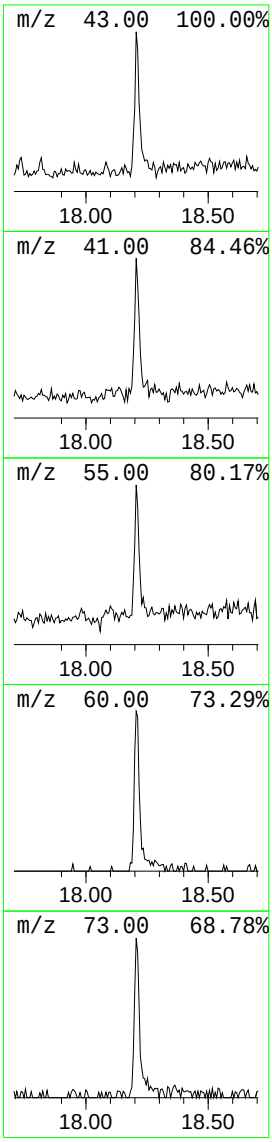
**********

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.205 | 6.46 ng | 140383 | Phenanthrene-d10 | 17.306 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 46 |
| 4 | 11-Bromoundecanoic acid | 264 | C11H21BrO2 | 002834-05-1 | 43 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 43 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

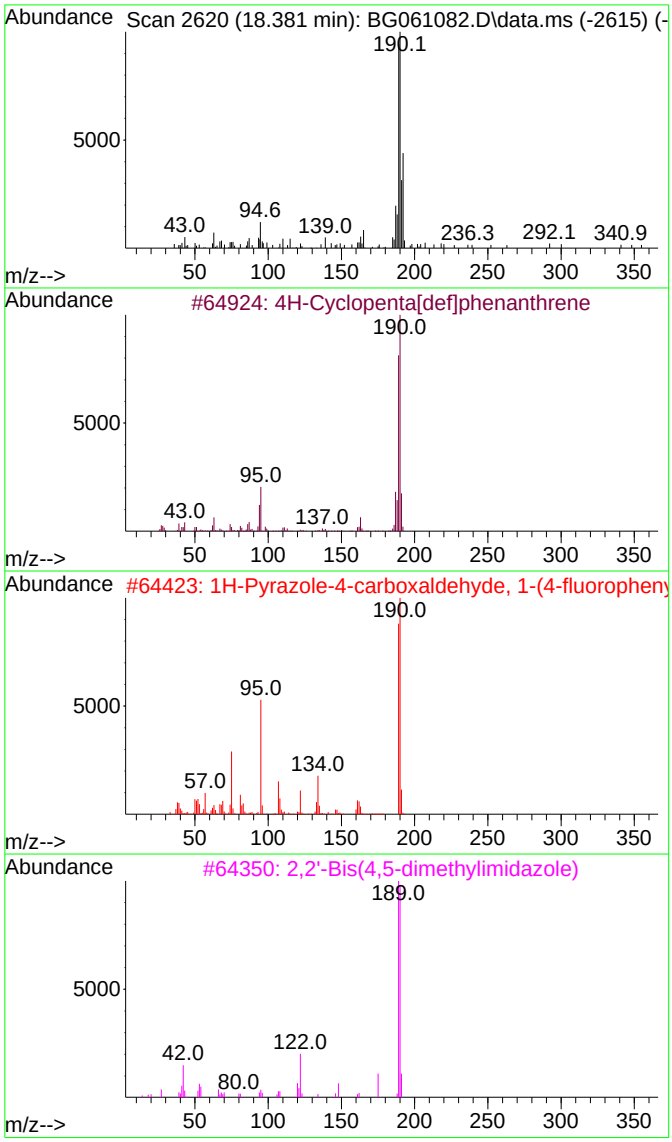
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

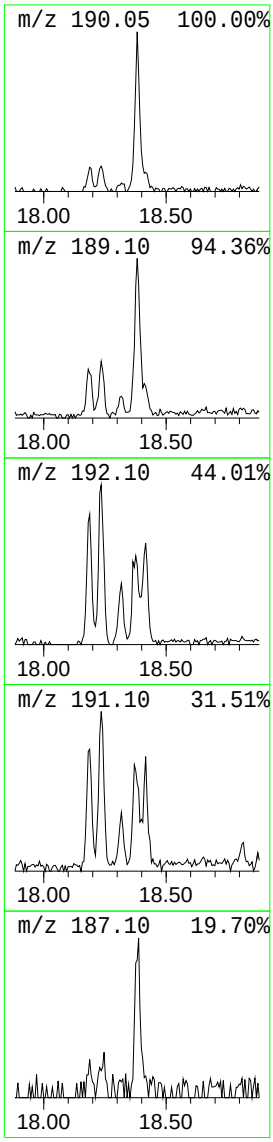
**********

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.381 | 3.48 ng | 75542 | Phenanthrene-d10 | 17.306 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 70 |
| 2 | 1H-Pyrazole-4-carboxaldehyde, 1-... | 190 | C10H7FN2O | 1000338-05-6 | 49 |
| 3 | 2,2'-Bis(4,5-dimethylimidazole) | 190 | C10H14N4 | 069286-06-2 | 47 |
| 4 | 6H-Cyclobuta[jk]phenanthrene | 190 | C15H10 | 083469-43-6 | 45 |
| 5 | Carbonic acid, 2-formyl-4,6-dich... | 276 | C11H10Cl2O4 | 1000331-39-3 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

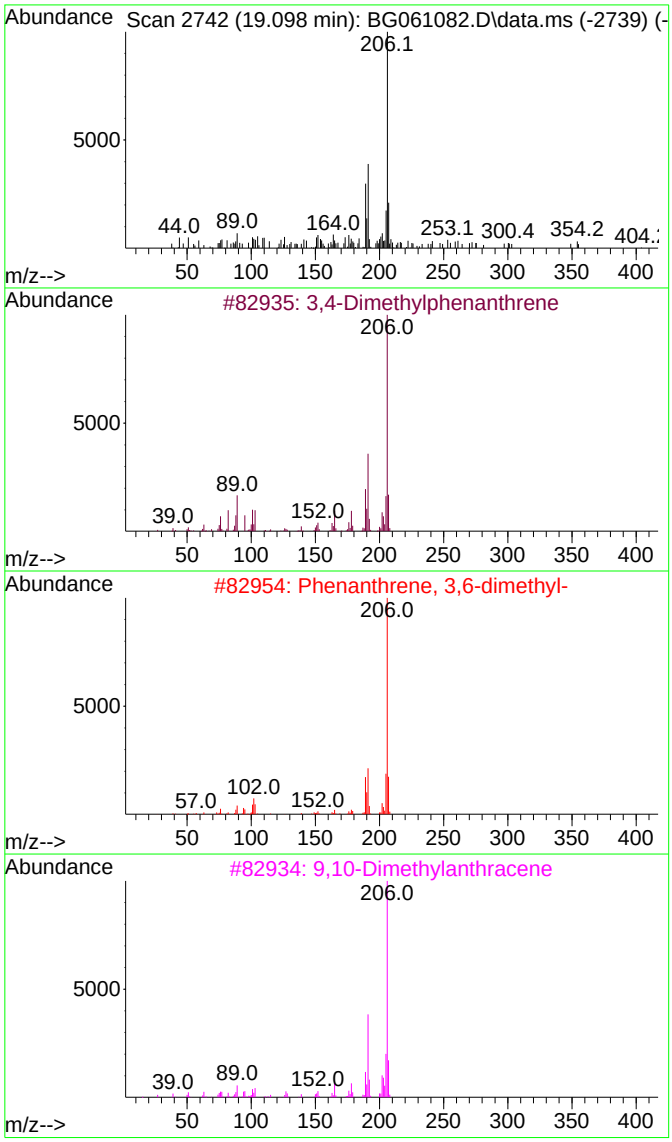
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

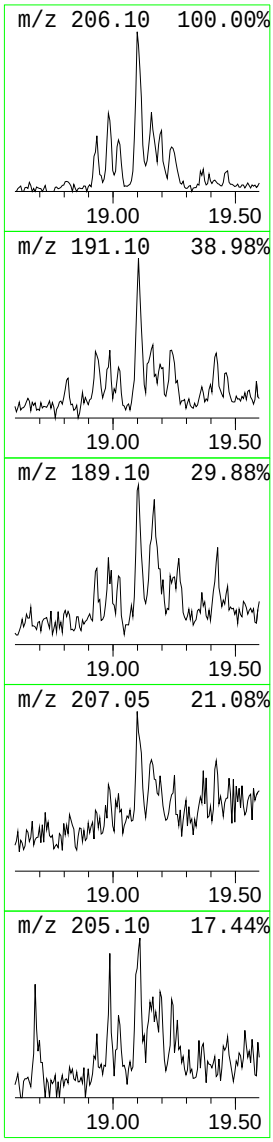
**********

Peak Number 5 3,4-Dimethylphenanthrene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.098 | 2.23 ng | 48483 | Phenanthrene-d10 | 17.306 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,4-Dimethylphenanthrene | 206 | C16H14 | 1000452-24-5 | 87 |
| 2 | Phenanthrene, 3,6-dimethyl- | 206 | C16H14 | 001576-67-6 | 86 |
| 3 | 9,10-Dimethylanthracene | 206 | C16H14 | 000781-43-1 | 74 |
| 4 | 3-Methyl-1-phenyl-1H-indene | 206 | C16H14 | 022360-63-0 | 72 |
| 5 | Phenanthrene, 2,3-dimethyl- | 206 | C16H14 | 003674-65-5 | 72 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

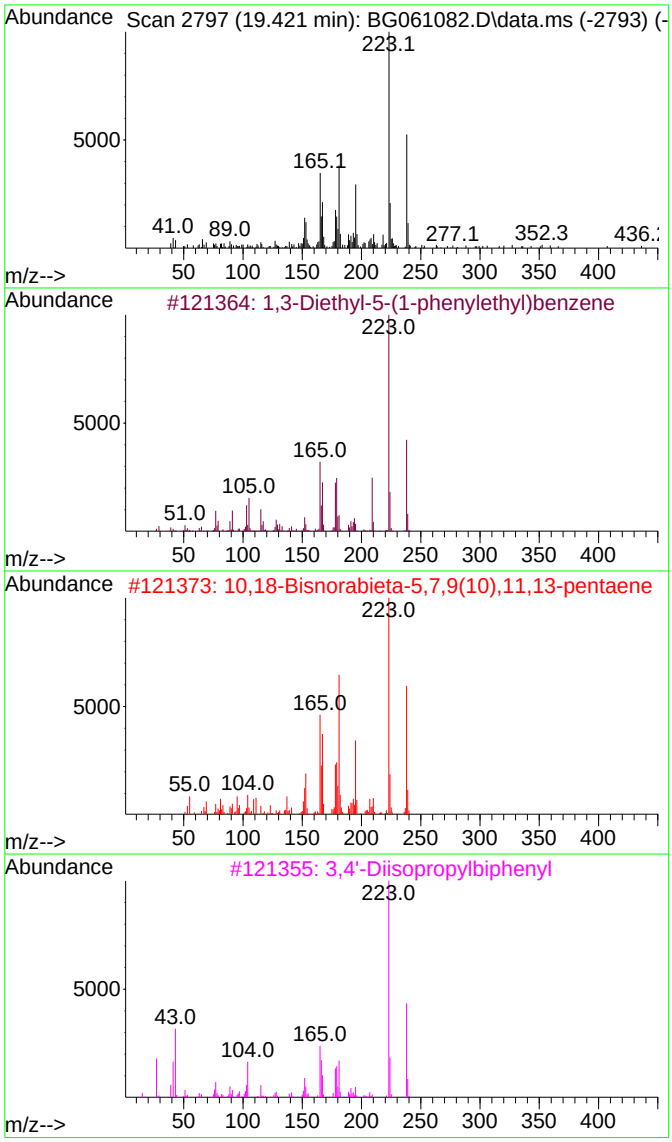
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

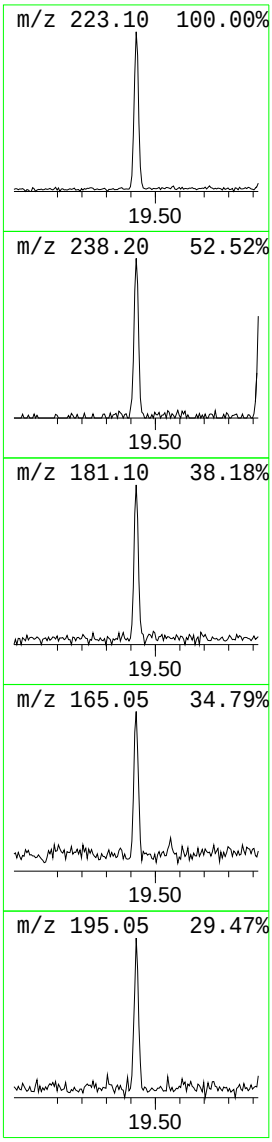
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 1,3-Diethyl-5-(1-phenylethy... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.421 | 6.21 ng | 134840 | Phenanthrene-d10 | 17.306 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Diethyl-5-(1-phenylethyl)ben... | 238 | C18H22 | 1000482-32-6 | 89 |
| 2 | 10,18-Bisnorabieta-5,7,9(10),11,... | 238 | C18H22 | 006566-19-4 | 86 |
| 3 | 3,4'-Diisopropylbiphenyl | 238 | C18H22 | 061434-46-6 | 76 |
| 4 | 3,3'-Diacetylbiphenyl | 238 | C16H14O2 | 094113-07-2 | 60 |
| 5 | Anthracene, 9,10-dimethoxy- | 238 | C16H14O2 | 002395-97-3 | 60 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050124\
Data File : BG061082.D
Acq On : 1 May 2024 18:51
Operator : MA/JU
Sample : P2330-05 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
F-1(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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 |
| unknown3.158 | 3.158 | 2.3 | ng | 23453 | 1 | 7.935 | 201674 | 20.0 |
| Benzene, 5-hept... | 15.608 | 2.2 | ng | 38716 | 3 | 14.562 | 355465 | 20.0 |
| n-Hexadecanoic ... | 18.205 | 6.5 | ng | 140383 | 4 | 17.306 | 434506 | 20.0 |
| 4H-Cyclopenta[d... | 18.381 | 3.5 | ng | 75542 | 4 | 17.306 | 434506 | 20.0 |
| 3,4-Dimethylphe... | 19.098 | 2.2 | ng | 48483 | 4 | 17.306 | 434506 | 20.0 |
| 1,3-Diethyl-5-(... | 19.421 | 6.2 | ng | 134840 | 4 | 17.306 | 434506 | 20.0 |