LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054439.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.567 | 433 | 439 | 452 | rVB | 88100 | 156173 | 2.11% | 1.100% |
| 2 | 5.961 | 499 | 506 | 515 | rVB | 90820 | 158362 | 2.13% | 1.115% |
| 3 | 7.177 | 707 | 713 | 725 | rVB2 | 94947 | 197873 | 2.67% | 1.394% |
| 4 | 7.988 | 845 | 851 | 857 | rBV | 65647 | 111753 | 1.51% | 0.787% |
| 5 | 9.151 | 1043 | 1049 | 1056 | rVB2 | 58506 | 105116 | 1.42% | 0.740% |
| 6 | 10.796 | 1320 | 1329 | 1335 | rBV | 84063 | 157546 | 2.12% | 1.110% |
| 7 | 13.240 | 1739 | 1745 | 1754 | rVB | 190713 | 305053 | 4.11% | 2.148% |
| 8 | 14.621 | 1972 | 1980 | 1986 | rBV | 145470 | 237885 | 3.21% | 1.675% |
| 9 | 16.113 | 2227 | 2234 | 2240 | rBV2 | 177000 | 288149 | 3.88% | 2.029% |
| 10 | 17.371 | 2442 | 2448 | 2451 | rBV | 188975 | 295140 | 3.98% | 2.079% |
| 11 | 17.412 | 2451 | 2455 | 2463 | rVV | 196199 | 321030 | 4.33% | 2.261% |
| 12 | 17.500 | 2464 | 2470 | 2476 | rVB | 52736 | 79787 | 1.08% | 0.562% |
| 13 | 18.252 | 2590 | 2598 | 2602 | rBV2 | 61237 | 112104 | 1.51% | 0.789% |
| 14 | 18.440 | 2624 | 2630 | 2634 | rBV3 | 40295 | 78318 | 1.06% | 0.552% |
| 15 | 19.251 | 2763 | 2768 | 2773 | rVB2 | 75980 | 103153 | 1.39% | 0.726% |
| 16 | 19.421 | 2790 | 2797 | 2803 | rBV | 347345 | 553547 | 7.46% | 3.898% |
| 17 | 19.527 | 2811 | 2815 | 2825 | rBV6 | 49887 | 103131 | 1.39% | 0.726% |
| 18 | 19.750 | 2849 | 2853 | 2855 | rBV2 | 66095 | 93370 | 1.26% | 0.658% |
| 19 | 19.786 | 2855 | 2859 | 2863 | rVV | 281320 | 427139 | 5.76% | 3.008% |
| 20 | 19.974 | 2886 | 2891 | 2896 | rBV | 391501 | 539433 | 7.27% | 3.799% |
| 21 | 20.273 | 2939 | 2942 | 2947 | rVB | 56843 | 89205 | 1.20% | 0.628% |
| 22 | 20.690 | 3009 | 3013 | 3016 | rBV | 76156 | 87232 | 1.18% | 0.614% |
| 23 | 21.260 | 3107 | 3110 | 3116 | rVB3 | 85222 | 115980 | 1.56% | 0.817% |
| 24 | 21.531 | 3147 | 3156 | 3163 | rBV | 4552774 | 7418306 | 100.00% | 52.243% |
| 25 | 21.631 | 3166 | 3173 | 3178 | rVV2 | 288741 | 708994 | 9.56% | 4.993% |
| 26 | 21.683 | 3179 | 3182 | 3192 | rVB | 132706 | 217099 | 2.93% | 1.529% |
| 27 | 21.836 | 3204 | 3208 | 3216 | rVB3 | 77637 | 133263 | 1.80% | 0.938% |
| 28 | 21.913 | 3216 | 3221 | 3226 | rBV2 | 71393 | 117915 | 1.59% | 0.830% |
| 29 | 22.706 | 3352 | 3356 | 3361 | rBV | 80092 | 116341 | 1.57% | 0.819% |
| 30 | 23.828 | 3542 | 3547 | 3554 | rBV2 | 68824 | 197152 | 2.66% | 1.388% |
| 31 | 24.263 | 3615 | 3621 | 3629 | rVB | 144412 | 325293 | 4.39% | 2.291% |
| 32 | 24.844 | 3714 | 3720 | 3729 | rVB2 | 96776 | 248812 | 3.35% | 1.752% |

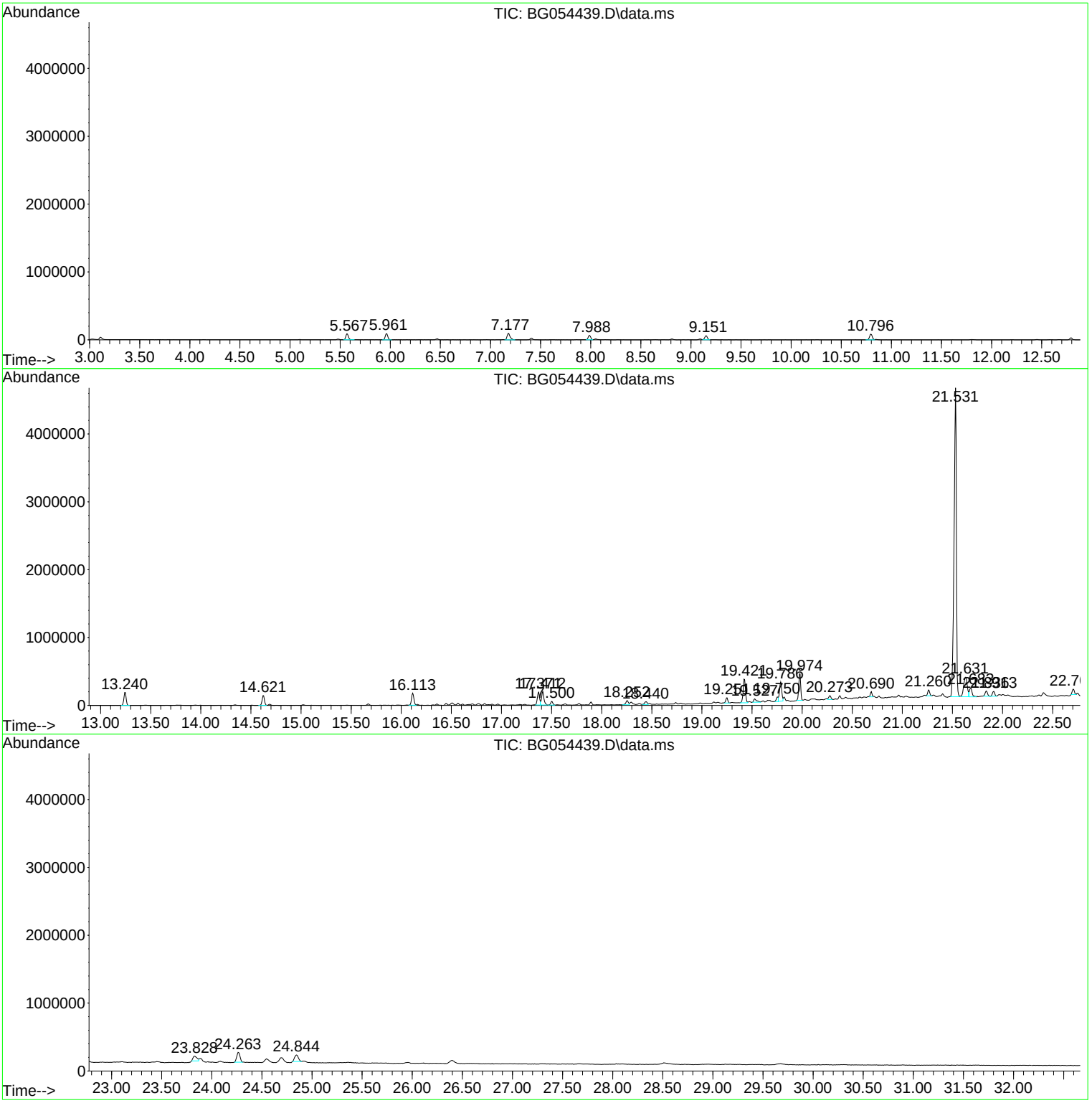
Sum of corrected areas: 14199654

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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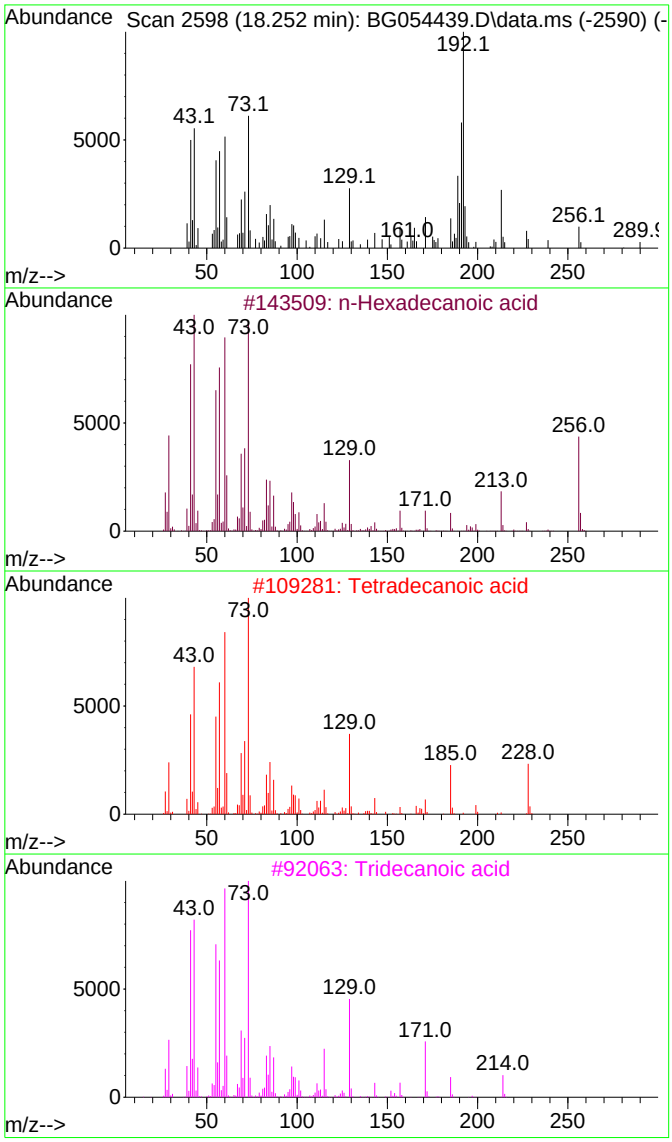
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

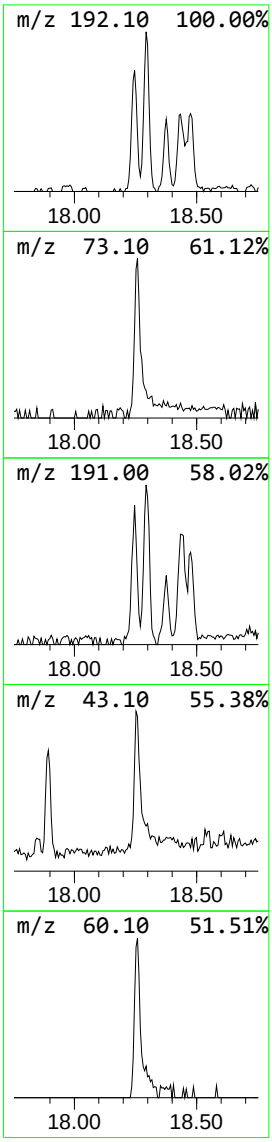
**********

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.252 | 7.60 ng | 112104 | Phenanthrene-d10 | 17.371 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 90 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 59 |
| 4 | Phenanthrene, 2-methyl- | 192 | C15H12 | 002531-84-2 | 55 |
| 5 | 1H-Indene, 2-phenyl- | 192 | C15H12 | 004505-48-0 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

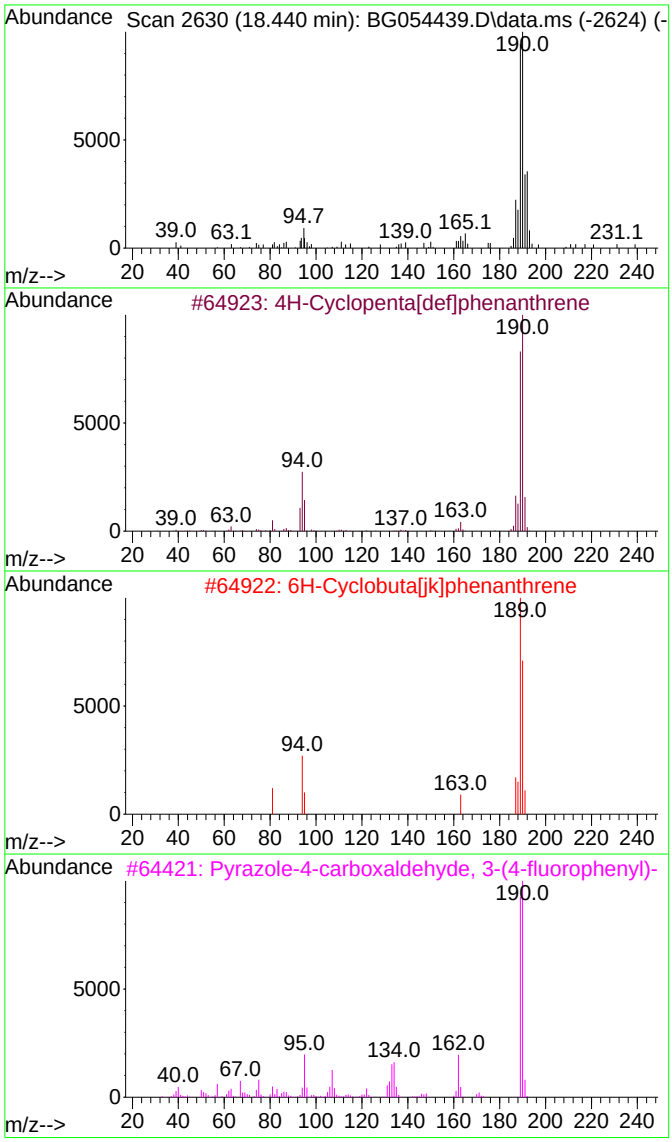
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

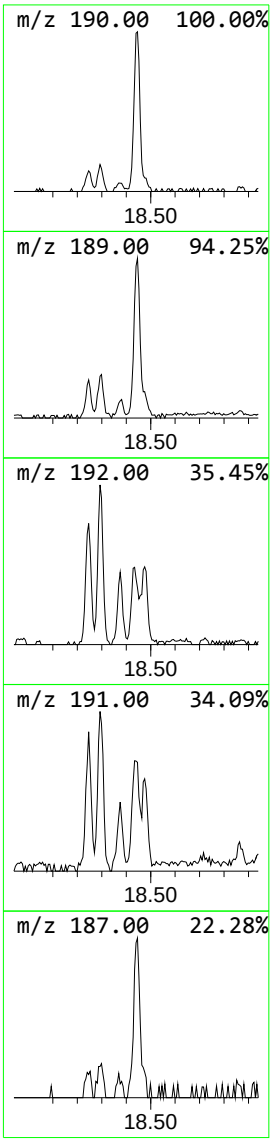
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.440 | 5.31 ng | 78318 | Phenanthrene-d10 | 17.371 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 87 |
| 2 | 6H-Cyclobuta[jk]phenanthrene | 190 | C15H10 | 083469-43-6 | 64 |
| 3 | Pyrazole-4-carboxaldehyde, 3-(4-... | 190 | C10H7FN2O | 306936-57-2 | 42 |
| 4 | 2,2'-Bis(4,5-dimethylimidazole) | 190 | C10H14N4 | 069286-06-2 | 36 |
| 5 | Pyrimidine, 6-oxo-4-(3-fluorophe... | 190 | C10H7FN2O | 085979-55-1 | 32 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

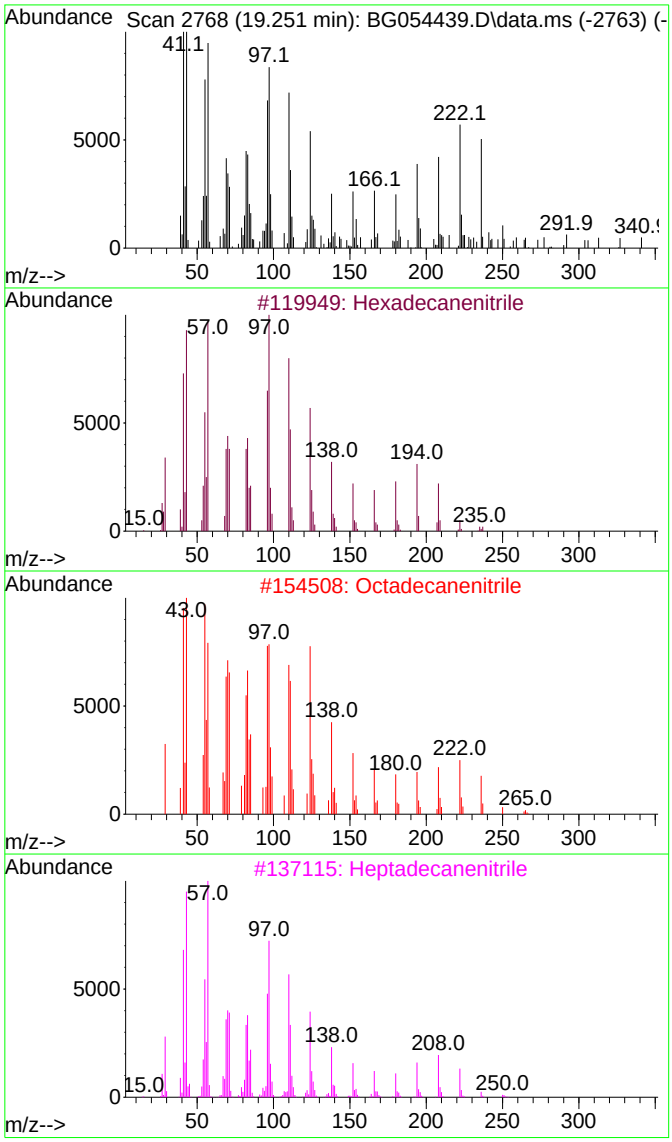
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

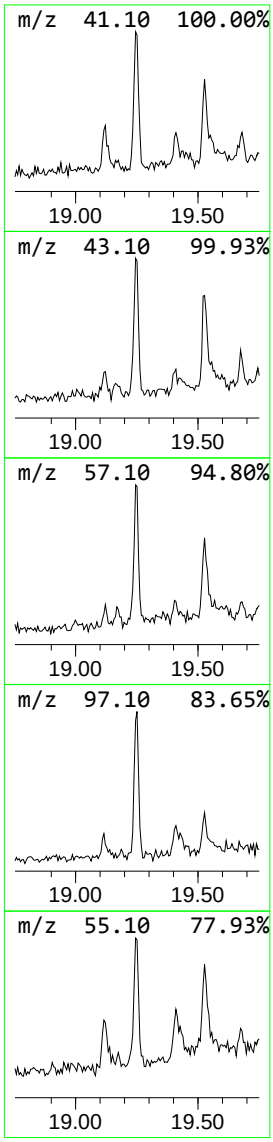
**********

Peak Number 4 Hexadecanenitrile Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.251 | 6.99 ng | 103153 | Phenanthrene-d10 | 17.371 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanenitrile | 237 | C16H31N | 000629-79-8 | 98 |
| 2 | Octadecanenitrile | 265 | C18H35N | 000638-65-3 | 83 |
| 3 | Heptadecanenitrile | 251 | C17H33N | 005399-02-0 | 68 |
| 4 | Undecanenitrile | 167 | C11H21N | 002244-07-7 | 64 |
| 5 | Pentadecanenitrile | 223 | C15H29N | 018300-91-9 | 55 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

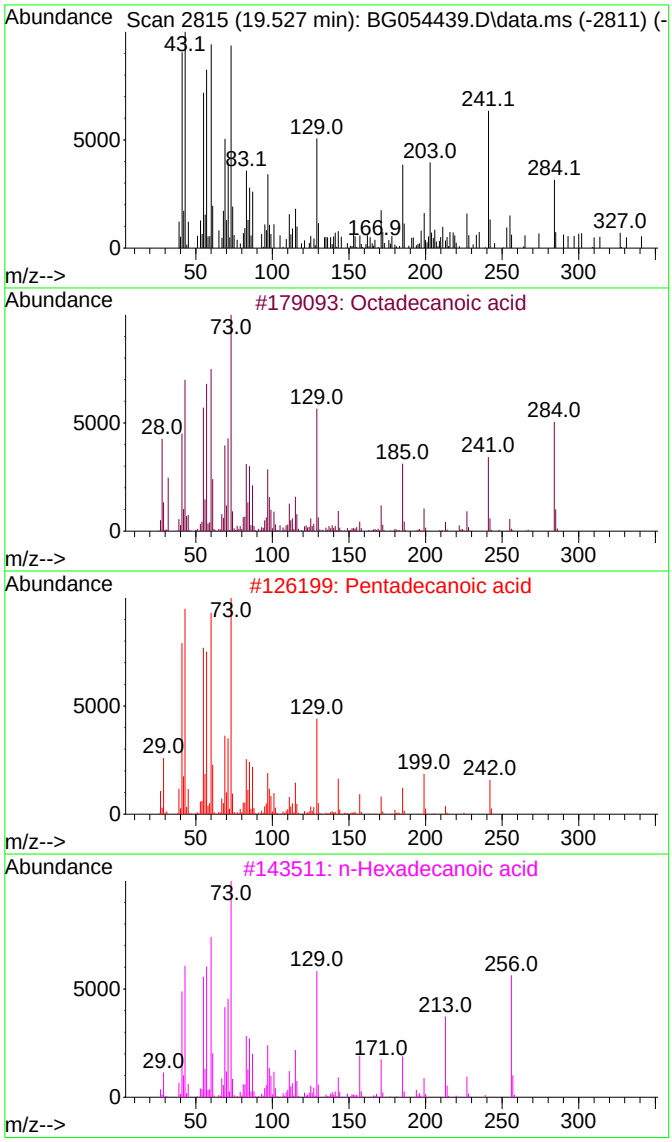
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

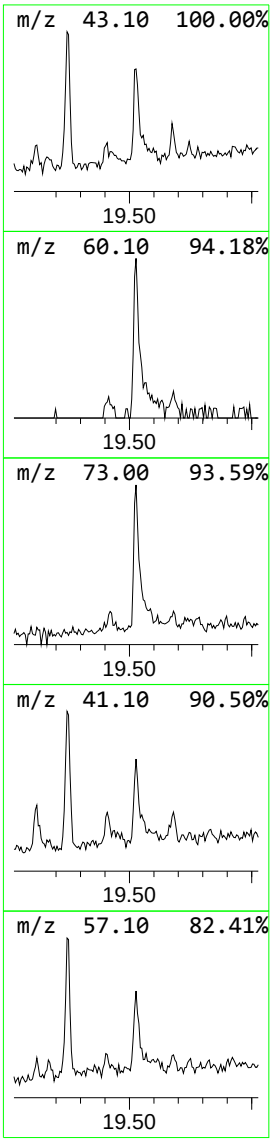
**********

Peak Number 5 Octadecanoic acid Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.527 | 2.91 ng | 103131 | Chrysene-d12 | 21.636 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 91 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 3 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 64 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 49 |
| 5 | Octadecanoic acid, 2-hydroxy-1,3... | 625 | C39H76O5 | 000504-40-5 | 43 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

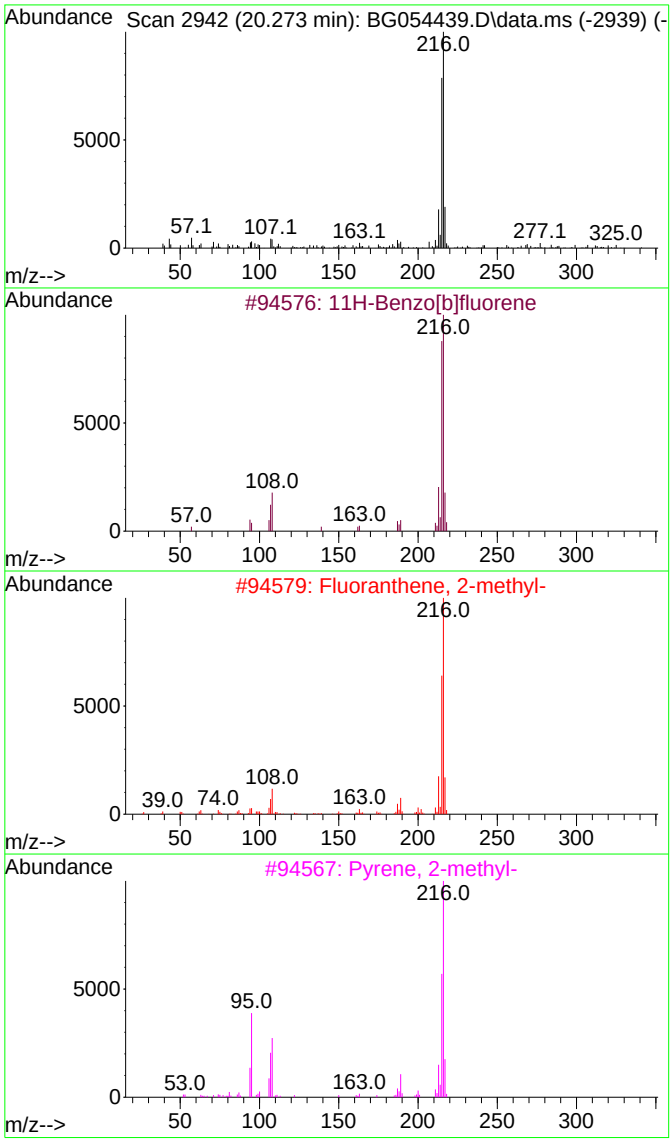
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

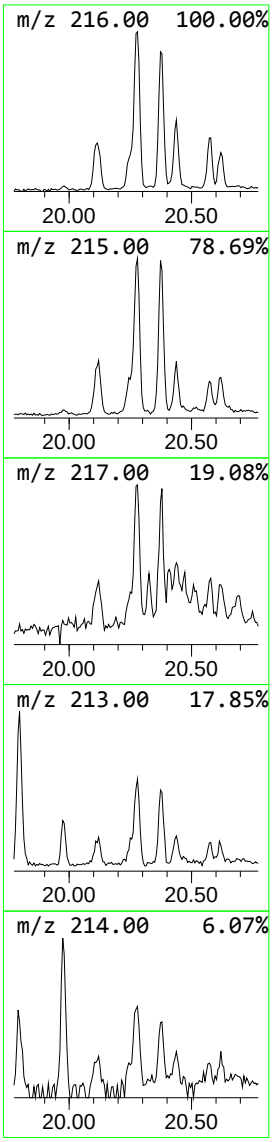
**********

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.273 | 2.52 ng | 89205 | Chrysene-d12 | 21.636 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 11H-Benzo[b]fluorene | 216 | C17H12 | 000243-17-4 | 90 |
| 2 | Fluoranthene, 2-methyl- | 216 | C17H12 | 033543-31-6 | 90 |
| 3 | Pyrene, 2-methyl- | 216 | C17H12 | 003442-78-2 | 90 |
| 4 | 11H-Benzo[a]fluorene | 216 | C17H12 | 000238-84-6 | 87 |
| 5 | Pyrene, 1-methyl- | 216 | C17H12 | 002381-21-7 | 86 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

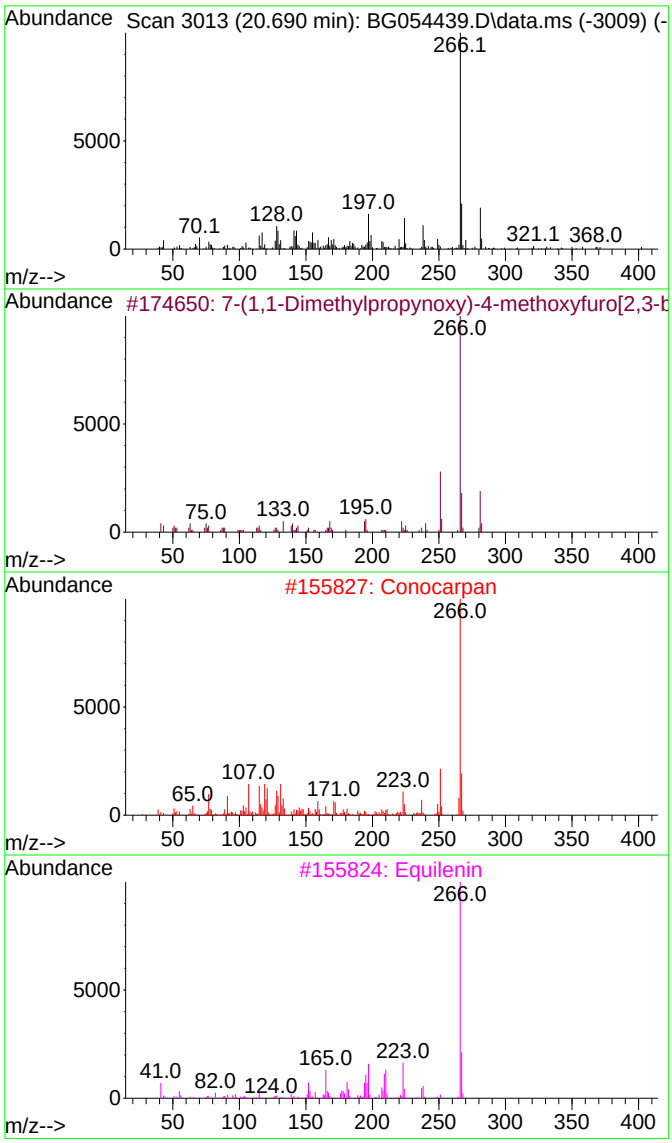
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

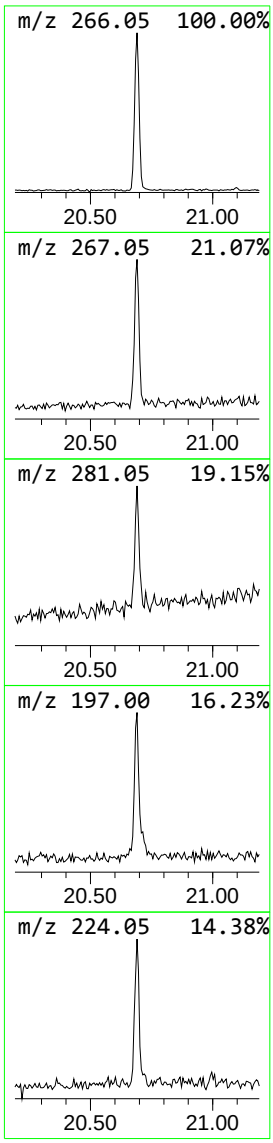
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 7-(1,1-Dimethylpropynoxy)-4... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.690 | 2.46 ng | 87232 | Chrysene-d12 | 21.636 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7-(1,1-Dimethylpropynoxy)-4-meth... | 281 | C17H15NO3 | 081781-88-6 | 59 |
| 2 | Conocarpan | 266 | C18H18O2 | 056319-02-9 | 53 |
| 3 | Equilenin | 266 | C18H18O2 | 000517-09-9 | 52 |
| 4 | Phthalic acid, diamide, N,N'-die... | 400 | C26H28N2O2 | 1010309-86-3 | 50 |
| 5 | Perylene, 1,2,3,3a,4,5,6,7,8,9,9... | 266 | C20H26 | 007594-86-7 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

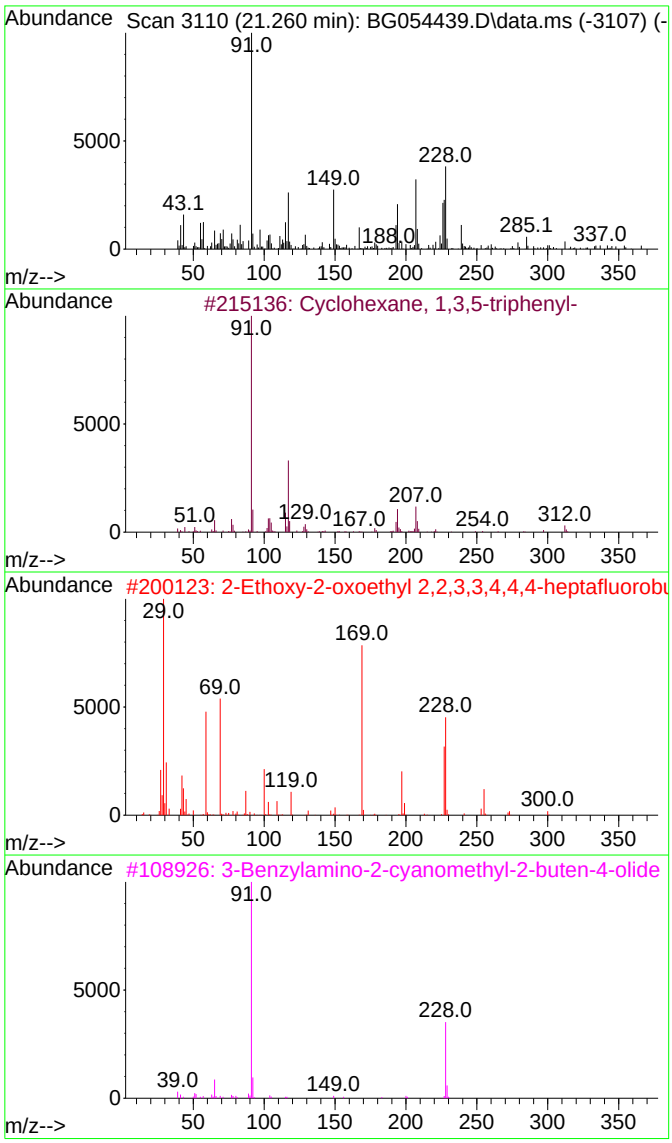
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

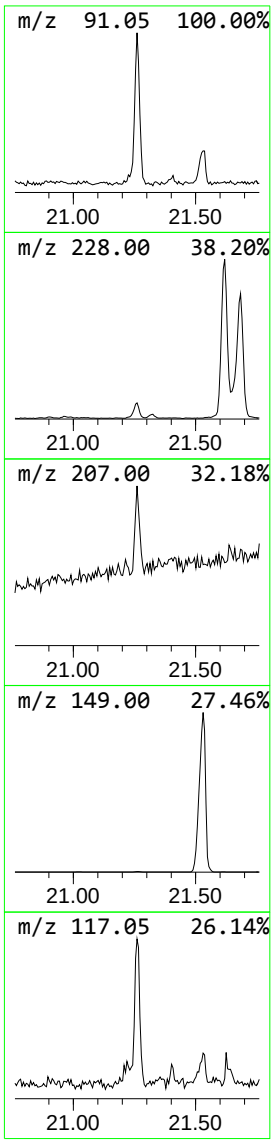
**********

Peak Number 8 unknown21.260 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.260 | 3.27 ng | 115980 | Chrysene-d12 | 21.636 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane, 1,3,5-triphenyl- | 312 | C24H24 | 028336-57-4 | 25 |
| 2 | 2-Ethoxy-2-oxoethyl 2,2,3,3,4,4,... | 300 | C8H7F7O4 | 1000366-75-2 | 10 |
| 3 | 3-Benzylamino-2-cyanomethyl-2-bu... | 228 | C13H12N2O2 | 1000430-46-9 | 10 |
| 4 | Benzoic acid, 2-[(phenylmethyl)a... | 227 | C14H13NO2 | 006622-55-5 | 9 |
| 5 | Perhydroisoquinoline-3-acetaldeh... | 315 | C19H25NO3 | 1000195-70-1 | 9 |



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Misc :
ALS Vial : 15 Sample Multiplier: 1

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**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

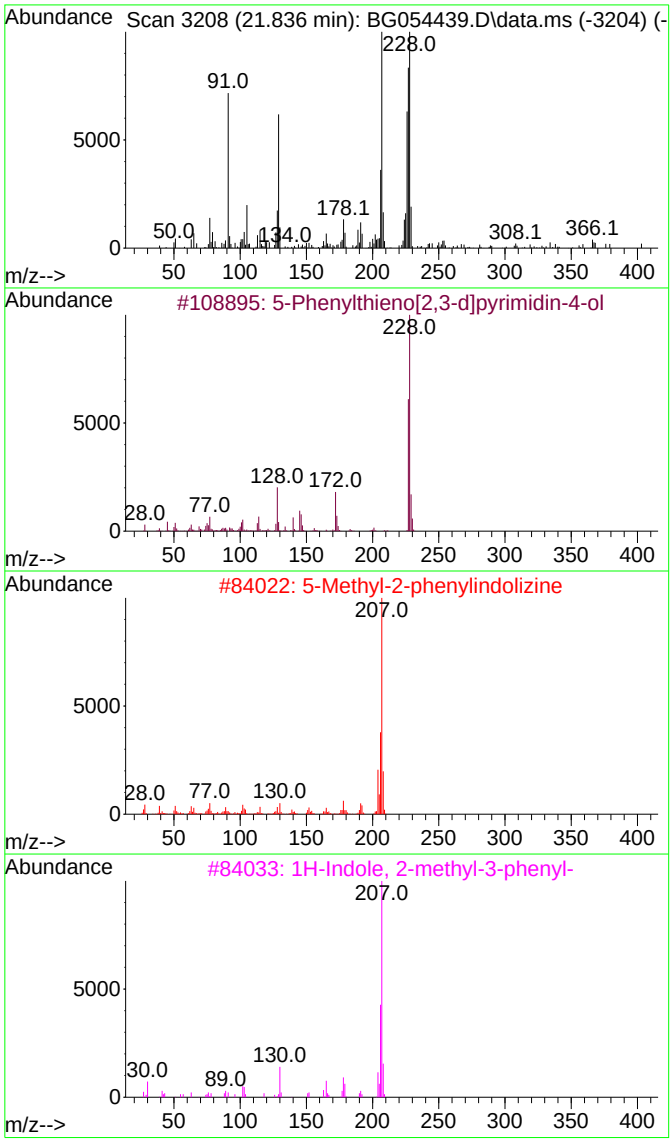
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

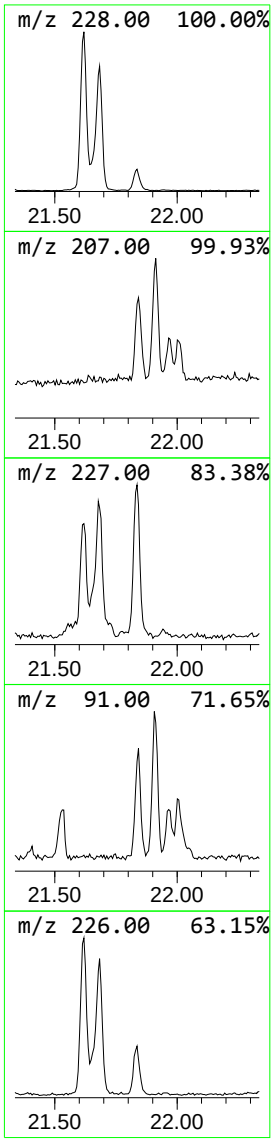
**********

Peak Number 9 unknown21.836 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.836 | 3.76 ng | 133263 | Chrysene-d12 | 21.636 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Phenylthieno[2,3-d]pyrimidin-4-ol | 228 | C12H8N2OS | 035978-39-3 | 35 |
| 2 | 5-Methyl-2-phenylindolizine | 207 | C15H13N | 036944-99-7 | 25 |
| 3 | 1H-Indole, 2-methyl-3-phenyl- | 207 | C15H13N | 004757-69-1 | 25 |
| 4 | 1-Propene, 3-(2-cyclopentenyl)-2... | 274 | C21H22 | 1010154-23-3 | 22 |
| 5 | 3-Chloro-9-methylacridine | 227 | C14H10ClN | 035422-72-1 | 18 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

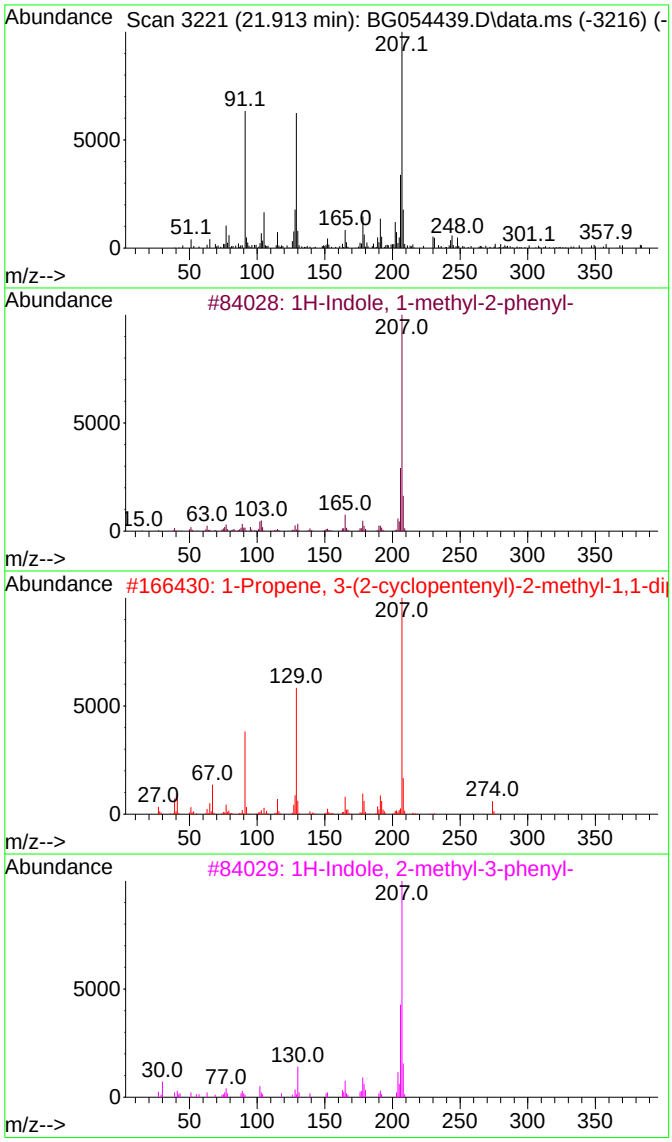
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

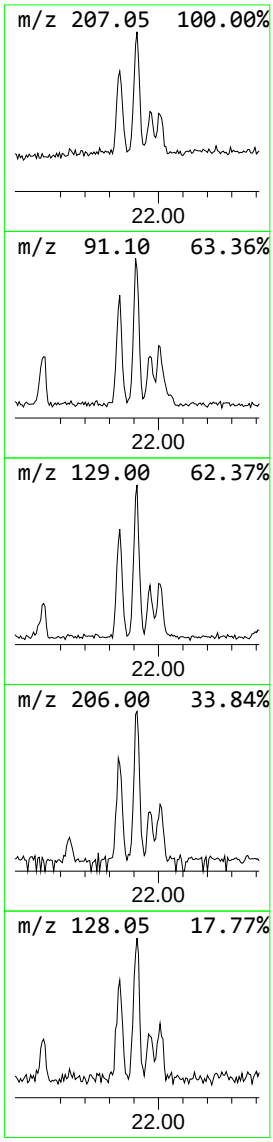
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 1H-Indole, 1-methyl-2-phenyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.913 | 3.33 ng | 117915 | Chrysene-d12 | 21.636 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Indole, 1-methyl-2-phenyl- | 207 | C15H13N | 003558-24-5 | 60 |
| 2 | 1-Propene, 3-(2-cyclopentenyl)-2... | 274 | C21H22 | 1010154-23-3 | 59 |
| 3 | 1H-Indole, 2-methyl-3-phenyl- | 207 | C15H13N | 004757-69-1 | 53 |
| 4 | 2-(4-Methylphenyl)-1H-indole | 207 | C15H13N | 055577-25-8 | 53 |
| 5 | 5-Methyl-2-phenylindolizine | 207 | C15H13N | 036944-99-7 | 52 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

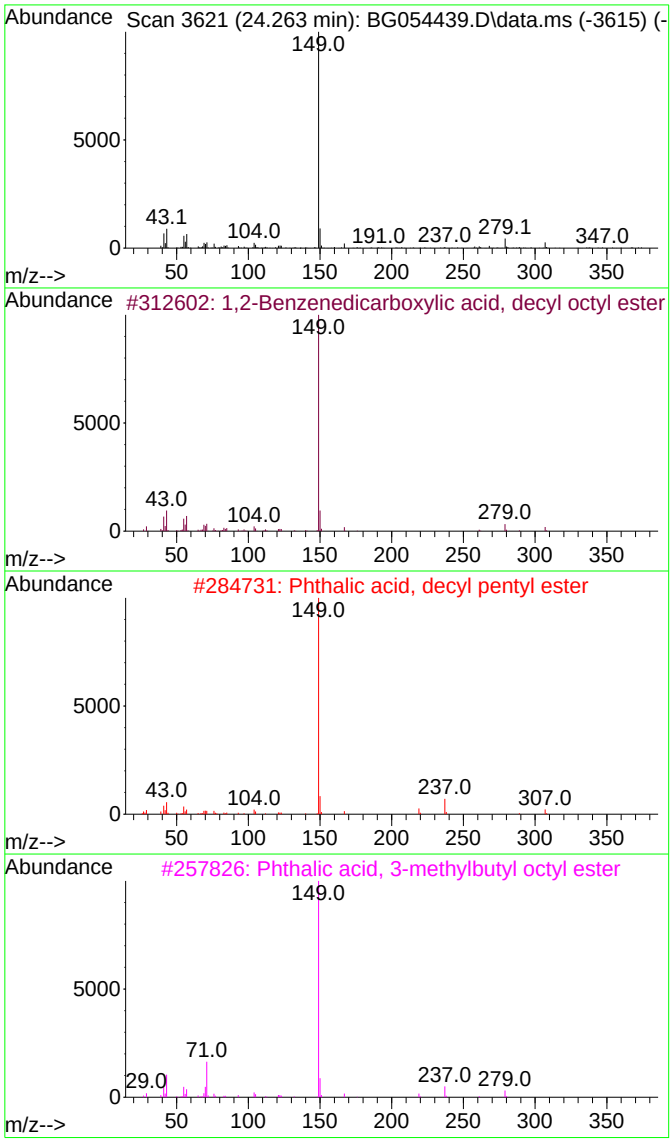
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

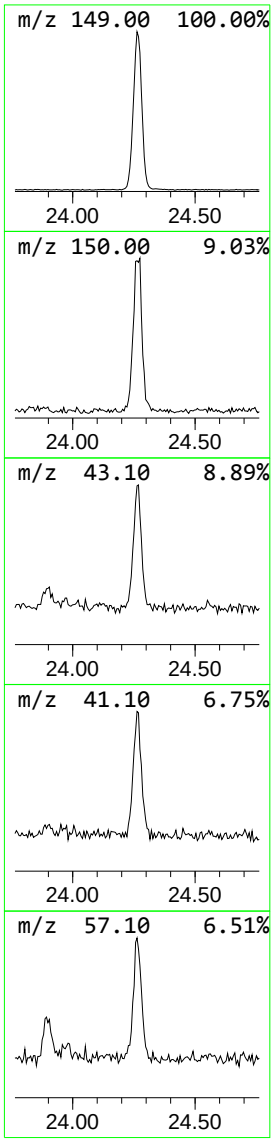
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 11 1,2-Benzenedicarboxylic aci... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.263 | 26.15 ng | 325293 | Perylene-d12 | 24.844 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Benzenedicarboxylic acid, de... | 418 | C26H42O4 | 000119-07-3 | 90 |
| 2 | Phthalic acid, decyl pentyl ester | 376 | C23H36O4 | 1000309-00-9 | 80 |
| 3 | Phthalic acid, 3-methylbutyl oct... | 348 | C21H32O4 | 1000356-80-9 | 80 |
| 4 | Phthalic acid, 6-ethyl-3-octyl h... | 404 | C25H40O4 | 1000315-17-7 | 80 |
| 5 | Phthalic acid, 6-methylhept-2-yl... | 390 | C24H38O4 | 1000377-96-2 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072822\
Data File : BG054439.D
Acq On : 28 Jul 2022 19:59
Operator : CG/JU
Sample : N3857-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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 |
| n-Hexadecanoic ... | 18.252 | 7.6 | ng | 112104 | 4 | 17.371 | 295140 | 20.0 |
| 4H-Cyclopenta[d... | 18.440 | 5.3 | ng | 78318 | 4 | 17.371 | 295140 | 20.0 |
| Hexadecanenitrile | 19.251 | 7.0 | ng | 103153 | 4 | 17.371 | 295140 | 20.0 |
| Octadecanoic acid | 19.527 | 2.9 | ng | 103131 | 5 | 21.636 | 708994 | 20.0 |
| 11H-Benzo[b]flu... | 20.273 | 2.5 | ng | 89205 | 5 | 21.636 | 708994 | 20.0 |
| 7-(1,1-Dimethyl... | 20.690 | 2.5 | ng | 87232 | 5 | 21.636 | 708994 | 20.0 |
| unknown21.260 | 21.260 | 3.3 | ng | 115980 | 5 | 21.636 | 708994 | 20.0 |
| unknown21.836 | 21.836 | 3.8 | ng | 133263 | 5 | 21.636 | 708994 | 20.0 |
| 1H-Indole, 1-me... | 21.913 | 3.3 | ng | 117915 | 5 | 21.636 | 708994 | 20.0 |
| 1,2-Benzenedica... | 24.263 | 26.1 | ng | 325293 | 6 | 24.844 | 248812 | 20.0 |