

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG052622\  
 Data File : BG053715.D  
 Acq On : 26 May 2022 13:44  
 Operator : CG/JU  
 Sample : N3028-01  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 TP-1-1-5FT

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053715.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 3.093       | 13            | 18          | 33           | rVB      | 173165         | 320058        | 23.19%          | 3.343%        |
| 2         | 3.528       | 85            | 92          | 103          | rVB2     | 21873          | 39096         | 2.83%           | 0.408%        |
| 3         | 3.686       | 108           | 119         | 135          | rBV      | 609350         | 1380039       | 100.00%         | 14.416%       |
| 4         | 5.554       | 431           | 437         | 448          | rBV      | 324616         | 537273        | 38.93%          | 5.613%        |
| 5         | 7.164       | 704           | 711         | 724          | rBV      | 336865         | 600760        | 43.53%          | 6.276%        |
| 6         | 7.980       | 844           | 850         | 857          | rBV      | 87932          | 144752        | 10.49%          | 1.512%        |
| 7         | 9.149       | 1041          | 1049        | 1058         | rBV      | 213381         | 380670        | 27.58%          | 3.977%        |
| 8         | 10.794      | 1321          | 1329        | 1337         | rBV      | 106790         | 194643        | 14.10%          | 2.033%        |
| 9         | 13.244      | 1737          | 1746        | 1753         | rBV      | 513696         | 810873        | 58.76%          | 8.471%        |
| 10        | 14.619      | 1975          | 1980        | 1986         | rVB      | 170306         | 262611        | 19.03%          | 2.743%        |
| 11        | 16.111      | 2228          | 2234        | 2246         | rBV      | 446241         | 728396        | 52.78%          | 7.609%        |
| 12        | 17.368      | 2441          | 2448        | 2454         | rBV      | 217269         | 331748        | 24.04%          | 3.466%        |
| 13        | 18.020      | 2555          | 2559        | 2564         | rBV3     | 23048          | 30821         | 2.23%           | 0.322%        |
| 14        | 18.255      | 2591          | 2599        | 2618         | rVB      | 243781         | 650421        | 47.13%          | 6.794%        |
| 15        | 19.424      | 2789          | 2798        | 2802         | rBV9     | 30030          | 104285        | 7.56%           | 1.089%        |
| 16        | 19.524      | 2806          | 2815        | 2835         | rVB      | 292660         | 777986        | 56.37%          | 8.127%        |
| 17        | 19.976      | 2886          | 2892        | 2897         | rBV      | 955812         | 1258670       | 91.21%          | 13.148%       |
| 18        | 20.875      | 3042          | 3045        | 3052         | rVB5     | 16094          | 29998         | 2.17%           | 0.313%        |
| 19        | 21.262      | 3107          | 3111        | 3122         | rBV3     | 51437          | 93466         | 6.77%           | 0.976%        |
| 20        | 21.503      | 3149          | 3152        | 3156         | rVB2     | 28323          | 35213         | 2.55%           | 0.368%        |
| 21        | 21.633      | 3168          | 3174        | 3180         | rBV      | 235323         | 395866        | 28.69%          | 4.135%        |
| 22        | 21.803      | 3199          | 3203        | 3208         | rVB2     | 26234          | 37855         | 2.74%           | 0.395%        |
| 23        | 24.834      | 3709          | 3719        | 3729         | rBV2     | 154921         | 427287        | 30.96%          | 4.464%        |

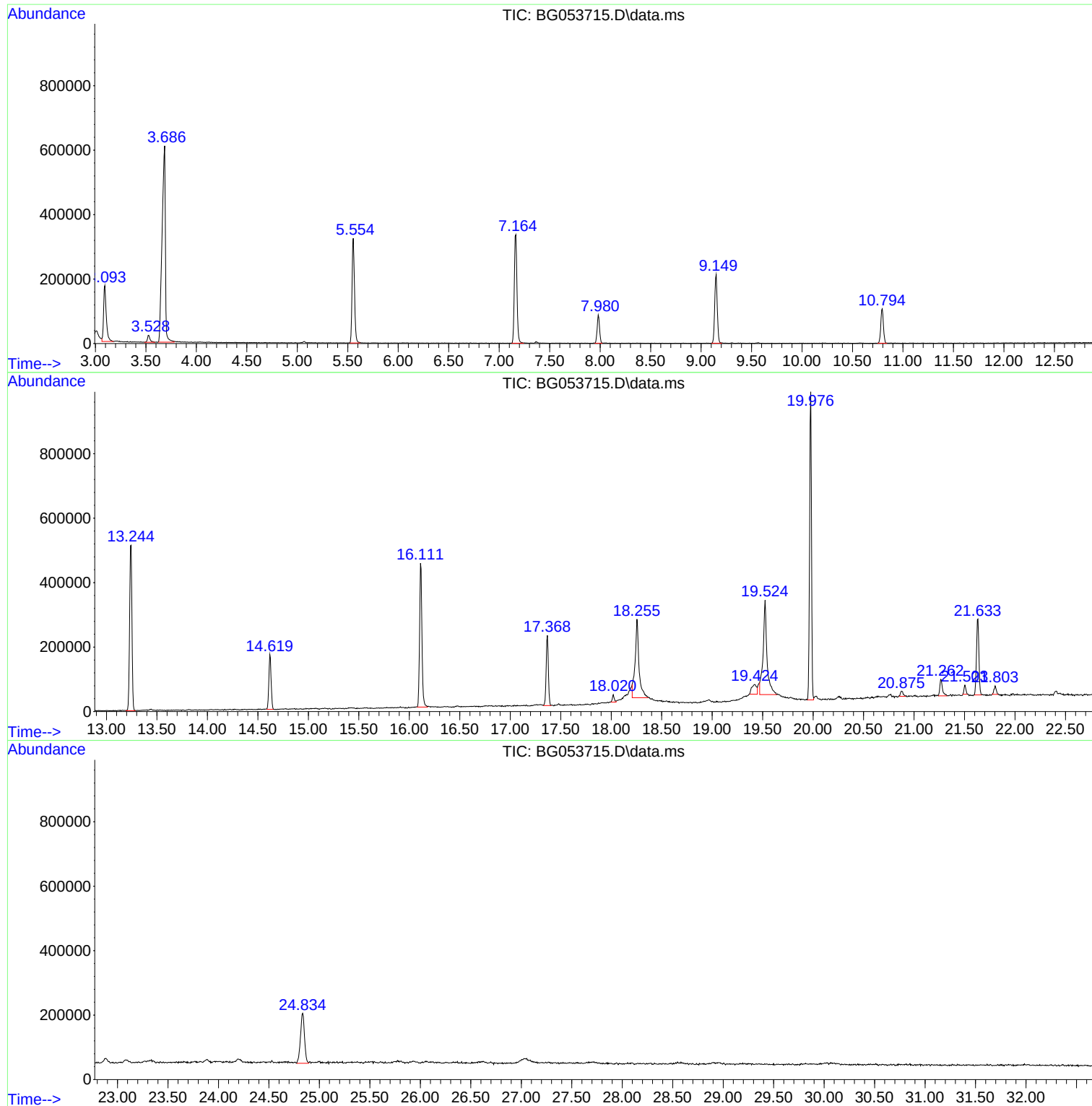
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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG050522.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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BNA\_G  
ClientSampleId :  
TP-1-1-5FT

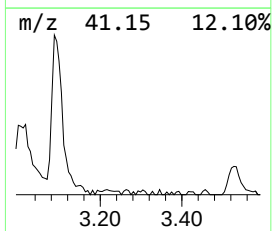
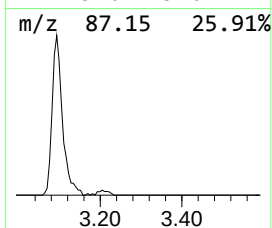
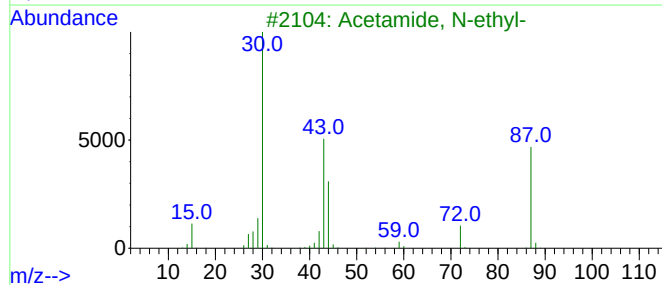
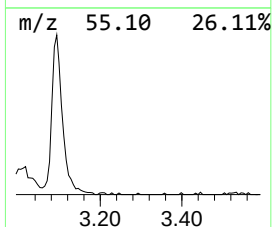
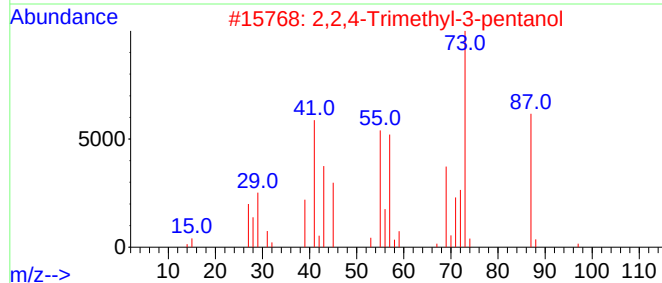
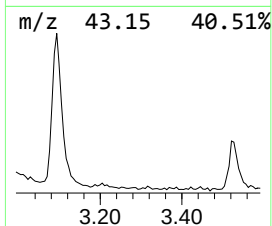
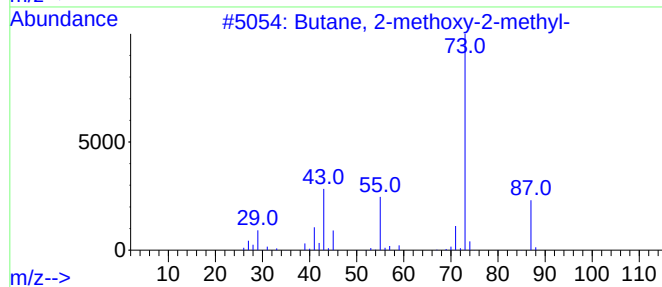
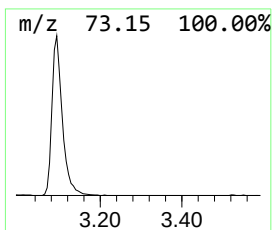
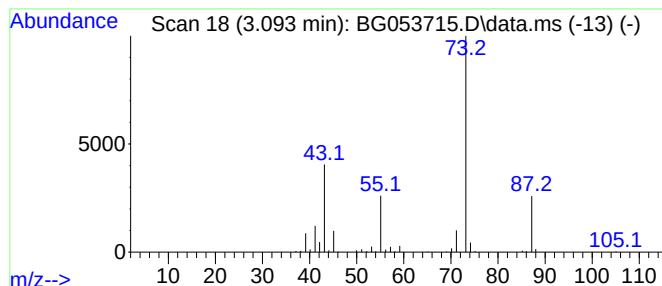
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 3.093 | 44.22 ng | 320058 | 1,4-Dichlorobenzene-d4 | 7.980 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 78   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 27   |
| 4    |    |   | 2-Methyl-5-hexen-3-ol       | 114 | C7H14O  | 032815-70-6 | 25   |
| 5    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |



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Sample : N3028-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG050522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

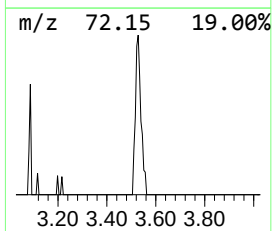
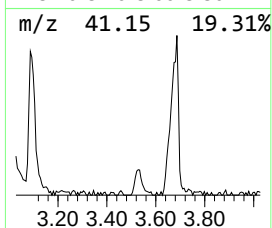
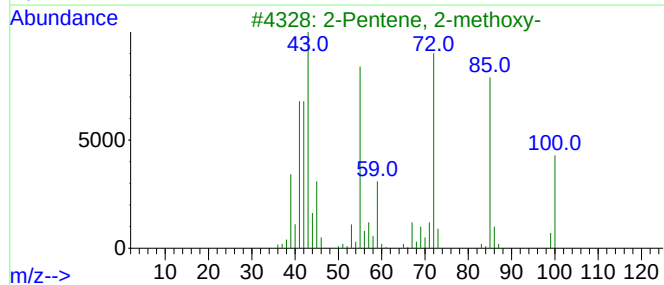
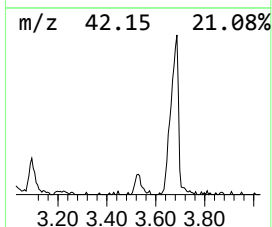
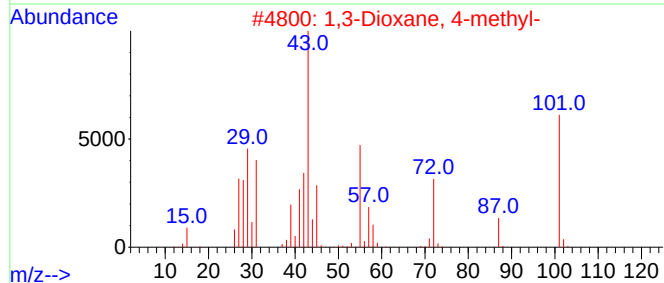
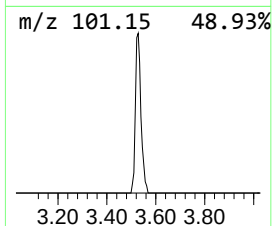
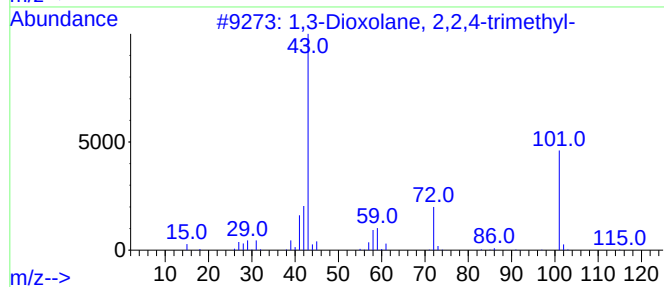
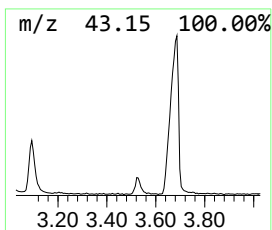
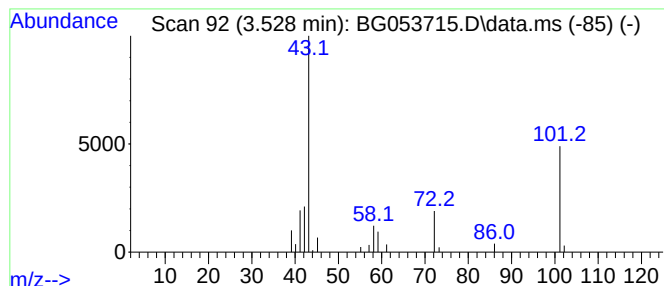
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 3.528 | 5.40 ng | 39096 | 1,4-Dichlorobenzene-d4 | 7.980 |

| Hit# of 5 | Tentative ID                    | MW  | MolForm | CAS#        | Qual |
|-----------|---------------------------------|-----|---------|-------------|------|
| 1         | 1,3-Dioxolane, 2,2,4-trimethyl- | 116 | C6H12O2 | 001193-11-9 | 83   |
| 2         | 1,3-Dioxane, 4-methyl-          | 102 | C5H10O2 | 001120-97-4 | 45   |
| 3         | 2-Pentene, 2-methoxy-           | 100 | C6H12O  | 061142-47-0 | 12   |
| 4         | Butane                          | 58  | C4H10   | 000106-97-8 | 9    |
| 5         | Butane, 2,3-dimethyl-           | 86  | C6H14   | 000079-29-8 | 9    |



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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

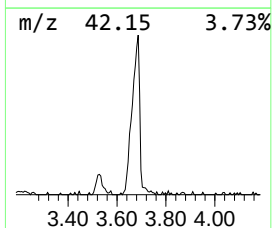
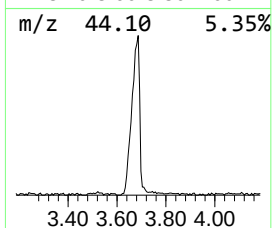
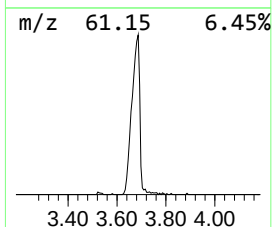
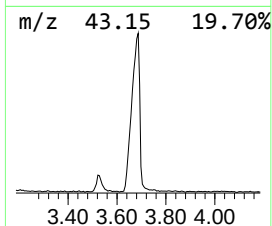
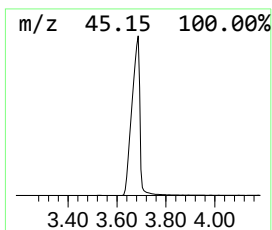
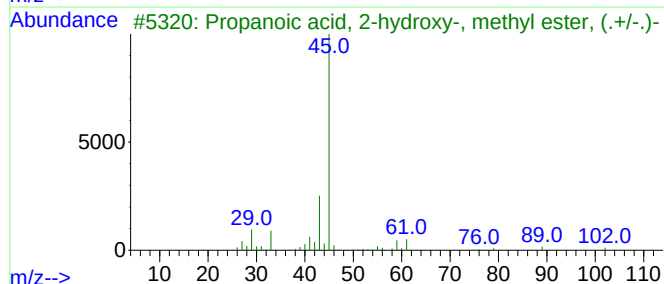
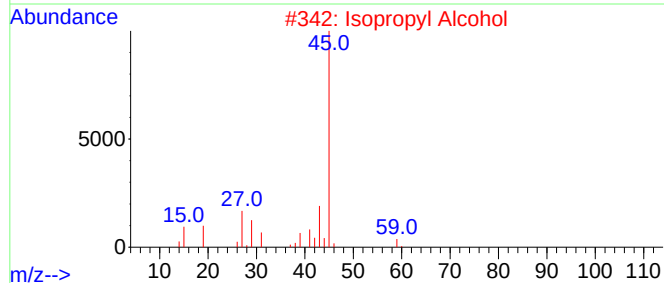
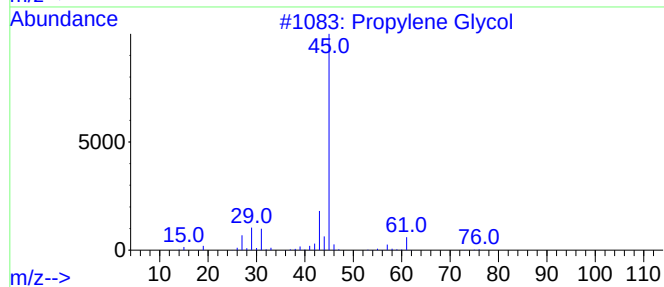
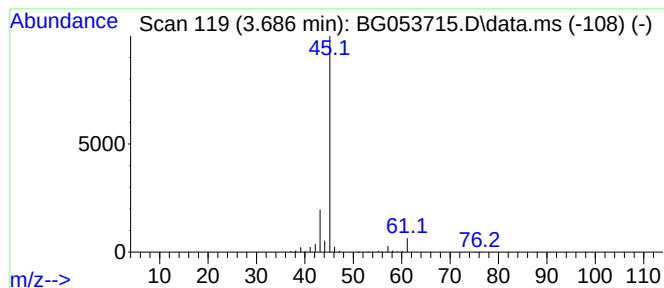
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG050522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Propylene Glycol Concentration Rank 1

| R.T.  | EstConc   | Area    | Relative to ISTD       | R.T.  |
|-------|-----------|---------|------------------------|-------|
| 3.686 | 190.68 ng | 1380040 | 1,4-Dichlorobenzene-d4 | 7.980 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Propylene Glycol                    | 76  | C3H8O2  | 000057-55-6 | 90   |
| 2    |    |   | Isopropyl Alcohol                   | 60  | C3H8O   | 000067-63-0 | 56   |
| 3    |    |   | Propanoic acid, 2-hydroxy-, meth... | 104 | C4H8O3  | 000547-64-8 | 40   |
| 4    |    |   | R-(-)-1,2-propanediol               | 76  | C3H8O2  | 004254-14-2 | 9    |
| 5    |    |   | 2-Butanol, 3-methyl-                | 88  | C5H12O  | 000598-75-4 | 9    |



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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

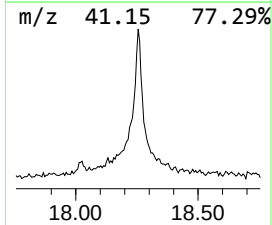
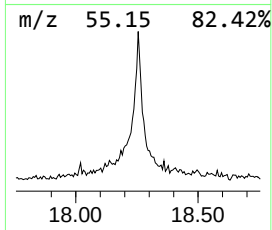
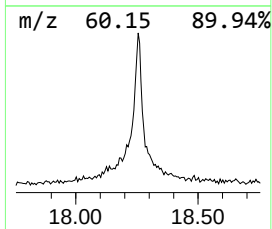
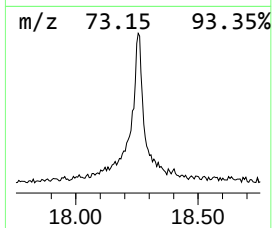
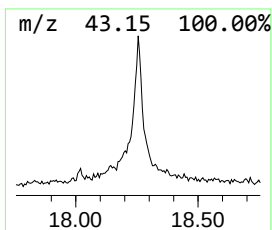
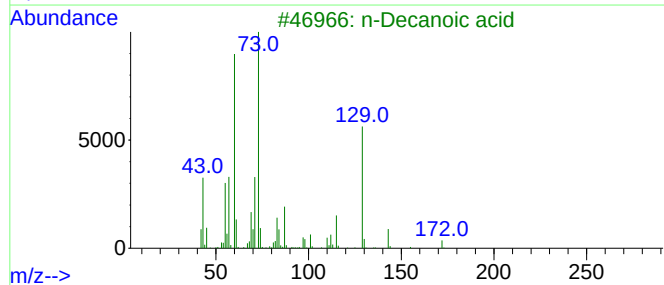
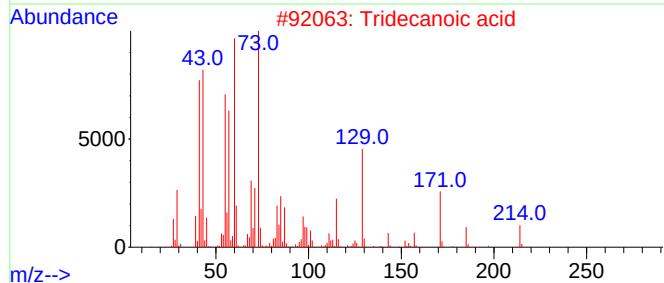
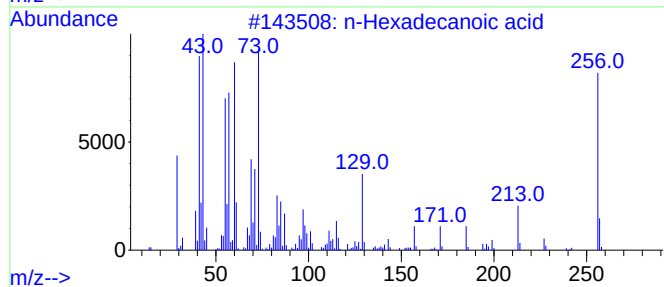
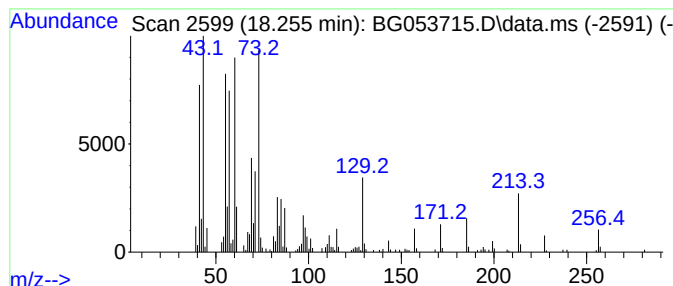
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG050522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 18.255 | 39.21 ng | 650421 | Phenanthrene-d10 | 17.368 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 91   |
| 3    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 83   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 74   |
| 5    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 72   |



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Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

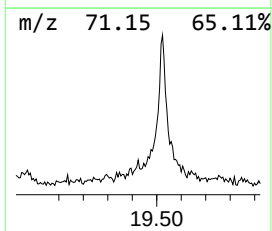
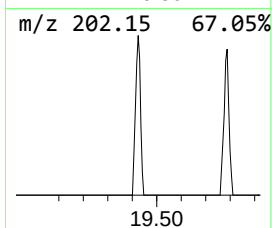
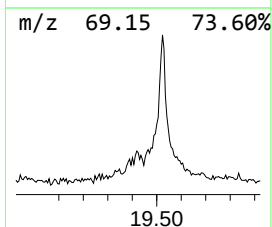
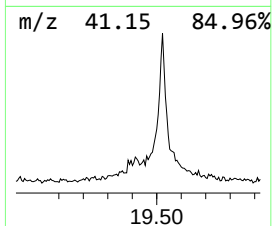
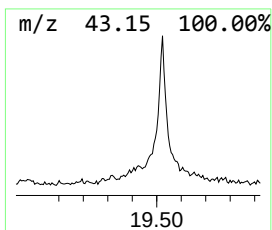
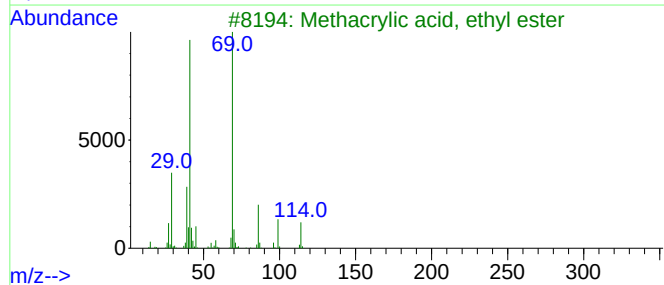
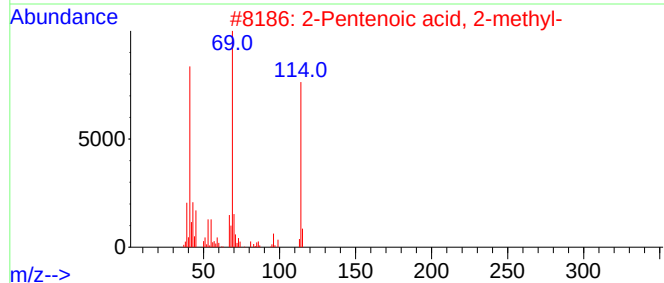
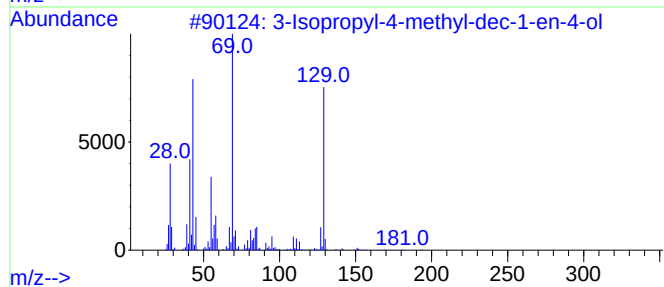
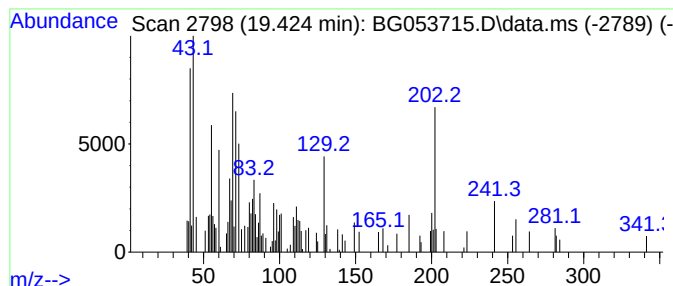
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG050522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 unknown19.424 Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.424 | 6.29 ng | 104285 | Phenanthrene-d10 | 17.368 |

| Hit# | of                                 | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 3-Isopropyl-4-methyl-dec-1-en-4-ol | 212 | C14H28O      | 1000194-91-8 | 27      |      |      |
| 2    | 2-Pentenoic acid, 2-methyl-        | 114 | C6H10O2      | 003142-72-1  | 18      |      |      |
| 3    | Methacrylic acid, ethyl ester      | 114 | C6H10O2      | 000097-63-2  | 18      |      |      |
| 4    | 1,22-Docosanediol                  | 342 | C22H46O2     | 022513-81-1  | 18      |      |      |
| 5    | 4-Nonanol, 2,6,8-trimethyl-        | 186 | C12H26O      | 000123-17-1  | 16      |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG052622\  
Data File : BG053715.D  
Acq On : 26 May 2022 13:44  
Operator : CG/JU  
Sample : N3028-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

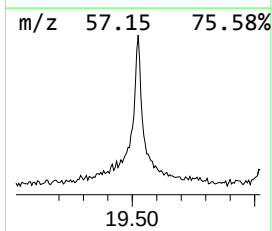
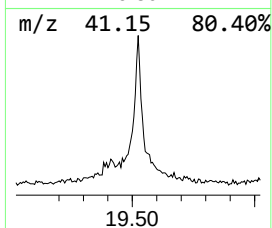
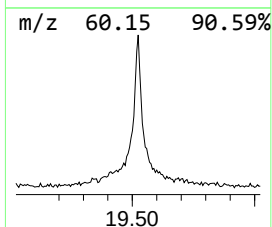
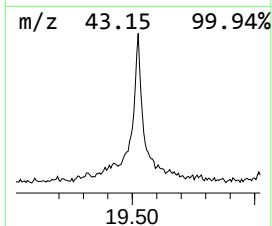
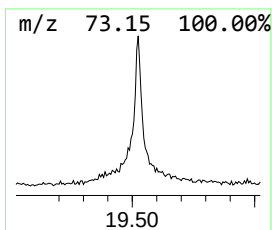
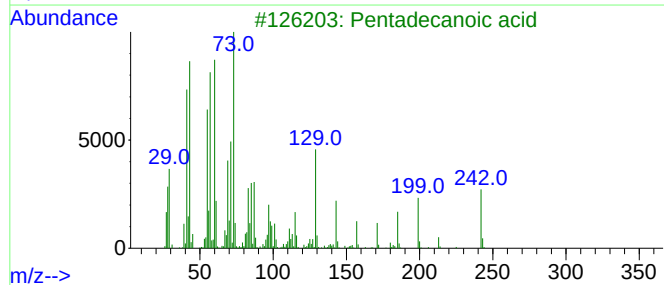
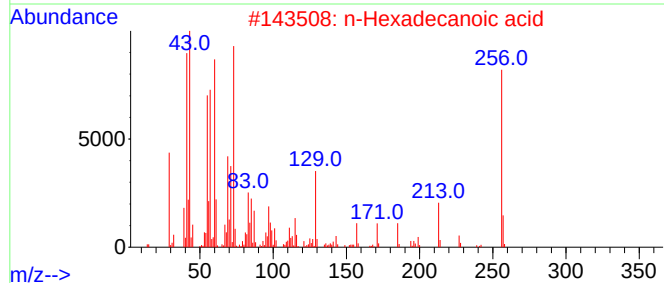
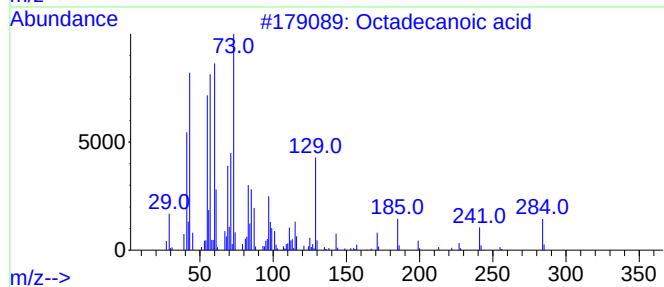
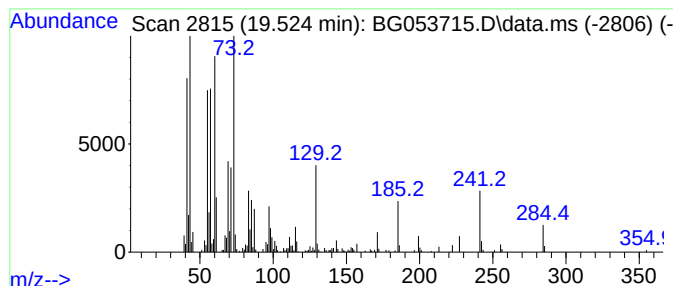
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Octadecanoic acid Concentration Rank 3

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 19.524 | 39.31 ng | 777986 | Chrysene-d12     | 21.633 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 98   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 89   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 5    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 72   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG052622\  
Data File : BG053715.D  
Acq On : 26 May 2022 13:44  
Operator : CG/JU  
Sample : N3028-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

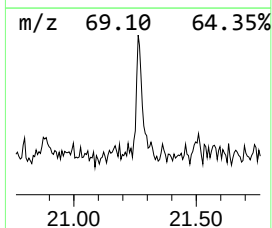
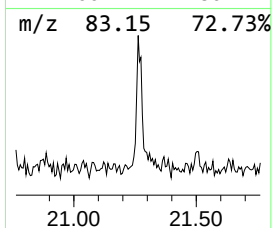
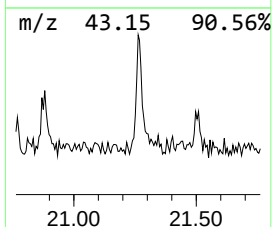
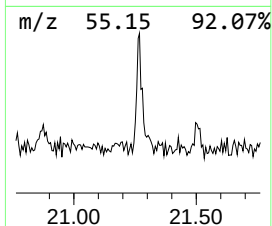
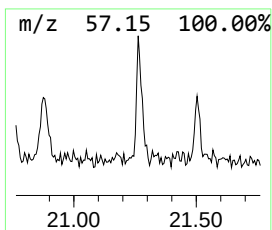
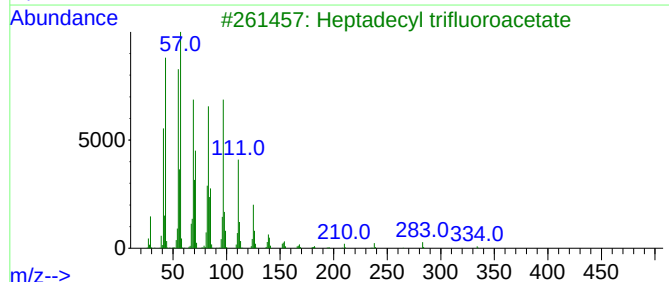
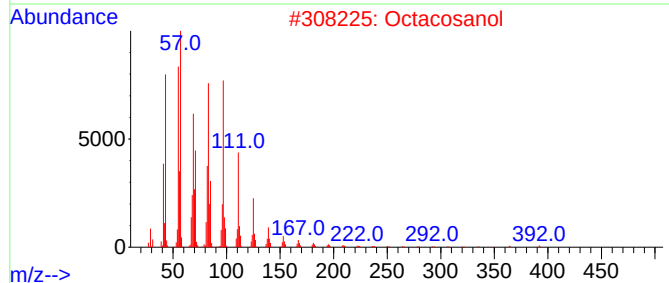
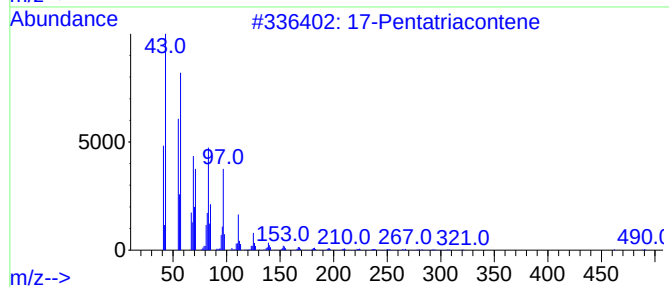
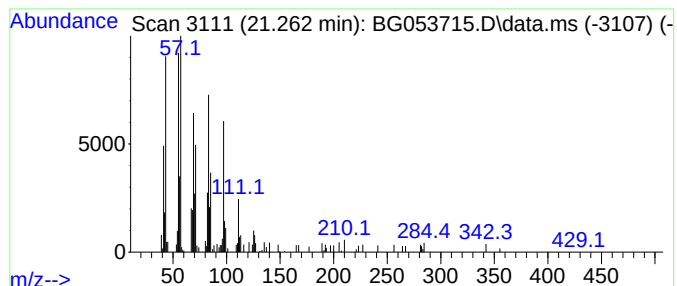
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 17-Pentatriacontene Concentration Rank 7

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.262 | 4.72 ng | 93466 | Chrysene-d12     | 21.633 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 17-Pentatriacontene                 | 491 | C35H70     | 006971-40-0  | 90   |
| 2    |    |   | Octacosanol                         | 410 | C28H58O    | 000557-61-9  | 87   |
| 3    |    |   | Heptadecyl trifluoroacetate         | 352 | C19H35F3O2 | 1010351-87-0 | 87   |
| 4    |    |   | n-Tetracosanol-1                    | 354 | C24H50O    | 000506-51-4  | 87   |
| 5    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5  | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG052622\  
Data File : BG053715.D  
Acq On : 26 May 2022 13:44  
Operator : CG/JU  
Sample : N3028-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-1-1-5FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG050522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 3.093  | 44.2    | ng    | 320058   | 1                     | 7.980  | 144752 | 20.0 |
| 1,3-Dioxolane, ... | 3.528  | 5.4     | ng    | 39096    | 1                     | 7.980  | 144752 | 20.0 |
| Propylene Glycol   | 3.686  | 190.7   | ng    | 1380040  | 1                     | 7.980  | 144752 | 20.0 |
| n-Hexadecanoic ... | 18.255 | 39.2    | ng    | 650421   | 4                     | 17.368 | 331748 | 20.0 |
| unknown19.424      | 19.424 | 6.3     | ng    | 104285   | 4                     | 17.368 | 331748 | 20.0 |
| Octadecanoic acid  | 19.524 | 39.3    | ng    | 777986   | 5                     | 21.633 | 395866 | 20.0 |
| 17-Pentatriacon... | 21.262 | 4.7     | ng    | 93466    | 5                     | 21.633 | 395866 | 20.0 |