

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG041321\  
 Data File : BG048683.D  
 Acq On : 13 Apr 2021 21:03  
 Operator : CG/JU  
 Sample : M1967-12  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 EB 2021-04-06\_SO

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-BG033021.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048683.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         | 5.631       | 382           | 390         | 399          | rBV      | 154271         | 249466        | 12.49%          | 3.956%        |
| 2         | 7.241       | 657           | 664         | 676          | rVB      | 100169         | 178912        | 8.95%           | 2.837%        |
| 3         | 8.081       | 798           | 807         | 813          | rBV2     | 66378          | 108590        | 5.43%           | 1.722%        |
| 4         | 9.256       | 998           | 1007        | 1015         | rBV      | 224506         | 411745        | 20.61%          | 6.530%        |
| 5         | 10.913      | 1280          | 1289        | 1296         | rBV      | 80095          | 143373        | 7.18%           | 2.274%        |
| 6         | 13.357      | 1698          | 1705        | 1712         | rBV      | 624850         | 929575        | 46.53%          | 14.742%       |
| 7         | 14.738      | 1934          | 1940        | 1948         | rVB      | 139305         | 215331        | 10.78%          | 3.415%        |
| 8         | 16.230      | 2187          | 2194        | 2201         | rBV      | 629215         | 911333        | 45.61%          | 14.453%       |
| 9         | 17.493      | 2403          | 2409        | 2417         | rBV      | 206681         | 309226        | 15.48%          | 4.904%        |
| 10        | 18.375      | 2552          | 2559        | 2566         | rBV4     | 25348          | 41375         | 2.07%           | 0.656%        |
| 11        | 20.102      | 2847          | 2853        | 2859         | rBV      | 1551043        | 1997994       | 100.00%         | 31.687%       |
| 12        | 21.407      | 3069          | 3075        | 3085         | rBV3     | 46443          | 94300         | 4.72%           | 1.496%        |
| 13        | 21.788      | 3133          | 3140        | 3150         | rVB      | 225421         | 364846        | 18.26%          | 5.786%        |
| 14        | 25.126      | 3700          | 3708        | 3719         | rVB2     | 117411         | 349439        | 17.49%          | 5.542%        |

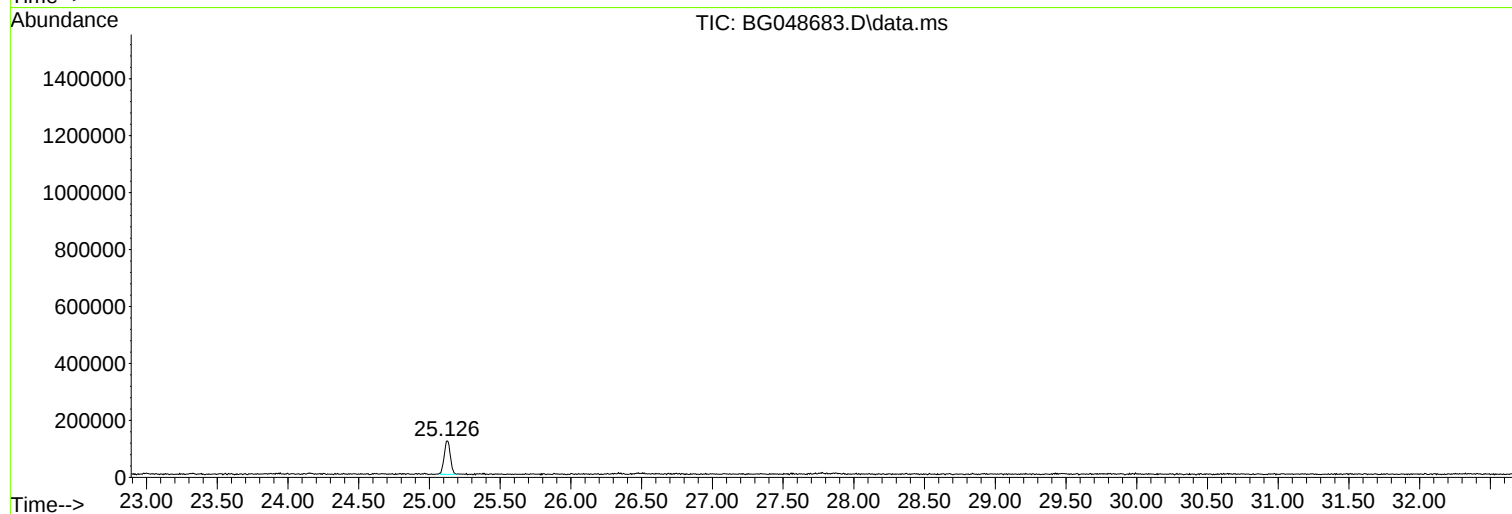
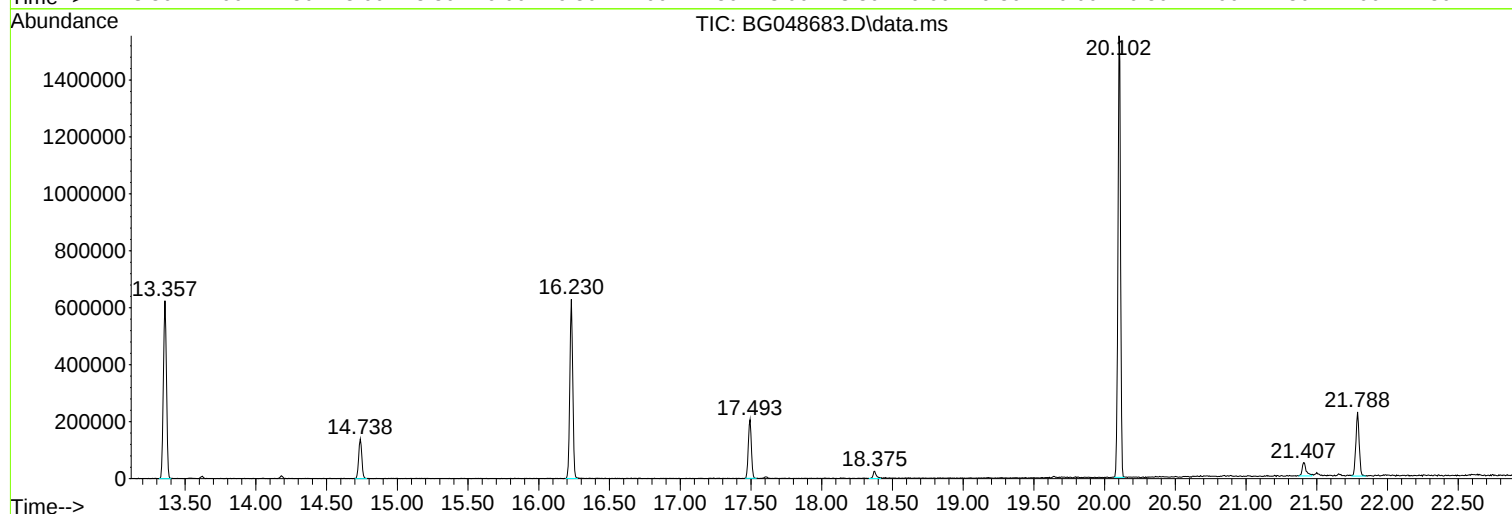
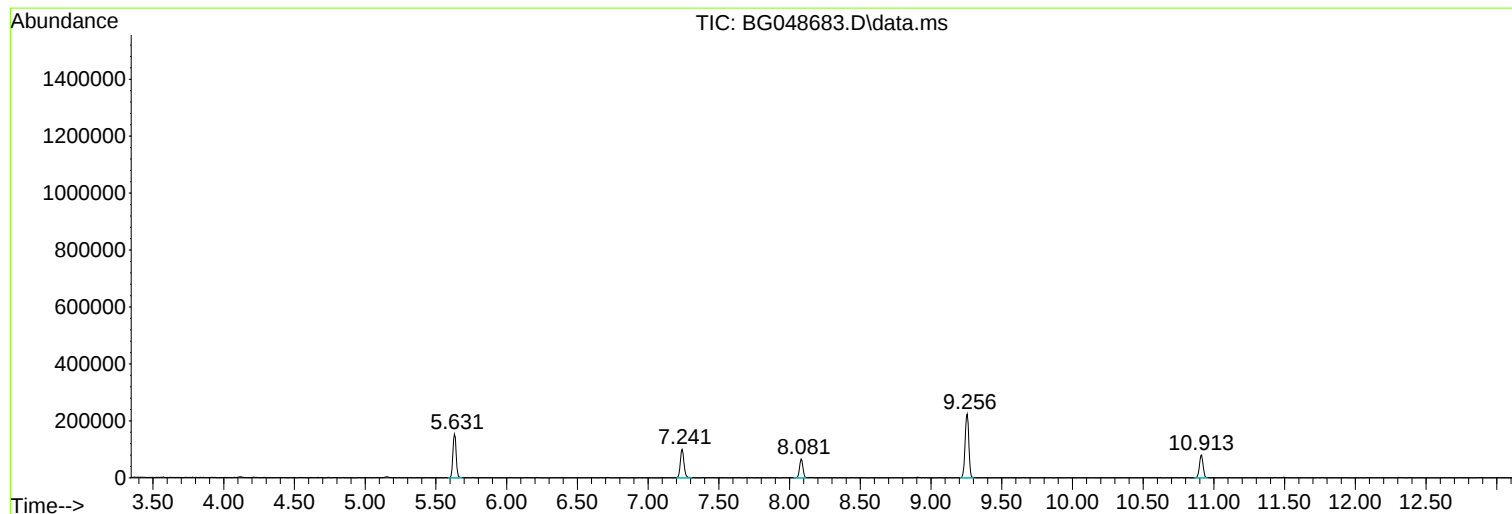
Sum of corrected areas: 6305505

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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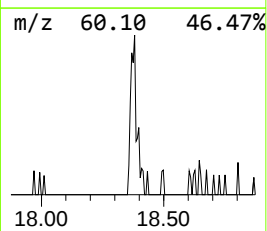
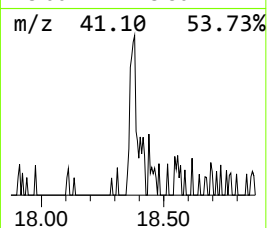
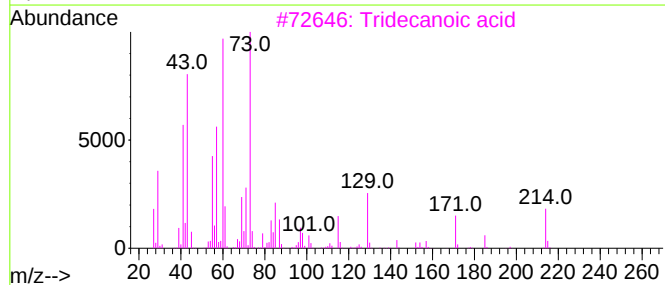
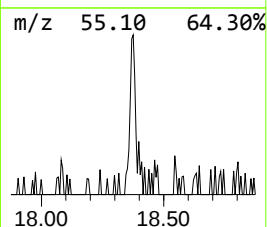
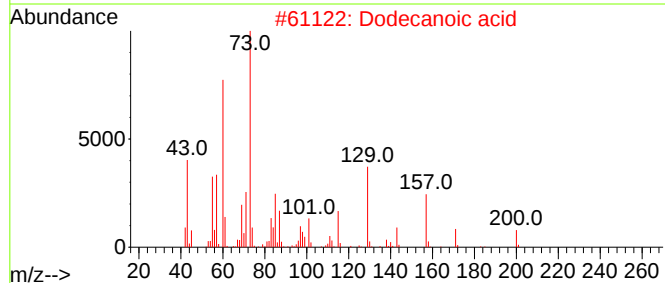
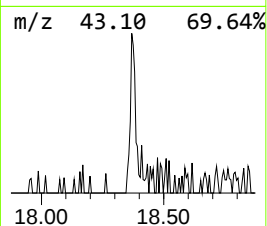
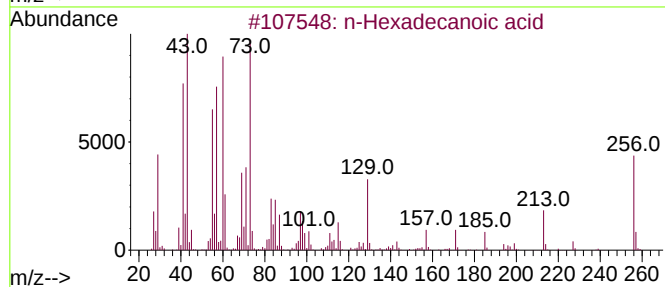
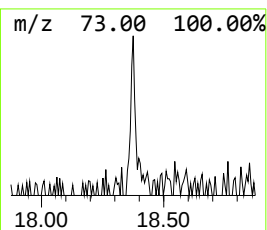
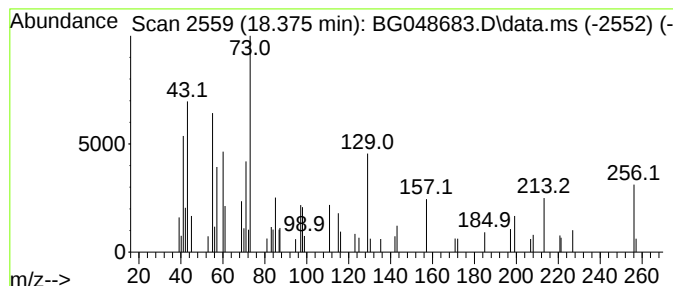
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG033021.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 18.375 | 2.68 ng | 41375 | Phenanthrene-d10 | 17.494 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|------|---------------------|-----|----------|-------------|------|
| 1    |      | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 58   |
| 2    |      | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 50   |
| 3    |      | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 37   |
| 4    |      | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 37   |
| 5    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 35   |



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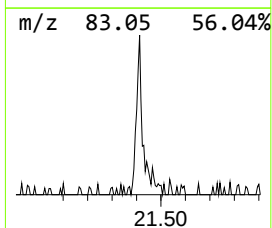
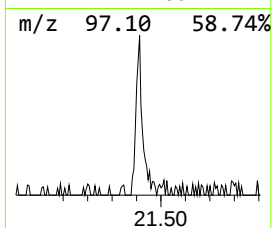
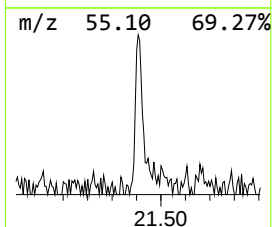
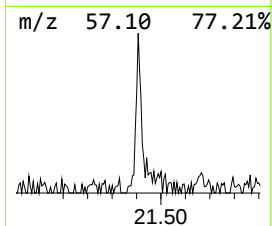
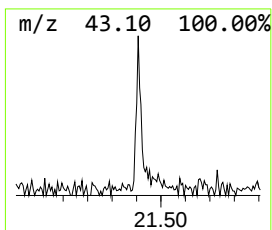
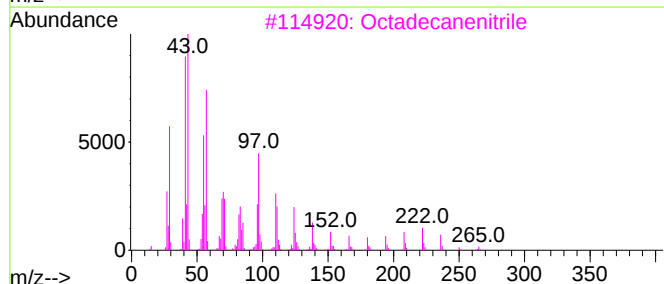
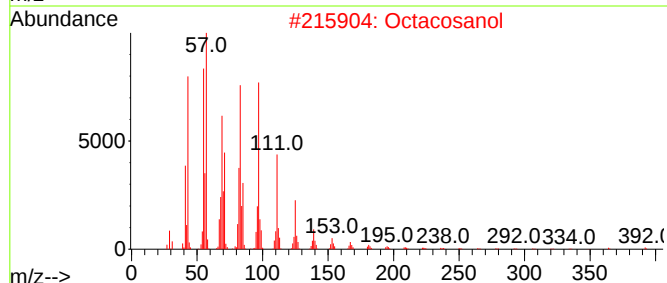
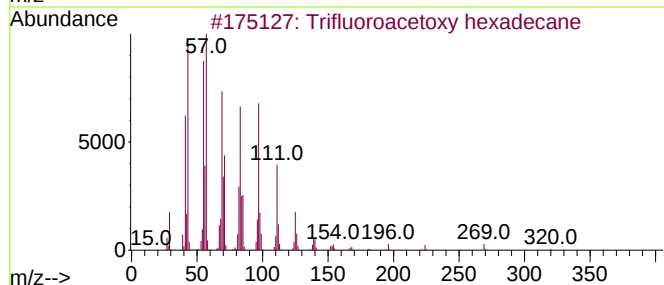
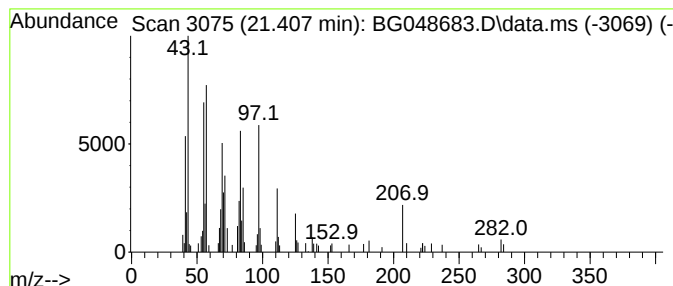
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Peak Number 2 Trifluoroacetoxy hexadecane Concentration Rank 1

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.407 | 5.17 ng | 94300 | Chrysene-d12     | 21.788 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------|-----|------------|--------------|------|
| 1    |    |   | Trifluoroacetoxy hexadecane    | 338 | C18H33F3O2 | 006222-03-3  | 64   |
| 2    |    |   | Octacosanol                    | 410 | C28H58O    | 000557-61-9  | 62   |
| 3    |    |   | Octadecanenitrile              | 265 | C18H35N    | 000638-65-3  | 60   |
| 4    |    |   | Tricosyl pentafluoropropionate | 486 | C26H47F5O2 | 1000351-81-0 | 58   |
| 5    |    |   | Heptadecyl trifluoroacetate    | 352 | C19H35F3O2 | 1000351-87-0 | 58   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| n-Hexadecanoic ... | 18.375 | 2.7     | ng    | 41375    | 4                     | 17.494 | 309226 | 20.0 |
| Trifluoroacetox... | 21.407 | 5.2     | ng    | 94300    | 5                     | 21.788 | 364846 | 20.0 |