

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF061323\  
 Data File : BF133738.D  
 Acq On : 13 Jun 2023 19:02  
 Operator : CG\JU  
 Sample : 03069-09  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TWP08

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\_F\Methods\8270-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133738.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         | 5.446       | 566           | 571         | 574          | rBV      | 1224232        | 1179529       | 53.32%          | 9.687%        |
| 2         | 6.452       | 739           | 742         | 748          | rBV      | 802409         | 694267        | 31.38%          | 5.702%        |
| 3         | 6.828       | 803           | 806         | 809          | rBV      | 584466         | 512849        | 23.18%          | 4.212%        |
| 4         | 6.863       | 809           | 812         | 815          | rVB      | 232447         | 173693        | 7.85%           | 1.426%        |
| 5         | 7.393       | 898           | 902         | 905          | rBV      | 1487422        | 1344840       | 60.79%          | 11.044%       |
| 6         | 8.116       | 1021          | 1025        | 1028         | rBV      | 661336         | 547783        | 24.76%          | 4.499%        |
| 7         | 9.187       | 1204          | 1207        | 1211         | rBV      | 2133948        | 1933427       | 87.40%          | 15.878%       |
| 8         | 9.869       | 1319          | 1323        | 1326         | rBV      | 656388         | 512804        | 23.18%          | 4.211%        |
| 9         | 10.581      | 1441          | 1444        | 1448         | rBV      | 170630         | 141639        | 6.40%           | 1.163%        |
| 10        | 10.657      | 1453          | 1457        | 1461         | rBV      | 1407556        | 1225576       | 55.40%          | 10.065%       |
| 11        | 10.892      | 1494          | 1497        | 1504         | rVB2     | 39090          | 33158         | 1.50%           | 0.272%        |
| 12        | 11.357      | 1572          | 1576        | 1580         | rBV      | 670129         | 519912        | 23.50%          | 4.270%        |
| 13        | 11.881      | 1661          | 1665        | 1669         | rBV2     | 32391          | 32475         | 1.47%           | 0.267%        |
| 14        | 12.951      | 1842          | 1847        | 1850         | rBV      | 2489503        | 2212134       | 100.00%         | 18.167%       |
| 15        | 13.845      | 1995          | 1999        | 2005         | rBV      | 46938          | 65532         | 2.96%           | 0.538%        |
| 16        | 14.004      | 2022          | 2026        | 2031         | rVB      | 661901         | 587253        | 26.55%          | 4.823%        |
| 17        | 14.480      | 2104          | 2107        | 2110         | rVB3     | 48436          | 46417         | 2.10%           | 0.381%        |
| 18        | 15.463      | 2269          | 2274        | 2281         | rBV      | 329768         | 413312        | 18.68%          | 3.394%        |

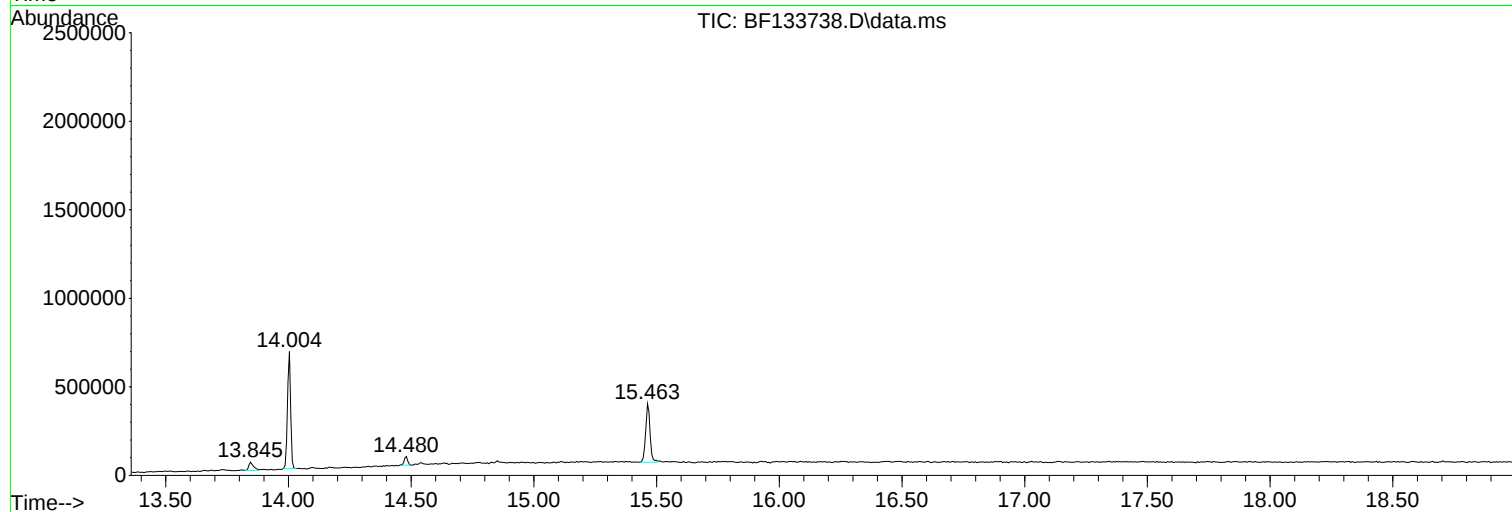
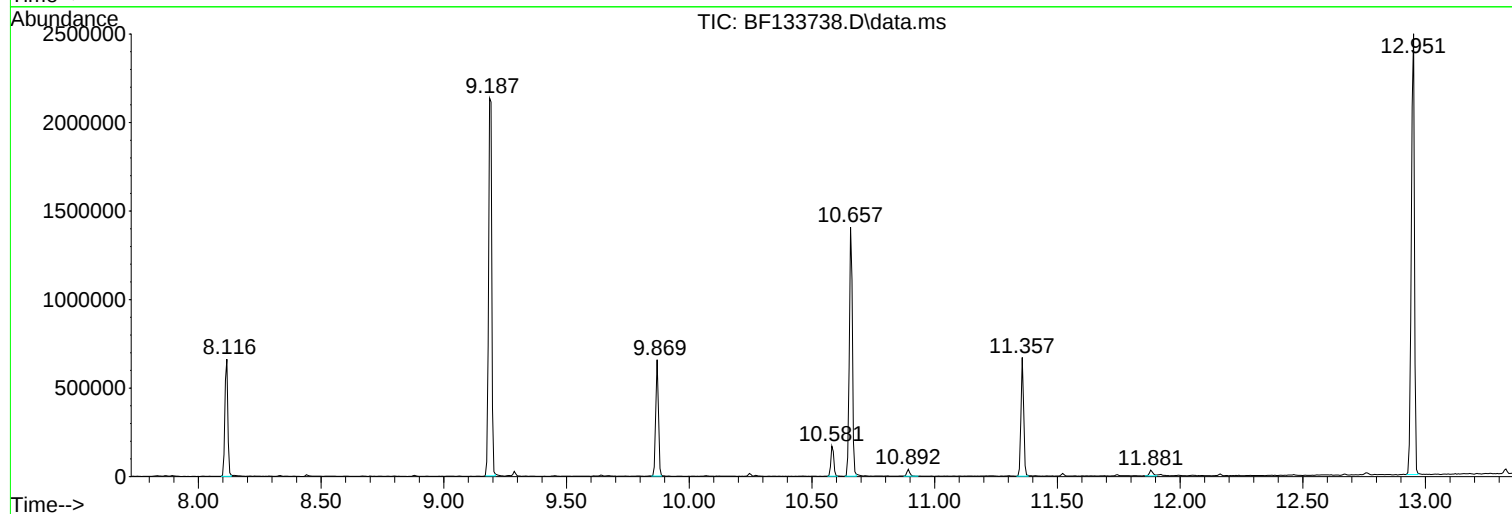
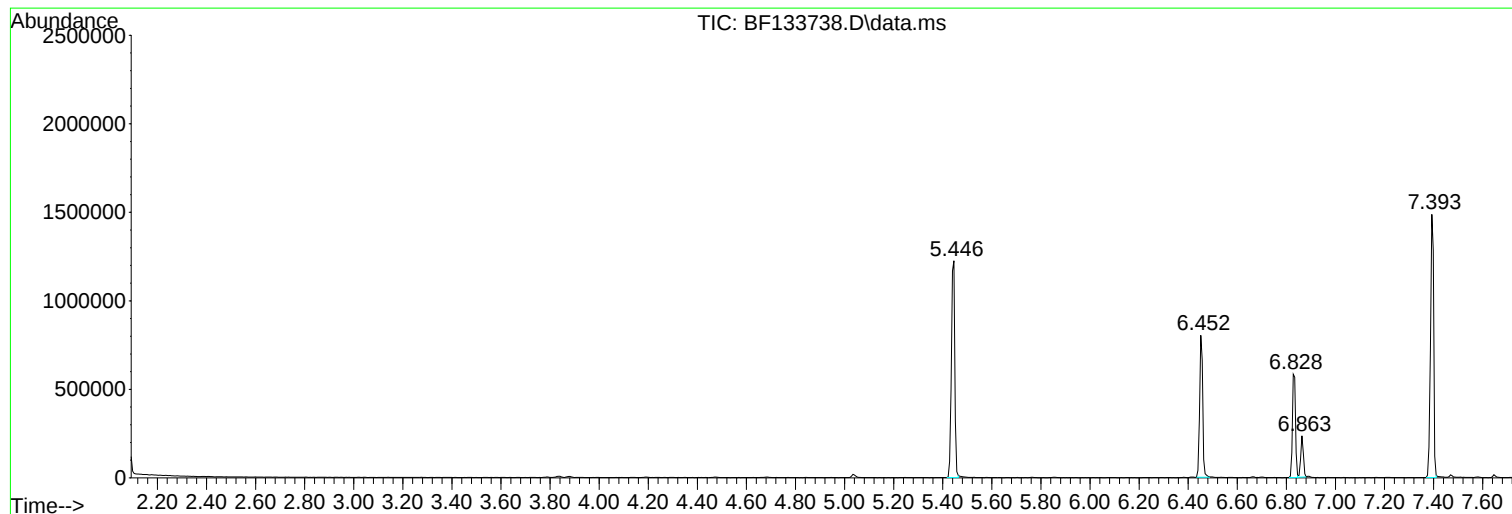
Sum of corrected areas: 12176600

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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.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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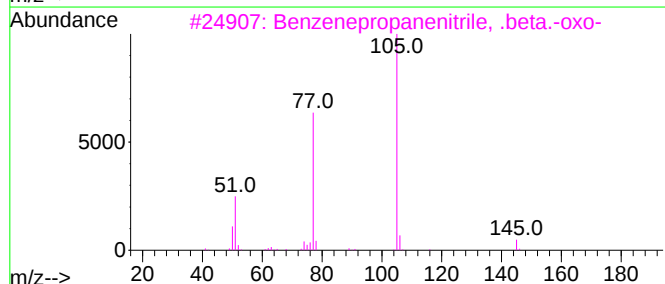
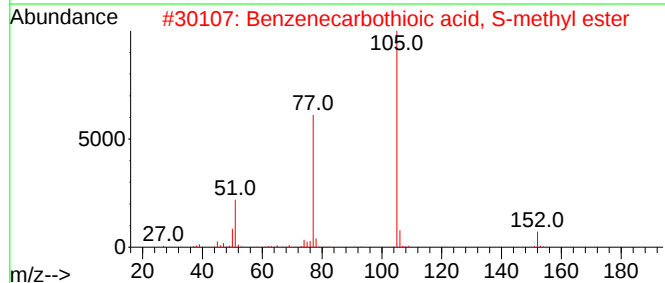
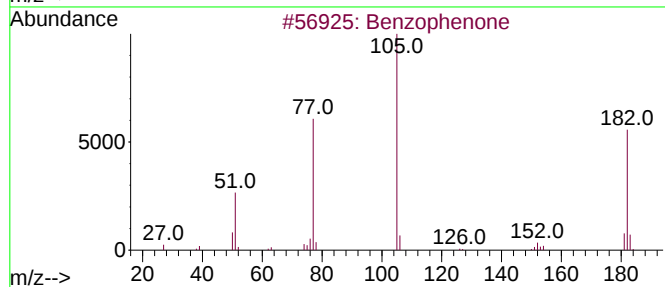
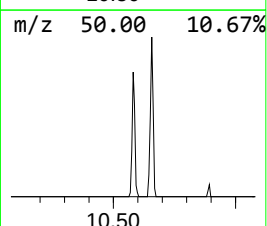
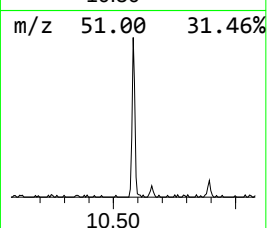
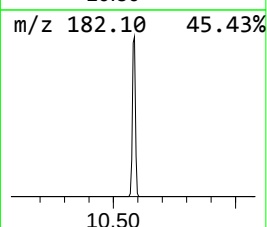
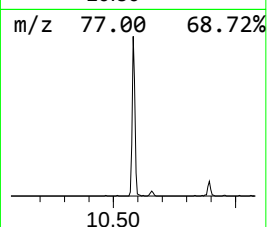
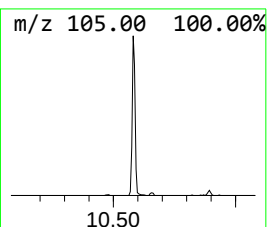
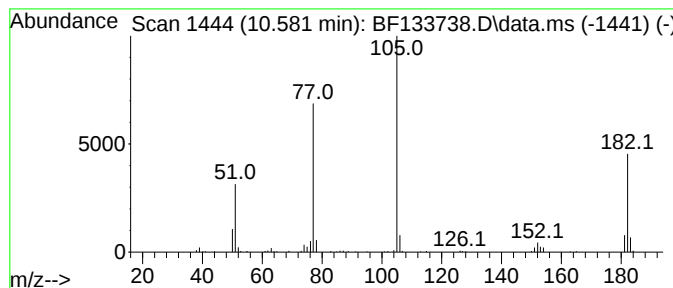
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Benzophenone Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.581 | 5.52 ng | 141639 | Acenaphthene-d10 | 9.869 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS   | 005925-68-8 | 52   |
| 3    |    |   | Benzenepropanenitrile, .beta.-oxo-  | 145 | C9H7NO   | 000614-16-4 | 52   |
| 4    |    |   | Benzenebutanoic acid, .gamma.-oxo-  | 178 | C10H10O3 | 002051-95-8 | 50   |
| 5    |    |   | 1,2-Propanedione, 1-phenyl-         | 148 | C9H8O2   | 000579-07-7 | 50   |



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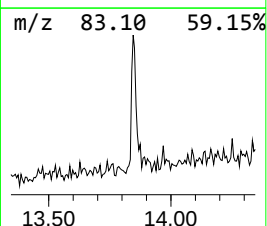
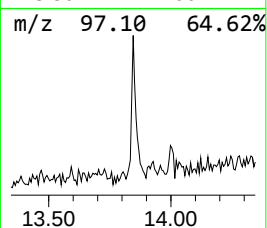
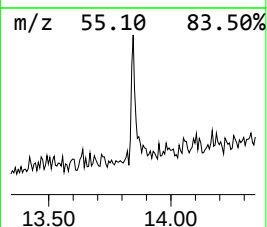
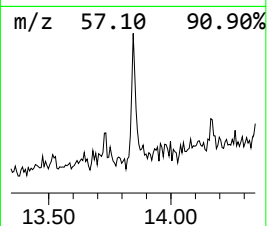
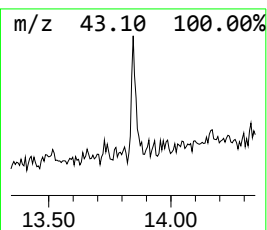
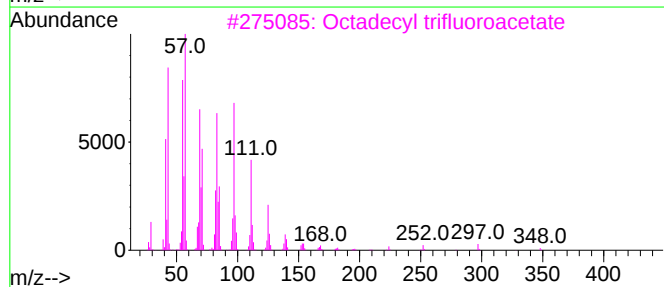
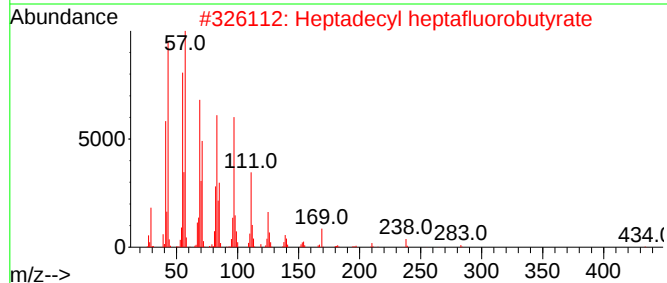
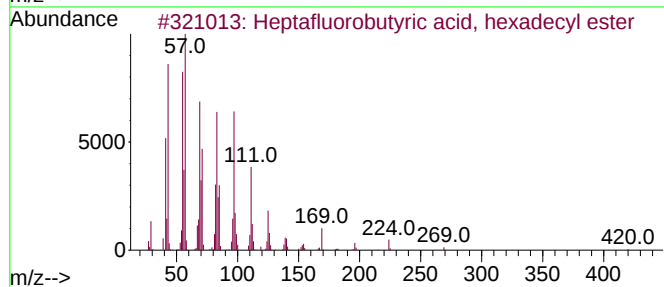
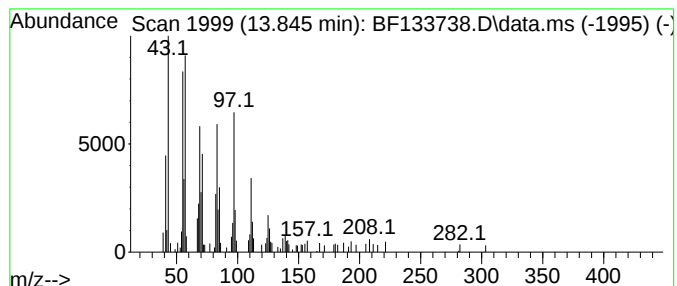
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Peak Number 2 Heptafluorobutyric acid, he... Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 13.845 | 2.23 ng | 65532 | Chrysene-d12     | 14.004 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 95   |
| 2    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2 | 959085-66-6 | 95   |
| 3    |    |   | Octadecyl trifluoroacetate          | 366 | C20H37F3O2 | 079392-43-1 | 95   |
| 4    |    |   | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 95   |
| 5    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 95   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Benzophenone       | 10.581 | 5.5     | ng    | 141639   | 3                     | 9.869  | 512804 | 20.0 |
| Heptafluorobuty... | 13.845 | 2.2     | ng    | 65532    | 5                     | 14.004 | 587253 | 20.0 |