

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF041322\  
 Data File : BF127787.D  
 Acq On : 13 Apr 2022 16:42  
 Operator : CG\JU  
 Sample : N2333-07  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MW-11R

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127787.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         | 2.387       | 12            | 17          | 22           | rBV      | 30687          | 42961         | 1.10%           | 0.233%        |
| 2         | 5.181       | 489           | 492         | 497          | rBV      | 96980          | 100687        | 2.57%           | 0.545%        |
| 3         | 5.575       | 555           | 559         | 562          | rBV      | 1685049        | 1456832       | 37.24%          | 7.886%        |
| 4         | 6.569       | 724           | 728         | 732          | rBV      | 1083317        | 892580        | 22.82%          | 4.832%        |
| 5         | 6.957       | 790           | 794         | 797          | rBV      | 888596         | 705733        | 18.04%          | 3.820%        |
| 6         | 7.522       | 885           | 890         | 893          | rVB      | 2373214        | 2275845       | 58.18%          | 12.319%       |
| 7         | 7.686       | 915           | 918         | 921          | rVB      | 52884          | 42945         | 1.10%           | 0.232%        |
| 8         | 7.722       | 921           | 924         | 930          | rBV3     | 48499          | 54740         | 1.40%           | 0.296%        |
| 9         | 8.239       | 1008          | 1012        | 1015         | rBV      | 1029079        | 866613        | 22.16%          | 4.691%        |
| 10        | 9.316       | 1190          | 1195        | 1198         | rBV      | 4445967        | 3911505       | 100.00%         | 21.173%       |
| 11        | 9.386       | 1203          | 1207        | 1210         | rVB      | 50525          | 46600         | 1.19%           | 0.252%        |
| 12        | 9.998       | 1307          | 1311        | 1314         | rBV      | 1093496        | 869456        | 22.23%          | 4.706%        |
| 13        | 10.028      | 1314          | 1316        | 1321         | rVB      | 111443         | 90517         | 2.31%           | 0.490%        |
| 14        | 10.786      | 1441          | 1445        | 1449         | rBV      | 2288736        | 2019768       | 51.64%          | 10.933%       |
| 15        | 11.486      | 1561          | 1564        | 1568         | rBV      | 848874         | 743698        | 19.01%          | 4.026%        |
| 16        | 13.074      | 1830          | 1834        | 1838         | rBV      | 2922701        | 2720436       | 69.55%          | 14.726%       |
| 17        | 14.004      | 1988          | 1992        | 2006         | rBV2     | 73507          | 164451        | 4.20%           | 0.890%        |
| 18        | 14.133      | 2010          | 2014        | 2018         | rVV      | 735641         | 640673        | 16.38%          | 3.468%        |
| 19        | 15.657      | 2267          | 2273        | 2284         | rVB      | 638164         | 828082        | 21.17%          | 4.482%        |

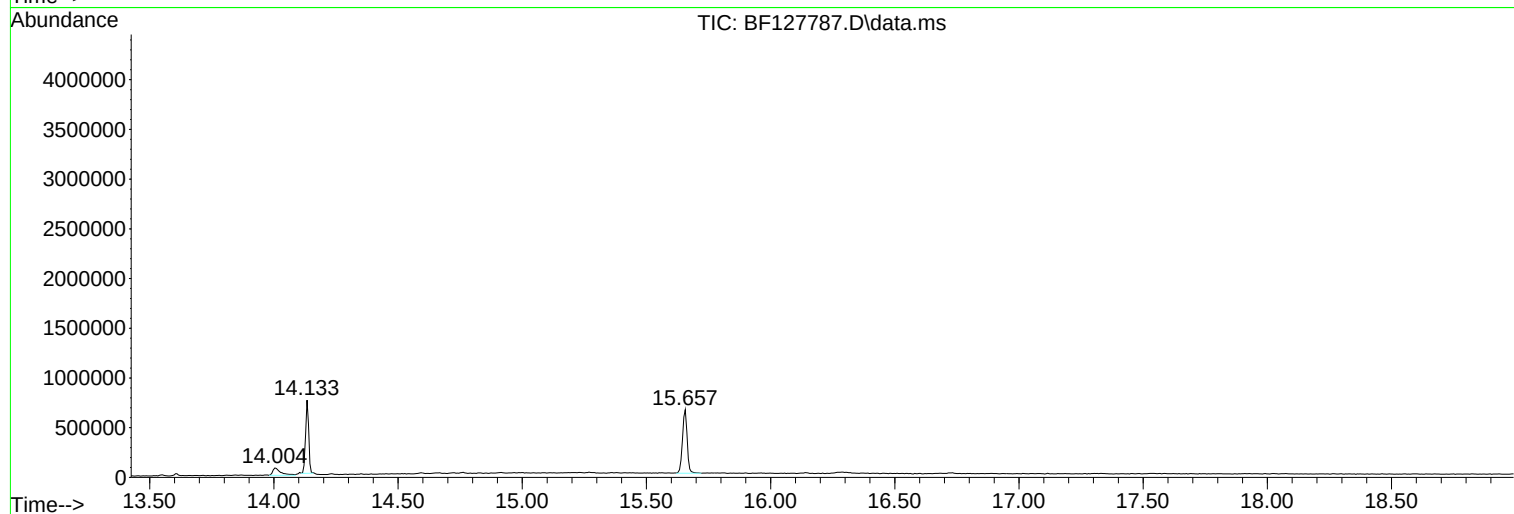
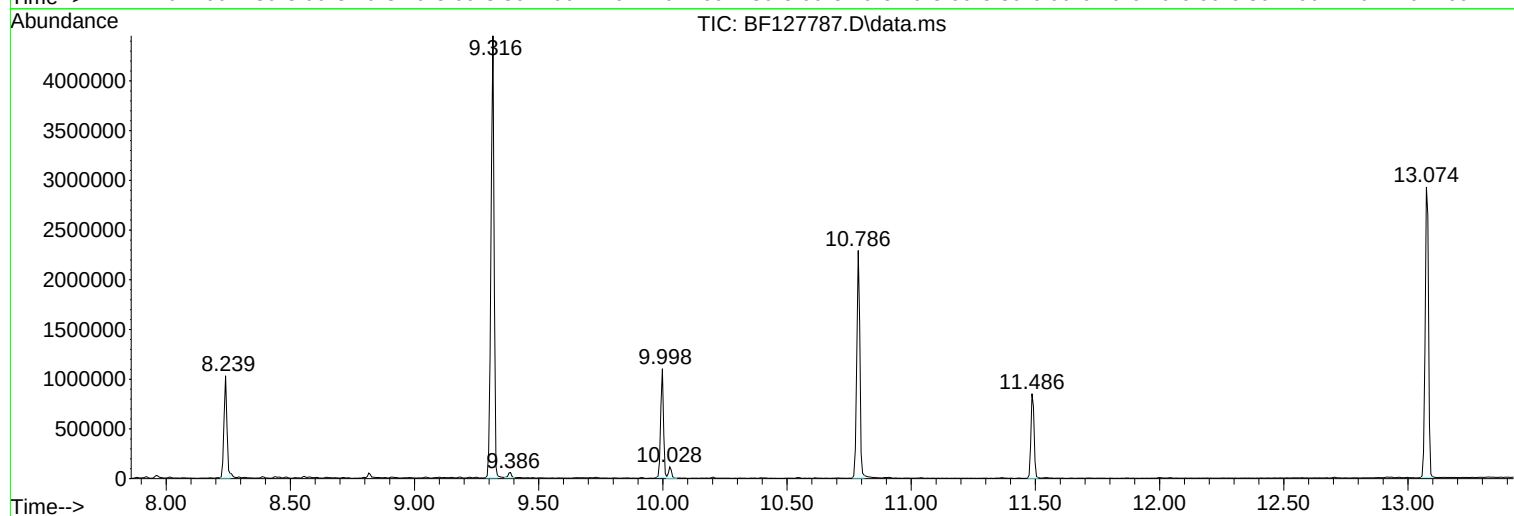
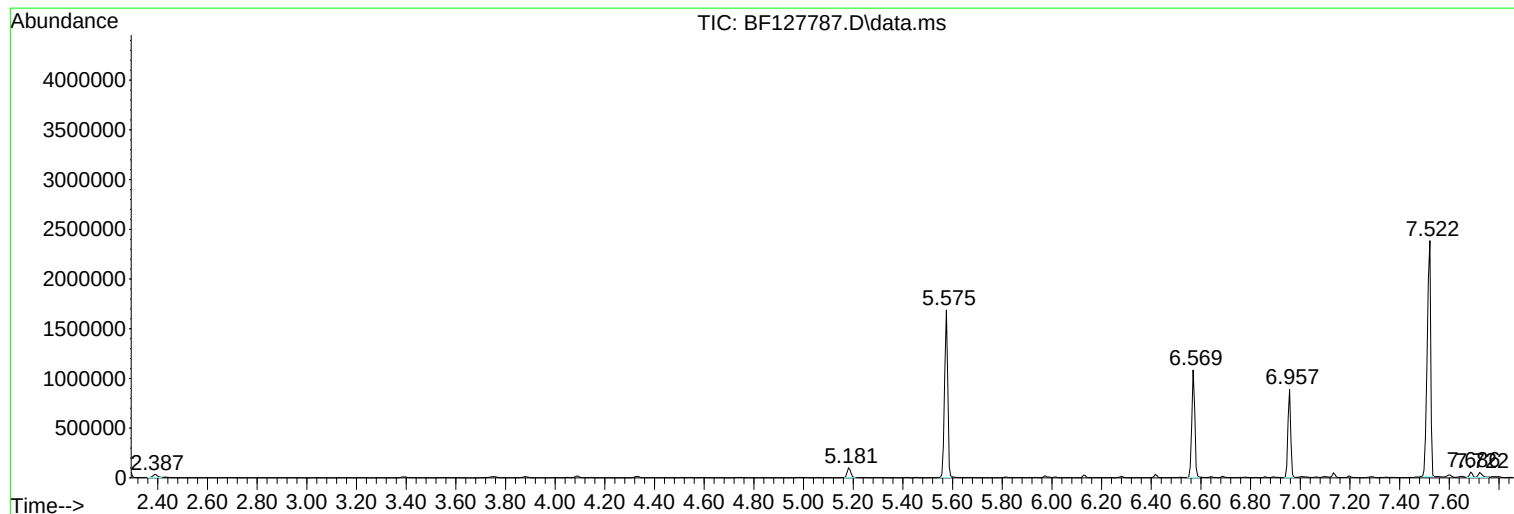
Sum of corrected areas: 18474122

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Instrument :  
BNA\_F  
ClientSampleId :  
MW-11R

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF040622.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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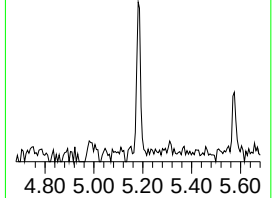
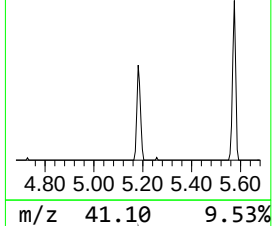
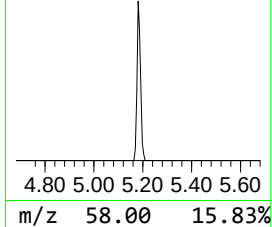
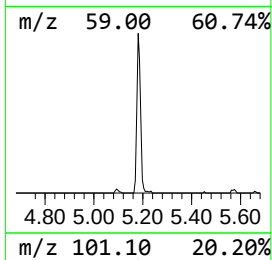
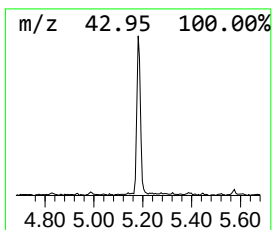
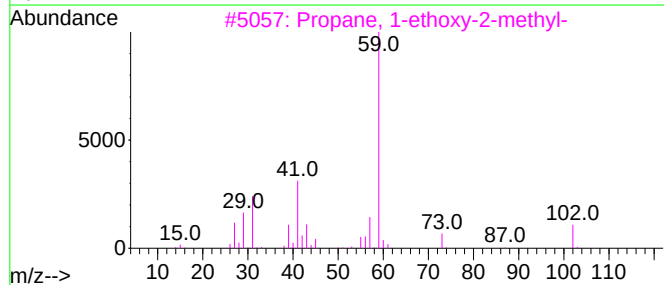
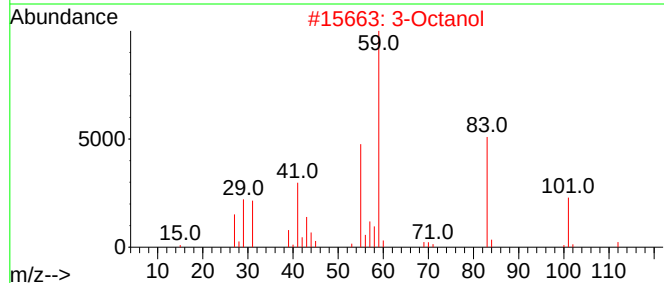
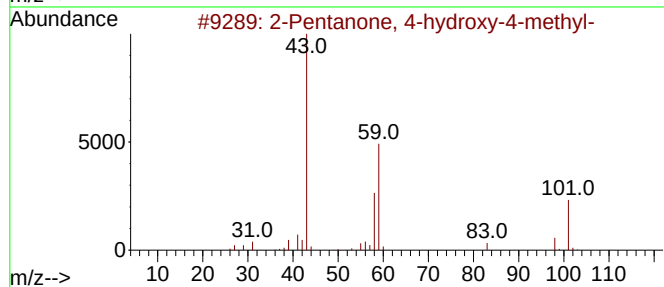
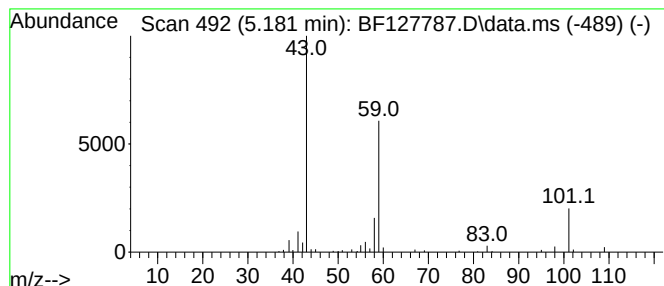
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.181 | 2.85 ng | 100687 | 1,4-Dichlorobenzene-d4 | 6.957 |

| Hit# | of                               | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|----------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | 3-Octanol                        | 130 | C8H18O       | 000589-98-0 | 36      |      |      |
| 3    | Propane, 1-ethoxy-2-methyl-      | 102 | C6H14O       | 000627-02-1 | 25      |      |      |
| 4    | 3-Hydroxy-3-methyl-2-butanone    | 102 | C5H10O2      | 000115-22-0 | 17      |      |      |
| 5    | 2,3-Butanediol, 2,3-dimethyl-    | 118 | C6H14O2      | 000076-09-5 | 17      |      |      |



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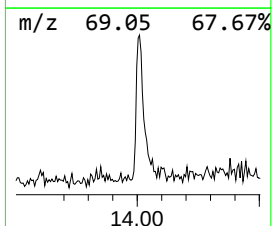
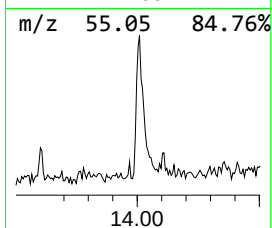
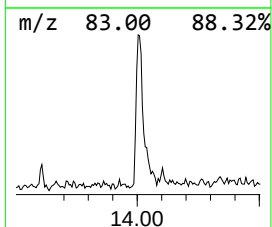
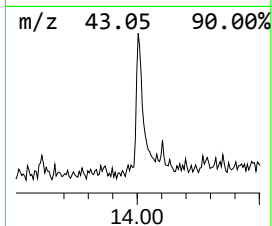
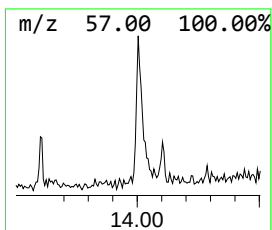
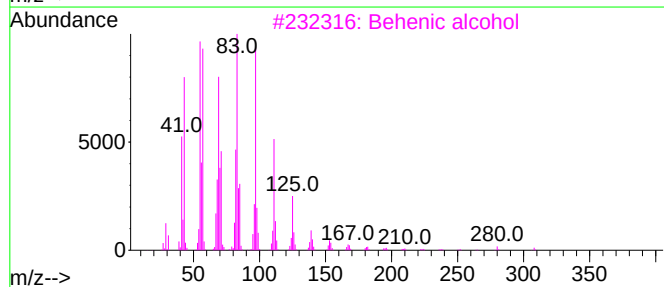
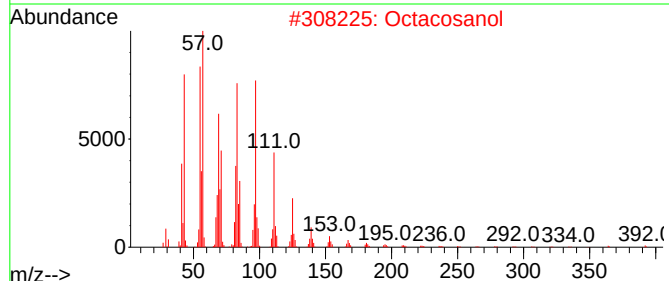
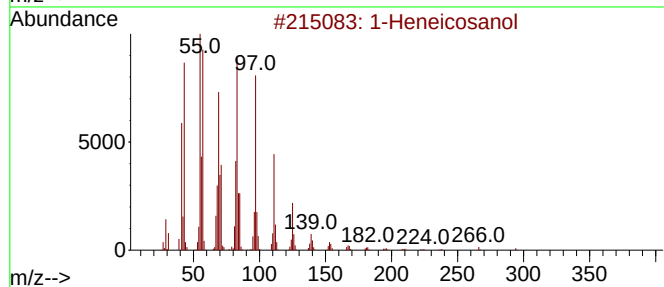
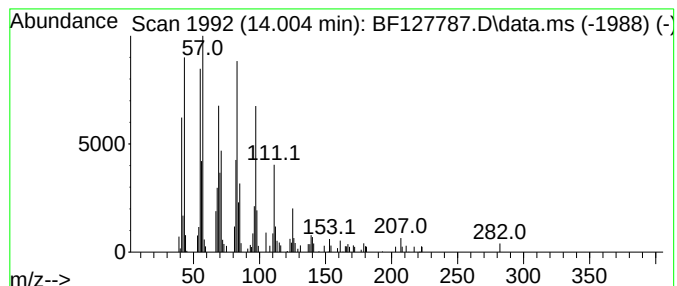
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Peak Number 2 1-Heneicosanol Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.004 | 5.13 ng | 164451 | Chrysene-d12     | 14.133 |

| Hit# | of 5 | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|------|------|------------------|-----|---------|-------------|------|
| 1    |      | 1-Heneicosanol   | 312 | C21H44O | 015594-90-8 | 95   |
| 2    |      | Octacosanol      | 410 | C28H58O | 000557-61-9 | 95   |
| 3    |      | Behenic alcohol  | 326 | C22H46O | 000661-19-8 | 95   |
| 4    |      | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 95   |
| 5    |      | 1-Heptacosanol   | 396 | C27H56O | 002004-39-9 | 94   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.181  | 2.9     | ng    | 100687   | 1                     | 6.957  | 705733 | 20.0 |
| 1-Heneicosanol     | 14.004 | 5.1     | ng    | 164451   | 5                     | 14.133 | 640673 | 20.0 |