

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011224\  
 Data File : BF137048.D  
 Acq On : 12 Jan 2024 15:01  
 Operator : CG\JU  
 Sample : P1119-01  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MH-J

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137048.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         | 2.163       | 9             | 13          | 20           | rVB2     | 12535          | 16629         | 1.49%           | 0.216%        |
| 2         | 5.016       | 494           | 498         | 510          | rVB      | 53248          | 63583         | 5.69%           | 0.827%        |
| 3         | 5.428       | 565           | 568         | 585          | rBV      | 864796         | 868963        | 77.79%          | 11.301%       |
| 4         | 6.434       | 735           | 739         | 755          | rBV      | 971452         | 860607        | 77.04%          | 11.192%       |
| 5         | 6.781       | 795           | 798         | 802          | rBV      | 397015         | 330643        | 29.60%          | 4.300%        |
| 6         | 7.345       | 890           | 894         | 897          | rBV      | 659940         | 554819        | 49.67%          | 7.216%        |
| 7         | 8.057       | 1012          | 1015        | 1019         | rBV      | 505438         | 424985        | 38.04%          | 5.527%        |
| 8         | 8.392       | 1068          | 1072        | 1085         | rVB4     | 5898           | 16132         | 1.44%           | 0.210%        |
| 9         | 9.133       | 1194          | 1198        | 1202         | rBV      | 1324524        | 1117116       | 100.00%         | 14.528%       |
| 10        | 9.816       | 1310          | 1314        | 1327         | rBV      | 580168         | 480376        | 43.00%          | 6.247%        |
| 11        | 10.610      | 1446          | 1449        | 1464         | rBV      | 652620         | 612948        | 54.87%          | 7.972%        |
| 12        | 11.310      | 1564          | 1568        | 1571         | rBV      | 574645         | 462872        | 41.43%          | 6.020%        |
| 13        | 11.839      | 1655          | 1658        | 1671         | rBV2     | 112130         | 130324        | 11.67%          | 1.695%        |
| 14        | 12.533      | 1773          | 1776        | 1779         | rBV      | 21110          | 18811         | 1.68%           | 0.245%        |
| 15        | 12.633      | 1790          | 1793        | 1806         | rBV3     | 25029          | 40360         | 3.61%           | 0.525%        |
| 16        | 12.763      | 1810          | 1815        | 1819         | rVB      | 16729          | 18691         | 1.67%           | 0.243%        |
| 17        | 12.904      | 1835          | 1839        | 1842         | rBV      | 1097655        | 908718        | 81.34%          | 11.818%       |
| 18        | 13.874      | 1999          | 2004        | 2005         | rBV5     | 13969          | 18805         | 1.68%           | 0.245%        |
| 19        | 13.968      | 2016          | 2020        | 2028         | rVB      | 316692         | 307162        | 27.50%          | 3.995%        |
| 20        | 14.433      | 2095          | 2099        | 2102         | rBV5     | 12020          | 15905         | 1.42%           | 0.207%        |
| 21        | 14.745      | 2149          | 2152        | 2156         | rBV5     | 10631          | 13182         | 1.18%           | 0.171%        |
| 22        | 14.815      | 2161          | 2164        | 2167         | rBV2     | 13472          | 14652         | 1.31%           | 0.191%        |
| 23        | 15.392      | 2260          | 2262        | 2268         | rVB6     | 8171           | 13141         | 1.18%           | 0.171%        |
| 24        | 15.457      | 2268          | 2273        | 2285         | rBV      | 244422         | 364116        | 32.59%          | 4.735%        |
| 25        | 15.921      | 2349          | 2352        | 2358         | rBV8     | 8473           | 15619         | 1.40%           | 0.203%        |

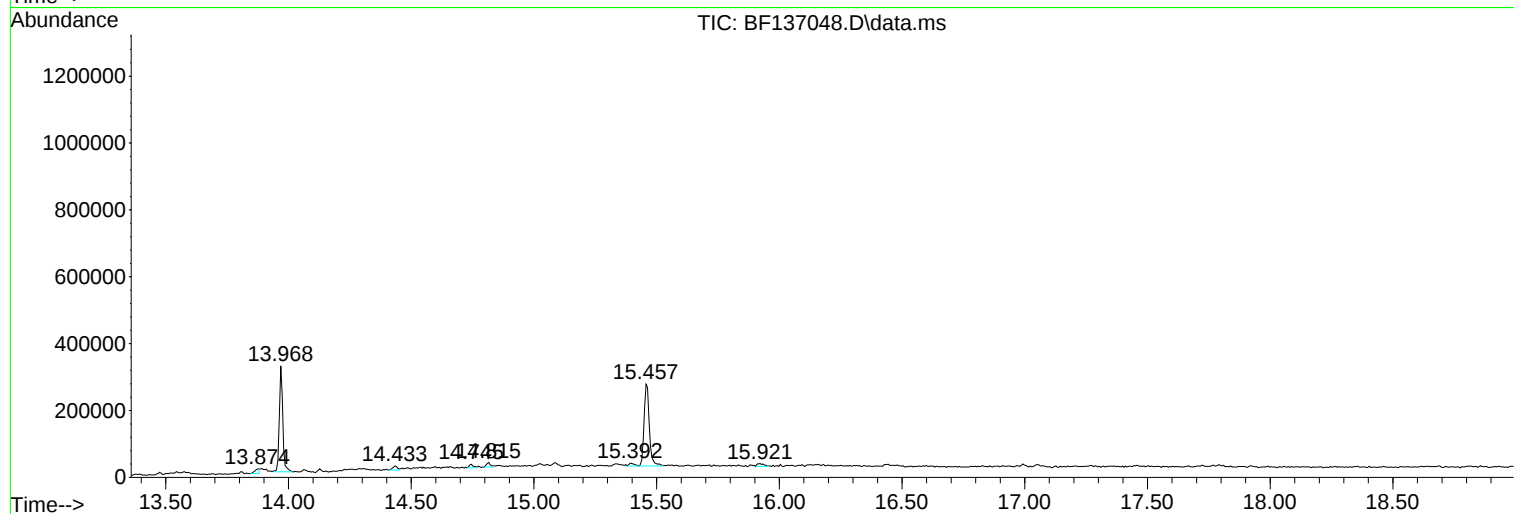
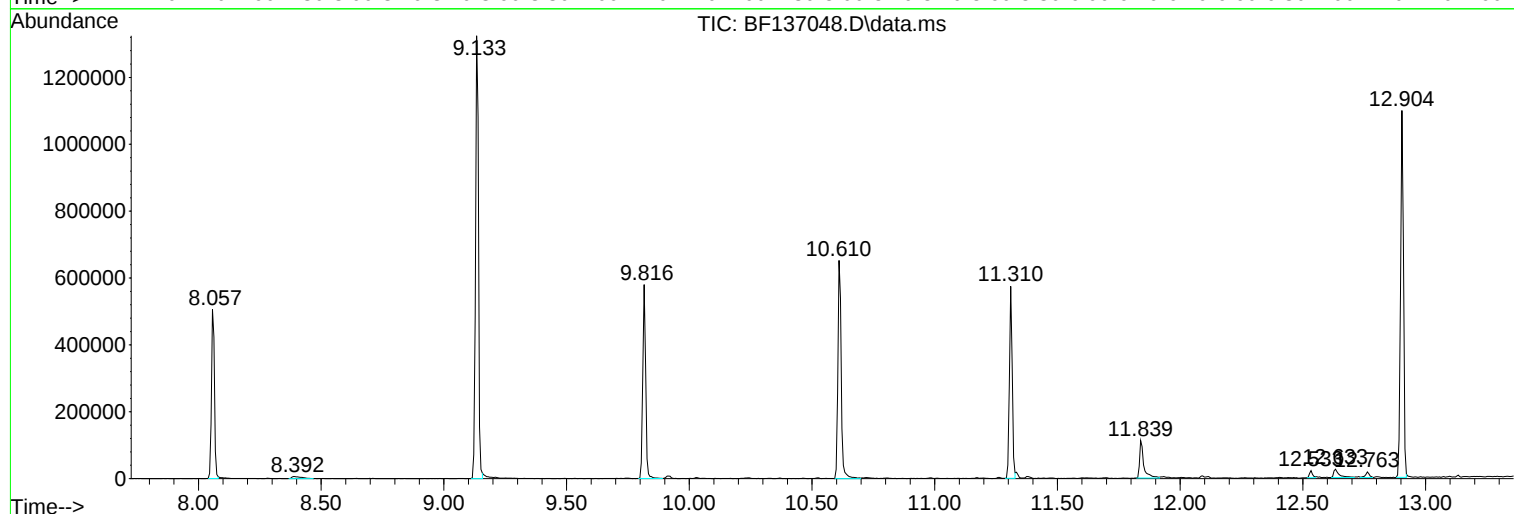
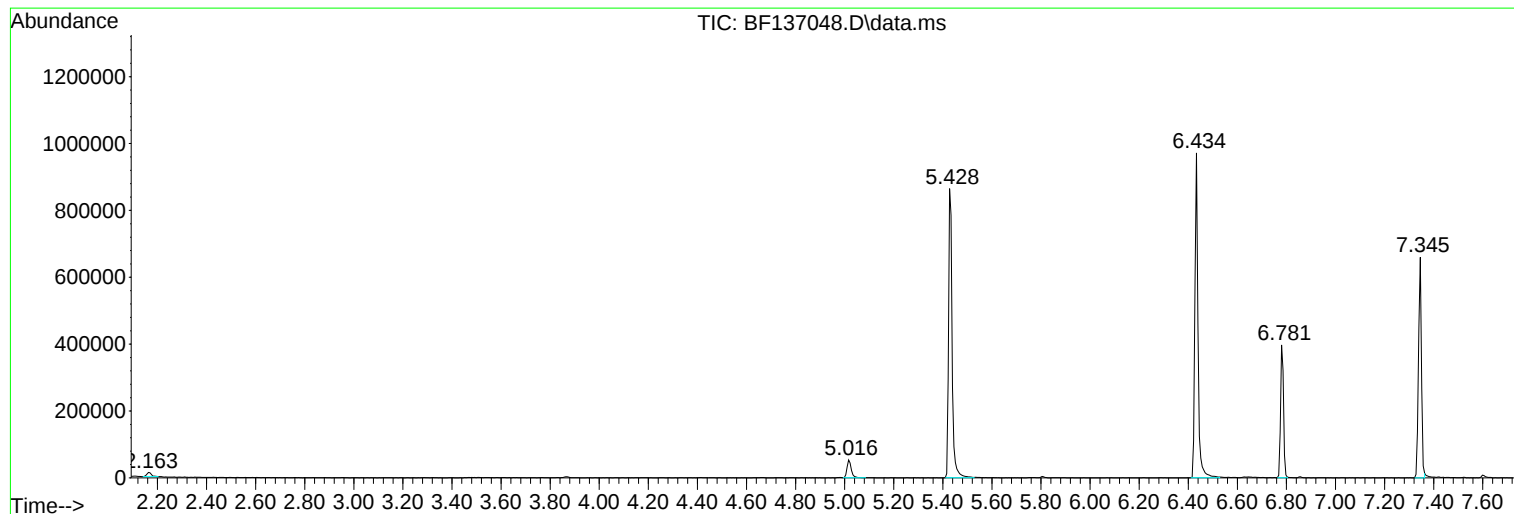
Sum of corrected areas: 7689159

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011224\  
Data File : BF137048.D  
Acq On : 12 Jan 2024 15:01  
Operator : CG\JU  
Sample : P1119-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MH-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011224\  
Data File : BF137048.D  
Acq On : 12 Jan 2024 15:01  
Operator : CG\JU  
Sample : P1119-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MH-J

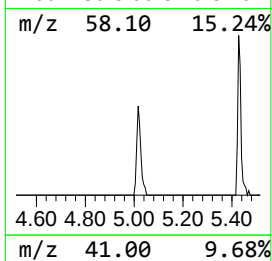
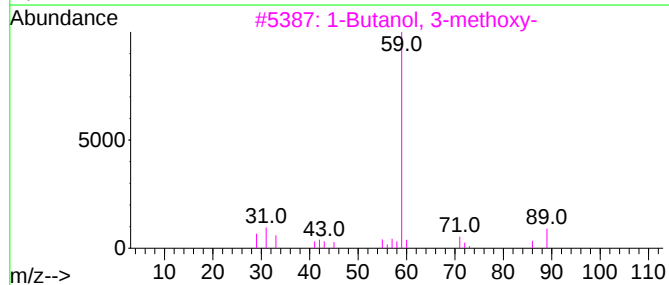
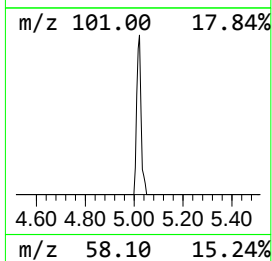
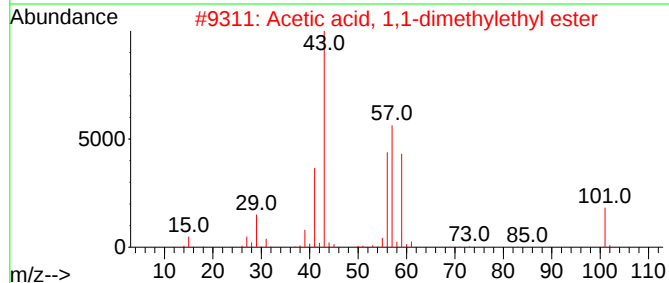
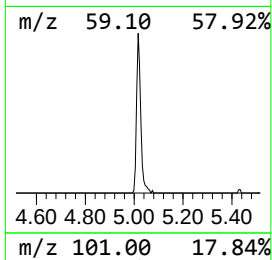
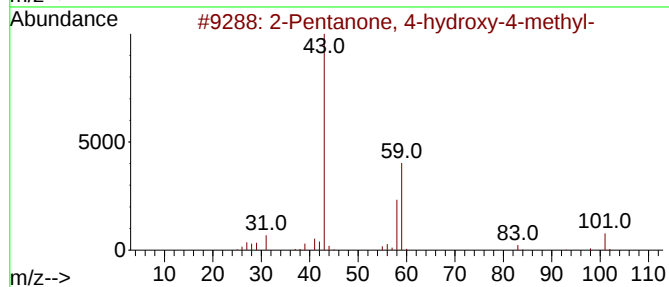
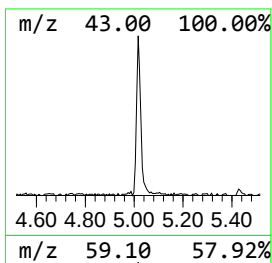
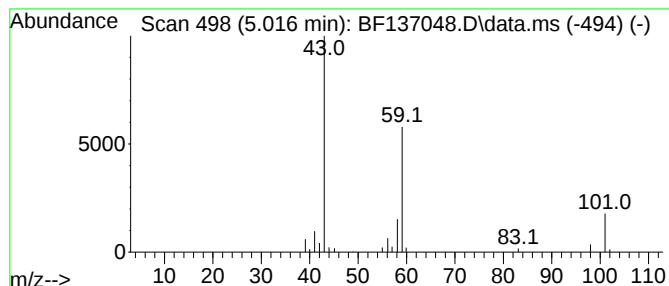
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.016 | 3.85 ng | 63583 | 1,4-Dichlorobenzene-d4 | 6.781 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 50      |      |      |
| 2    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2      | 000540-88-5 | 45      |      |      |
| 3    | 1-Butanol, 3-methoxy-               | 104 | C5H12O2      | 002517-43-3 | 17      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Butane, 1-ethoxy-                   | 102 | C6H14O       | 000628-81-9 | 9       |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011224\  
Data File : BF137048.D  
Acq On : 12 Jan 2024 15:01  
Operator : CG\JU  
Sample : P1119-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MH-J

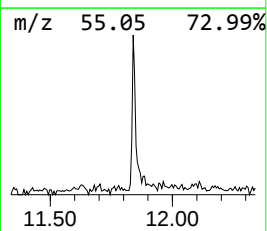
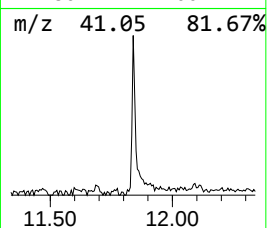
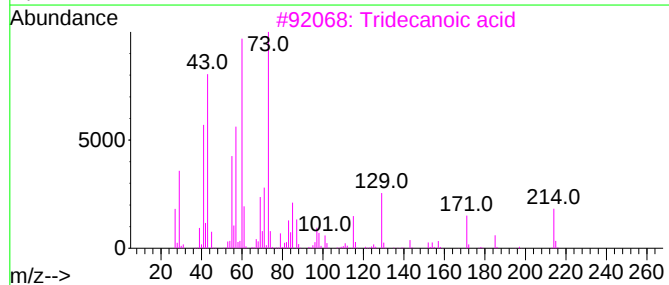
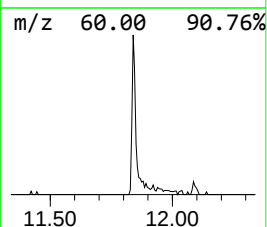
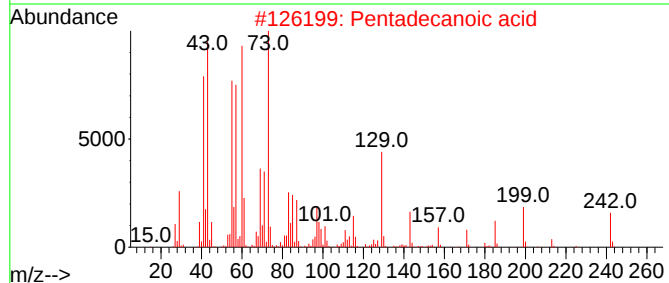
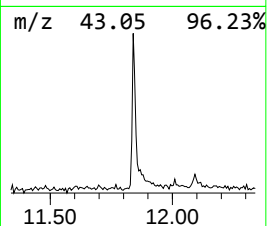
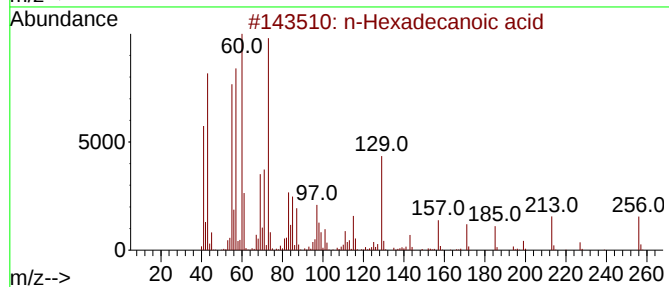
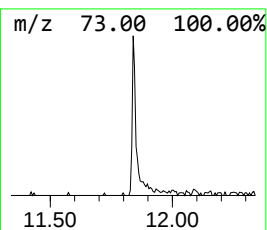
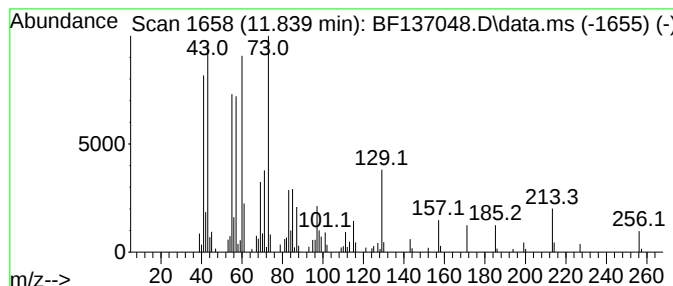
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.839 | 5.63 ng | 130324 | Phenanthrene-d10 | 11.310 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 91   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 87   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 50   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011224\  
Data File : BF137048.D  
Acq On : 12 Jan 2024 15:01  
Operator : CG\JU  
Sample : P1119-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MH-J

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.016  | 3.9     | ng    | 63583    | 1                     | 6.781  | 330643 | 20.0 |
| n-Hexadecanoic ... | 11.839 | 5.6     | ng    | 130324   | 4                     | 11.310 | 462872 | 20.0 |