

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111522\  
 Data File : BG055620.D  
 Acq On : 15 Nov 2022 12:39  
 Operator : CG/JU  
 Sample : PB148810BL  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB148810BL

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055620.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         | 5.310       | 337           | 344         | 351          | rBV      | 189723         | 288763        | 8.11%           | 1.913%        |
| 2         | 5.786       | 417           | 425         | 437          | rBV      | 728837         | 1157348       | 32.49%          | 7.668%        |
| 3         | 7.395       | 691           | 699         | 713          | rBV      | 737450         | 1256815       | 35.28%          | 8.327%        |
| 4         | 8.259       | 839           | 846         | 852          | rBV      | 142008         | 239006        | 6.71%           | 1.584%        |
| 5         | 9.428       | 1037          | 1045        | 1053         | rBV      | 431461         | 748672        | 21.02%          | 4.960%        |
| 6         | 11.085      | 1320          | 1327        | 1338         | rVB      | 215598         | 376275        | 10.56%          | 2.493%        |
| 7         | 13.506      | 1732          | 1739        | 1746         | rBV      | 1275633        | 1891653       | 53.10%          | 12.533%       |
| 8         | 14.881      | 1966          | 1973        | 1981         | rVB      | 374555         | 588054        | 16.51%          | 3.896%        |
| 9         | 16.361      | 2218          | 2225        | 2243         | rBV      | 1158729        | 1750085       | 49.13%          | 11.595%       |
| 10        | 17.625      | 2433          | 2440        | 2450         | rBV      | 537867         | 838496        | 23.54%          | 5.555%        |
| 11        | 20.210      | 2874          | 2880        | 2886         | rBV      | 2665789        | 3562341       | 100.00%         | 23.602%       |
| 12        | 21.920      | 3164          | 3171        | 3178         | rBV      | 555996         | 929465        | 26.09%          | 6.158%        |
| 13        | 23.482      | 3432          | 3437        | 3442         | rBV2     | 25055          | 47624         | 1.34%           | 0.316%        |
| 14        | 24.346      | 3579          | 3584        | 3591         | rVB      | 32509          | 68956         | 1.94%           | 0.457%        |
| 15        | 25.339      | 3742          | 3753        | 3767         | rVB2     | 334790         | 1087190       | 30.52%          | 7.203%        |
| 16        | 26.585      | 3958          | 3965        | 3975         | rVB4     | 40143          | 125094        | 3.51%           | 0.829%        |
| 17        | 28.054      | 4207          | 4215        | 4225         | rVB5     | 38862          | 137519        | 3.86%           | 0.911%        |

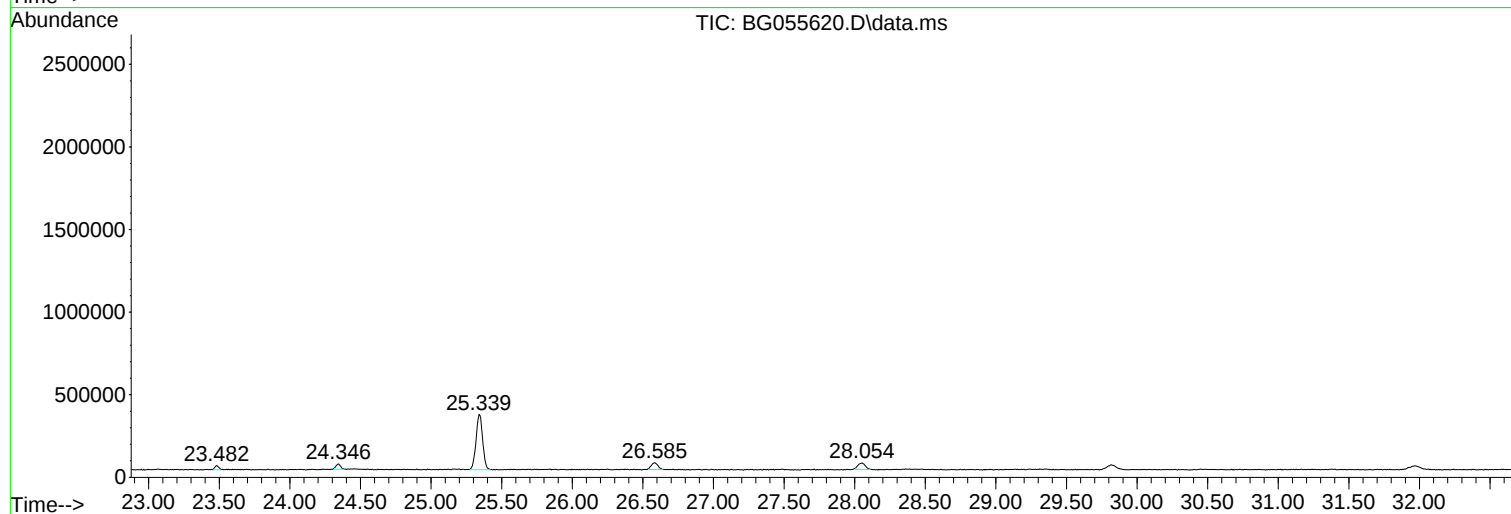
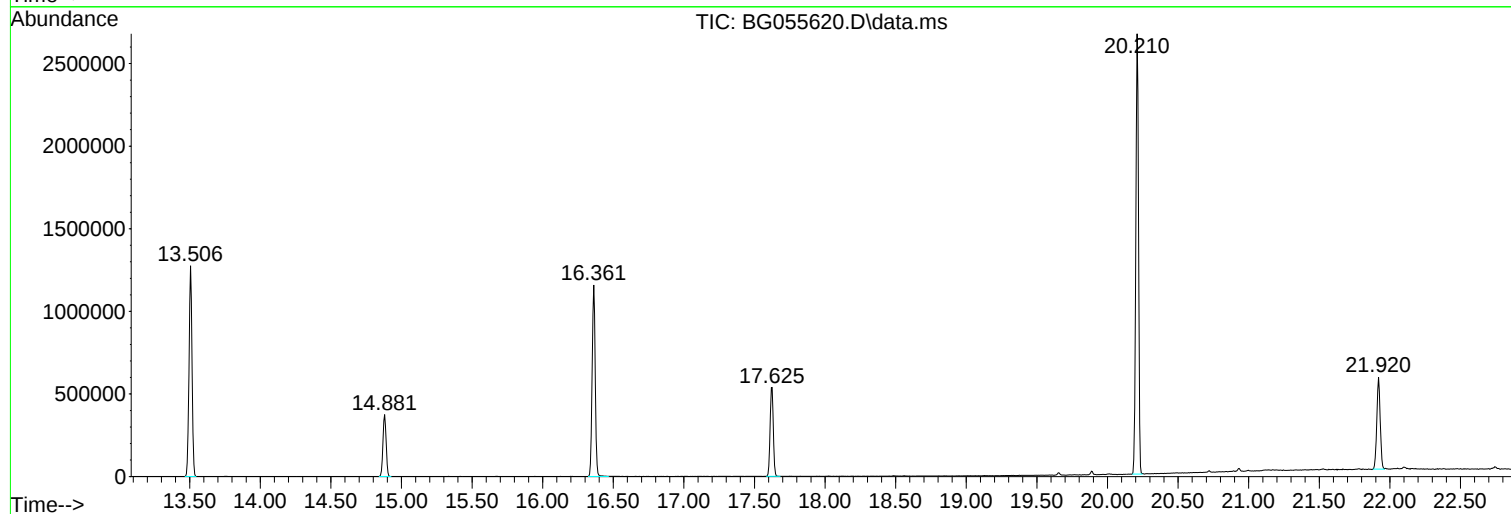
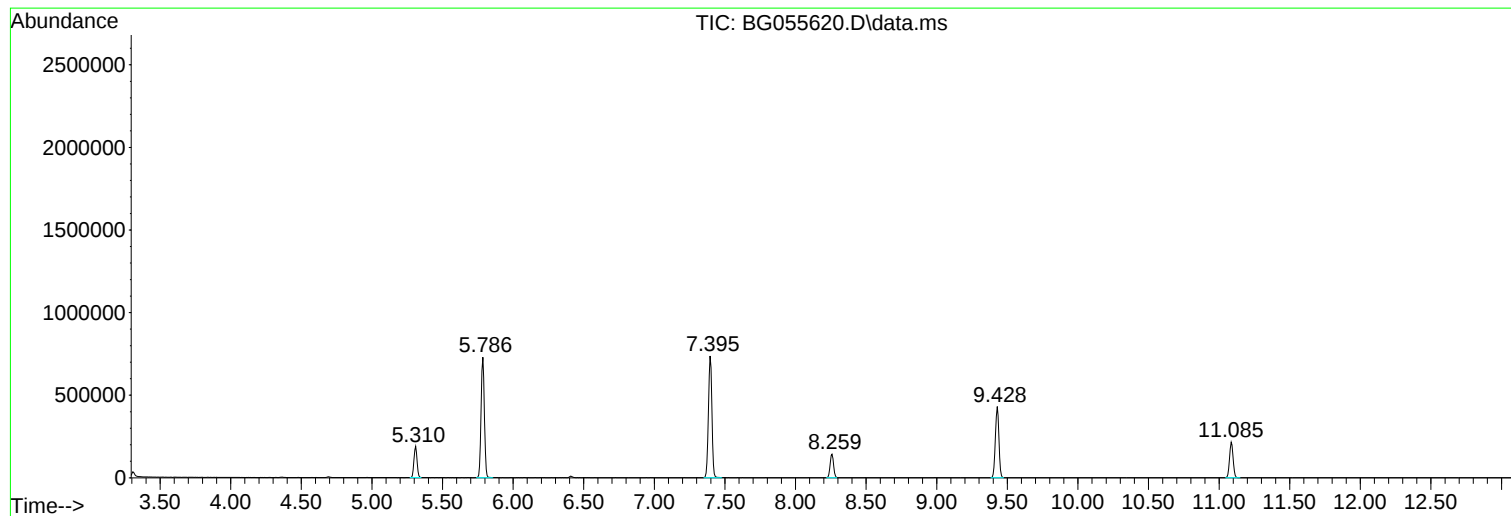
Sum of corrected areas: 15093356

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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.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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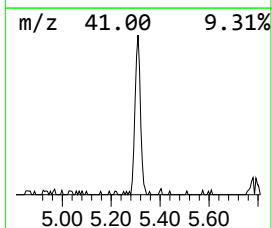
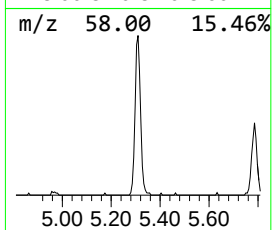
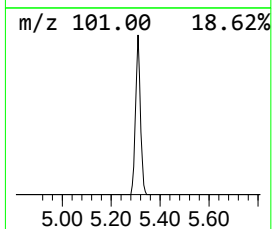
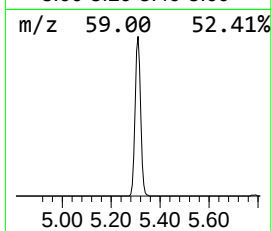
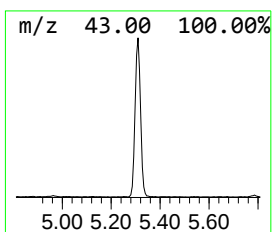
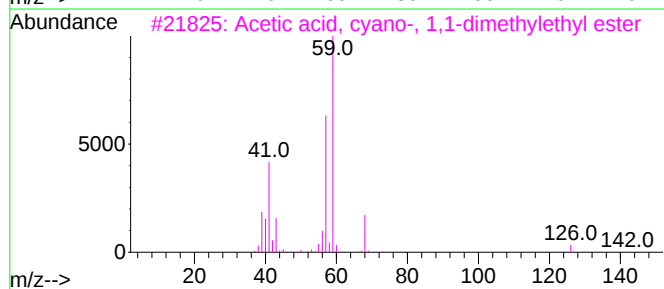
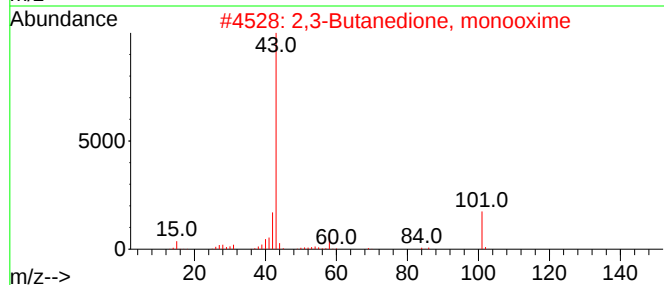
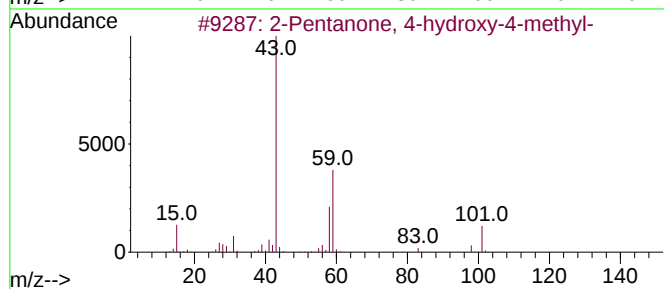
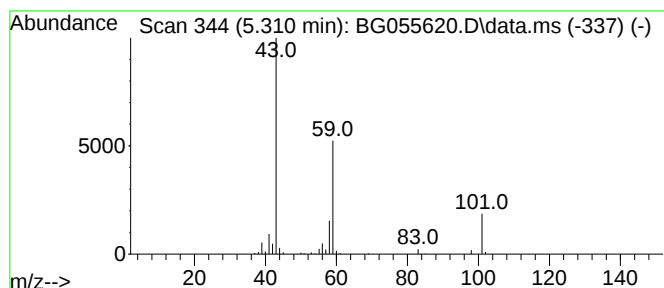
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.310 | 24.16 ng | 288763 | 1,4-Dichlorobenzene-d4 | 8.259 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2  | 64      |      |      |
| 2    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6  | 27      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9  | 25      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5  | 12      |      |      |
| 5    | n-Propyl t-butyl ether              | 116 | C7H16O       | 1000334-81-9 | 9       |      |      |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

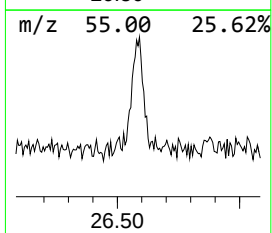
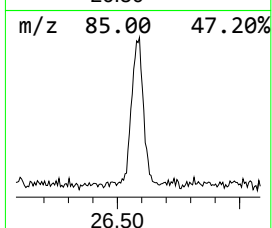
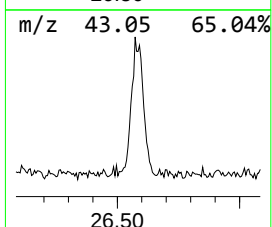
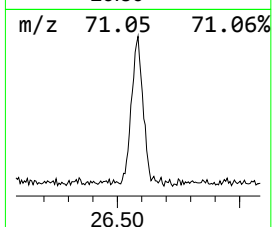
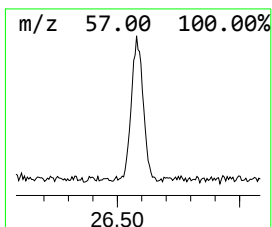
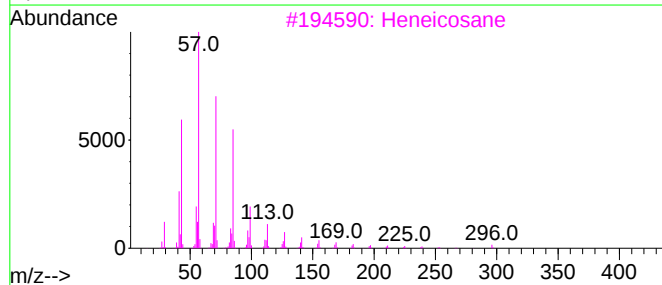
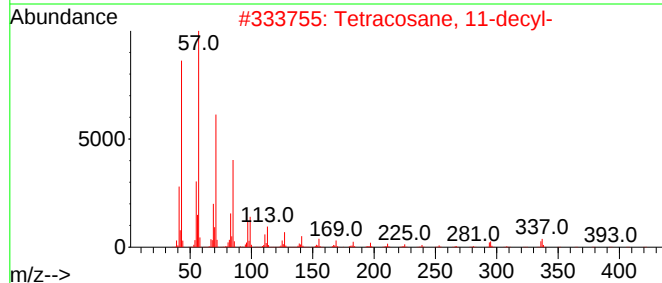
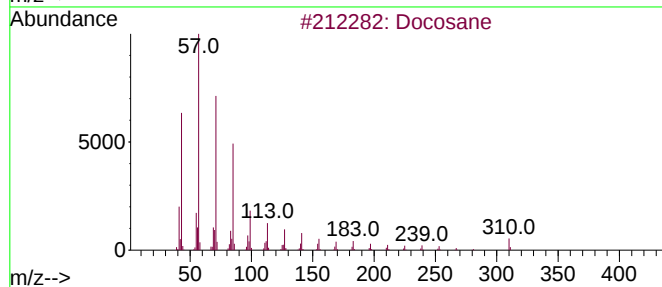
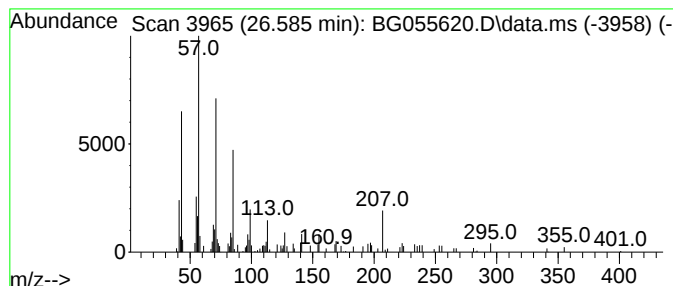
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Peak Number 2 Docosane Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 26.585 | 2.30 ng | 125094 | Perylene-d12     | 25.339 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------|-----|---------|-------------|------|
| 1    |    |   | Docosane               | 310 | C22H46  | 000629-97-0 | 81   |
| 2    |    |   | Tetracosane, 11-decyl- | 479 | C34H70  | 055429-84-0 | 80   |
| 3    |    |   | Heneicosane            | 296 | C21H44  | 000629-94-7 | 74   |
| 4    |    |   | Heptadecane            | 240 | C17H36  | 000629-78-7 | 74   |
| 5    |    |   | Octacosane             | 394 | C28H58  | 000630-02-4 | 74   |



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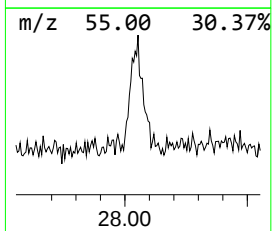
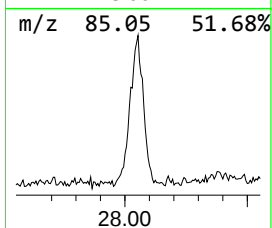
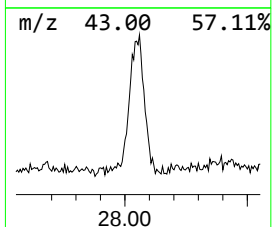
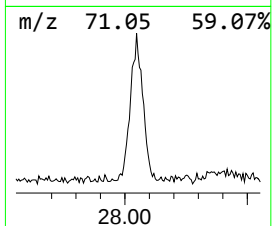
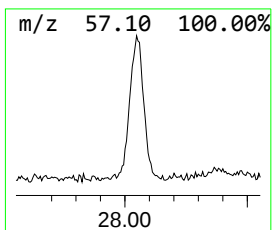
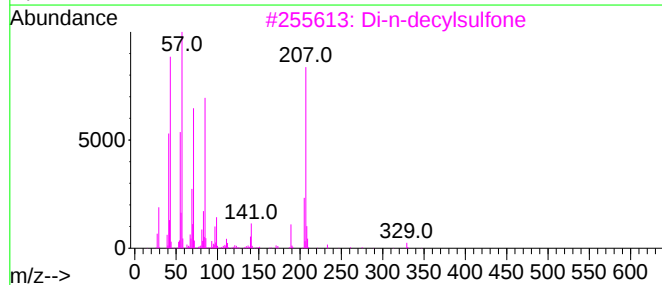
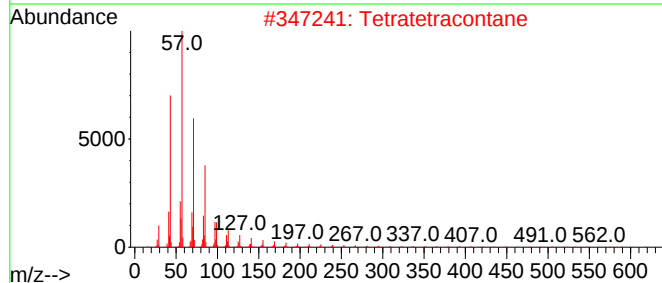
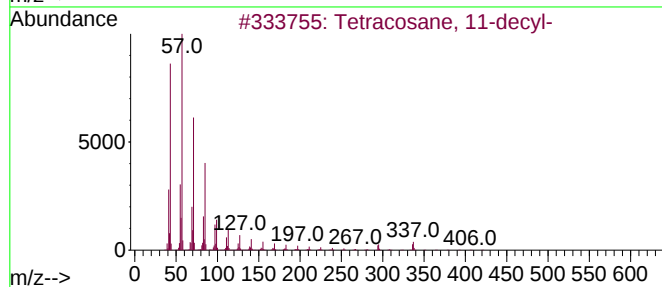
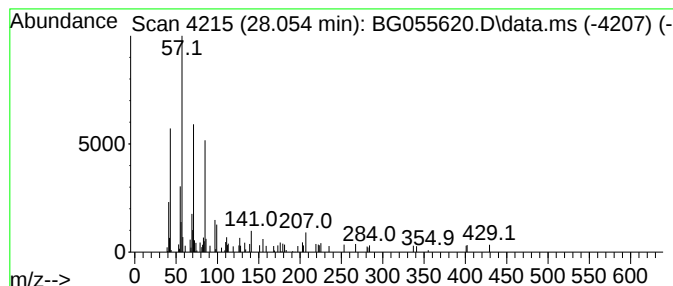
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Tetracosane, 11-decyl- Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 28.054 | 2.53 ng | 137519 | Perylene-d12     | 25.339 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm   | CAS#        | Qual |
|------|----|---|------------------------|-----|-----------|-------------|------|
| 1    |    |   | Tetracosane, 11-decyl- | 479 | C34H70    | 055429-84-0 | 72   |
| 2    |    |   | Tetratetracontane      | 619 | C44H90    | 007098-22-8 | 72   |
| 3    |    |   | Di-n-decylsulfone      | 346 | C20H42O2S | 111530-37-1 | 72   |
| 4    |    |   | Eicosane               | 282 | C20H42    | 000112-95-8 | 68   |
| 5    |    |   | Heptacosane            | 380 | C27H56    | 000593-49-7 | 64   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 5.310  | 24.2    | ng    | 288763   | 1                     | 8.259  | 239006  | 20.0 |
| Docosane           | 26.585 | 2.3     | ng    | 125094   | 6                     | 25.339 | 1087190 | 20.0 |
| Tetracosane, 11... | 28.054 | 2.5     | ng    | 137519   | 6                     | 25.339 | 1087190 | 20.0 |