

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062223\  
 Data File : BF133890.D  
 Acq On : 22 Jun 2023 09:00  
 Operator : CG\JU  
 Sample : PB153533BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB153533BL

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: BF133890.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         | 2.199       | 12            | 19          | 24           | rVB      | 61116          | 83607         | 1.98%           | 0.314%        |
| 2         | 4.498       | 405           | 410         | 422          | rBV      | 313323         | 349707        | 8.30%           | 1.312%        |
| 3         | 5.110       | 509           | 514         | 525          | rBV      | 796332         | 1104148       | 26.21%          | 4.143%        |
| 4         | 5.504       | 576           | 581         | 584          | rBV      | 3249046        | 3454546       | 82.00%          | 12.962%       |
| 5         | 5.881       | 642           | 645         | 652          | rVB      | 62390          | 57973         | 1.38%           | 0.218%        |
| 6         | 6.504       | 745           | 751         | 754          | rBV      | 2973800        | 3493821       | 82.93%          | 13.110%       |
| 7         | 6.857       | 808           | 811         | 815          | rBV      | 840193         | 660940        | 15.69%          | 2.480%        |
| 8         | 7.428       | 902           | 908         | 910          | rBV      | 2231212        | 2301205       | 54.62%          | 8.635%        |
| 9         | 8.139       | 1025          | 1029        | 1032         | rBV      | 1074529        | 860254        | 20.42%          | 3.228%        |
| 10        | 9.222       | 1207          | 1213        | 1216         | rBV      | 4327398        | 4070687       | 96.63%          | 15.274%       |
| 11        | 9.898       | 1324          | 1328        | 1331         | rBV      | 1172628        | 957117        | 22.72%          | 3.591%        |
| 12        | 10.692      | 1458          | 1463        | 1466         | rBV      | 2971704        | 2692733       | 63.92%          | 10.104%       |
| 13        | 11.392      | 1578          | 1582        | 1585         | rBV      | 1163633        | 1018709       | 24.18%          | 3.822%        |
| 14        | 12.992      | 1849          | 1854        | 1857         | rBV      | 4294847        | 4212786       | 100.00%         | 15.807%       |
| 15        | 14.051      | 2027          | 2034        | 2044         | rBV      | 720466         | 716574        | 17.01%          | 2.689%        |
| 16        | 15.557      | 2285          | 2290        | 2294         | rBV      | 441251         | 569389        | 13.52%          | 2.136%        |
| 17        | 16.057      | 2373          | 2375        | 2384         | rVB4     | 25874          | 46444         | 1.10%           | 0.174%        |

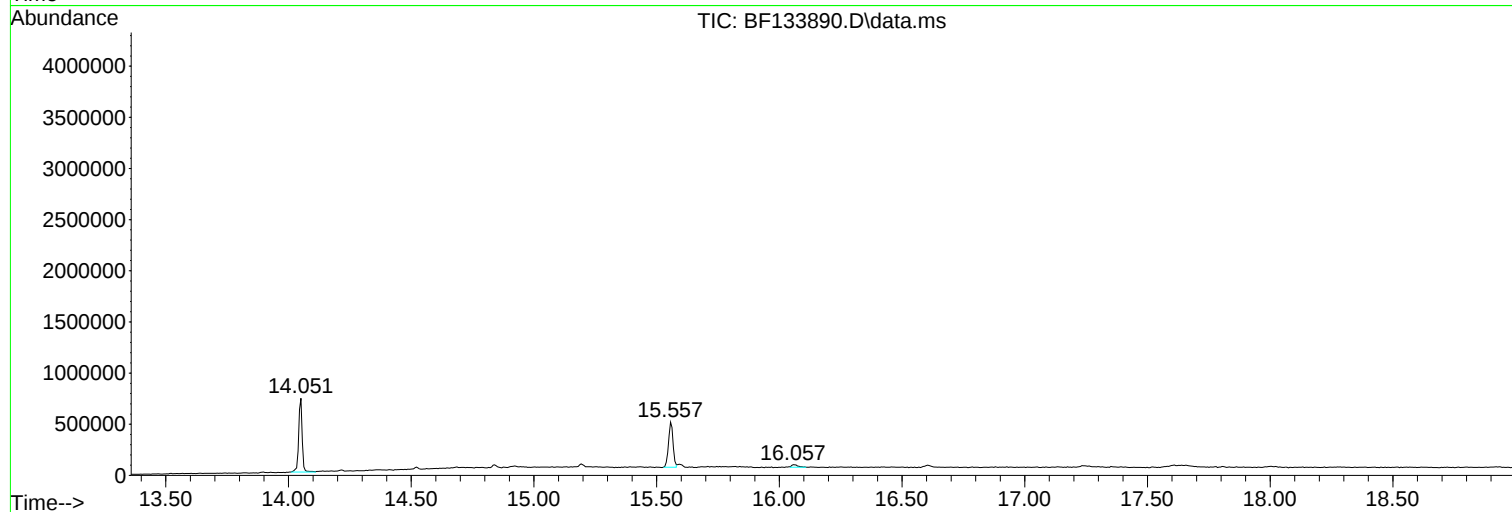
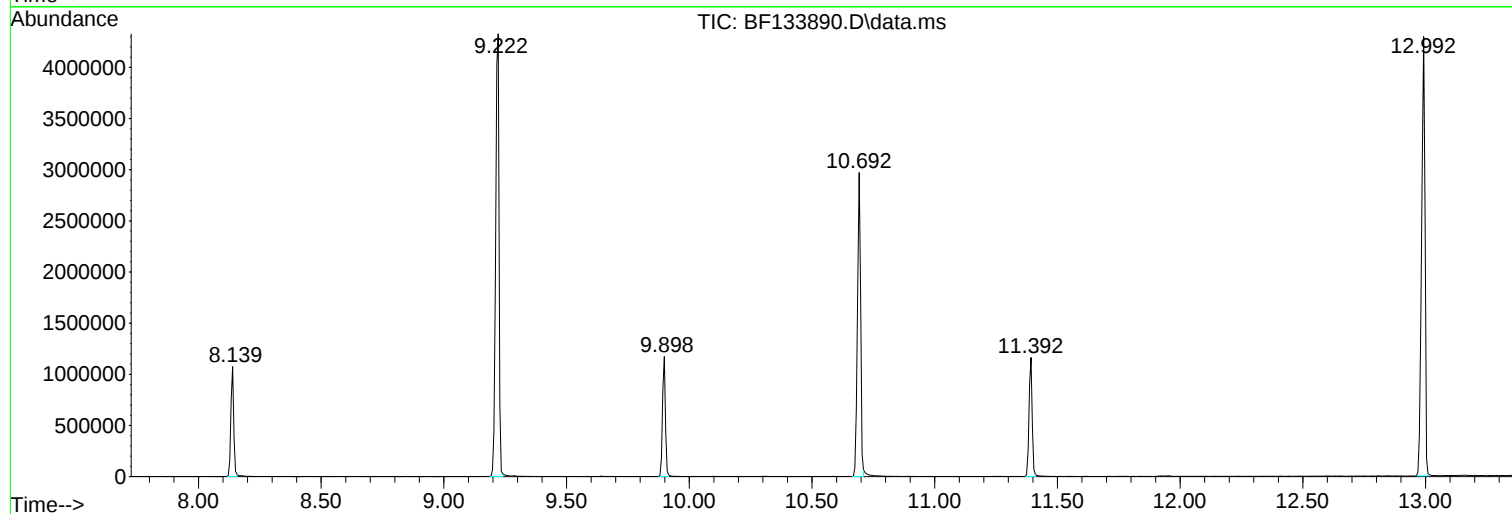
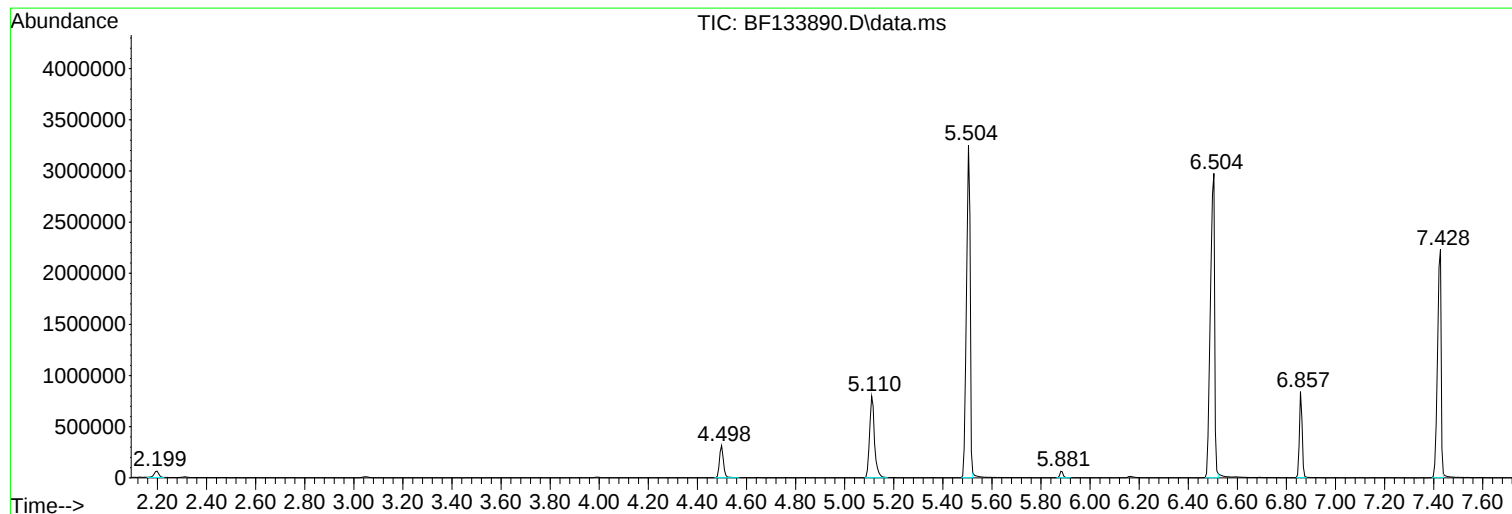
Sum of corrected areas: 26650640

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BNA\_F  
ClientSampleId :  
PB153533BL

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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Instrument :  
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ClientSampleId :  
PB153533BL

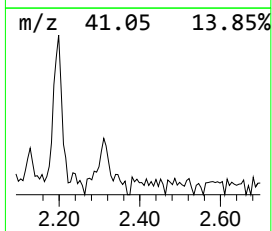
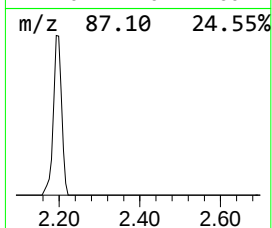
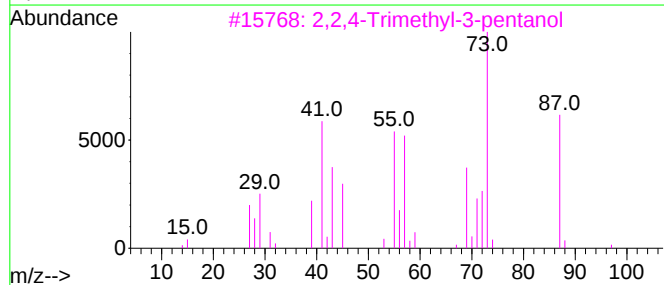
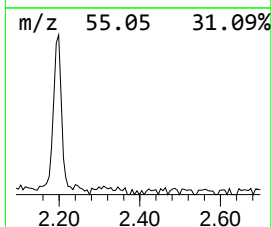
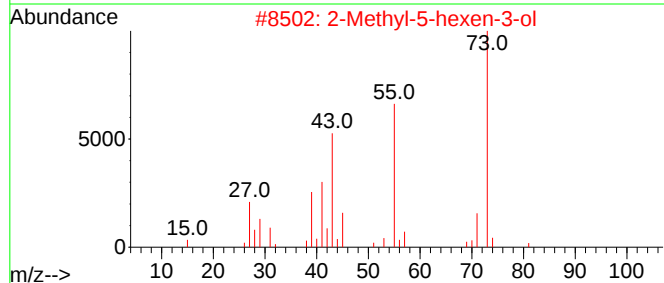
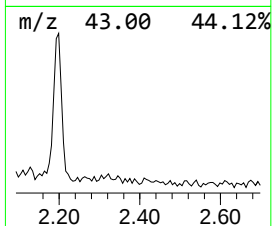
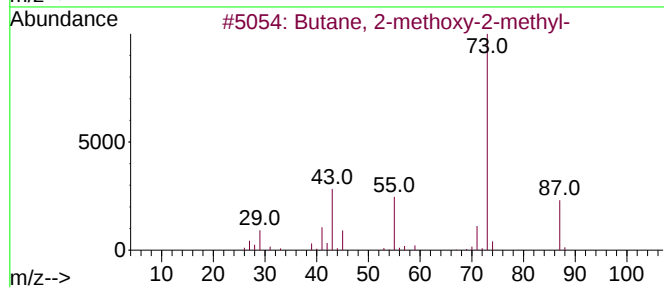
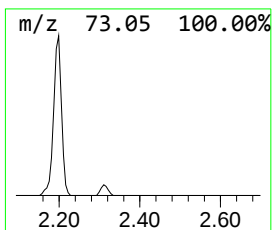
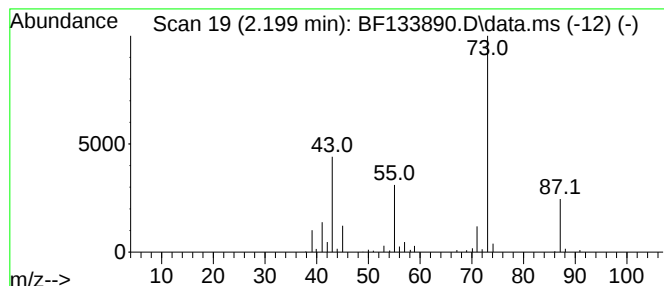
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 2.199 | 2.53 ng | 83607 | 1,4-Dichlorobenzene-d4 | 6.857 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2-Methyl-5-hexen-3-ol       | 114 | C7H14O  | 032815-70-6 | 50   |
| 3    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 4    |    |   | Borane, dimethoxy-          | 74  | C2H7BO2 | 004542-61-4 | 27   |
| 5    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 17   |



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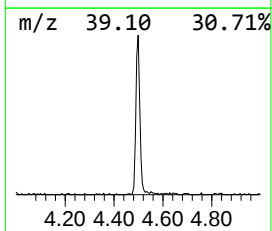
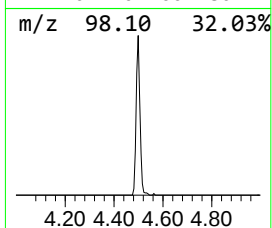
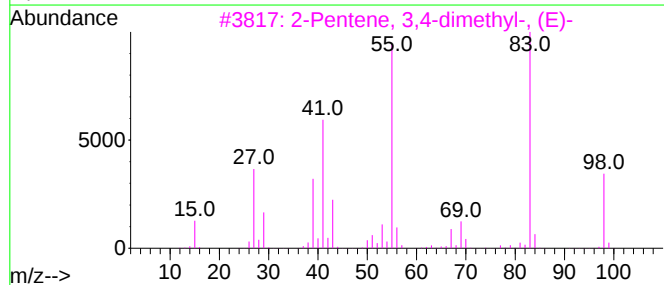
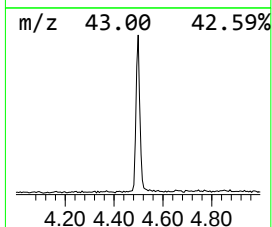
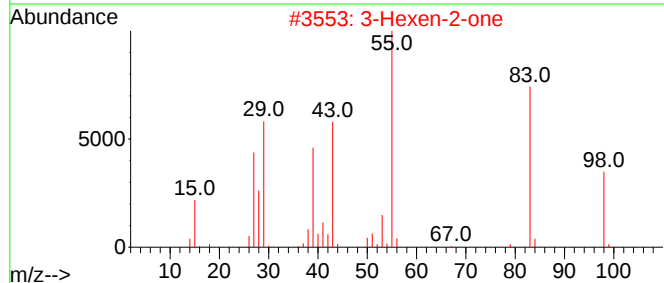
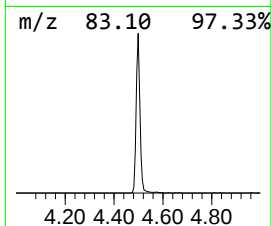
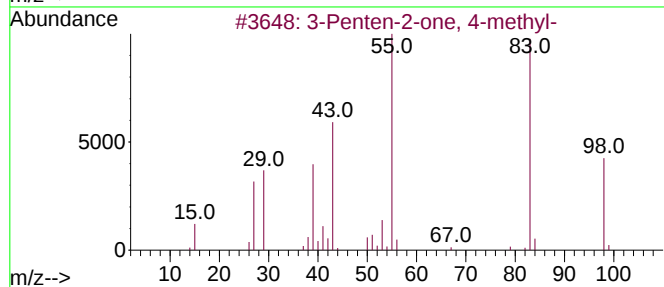
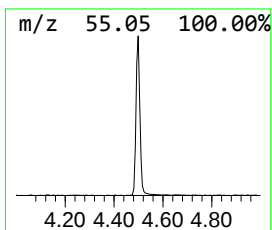
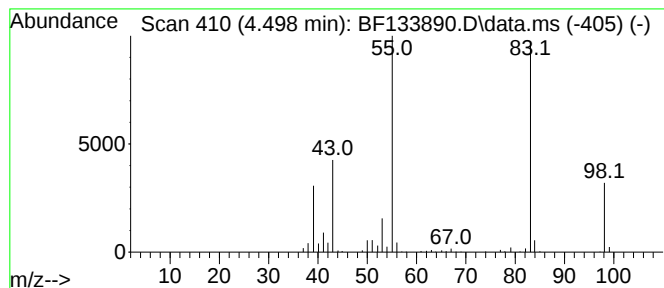
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 4.498 | 10.58 ng | 349707 | 1,4-Dichlorobenzene-d4 | 6.857 |

| Hit# | of 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|------|--------------------------------|----|---------|-------------|------|
| 1    |      | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |      | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |      | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 4    |      | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |
| 5    |      | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 86   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
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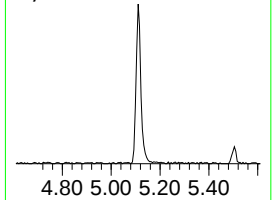
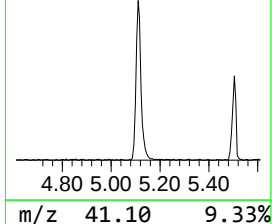
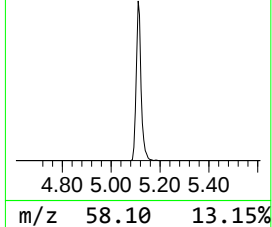
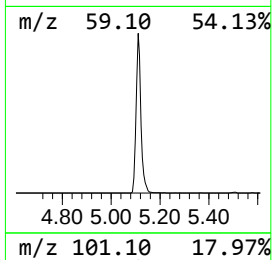
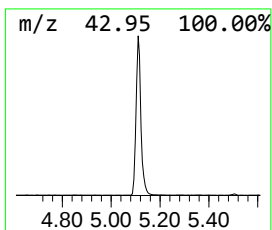
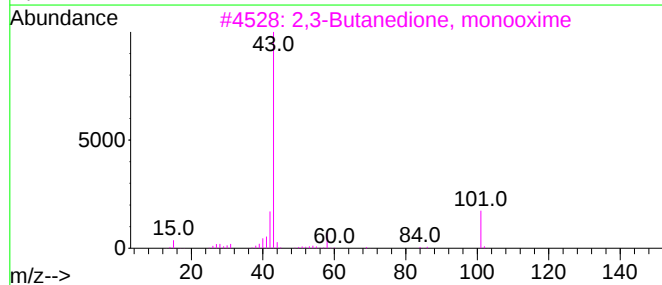
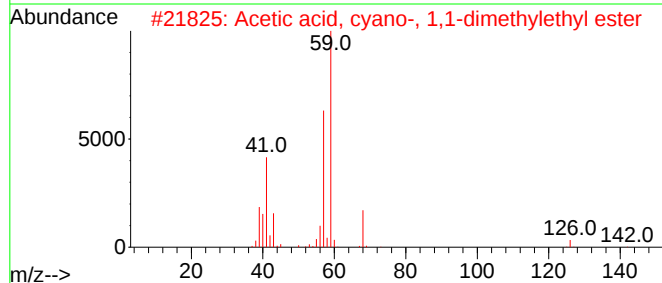
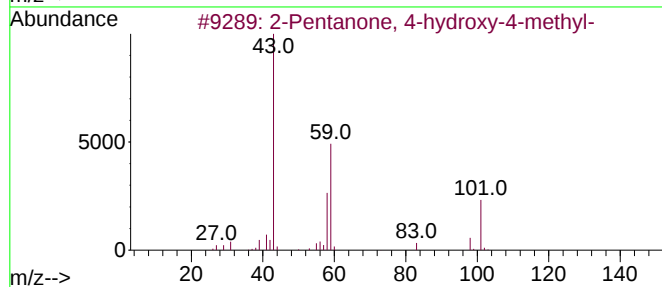
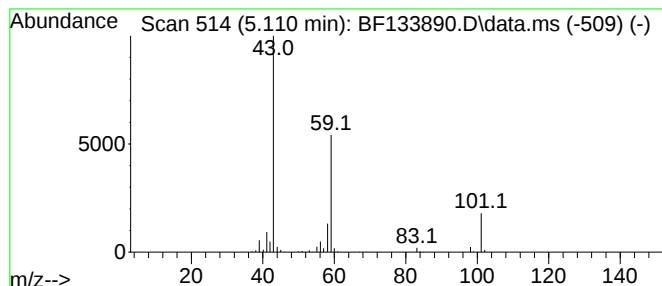
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 5.110 | 33.41 ng | 1104150 | 1,4-Dichlorobenzene-d4 | 6.857 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 72   |
| 2    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 3    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 16   |
| 4    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 12   |
| 5    |    |   | 3-Hydroxy-3-methyl-2-butanone       | 102 | C5H10O2  | 000115-22-0 | 9    |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Butane, 2-metho... | 2.199 | 2.5     | ng    | 83607    | 1                     | 6.857 | 660940 | 20.0 |
| 3-Penten-2-one,... | 4.498 | 10.6    | ng    | 349707   | 1                     | 6.857 | 660940 | 20.0 |
| 2-Pentanone, 4-... | 5.110 | 33.4    | ng    | 1104150  | 1                     | 6.857 | 660940 | 20.0 |