

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF070616\  
 Data File : BF088737.D  
 Acq On : 6 Jul 2016 14:41  
 Operator : UM/SJ  
 Sample : PB91761BL  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB91761BL

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 1.644       | 3             | 5           | 8            | rVB      | 4648360        | 7359947       | 100.00%         | 22.499%       |
| 2         | 1.701       | 8             | 10          | 19           | rVV      | 466577         | 714899        | 9.71%           | 2.185%        |
| 3         | 1.827       | 19            | 21          | 62           | rVB      | 1247396        | 2515396       | 34.18%          | 7.689%        |
| 4         | 4.936       | 290           | 293         | 298          | rBV      | 72804          | 107388        | 1.46%           | 0.328%        |
| 5         | 5.359       | 327           | 330         | 332          | rBV      | 2194828        | 2353504       | 31.98%          | 7.194%        |
| 6         | 6.399       | 417           | 421         | 423          | rBV      | 2174751        | 2527345       | 34.34%          | 7.726%        |
| 7         | 6.525       | 429           | 432         | 434          | rBV      | 2385762        | 2306103       | 31.33%          | 7.050%        |
| 8         | 6.753       | 450           | 452         | 454          | rVB      | 603918         | 513347        | 6.97%           | 1.569%        |
| 9         | 6.913       | 463           | 466         | 468          | rBV      | 2158828        | 1874473       | 25.47%          | 5.730%        |
| 10        | 7.325       | 499           | 502         | 504          | rBV      | 1401006        | 1727237       | 23.47%          | 5.280%        |
| 11        | 8.045       | 562           | 565         | 567          | rBV      | 529984         | 694128        | 9.43%           | 2.122%        |
| 12        | 9.119       | 656           | 659         | 661          | rBV      | 2884783        | 2906177       | 39.49%          | 8.884%        |
| 13        | 9.793       | 715           | 718         | 720          | rBV      | 800212         | 834043        | 11.33%          | 2.550%        |
| 14        | 10.571      | 784           | 786         | 789          | rBV      | 877895         | 905676        | 12.31%          | 2.769%        |
| 15        | 11.268      | 844           | 847         | 849          | rBV      | 1052966        | 900685        | 12.24%          | 2.753%        |
| 16        | 12.857      | 983           | 986         | 988          | rBV      | 3073538        | 3147452       | 42.76%          | 9.621%        |
| 17        | 13.885      | 1074          | 1076        | 1079         | rBV      | 748556         | 756745        | 10.28%          | 2.313%        |
| 18        | 15.268      | 1195          | 1197        | 1200         | rBV      | 396274         | 568224        | 7.72%           | 1.737%        |

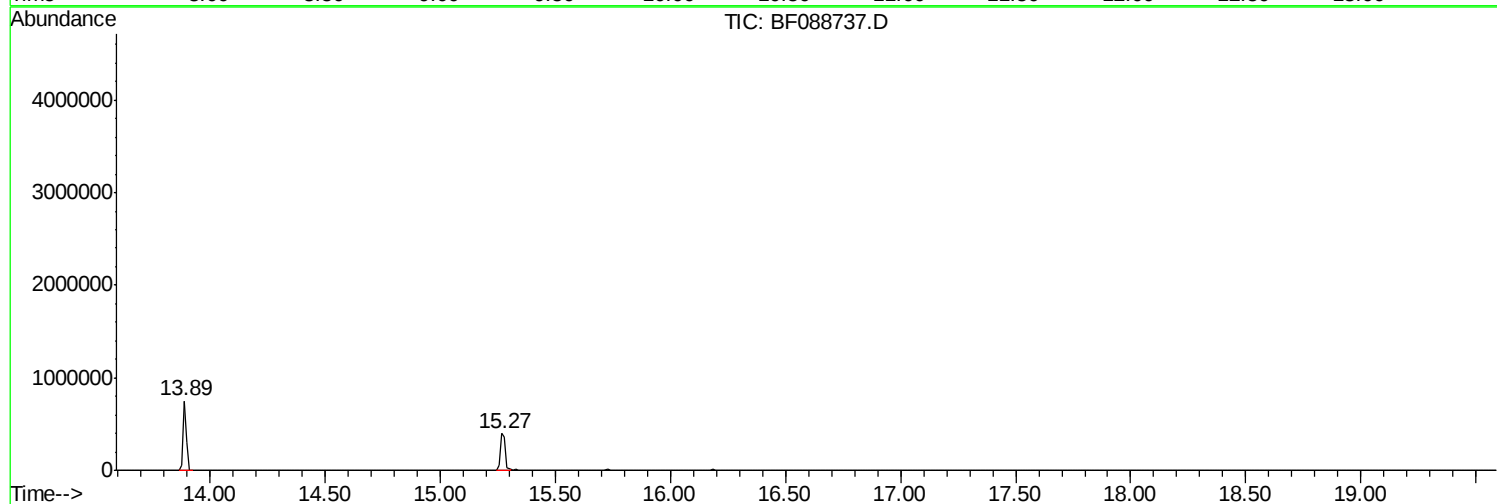
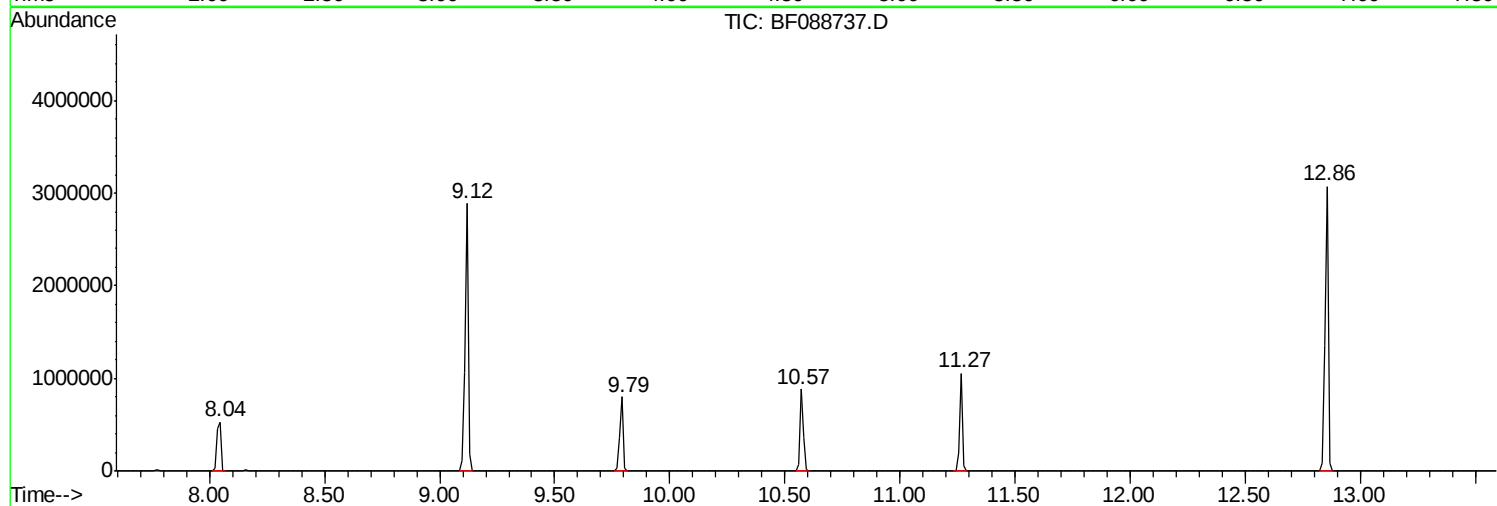
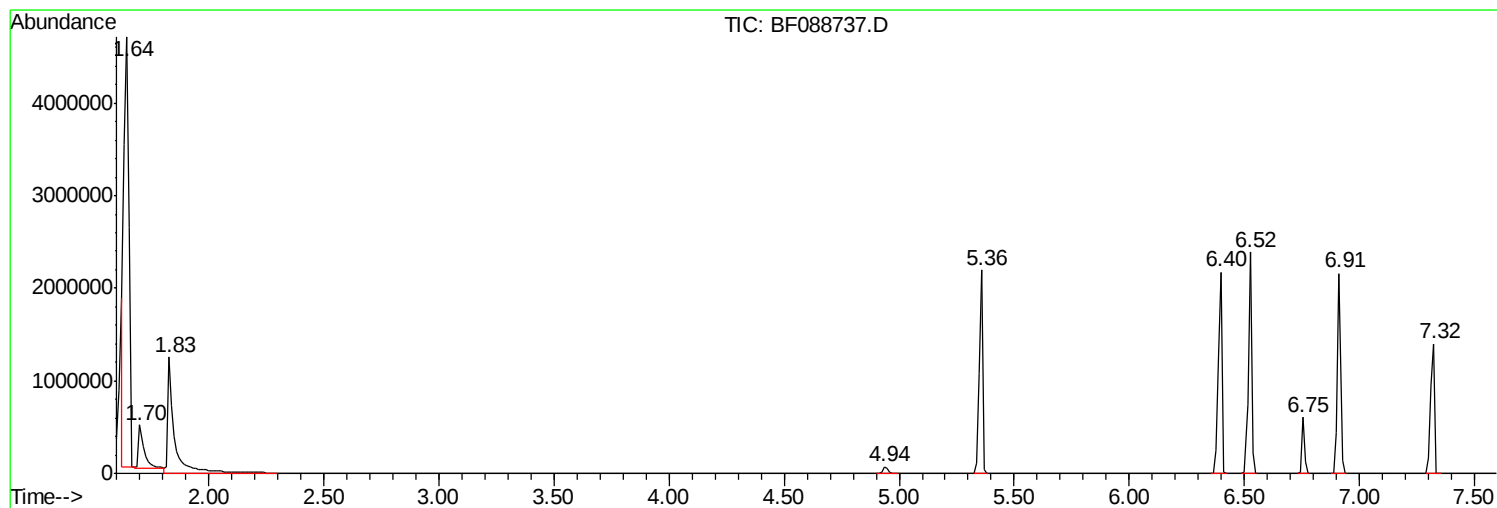
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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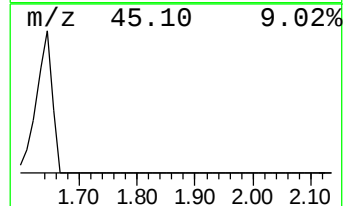
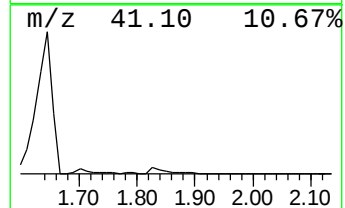
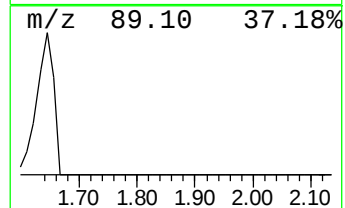
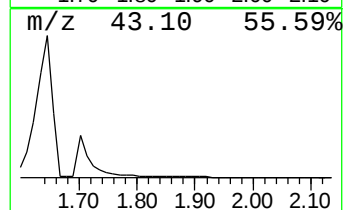
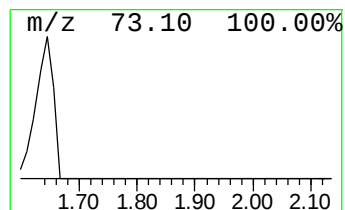
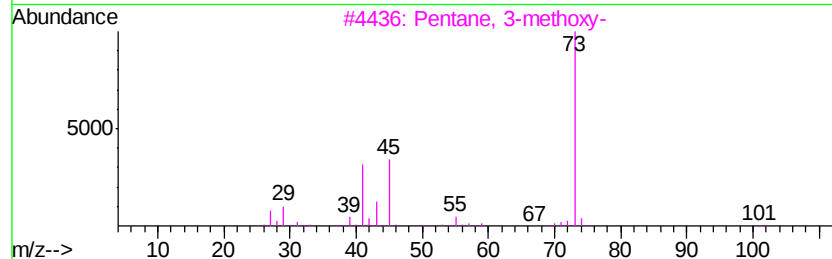
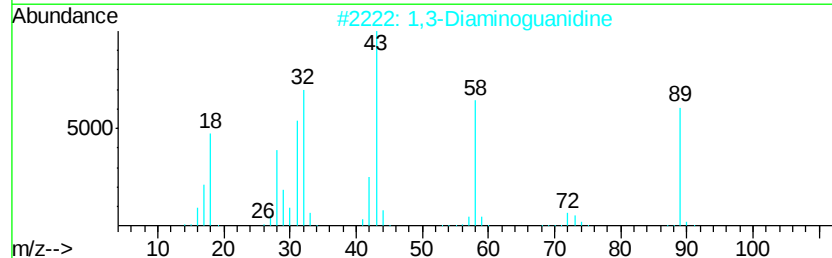
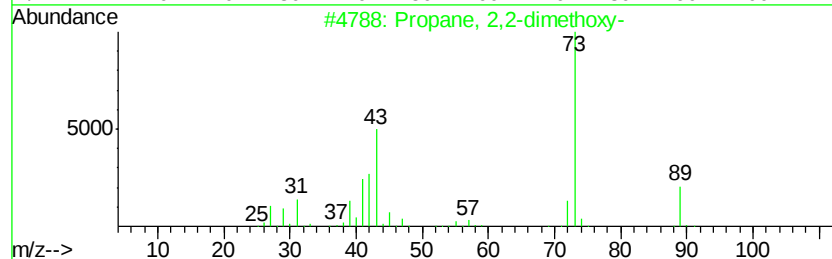
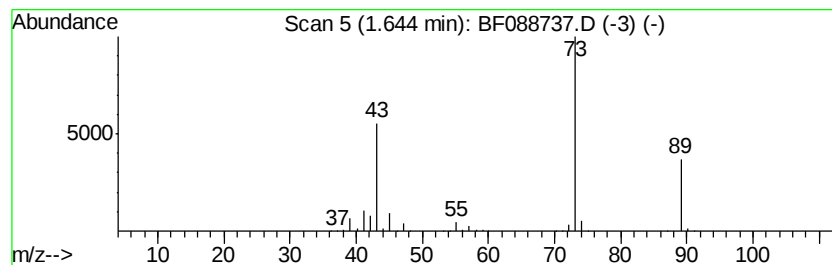
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TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown1.64 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 1.64 | 286.74 ng | 7359950 | 1,4-Dichlorobenzene-d4 | 6.75 |

| Hit# | of | Tentative ID            | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 40   |
| 2    |    | 1,3-Diaminoguanidine    | 89  | CH7N5   | 004364-78-7 | 25   |
| 3    |    | Pentane, 3-methoxy-     | 102 | C6H14O  | 036839-67-5 | 17   |
| 4    |    | N-Ethylformamide        | 73  | C3H7NO  | 000627-45-2 | 9    |
| 5    |    | 1-Propanol, 2-methyl-   | 74  | C4H10O  | 000078-83-1 | 9    |



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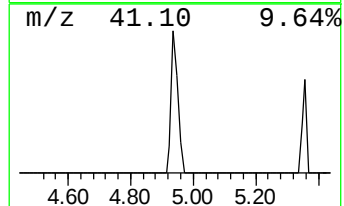
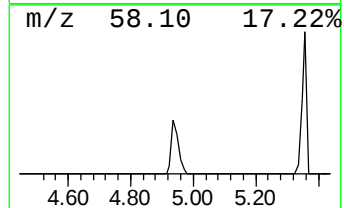
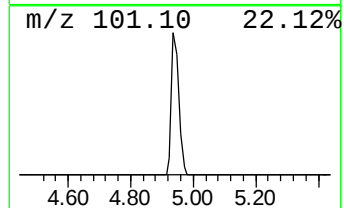
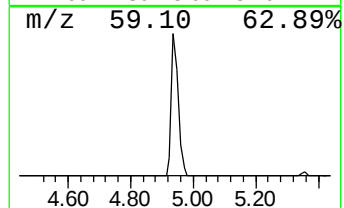
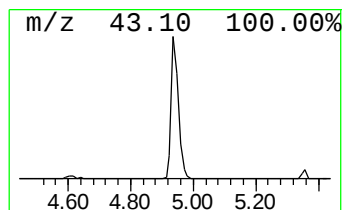
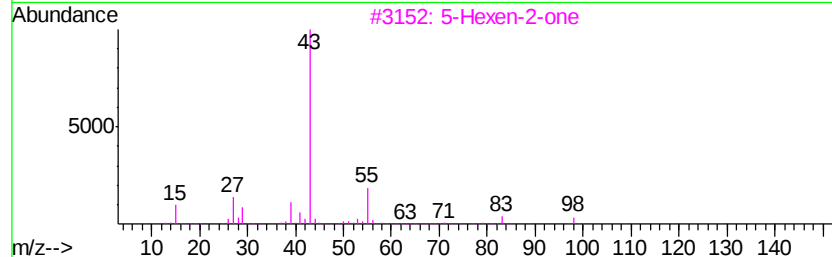
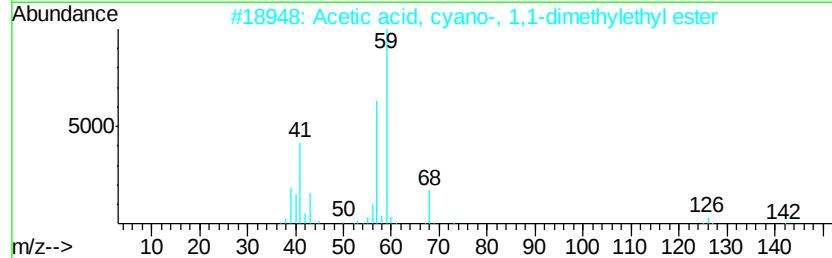
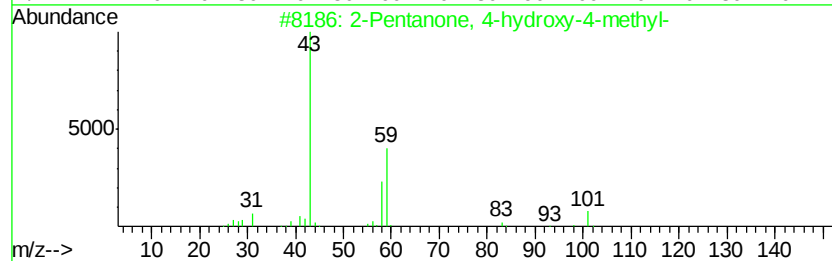
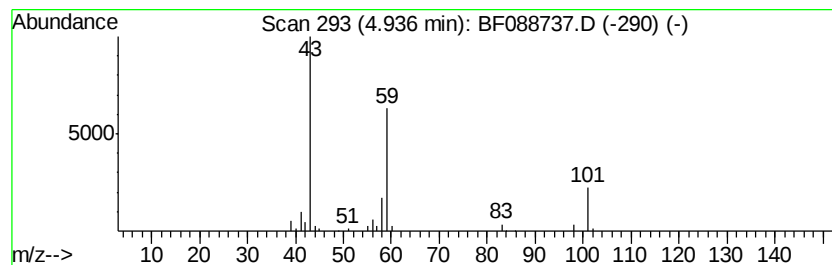
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.94 | 4.18 ng | 107388 | 1,4-Dichlorobenzene-d4 | 6.75 |

| Hit# of | 5                                   | Tentative ID | MW       | MolForm     | CAS# | Qual |
|---------|-------------------------------------|--------------|----------|-------------|------|------|
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-    | 116          | C6H12O2  | 000123-42-2 | 56   |      |
| 2       | Acetic acid, cyano-, 1,1-dimethy... | 141          | C7H11NO2 | 001116-98-9 | 23   |      |
| 3       | 5-Hexen-2-one                       | 98           | C6H10O   | 000109-49-9 | 9    |      |
| 4       | Morpholine, 4-methyl-               | 101          | C5H11NO  | 000109-02-4 | 9    |      |
| 5       | 2,3-Butanedione, monooxime          | 101          | C4H7NO2  | 000057-71-6 | 9    |      |



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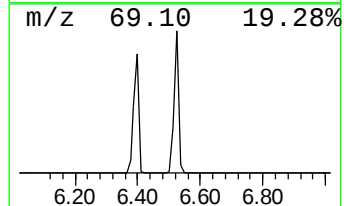
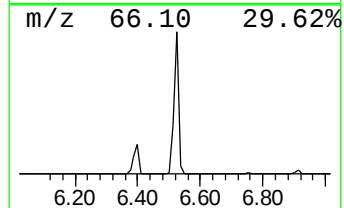
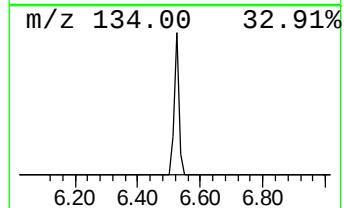
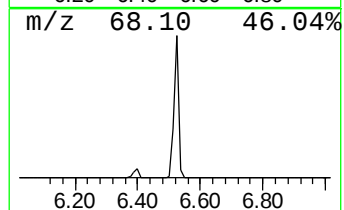
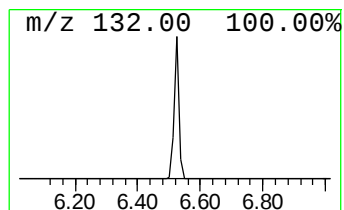
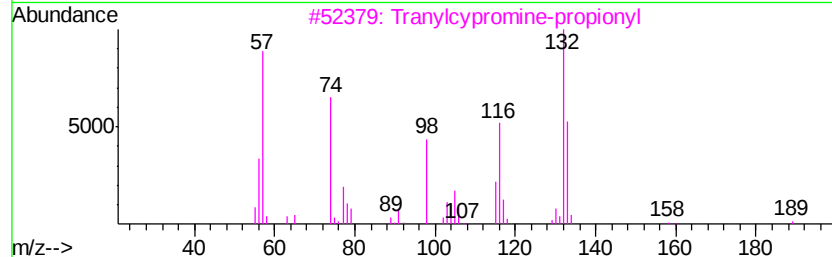
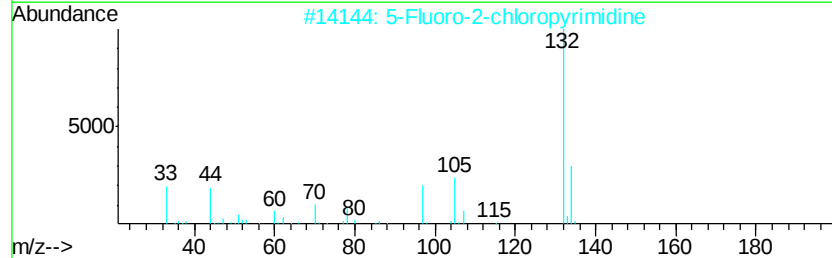
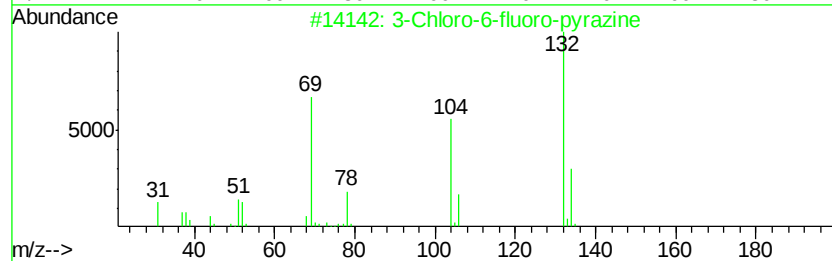
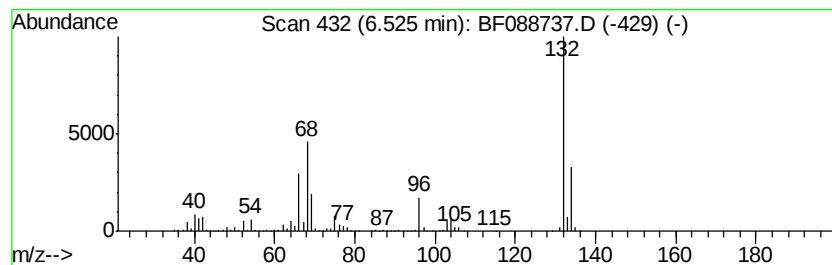
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Peak Number 5 unknown6.52 Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.52 | 89.85 ng | 2306100 | 1,4-Dichlorobenzene-d4 | 6.75 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 16   |
| 3    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| unknown1.64          | 1.64 | 286.7   | ng    | 7359950  | 1                     | 6.75 | 513347 | 20.0 |
| 2-Pentanone, 4-hy... | 4.94 | 4.2     | ng    | 107388   | 1                     | 6.75 | 513347 | 20.0 |
| unknown6.52          | 6.52 | 89.8    | ng    | 2306100  | 1                     | 6.75 | 513347 | 20.0 |