

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112223\  
 Data File : BG059821.D  
 Acq On : 22 Nov 2023 17:00  
 Operator : MA/JU  
 Sample : PB157329BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB157329BL

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059821.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         | 4.732       | 223           | 229         | 235          | rBV      | 64272          | 96531         | 2.03%           | 0.647%        |
| 2         | 5.367       | 330           | 337         | 343          | rBV      | 108678         | 174380        | 3.66%           | 1.169%        |
| 3         | 5.825       | 408           | 415         | 423          | rBV      | 547784         | 868963        | 18.24%          | 5.827%        |
| 4         | 7.453       | 680           | 692         | 700          | rBV      | 562636         | 979378        | 20.56%          | 6.567%        |
| 5         | 8.328       | 835           | 841         | 849          | rVB2     | 111001         | 199354        | 4.18%           | 1.337%        |
| 6         | 9.533       | 1038          | 1046        | 1053         | rBV      | 366751         | 651601        | 13.68%          | 4.369%        |
| 7         | 11.178      | 1319          | 1326        | 1333         | rBV2     | 148777         | 277437        | 5.82%           | 1.860%        |
| 8         | 13.587      | 1729          | 1736        | 1742         | rBV      | 1314851        | 2014636       | 42.28%          | 13.509%       |
| 9         | 14.962      | 1963          | 1970        | 1978         | rVB3     | 334340         | 561105        | 11.78%          | 3.763%        |
| 10        | 16.448      | 2213          | 2223        | 2231         | rBV2     | 1309277        | 2065385       | 43.35%          | 13.850%       |
| 11        | 17.711      | 2432          | 2438        | 2446         | rBV      | 476359         | 724764        | 15.21%          | 4.860%        |
| 12        | 20.291      | 2871          | 2877        | 2884         | rBV      | 3856929        | 4764443       | 100.00%         | 31.949%       |
| 13        | 22.042      | 3168          | 3175        | 3182         | rBV2     | 431075         | 751428        | 15.77%          | 5.039%        |
| 14        | 25.626      | 3777          | 3785        | 3798         | rVB2     | 243786         | 783448        | 16.44%          | 5.254%        |

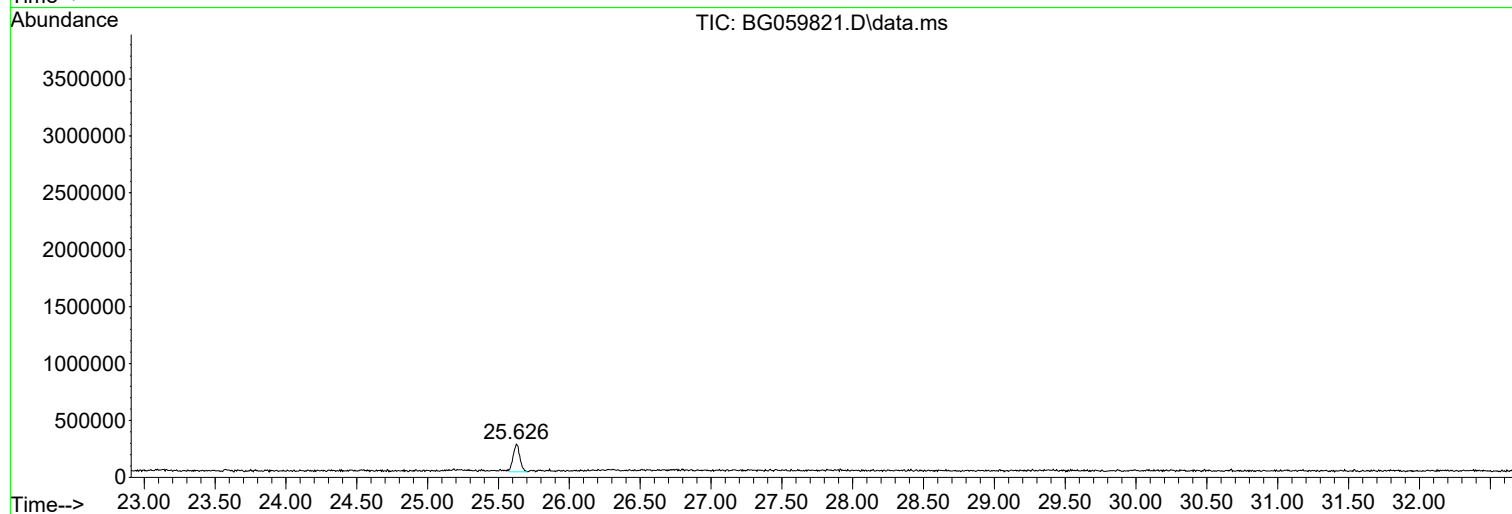
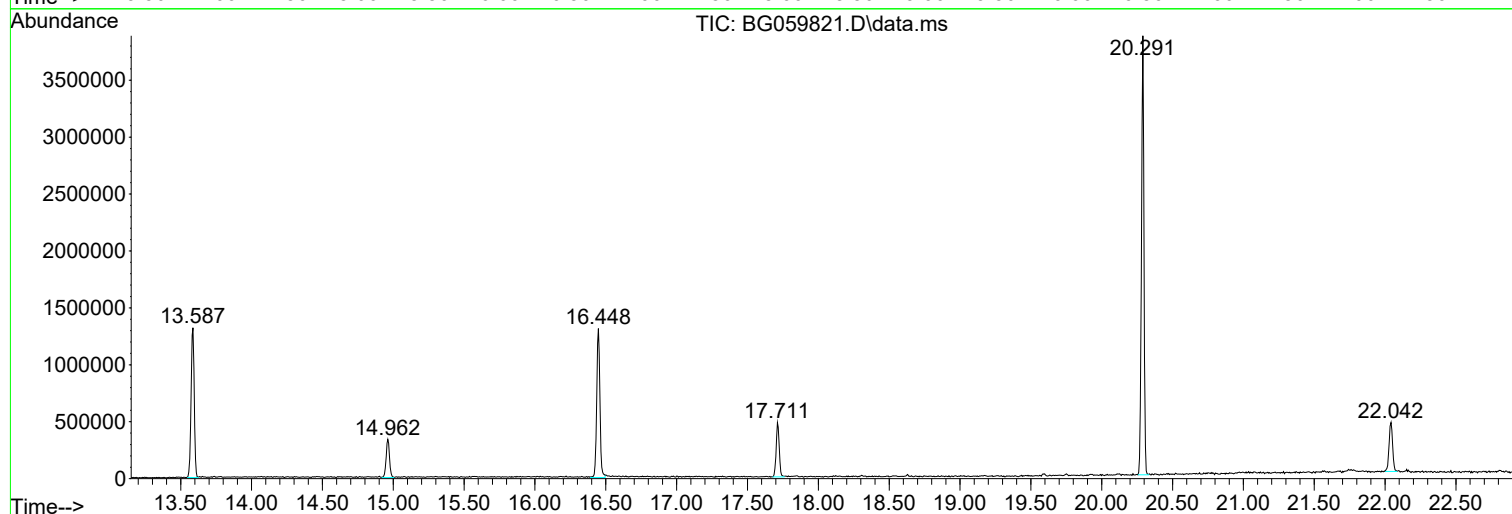
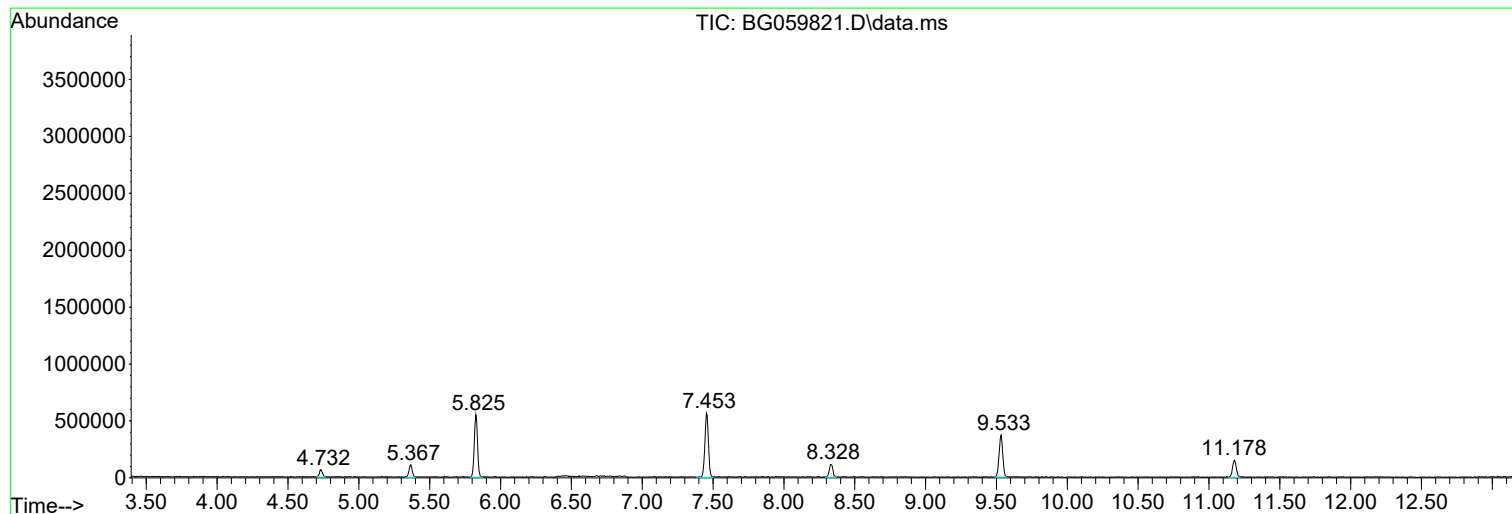
Sum of corrected areas: 14912853

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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111623.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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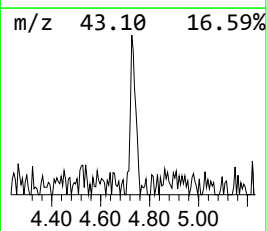
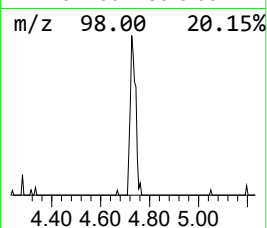
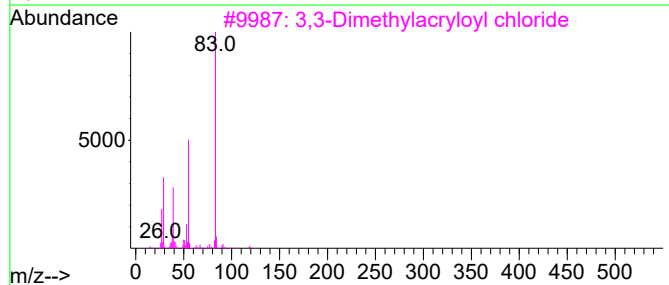
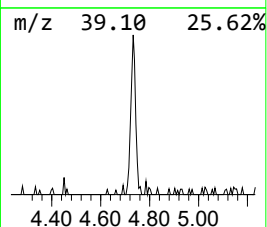
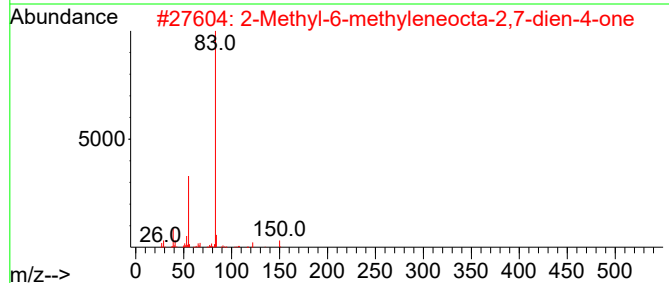
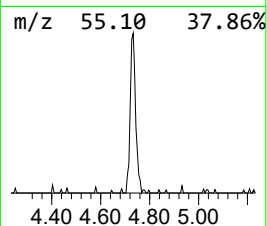
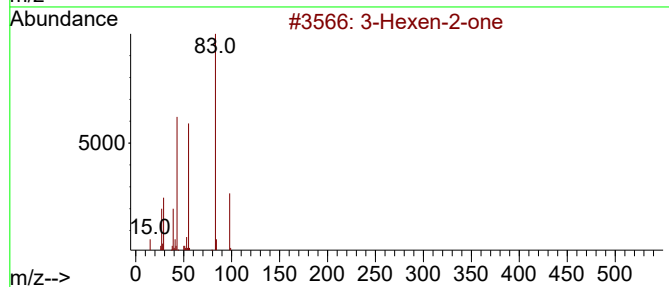
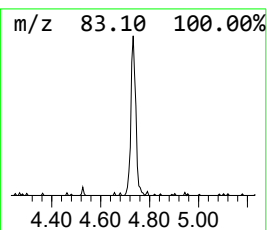
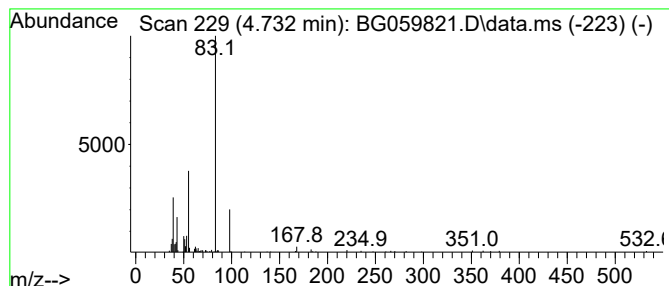
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Hexen-2-one Concentration Rank 2

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.732 | 9.68 ng | 96531 | 1,4-Dichlorobenzene-d4 | 8.328 |

| Hit# | of | 5 | Tentative ID                            | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-----------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | 3-Hexen-2-one                           | 98  | C6H10O    | 000763-93-9 | 50   |
| 2    |    |   | 2-Methyl-6-methyleneocta-2,7-dien-4-one | 150 | C10H14O   | 000539-70-8 | 40   |
| 3    |    |   | 3,3-Dimethylacryloyl chloride           | 118 | C5H7ClO   | 003350-78-5 | 33   |
| 4    |    |   | Phosphorous acid, dicyclohexyl ester    | 246 | C12H23O3P | 000139-69-5 | 33   |
| 5    |    |   | 3-Methyl-2-butenic acid, phenyl ester   | 176 | C11H12O2  | 054897-52-8 | 33   |



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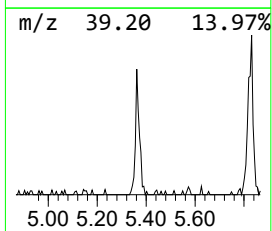
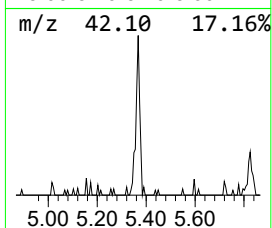
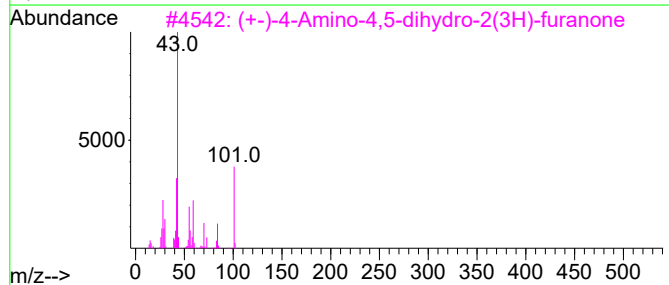
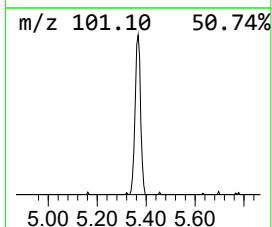
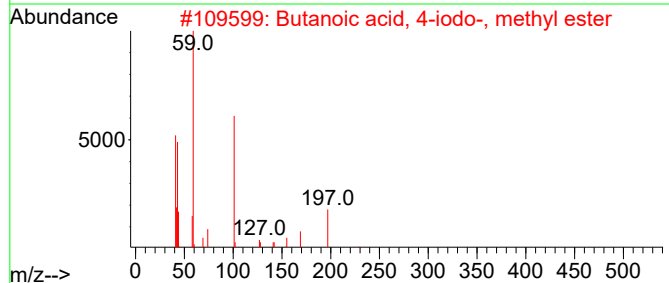
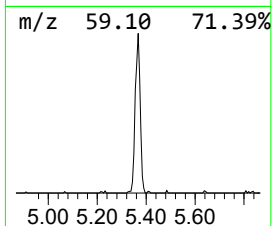
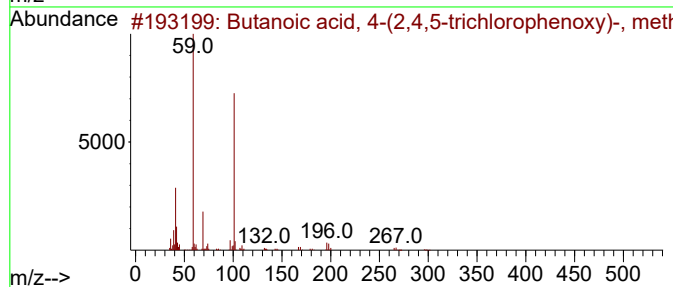
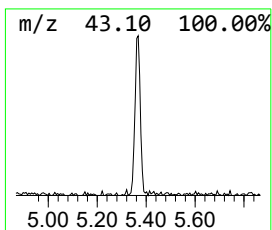
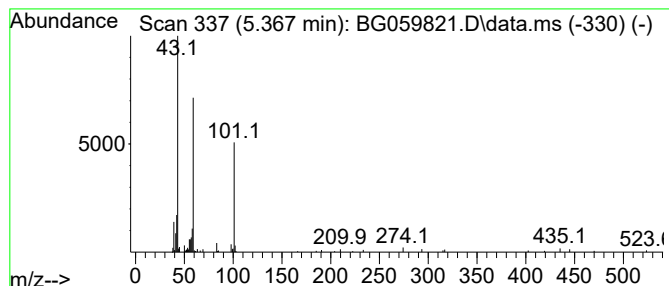
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\*\*\*\*\*  
Peak Number 2 Butanoic acid, 4-(2,4,5-tri... Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.367 | 17.49 ng | 174380 | 1,4-Dichlorobenzene-d4 | 8.328 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-------------|-------------|------|
| 1    |    |   | Butanoic acid, 4-(2,4,5-trichlor... | 296 | C11H11Cl3O3 | 025333-21-5 | 50   |
| 2    |    |   | Butanoic acid, 4-iodo-, methyl e... | 228 | C5H9IO2     | 014273-85-9 | 50   |
| 3    |    |   | (+)-4-Amino-4,5-dihydro-2(3H)-f...  | 101 | C4H7NO2     | 016504-58-8 | 50   |
| 4    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2     | 000123-42-2 | 39   |
| 5    |    |   | Isopropyl isothiocyanate            | 101 | C4H7NS      | 002253-73-8 | 23   |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| 3-Hexen-2-one      | 4.732 | 9.7     | ng    | 96531    | 1                     | 8.328 | 199354 | 20.0 |
| Butanoic acid, ... | 5.367 | 17.5    | ng    | 174380   | 1                     | 8.328 | 199354 | 20.0 |