

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP070921\  
 Data File : BP006159.D  
 Acq On : 09 Jul 2021 14:02  
 Operator : CG/JU  
 Sample : PB137592BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 PB137592BL

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\_P\Methods\8270E-BP070721.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006159.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         | 5.446       | 395           | 401         | 423          | rBV      | 2725554        | 4230575       | 43.88%          | 10.134%       |
| 2         | 7.058       | 668           | 675         | 702          | rBV      | 2307742        | 4081960       | 42.34%          | 9.778%        |
| 3         | 7.869       | 806           | 813         | 830          | rBV      | 502770         | 838623        | 8.70%           | 2.009%        |
| 4         | 9.040       | 1005          | 1012        | 1042         | rBV      | 1317807        | 2541738       | 26.36%          | 6.089%        |
| 5         | 10.681      | 1281          | 1291        | 1309         | rBV      | 493552         | 1047980       | 10.87%          | 2.510%        |
| 6         | 13.140      | 1697          | 1709        | 1736         | rBV      | 3412664        | 5674562       | 58.86%          | 13.593%       |
| 7         | 14.516      | 1936          | 1943        | 1960         | rBV      | 851835         | 1460939       | 15.15%          | 3.500%        |
| 8         | 16.010      | 2188          | 2197        | 2219         | rBV      | 2788708        | 4555579       | 47.25%          | 10.913%       |
| 9         | 17.269      | 2404          | 2411        | 2429         | rBV      | 976506         | 1683372       | 17.46%          | 4.032%        |
| 10        | 19.816      | 2839          | 2844        | 2854         | rBV      | 7851978        | 9640840       | 100.00%         | 23.094%       |
| 11        | 21.016      | 3043          | 3048        | 3052         | rBV      | 216026         | 398333        | 4.13%           | 0.954%        |
| 12        | 21.063      | 3053          | 3056        | 3061         | rVV      | 290575         | 424008        | 4.40%           | 1.016%        |
| 13        | 21.122      | 3062          | 3066        | 3074         | rVV      | 671642         | 985463        | 10.22%          | 2.361%        |
| 14        | 21.345      | 3100          | 3104        | 3112         | rBV      | 1376234        | 1946352       | 20.19%          | 4.662%        |
| 15        | 23.751      | 3507          | 3513        | 3523         | rVB2     | 1052615        | 2235971       | 23.19%          | 5.356%        |

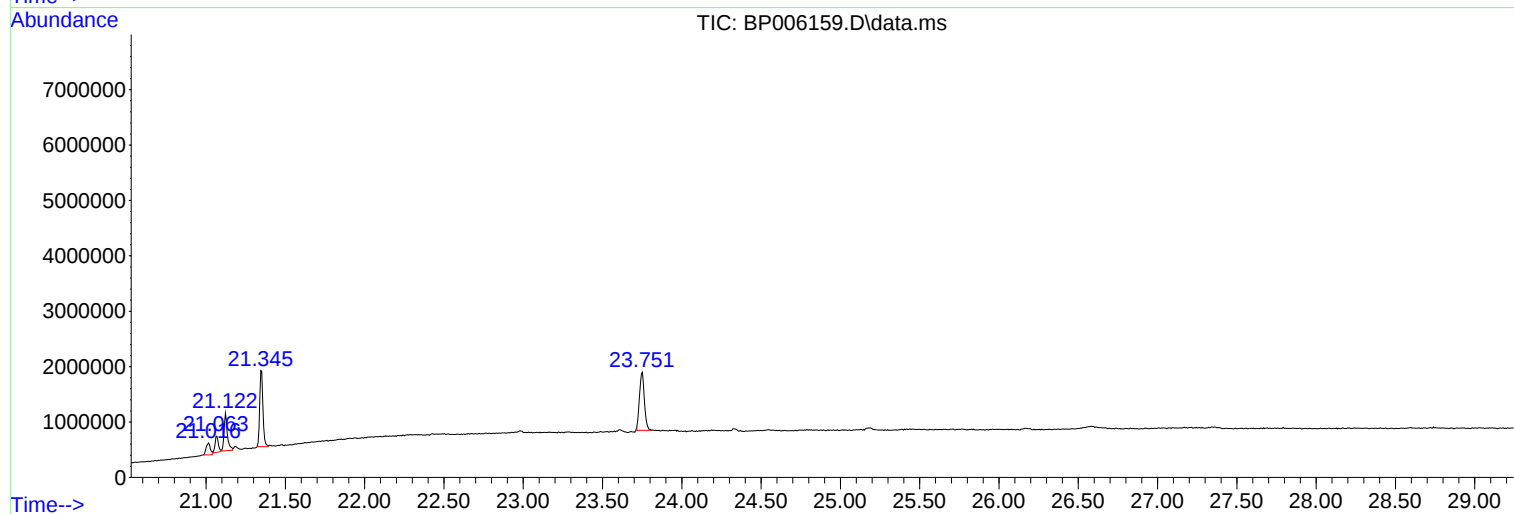
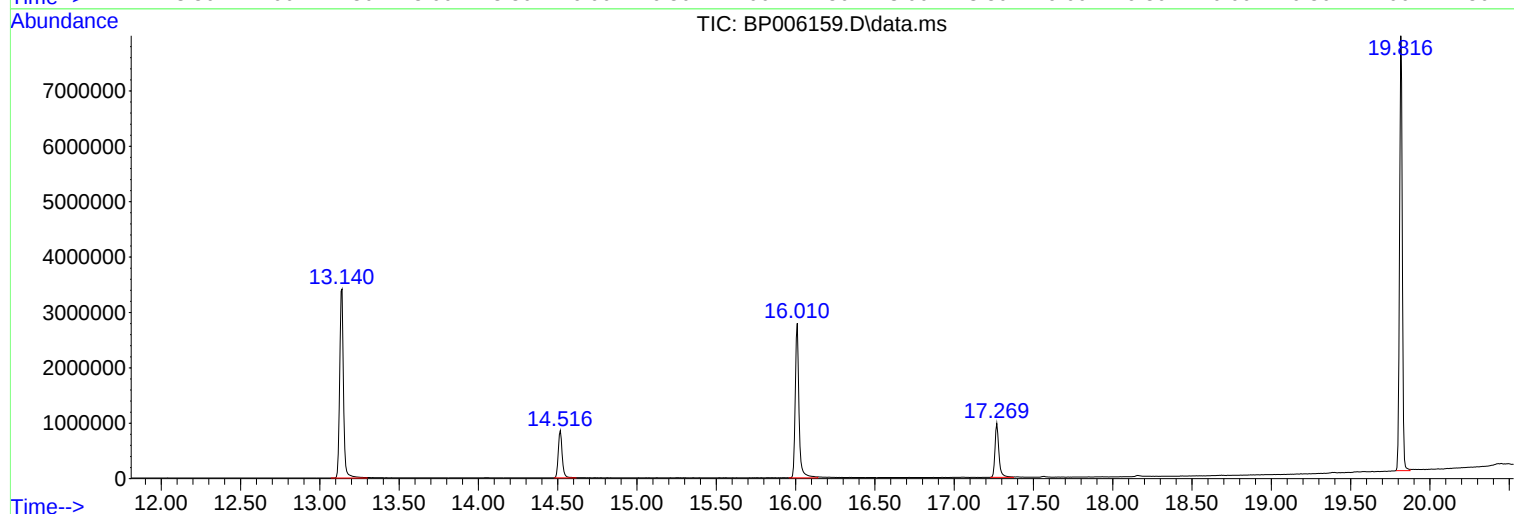
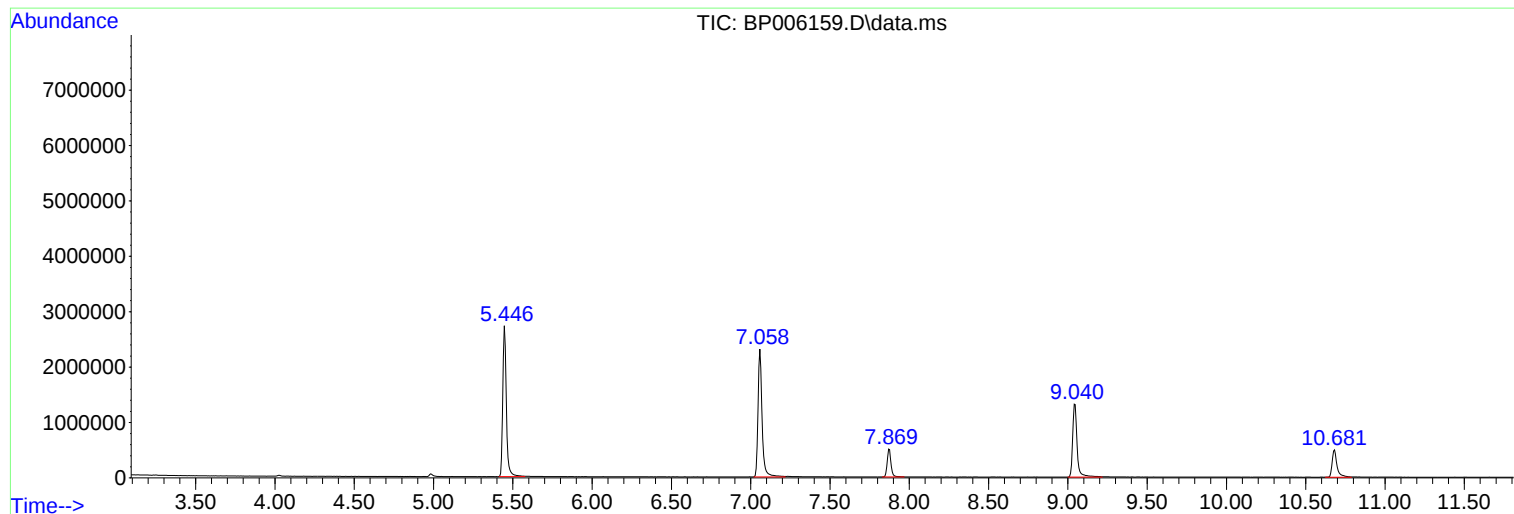
Sum of corrected areas: 41746295

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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP070721.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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ClientSampleId :  
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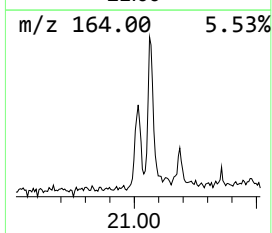
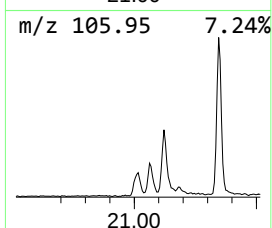
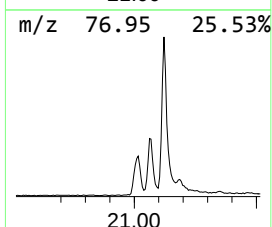
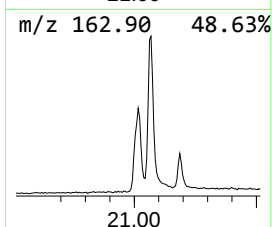
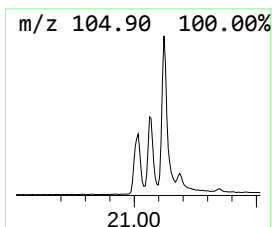
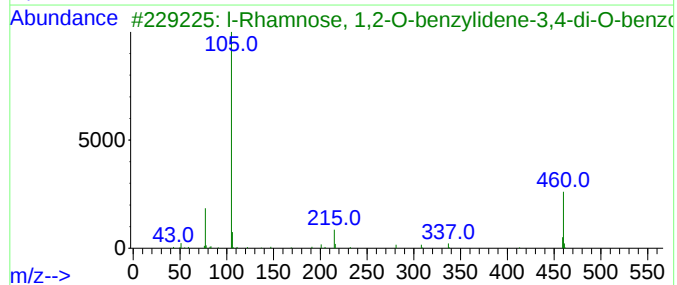
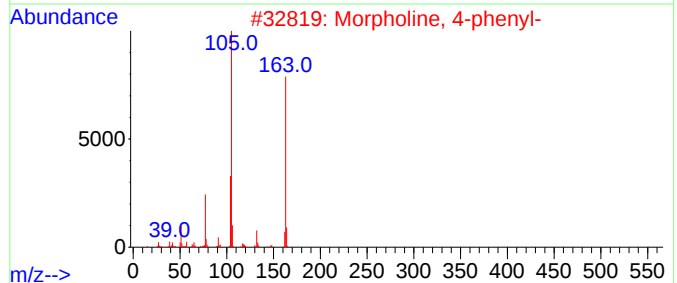
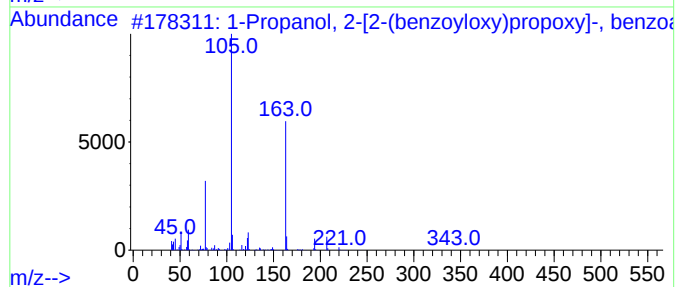
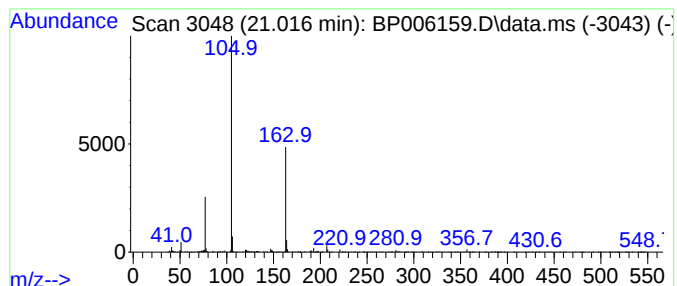
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP070721.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown21.016 Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.016 | 4.09 ng | 398333 | Chrysene-d12     | 21.345 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 1-Propanol, 2-[2-(benzyloxy)pro...  | 342 | C20H22O5     | 020109-39-1  | 40      |      |      |
| 2    | Morpholine, 4-phenyl-               | 163 | C10H13NO     | 000092-53-5  | 40      |      |      |
| 3    | l-Rhamnose, 1,2-O-benzylidene-3,... | 460 | C27H24O7     | 1000128-99-1 | 35      |      |      |
| 4    | Benzoic acid, 2-benzyloxy-3-brom... | 348 | C17H17BrO3   | 1000191-33-3 | 33      |      |      |
| 5    | 1,3-Dibenzoyl-4-oxo-2-thioxoimid... | 324 | C17H12N2O3S  | 083800-63-9  | 27      |      |      |



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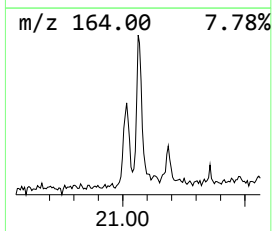
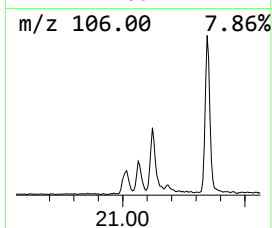
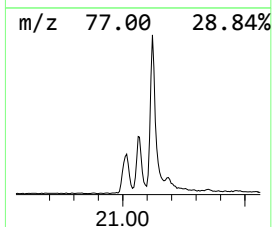
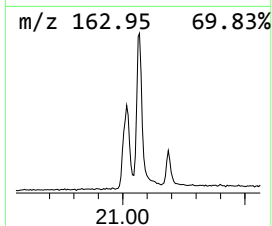
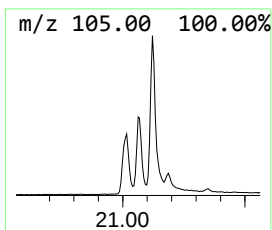
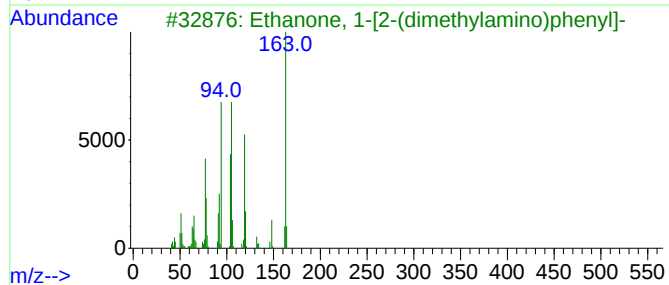
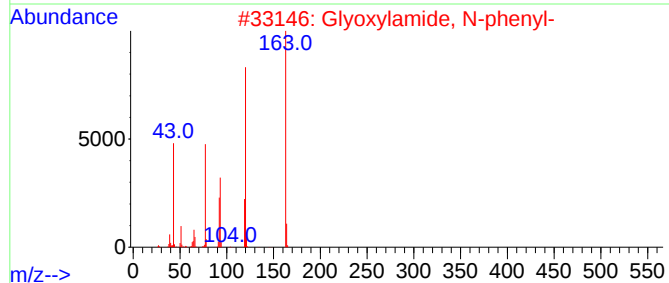
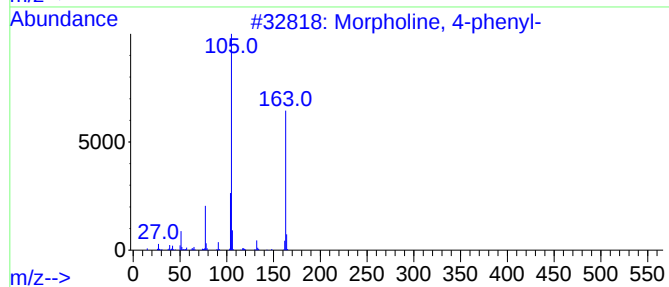
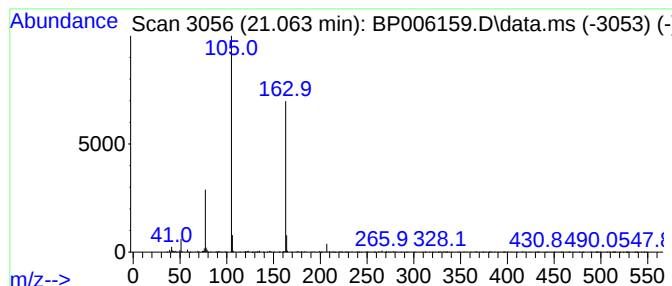
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Morpholine, 4-phenyl- Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.063 | 4.36 ng | 424008 | Chrysene-d12     | 21.345 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Morpholine, 4-phenyl-               | 163 | C10H13NO | 000092-53-5 | 50   |
| 2    |    |   | Glyoxylamide, N-phenyl-             | 163 | C9H9NO2  | 032331-52-5 | 47   |
| 3    |    |   | Ethanone, 1-[2-(dimethylamino)ph... | 163 | C10H13NO | 010336-55-7 | 42   |
| 4    |    |   | 1-Propanol, 2-[2-(benzoyloxy)pro... | 342 | C20H22O5 | 020109-39-1 | 39   |
| 5    |    |   | .delta.2-1,3,4-Oxadiazolin-5-one... | 163 | C7H5N3O2 | 002845-82-1 | 35   |



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ClientSampleId :  
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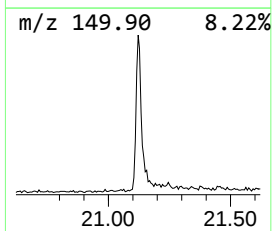
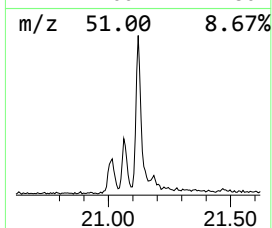
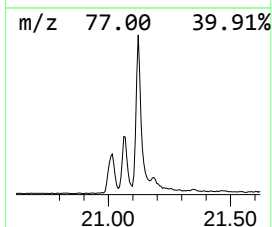
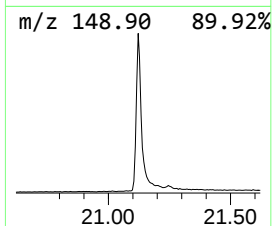
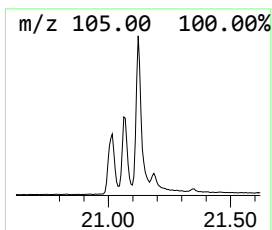
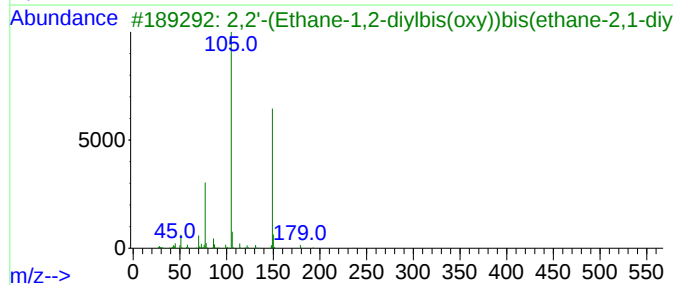
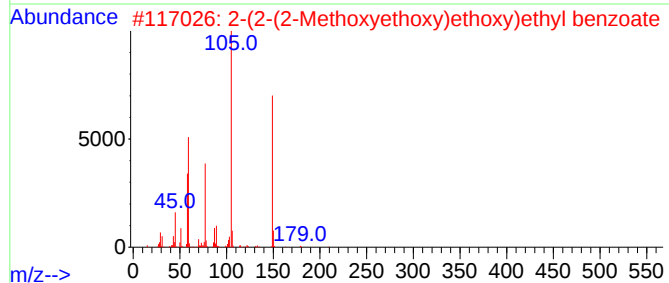
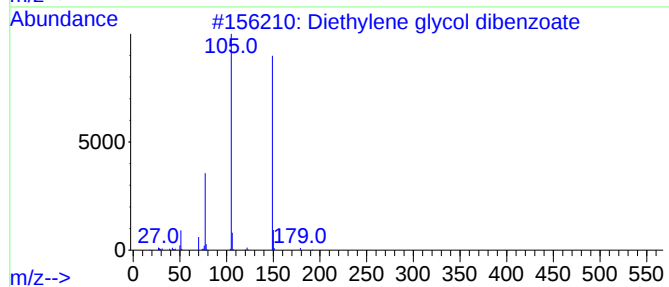
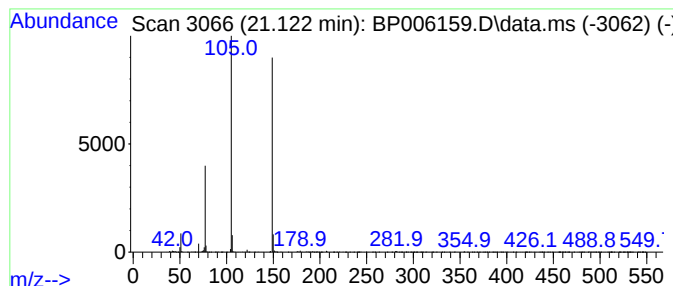
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Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 21.122 | 10.13 ng | 985463 | Chrysene-d12     | 21.345 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Diethylene glycol dibenzoate        | 314 | C18H18O5  | 000120-55-8  | 86   |
| 2    |    |   | 2-(2-(2-Methoxyethoxy)ethoxy)eth... | 268 | C14H20O5  | 1000366-99-1 | 64   |
| 3    |    |   | 2,2'-(Ethane-1,2-diylbis(oxy))bi... | 358 | C20H22O6  | 1000366-99-4 | 64   |
| 4    |    |   | 1,3-Dioxolane, 2-(methoxymethyl)... | 194 | C11H14O3  | 1000156-71-2 | 64   |
| 5    |    |   | Benzoic acid, 2-(4-nitrophenoxy)... | 287 | C15H13NO5 | 1000368-92-7 | 56   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| unknown21.016      | 21.016 | 4.1     | ng    | 398333   | 5                     | 21.345 | 1946350 | 20.0 |
| Morpholine, 4-p... | 21.063 | 4.4     | ng    | 424008   | 5                     | 21.345 | 1946350 | 20.0 |
| Diethylene glyc... | 21.122 | 10.1    | ng    | 985463   | 5                     | 21.345 | 1946350 | 20.0 |