

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN061021\  
 Data File : VN067276.D  
 Acq On : 10 Jun 2021 17:01  
 Operator : JC/MD  
 Sample : M2659-01 20X  
 Misc : 1.10g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 31454

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:\voasrv\HPCHEM1\MSVOA\_N\methods\82N061021W.M

Title : SW846 8260

Signal : TIC: VN067276.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         | 8.021       | 2229          | 2249        | 2260         | rBV2     | 296621         | 704889        | 13.47%          | 2.906%        |
| 2         | 8.086       | 2261          | 2273        | 2299         | rVB      | 561470         | 1281485       | 24.48%          | 5.283%        |
| 3         | 8.440       | 2385          | 2405        | 2432         | rBV      | 380275         | 869782        | 16.62%          | 3.586%        |
| 4         | 8.968       | 2584          | 2602        | 2631         | rBV      | 827486         | 1733943       | 33.13%          | 7.149%        |
| 5         | 10.443      | 3136          | 3152        | 3182         | rBV      | 1314452        | 2450641       | 46.82%          | 10.104%       |
| 6         | 11.747      | 3624          | 3638        | 3659         | rBV      | 1203195        | 2156700       | 41.20%          | 8.892%        |
| 7         | 12.734      | 3993          | 4006        | 4025         | rVB      | 987219         | 1703785       | 32.55%          | 7.025%        |
| 8         | 13.675      | 4347          | 4357        | 4379         | rVB      | 1111383        | 2129890       | 40.69%          | 8.781%        |
| 9         | 13.997      | 4468          | 4477        | 4491         | rBV5     | 636137         | 1156261       | 22.09%          | 4.767%        |
| 10        | 14.383      | 4612          | 4621        | 4636         | rBV7     | 662422         | 1260451       | 24.08%          | 5.197%        |
| 11        | 14.538      | 4661          | 4679        | 4702         | rVB2     | 1998111        | 5234259       | 100.00%         | 21.580%       |
| 12        | 14.850      | 4787          | 4795        | 4809         | rVB      | 2364136        | 3572785       | 68.26%          | 14.730%       |

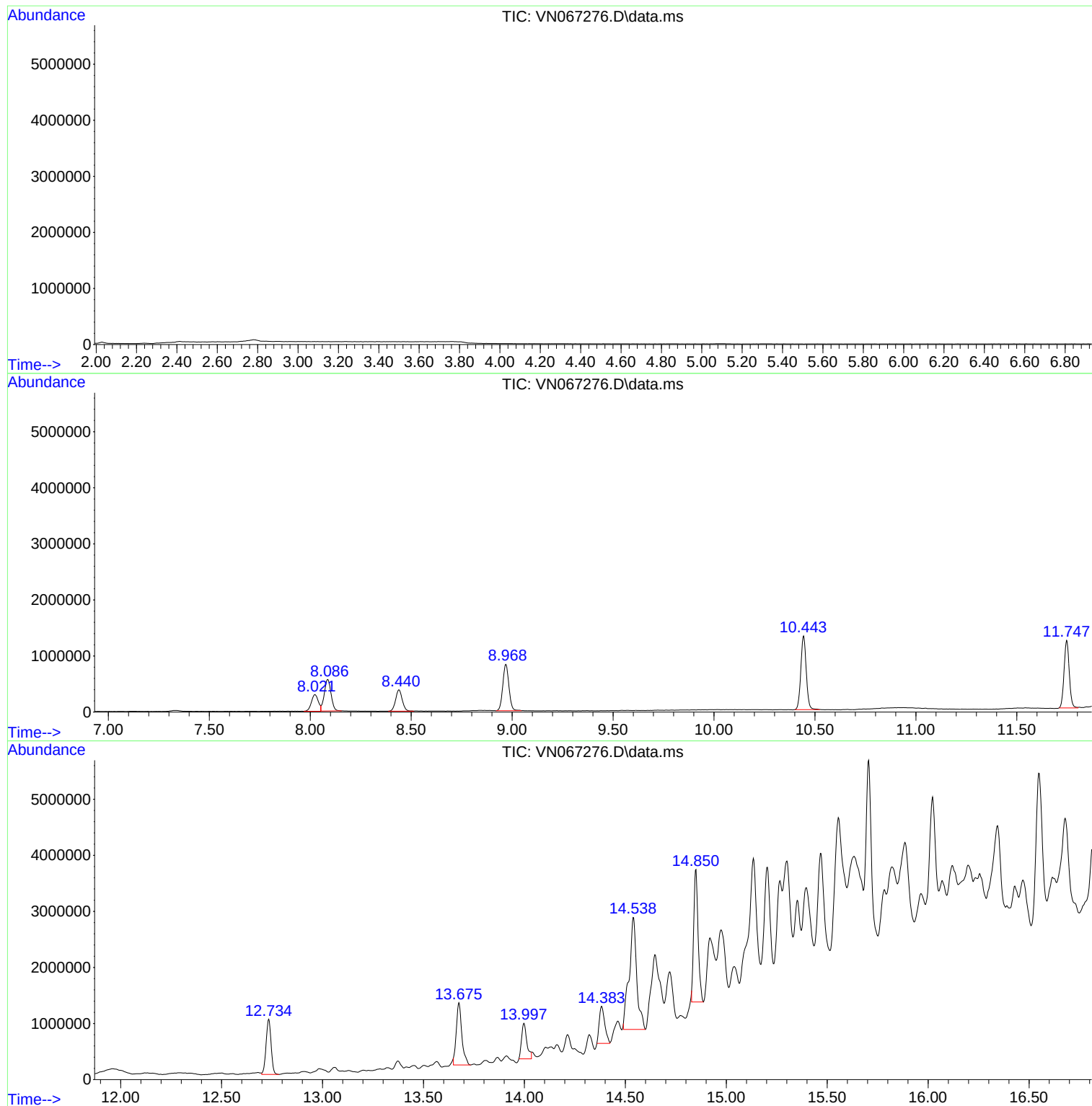
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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N061021W.M  
Quant Title : SW846 8260

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



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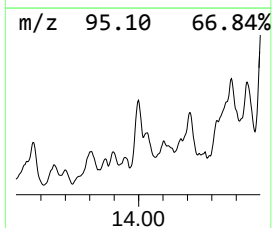
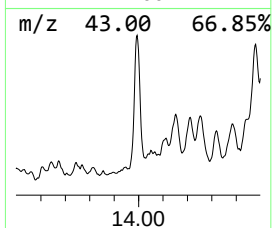
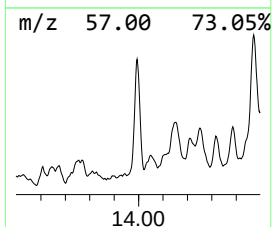
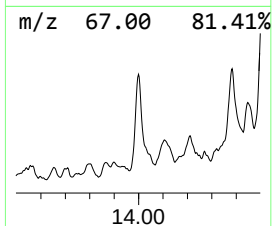
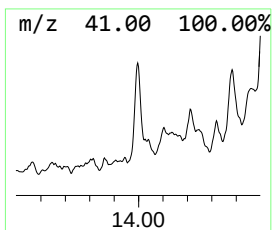
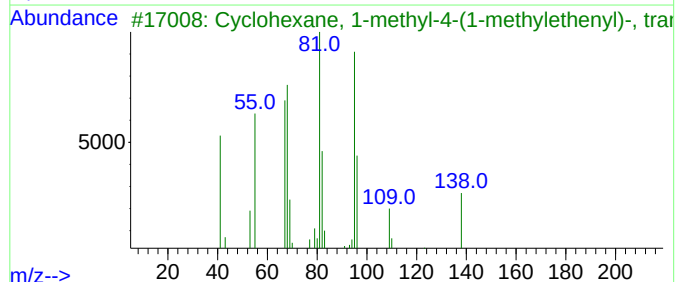
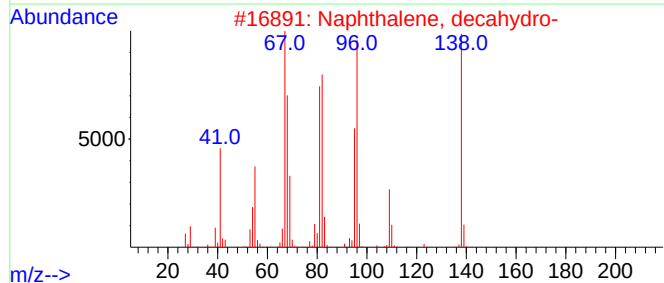
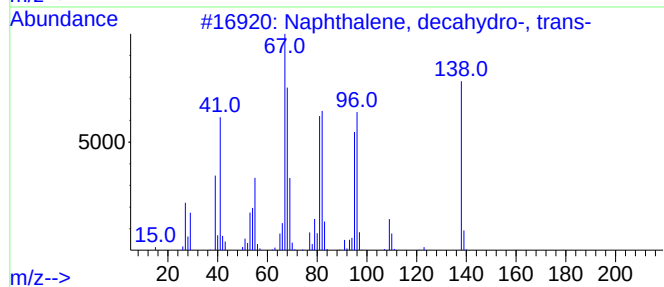
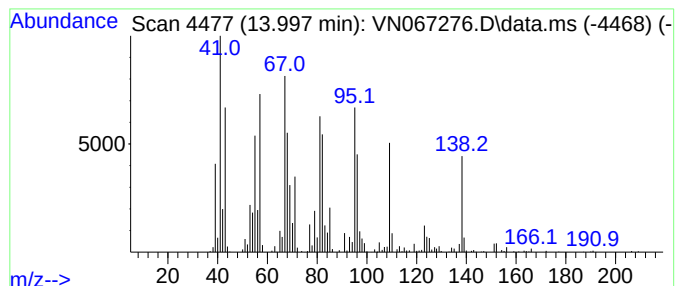
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N061021W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Naphthalene, decahydro-, tr... Concentration Rank 4

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 13.997 | 27.14 ug/l | 1156260 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Naphthalene, decahydro-, trans-     | 138 | C10H18  | 000493-02-7 | 93   |
| 2    |    |   | Naphthalene, decahydro-             | 138 | C10H18  | 000091-17-8 | 89   |
| 3    |    |   | Cyclohexane, 1-methyl-4-(1-methy... | 138 | C10H18  | 001124-25-0 | 78   |
| 4    |    |   | Naphthalene, decahydro-, cis-       | 138 | C10H18  | 000493-01-6 | 70   |
| 5    |    |   | Cyclohexane, 1-methyl-3-(1-methy... | 138 | C10H18  | 024399-15-3 | 64   |



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Instrument :  
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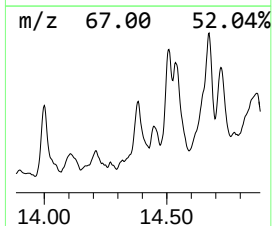
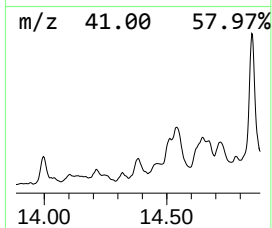
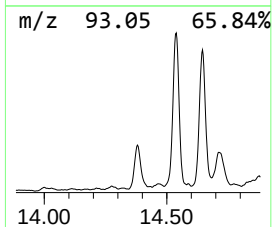
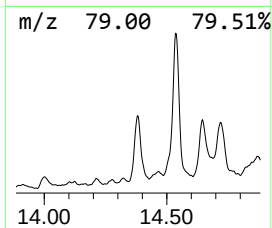
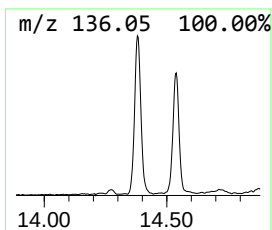
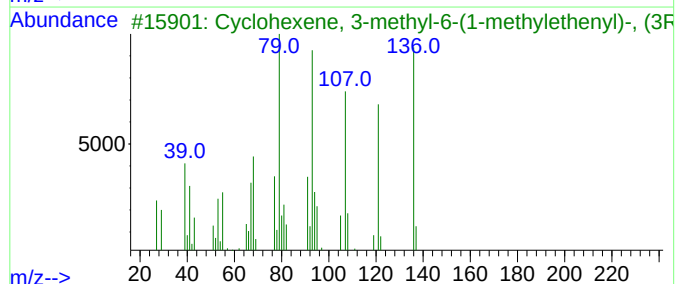
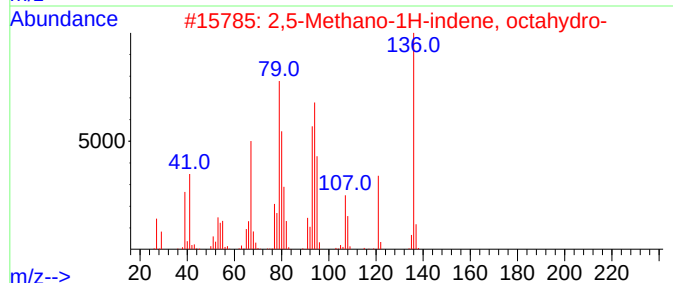
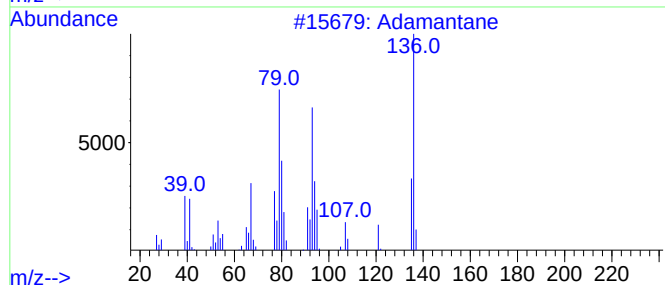
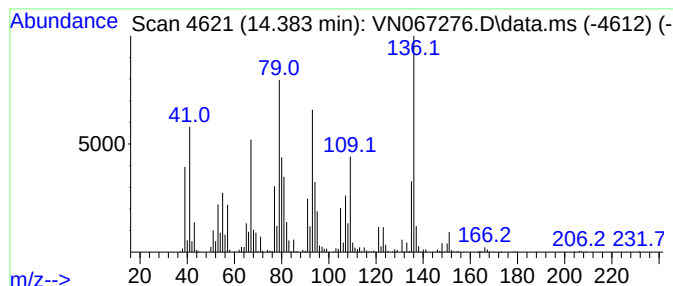
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N061021W.M  
Quant Title : SW846 8260

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

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Peak Number 2 Adamantane Concentration Rank 3

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 14.383 | 29.59 ug/l | 1260450 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Adamantane                          | 136 | C10H16  | 000281-23-2 | 96   |
| 2    |    |   | 2,5-Methano-1H-indene, octahydro-   | 136 | C10H16  | 019026-94-9 | 76   |
| 3    |    |   | Cyclohexene, 3-methyl-6-(1-methy... | 136 | C10H16  | 005113-87-1 | 64   |
| 4    |    |   | 2-Methyl-3(2-furyl)acrolein         | 136 | C8H8O2  | 000874-66-8 | 43   |
| 5    |    |   | Bicyclo[3.2.0]heptane, 2-methylene- | 108 | C8H12   | 089243-94-7 | 41   |



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Instrument :  
MSVOA\_N  
ClientSampleId :  
31454

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N061021W.M  
Quant Title : SW846 8260

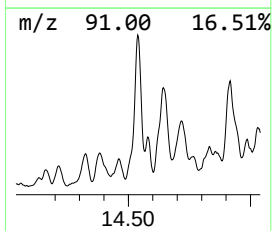
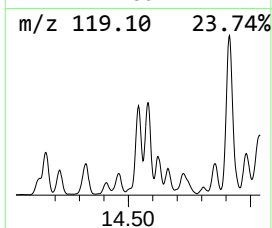
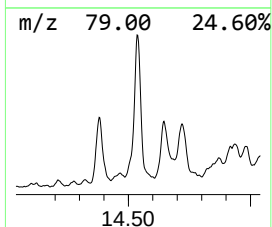
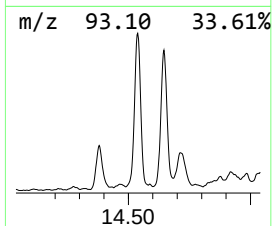
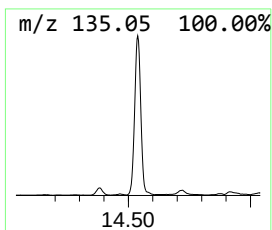
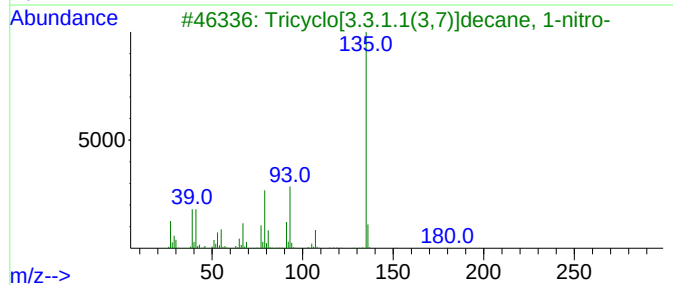
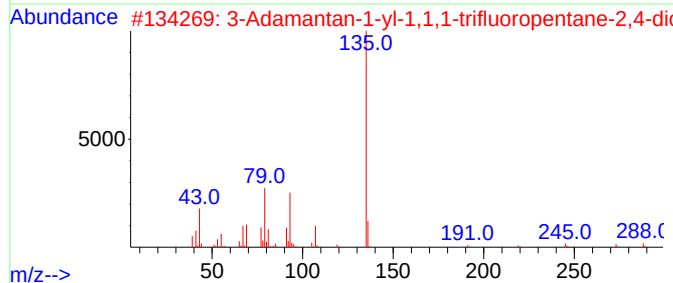
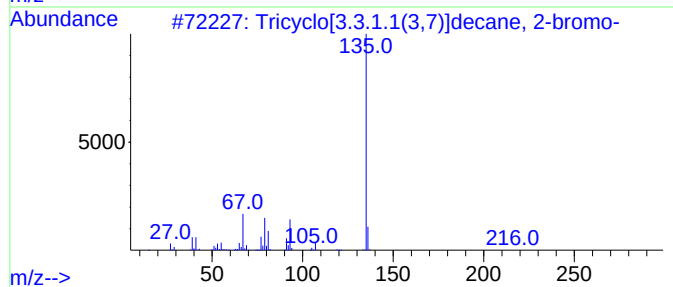
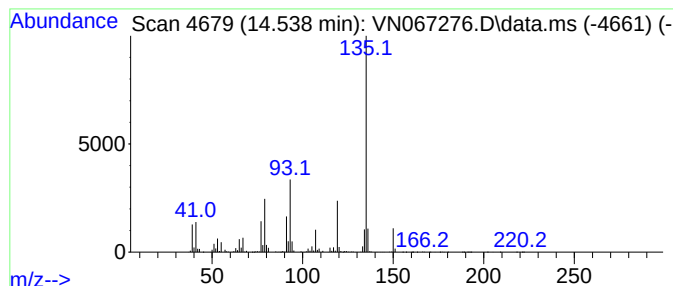
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Tricyclo[3.3.1.1(3,7)]decan... Concentration Rank 1

| R.T.   | EstConc     | Area    | Relative to ISTD       | R.T.   |
|--------|-------------|---------|------------------------|--------|
| 14.539 | 122.88 ug/l | 5234260 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Tricyclo[3.3.1.1(3,7)]decane, 2-... | 214 | C10H15Br   | 007314-85-4  | 64   |
| 2    |    |   | 3-Adamantan-1-yl-1,1,1-trifluoro... | 288 | C15H19F3O2 | 1000311-44-8 | 59   |
| 3    |    |   | Tricyclo[3.3.1.1(3,7)]decane, 1-... | 181 | C10H15NO2  | 007575-82-8  | 59   |
| 4    |    |   | 1-Adamantanecarboxylic acid chlo... | 198 | C11H15ClO  | 002094-72-6  | 58   |
| 5    |    |   | 1-Bromoadamantane                   | 214 | C10H15Br   | 000768-90-1  | 53   |



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Quant Title : SW846 8260

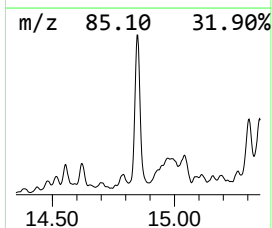
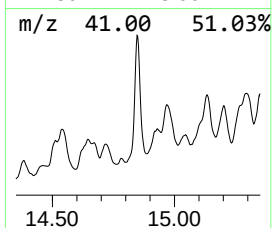
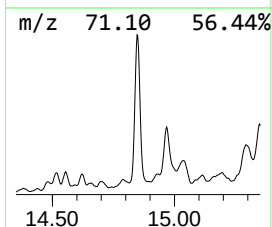
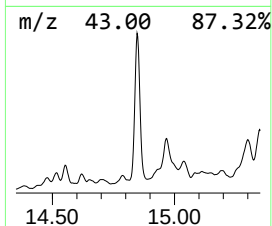
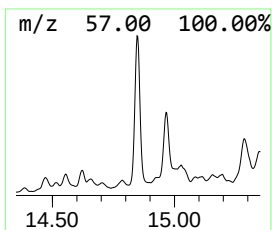
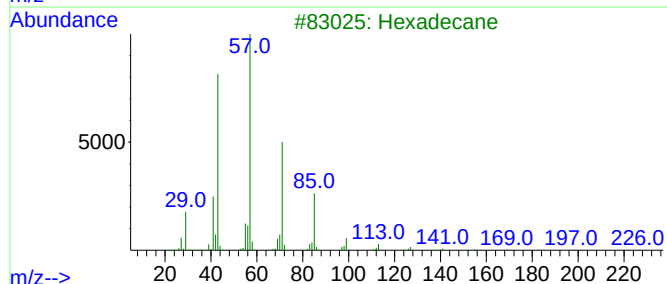
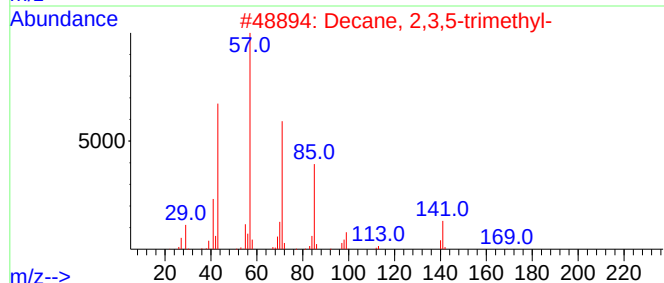
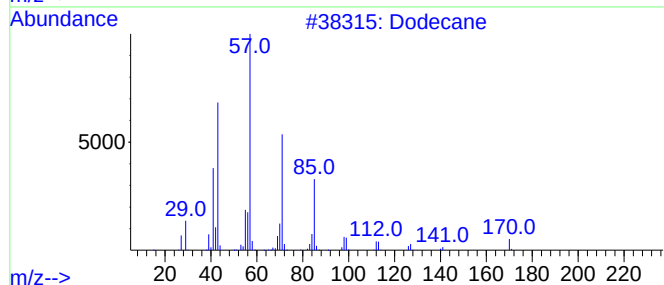
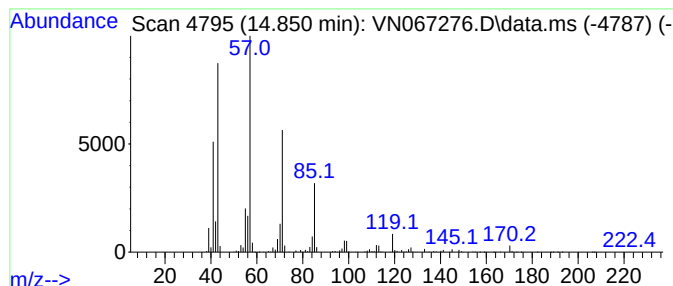
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Dodecane Concentration Rank 2

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 14.850 | 83.87 ug/l | 3572790 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# | of | 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|-----|---------|-------------|------|
| 1    |    |   | Dodecane                 | 170 | C12H26  | 000112-40-3 | 95   |
| 2    |    |   | Decane, 2,3,5-trimethyl- | 184 | C13H28  | 062238-11-3 | 86   |
| 3    |    |   | Hexadecane               | 226 | C16H34  | 000544-76-3 | 86   |
| 4    |    |   | Tridecane                | 184 | C13H28  | 000629-50-5 | 80   |
| 5    |    |   | Undecane                 | 156 | C11H24  | 001120-21-4 | 80   |



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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Naphthalene, de... | 13.997 | 27.1    | ug/l  | 1156260  | 4                     | 13.675 | 2129890 | 50.0 |
| Adamantane         | 14.383 | 29.6    | ug/l  | 1260450  | 4                     | 13.675 | 2129890 | 50.0 |
| Tricyclo[3.3.1.... | 14.539 | 122.9   | ug/l  | 5234260  | 4                     | 13.675 | 2129890 | 50.0 |
| Dodecane           | 14.850 | 83.9    | ug/l  | 3572790  | 4                     | 13.675 | 2129890 | 50.0 |