

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG061923\  
 Data File : BG057762.D  
 Acq On : 19 Jun 2023 19:41  
 Operator : CG/JU  
 Sample : PB153461BL  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB153461BL

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057762.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         | 5.032       | 326           | 331         | 341          | rVB      | 59527          | 90778         | 3.06%           | 0.730%        |
| 2         | 5.502       | 403           | 411         | 421          | rBV      | 716941         | 1126578       | 38.03%          | 9.061%        |
| 3         | 7.088       | 673           | 681         | 694          | rVB      | 719487         | 1205878       | 40.71%          | 9.699%        |
| 4         | 7.928       | 818           | 824         | 832          | rVB      | 109078         | 182820        | 6.17%           | 1.470%        |
| 5         | 9.086       | 1013          | 1021        | 1030         | rBV      | 408502         | 696355        | 23.51%          | 5.601%        |
| 6         | 10.731      | 1293          | 1301        | 1308         | rBV      | 157545         | 279528        | 9.44%           | 2.248%        |
| 7         | 13.187      | 1711          | 1719        | 1729         | rBV      | 1029576        | 1581840       | 53.40%          | 12.722%       |
| 8         | 14.556      | 1946          | 1952        | 1960         | rVB      | 260308         | 407127        | 13.74%          | 3.274%        |
| 9         | 16.042      | 2198          | 2205        | 2217         | rBV      | 915310         | 1363926       | 46.04%          | 10.970%       |
| 10        | 17.300      | 2412          | 2419        | 2426         | rBV      | 411039         | 590217        | 19.92%          | 4.747%        |
| 11        | 19.920      | 2859          | 2865        | 2870         | rBV      | 2265555        | 2962468       | 100.00%         | 23.826%       |
| 12        | 21.554      | 3137          | 3143        | 3153         | rBV      | 421862         | 661335        | 22.32%          | 5.319%        |
| 13        | 23.193      | 3417          | 3422        | 3428         | rVB5     | 19114          | 36511         | 1.23%           | 0.294%        |
| 14        | 24.227      | 3591          | 3598        | 3608         | rVB3     | 33020          | 85364         | 2.88%           | 0.687%        |
| 15        | 24.703      | 3668          | 3679        | 3694         | rVB      | 270424         | 730326        | 24.65%          | 5.874%        |
| 16        | 25.508      | 3806          | 3816        | 3829         | rVB4     | 41164          | 139659        | 4.71%           | 1.123%        |
| 17        | 27.100      | 4076          | 4087        | 4103         | rBV6     | 39378          | 172747        | 5.83%           | 1.389%        |
| 18        | 29.109      | 4410          | 4429        | 4431         | rBV5     | 32916          | 120045        | 4.05%           | 0.965%        |

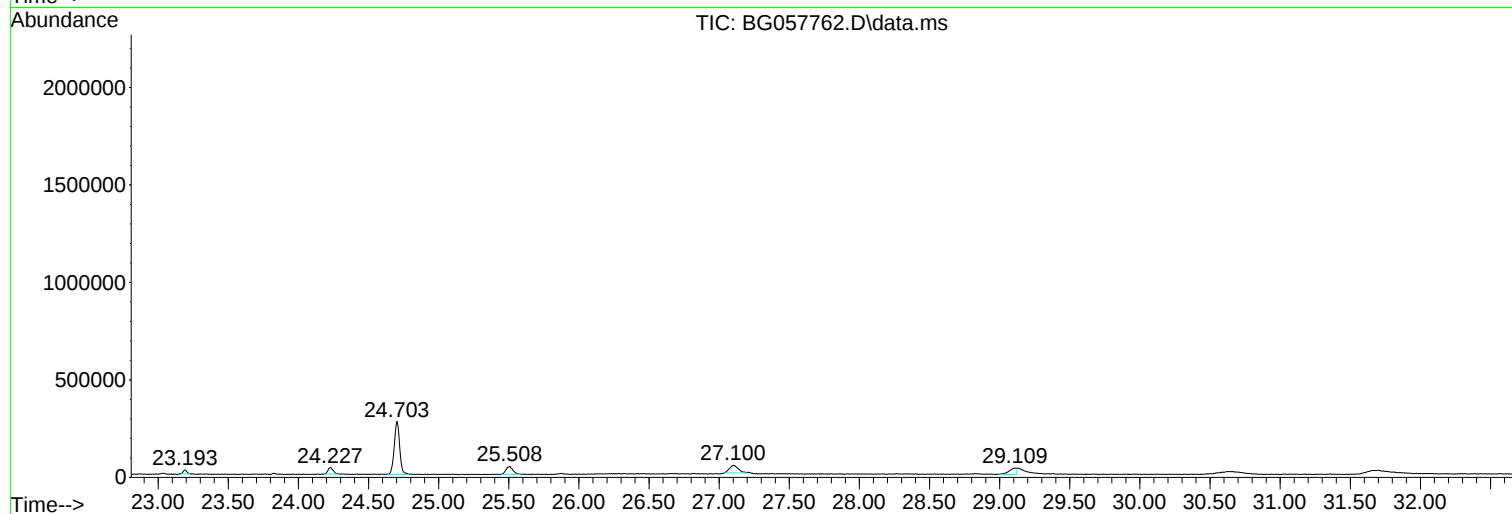
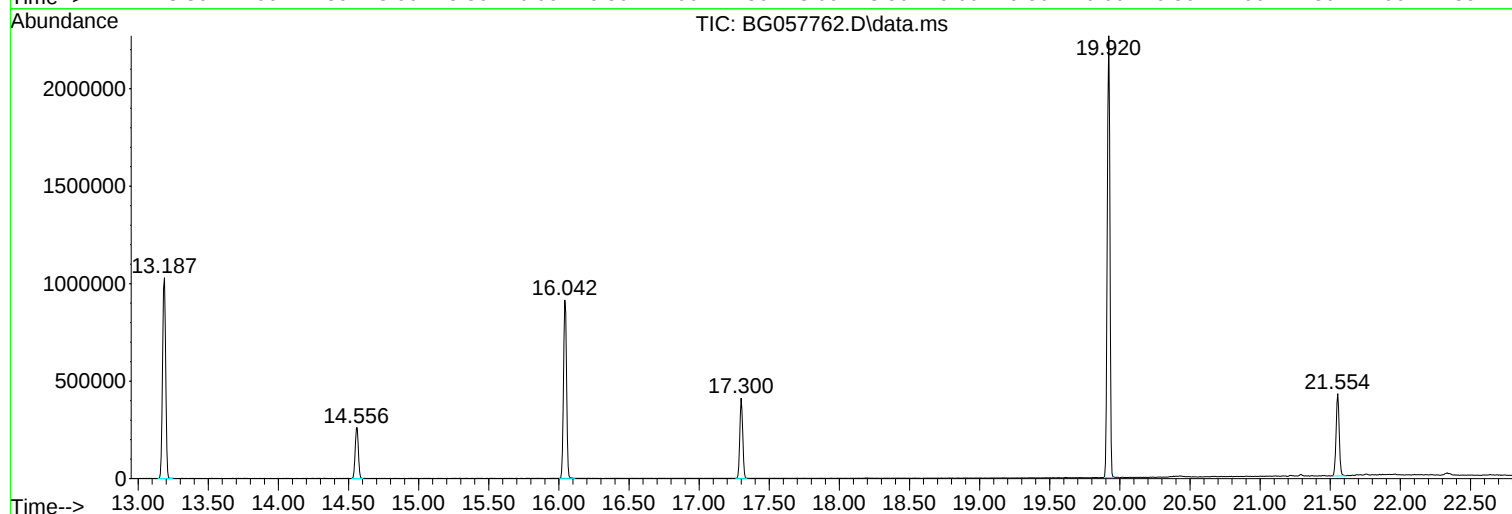
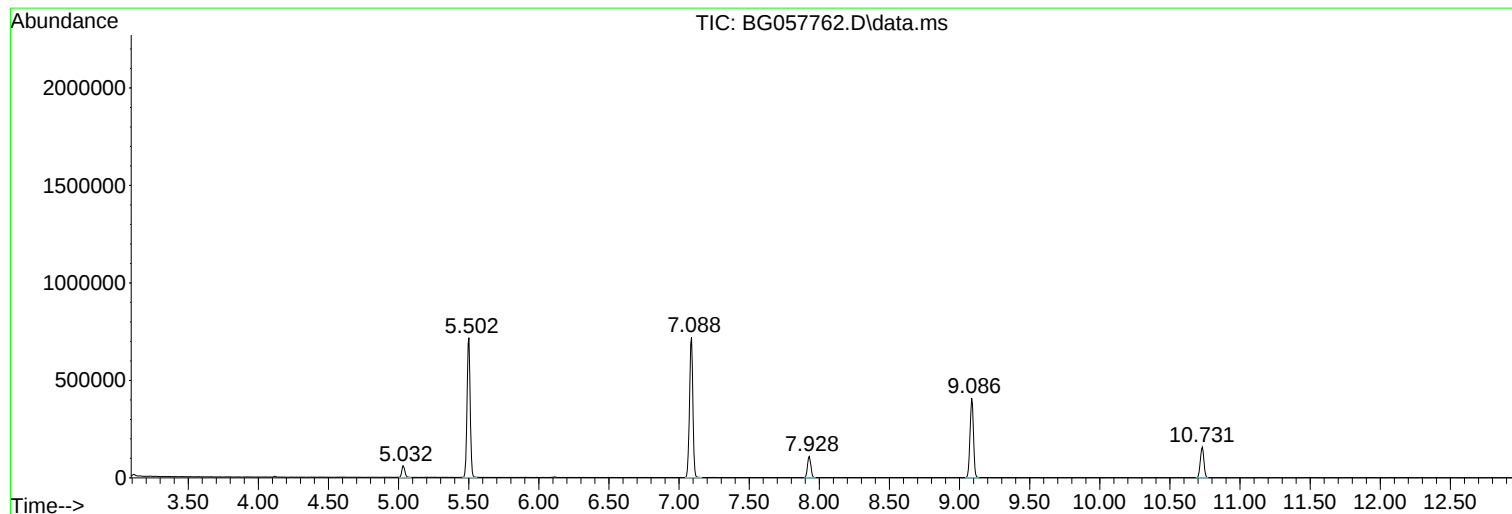
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG061923\  
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Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153461BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG061923\  
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

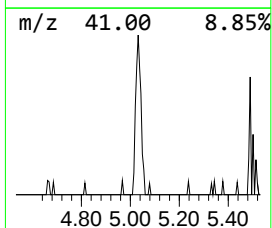
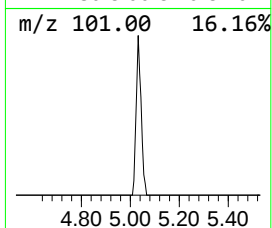
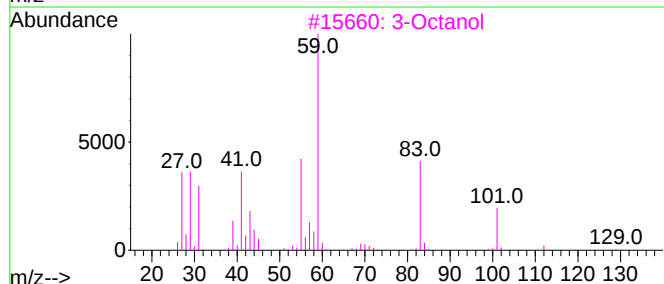
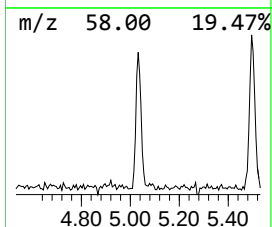
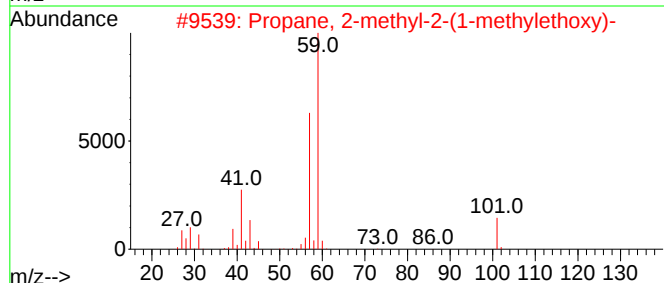
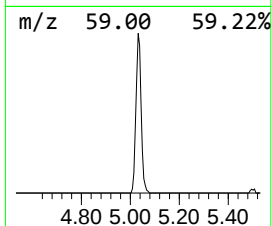
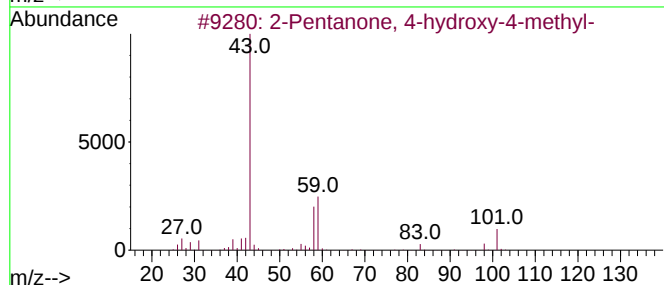
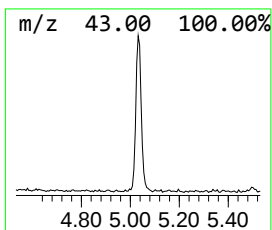
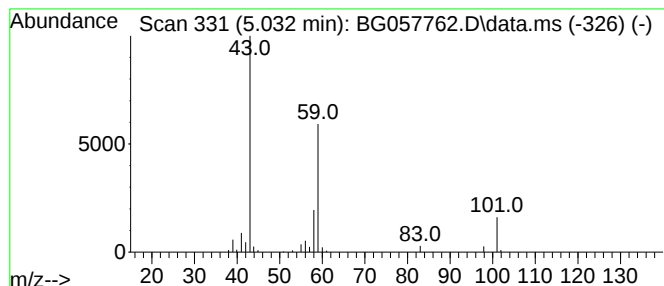
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.032 | 9.93 ng | 90778 | 1,4-Dichlorobenzene-d4 | 7.928 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 59      |      |      |
| 2    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O       | 017348-59-3 | 33      |      |      |
| 3    | 3-Octanol                           | 130 | C8H18O       | 000589-98-0 | 25      |      |      |
| 4    | 2-Hexanol, 2-methyl-                | 116 | C7H16O       | 000625-23-0 | 25      |      |      |
| 5    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 23      |      |      |



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Instrument :  
BNA\_G  
ClientSampleId :  
PB153461BL

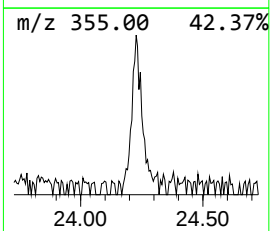
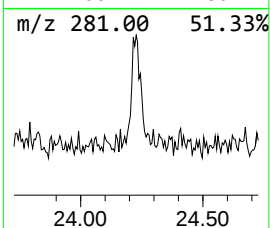
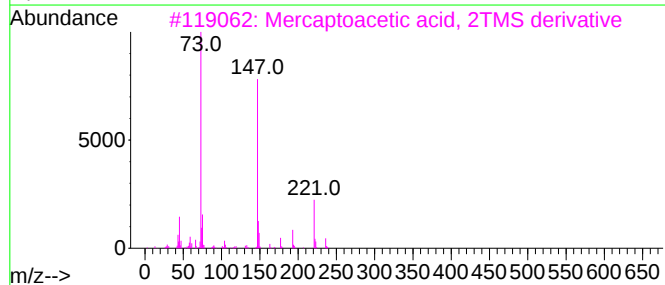
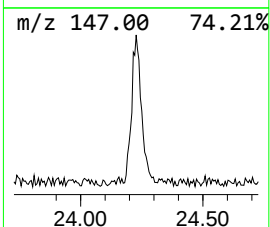
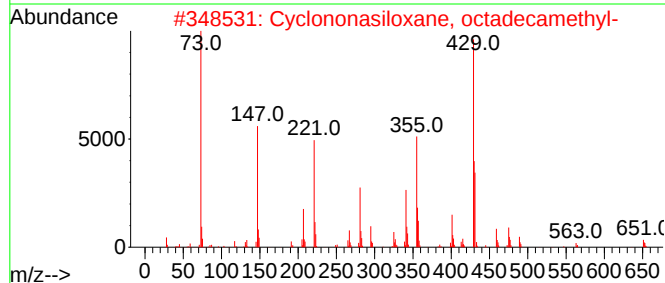
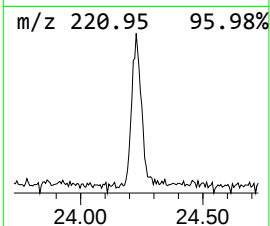
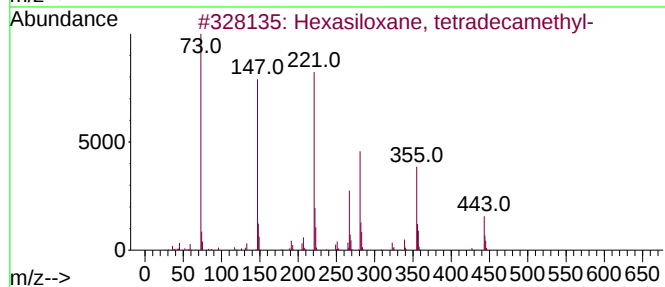
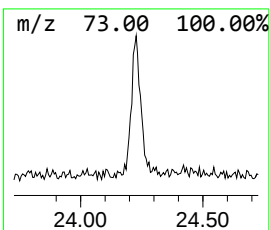
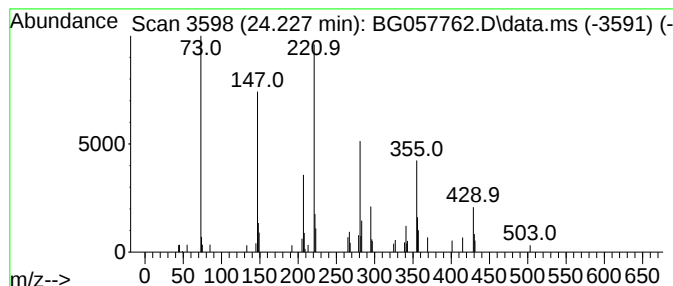
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Hexasiloxane, tetradecamethyl- Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 24.227 | 2.34 ng | 85364 | Perylene-d12     | 24.703 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|------|-------------------------------------|-----|-------------|-------------|------|
| 1    |      | Hexasiloxane, tetradecamethyl-      | 458 | C14H42O5Si6 | 000107-52-8 | 72   |
| 2    |      | Cyclononasiloxane, octadecamethyl-  | 666 | C18H54O9Si9 | 000556-71-8 | 45   |
| 3    |      | Mercaptoacetic acid, 2TMS deriva... | 236 | C8H20O2SSi2 | 006398-62-5 | 32   |
| 4    |      | Heptasiloxane, hexadecamethyl-      | 532 | C16H48O6Si7 | 000541-01-5 | 32   |
| 5    |      | 3,6-Dioxa-2,4,5,7-tetrasilaoctan... | 294 | C10H30O2Si4 | 004342-25-0 | 27   |



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ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153461BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

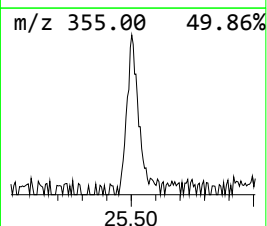
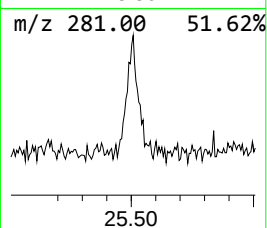
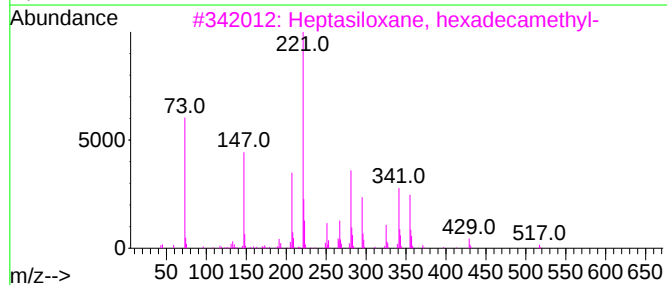
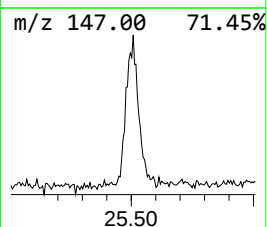
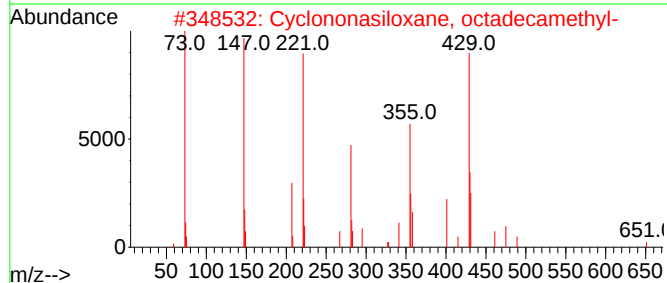
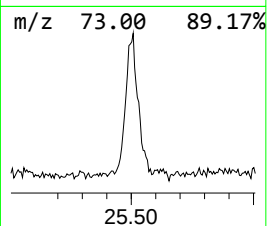
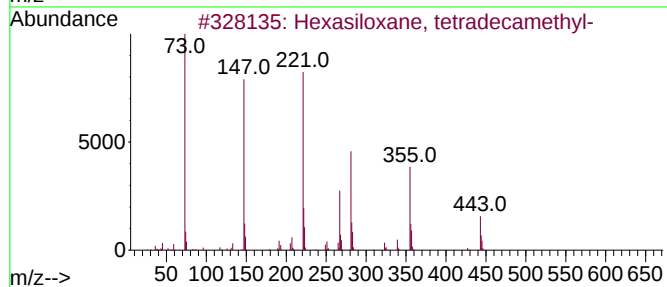
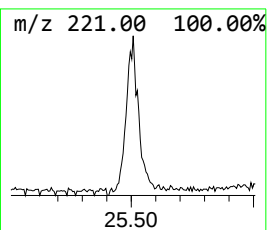
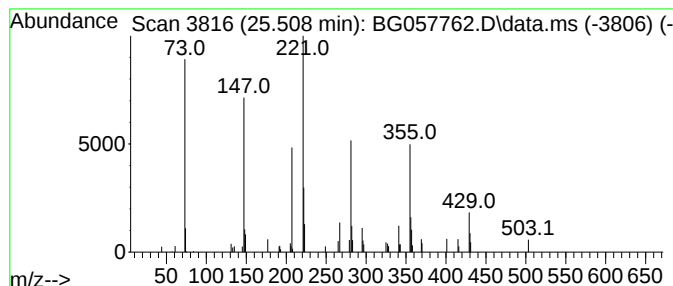
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown25.508 Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 25.508 | 3.82 ng | 139659 | Perylene-d12     | 24.703 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-------------|-------------|------|
| 1    |    |   | Hexasiloxane, tetradecamethyl-      | 458 | C14H42O5Si6 | 000107-52-8 | 52   |
| 2    |    |   | Cyclononasiloxane, octadecamethyl-  | 666 | C18H54O9Si9 | 000556-71-8 | 46   |
| 3    |    |   | Heptasiloxane, hexadecamethyl-      | 532 | C16H48O6Si7 | 000541-01-5 | 42   |
| 4    |    |   | 1,1,1,5,7,7,7-Heptamethyl-3,3-bi... | 444 | C13H40O5Si6 | 038147-00-1 | 25   |
| 5    |    |   | Boric acid, 3TMS derivative         | 278 | C9H27B03Si3 | 004325-85-3 | 16   |



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Sample : PB153461BL  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153461BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

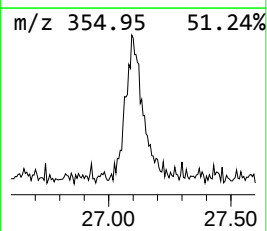
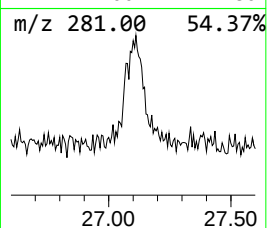
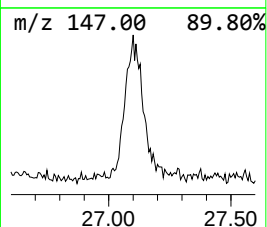
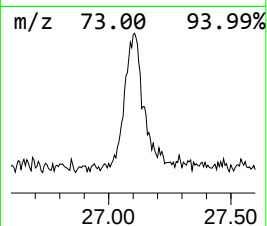
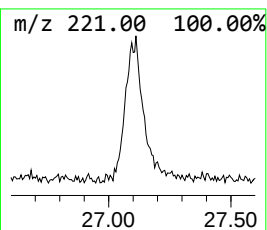
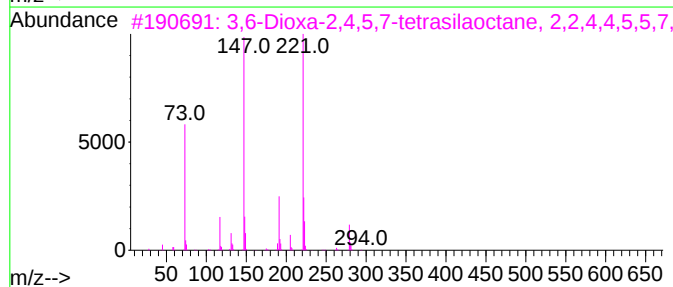
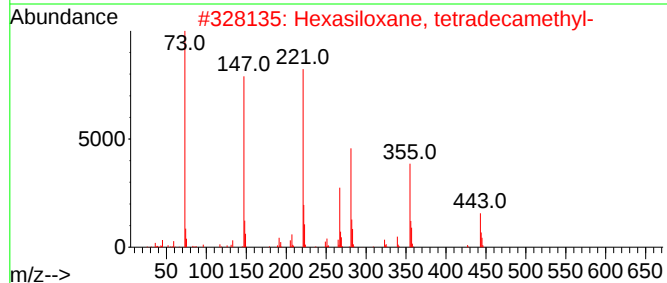
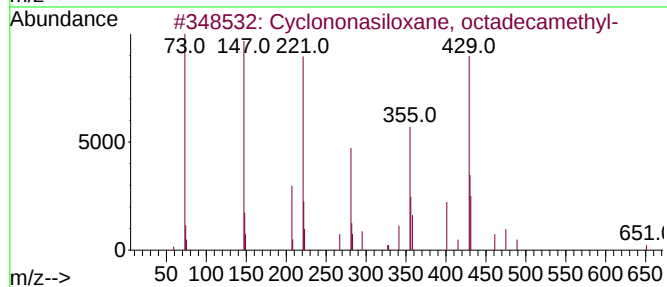
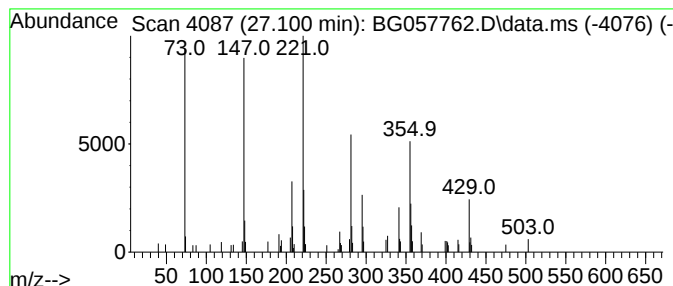
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Cyclononasiloxane, octadeca... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 27.100 | 4.73 ng | 172747 | Perylene-d12     | 24.703 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Cyclononasiloxane, octadecamethyl-  | 666 | C18H54O9Si9 | 000556-71-8  | 74   |
| 2    |    |   | Hexasiloxane, tetradecamethyl-      | 458 | C14H42O5Si6 | 000107-52-8  | 59   |
| 3    |    |   | 3,6-Dioxa-2,4,5,7-tetrasilaoctan... | 294 | C10H30O2Si4 | 004342-25-0  | 32   |
| 4    |    |   | N-Benzyl-N-ethyl-p-isopropylbenz... | 281 | C19H23NO    | 015089-22-2  | 25   |
| 5    |    |   | benzenamine, N-[bis(2,4,6-trimet... | 341 | C24H28BN    | 1000398-20-2 | 22   |



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Instrument :  
BNA\_G  
ClientSampleId :  
PB153461BL

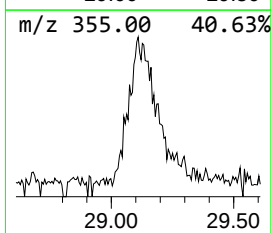
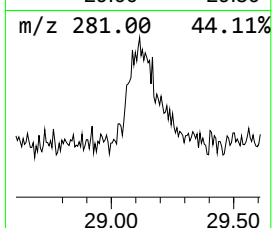
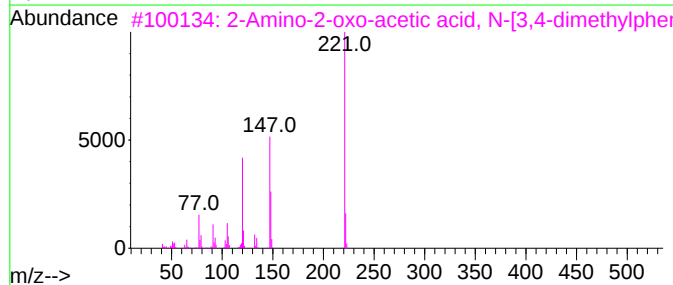
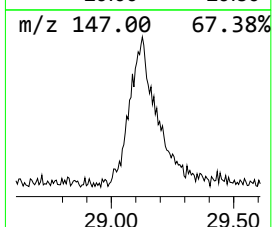
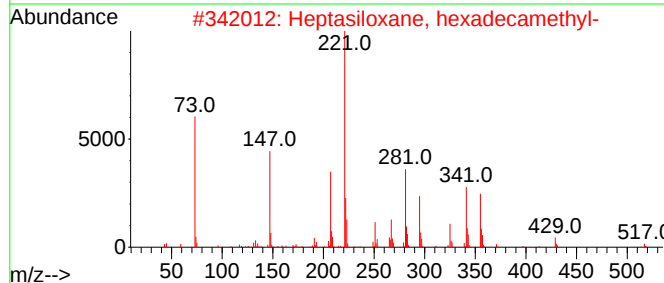
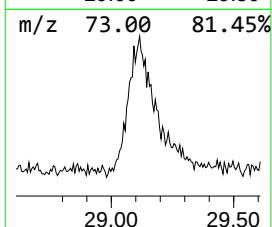
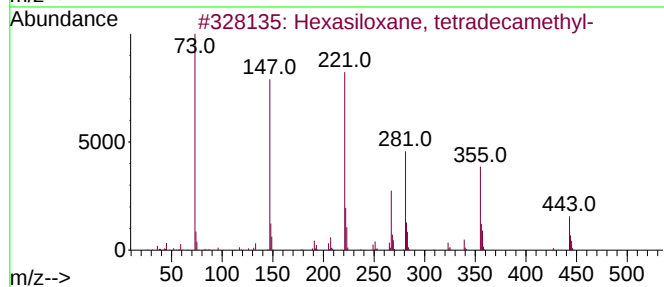
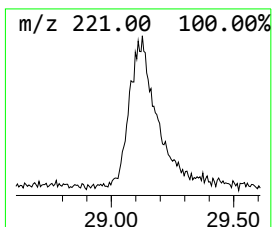
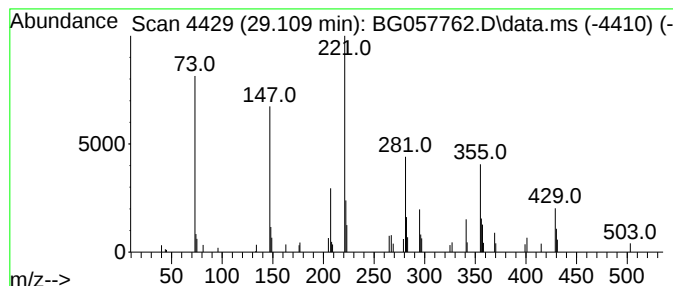
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 unknown29.109 Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 29.109 | 3.29 ng | 120045 | Perylene-d12     | 24.703 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm      | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|--------------|--------------|------|
| 1    |    |   | Hexasiloxane, tetradecamethyl-      | 458 | C14H42O5Si6  | 000107-52-8  | 59   |
| 2    |    |   | Heptasiloxane, hexadecamethyl-      | 532 | C16H48O6Si7  | 000541-01-5  | 45   |
| 3    |    |   | 2-Amino-2-oxo-acetic acid, N-[3,... | 221 | C12H15NO3    | 024451-17-0  | 38   |
| 4    |    |   | Cyclononasiloxane, octadecamethyl-  | 666 | C18H54O9Si9  | 000556-71-8  | 38   |
| 5    |    |   | 2,6-Dimethyl-3,4-bis(trimethylsi... | 311 | C15H29NO2Si2 | 1000079-52-1 | 32   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG061923\  
Data File : BG057762.D  
Acq On : 19 Jun 2023 19:41  
Operator : CG/JU  
Sample : PB153461BL  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153461BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.032  | 9.9     | ng    | 90778    | 1                     | 7.928  | 182820 | 20.0 |
| Hexasiloxane, t... | 24.227 | 2.3     | ng    | 85364    | 6                     | 24.703 | 730326 | 20.0 |
| unknown25.508      | 25.508 | 3.8     | ng    | 139659   | 6                     | 24.703 | 730326 | 20.0 |
| Cyclononasiloxa... | 27.100 | 4.7     | ng    | 172747   | 6                     | 24.703 | 730326 | 20.0 |
| unknown29.109      | 29.109 | 3.3     | ng    | 120045   | 6                     | 24.703 | 730326 | 20.0 |