LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043681.D
Acq On : 18 Nov 2019 20:13
Operator : JU
Sample : K5833-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 8-(12-13)

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-BG102119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.154 | 7 | 11 | 24 | rVB | 54479 | 96121 | 5.13% | 1.079% |
| 2 | 5.098 | 337 | 342 | 353 | rBV | 68228 | 108654 | 5.80% | 1.219% |
| 3 | 5.586 | 417 | 425 | 443 | rBV | 305203 | 547070 | 29.19% | 6.140% |
| 4 | 7.190 | 689 | 698 | 709 | rBV | 312141 | 610764 | 32.59% | 6.855% |
| 5 | 7.537 | 748 | 757 | 767 | rBV | 343477 | 613231 | 32.72% | 6.883% |
| 6 | 7.989 | 827 | 834 | 844 | rBV | 90801 | 163935 | 8.75% | 1.840% |
| 7 | 8.318 | 882 | 890 | 902 | rBV | 266725 | 490841 | 26.19% | 5.509% |
| 8 | 9.158 | 1026 | 1033 | 1053 | rBV | 159956 | 352284 | 18.80% | 3.954% |
| 9 | 10.798 | 1305 | 1312 | 1321 | rBV | 88538 | 191151 | 10.20% | 2.145% |
| 10 | 13.248 | 1722 | 1729 | 1742 | rBV | 537051 | 941496 | 50.24% | 10.567% |
| 11 | 14.082 | 1864 | 1871 | 1883 | rBV2 | 41164 | 90638 | 4.84% | 1.017% |
| 12 | 14.622 | 1956 | 1963 | 1978 | rBV | 193519 | 332025 | 17.72% | 3.727% |
| 13 | 16.115 | 2210 | 2217 | 2233 | rBV | 424342 | 810948 | 43.28% | 9.102% |
| 14 | 17.372 | 2424 | 2431 | 2448 | rBV | 230402 | 426582 | 22.76% | 4.788% |
| 15 | 19.981 | 2869 | 2875 | 2890 | rBV | 1354129 | 1873924 | 100.00% | 21.032% |
| 16 | 21.279 | 3092 | 3096 | 3105 | rBV8 | 19972 | 60621 | 3.23% | 0.680% |
| 17 | 21.638 | 3150 | 3157 | 3165 | rBV2 | 279968 | 548443 | 29.27% | 6.156% |
| 18 | 22.413 | 3284 | 3289 | 3295 | rBV5 | 12589 | 23498 | 1.25% | 0.264% |
| 19 | 23.089 | 3399 | 3404 | 3409 | rBV5 | 15061 | 26122 | 1.39% | 0.293% |
| 20 | 24.816 | 3688 | 3698 | 3710 | rBV | 200785 | 601408 | 32.09% | 6.750% |

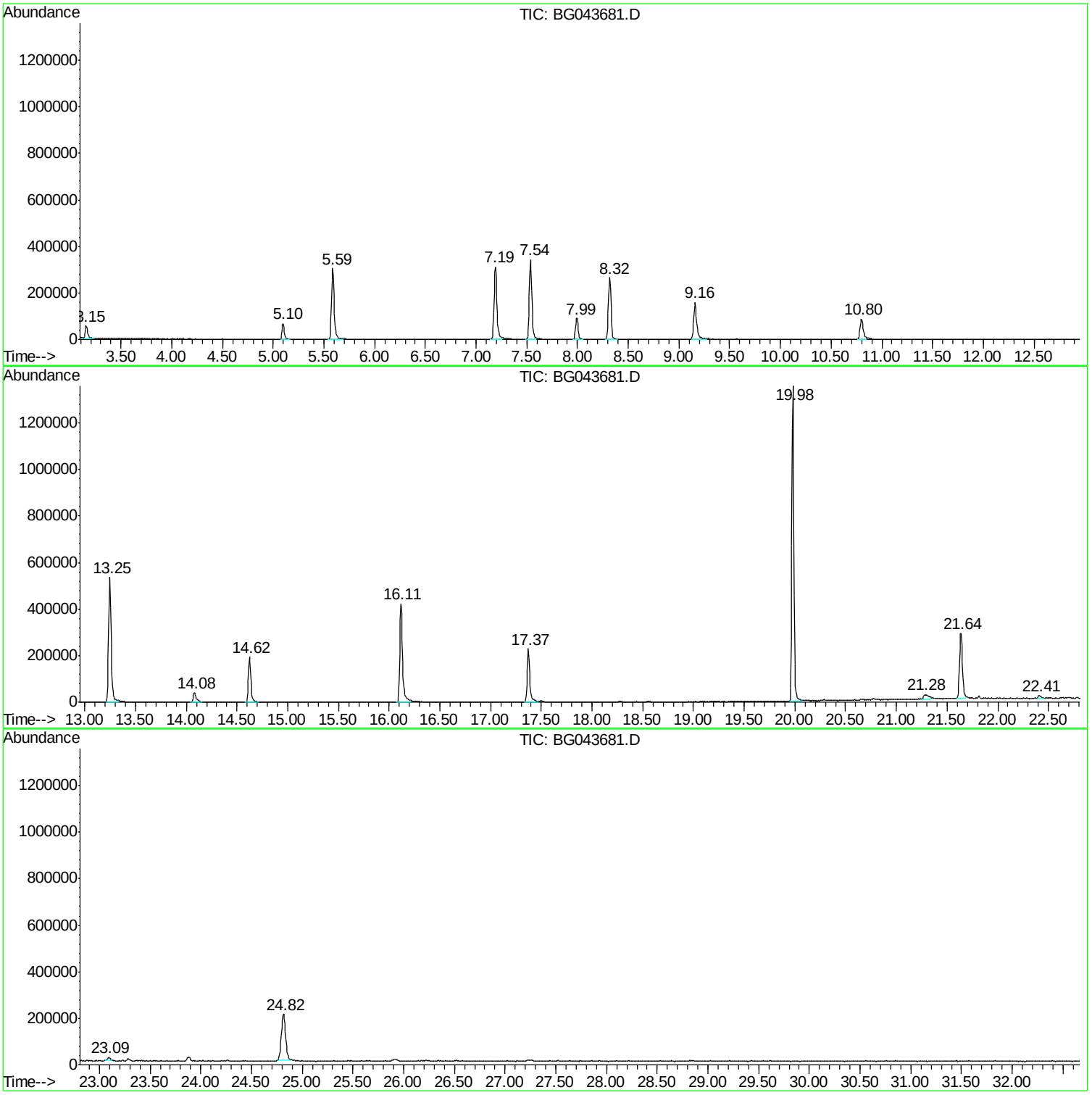
Sum of corrected areas: 8909756

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043681.D
Acq On : 18 Nov 2019 20:13
Operator : JU
Sample : K5833-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
8-(12-13)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043681.D
Acq On : 18 Nov 2019 20:13
Operator : JU
Sample : K5833-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 8-(12-13)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

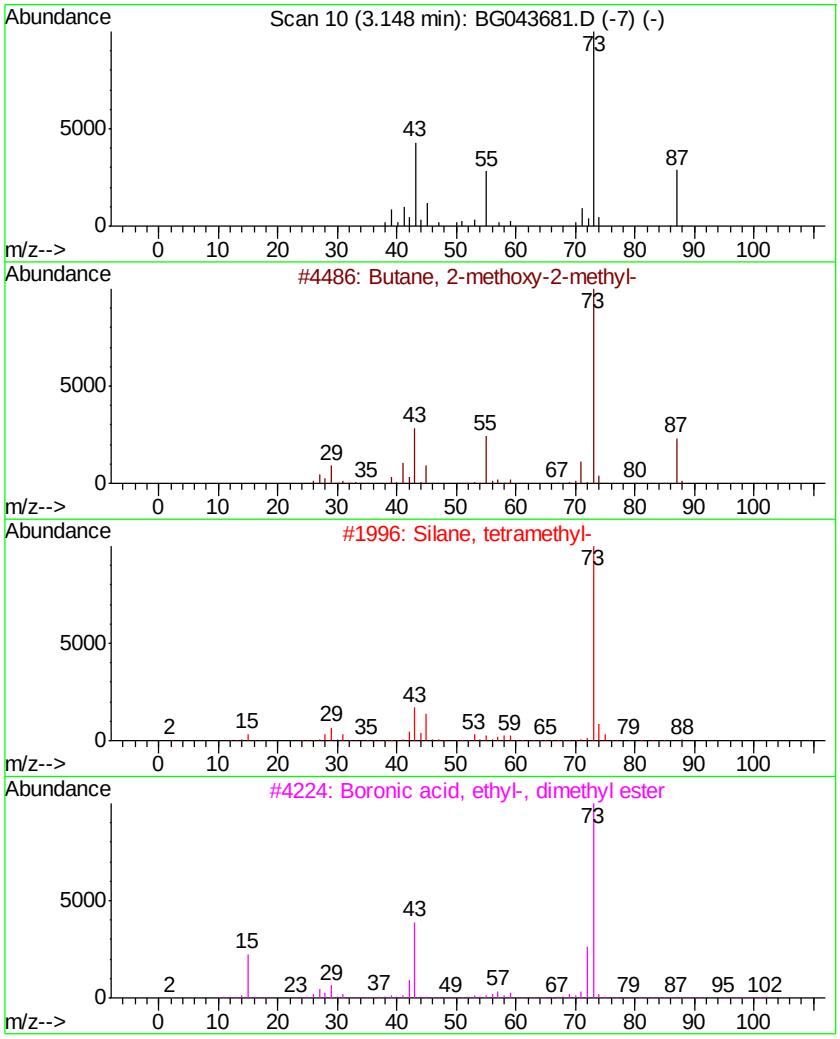
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

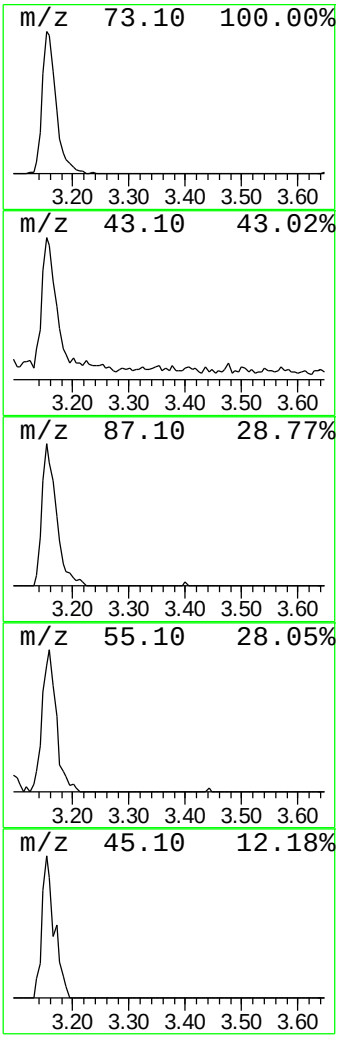
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.15 | 11.73 ng | 96121 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 72 |
| 2 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 32 |
| 3 | Boronic acid, ethyl-, dimethyl e... | 102 | C4H11BO2 | 007318-82-3 | 12 |
| 4 | Silane, ethyltrimethyl- | 102 | C5H14Si | 003439-38-1 | 9 |
| 5 | Acetic acid, 3-[1,3]dioxolan-2-y... | 174 | C8H14O4 | 1000186-02-3 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043681.D
Acq On : 18 Nov 2019 20:13
Operator : JU
Sample : K5833-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 8-(12-13)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

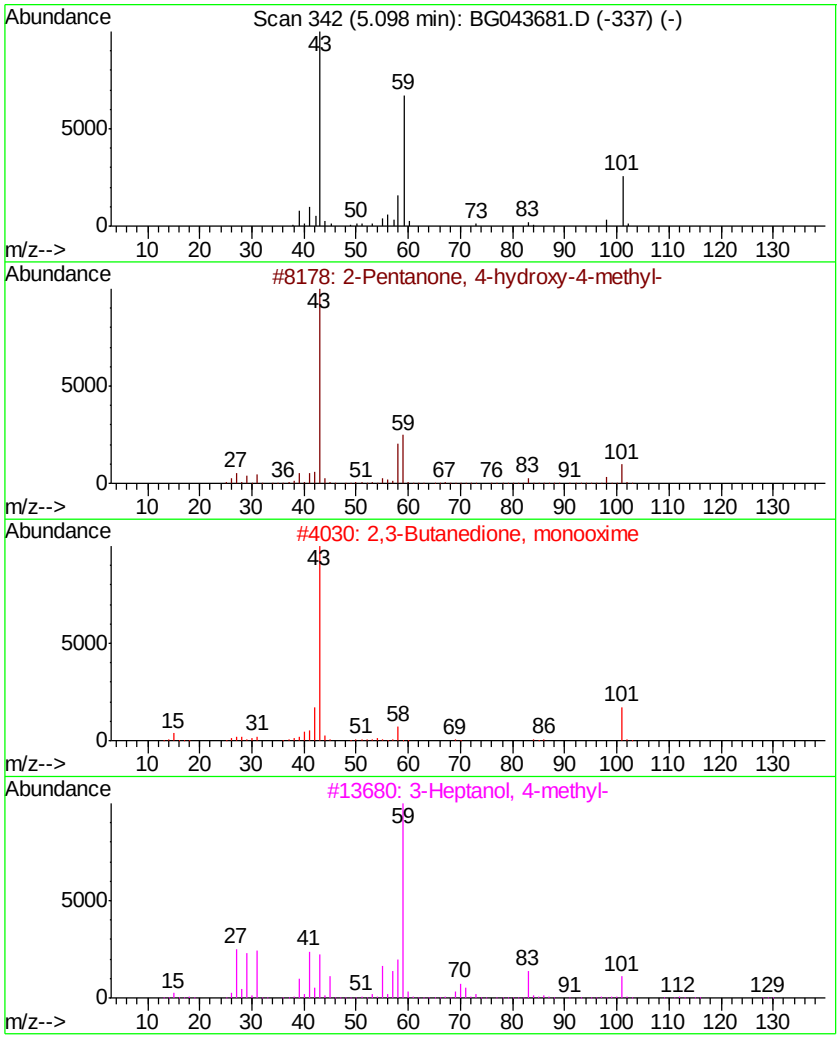
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

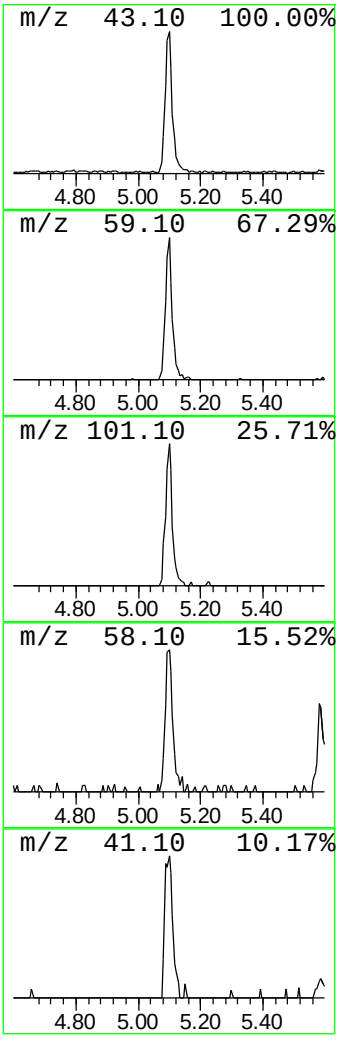
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.10 | 13.26 ng | 108654 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |
| 3 | 3-Heptanol, 4-methyl- | 130 | C8H18O | 014979-39-6 | 23 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043681.D
Acq On : 18 Nov 2019 20:13
Operator : JU
Sample : K5833-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 8-(12-13)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

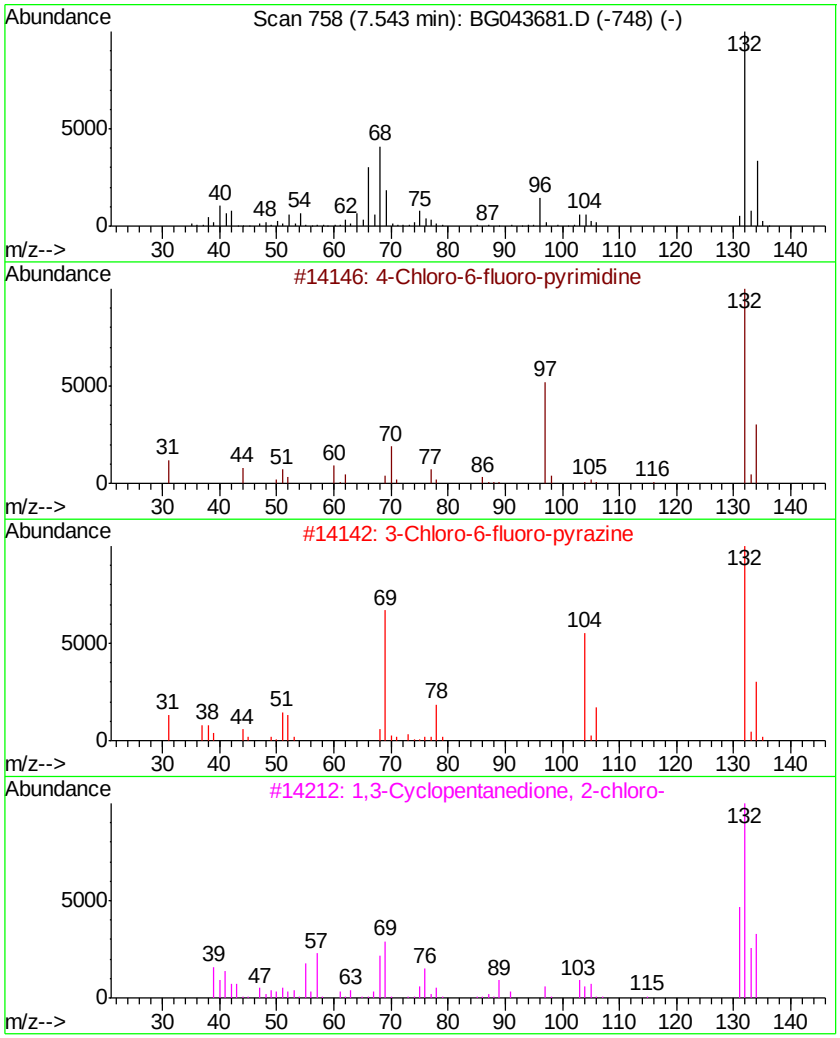
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

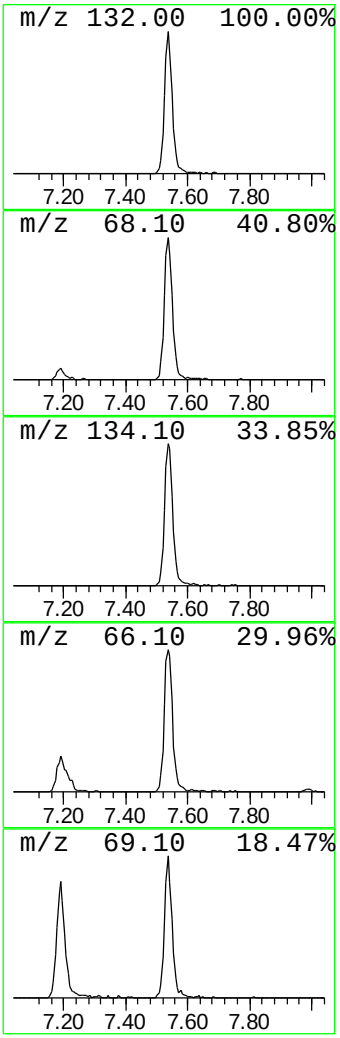
**********

Peak Number 3 unknown7.54 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.54 | 74.81 ng | 613231 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 3 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 13 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 12 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043681.D
Acq On : 18 Nov 2019 20:13
Operator : JU
Sample : K5833-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 8-(12-13)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

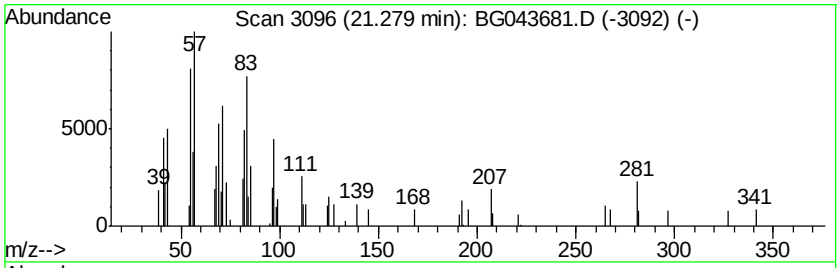
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

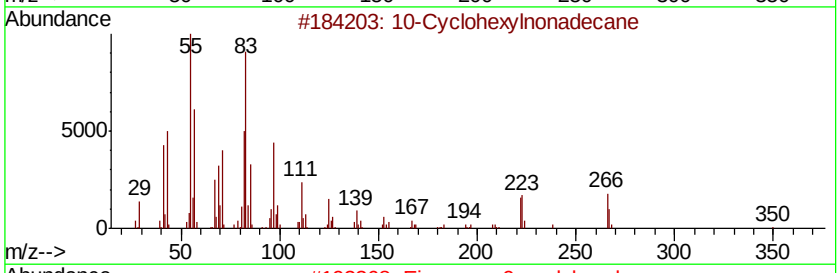
**********

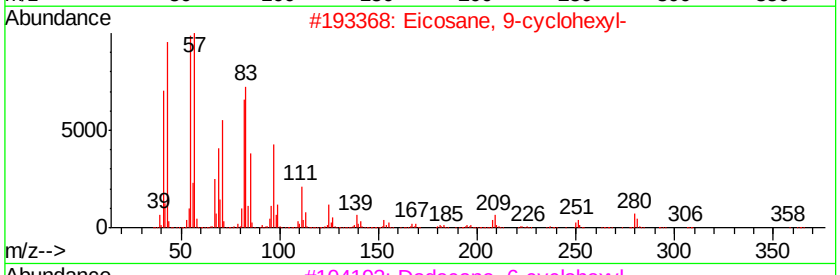
Peak Number 5 10-Cyclohexylnonadecane Concentration Rank 5

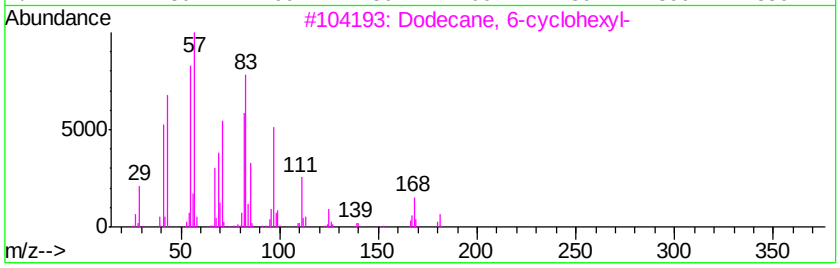
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.28 | 2.21 ng | 60621 | Chrysene-d12 | 21.64 |

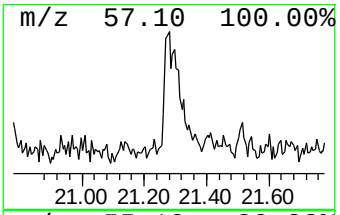
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 10-Cyclohexylnonadecane | 350 | C25H50 | 1000357-25-5 | 58 |
| 2 | Eicosane, 9-cyclohexyl- | 364 | C26H52 | 004443-61-2 | 58 |
| 3 | Dodecane, 6-cyclohexyl- | 252 | C18H36 | 013151-86-5 | 58 |
| 4 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 49 |
| 5 | 1-Hentetracontanol | 593 | C41H84O | 040710-42-7 | 46 |

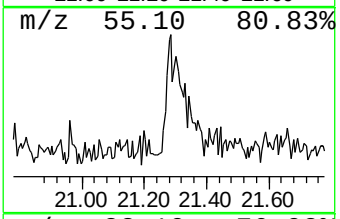


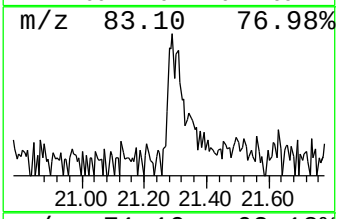



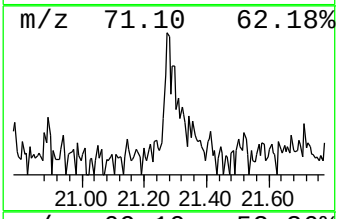



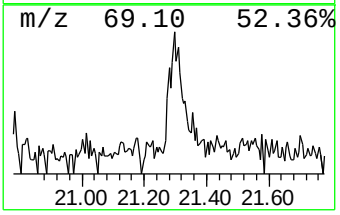



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111819\
Data File : BG043681.D
Acq On : 18 Nov 2019 20:13
Operator : JU
Sample : K5833-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 8-(12-13)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 3.15 | 11.7 | ng | 96121 | 1 | 7.99 | 163935 | 20.0 |
| 2-Pentanone, 4-hy... | 5.10 | 13.3 | ng | 108654 | 1 | 7.99 | 163935 | 20.0 |
| unknown7.54 | 7.54 | 74.8 | ng | 613231 | 1 | 7.99 | 163935 | 20.0 |
| 10-Cyclohexylnona... | 21.28 | 2.2 | ng | 60621 | 5 | 21.64 | 548443 | 20.0 |