LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044035.D
Acq On : 14 Jan 2020 13:54
Operator : JU
Sample : PB126078BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126078BL

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-BG123019.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 | 3.130 | 3 | 7 | 20 | rVB | 281759 | 477375 | 6.47% | 1.106% |
| 2 | 5.051 | 328 | 334 | 347 | rBV | 451220 | 709619 | 9.62% | 1.643% |
| 3 | 5.527 | 407 | 415 | 428 | rBV | 1943903 | 3223461 | 43.70% | 7.465% |
| 4 | 7.113 | 676 | 685 | 704 | rBV | 2055830 | 3701674 | 50.19% | 8.573% |
| 5 | 7.483 | 739 | 748 | 756 | rBV | 2088786 | 3651216 | 49.50% | 8.456% |
| 6 | 7.947 | 819 | 827 | 834 | rBV | 393988 | 675636 | 9.16% | 1.565% |
| 7 | 8.271 | 873 | 882 | 892 | rBV | 1598525 | 2813620 | 38.15% | 6.516% |
| 8 | 9.099 | 1016 | 1023 | 1041 | rBV | 1213396 | 2251924 | 30.53% | 5.215% |
| 9 | 10.744 | 1295 | 1303 | 1317 | rBV | 521589 | 974917 | 13.22% | 2.258% |
| 10 | 13.206 | 1714 | 1722 | 1734 | rBV | 3296789 | 5328592 | 72.25% | 12.340% |
| 11 | 14.029 | 1857 | 1862 | 1868 | rBV | 72855 | 111658 | 1.51% | 0.259% |
| 12 | 14.575 | 1948 | 1955 | 1965 | rBV2 | 857303 | 1398010 | 18.95% | 3.238% |
| 13 | 16.067 | 2201 | 2209 | 2230 | rBV | 2561251 | 4154742 | 56.33% | 9.622% |
| 14 | 17.319 | 2414 | 2422 | 2433 | rBV | 1016362 | 1610034 | 21.83% | 3.729% |
| 15 | 19.933 | 2861 | 2867 | 2882 | rBV | 5182065 | 7375618 | 100.00% | 17.081% |
| 16 | 21.238 | 3084 | 3089 | 3097 | rBV | 291609 | 475432 | 6.45% | 1.101% |
| 17 | 21.302 | 3097 | 3100 | 3112 | rVB | 60788 | 110602 | 1.50% | 0.256% |
| 18 | 21.567 | 3138 | 3145 | 3158 | rBV | 1048342 | 1690342 | 22.92% | 3.915% |
| 19 | 21.784 | 3177 | 3182 | 3187 | rVB | 54352 | 77437 | 1.05% | 0.179% |
| 20 | 22.378 | 3277 | 3283 | 3296 | rBV | 80726 | 164364 | 2.23% | 0.381% |
| 21 | 23.053 | 3392 | 3398 | 3406 | rBV | 84683 | 161464 | 2.19% | 0.374% |
| 22 | 23.835 | 3525 | 3531 | 3540 | rVB2 | 82099 | 173121 | 2.35% | 0.401% |
| 23 | 24.681 | 3664 | 3675 | 3684 | rBV2 | 596932 | 1720015 | 23.32% | 3.983% |
| 24 | 25.850 | 3867 | 3874 | 3885 | rVB4 | 51302 | 148861 | 2.02% | 0.345% |

Sum of corrected areas: 43179734

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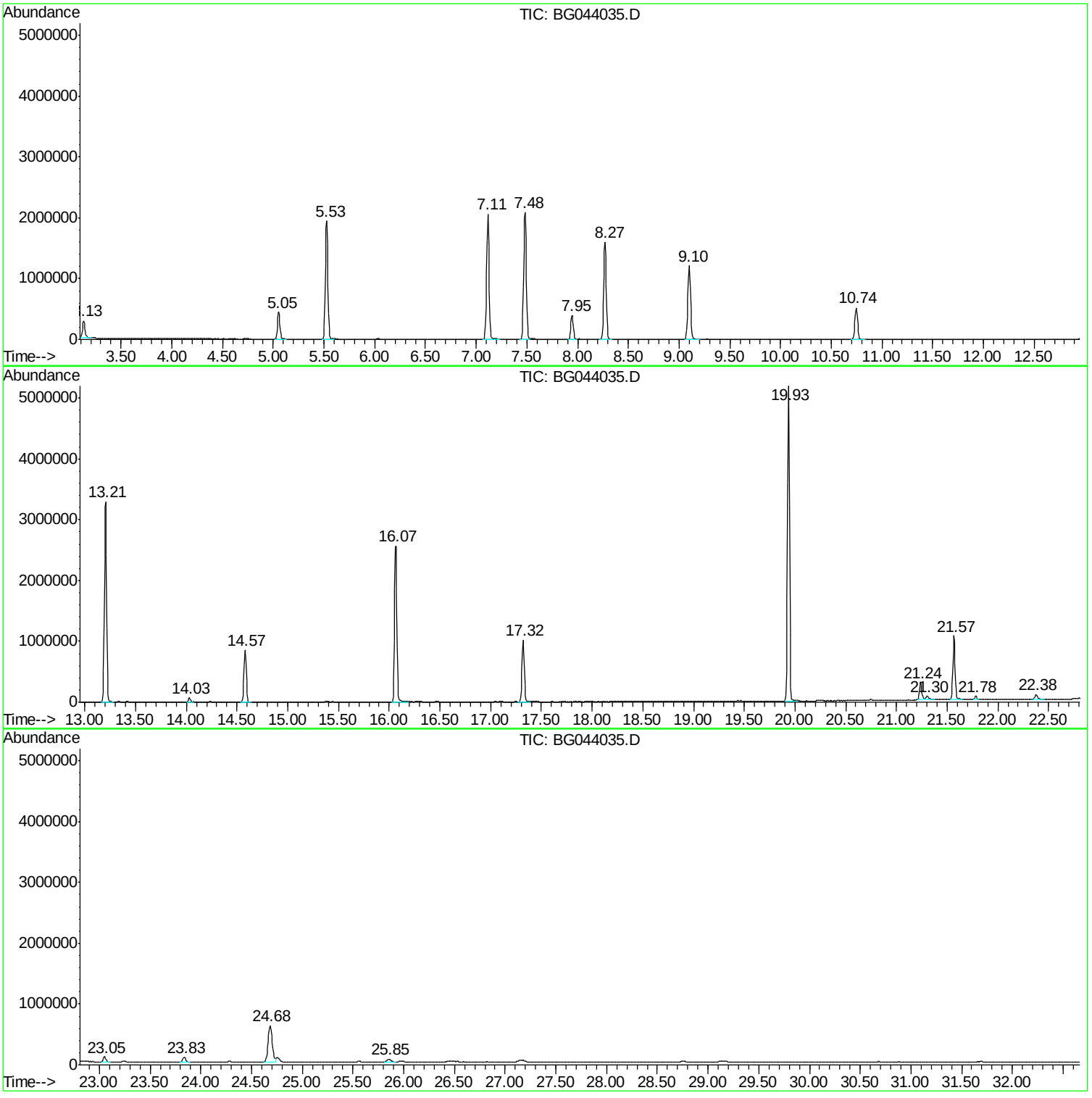
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
PB126078BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044035.D
Acq On : 14 Jan 2020 13:54
Operator : JU
Sample : PB126078BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126078BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

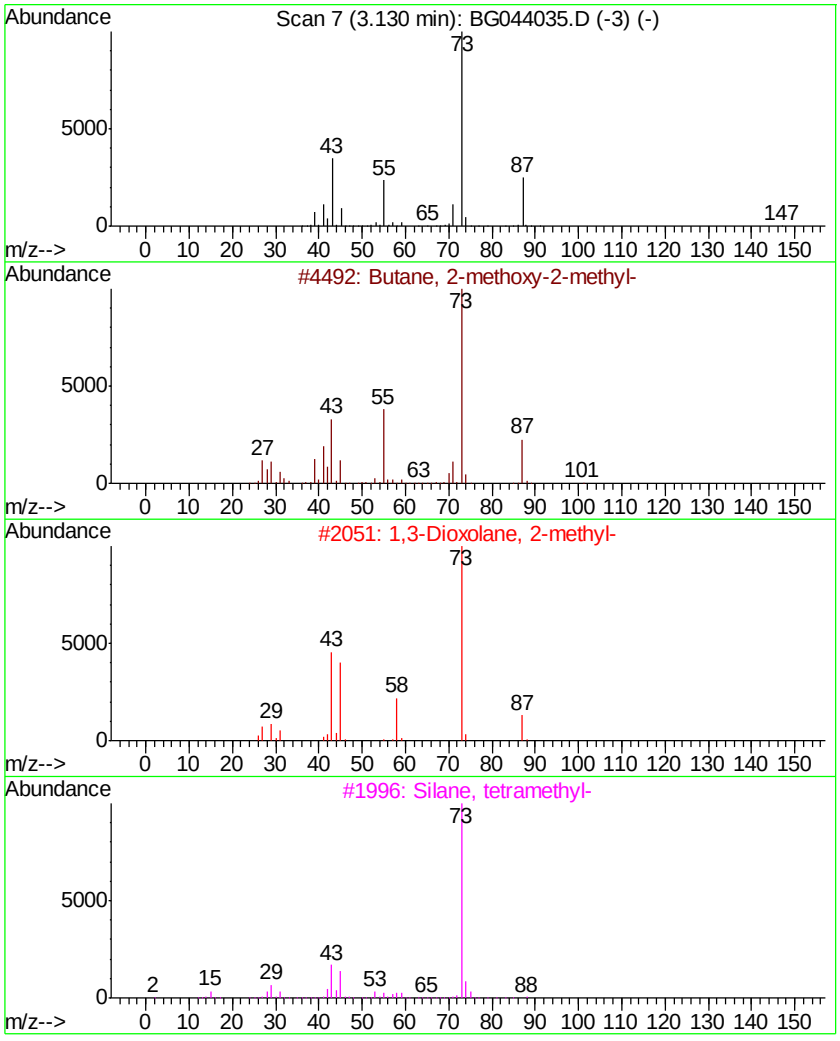
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

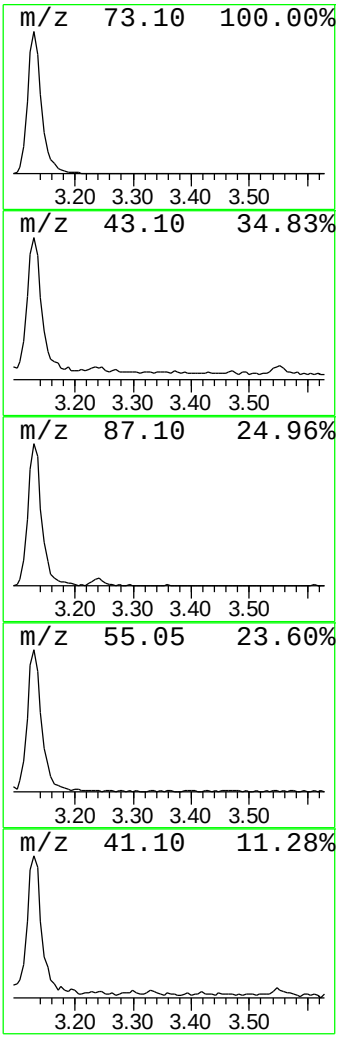
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.13 | 14.13 ng | 477375 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 25 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 10 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044035.D
Acq On : 14 Jan 2020 13:54
Operator : JU
Sample : PB126078BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126078BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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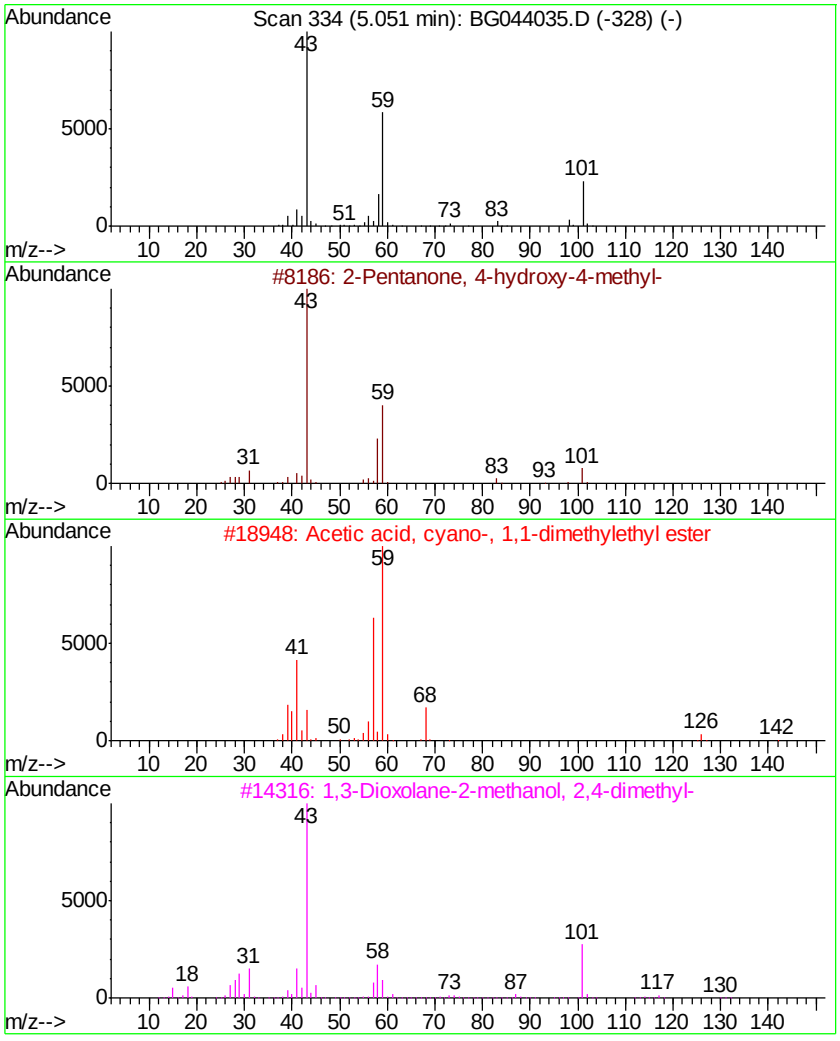
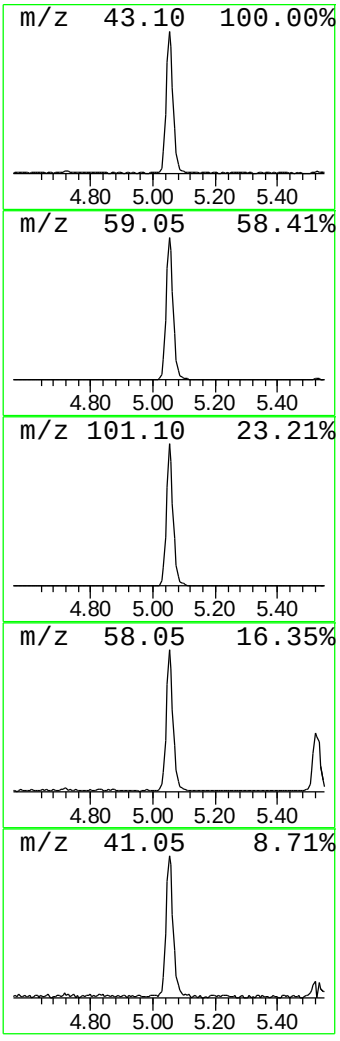
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.05 | 21.01 ng | 709619 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |
| 3 | 1,3-Dioxolane-2-methanol, 2,4-di... | 132 | C6H12O3 | 053951-43-2 | 28 |
| 4 | Tetraglyme | 222 | C10H22O5 | 000143-24-8 | 25 |
| 5 | 2,5,8,11-Tetraoxadodecane | 178 | C8H18O4 | 000112-49-2 | 23 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044035.D
Acq On : 14 Jan 2020 13:54
Operator : JU
Sample : PB126078BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126078BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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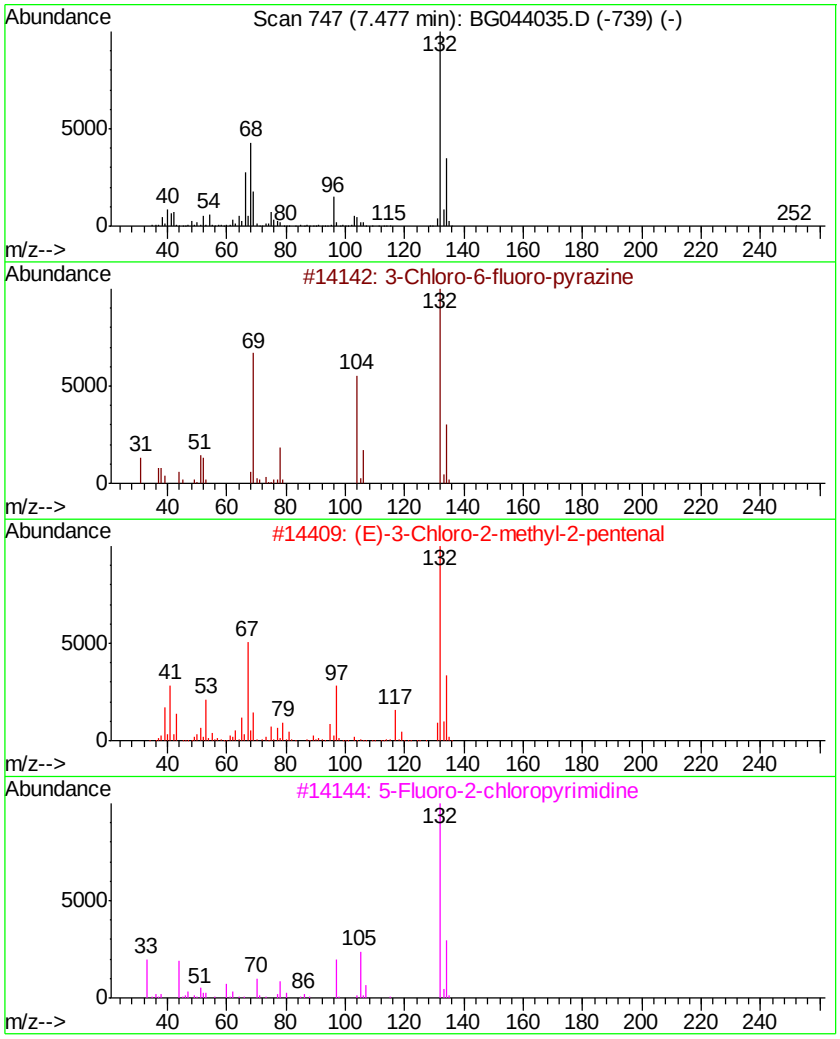
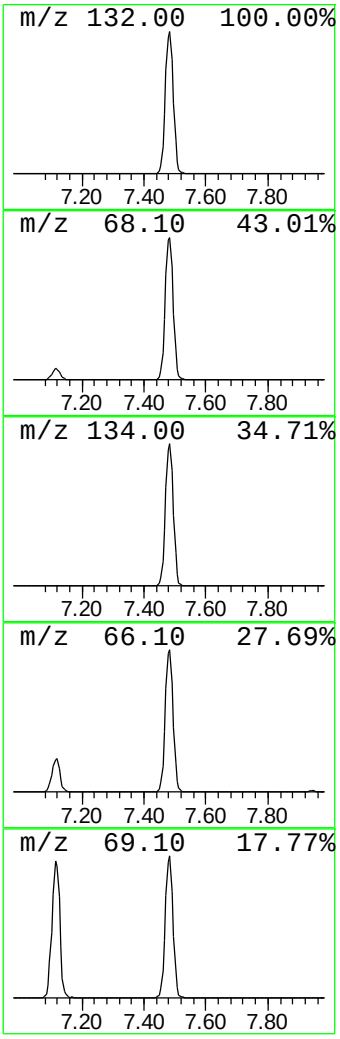
Peak Number 3 unknown7.48 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.48 | 108.08 ng | 3651220 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 12 |
| 5 | 1-Isoquinolinemethanol, .alpha.-... | 191 | C12H17NO | 114608-92-3 | 12 |



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Data File : BG044035.D
Acq On : 14 Jan 2020 13:54
Operator : JU
Sample : PB126078BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126078BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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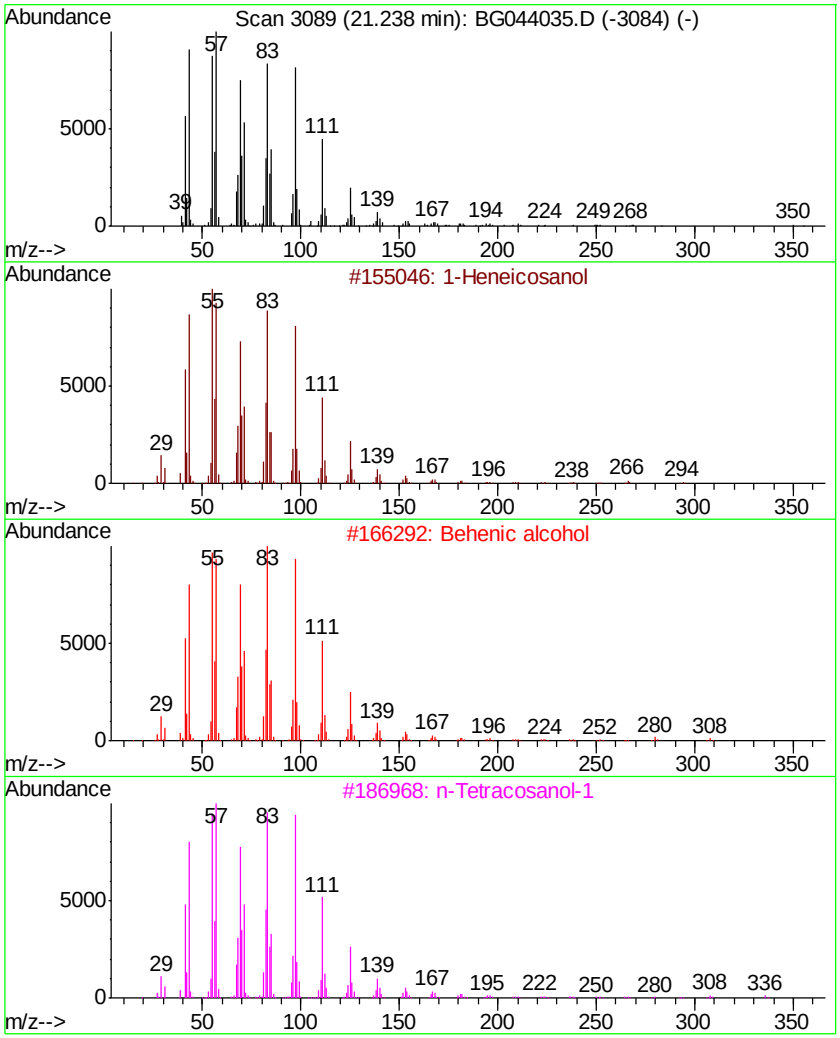
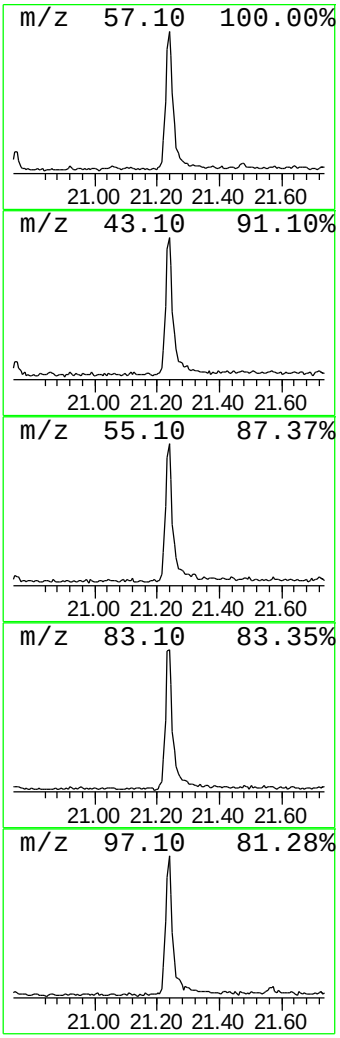
Peak Number 5 1-Heneicosanol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.24 | 5.63 ng | 475432 | Chrysene-d12 | 21.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 2 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 93 |
| 4 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 91 |
| 5 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 91 |



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Data File : BG044035.D
Acq On : 14 Jan 2020 13:54
Operator : JU
Sample : PB126078BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126078BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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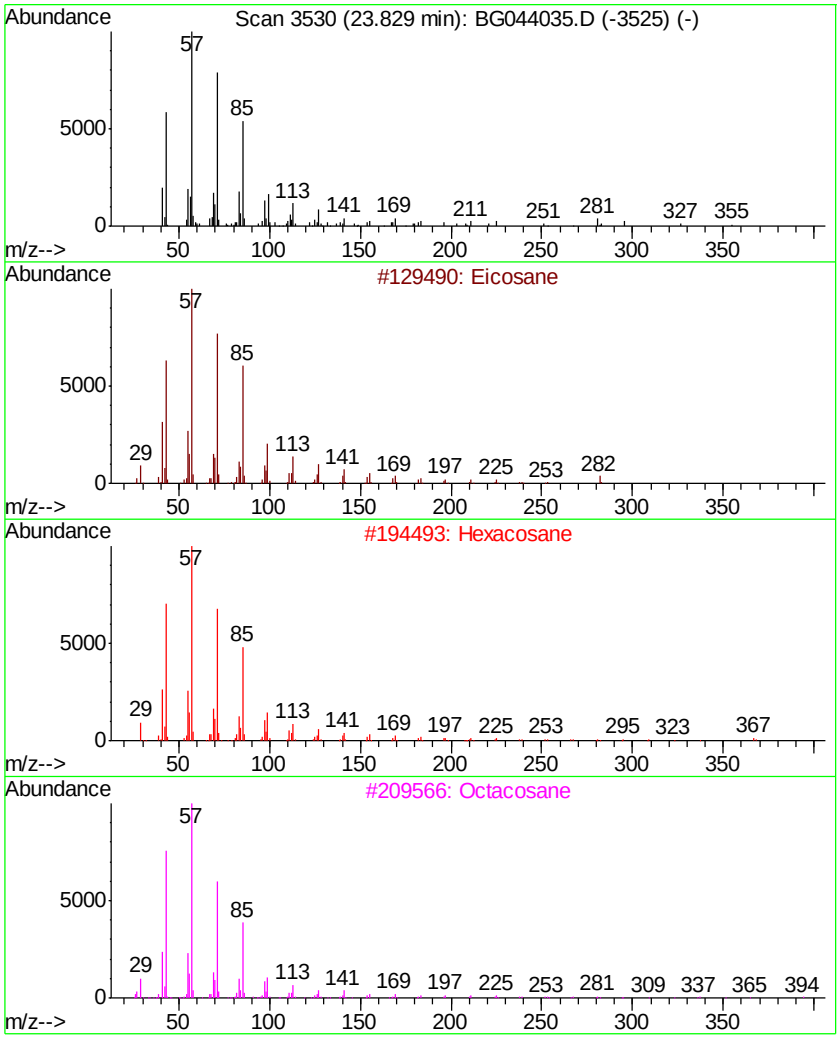
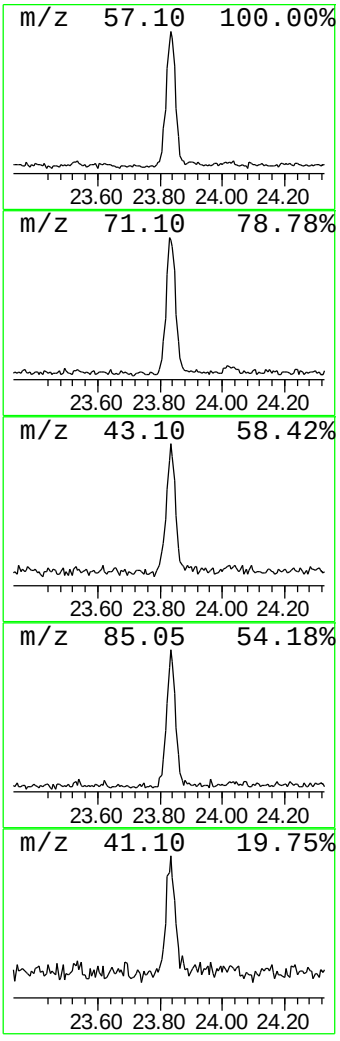
Peak Number 6 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.83 | 2.01 ng | 173121 | Perylene-d12 | 24.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 97 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 4 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |



Tentatively Identified Compound (LSC) summary

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Data File : BG044035.D
Acq On : 14 Jan 2020 13:54
Operator : JU
Sample : PB126078BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126078BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
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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... | 3.13 | 14.1 | ng | 477375 | 1 | 7.95 | 675636 | 20.0 |
| 2-Pentanone, 4-hy... | 5.05 | 21.0 | ng | 709619 | 1 | 7.95 | 675636 | 20.0 |
| unknown7.48 | 7.48 | 108.1 | ng | 3651220 | 1 | 7.95 | 675636 | 20.0 |
| 1-Heneicosanol | 21.24 | 5.6 | ng | 475432 | 5 | 21.57 | 1690340 | 20.0 |
| Eicosane | 23.83 | 2.0 | ng | 173121 | 6 | 24.69 | 1720020 | 20.0 |