# LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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 | 5.036 | 326 | 331 | 339 | rVB | 95797 | 141726 | 2.58% | 0.465% |
| 2 | 5.512 | 404 | 412 | 427 | rBV | 702136 | 1166340 | 21.21% | 3.826% |
| 3 | 7.104 | 674 | 683 | 694 | rBV | 455957 | 880397 | 16.01% | 2.888% |
| 4 | 7.468 | 736 | 745 | 754 | rBV | 1354932 | 2355248 | 42.83% | 7.726% |
| 5 | 7.932 | 817 | 824 | 831 | rBV | 256429 | 429782 | 7.82% | 1.410% |
| 6 | 8.256 | 870 | 879 | 888 | rBV | 1084120 | 1883329 | 34.25% | 6.178% |
| 7 | 9.090 | 1010 | 1021 | 1033 | rBV | 861234 | 1608363 | 29.25% | 5.276% |
| 8 | 10.382 | 1235 | 1241 | 1250 | rBV | 76033 | 115769 | 2.11% | 0.380% |
| 9 | 10.735 | 1291 | 1301 | 1314 | rBV | 361084 | 665845 | 12.11% | 2.184% |
| 10 | 13.191 | 1711 | 1719 | 1734 | rBV | 2568894 | 4091595 | 74.40% | 13.421% |
| 11 | 14.019 | 1854 | 1860 | 1872 | rBV | 155175 | 253441 | 4.61% | 0.831% |
| 12 | 14.566 | 1944 | 1953 | 1968 | rBV | 665068 | 1072571 | 19.50% | 3.518% |
| 13 | 16.058 | 2199 | 2207 | 2223 | rBV | 2174207 | 3420219 | 62.19% | 11.219% |
| 14 | 17.310 | 2413 | 2420 | 2429 | rBV | 793065 | 1227399 | 22.32% | 4.026% |
| 15 | 17.985 | 2529 | 2535 | 2540 | rBV2 | 60483 | 82189 | 1.49% | 0.270% |
| 16 | 19.713 | 2826 | 2829 | 2833 | rBV | 57027 | 69914 | 1.27% | 0.229% |
| 17 | 19.930 | 2859 | 2866 | 2871 | rBV | 3888571 | 5499445 | 100.00% | 18.039% |
| 18 | 20.247 | 2916 | 2920 | 2925 | rVB | 94724 | 108795 | 1.98% | 0.357% |
| 19 | 20.735 | 3000 | 3003 | 3008 | rVB | 79840 | 95413 | 1.73% | 0.313% |
| 20 | 21.229 | 3082 | 3087 | 3107 | rBV | 487500 | 903735 | 16.43% | 2.964% |
| 21 | 21.558 | 3137 | 3143 | 3152 | rBV2 | 767454 | 1233678 | 22.43% | 4.047% |
| 22 | 21.769 | 3175 | 3179 | 3187 | rVB | 122043 | 180214 | 3.28% | 0.591% |
| 23 | 22.363 | 3275 | 3280 | 3294 | rVB | 161051 | 304849 | 5.54% | 1.000% |
| 24 | 23.032 | 3389 | 3394 | 3401 | rVB | 181870 | 338987 | 6.16% | 1.112% |
| 25 | 23.220 | 3423 | 3426 | 3431 | rVB2 | 41848 | 67759 | 1.23% | 0.222% |
| 26 | 23.814 | 3521 | 3527 | 3535 | rBV | 166877 | 348346 | 6.33% | 1.143% |
| 27 | 24.666 | 3662 | 3672 | 3679 | rBV2 | 458293 | 1295065 | 23.55% | 4.248% |
| 28 | 24.736 | 3679 | 3684 | 3693 | rVB2 | 142189 | 336197 | 6.11% | 1.103% |
| 29 | 25.829 | 3862 | 3870 | 3881 | rVB4 | 101152 | 309004 | 5.62% | 1.014% |

Sum of corrected areas: 30485614

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
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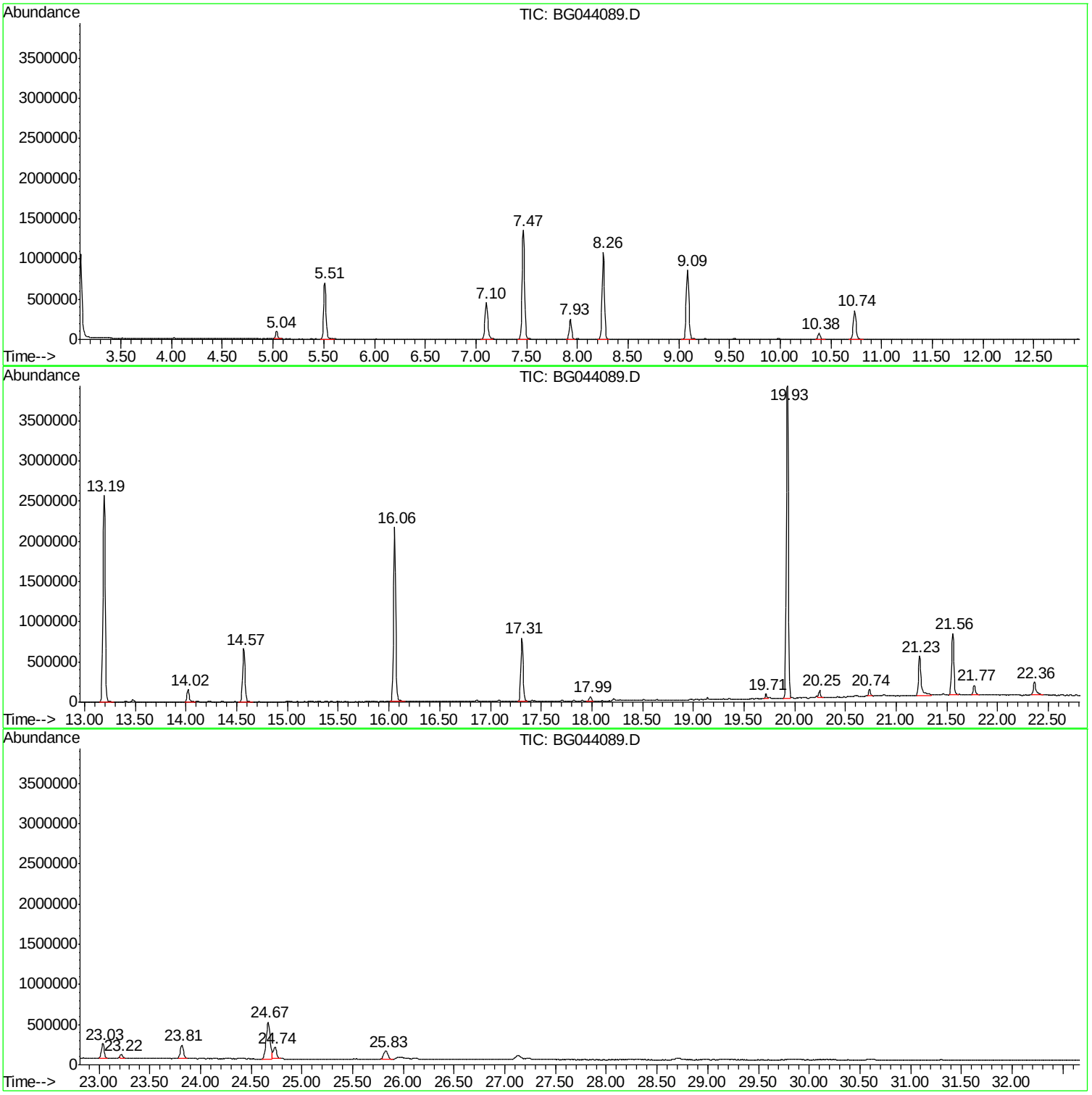
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
CBH-591

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

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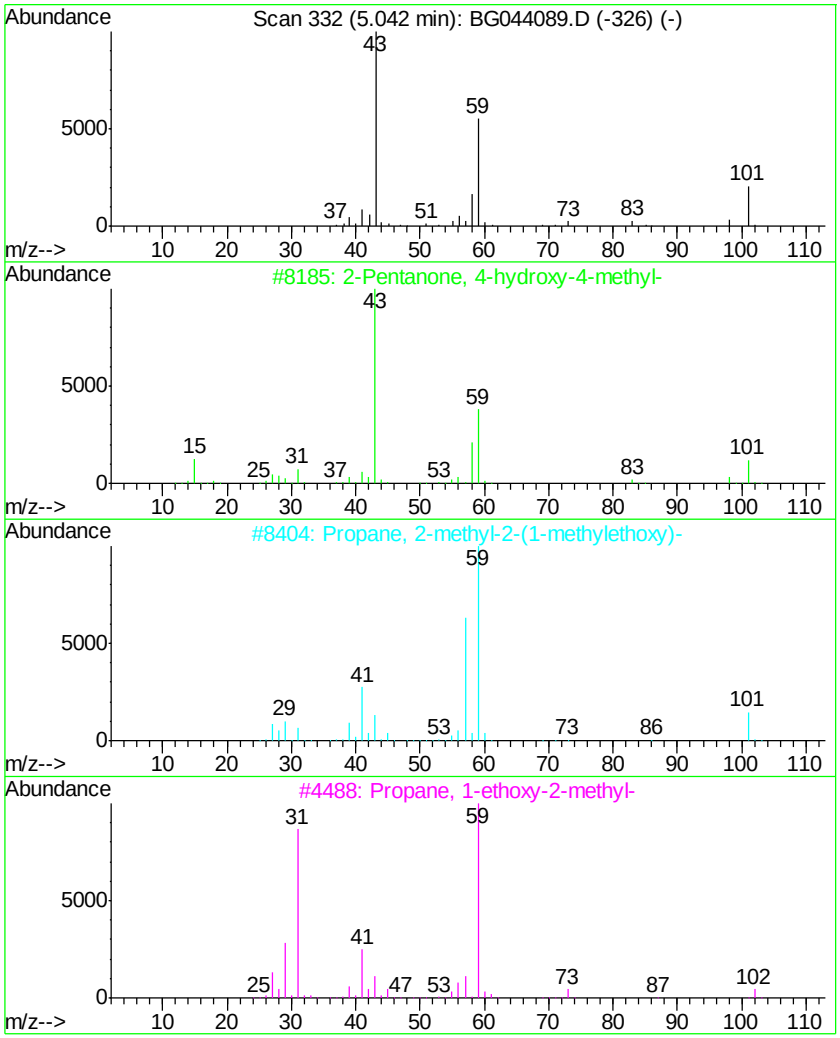
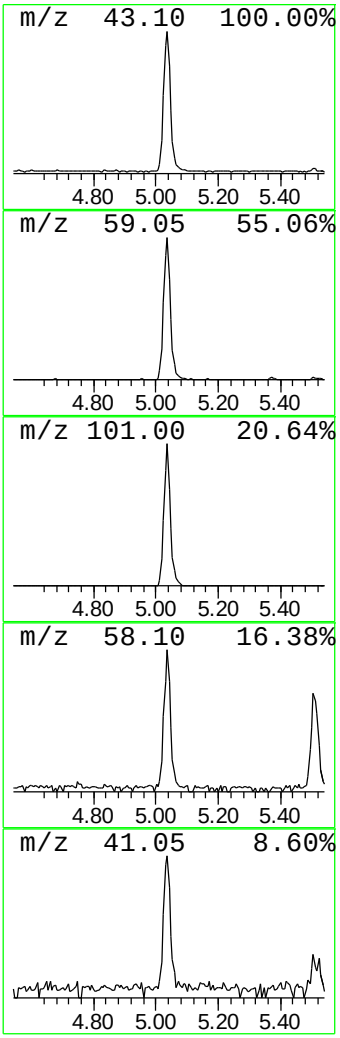
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.04 | 6.60 ng | 141726 | 1,4-Dichlorobenzene-d4 | 7.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 33 |
| 3 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 32 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 5 | Propane, 2-ethoxy-2-methyl- | 102 | C6H14O | 000637-92-3 | 17 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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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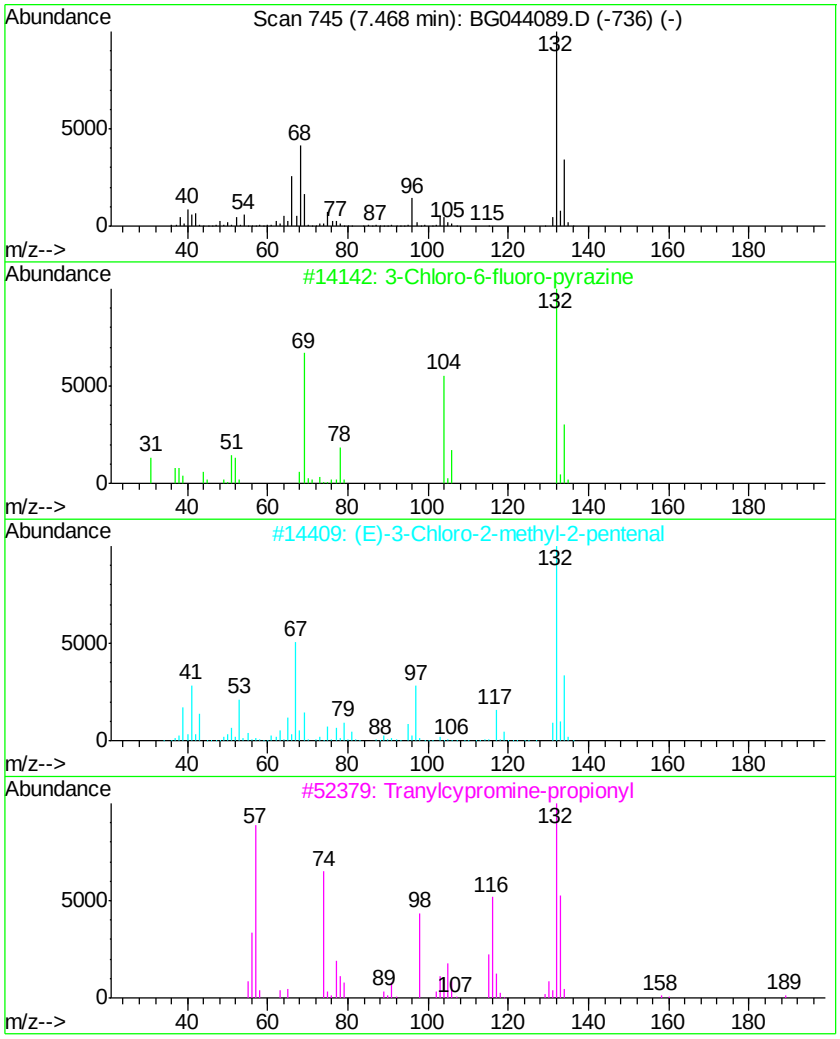
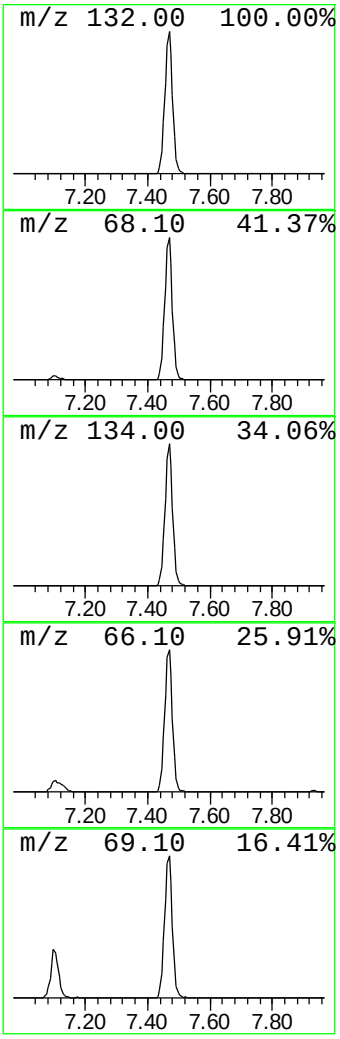
Peak Number 2 unknown7.47 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.47 | 109.60 ng | 2355250 | 1,4-Dichlorobenzene-d4 | 7.93 |

| 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 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



Library Search Compound Report

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Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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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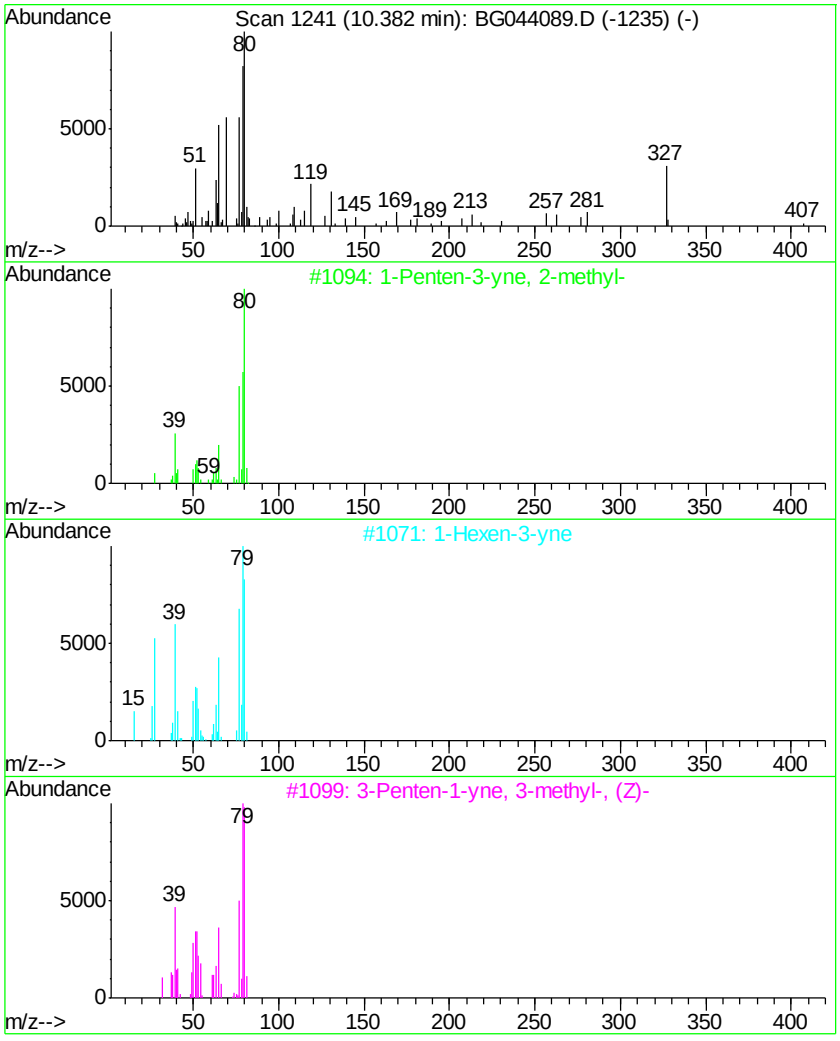
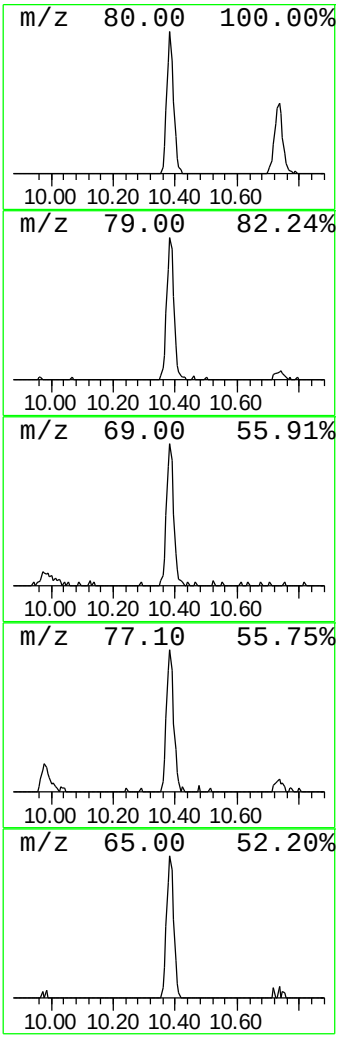
Peak Number 4 1-Penten-3-yne, 2-methyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.38 | 3.48 ng | 115769 | Naphthalene-d8 | 10.73 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Penten-3-yne, 2-methyl- | 80 | C6H8 | 000926-55-6 | 56 |
| 2 | 1-Hexen-3-yne | 80 | C6H8 | 013721-54-5 | 56 |
| 3 | 3-Penten-1-yne, 3-methyl-, (Z)- | 80 | C6H8 | 014272-81-2 | 47 |
| 4 | 3-Penten-1-yne, 3-methyl- | 80 | C6H8 | 001574-33-0 | 47 |
| 5 | Bicyclo[3.2.0]hept-2-ene, 2-methyl- | 108 | C8H12 | 094122-58-4 | 43 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
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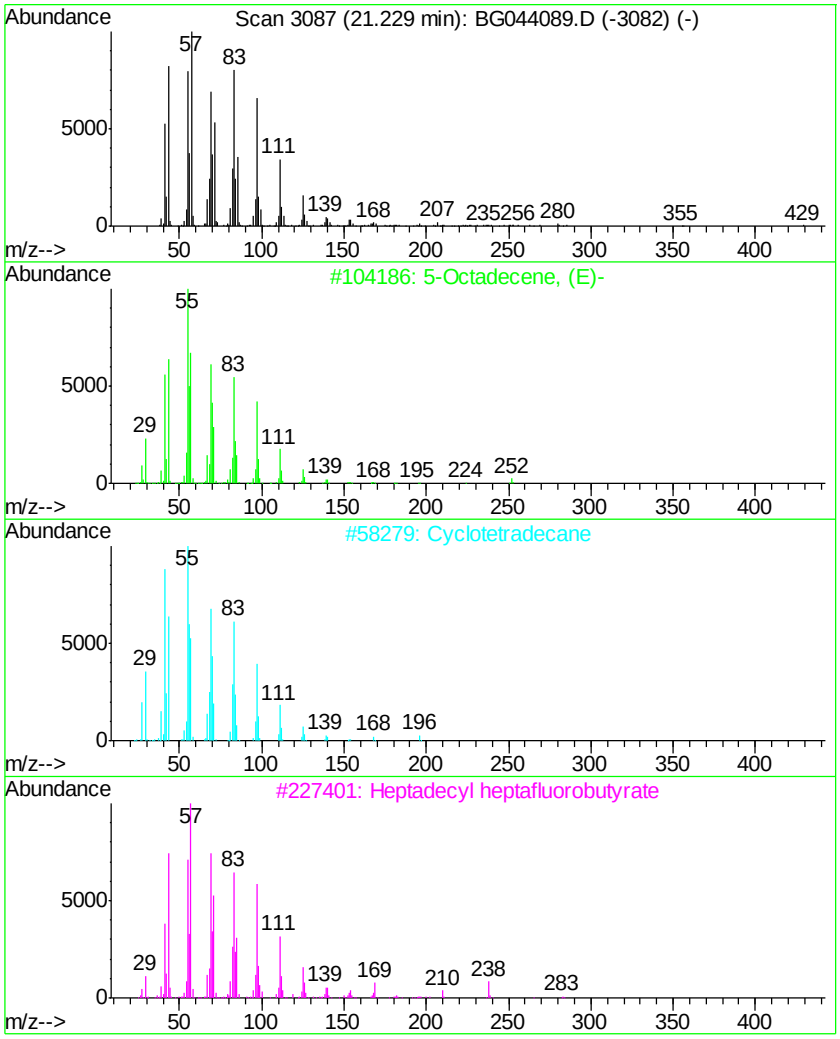
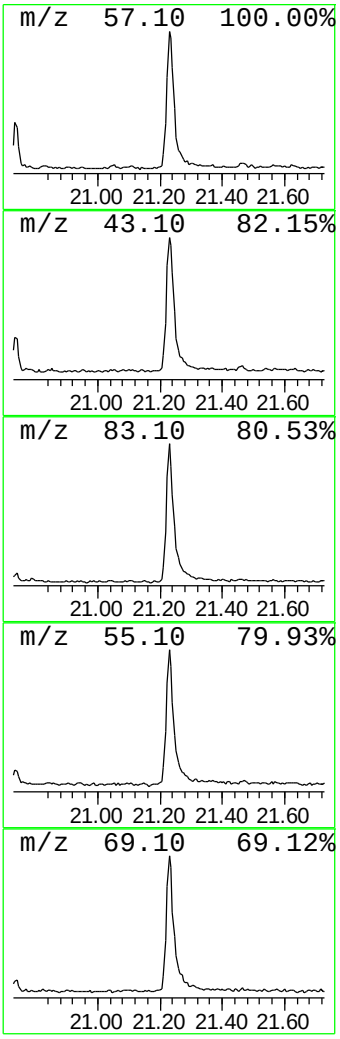
Peak Number 5 5-Octadecene, (E)- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.23 | 14.65 ng | 903735 | Chrysene-d12 | 21.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Octadecene, (E)- | 252 | C18H36 | 007206-21-5 | 95 |
| 2 | Cyclotetradecane | 196 | C14H28 | 000295-17-0 | 95 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 4 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 94 |
| 5 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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
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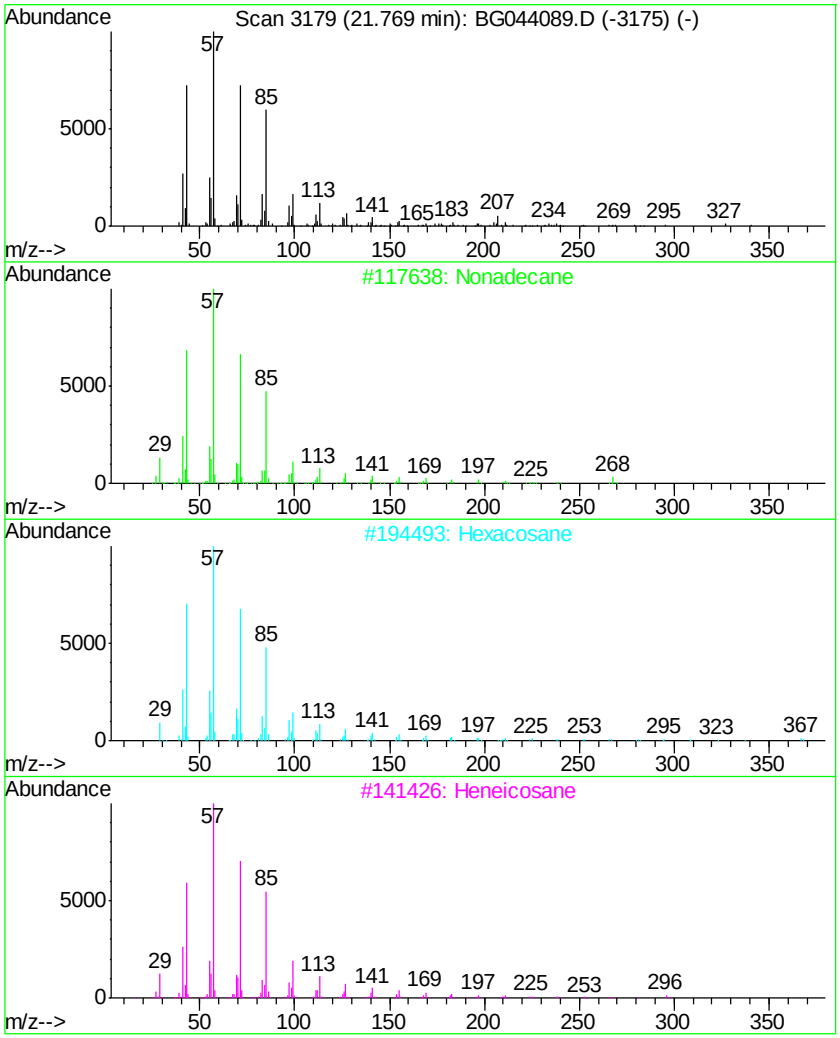
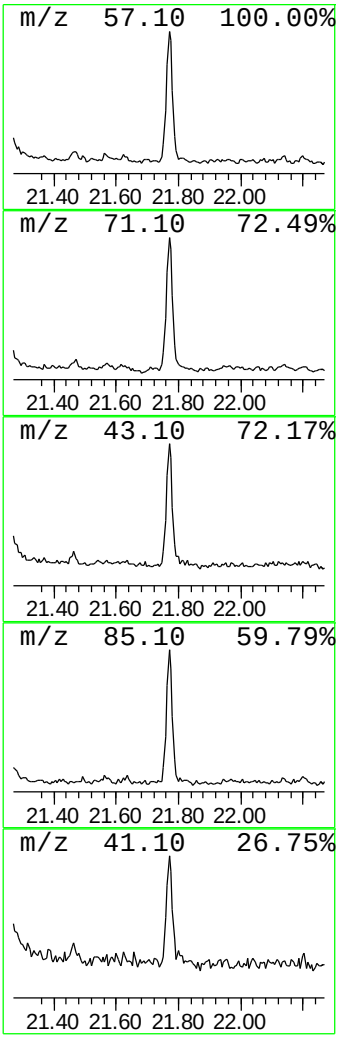
Peak Number 6 Nonadecane Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.77 | 2.92 ng | 180214 | Chrysene-d12 | 21.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecane | 268 | C19H40 | 000629-92-5 | 93 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 76 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 68 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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

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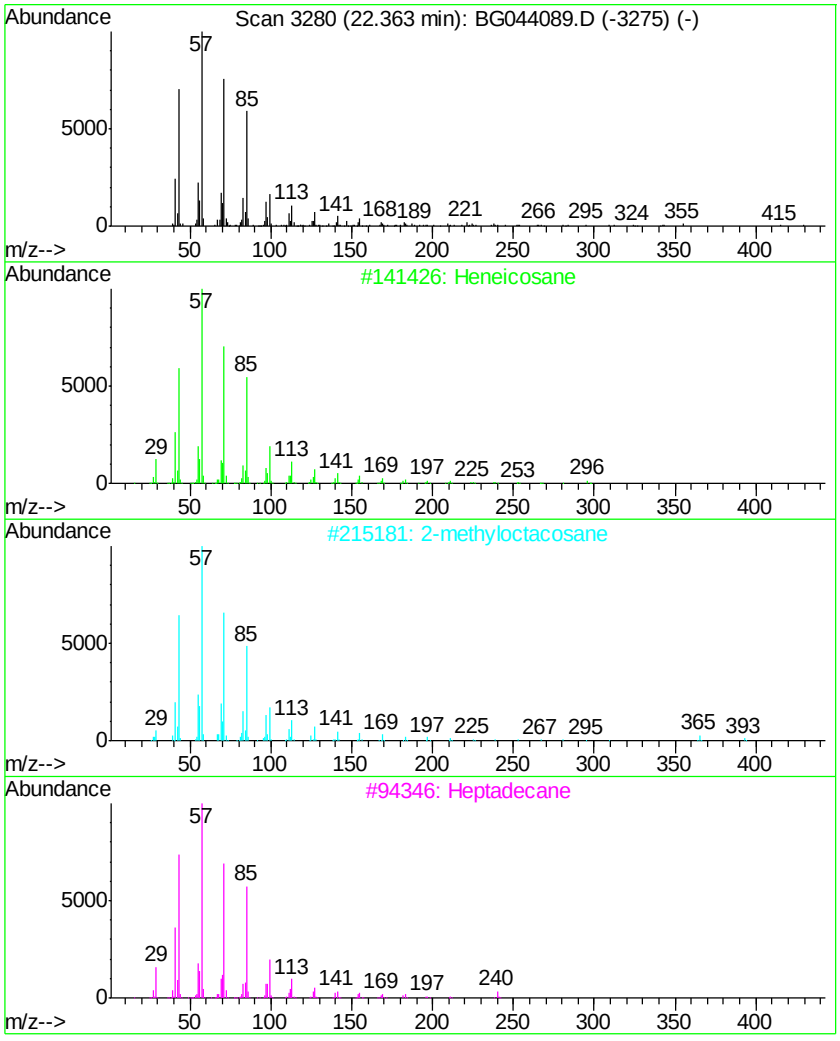
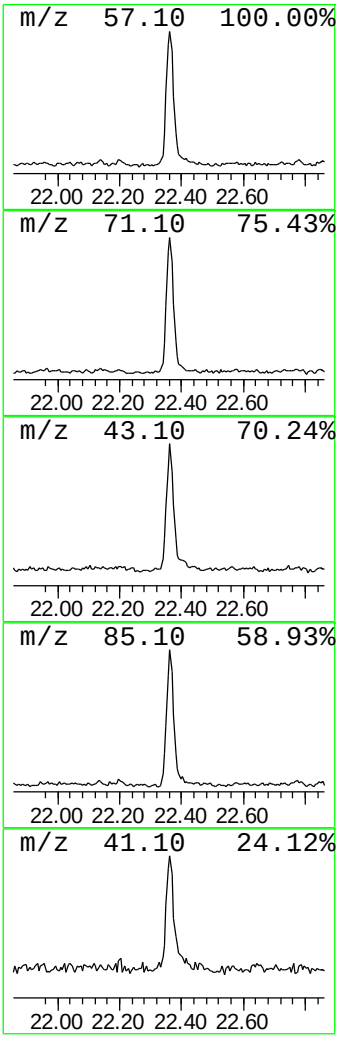
Peak Number 7 Heneicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.36 | 4.94 ng | 304849 | Chrysene-d12 | 21.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |



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Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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**ClientSampleId :** CBH-591

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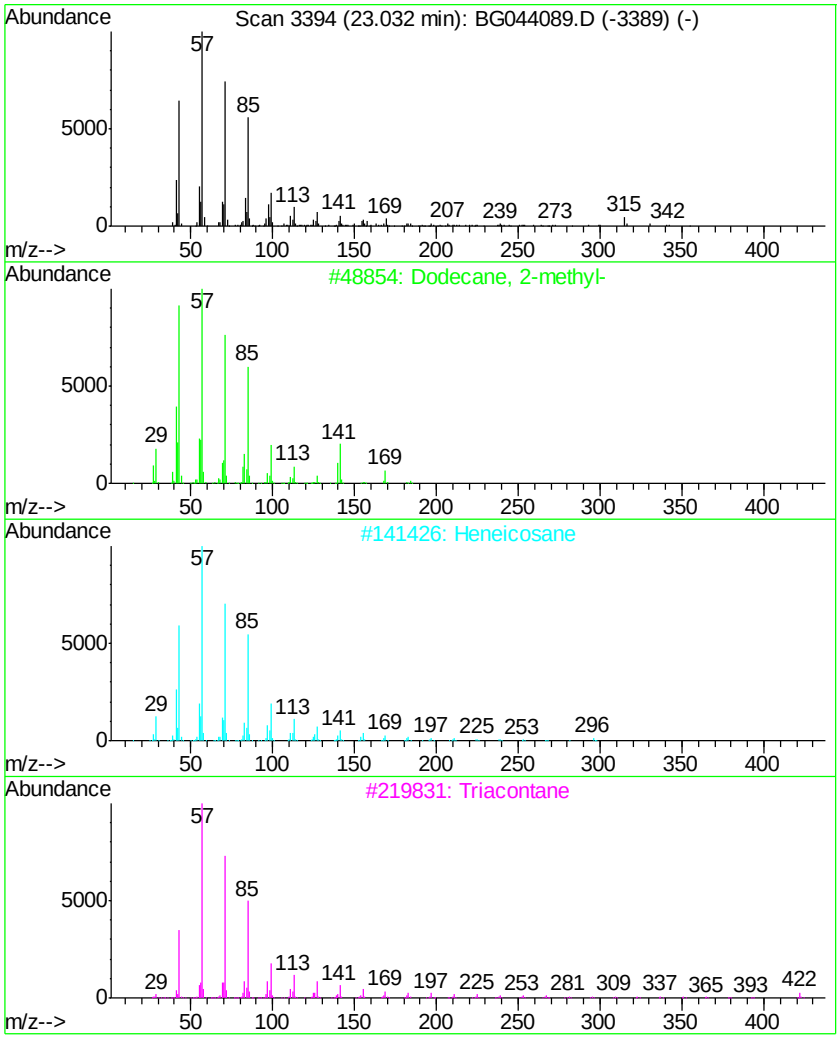
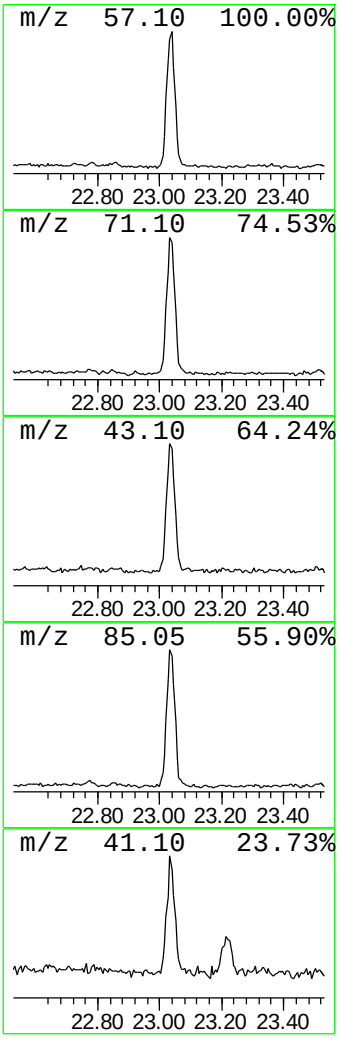
Peak Number 8 Dodecane, 2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.03 | 5.50 ng | 338987 | Chrysene-d12 | 21.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecane, 2-methyl- | 184 | C13H28 | 001560-97-0 | 90 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 3 | Triacontane | 422 | C30H62 | 000638-68-6 | 87 |
| 4 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 5 | Docosane, 7-hexyl- | 394 | C28H58 | 055373-86-9 | 86 |



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ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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TIC Library : C:\Database\NIST11.L
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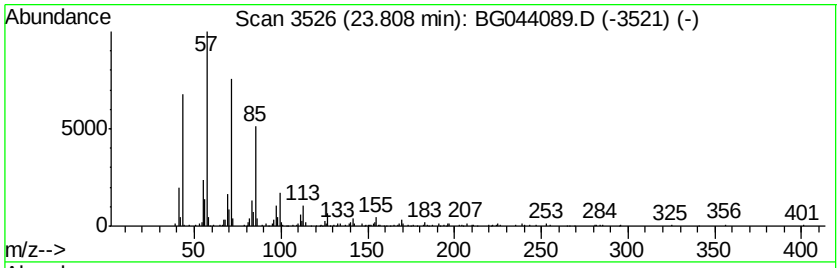
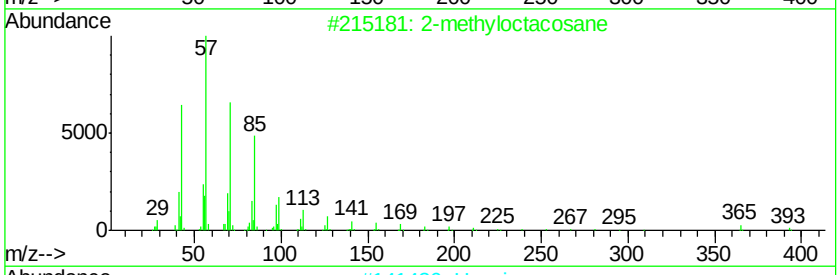
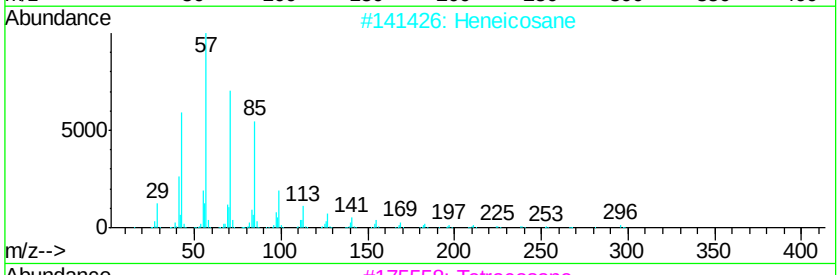
Peak Number 9 2-methyloctacosane Concentration Rank 6

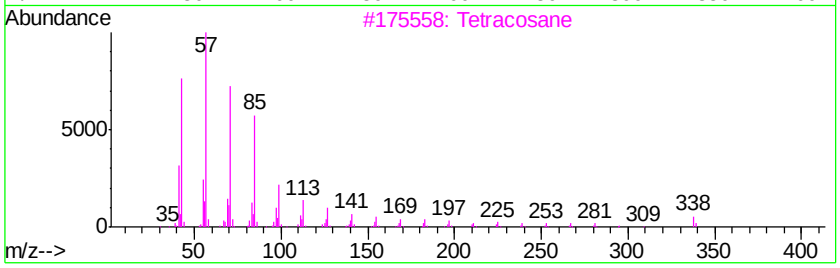
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.81 | 5.38 ng | 348346 | Perylene-d12 | 24.67 |

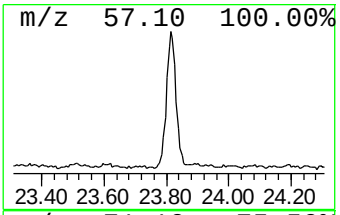
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 4 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 90 |
| 5 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 86 |

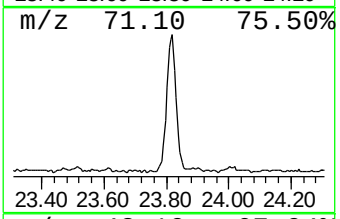


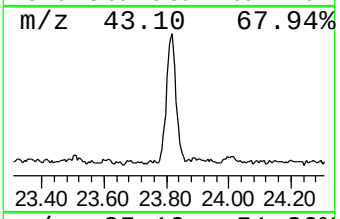



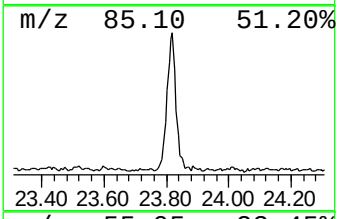



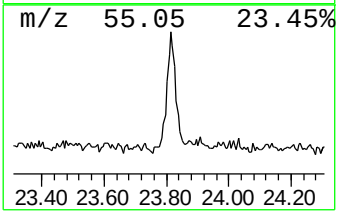



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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

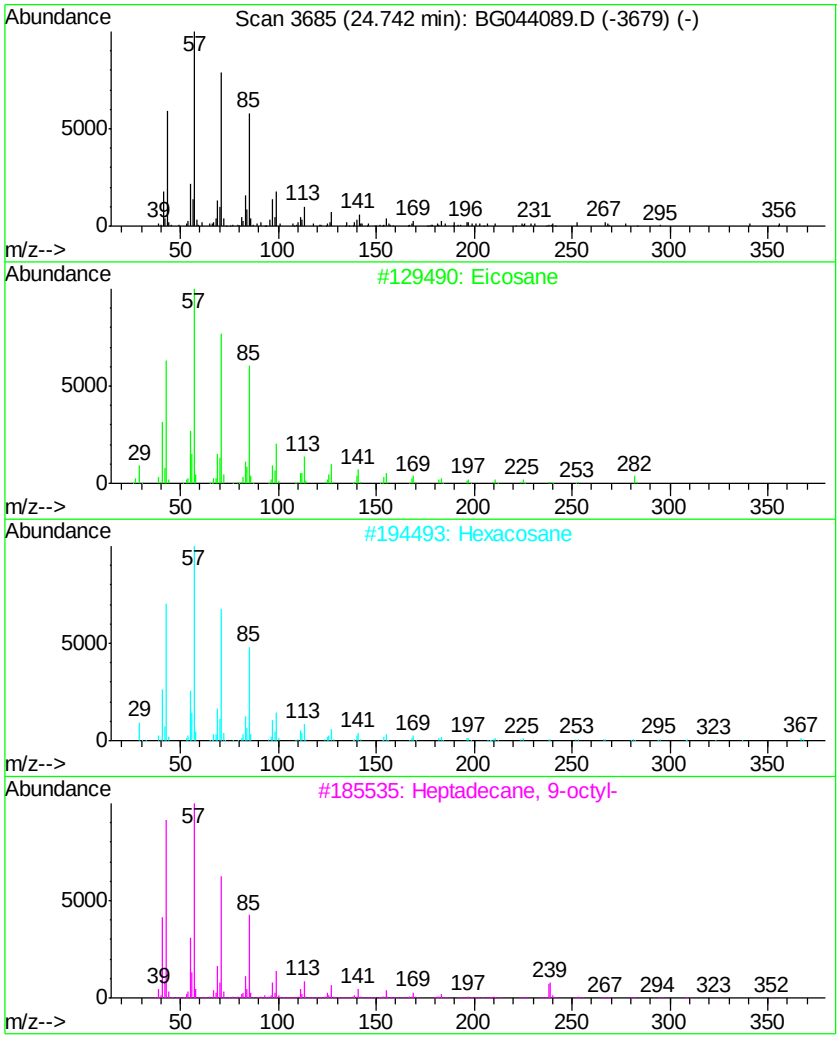
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

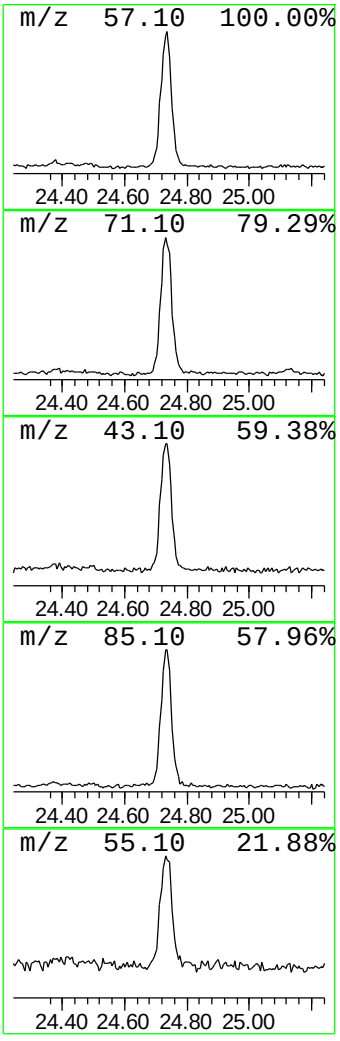
**********

Peak Number 10 Hexacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.74 | 5.19 ng | 336197 | Perylene-d12 | 24.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 94 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 3 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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

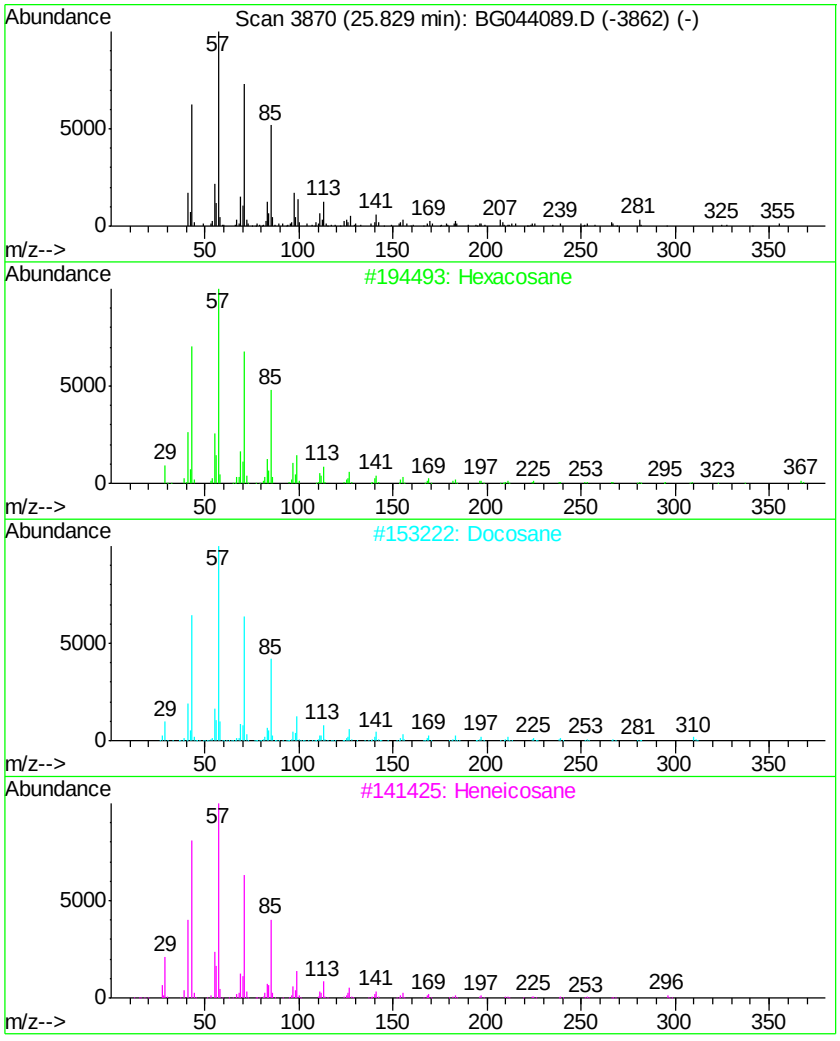
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

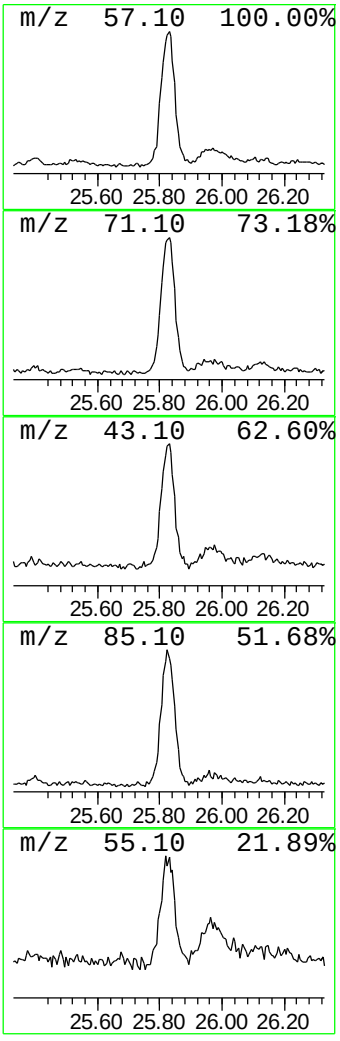
**********

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 25.83 | 4.77 ng | 309004 | Perylene-d12 | 24.67 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 2 | Docosane | 310 | C22H46 | 000629-97-0 | 87 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 4 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 87 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011720\
Data File : BG044089.D
Acq On : 18 Jan 2020 00:32
Operator : JU
Sample : L1162-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** CBH-591

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.04 | 6.6 | ng | 141726 | 1 | 7.93 | 429782 | 20.0 |
| unknown7.47 | 7.47 | 109.6 | ng | 2355250 | 1 | 7.93 | 429782 | 20.0 |
| 1-Penten-3-yne, 2... | 10.38 | 3.5 | ng | 115769 | 2 | 10.73 | 665845 | 20.0 |
| 5-Octadecene, (E)- | 21.23 | 14.7 | ng | 903735 | 5 | 21.56 | 1233680 | 20.0 |
| Nonadecane | 21.77 | 2.9 | ng | 180214 | 5 | 21.56 | 1233680 | 20.0 |
| Heneicosane | 22.36 | 4.9 | ng | 304849 | 5 | 21.56 | 1233680 | 20.0 |
| Dodecane, 2-methyl- | 23.03 | 5.5 | ng | 338987 | 5 | 21.56 | 1233680 | 20.0 |
| 2-methyloctacosane | 23.81 | 5.4 | ng | 348346 | 6 | 24.67 | 1295070 | 20.0 |
| Hexacosane | 24.74 | 5.2 | ng | 336197 | 6 | 24.67 | 1295070 | 20.0 |
| Heptadecane, 9-oc... | 25.83 | 4.8 | ng | 309004 | 6 | 24.67 | 1295070 | 20.0 |