LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

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-BG111318.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 | 3.753 | 75 | 79 | 89 | rBV | 27698 | 53194 | 1.83% | 0.276% |
| 2 | 5.169 | 314 | 320 | 328 | rBV | 38948 | 66555 | 2.29% | 0.345% |
| 3 | 5.627 | 391 | 398 | 409 | rBV | 841080 | 1387452 | 47.71% | 7.194% |
| 4 | 7.231 | 662 | 671 | 686 | rBV | 903009 | 1651041 | 56.78% | 8.561% |
| 5 | 7.613 | 728 | 736 | 745 | rBV | 826370 | 1470918 | 50.58% | 7.627% |
| 6 | 8.083 | 809 | 816 | 829 | rVB | 149253 | 267984 | 9.22% | 1.389% |
| 7 | 8.406 | 863 | 871 | 879 | rBV | 589157 | 1070014 | 36.80% | 5.548% |
| 8 | 9.264 | 1008 | 1017 | 1027 | rBV | 521172 | 964130 | 33.15% | 4.999% |
| 9 | 10.903 | 1288 | 1296 | 1301 | rBV | 220869 | 410514 | 14.12% | 2.128% |
| 10 | 10.956 | 1301 | 1305 | 1311 | rVB | 78615 | 135927 | 4.67% | 0.705% |
| 11 | 12.554 | 1570 | 1577 | 1583 | rVB | 26173 | 41113 | 1.41% | 0.213% |
| 12 | 13.342 | 1703 | 1711 | 1721 | rVB | 1369429 | 2216013 | 76.21% | 11.490% |
| 13 | 14.164 | 1845 | 1851 | 1856 | rVB | 191590 | 285522 | 9.82% | 1.480% |
| 14 | 14.717 | 1939 | 1945 | 1954 | rVB2 | 354012 | 610876 | 21.01% | 3.167% |
| 15 | 16.209 | 2192 | 2199 | 2207 | rBV | 1043986 | 1656616 | 56.97% | 8.589% |
| 16 | 16.385 | 2225 | 2229 | 2240 | rVB2 | 22376 | 39138 | 1.35% | 0.203% |
| 17 | 17.466 | 2405 | 2413 | 2424 | rBV2 | 484269 | 760425 | 26.15% | 3.943% |
| 18 | 18.324 | 2554 | 2559 | 2565 | rBV2 | 51926 | 87608 | 3.01% | 0.454% |
| 19 | 19.235 | 2710 | 2714 | 2718 | rBV2 | 23593 | 32241 | 1.11% | 0.167% |
| 20 | 19.587 | 2771 | 2774 | 2781 | rBV5 | 14286 | 29387 | 1.01% | 0.152% |
| 21 | 19.811 | 2807 | 2812 | 2815 | rBV3 | 21652 | 29931 | 1.03% | 0.155% |
| 22 | 20.069 | 2849 | 2856 | 2863 | rBV | 2044849 | 2907962 | 100.00% | 15.078% |
| 23 | 20.833 | 2982 | 2986 | 2990 | rVB2 | 26768 | 29651 | 1.02% | 0.154% |
| 24 | 21.344 | 3068 | 3073 | 3079 | rBV2 | 29706 | 42512 | 1.46% | 0.220% |
| 25 | 21.749 | 3135 | 3142 | 3151 | rVB | 464104 | 796052 | 27.37% | 4.127% |
| 26 | 21.896 | 3160 | 3167 | 3173 | rVB | 58999 | 84195 | 2.90% | 0.437% |
| 27 | 22.513 | 3266 | 3272 | 3280 | rBV | 91585 | 153478 | 5.28% | 0.796% |
| 28 | 23.218 | 3385 | 3392 | 3400 | rVB | 134282 | 252803 | 8.69% | 1.311% |
| 29 | 24.041 | 3522 | 3532 | 3540 | rBV | 142149 | 328530 | 11.30% | 1.703% |
| 30 | 25.016 | 3687 | 3698 | 3700 | rBV2 | 128901 | 315541 | 10.85% | 1.636% |
| 31 | 25.063 | 3701 | 3706 | 3720 | rVB | 255377 | 730190 | 25.11% | 3.786% |
| 32 | 26.174 | 3884 | 3895 | 3905 | rBV2 | 79660 | 252092 | 8.67% | 1.307% |
| 33 | 27.554 | 4120 | 4130 | 4142 | rBV5 | 33657 | 126957 | 4.37% | 0.658% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

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-BG111318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

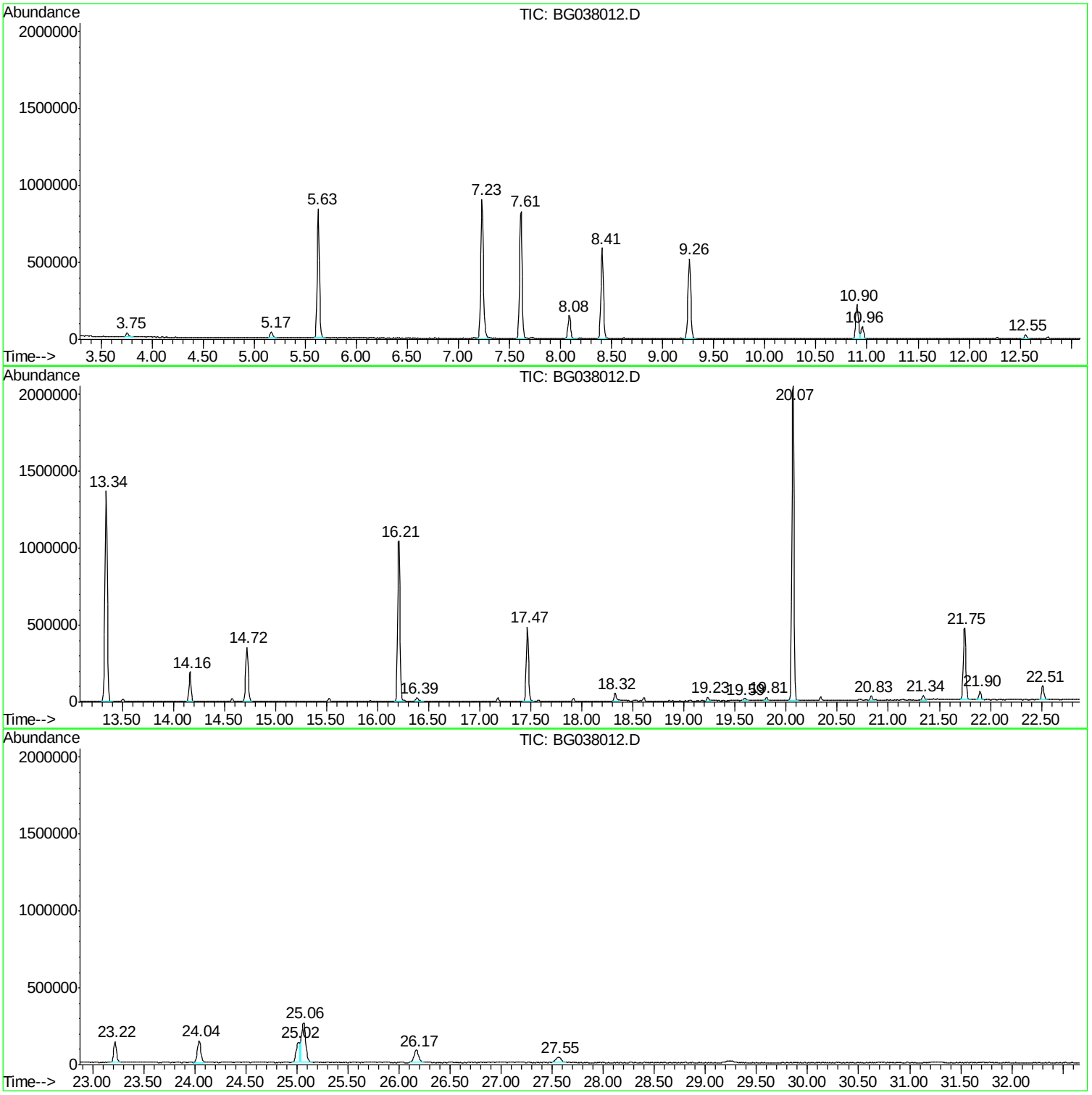
Sum of corrected areas: 19286562

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

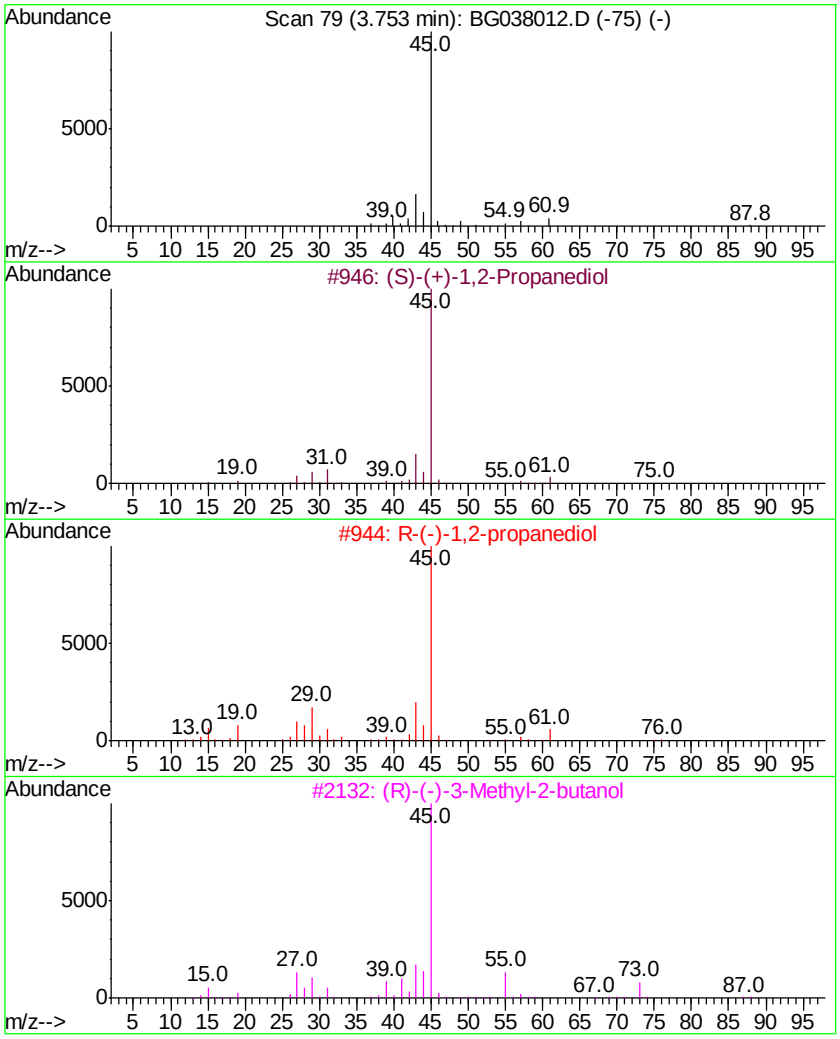
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

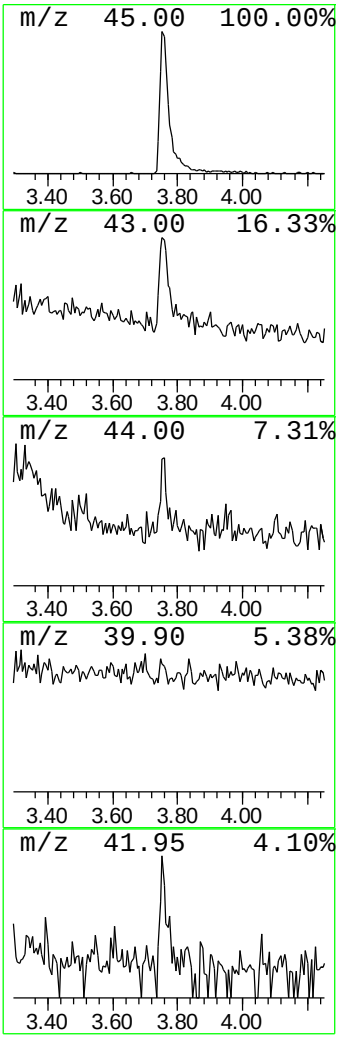
**********

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.75 | 3.97 ng | 53194 | 1,4-Dichlorobenzene-d4 | 8.08 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (S)-(+)-1,2-Propanediol | 76 | C3H8O2 | 004254-15-3 | 56 |
| 2 | R-(-)-1,2-propanediol | 76 | C3H8O2 | 004254-14-2 | 43 |
| 3 | (R)-(-)-3-Methyl-2-butanol | 88 | C5H12O | 001572-93-6 | 40 |
| 4 | 3-Ethyl-2-pentanol | 116 | C7H16O | 000609-27-8 | 40 |
| 5 | 2-Butanol, 3-methyl- | 88 | C5H12O | 000598-75-4 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

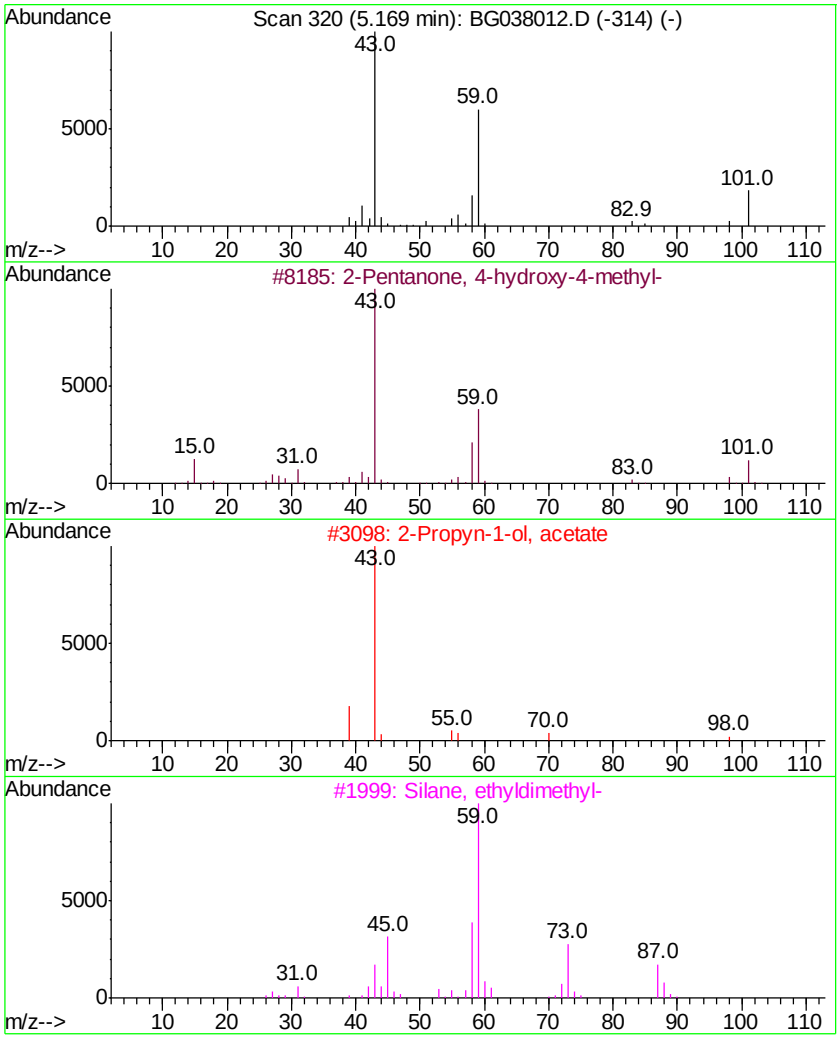
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

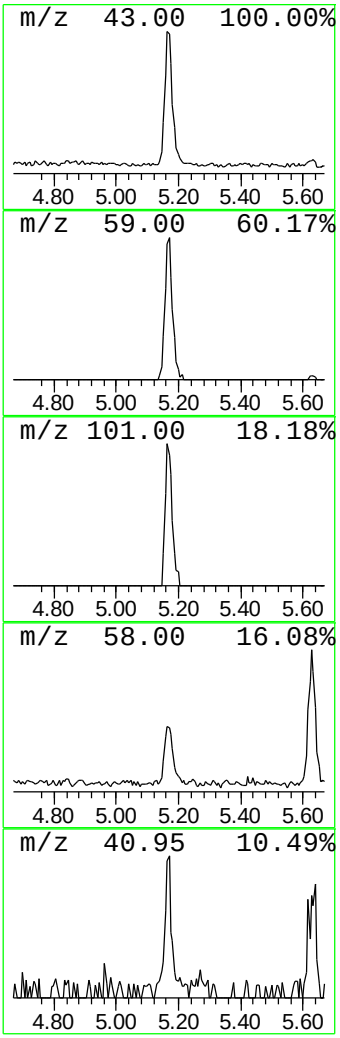
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.17 | 4.97 ng | 66555 | 1,4-Dichlorobenzene-d4 | 8.08 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 2-Propyn-1-ol, acetate | 98 | C5H6O2 | 000627-09-8 | 9 |
| 3 | Silane, ethyldimethyl- | 88 | C4H12Si | 000758-21-4 | 9 |
| 4 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |
| 5 | Ethyl ether | 74 | C4H10O | 000060-29-7 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

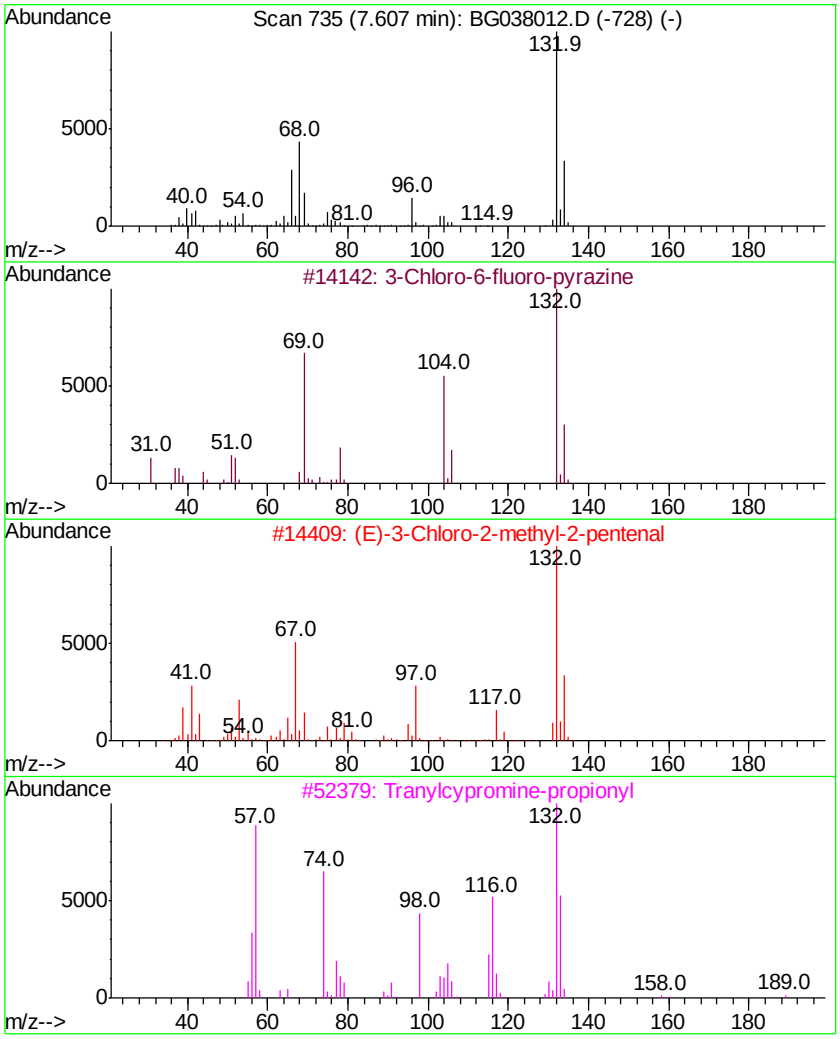
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

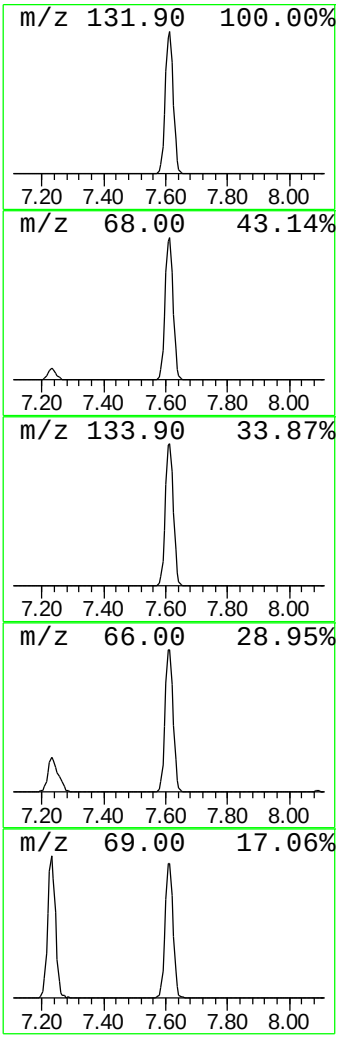
**********

Peak Number 3 unknown7.61 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.61 | 109.78 ng | 1470920 | 1,4-Dichlorobenzene-d4 | 8.08 |

| 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 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

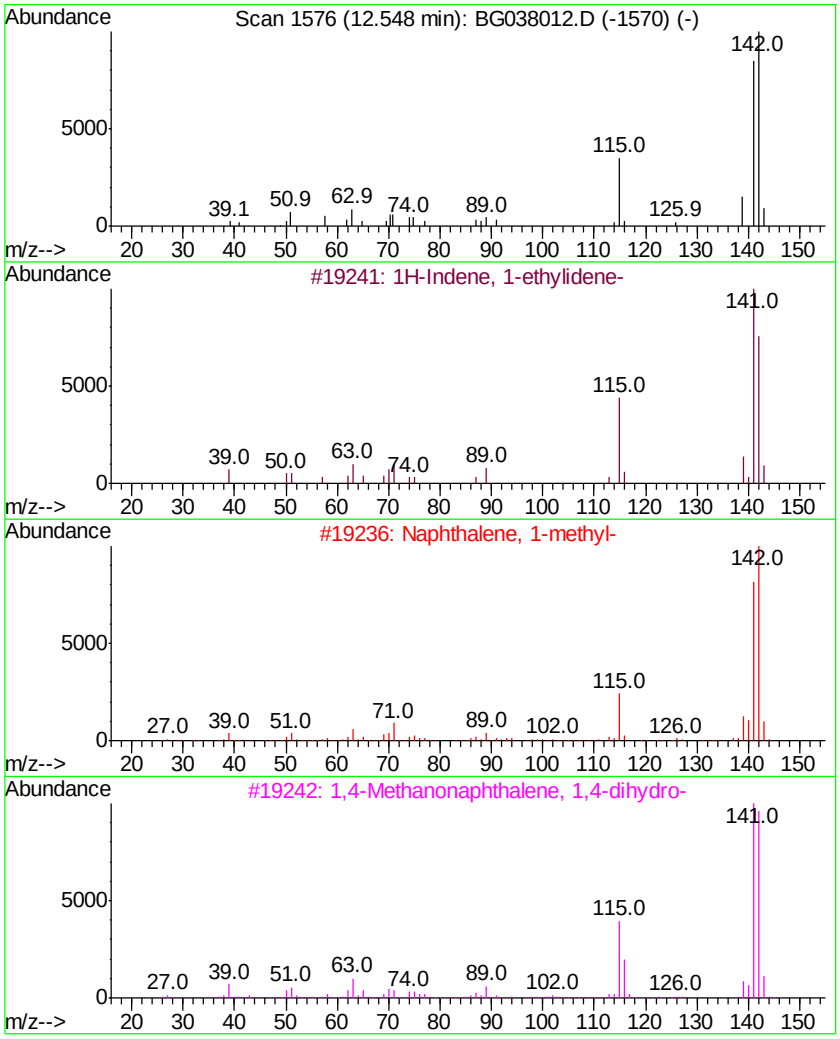
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

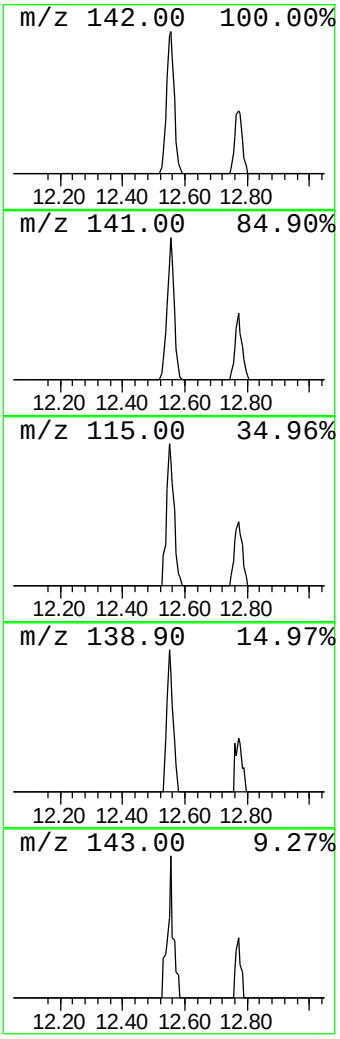
**********

Peak Number 5 1H-Indene, 1-ethylidene- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.55 | 2.00 ng | 41113 | Naphthalene-d8 | 10.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Indene, 1-ethylidene- | 142 | C11H10 | 002471-83-2 | 91 |
| 2 | Naphthalene, 1-methyl- | 142 | C11H10 | 000090-12-0 | 90 |
| 3 | 1,4-Methanonaphthalene, 1,4-dihy... | 142 | C11H10 | 004453-90-1 | 90 |
| 4 | Naphthalene, 2-methyl- | 142 | C11H10 | 000091-57-6 | 90 |
| 5 | Benzocycloheptatriene | 142 | C11H10 | 000264-09-5 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

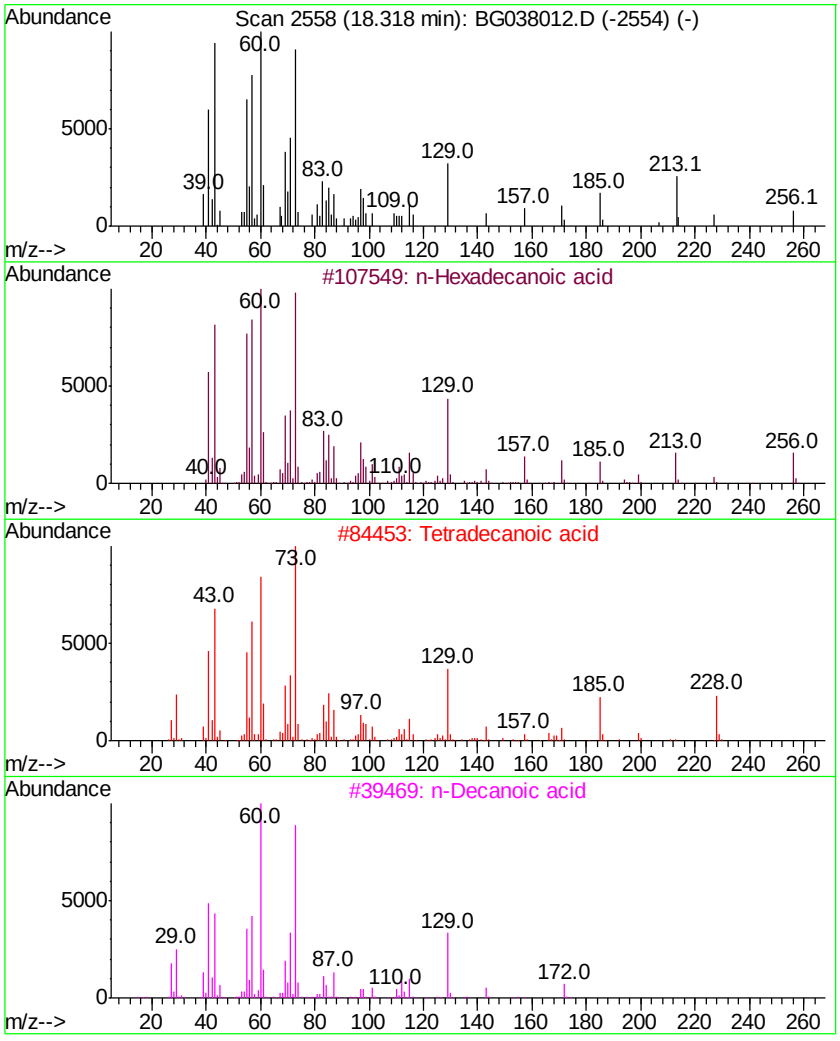
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

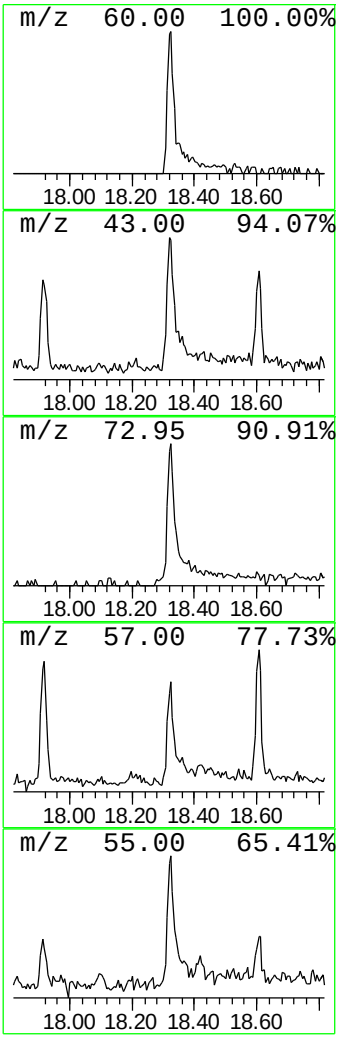
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.32 | 2.30 ng | 87608 | Phenanthrene-d10 | 17.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 68 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 64 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

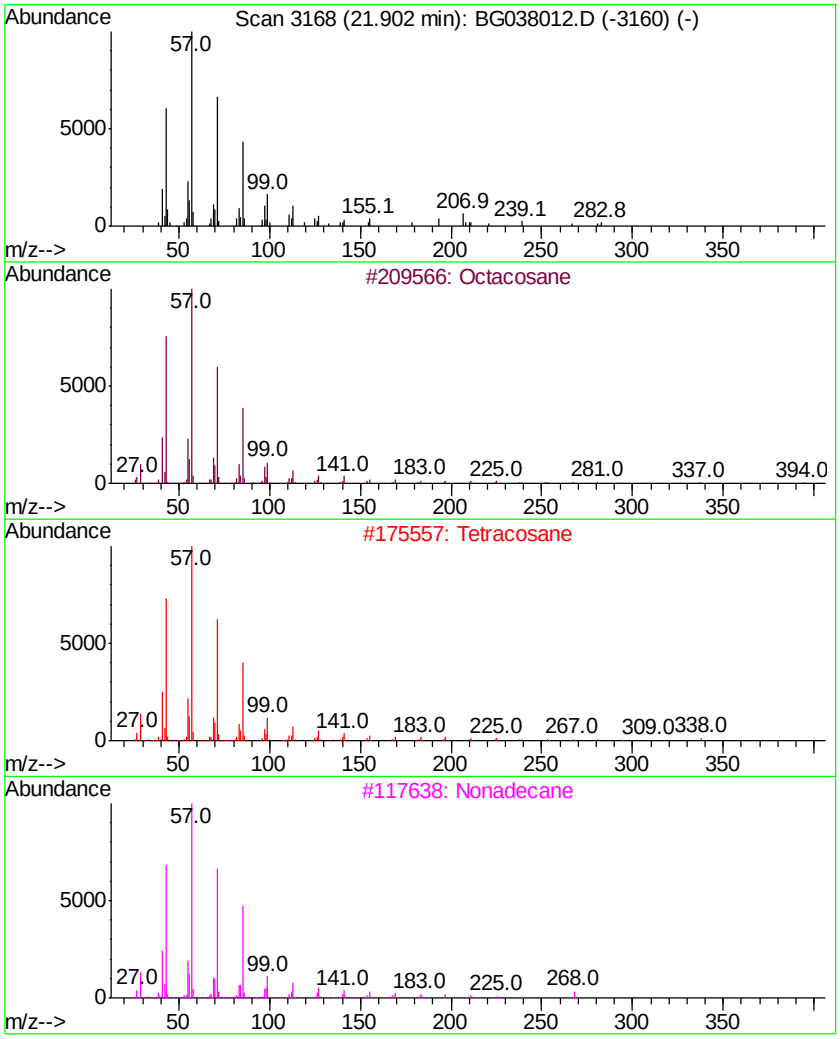
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

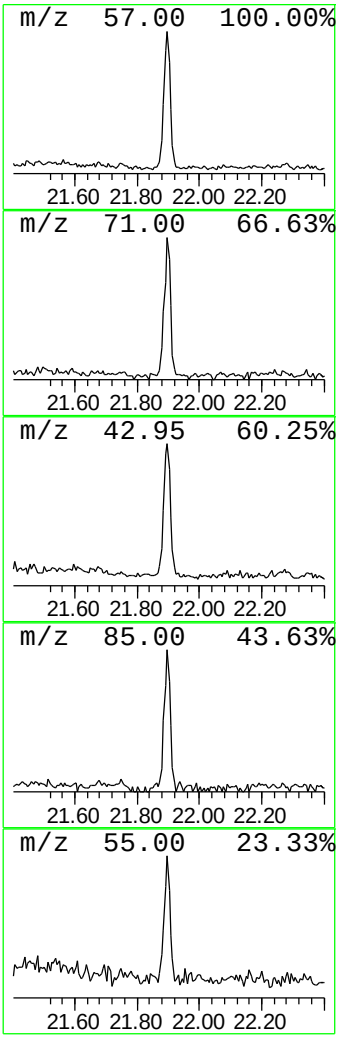
**********

Peak Number 7 Octacosane Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.90 | 2.12 ng | 84195 | Chrysene-d12 | 21.75 |

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

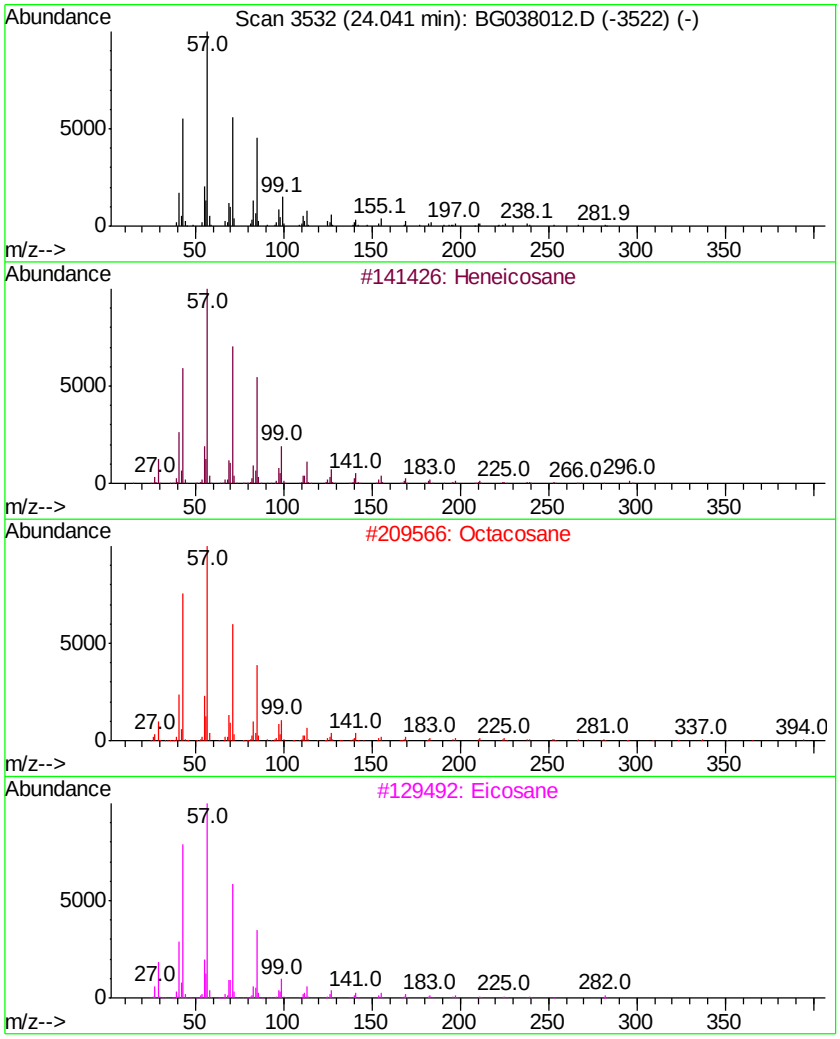
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

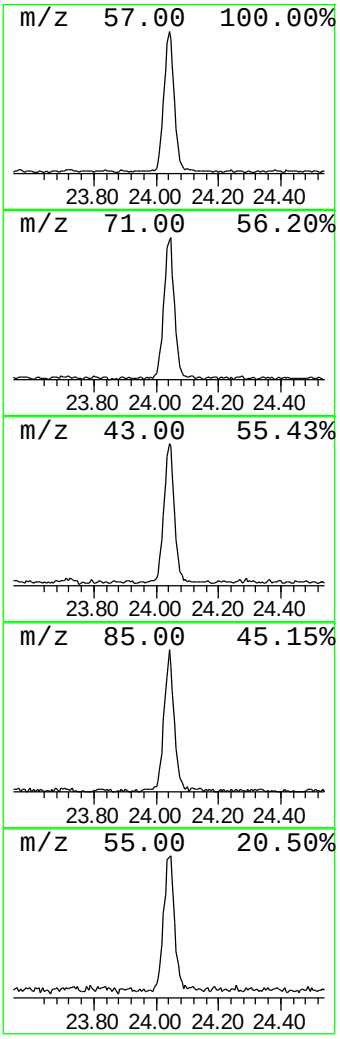
**********

Peak Number 10 Heneicosane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 24.04 | 9.00 ng | 328530 | Perylene-d12 | 25.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

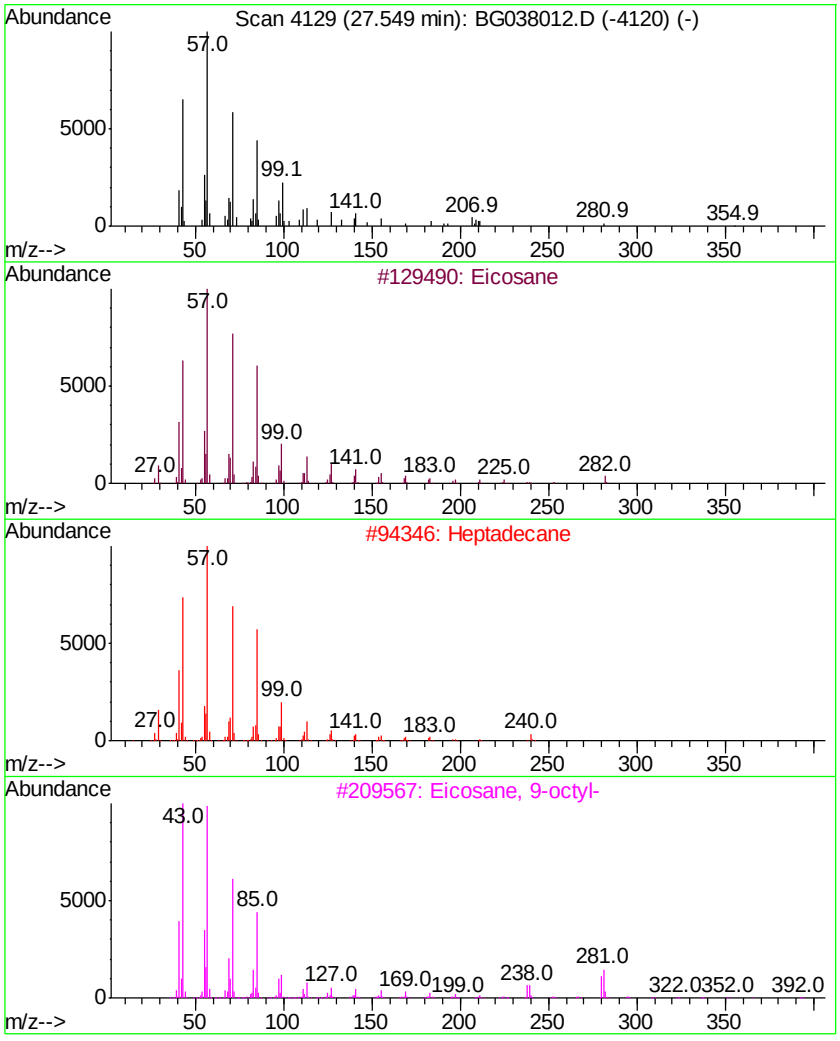
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

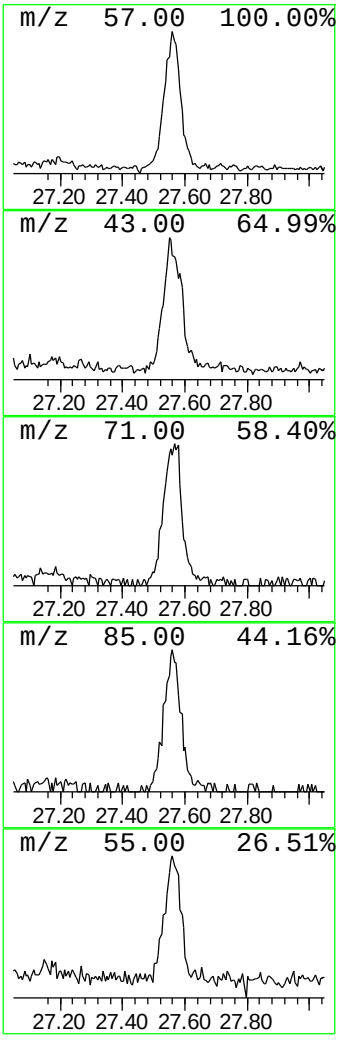
**********

Peak Number 12 Eicosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 27.55 | 3.48 ng | 126957 | Perylene-d12 | 25.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 94 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 3 | Eicosane, 9-octyl- | 394 | C28H58 | 013475-77-9 | 80 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 74 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 72 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111418\
Data File : BG038012.D
Acq On : 15 Nov 2018 00:53
Operator : JU/SJ
Sample : J5889-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** BOTTOM-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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 |
| (S)-(+)-1,2-Propa... | 3.75 | 4.0 | ng | 53194 | 1 | 8.08 | 267984 | 20.0 |
| 2-Pentanone, 4-hy... | 5.17 | 5.0 | ng | 66555 | 1 | 8.08 | 267984 | 20.0 |
| unknown7.61 | 7.61 | 109.8 | ng | 1470920 | 1 | 8.08 | 267984 | 20.0 |
| 1H-Indene, 1-ethy... | 12.55 | 2.0 | ng | 41113 | 2 | 10.90 | 410514 | 20.0 |
| n-Hexadecanoic acid | 18.32 | 2.3 | ng | 87608 | 4 | 17.47 | 760425 | 20.0 |
| Octacosane | 21.90 | 2.1 | ng | 84195 | 5 | 21.75 | 796052 | 20.0 |
| Heneicosane | 24.04 | 9.0 | ng | 328530 | 6 | 25.06 | 730190 | 20.0 |
| Eicosane | 27.55 | 3.5 | ng | 126957 | 6 | 25.06 | 730190 | 20.0 |