LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072319\
Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

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-BG071519.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 | 3.203 | 13 | 19 | 36 | rVB | 766146 | 1588259 | 28.90% | 5.388% |
| 2 | 5.606 | 422 | 428 | 440 | rVB | 358140 | 587162 | 10.68% | 1.992% |
| 3 | 7.192 | 691 | 698 | 710 | rVB | 228669 | 418652 | 7.62% | 1.420% |
| 4 | 7.574 | 755 | 763 | 771 | rBV | 731895 | 1230008 | 22.38% | 4.172% |
| 5 | 8.044 | 836 | 843 | 853 | rBV | 357038 | 598650 | 10.89% | 2.031% |
| 6 | 8.367 | 891 | 898 | 906 | rBV | 1086388 | 1843928 | 33.55% | 6.255% |
| 7 | 9.202 | 1032 | 1040 | 1048 | rBV | 817739 | 1471480 | 26.78% | 4.991% |
| 8 | 10.847 | 1312 | 1320 | 1332 | rBV | 441635 | 811399 | 14.76% | 2.752% |
| 9 | 13.291 | 1728 | 1736 | 1747 | rBV | 2303976 | 3634650 | 66.14% | 12.329% |
| 10 | 14.108 | 1869 | 1875 | 1882 | rBV | 206764 | 301650 | 5.49% | 1.023% |
| 11 | 14.660 | 1960 | 1969 | 1976 | rBV2 | 765149 | 1183896 | 21.54% | 4.016% |
| 12 | 16.140 | 2214 | 2221 | 2231 | rBV | 1184639 | 1840377 | 33.49% | 6.243% |
| 13 | 17.163 | 2390 | 2395 | 2401 | rBV3 | 47843 | 83589 | 1.52% | 0.284% |
| 14 | 17.398 | 2428 | 2435 | 2443 | rBV | 895724 | 1391264 | 25.32% | 4.719% |
| 15 | 17.897 | 2517 | 2520 | 2531 | rVB3 | 55320 | 94814 | 1.73% | 0.322% |
| 16 | 18.291 | 2581 | 2587 | 2604 | rBV | 642968 | 1116938 | 20.32% | 3.789% |
| 17 | 18.585 | 2634 | 2637 | 2641 | rBV2 | 55390 | 66428 | 1.21% | 0.225% |
| 18 | 19.213 | 2741 | 2744 | 2747 | rBV2 | 49076 | 56305 | 1.02% | 0.191% |
| 19 | 19.554 | 2798 | 2802 | 2813 | rBV | 768032 | 1230349 | 22.39% | 4.174% |
| 20 | 20.001 | 2872 | 2878 | 2885 | rBV | 4141953 | 5495492 | 100.00% | 18.642% |
| 21 | 21.311 | 3098 | 3101 | 3119 | rVB2 | 245950 | 608596 | 11.07% | 2.064% |
| 22 | 21.546 | 3138 | 3141 | 3151 | rVB | 172688 | 243323 | 4.43% | 0.825% |
| 23 | 21.646 | 3152 | 3158 | 3166 | rBV | 1029772 | 1735566 | 31.58% | 5.887% |
| 24 | 23.162 | 3412 | 3416 | 3424 | rVB | 124932 | 232270 | 4.23% | 0.788% |
| 25 | 24.842 | 3693 | 3702 | 3710 | rBV2 | 581462 | 1614713 | 29.38% | 5.477% |

Sum of corrected areas: 29479758

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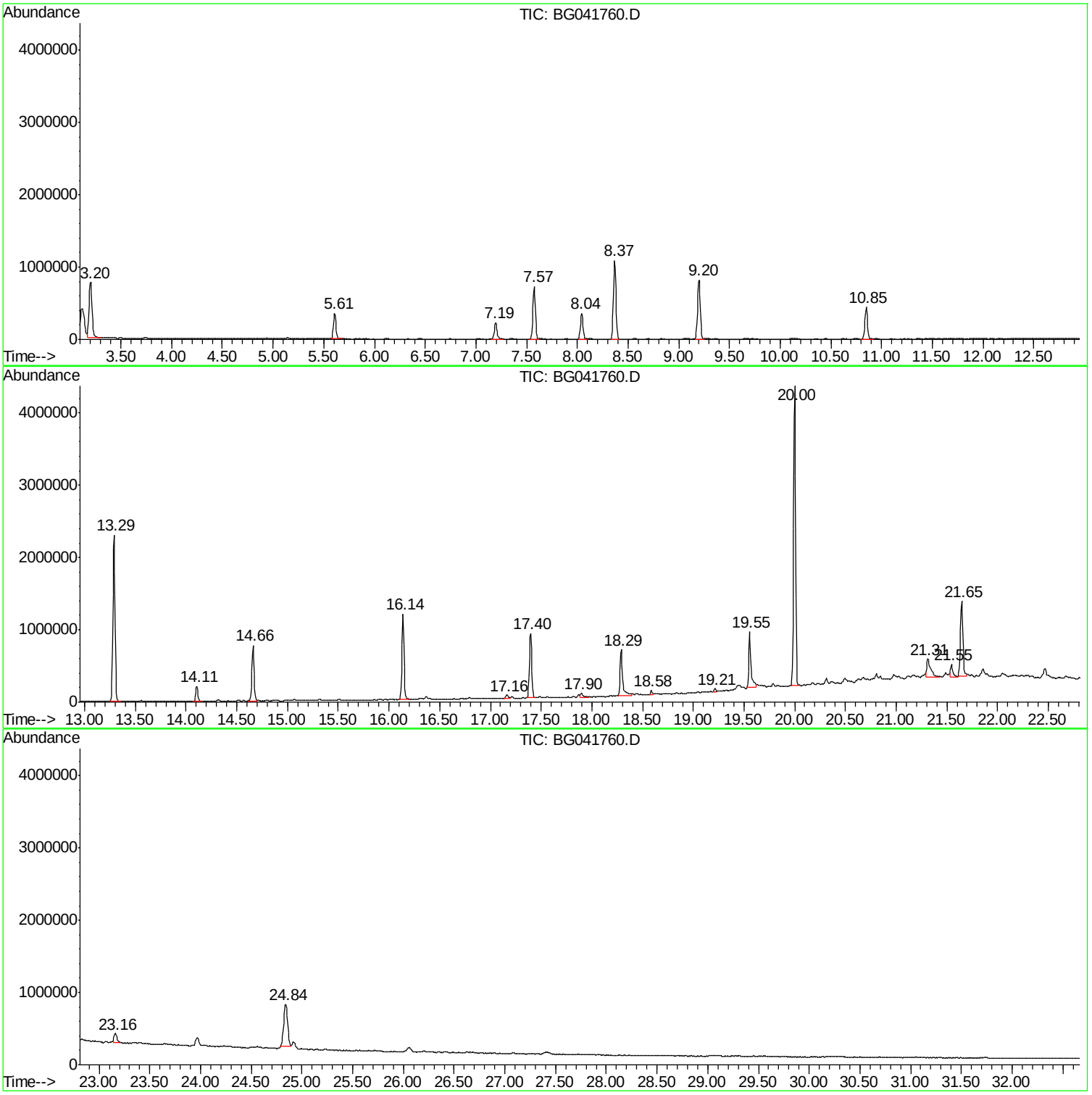
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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\BG072319\
Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

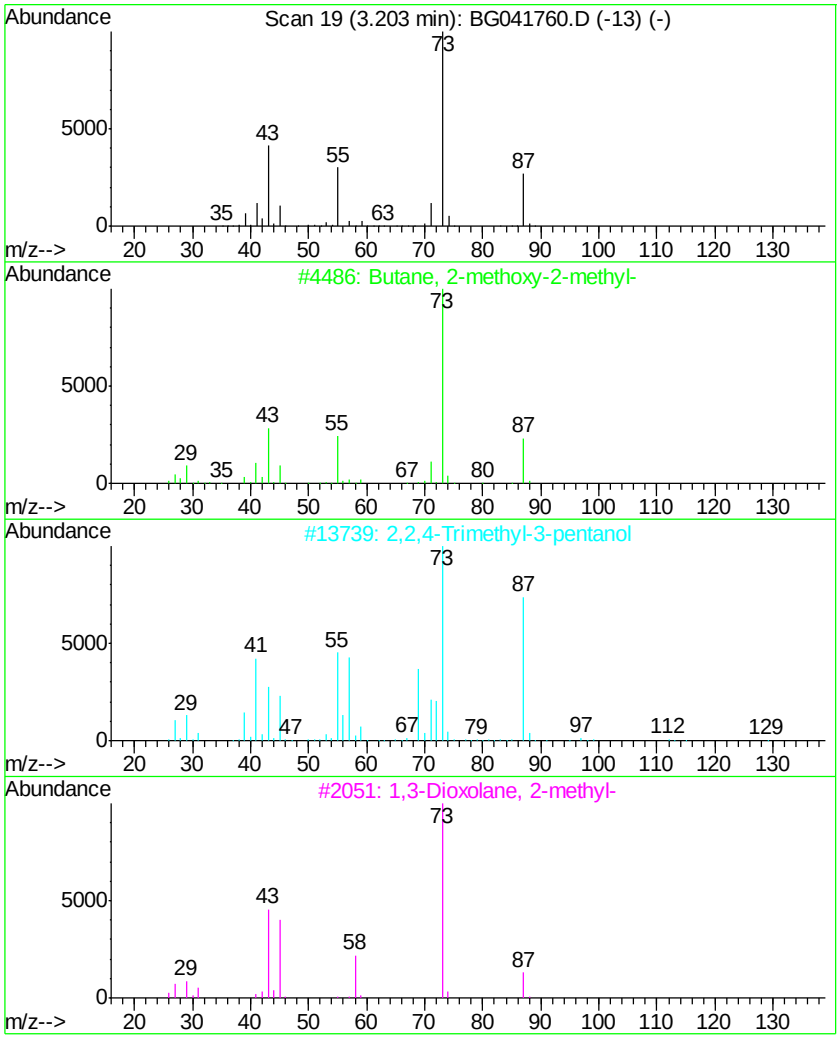
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

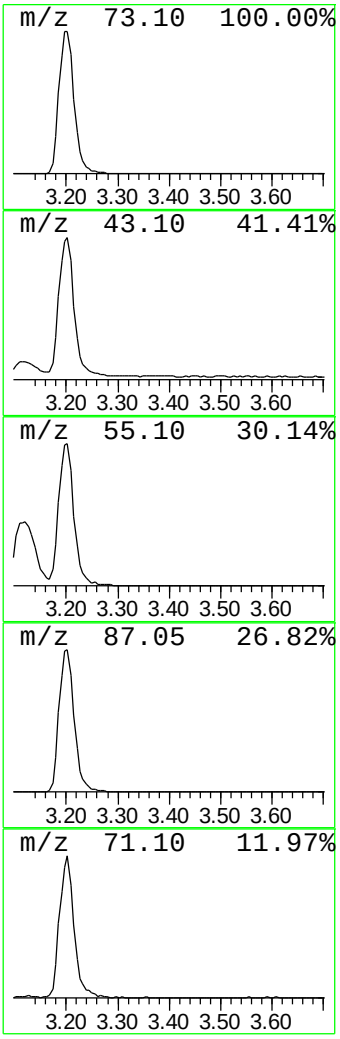
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.20 | 53.06 ng | 1588260 | 1,4-Dichlorobenzene-d4 | 8.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 38 |
| 3 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 38 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072319\
Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

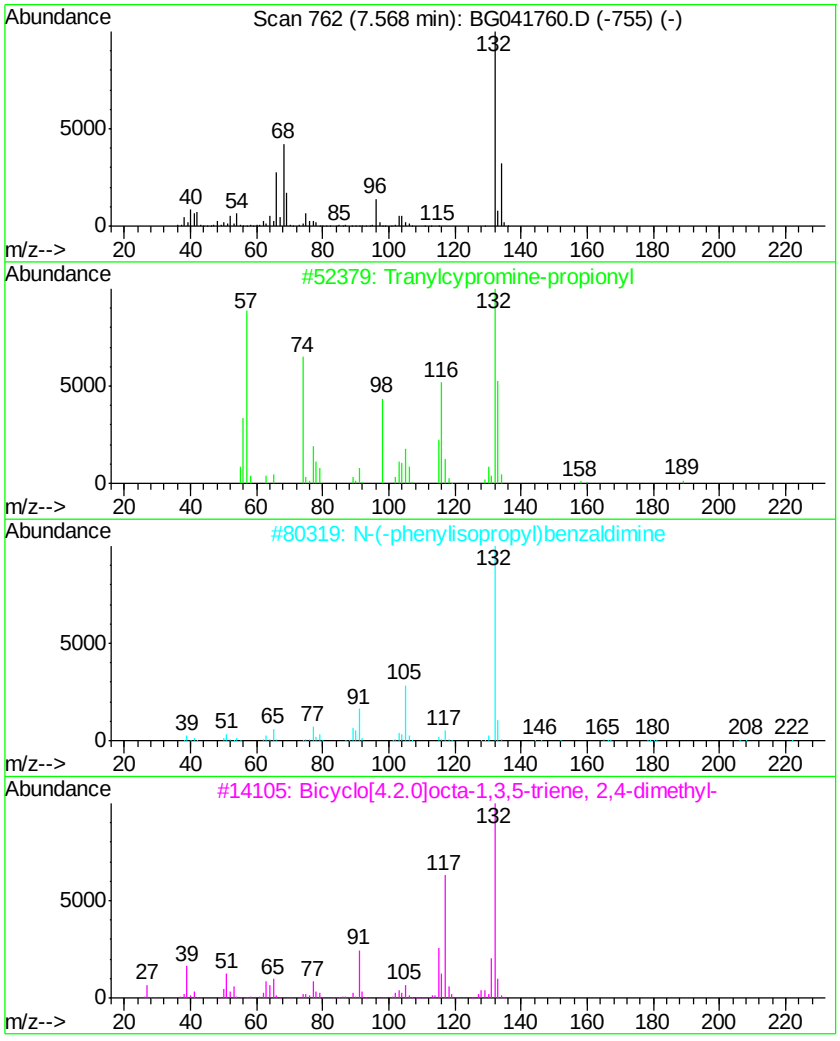
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

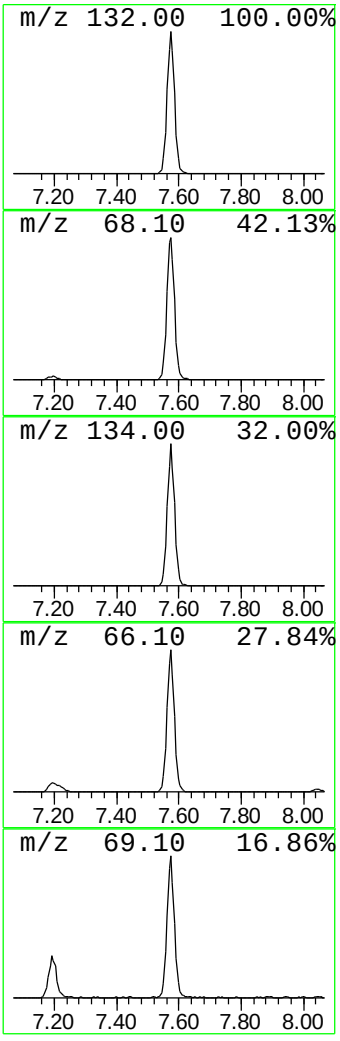
**********

Peak Number 2 unknown7.57 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.57 | 41.09 ng | 1230010 | 1,4-Dichlorobenzene-d4 | 8.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 2 | N-(-phenylisopropyl)benzaldimine | 223 | C16H17N | 1000379-01-3 | 10 |
| 3 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 4 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |
| 5 | Xenon | 132 | Xe | 007440-63-3 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072319\
Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

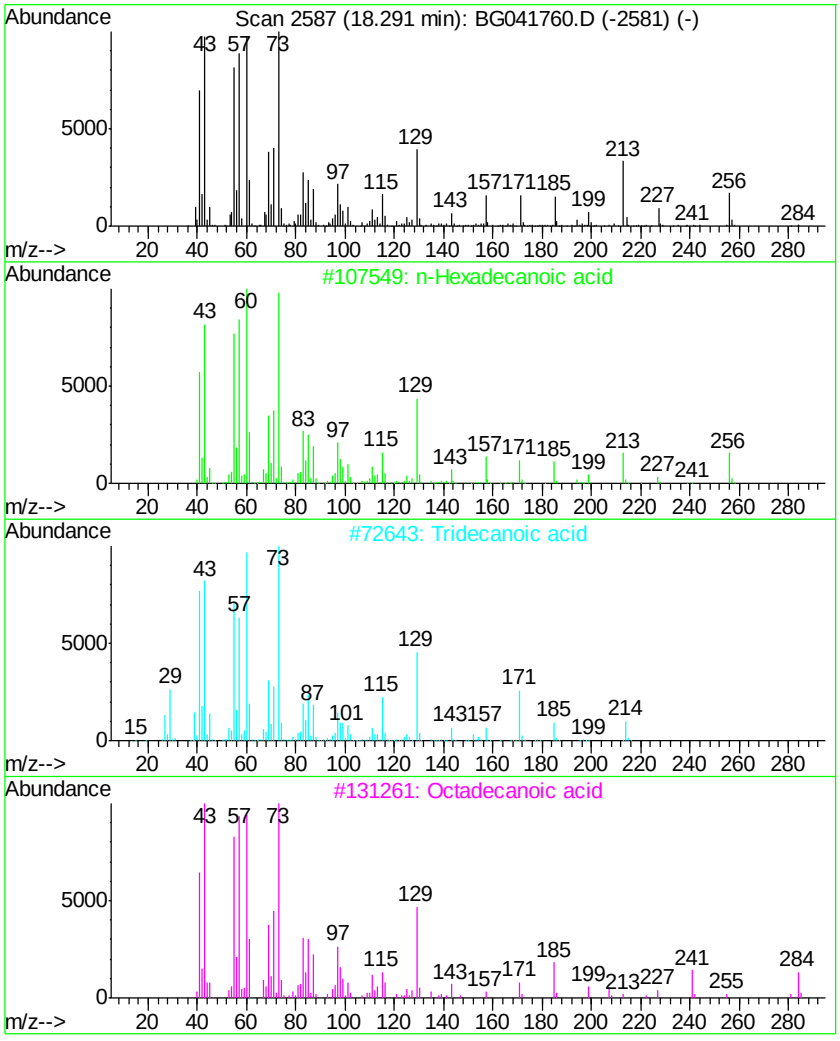
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

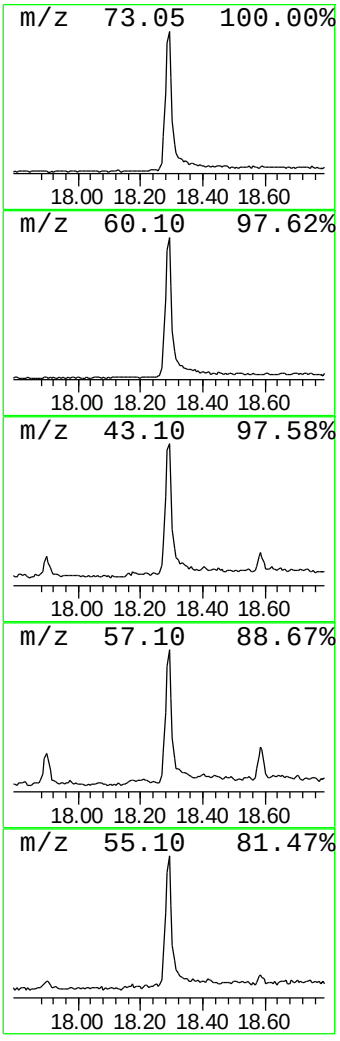
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.29 | 16.06 ng | 1116940 | Phenanthrene-d10 | 17.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 93 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 91 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072319\
Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

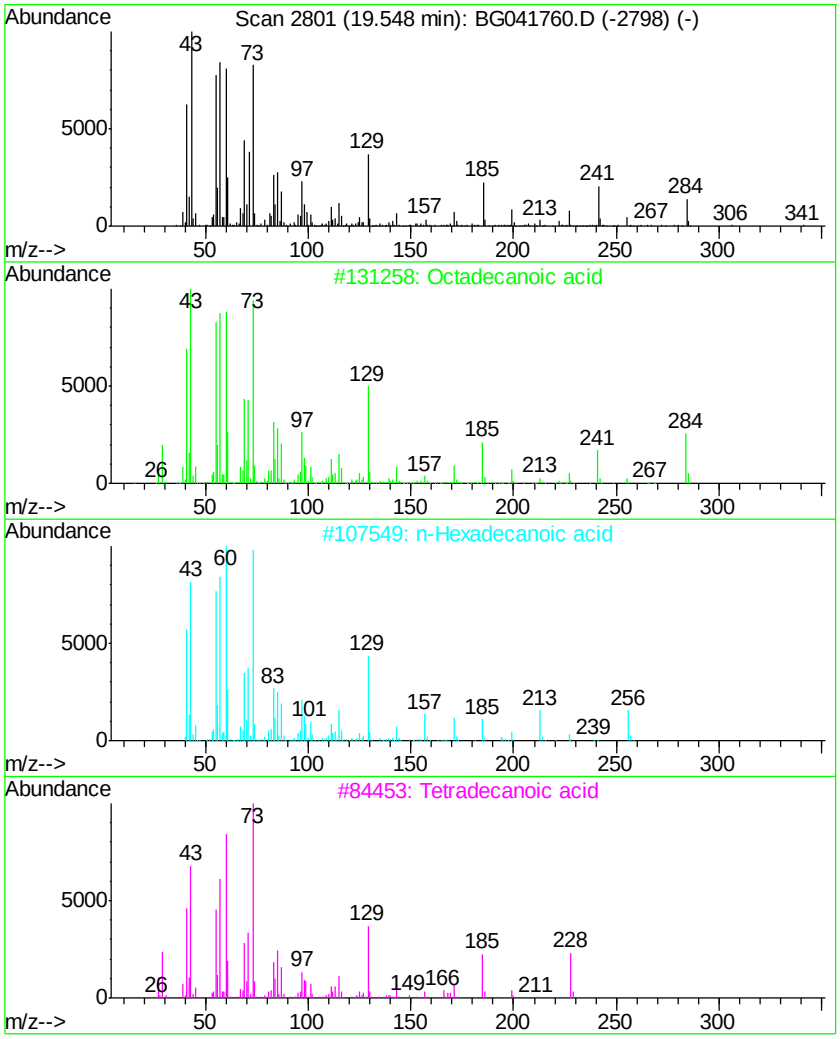
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

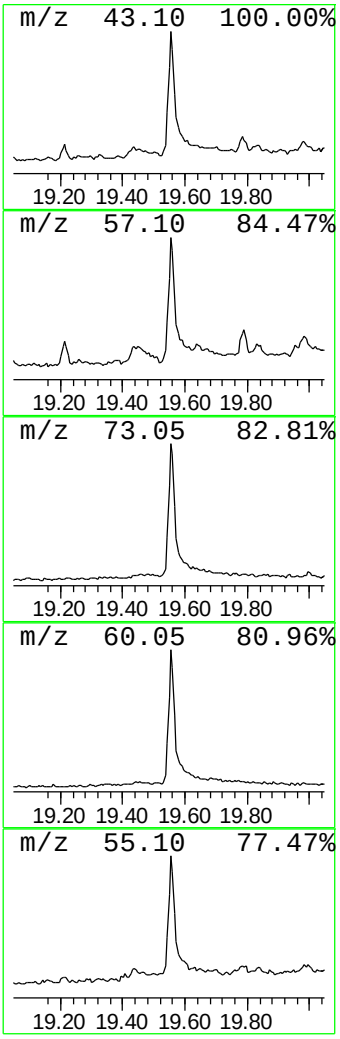
**********

Peak Number 5 Octadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.55 | 14.18 ng | 1230350 | Chrysene-d12 | 21.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 83 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 74 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 60 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 30 |



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Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

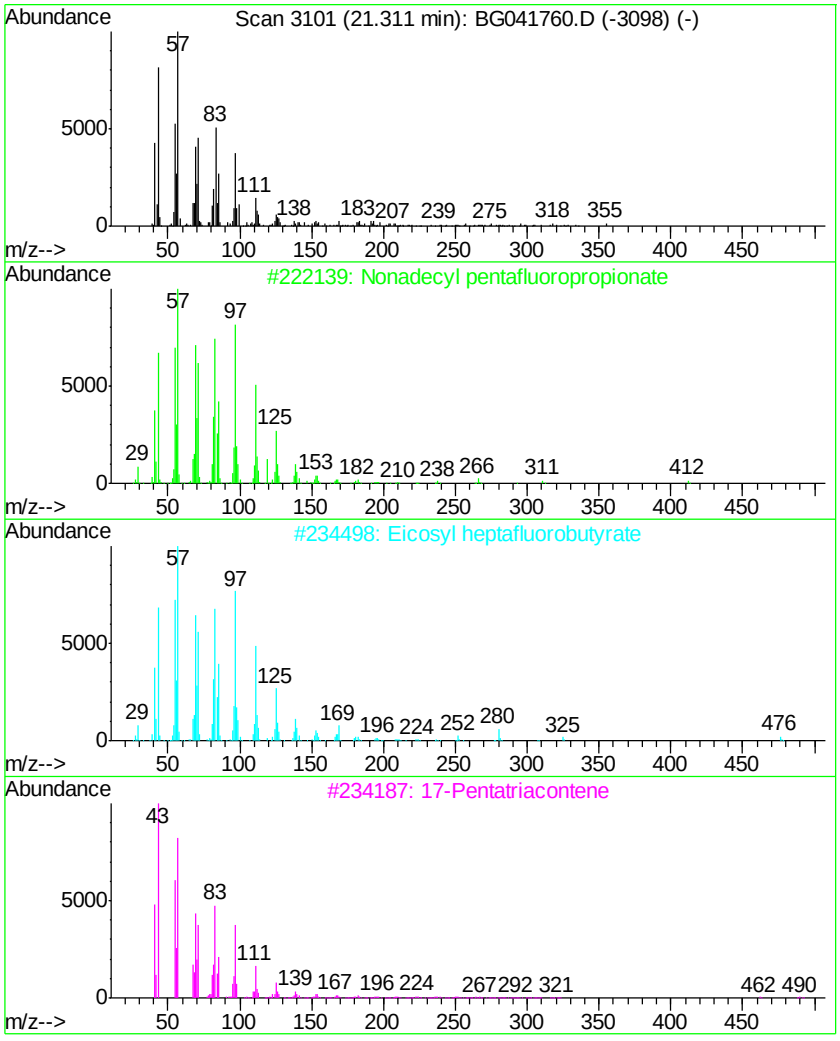
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

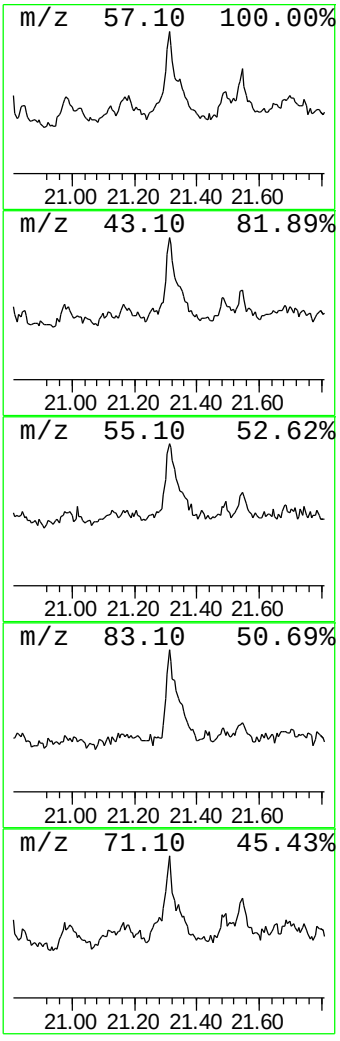
**********

Peak Number 6 Nonadecyl pentafluoropropio... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.31 | 7.01 ng | 608596 | Chrysene-d12 | 21.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 90 |
| 2 | Eicosyl heptafluorobutyrate | 494 | C24H41F7O2 | 1000351-83-5 | 90 |
| 3 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 87 |
| 4 | Trihexadecyl borate | 735 | C48H99BO3 | 002665-11-4 | 87 |
| 5 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 83 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG072319\
Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

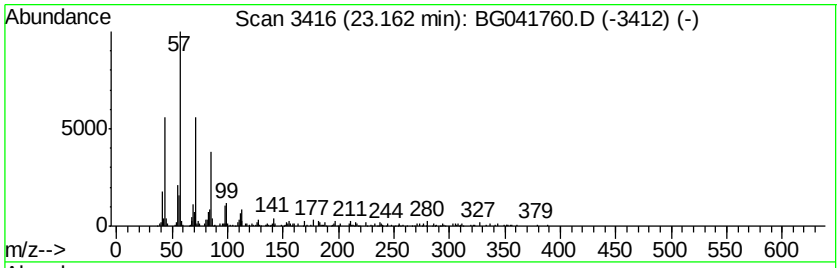
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

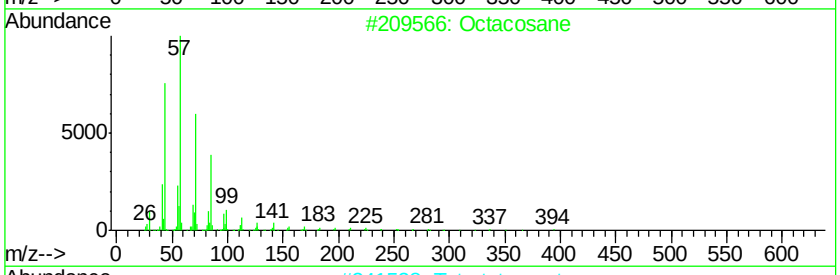
**********

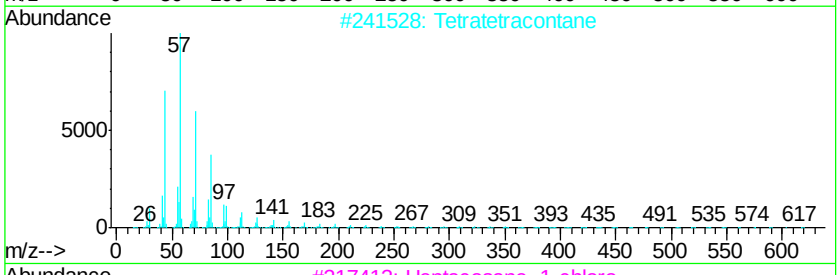
Peak Number 7 Octacosane Concentration Rank 7

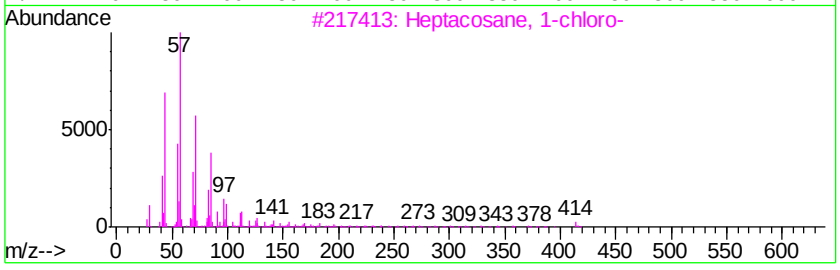
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.16 | 2.68 ng | 232270 | Chrysene-d12 | 21.65 |

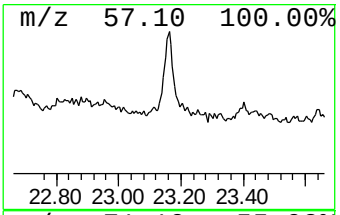
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 2 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 86 |
| 3 | Heptacosane, 1-chloro- | 414 | C27H55Cl | 062016-79-9 | 86 |
| 4 | Heneicosane, 11-decyl- | 437 | C31H64 | 055320-06-4 | 86 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 86 |

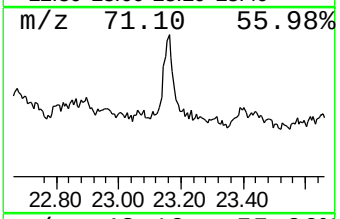


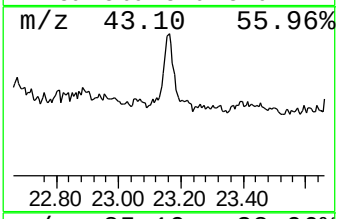



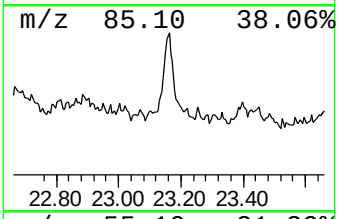



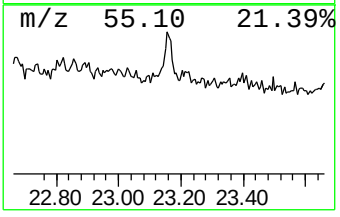



Tentatively Identified Compound (LSC) summary

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Data File : BG041760.D
Acq On : 23 Jul 2019 17:49
Operator : HP/JU
Sample : K3928-08
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TOTE-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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... | 3.20 | 53.1 | ng | 1588260 | 1 | 8.04 | 598650 | 20.0 |
| unknown7.57 | 7.57 | 41.1 | ng | 1230010 | 1 | 8.04 | 598650 | 20.0 |
| n-Hexadecanoic acid | 18.29 | 16.1 | ng | 1116940 | 4 | 17.40 | 1391260 | 20.0 |
| Octadecanoic acid | 19.55 | 14.2 | ng | 1230350 | 5 | 21.65 | 1735570 | 20.0 |
| Nonadecyl pentafl... | 21.31 | 7.0 | ng | 608596 | 5 | 21.65 | 1735570 | 20.0 |
| Octacosane | 23.16 | 2.7 | ng | 232270 | 5 | 21.65 | 1735570 | 20.0 |