LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

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_F\METHODS\8270-BF100818.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 | 4.887 | 473 | 476 | 488 | rBV | 68486 | 91419 | 2.26% | 0.402% |
| 2 | 5.310 | 545 | 548 | 576 | rBV | 453271 | 738666 | 18.27% | 3.252% |
| 3 | 6.339 | 720 | 723 | 741 | rBV | 286867 | 558758 | 13.82% | 2.460% |
| 4 | 6.463 | 741 | 744 | 776 | rVV | 1599890 | 1870178 | 46.26% | 8.233% |
| 5 | 6.692 | 780 | 783 | 805 | rVV | 470176 | 669616 | 16.57% | 2.948% |
| 6 | 6.851 | 805 | 810 | 839 | rVV | 2422452 | 2575172 | 63.70% | 11.337% |
| 7 | 7.263 | 875 | 880 | 914 | rBV | 1699988 | 2275413 | 56.29% | 10.017% |
| 8 | 7.975 | 997 | 1001 | 1028 | rBV | 649311 | 856095 | 21.18% | 3.769% |
| 9 | 9.051 | 1179 | 1184 | 1203 | rBV | 3611909 | 4042339 | 100.00% | 17.795% |
| 10 | 9.722 | 1294 | 1298 | 1320 | rBV | 969740 | 1003157 | 24.82% | 4.416% |
| 11 | 10.510 | 1428 | 1432 | 1460 | rBV | 1297310 | 1656225 | 40.97% | 7.291% |
| 12 | 11.198 | 1546 | 1549 | 1572 | rBV | 774288 | 989037 | 24.47% | 4.354% |
| 13 | 11.739 | 1638 | 1641 | 1644 | rBV | 42808 | 51452 | 1.27% | 0.227% |
| 14 | 12.786 | 1814 | 1819 | 1834 | rBV | 3279914 | 3612397 | 89.36% | 15.903% |
| 15 | 13.827 | 1992 | 1996 | 2013 | rVB | 577074 | 689065 | 17.05% | 3.033% |
| 16 | 14.592 | 2122 | 2126 | 2130 | rBV | 79813 | 75321 | 1.86% | 0.332% |
| 17 | 14.904 | 2173 | 2179 | 2188 | rBV | 97951 | 113413 | 2.81% | 0.499% |
| 18 | 15.227 | 2229 | 2234 | 2252 | rVB2 | 338660 | 663890 | 16.42% | 2.923% |
| 19 | 15.645 | 2299 | 2305 | 2313 | rBV | 81417 | 110922 | 2.74% | 0.488% |
| 20 | 16.098 | 2377 | 2382 | 2394 | rVB | 41195 | 73030 | 1.81% | 0.321% |

Sum of corrected areas: 22715565

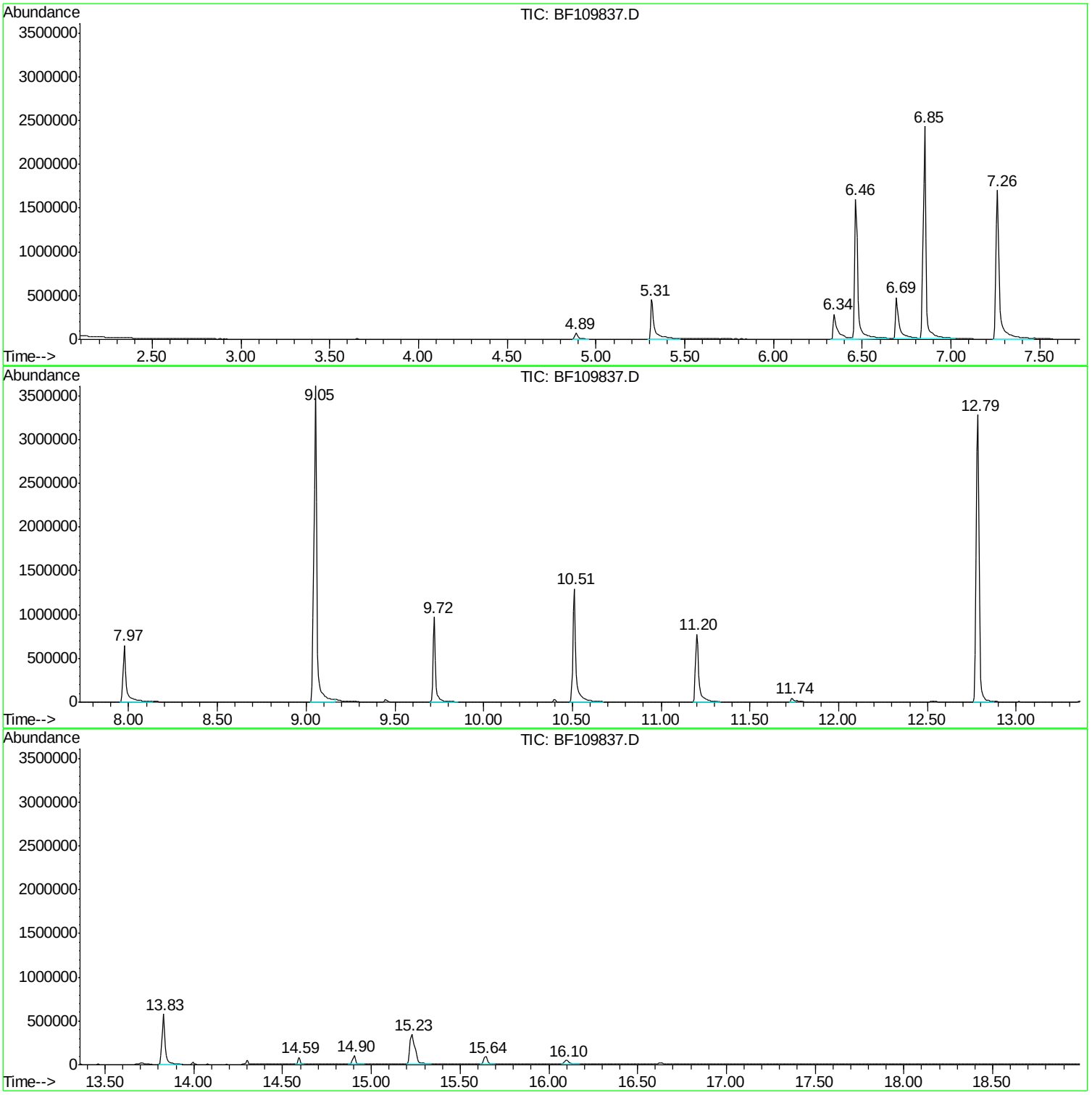
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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 F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

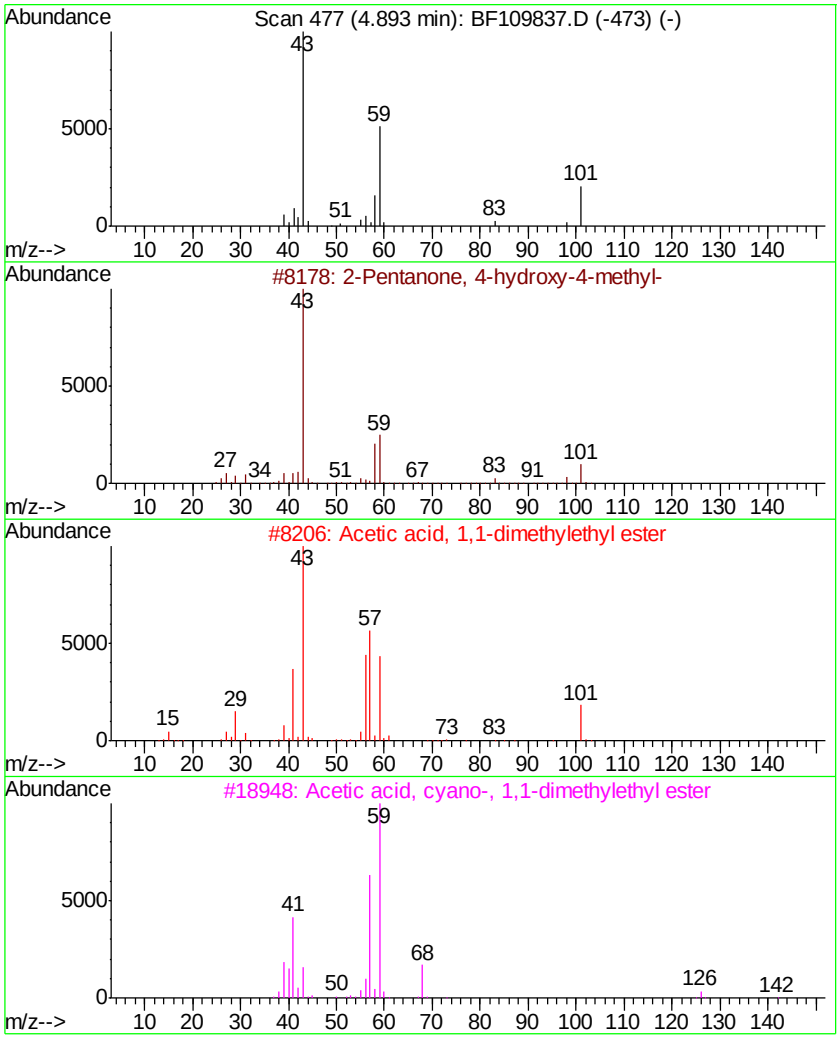
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

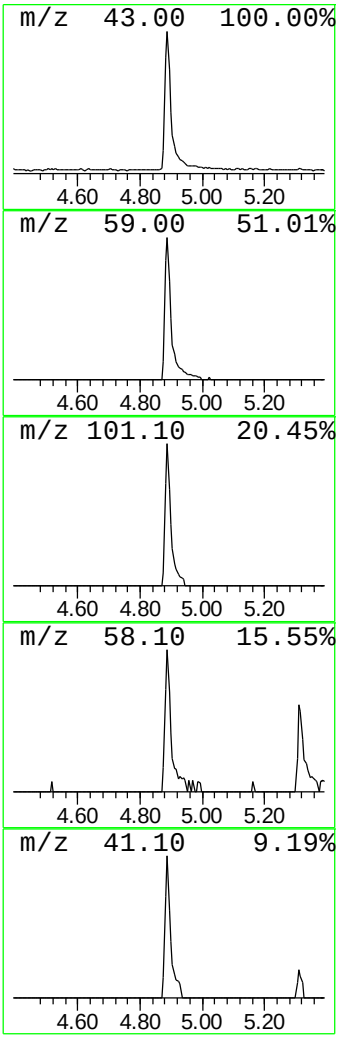
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.89 | 2.73 ng | 91419 | 1,4-Dichlorobenzene-d4 | 6.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 17 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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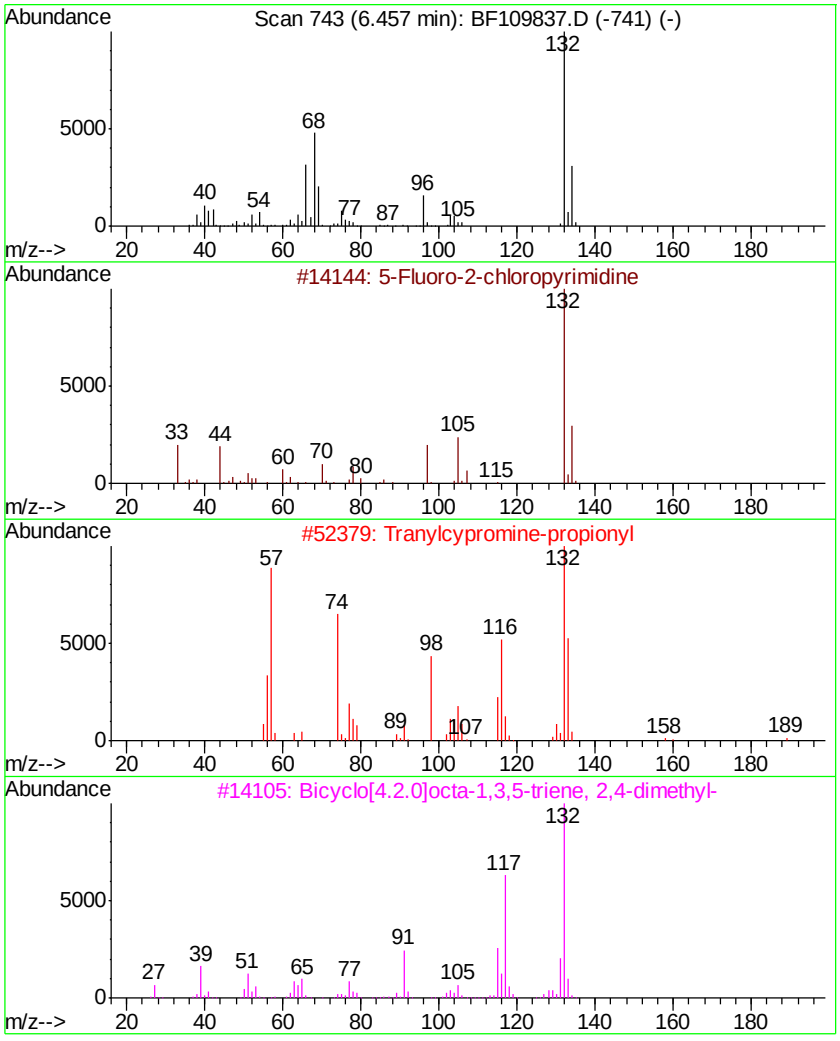
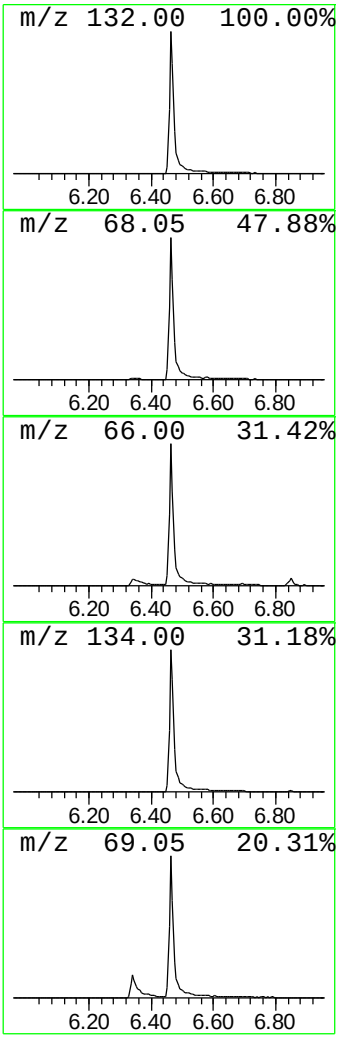
Peak Number 2 unknown6.46 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.46 | 55.86 ng | 1870180 | 1,4-Dichlorobenzene-d4 | 6.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 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 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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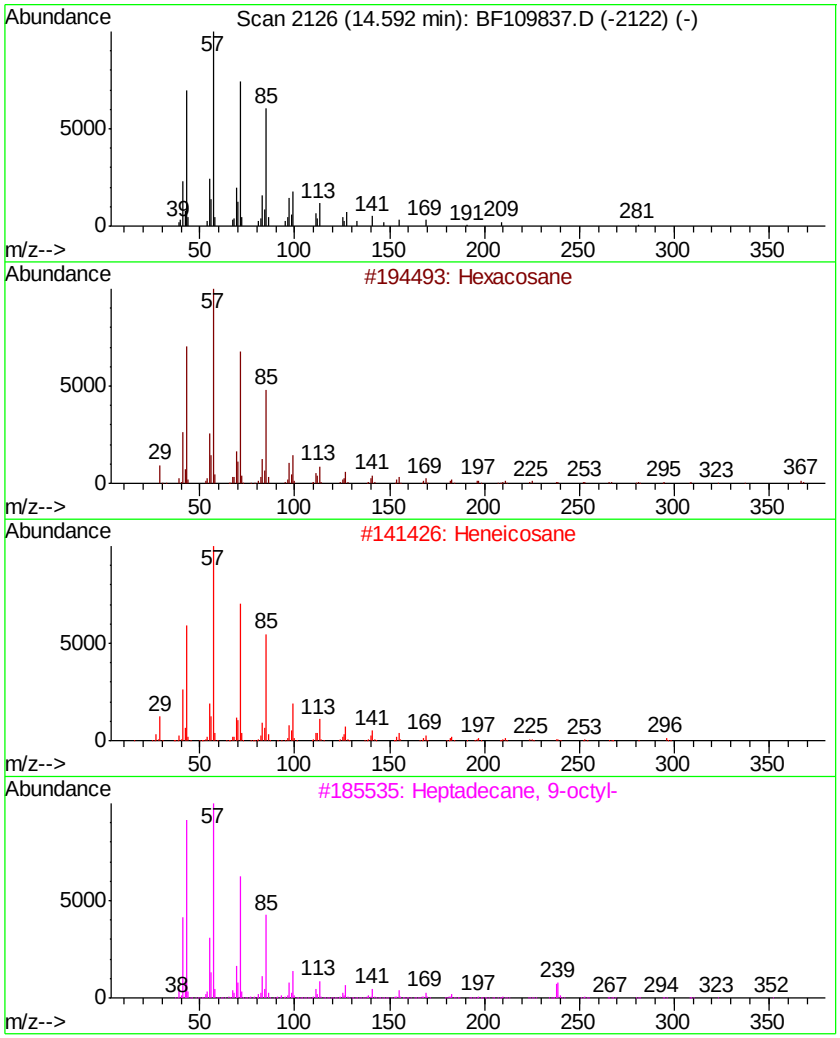
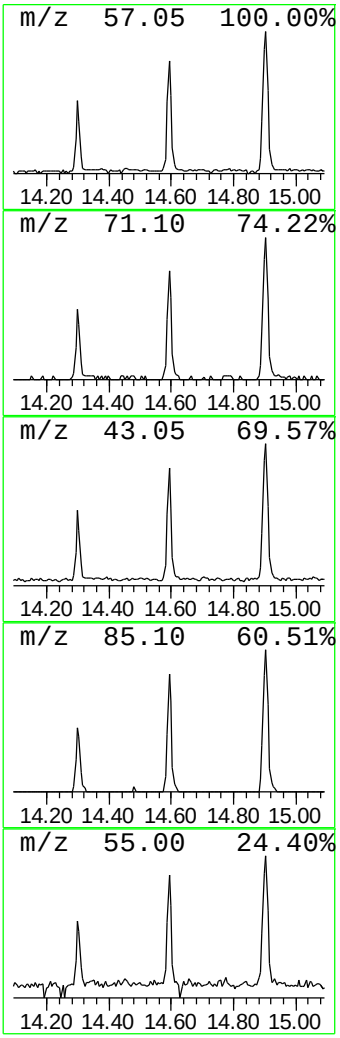
Peak Number 4 Hexacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.59 | 2.27 ng | 75321 | Perylene-d12 | 15.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 5 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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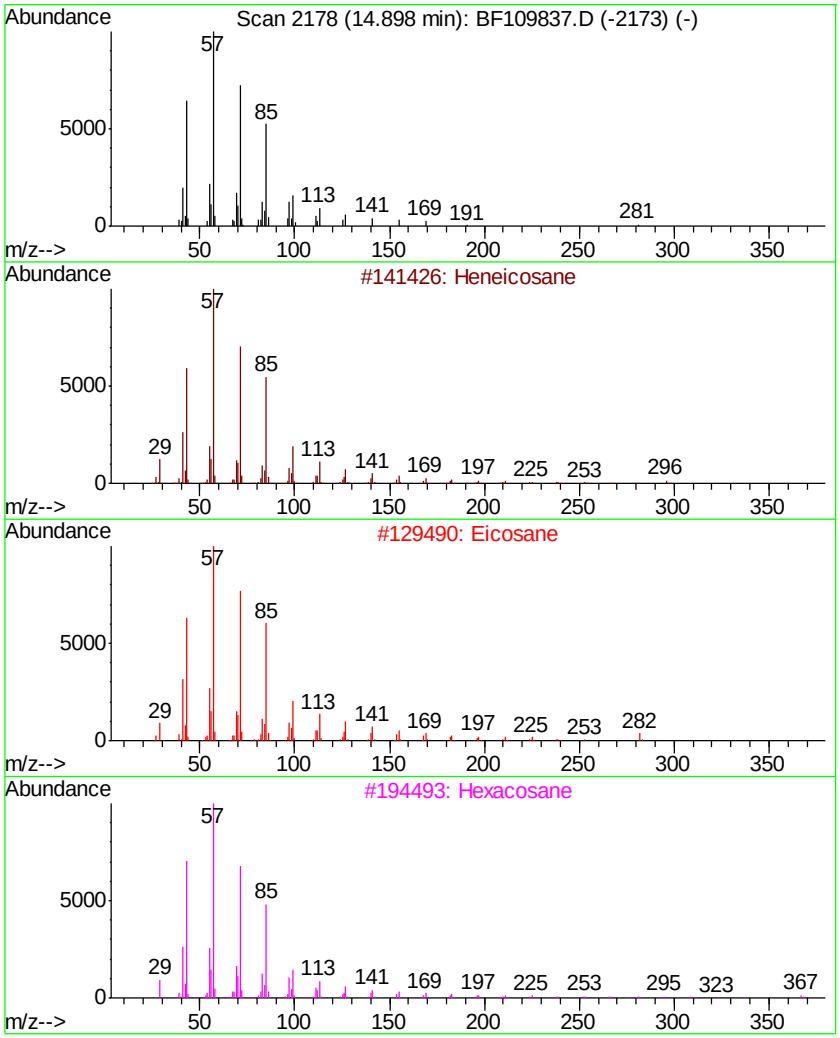
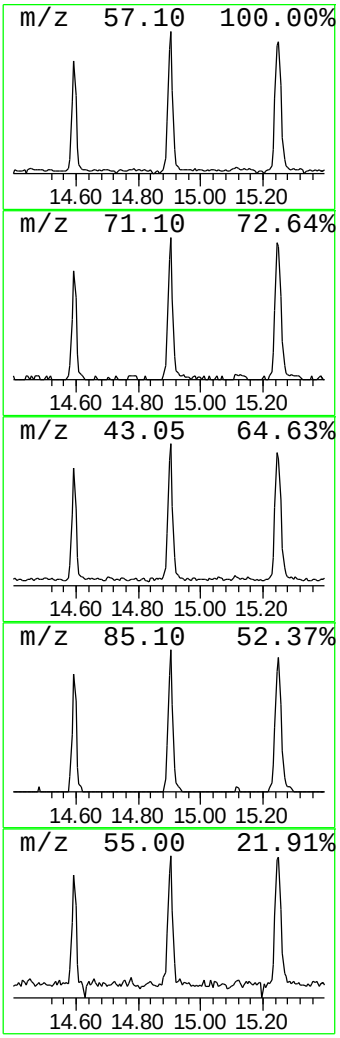
Peak Number 5 Heneicosane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.90 | 3.42 ng | 113413 | Perylene-d12 | 15.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 87 |
| 5 | 5-Ethyl-5-methylnonadecane | 310 | C22H46 | 1000360-42-7 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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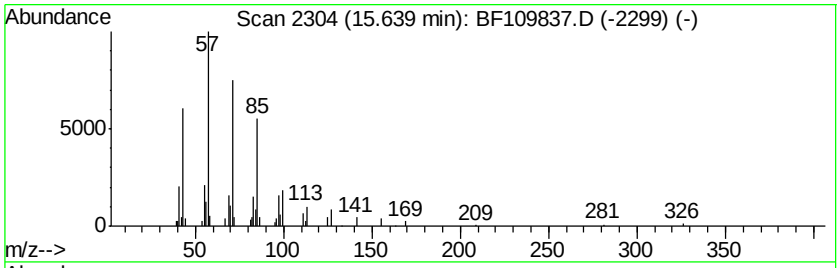
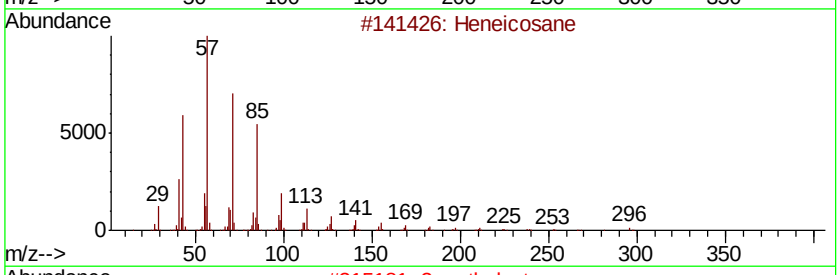
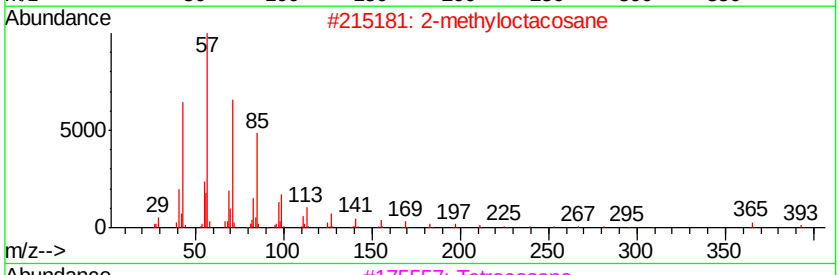
Peak Number 6 2-methyloctacosane Concentration Rank 4

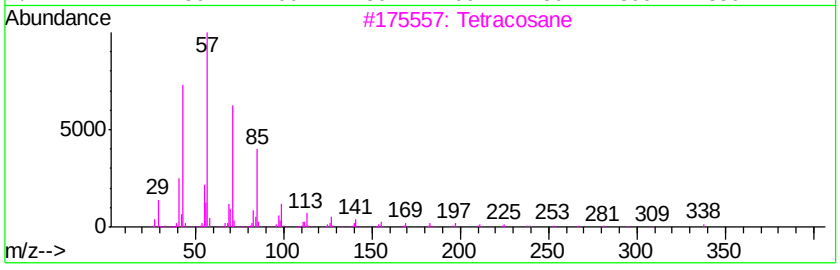
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.64 | 3.34 ng | 110922 | Perylene-d12 | 15.23 |

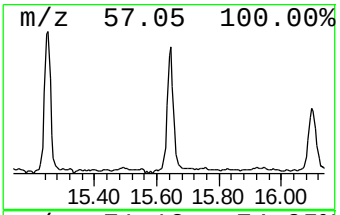
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 5 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 90 |

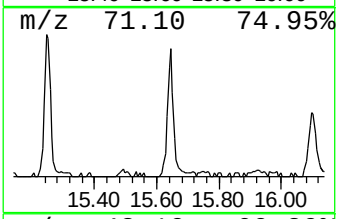


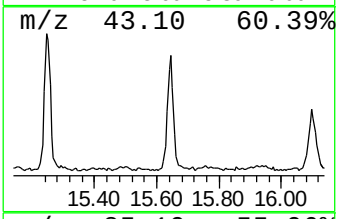



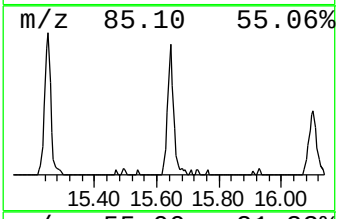



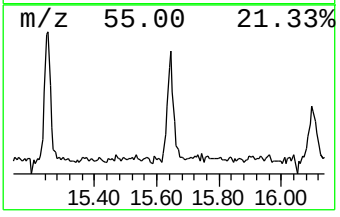



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

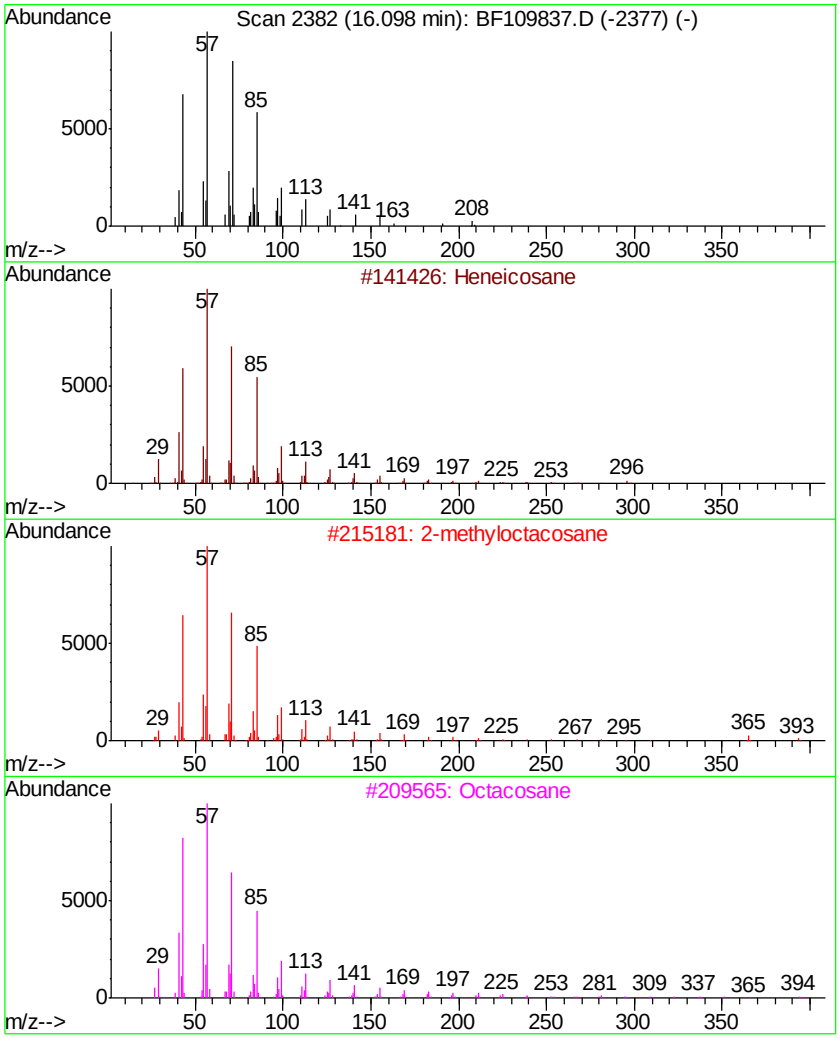
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

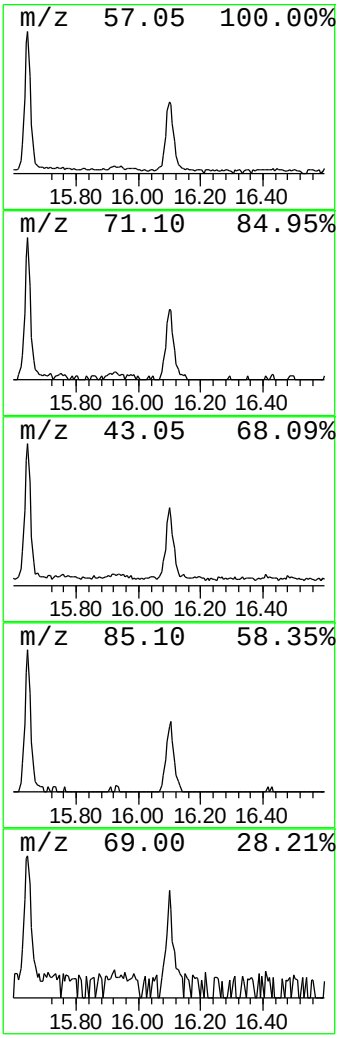
**********

Peak Number 7 Octacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.10 | 2.20 ng | 73030 | Perylene-d12 | 15.23 |

| 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 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 4 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 90 |
| 5 | 2-methyltetracosane | 352 | C25H52 | 1000376-72-6 | 90 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101218\
Data File : BF109837.D
Acq On : 12 Oct 2018 16:51
Operator : JU/SJ
Sample : J5371-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 100818-SIDI-E-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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... | 4.89 | 2.7 | ng | 91419 | 1 | 6.69 | 669616 | 20.0 |
| unknown6.46 | 6.46 | 55.9 | ng | 1870180 | 1 | 6.69 | 669616 | 20.0 |
| Hexacosane | 14.59 | 2.3 | ng | 75321 | 6 | 15.23 | 663890 | 20.0 |
| Heneicosane | 14.90 | 3.4 | ng | 113413 | 6 | 15.23 | 663890 | 20.0 |
| 2-methyloctacosane | 15.64 | 3.3 | ng | 110922 | 6 | 15.23 | 663890 | 20.0 |
| Octacosane | 16.10 | 2.2 | ng | 73030 | 6 | 15.23 | 663890 | 20.0 |