LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-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:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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 | 1.690 | 7 | 9 | 28 | rVB | 2087708 | 5077535 | 100.00% | 11.646% |
| 2 | 4.901 | 288 | 290 | 306 | rBV | 164930 | 525521 | 10.35% | 1.205% |
| 3 | 5.530 | 343 | 345 | 366 | rBV | 2492723 | 3785102 | 74.55% | 8.682% |
| 4 | 7.153 | 484 | 487 | 494 | rBV | 2624640 | 3824420 | 75.32% | 8.772% |
| 5 | 7.267 | 494 | 497 | 506 | rVB | 3102996 | 4038933 | 79.55% | 9.264% |
| 6 | 7.610 | 525 | 527 | 539 | rVB | 753044 | 1040464 | 20.49% | 2.386% |
| 7 | 7.850 | 545 | 548 | 564 | rVB | 1986181 | 2979730 | 58.68% | 6.834% |
| 8 | 8.525 | 604 | 607 | 625 | rBV | 1953222 | 2748609 | 54.13% | 6.304% |
| 9 | 9.645 | 702 | 705 | 717 | rBV | 897650 | 1386159 | 27.30% | 3.179% |
| 10 | 11.416 | 857 | 860 | 863 | rBV | 2761267 | 4441822 | 87.48% | 10.188% |
| 11 | 12.113 | 919 | 921 | 926 | rBV | 304580 | 386397 | 7.61% | 0.886% |
| 12 | 12.468 | 949 | 952 | 958 | rBV | 1099918 | 1639342 | 32.29% | 3.760% |
| 13 | 13.302 | 1021 | 1025 | 1028 | rBV | 131518 | 165683 | 3.26% | 0.380% |
| 14 | 13.656 | 1050 | 1056 | 1059 | rBV | 35048 | 81822 | 1.61% | 0.188% |
| 15 | 13.771 | 1062 | 1066 | 1072 | rBV | 1851964 | 2835448 | 55.84% | 6.504% |
| 16 | 14.079 | 1090 | 1093 | 1104 | rVB | 126566 | 244022 | 4.81% | 0.560% |
| 17 | 14.811 | 1154 | 1157 | 1160 | rBV | 52924 | 70025 | 1.38% | 0.161% |
| 18 | 14.879 | 1160 | 1163 | 1173 | rVB | 926062 | 1510278 | 29.74% | 3.464% |
| 19 | 17.051 | 1351 | 1353 | 1356 | rVB | 50700 | 52283 | 1.03% | 0.120% |
| 20 | 17.211 | 1364 | 1367 | 1370 | rBV | 3190767 | 3984950 | 78.48% | 9.140% |
| 21 | 18.503 | 1474 | 1480 | 1482 | rBV | 61873 | 174690 | 3.44% | 0.401% |
| 22 | 18.560 | 1482 | 1485 | 1487 | rVV | 758978 | 1264916 | 24.91% | 2.901% |
| 23 | 18.606 | 1487 | 1489 | 1496 | rVB | 132361 | 243467 | 4.79% | 0.558% |
| 24 | 19.577 | 1571 | 1574 | 1576 | rBV | 69885 | 92356 | 1.82% | 0.212% |
| 25 | 19.680 | 1580 | 1583 | 1586 | rBV | 139109 | 145618 | 2.87% | 0.334% |
| 26 | 20.217 | 1628 | 1630 | 1636 | rVV | 603520 | 859133 | 16.92% | 1.971% |

Sum of corrected areas: 43598725

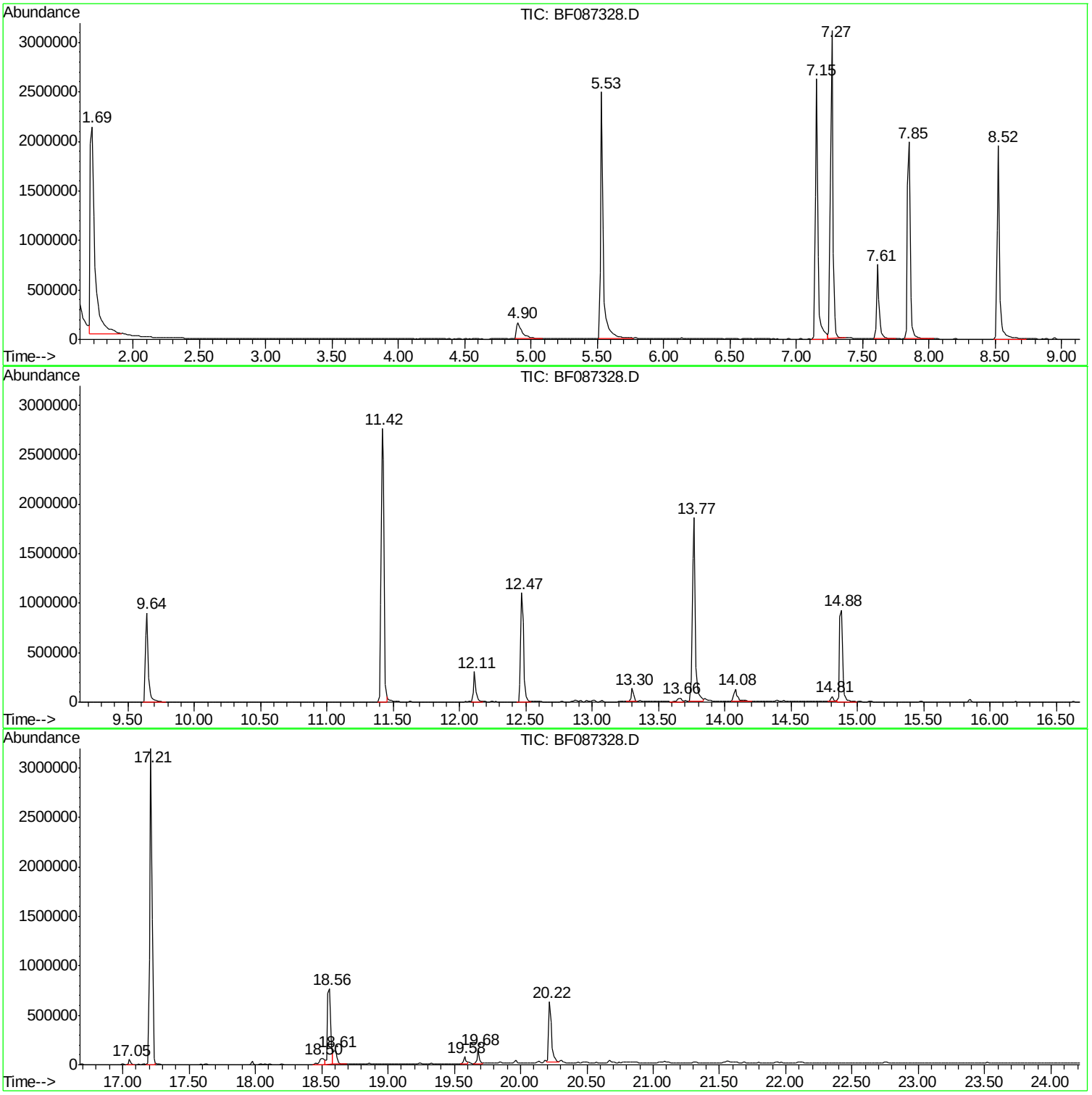
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

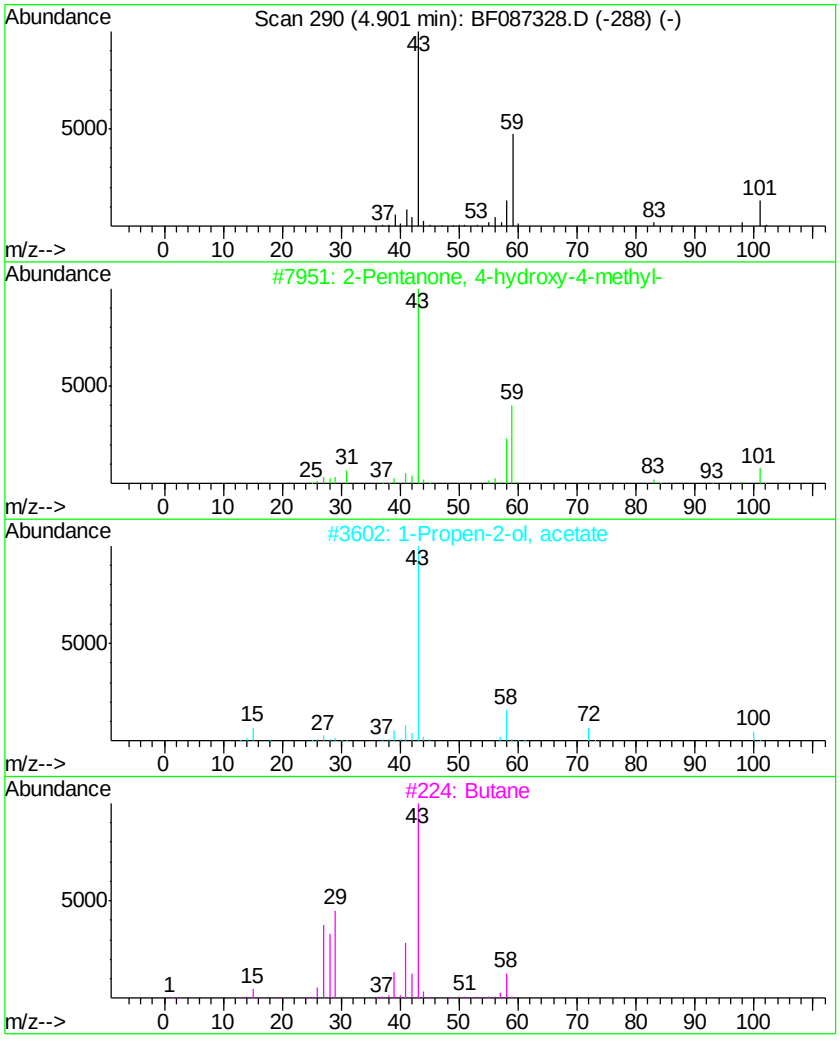
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

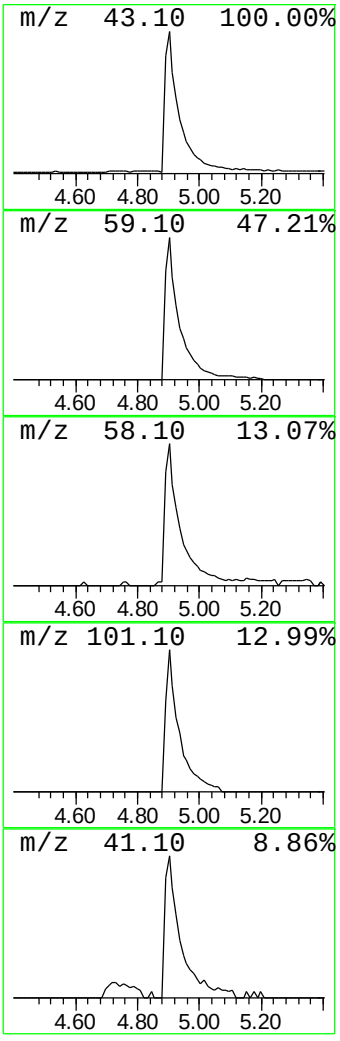
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.90 | 10.10 ng | 525521 | 1,4-Dichlorobenzene-d4 | 7.61 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 3 | Butane | 58 | C4H10 | 000106-97-8 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Diacetamide | 101 | C4H7NO2 | 000625-77-4 | 9 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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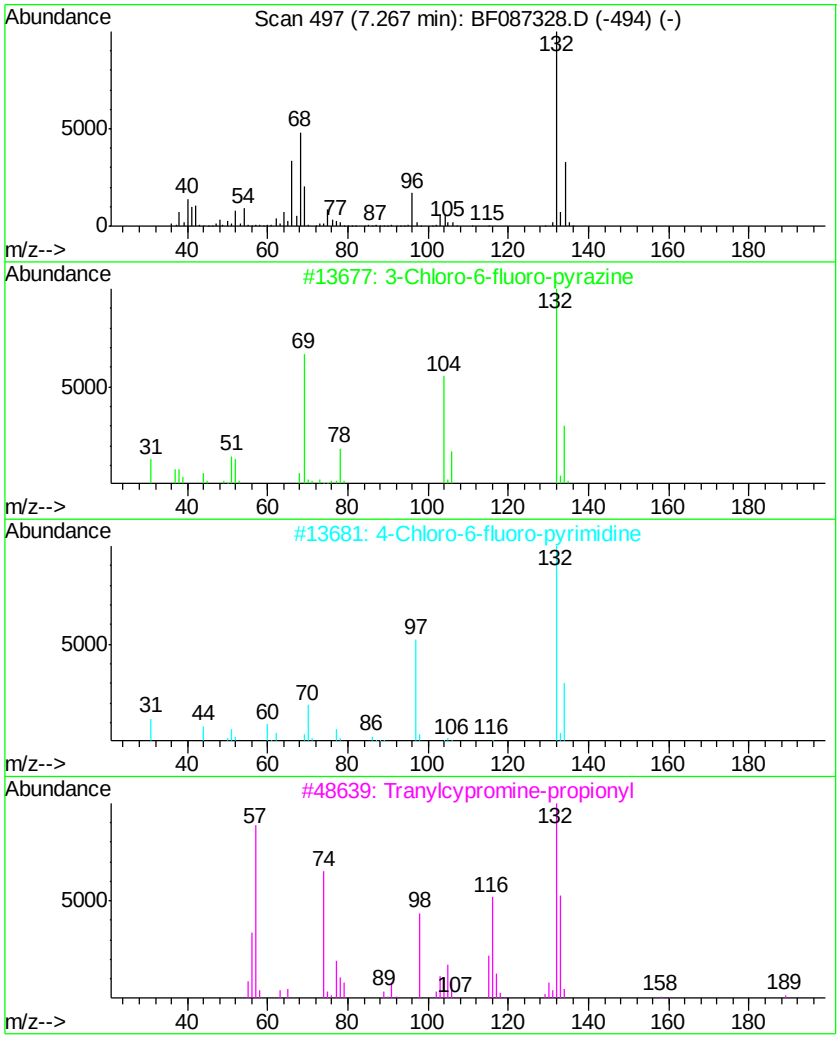
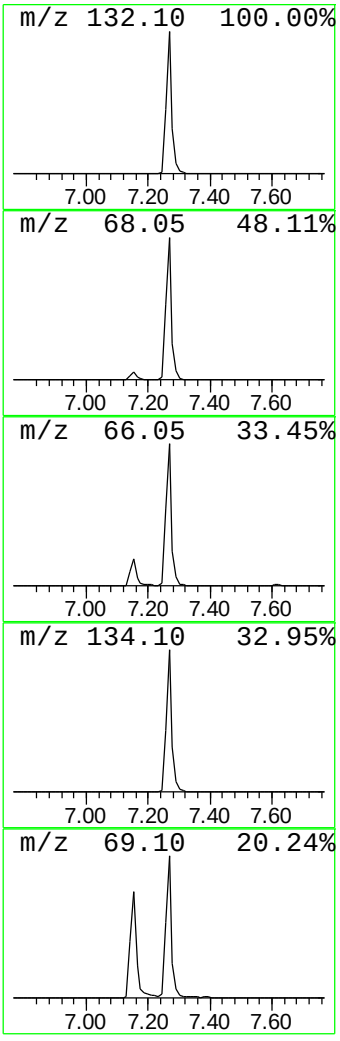
Peak Number 3 unknown7.27 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.27 | 77.64 ng | 4038930 | 1,4-Dichlorobenzene-d4 | 7.61 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 22 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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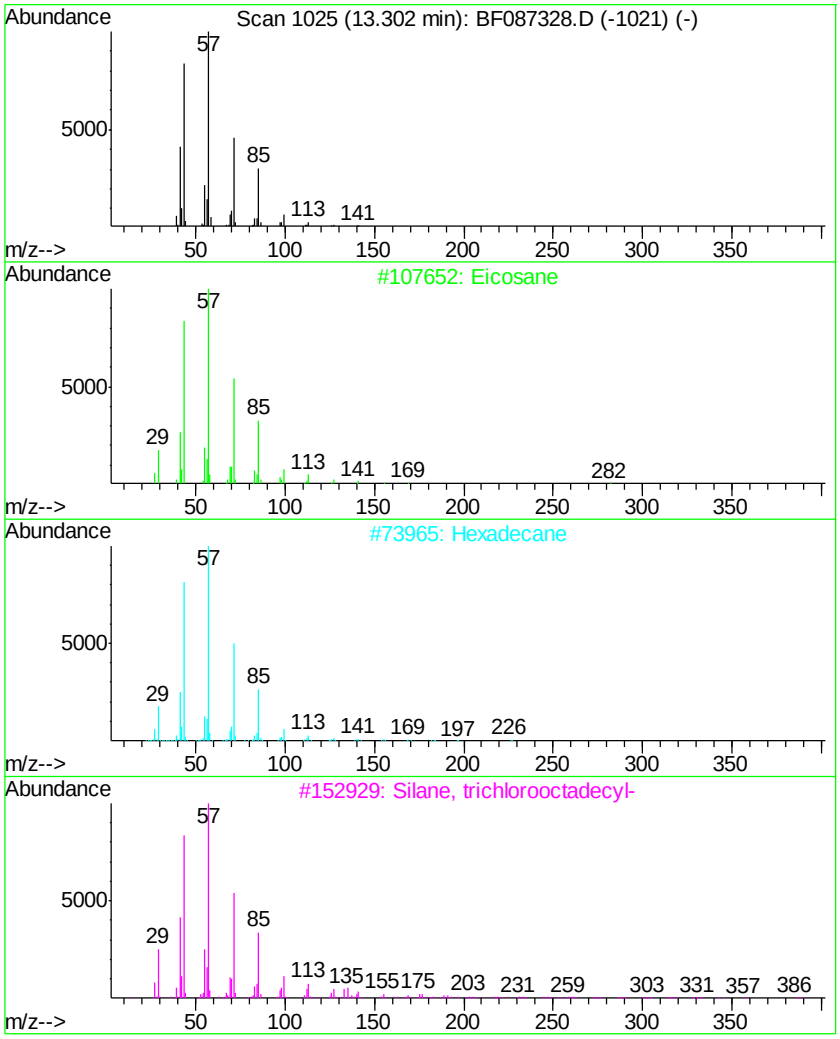
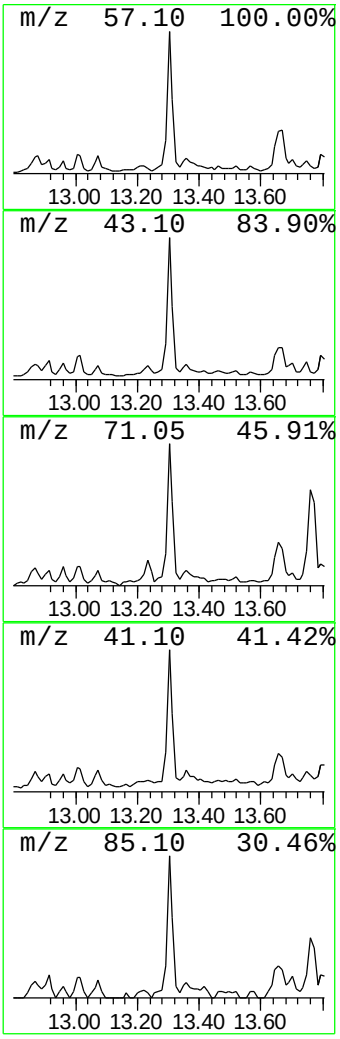
Peak Number 5 Eicosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.30 | 2.02 ng | 165683 | Acenaphthene-d10 | 12.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 3 | Silane, trichlorooctadecyl- | 386 | C18H37Cl3Si | 000112-04-9 | 90 |
| 4 | Tridecane | 184 | C13H28 | 000629-50-5 | 86 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 80 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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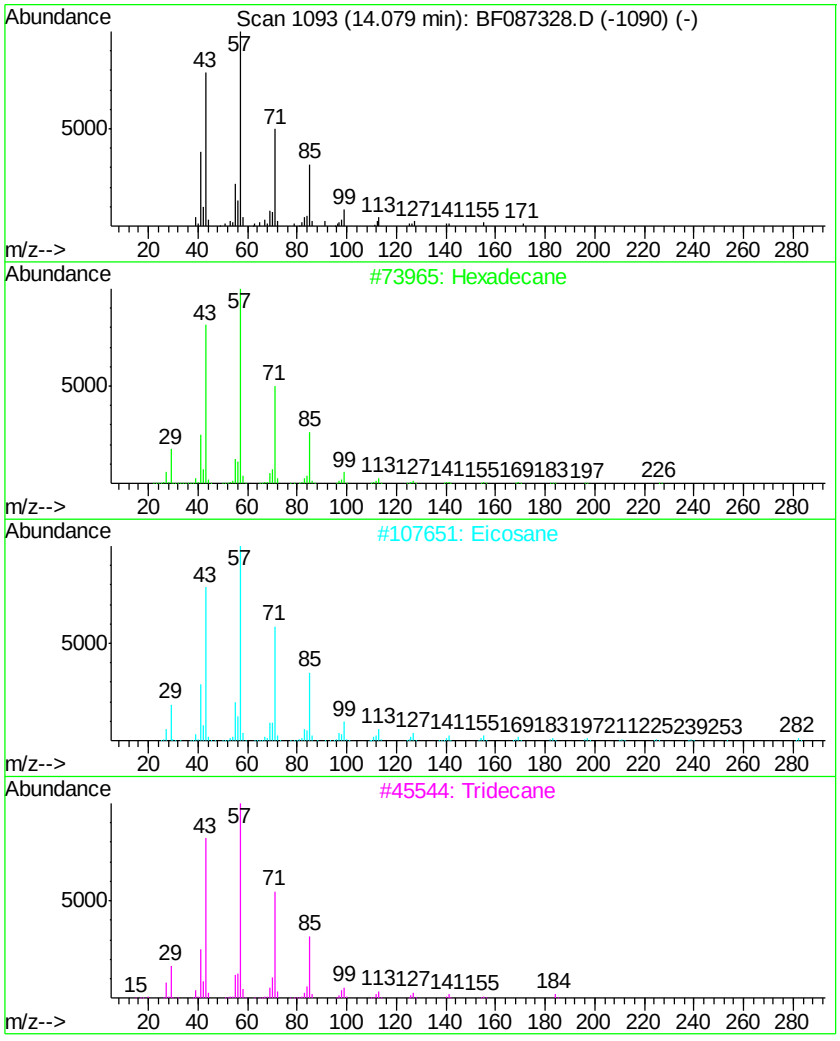
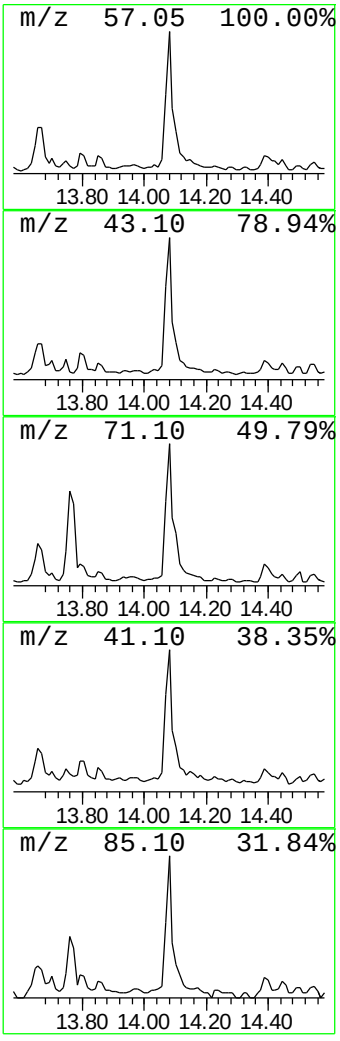
Peak Number 6 Hexadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.08 | 3.23 ng | 244022 | Phenanthrene-d10 | 14.88 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 86 |
| 3 | Tridecane | 184 | C13H28 | 000629-50-5 | 86 |
| 4 | Decane, 3-bromo- | 220 | C10H21Br | 030571-71-2 | 80 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 80 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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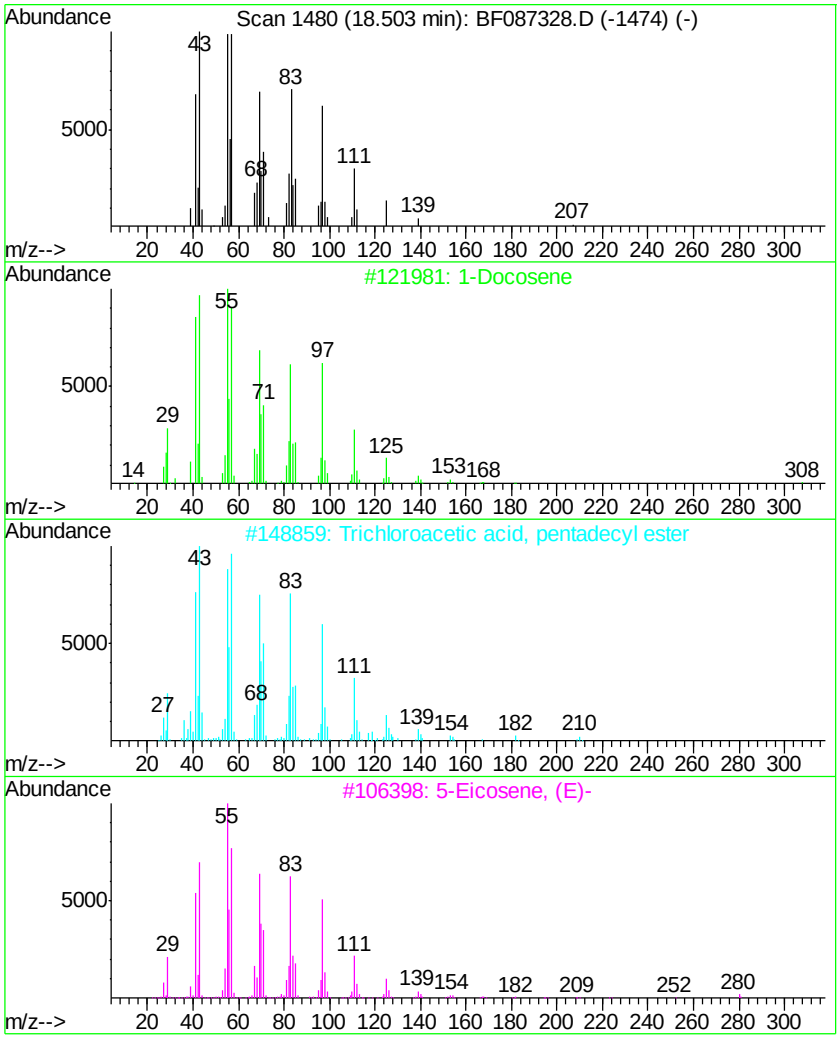
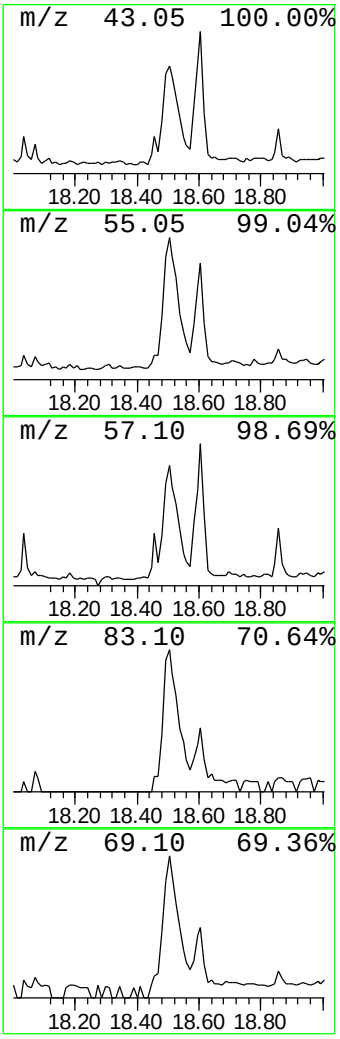
Peak Number 7 1-Docosene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.50 | 2.76 ng | 174690 | Chrysene-d12 | 18.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 94 |
| 2 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 3 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 91 |
| 4 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 91 |
| 5 | 1-Eicosanol | 298 | C20H42O | 000629-96-9 | 91 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
Data File : BF087328.D
Acq On : 24 May 2016 7:18
Operator : UM/SJ
Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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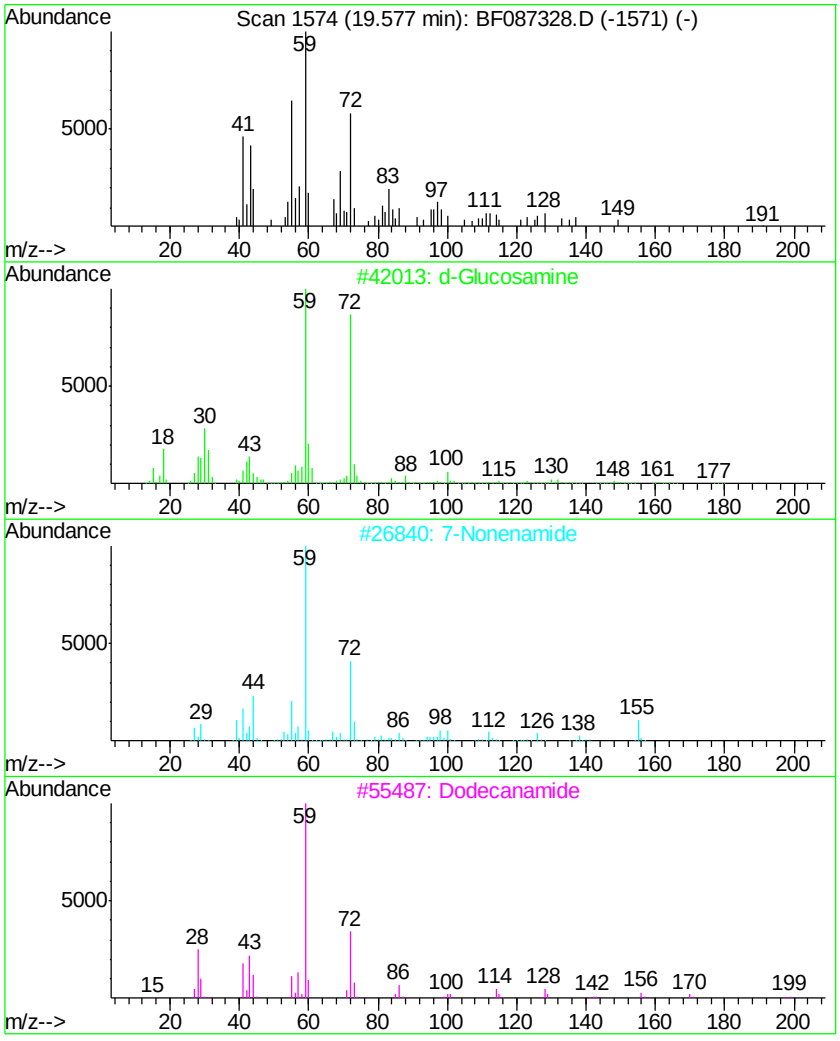
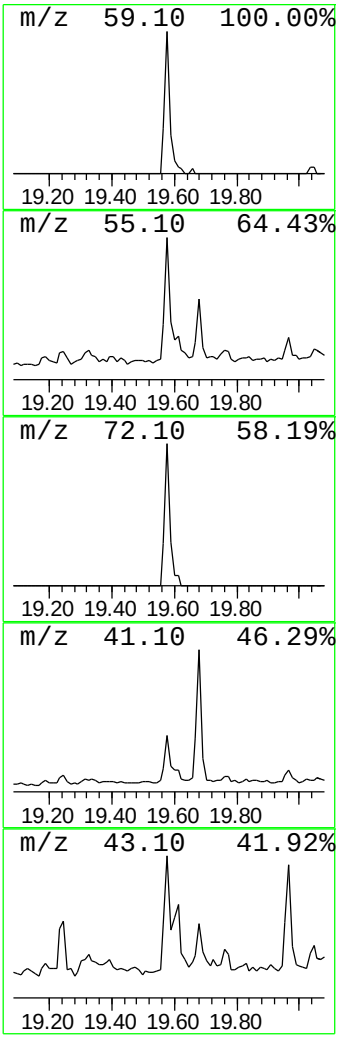
Peak Number 8 unknown19.58 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.58 | 2.15 ng | 92356 | Perylene-d12 | 20.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | d-Glucosamine | 179 | C6H13NO5 | 000090-77-7 | 47 |
| 2 | 7-Nonenamide | 155 | C9H17NO | 090949-53-4 | 47 |
| 3 | Dodecanamide | 199 | C12H25NO | 001120-16-7 | 47 |
| 4 | Cyclohexanecarboxamide | 127 | C7H13NO | 001122-56-1 | 35 |
| 5 | Mannosamine hydrochloride | 179 | C6H13NO5 | 1000127-68-8 | 27 |



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Data File : BF087328.D
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Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-19-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

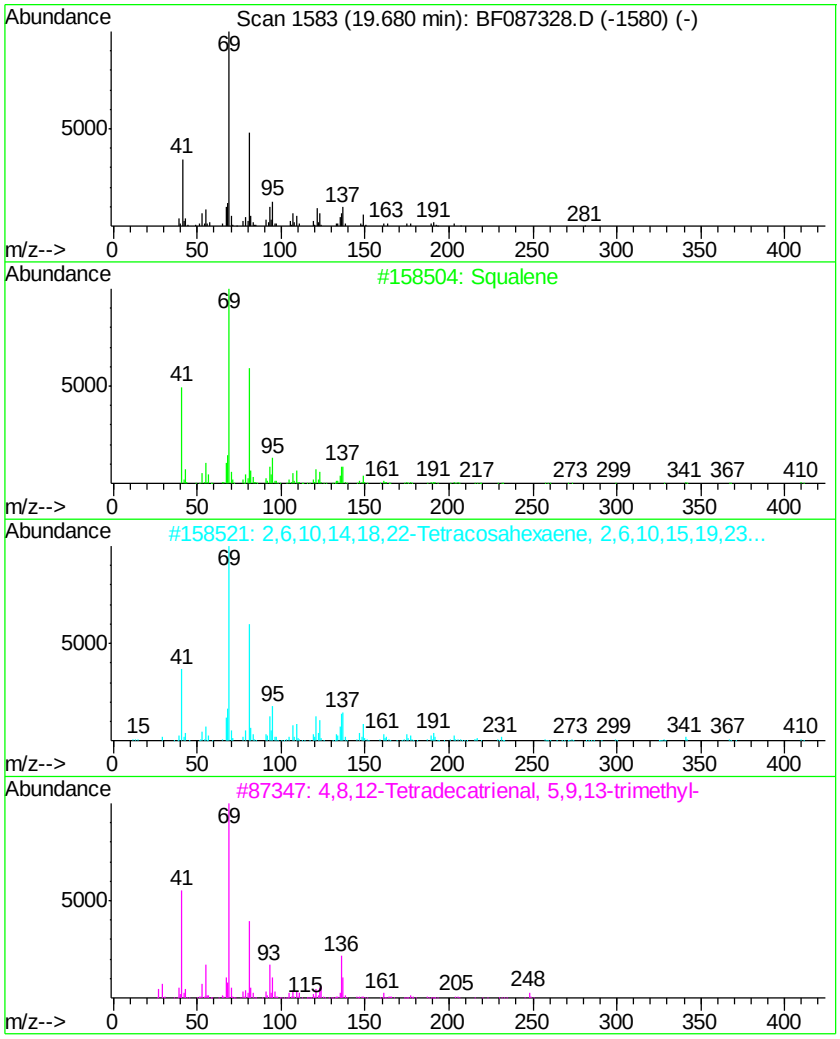
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

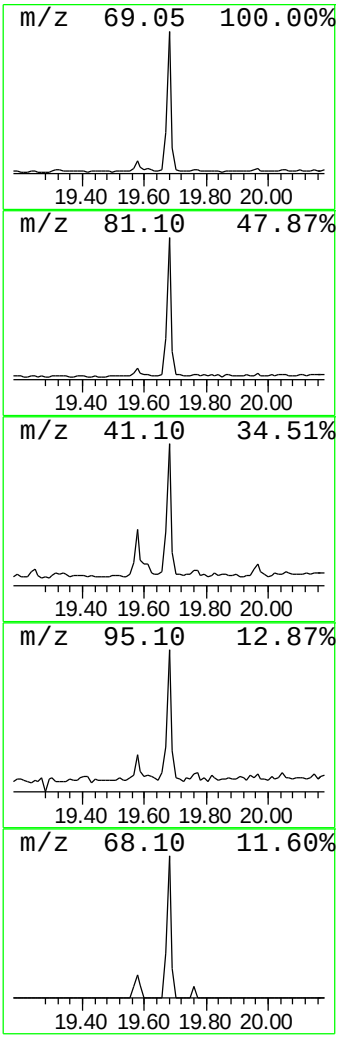
**********

Peak Number 9 Squalene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.68 | 3.39 ng | 145618 | Perylene-d12 | 20.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 007683-64-9 | 91 |
| 2 | 2,6,10,14,18,22-Tetracosahexaene... | 410 | C30H50 | 000111-02-4 | 91 |
| 3 | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O | 066408-55-7 | 78 |
| 4 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 72 |
| 5 | 2-Octene, 2-methyl-6-methylene- | 138 | C10H18 | 010054-09-8 | 50 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052316\
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Sample : H3168-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.90 | 10.1 | ng | 525521 | 1 | 7.61 | 1040460 | 20.0 |
| unknown7.27 | 7.27 | 77.6 | ng | 4038930 | 1 | 7.61 | 1040460 | 20.0 |
| Eicosane | 13.30 | 2.0 | ng | 165683 | 3 | 12.47 | 1639340 | 20.0 |
| Hexadecane | 14.08 | 3.2 | ng | 244022 | 4 | 14.88 | 1510280 | 20.0 |
| 1-Docosene | 18.50 | 2.8 | ng | 174690 | 5 | 18.56 | 1264920 | 20.0 |
| unknown19.58 | 19.58 | 2.1 | ng | 92356 | 6 | 20.22 | 859133 | 20.0 |
| Squalene | 19.68 | 3.4 | ng | 145618 | 6 | 20.22 | 859133 | 20.0 |