LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

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-BF080818.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 | 5.231 | 489 | 492 | 500 | rVB | 35763 | 38685 | 1.11% | 0.199% |
| 2 | 5.625 | 555 | 559 | 576 | rVB | 911125 | 827933 | 23.69% | 4.258% |
| 3 | 6.613 | 724 | 727 | 731 | rBV | 561131 | 504422 | 14.43% | 2.594% |
| 4 | 6.766 | 749 | 753 | 757 | rBV | 1856696 | 1667095 | 47.69% | 8.574% |
| 5 | 7.001 | 789 | 793 | 796 | rBV | 719627 | 644048 | 18.42% | 3.312% |
| 6 | 7.154 | 815 | 819 | 823 | rBV | 2612741 | 2517422 | 72.02% | 12.948% |
| 7 | 7.566 | 883 | 889 | 892 | rBV | 1983591 | 2011459 | 57.54% | 10.345% |
| 8 | 8.283 | 1007 | 1011 | 1023 | rBV | 840340 | 739848 | 21.17% | 3.805% |
| 9 | 9.354 | 1187 | 1193 | 1197 | rBV | 3676108 | 3495528 | 100.00% | 17.978% |
| 10 | 9.742 | 1256 | 1259 | 1267 | rBV | 90911 | 82982 | 2.37% | 0.427% |
| 11 | 10.042 | 1307 | 1310 | 1322 | rVB2 | 819604 | 706118 | 20.20% | 3.632% |
| 12 | 10.701 | 1419 | 1422 | 1426 | rBV | 71466 | 59300 | 1.70% | 0.305% |
| 13 | 10.836 | 1441 | 1445 | 1457 | rBV | 1113392 | 1056628 | 30.23% | 5.434% |
| 14 | 11.536 | 1561 | 1564 | 1573 | rBV | 691126 | 625458 | 17.89% | 3.217% |
| 15 | 13.124 | 1830 | 1834 | 1837 | rBV | 3006641 | 2588428 | 74.05% | 13.313% |
| 16 | 13.671 | 1923 | 1927 | 1930 | rBV2 | 63149 | 56454 | 1.62% | 0.290% |
| 17 | 14.001 | 1980 | 1983 | 1987 | rBV | 74743 | 62195 | 1.78% | 0.320% |
| 18 | 14.065 | 1987 | 1994 | 2001 | rBV8 | 14819 | 47236 | 1.35% | 0.243% |
| 19 | 14.189 | 2012 | 2015 | 2022 | rBV | 696457 | 689135 | 19.71% | 3.544% |
| 20 | 14.318 | 2033 | 2037 | 2040 | rBV | 100808 | 89577 | 2.56% | 0.461% |
| 21 | 14.624 | 2086 | 2089 | 2094 | rVB | 106233 | 103589 | 2.96% | 0.533% |
| 22 | 14.954 | 2141 | 2145 | 2148 | rVB | 89778 | 97686 | 2.79% | 0.502% |
| 23 | 15.036 | 2155 | 2159 | 2164 | rBV | 35143 | 39672 | 1.13% | 0.204% |
| 24 | 15.312 | 2202 | 2206 | 2210 | rBV | 77645 | 90779 | 2.60% | 0.467% |
| 25 | 15.748 | 2272 | 2280 | 2288 | rBV | 331371 | 536232 | 15.34% | 2.758% |
| 26 | 16.195 | 2351 | 2356 | 2361 | rVB2 | 40181 | 65384 | 1.87% | 0.336% |

Sum of corrected areas: 19443293

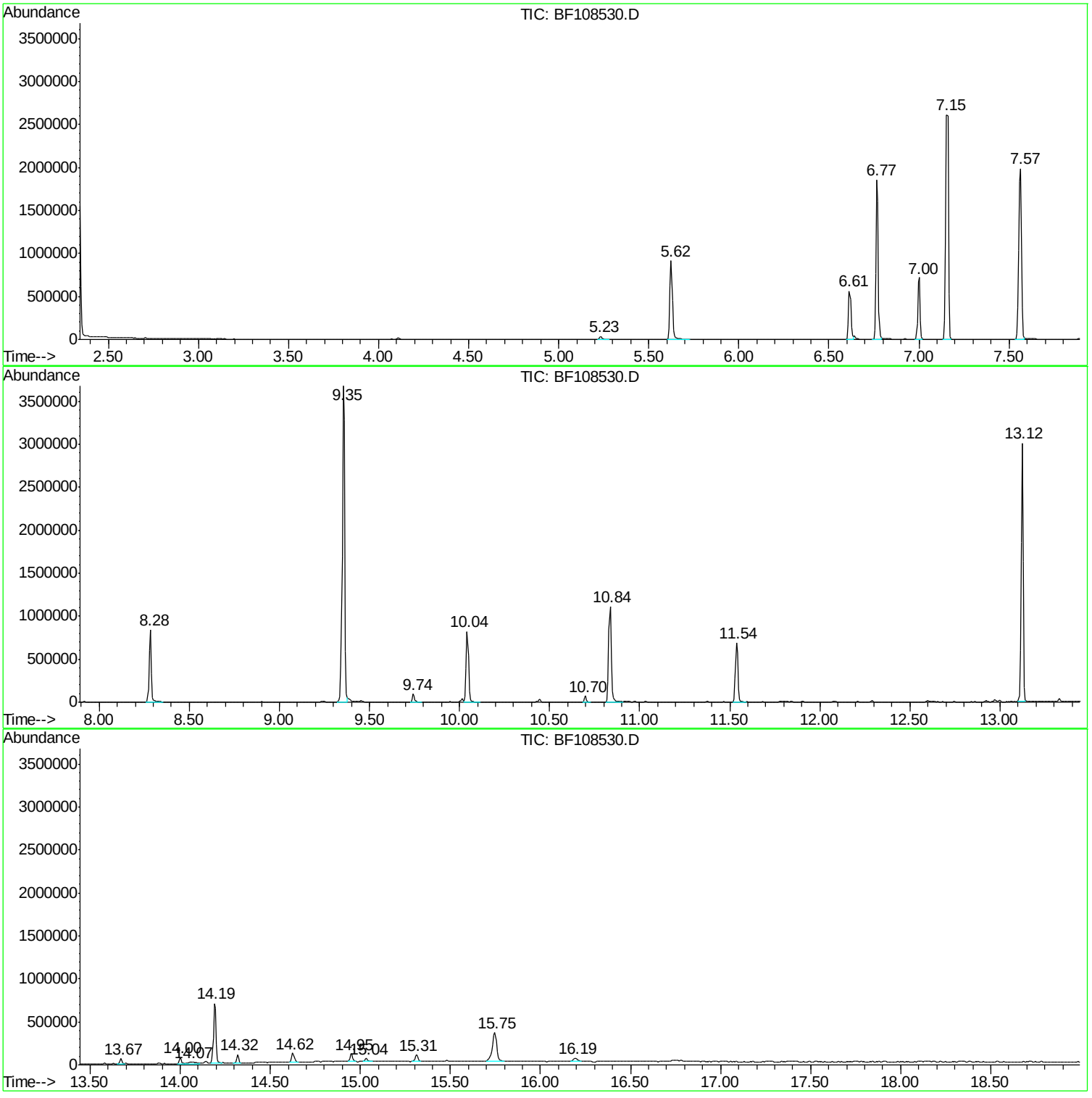
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

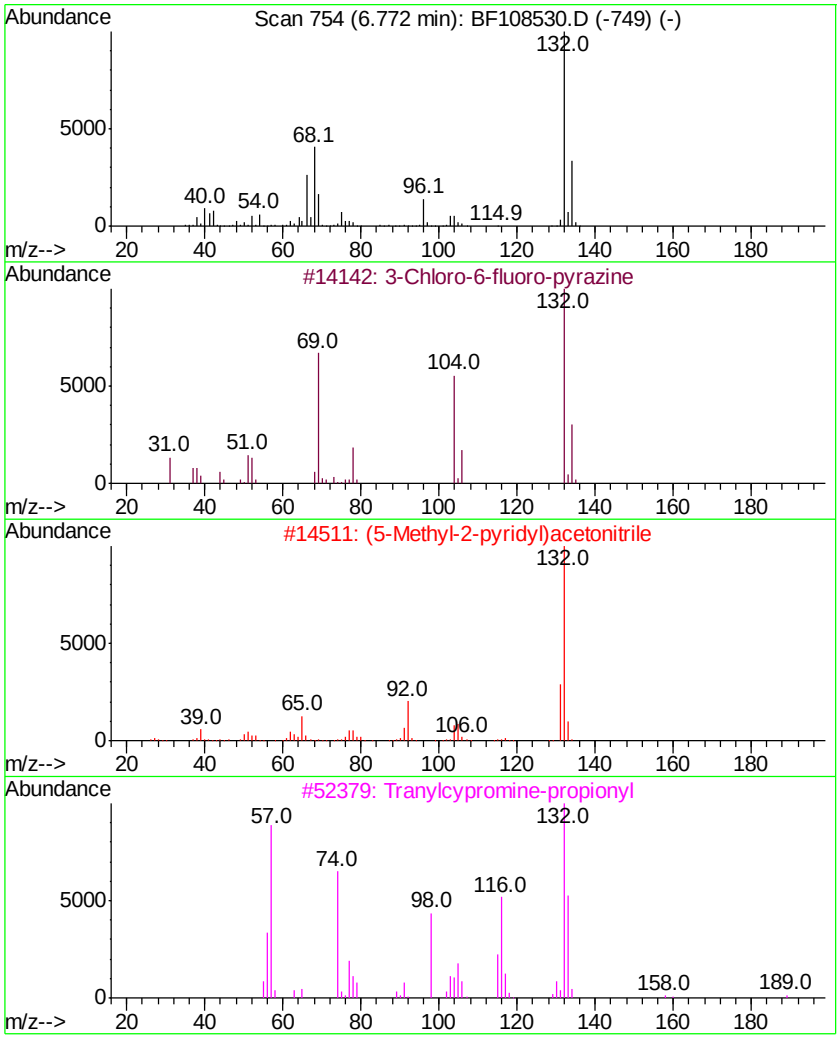
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

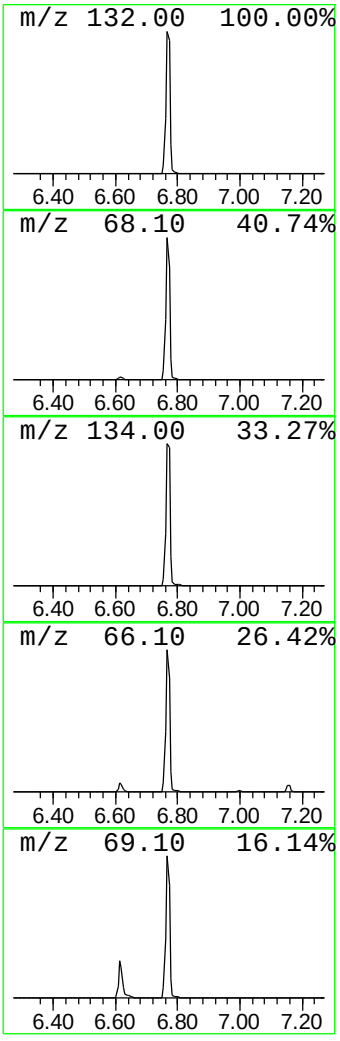
**********

Peak Number 1 unknown6.77 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.77 | 51.77 ng | 1667100 | 1,4-Dichlorobenzene-d4 | 7.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 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 F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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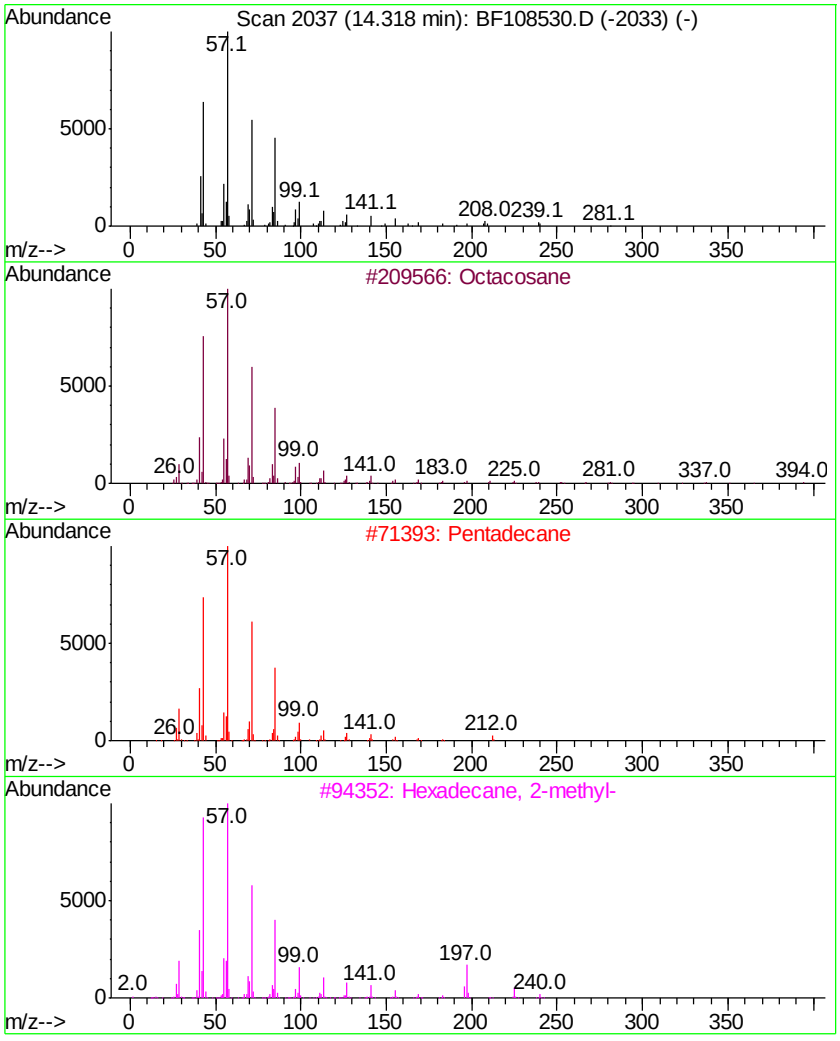
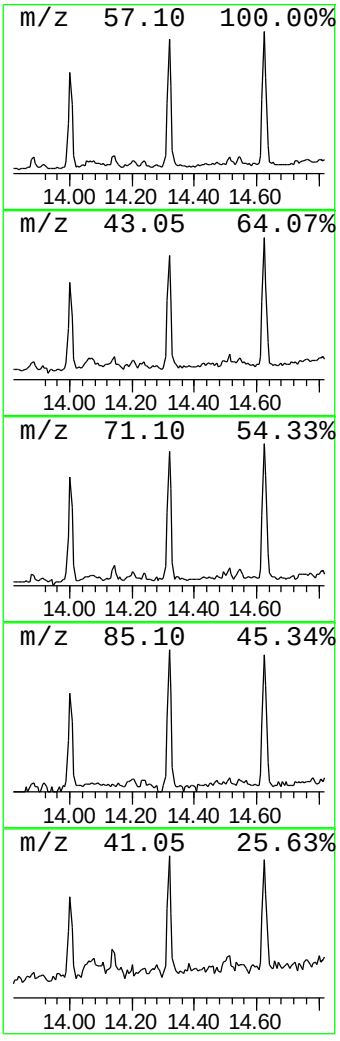
Peak Number 3 Octacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.32 | 2.60 ng | 89577 | Chrysene-d12 | 14.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 91 |
| 3 | Hexadecane, 2-methyl- | 240 | C17H36 | 001560-92-5 | 91 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 91 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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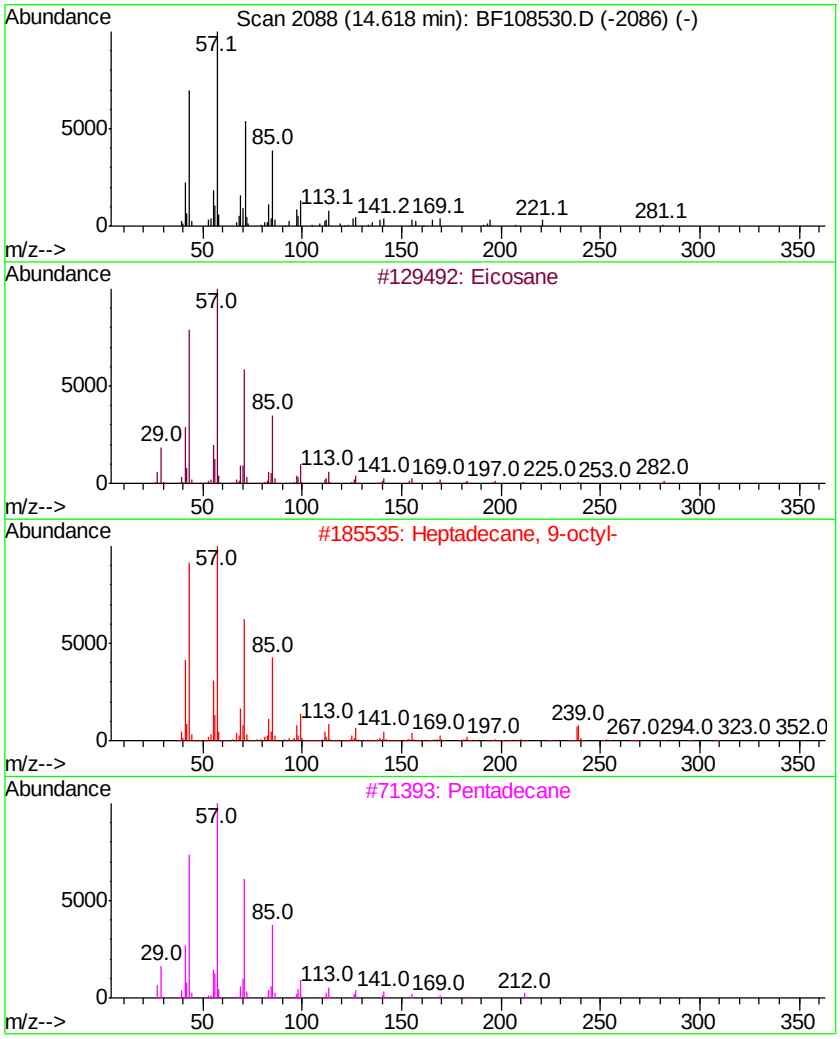
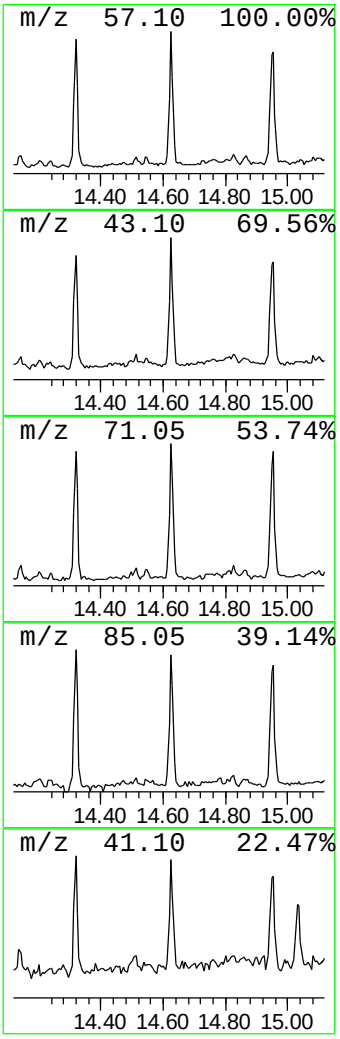
Peak Number 4 Eicosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.62 | 3.01 ng | 103589 | Chrysene-d12 | 14.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 98 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 91 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 5 | Docosane | 310 | C22H46 | 000629-97-0 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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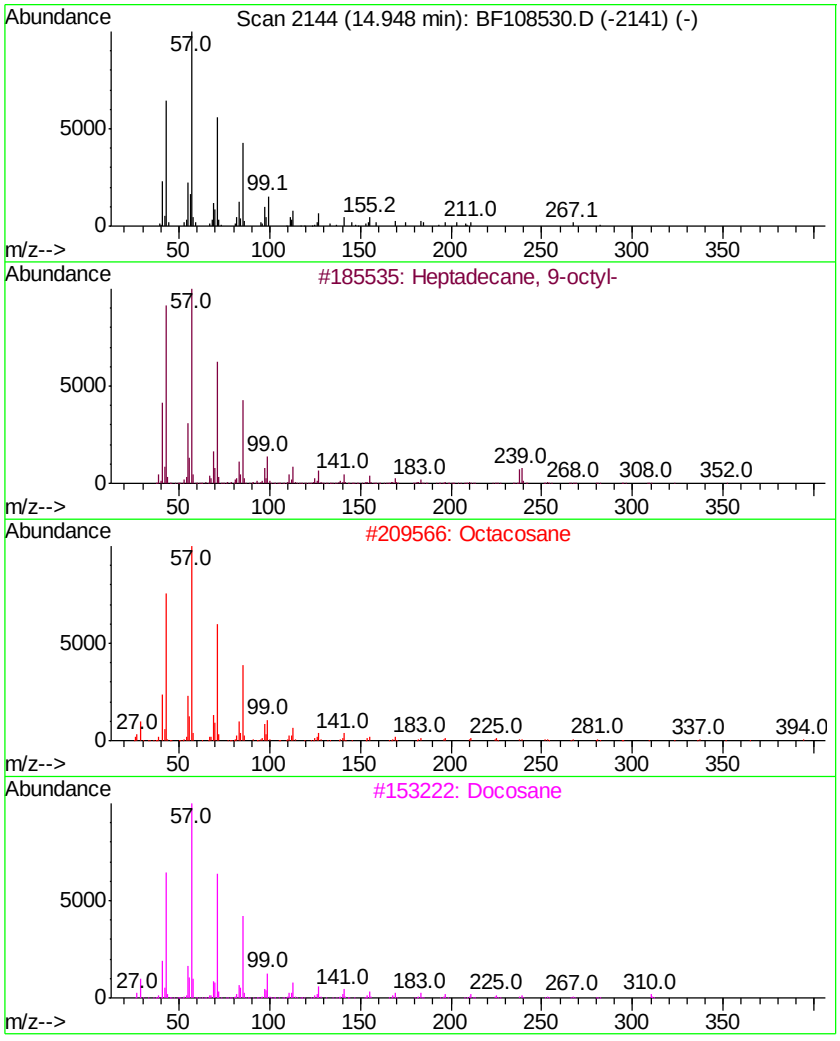
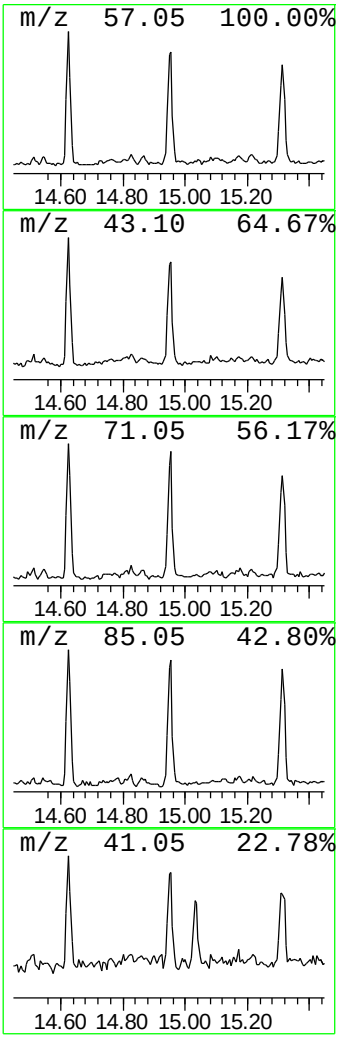
Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.95 | 2.84 ng | 97686 | Chrysene-d12 | 14.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Docosane | 310 | C22H46 | 000629-97-0 | 91 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 91 |
| 5 | Eicosane, 2-methyl- | 296 | C21H44 | 001560-84-5 | 90 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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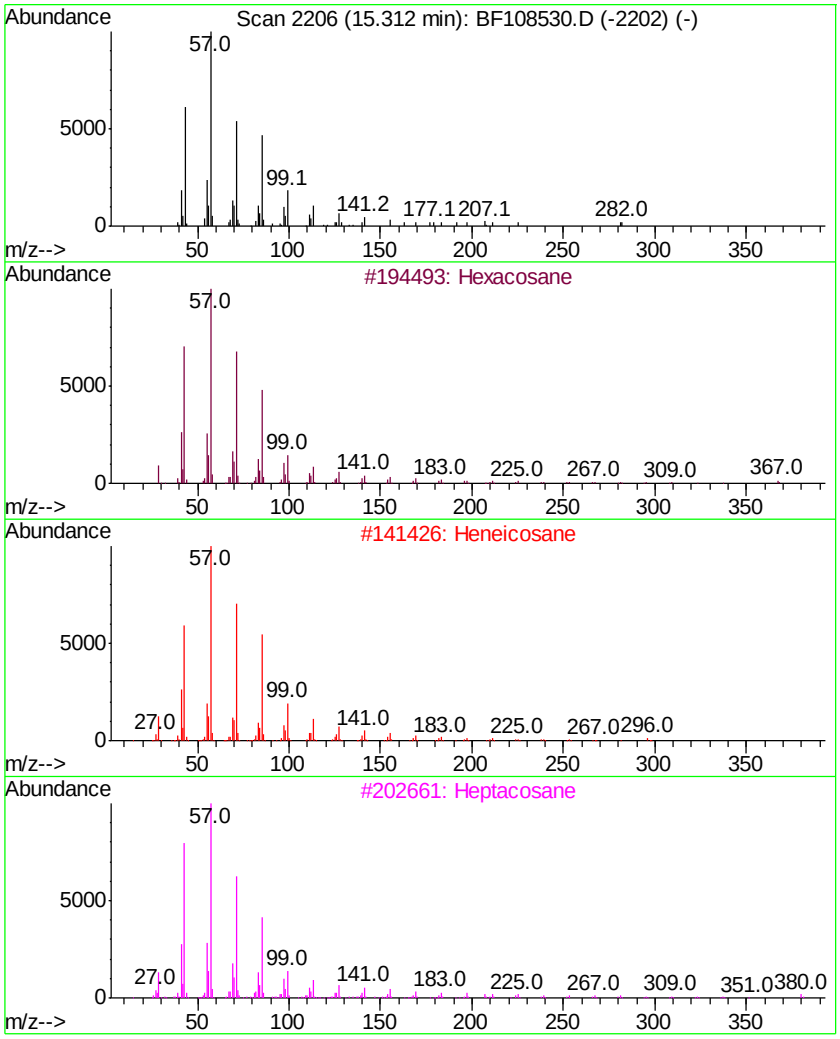
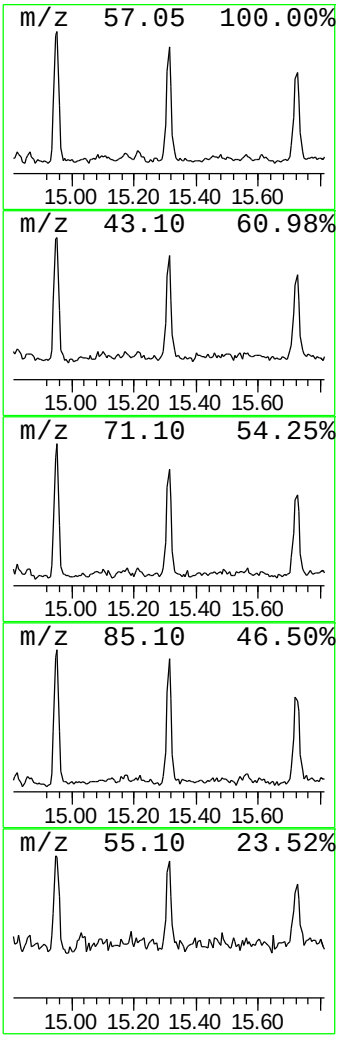
Peak Number 6 Hexacosane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.31 | 3.39 ng | 90779 | Perylene-d12 | 15.75 |

| 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 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

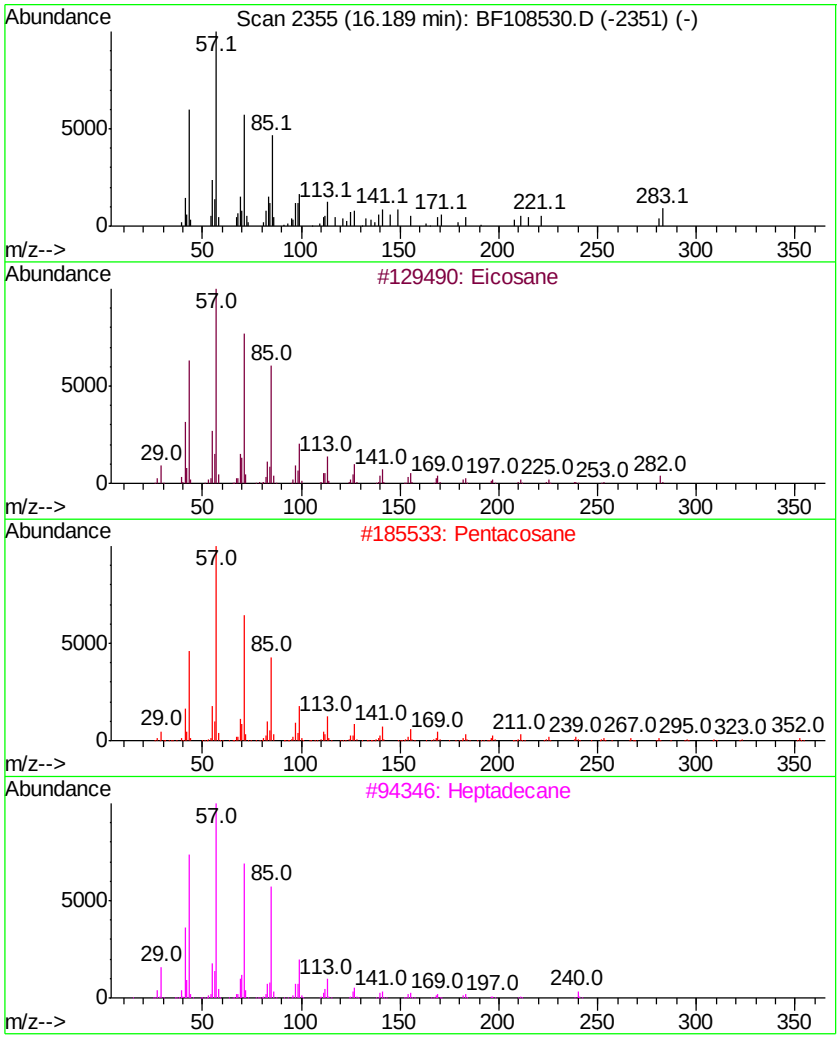
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

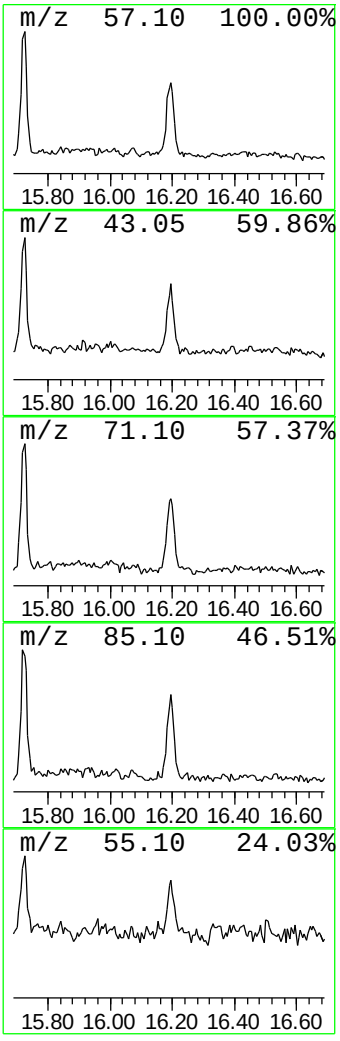
**********

Peak Number 7 Pentacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.19 | 2.44 ng | 65384 | Perylene-d12 | 15.75 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 2 | Pentacosane | 352 | C25H52 | 000629-99-2 | 87 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 86 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 86 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
Data File : BF108530.D
Acq On : 28 Aug 2018 1:01
Operator : JU/SJ
Sample : J4659-03
Misc :
ALS Vial : 32 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 082218-TIPC-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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 |
| unknown6.77 | 6.77 | 51.8 | ng | 1667100 | 1 | 7.00 | 644048 | 20.0 |
| Octacosane | 14.32 | 2.6 | ng | 89577 | 5 | 14.19 | 689135 | 20.0 |
| Eicosane | 14.62 | 3.0 | ng | 103589 | 5 | 14.19 | 689135 | 20.0 |
| Heptadecane, 9-oc... | 14.95 | 2.8 | ng | 97686 | 5 | 14.19 | 689135 | 20.0 |
| Hexacosane | 15.31 | 3.4 | ng | 90779 | 6 | 15.75 | 536232 | 20.0 |
| Pentacosane | 16.19 | 2.4 | ng | 65384 | 6 | 15.75 | 536232 | 20.0 |