LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
Data File : BF098047.D
Acq On : 25 Aug 2017 23:07
Operator : SJ/JU
Sample : I4955-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-SF-03-002-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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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 | 4.934 | 481 | 484 | 497 | rVB | 178630 | 244851 | 8.33% | 1.106% |
| 2 | 5.346 | 549 | 554 | 558 | rBV | 2493286 | 2702335 | 91.96% | 12.211% |
| 3 | 6.375 | 724 | 729 | 734 | rBV | 2487611 | 2938519 | 100.00% | 13.278% |
| 4 | 6.510 | 747 | 752 | 755 | rBV | 2874448 | 2664907 | 90.69% | 12.042% |
| 5 | 6.740 | 787 | 791 | 794 | rBV | 999257 | 789923 | 26.88% | 3.569% |
| 6 | 6.898 | 813 | 818 | 821 | rBV | 2048986 | 1858508 | 63.25% | 8.398% |
| 7 | 7.304 | 882 | 887 | 890 | rBV | 1805928 | 1606715 | 54.68% | 7.260% |
| 8 | 8.022 | 1004 | 1009 | 1015 | rBV | 1134315 | 947597 | 32.25% | 4.282% |
| 9 | 9.098 | 1187 | 1192 | 1195 | rBV | 2503902 | 2120781 | 72.17% | 9.583% |
| 10 | 9.492 | 1255 | 1259 | 1263 | rBV | 211804 | 189242 | 6.44% | 0.855% |
| 11 | 9.710 | 1294 | 1296 | 1300 | rVB2 | 53662 | 41161 | 1.40% | 0.186% |
| 12 | 9.775 | 1303 | 1307 | 1311 | rVV | 925896 | 785248 | 26.72% | 3.548% |
| 13 | 10.210 | 1378 | 1381 | 1384 | rVB | 70321 | 50465 | 1.72% | 0.228% |
| 14 | 10.428 | 1412 | 1418 | 1421 | rBV | 26949 | 36286 | 1.23% | 0.164% |
| 15 | 10.557 | 1436 | 1440 | 1449 | rBV | 1126156 | 985208 | 33.53% | 4.452% |
| 16 | 10.669 | 1455 | 1459 | 1460 | rBV | 61675 | 65568 | 2.23% | 0.296% |
| 17 | 10.680 | 1460 | 1461 | 1470 | rVB | 80890 | 77292 | 2.63% | 0.349% |
| 18 | 11.128 | 1534 | 1537 | 1540 | rBV2 | 40311 | 32537 | 1.11% | 0.147% |
| 19 | 11.251 | 1555 | 1558 | 1561 | rBV | 719399 | 658532 | 22.41% | 2.976% |
| 20 | 11.275 | 1561 | 1562 | 1565 | rVV | 66559 | 43373 | 1.48% | 0.196% |
| 21 | 12.463 | 1760 | 1764 | 1767 | rBV | 77535 | 69303 | 2.36% | 0.313% |
| 22 | 12.692 | 1797 | 1803 | 1805 | rBV | 60974 | 68362 | 2.33% | 0.309% |
| 23 | 12.839 | 1824 | 1828 | 1831 | rBV | 1789575 | 1563478 | 53.21% | 7.065% |
| 24 | 13.739 | 1978 | 1981 | 1988 | rBV2 | 122601 | 144506 | 4.92% | 0.653% |
| 25 | 13.886 | 2001 | 2006 | 2009 | rBV | 854395 | 792397 | 26.97% | 3.580% |
| 26 | 15.304 | 2243 | 2247 | 2251 | rBV | 447365 | 512086 | 17.43% | 2.314% |
| 27 | 16.227 | 2401 | 2404 | 2413 | rVB2 | 75217 | 141755 | 4.82% | 0.641% |

Sum of corrected areas: 22130935

LSC Report - Integrated Chromatogram

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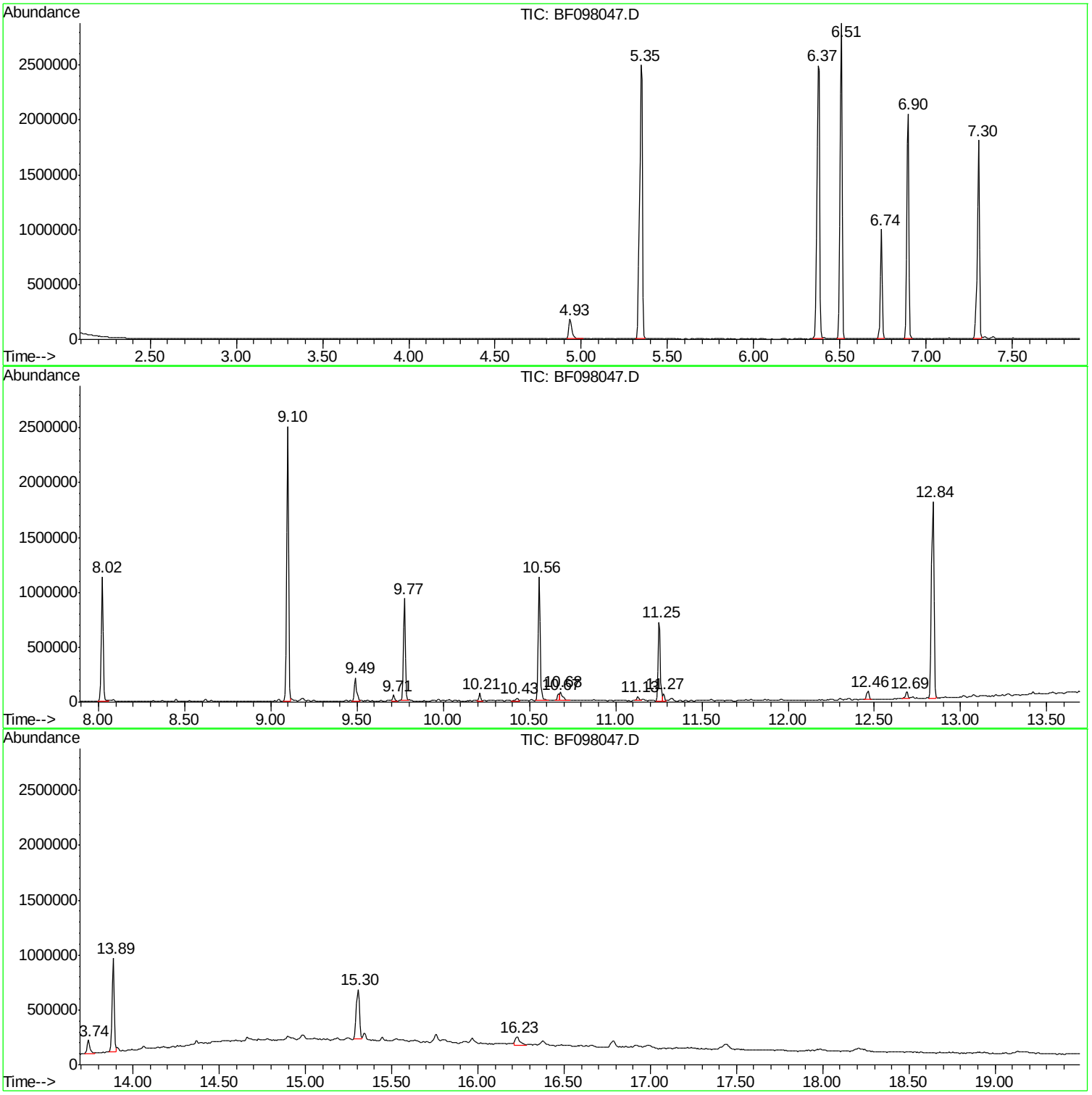
Data File : BF098047.D
Acq On : 25 Aug 2017 23:07
Operator : SJ/JU
Sample : I4955-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-SF-03-002-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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Data File : BF098047.D
Acq On : 25 Aug 2017 23:07
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**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

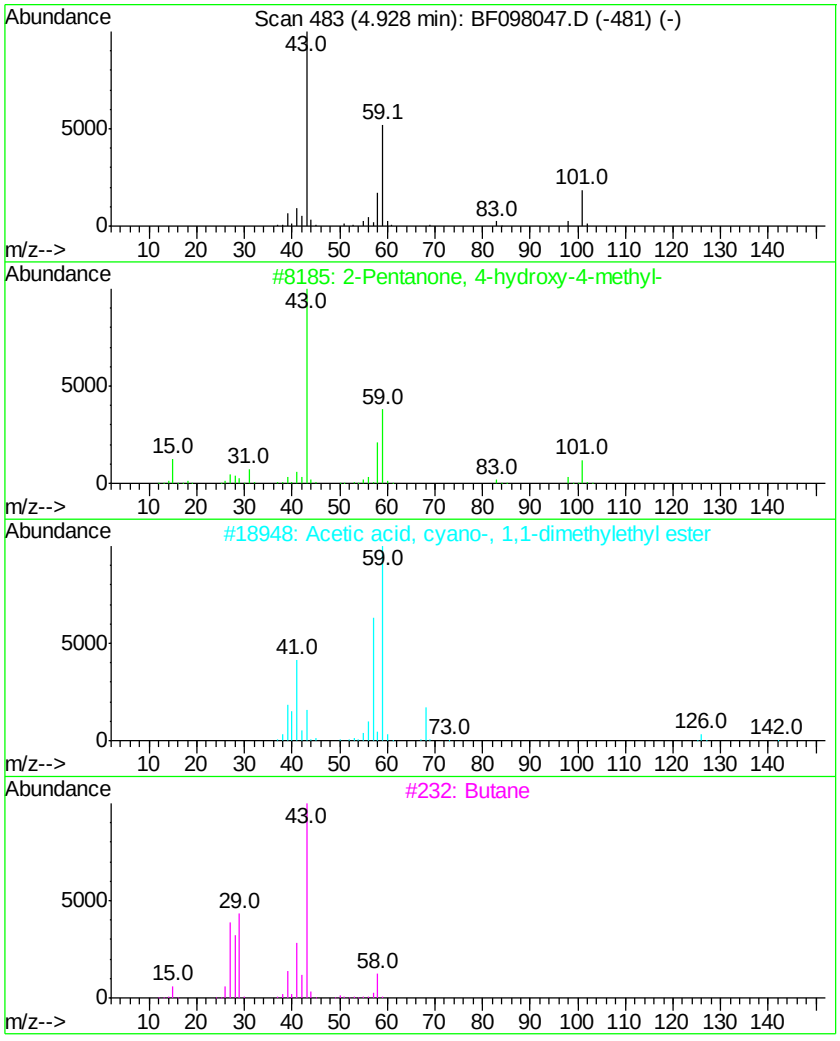
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

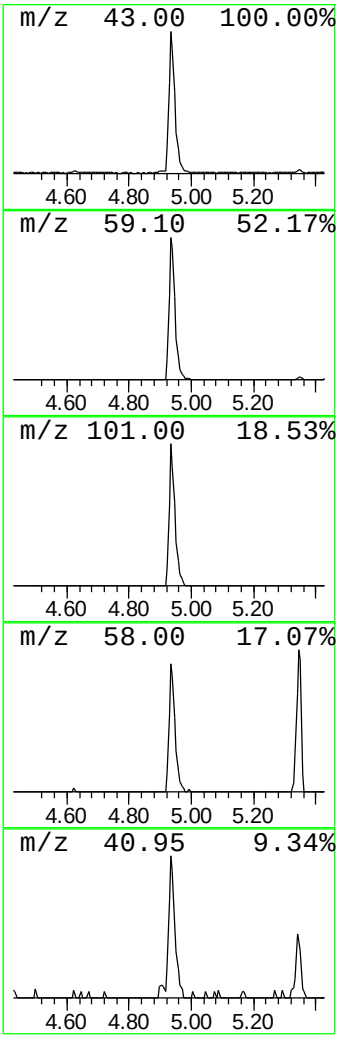
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.93 | 6.20 ng | 244851 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | Butane | 58 | C4H10 | 000106-97-8 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
Data File : BF098047.D
Acq On : 25 Aug 2017 23:07
Operator : SJ/JU
Sample : I4955-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-SF-03-002-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

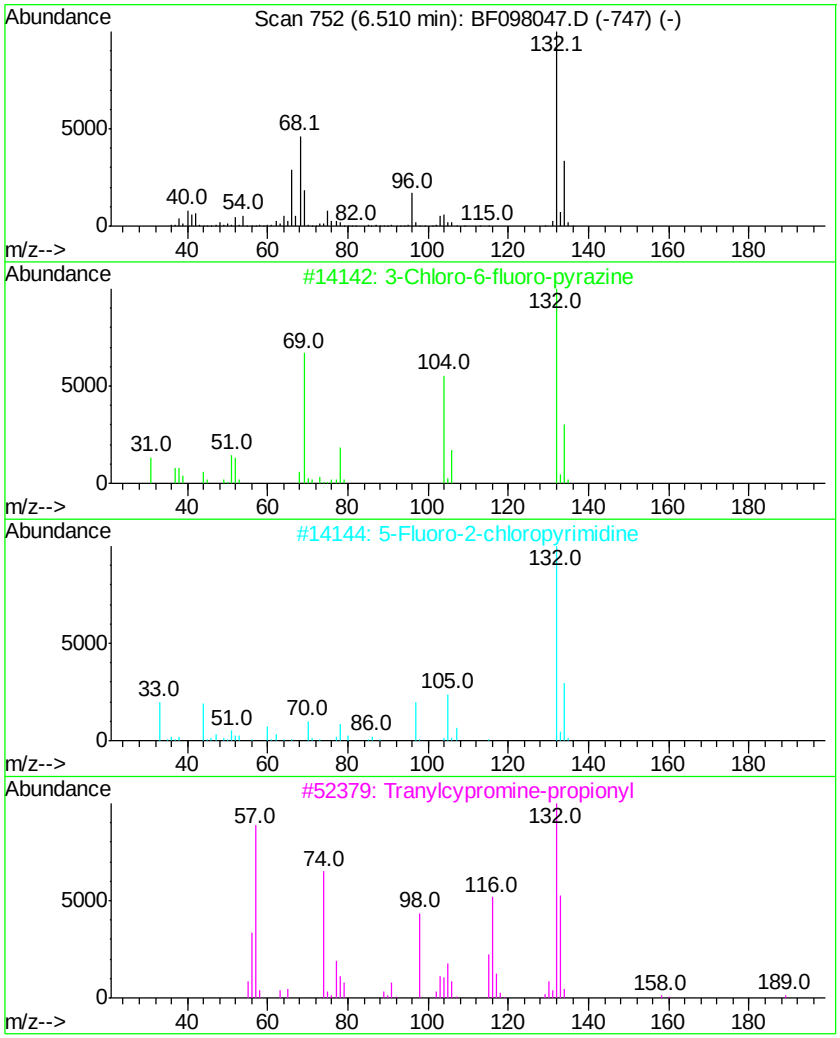
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

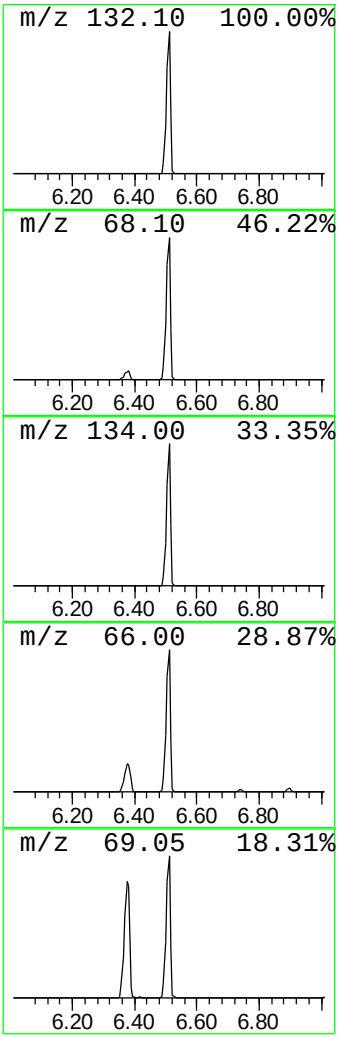
**********

Peak Number 2 unknown6.51 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.51 | 67.47 ng | 2664910 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082517\
Data File : BF098047.D
Acq On : 25 Aug 2017 23:07
Operator : SJ/JU
Sample : I4955-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-SF-03-002-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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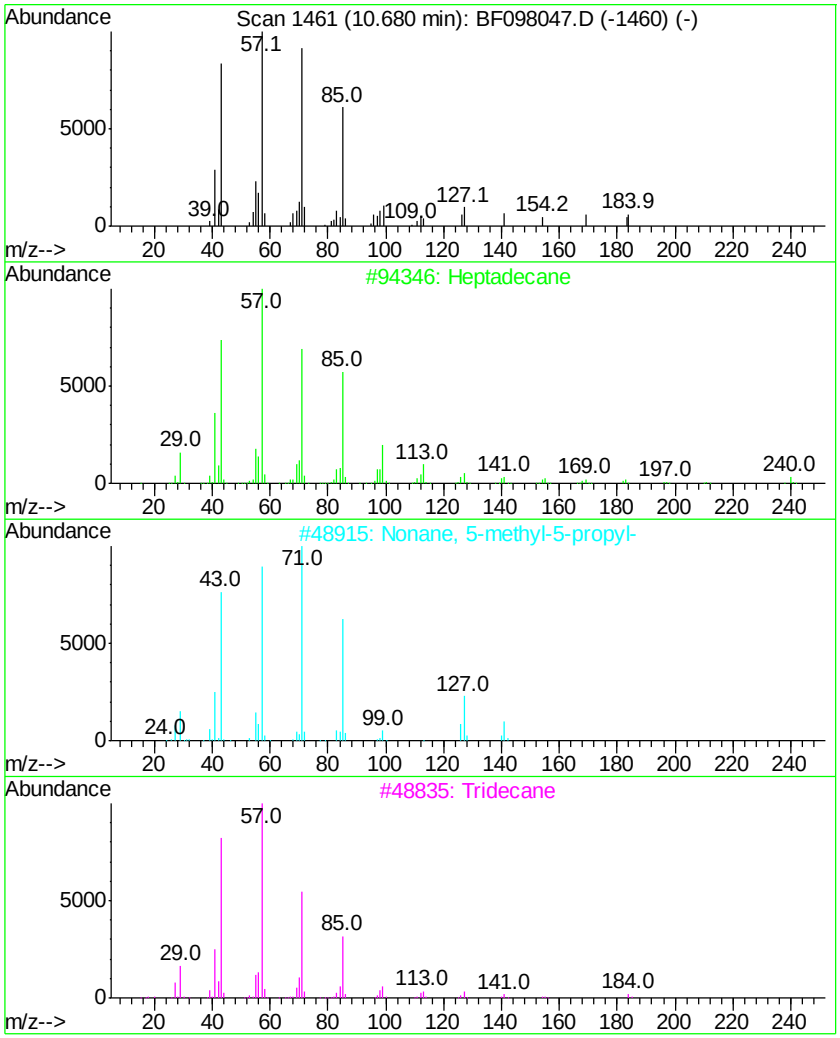
TIC Integration Parameters: LSCINT.P

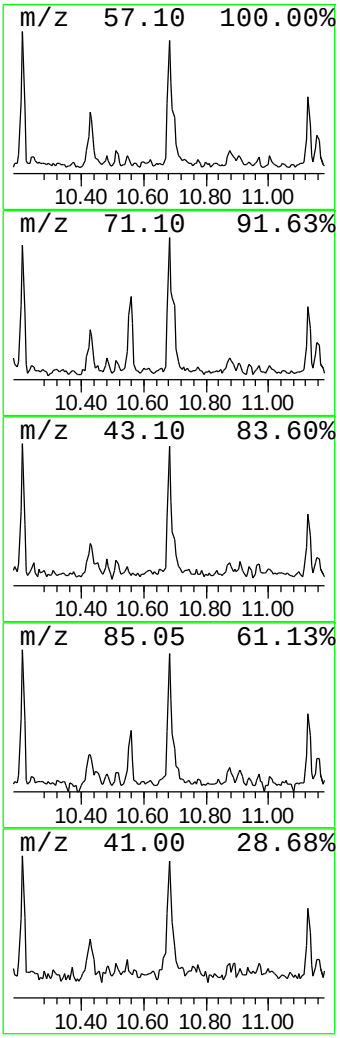
**********

Peak Number 4 Heptadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.68 | 2.35 ng | 77292 | Phenanthrene-d10 | 11.25 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 64 |
| 2 | Nonane, 5-methyl-5-propyl- | 184 | C13H28 | 017312-75-3 | 64 |
| 3 | Tridecane | 184 | C13H28 | 000629-50-5 | 64 |
| 4 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 59 |
| 5 | Nonane, 5-butyl- | 184 | C13H28 | 017312-63-9 | 47 |



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Operator : SJ/JU
Sample : I4955-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-SF-03-002-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

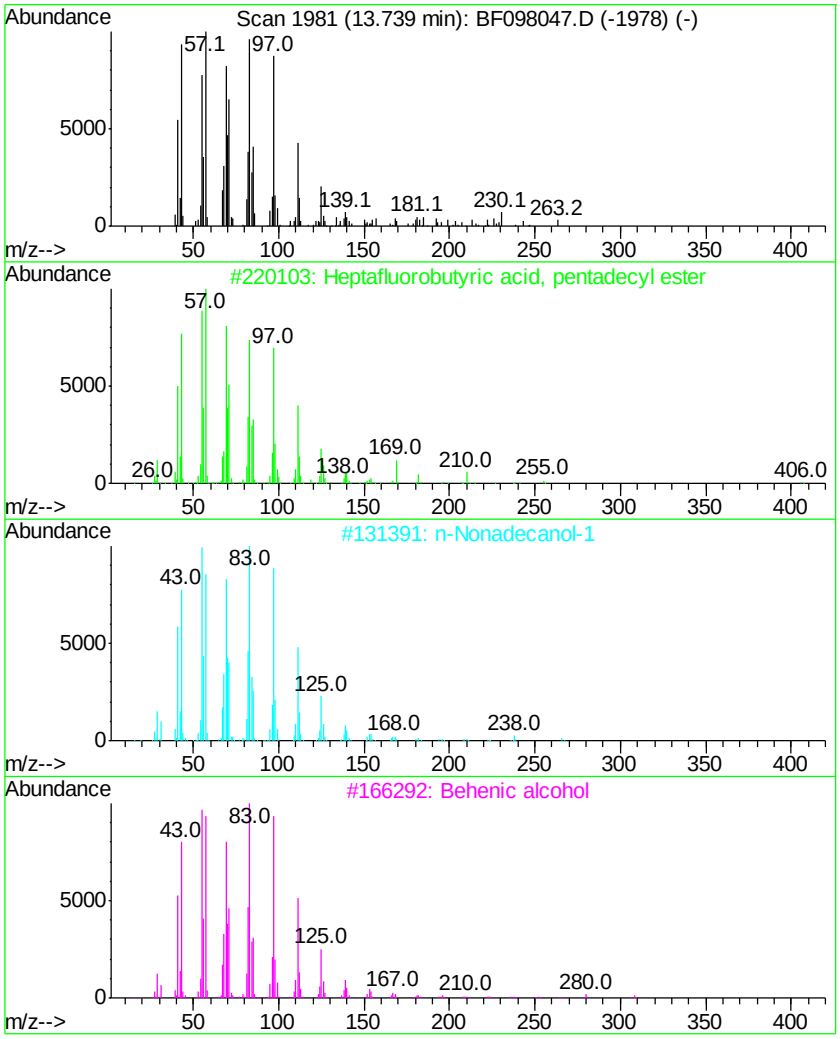
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

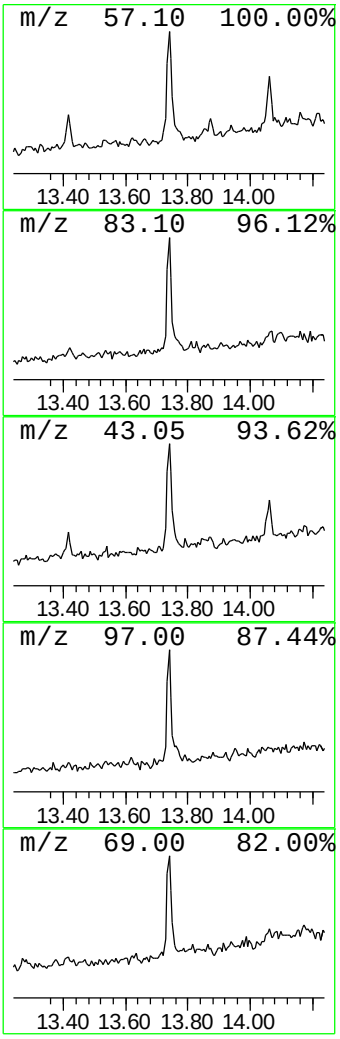
**********

Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.74 | 3.65 ng | 144506 | Chrysene-d12 | 13.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 91 |
| 2 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 90 |
| 3 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 87 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 87 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 81 |



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Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-SF-03-002-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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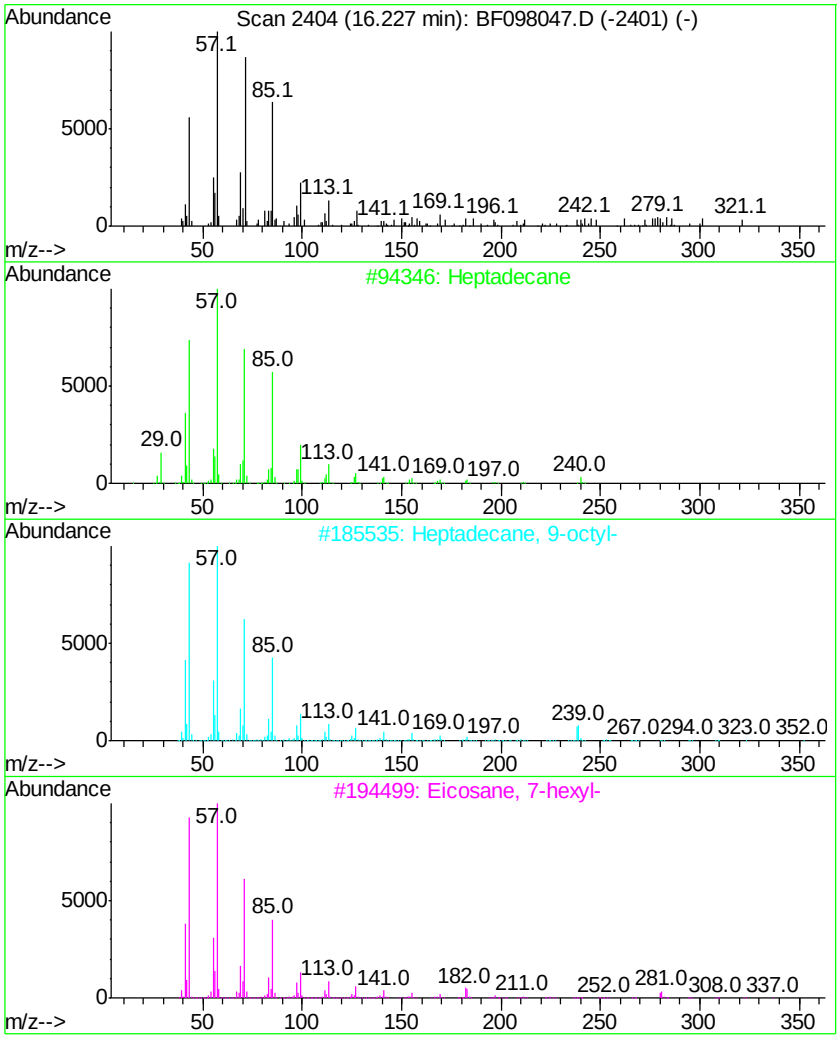
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

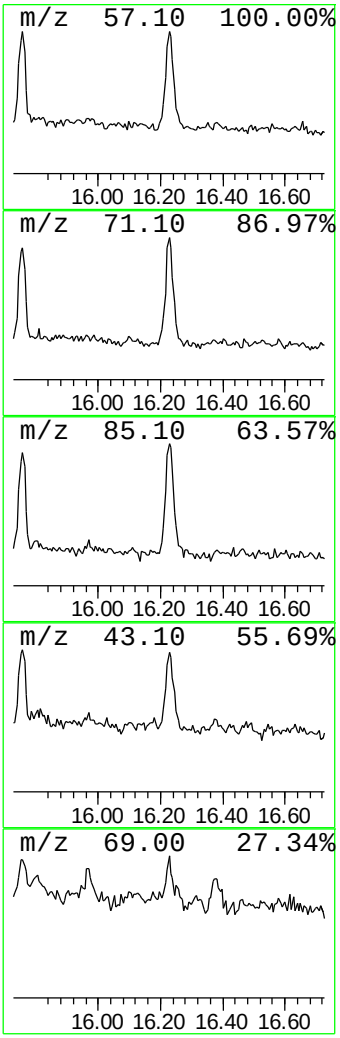
**********

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.23 | 5.54 ng | 141755 | Perylene-d12 | 15.30 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 72 |
| 3 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 72 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 64 |
| 5 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
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**Instrument :** BNA_F
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TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.93 | 6.2 | ng | 244851 | 1 | 6.74 | 789923 | 20.0 |
| unknown6.51 | 6.51 | 67.5 | ng | 2664910 | 1 | 6.74 | 789923 | 20.0 |
| Heptadecane | 10.68 | 2.4 | ng | 77292 | 4 | 11.25 | 658532 | 20.0 |
| Heptafluorobutyri... | 13.74 | 3.6 | ng | 144506 | 5 | 13.89 | 792397 | 20.0 |
| Heptadecane, 9-oc... | 16.23 | 5.5 | ng | 141755 | 6 | 15.30 | 512086 | 20.0 |