LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104413.D
Acq On : 10 Apr 2018 17:13
Operator : JU/SJ
Sample : J2297-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RO-3-1

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-BF040618.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 | 5.022 | 495 | 499 | 507 | rVB | 98393 | 119593 | 4.71% | 0.530% |
| 2 | 5.422 | 561 | 567 | 570 | rBV | 2553351 | 2477287 | 97.49% | 10.989% |
| 3 | 6.057 | 673 | 675 | 682 | rVB | 39977 | 50385 | 1.98% | 0.223% |
| 4 | 6.440 | 734 | 740 | 748 | rBV | 2389950 | 2465433 | 97.02% | 10.936% |
| 5 | 6.575 | 759 | 763 | 766 | rBV | 2683703 | 2541110 | 100.00% | 11.272% |
| 6 | 6.810 | 799 | 803 | 806 | rBV | 807941 | 710583 | 27.96% | 3.152% |
| 7 | 6.963 | 825 | 829 | 832 | rBV | 2311452 | 1969993 | 77.52% | 8.739% |
| 8 | 7.375 | 893 | 899 | 901 | rBV | 1485230 | 1529344 | 60.18% | 6.784% |
| 9 | 8.092 | 1017 | 1021 | 1024 | rBV | 1055598 | 904049 | 35.58% | 4.010% |
| 10 | 9.169 | 1199 | 1204 | 1207 | rBV | 2939171 | 2531740 | 99.63% | 11.230% |
| 11 | 9.557 | 1267 | 1270 | 1273 | rBV | 196897 | 168122 | 6.62% | 0.746% |
| 12 | 9.775 | 1304 | 1307 | 1310 | rBV | 69555 | 50722 | 2.00% | 0.225% |
| 13 | 9.845 | 1315 | 1319 | 1323 | rVB2 | 989073 | 853918 | 33.60% | 3.788% |
| 14 | 10.145 | 1366 | 1370 | 1373 | rBV2 | 88993 | 77811 | 3.06% | 0.345% |
| 15 | 10.275 | 1389 | 1392 | 1395 | rVB | 93377 | 68758 | 2.71% | 0.305% |
| 16 | 10.498 | 1423 | 1430 | 1432 | rBV | 23791 | 32221 | 1.27% | 0.143% |
| 17 | 10.633 | 1449 | 1453 | 1457 | rBV | 1330258 | 1206989 | 47.50% | 5.354% |
| 18 | 10.751 | 1470 | 1473 | 1482 | rVB | 71314 | 81574 | 3.21% | 0.362% |
| 19 | 11.333 | 1569 | 1572 | 1576 | rBV | 856206 | 678629 | 26.71% | 3.010% |
| 20 | 11.857 | 1658 | 1661 | 1665 | rBV | 34822 | 31867 | 1.25% | 0.141% |
| 21 | 12.922 | 1838 | 1842 | 1846 | rBV | 1910692 | 1871974 | 73.67% | 8.304% |
| 22 | 13.463 | 1930 | 1934 | 1937 | rBV | 266404 | 227903 | 8.97% | 1.011% |
| 23 | 13.816 | 1991 | 1994 | 2005 | rBV2 | 275395 | 275373 | 10.84% | 1.222% |
| 24 | 13.980 | 2018 | 2022 | 2025 | rBV | 781767 | 735224 | 28.93% | 3.261% |
| 25 | 14.457 | 2100 | 2103 | 2108 | rVB4 | 33316 | 44303 | 1.74% | 0.197% |
| 26 | 14.621 | 2128 | 2131 | 2136 | rBV5 | 41318 | 44488 | 1.75% | 0.197% |
| 27 | 15.392 | 2258 | 2262 | 2266 | rBV | 223025 | 277506 | 10.92% | 1.231% |
| 28 | 15.445 | 2266 | 2271 | 2275 | rBV | 445074 | 516842 | 20.34% | 2.293% |

Sum of corrected areas: 22543741

LSC Report - Integrated Chromatogram

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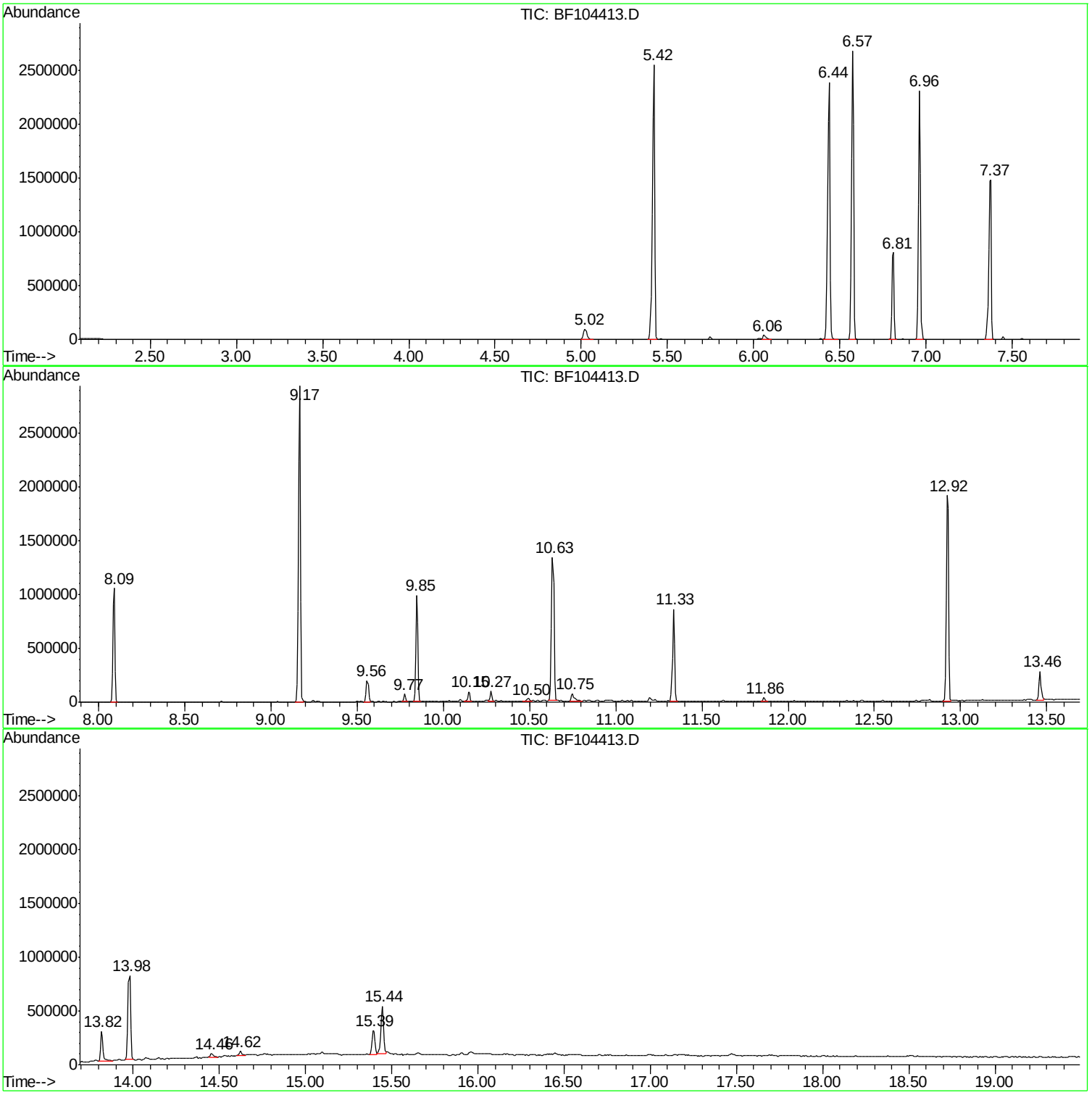
Operator : JU/SJ
Sample : J2297-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RO-3-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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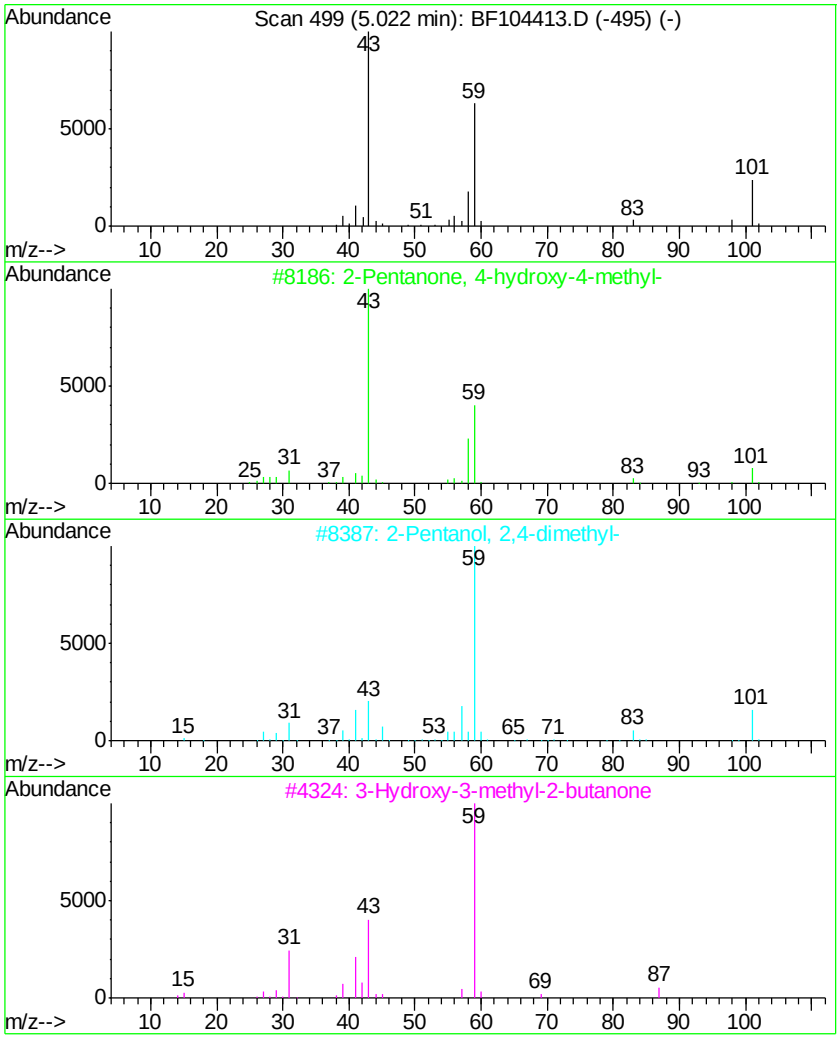
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

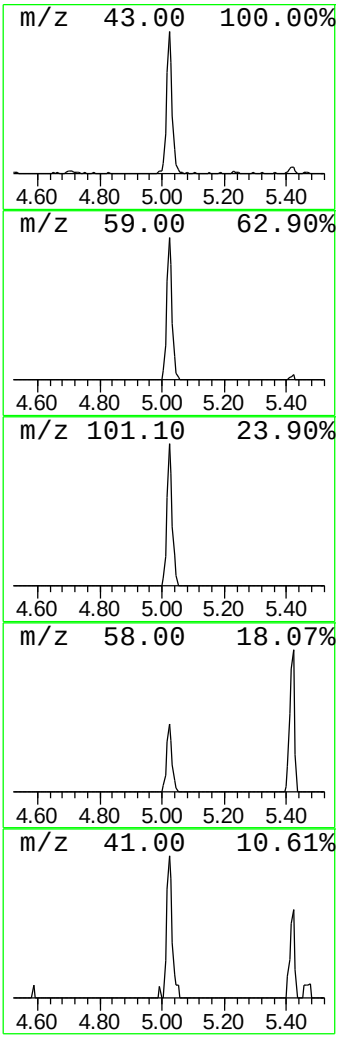
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.02 | 3.37 ng | 119593 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 38 |
| 3 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 25 |
| 4 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 23 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |



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Operator : JU/SJ
Sample : J2297-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RO-3-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

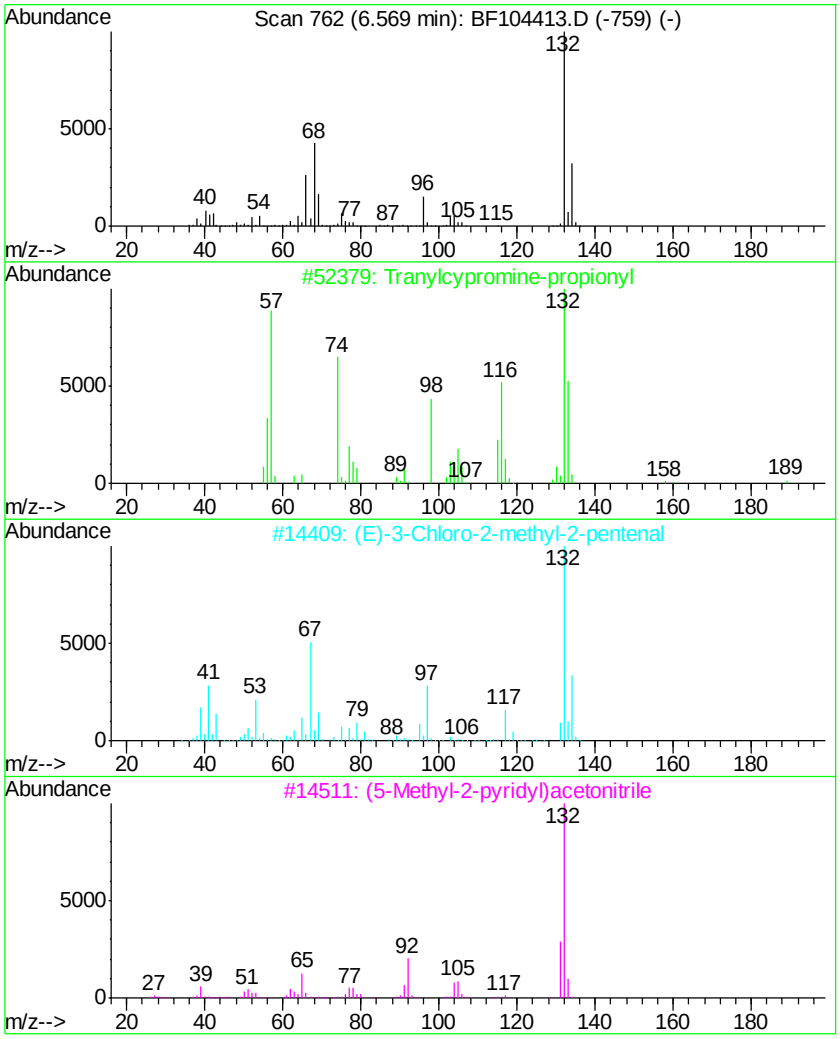
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

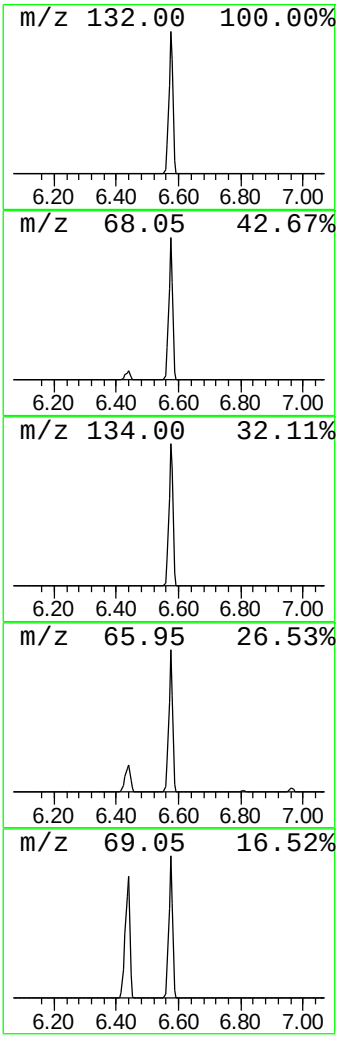
**********

Peak Number 2 unknown6.57 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.57 | 71.52 ng | 2541110 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 3 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 9 |
| 4 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104413.D
Acq On : 10 Apr 2018 17:13
Operator : JU/SJ
Sample : J2297-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RO-3-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

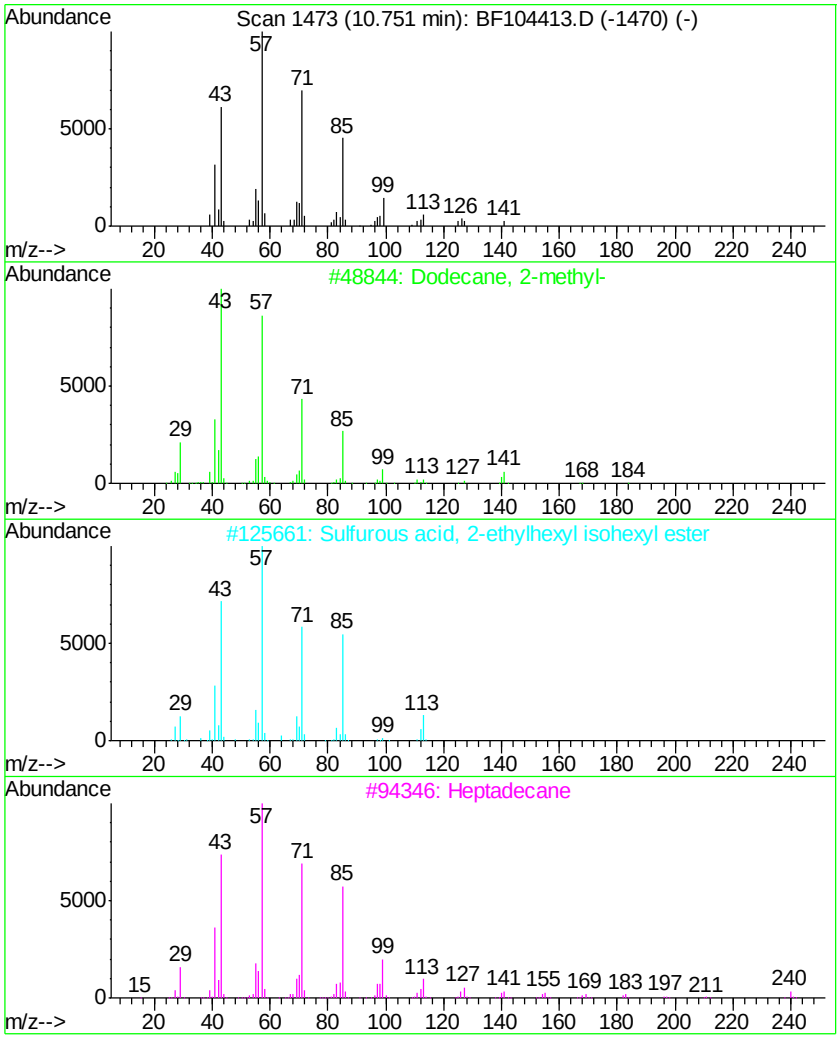
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

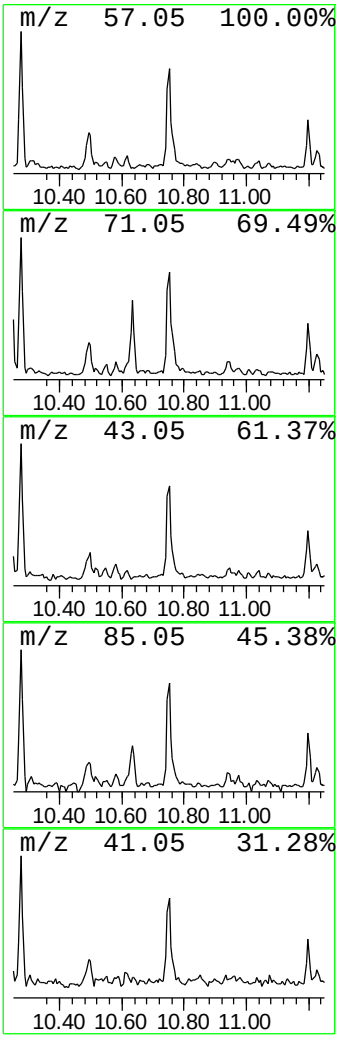
**********

Peak Number 4 Dodecane, 2-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.75 | 2.40 ng | 81574 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecane, 2-methyl- | 184 | C13H28 | 001560-97-0 | 86 |
| 2 | Sulfurous acid, 2-ethylhexyl iso... | 278 | C14H30O3S | 1000309-19-0 | 72 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 64 |
| 4 | Eicosane | 282 | C20H42 | 000112-95-8 | 59 |
| 5 | 1-Iodo-2-methylnonane | 268 | C10H21I | 1000101-47-9 | 53 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
Data File : BF104413.D
Acq On : 10 Apr 2018 17:13
Operator : JU/SJ
Sample : J2297-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RO-3-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

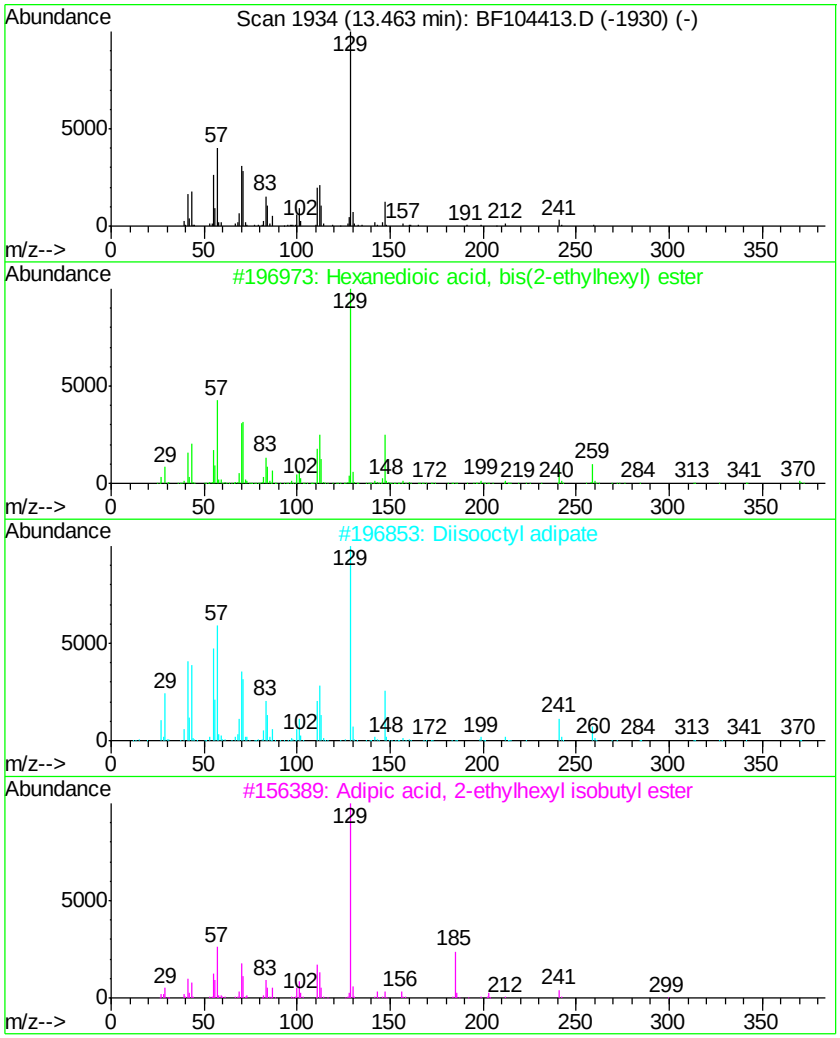
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

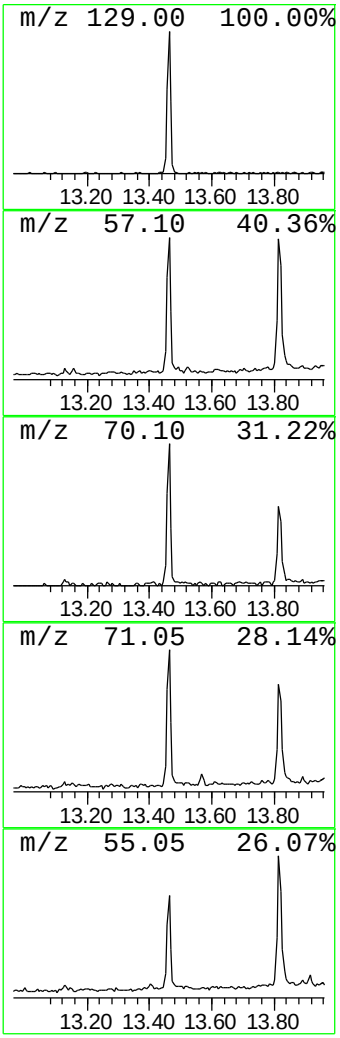
**********

Peak Number 5 Hexanedioic acid, bis(2-eth... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.46 | 6.20 ng | 227903 | Chrysene-d12 | 13.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanedioic acid, bis(2-ethylhex... | 370 | C22H42O4 | 000103-23-1 | 90 |
| 2 | Diisooctyl adipate | 370 | C22H42O4 | 001330-86-5 | 78 |
| 3 | Adipic acid, 2-ethylhexyl isobut... | 314 | C18H34O4 | 1000324-48-0 | 64 |
| 4 | Adipic acid, 2-ethylhexyl isohex... | 342 | C20H38O4 | 1000324-48-3 | 50 |
| 5 | Adipic acid, octyl trans-2-methy... | 354 | C21H38O4 | 1000324-75-1 | 50 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041018\
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Sample : J2297-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RO-3-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

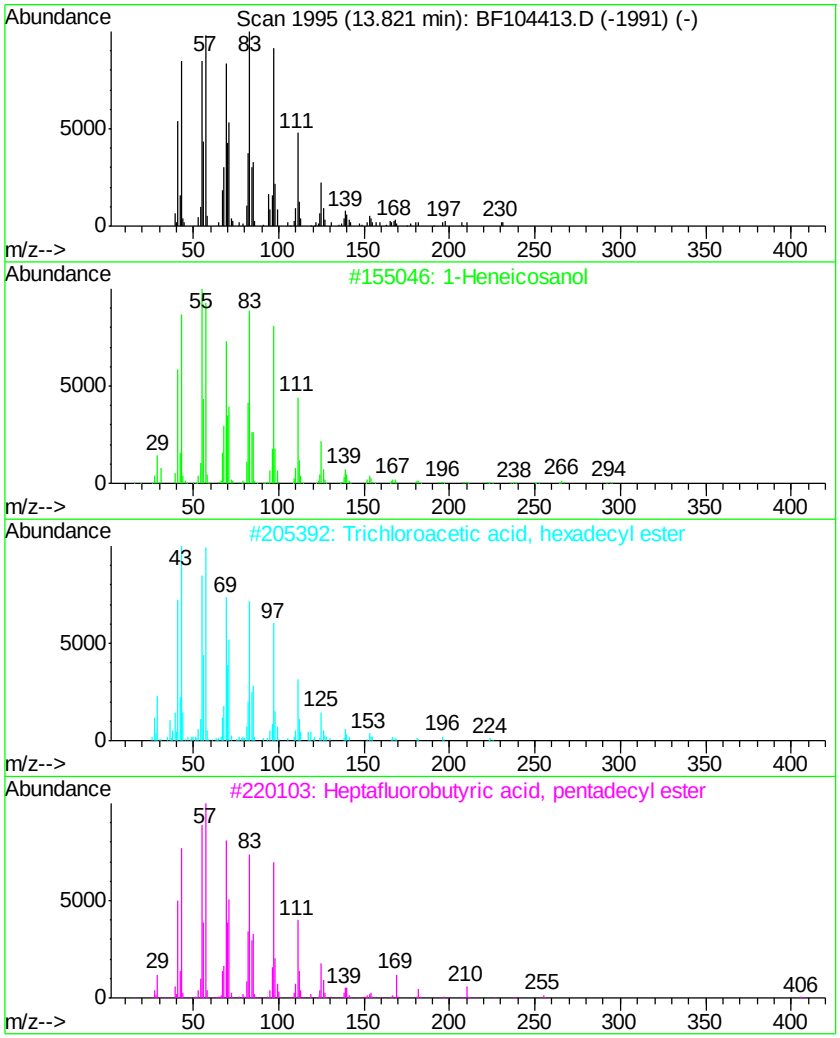
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

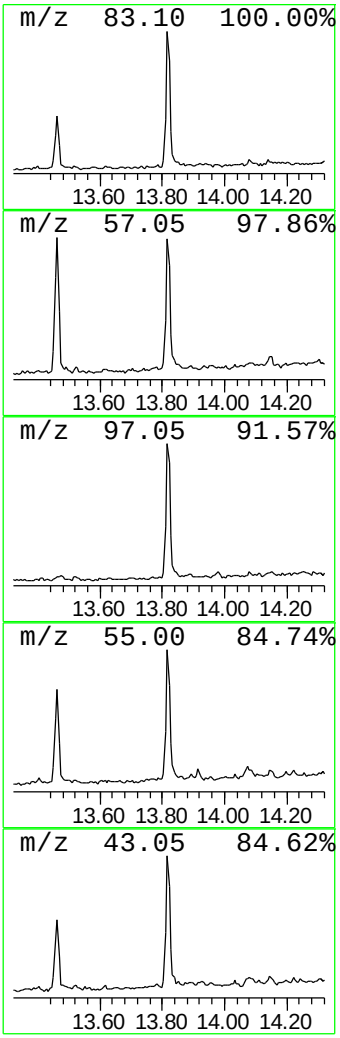
**********

Peak Number 6 1-Heneicosanol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.82 | 7.49 ng | 275373 | Chrysene-d12 | 13.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 2 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 3 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 94 |
| 5 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 91 |



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Sample : J2297-01
Misc :
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**Instrument :** BNA_F
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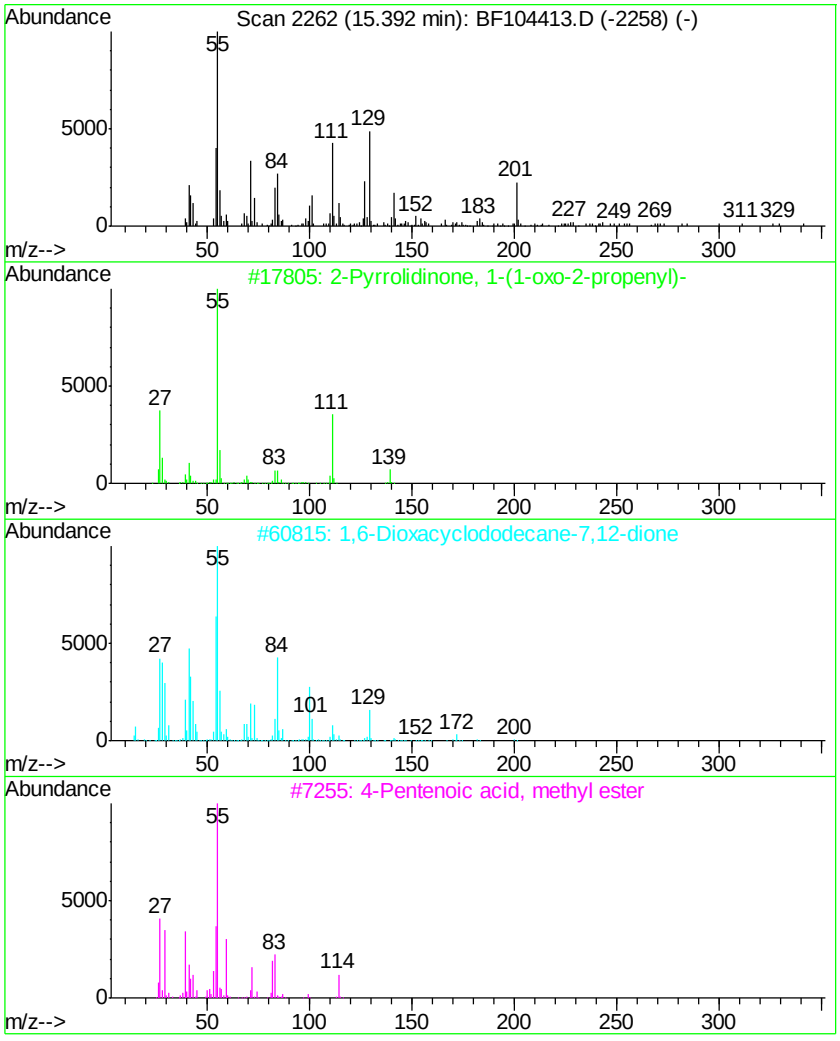
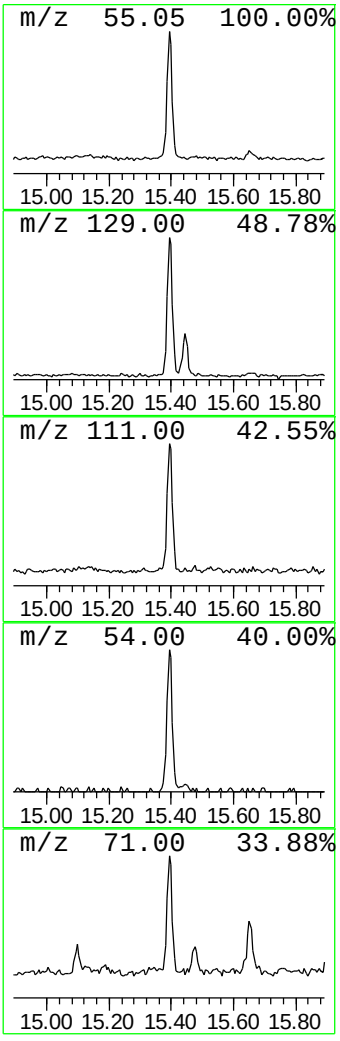
**********

Peak Number 7 unknown15.39 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.39 | 10.74 ng | 277506 | Perylene-d12 | 15.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pyrrolidinone, 1-(1-oxo-2-prop... | 139 | C7H9NO2 | 002043-26-7 | 10 |
| 2 | 1,6-Dioxacyclododecane-7,12-dione | 200 | C10H16O4 | 000777-95-7 | 10 |
| 3 | 4-Pentenoic acid, methyl ester | 114 | C6H10O2 | 000818-57-5 | 10 |
| 4 | 4-Pentenoic acid ethyl ester | 128 | C7H12O2 | 001968-40-7 | 9 |
| 5 | Cyclohexanamine, N-methylidene-N... | 127 | C7H13NO | 183969-41-7 | 9 |



Tentatively Identified Compound (LSC) summary

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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... | 5.02 | 3.4 | ng | 119593 | 1 | 6.81 | 710583 | 20.0 |
| unknown6.57 | 6.57 | 71.5 | ng | 2541110 | 1 | 6.81 | 710583 | 20.0 |
| Dodecane, 2-methyl- | 10.75 | 2.4 | ng | 81574 | 4 | 11.33 | 678629 | 20.0 |
| Hexanedioic acid,... | 13.46 | 6.2 | ng | 227903 | 5 | 13.98 | 735224 | 20.0 |
| 1-Heneicosanol | 13.82 | 7.5 | ng | 275373 | 5 | 13.98 | 735224 | 20.0 |
| unknown15.39 | 15.39 | 10.7 | ng | 277506 | 6 | 15.44 | 516842 | 20.0 |