# LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117501.D
Acq On : 23 Oct 2019 23:24
Operator : JU
Sample : K5497-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 169-90-(0-1.2)

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-BF101819.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 | 5.351 | 551 | 555 | 577 | rBV | 759204 | 880910 | 87.11% | 9.945% |
| 2 | 6.381 | 726 | 730 | 748 | rBV | 1001214 | 1011314 | 100.00% | 11.417% |
| 3 | 6.504 | 748 | 751 | 758 | rVV | 1136110 | 1009172 | 99.79% | 11.393% |
| 4 | 6.734 | 786 | 790 | 800 | rBV | 261462 | 264349 | 26.14% | 2.984% |
| 5 | 6.886 | 812 | 816 | 830 | rBV | 776569 | 667076 | 65.96% | 7.531% |
| 6 | 7.298 | 882 | 886 | 905 | rBV | 599655 | 593498 | 58.69% | 6.700% |
| 7 | 8.010 | 1004 | 1007 | 1034 | rBV | 360942 | 351060 | 34.71% | 3.963% |
| 8 | 9.086 | 1186 | 1190 | 1193 | rBV | 1115198 | 867020 | 85.73% | 9.788% |
| 9 | 9.480 | 1254 | 1257 | 1267 | rBV | 110665 | 94769 | 9.37% | 1.070% |
| 10 | 9.763 | 1301 | 1305 | 1318 | rBV | 494428 | 405963 | 40.14% | 4.583% |
| 11 | 10.551 | 1436 | 1439 | 1456 | rBV | 615295 | 611828 | 60.50% | 6.907% |
| 12 | 11.245 | 1554 | 1557 | 1567 | rBV | 367444 | 378797 | 37.46% | 4.276% |
| 13 | 11.780 | 1644 | 1648 | 1658 | rBV | 56632 | 66327 | 6.56% | 0.749% |
| 14 | 12.563 | 1778 | 1781 | 1785 | rBV | 13810 | 16236 | 1.61% | 0.183% |
| 15 | 12.692 | 1799 | 1803 | 1807 | rBV2 | 9334 | 10854 | 1.07% | 0.123% |
| 16 | 12.827 | 1822 | 1826 | 1830 | rBV | 849481 | 705469 | 69.76% | 7.964% |
| 17 | 13.733 | 1976 | 1980 | 1992 | rBV3 | 65396 | 146198 | 14.46% | 1.650% |
| 18 | 13.892 | 2003 | 2007 | 2014 | rBV | 247141 | 263292 | 26.03% | 2.972% |
| 19 | 14.039 | 2029 | 2032 | 2037 | rBV | 11021 | 12811 | 1.27% | 0.145% |
| 20 | 14.345 | 2080 | 2084 | 2087 | rBV3 | 22896 | 20486 | 2.03% | 0.231% |
| 21 | 14.639 | 2131 | 2134 | 2139 | rVB | 28032 | 28664 | 2.83% | 0.324% |
| 22 | 14.715 | 2143 | 2147 | 2152 | rVB | 16830 | 18431 | 1.82% | 0.208% |
| 23 | 14.957 | 2185 | 2188 | 2192 | rVB | 33806 | 36724 | 3.63% | 0.415% |
| 24 | 15.315 | 2245 | 2249 | 2257 | rVB | 215757 | 291373 | 28.81% | 3.289% |
| 25 | 15.715 | 2311 | 2317 | 2322 | rBV2 | 27771 | 41849 | 4.14% | 0.472% |
| 26 | 15.804 | 2326 | 2332 | 2333 | rBV5 | 9326 | 14172 | 1.40% | 0.160% |
| 27 | 16.186 | 2391 | 2397 | 2403 | rBV5 | 16999 | 32756 | 3.24% | 0.370% |
| 28 | 16.733 | 2486 | 2490 | 2497 | rVB7 | 7823 | 16803 | 1.66% | 0.190% |

Sum of corrected areas: 8858201

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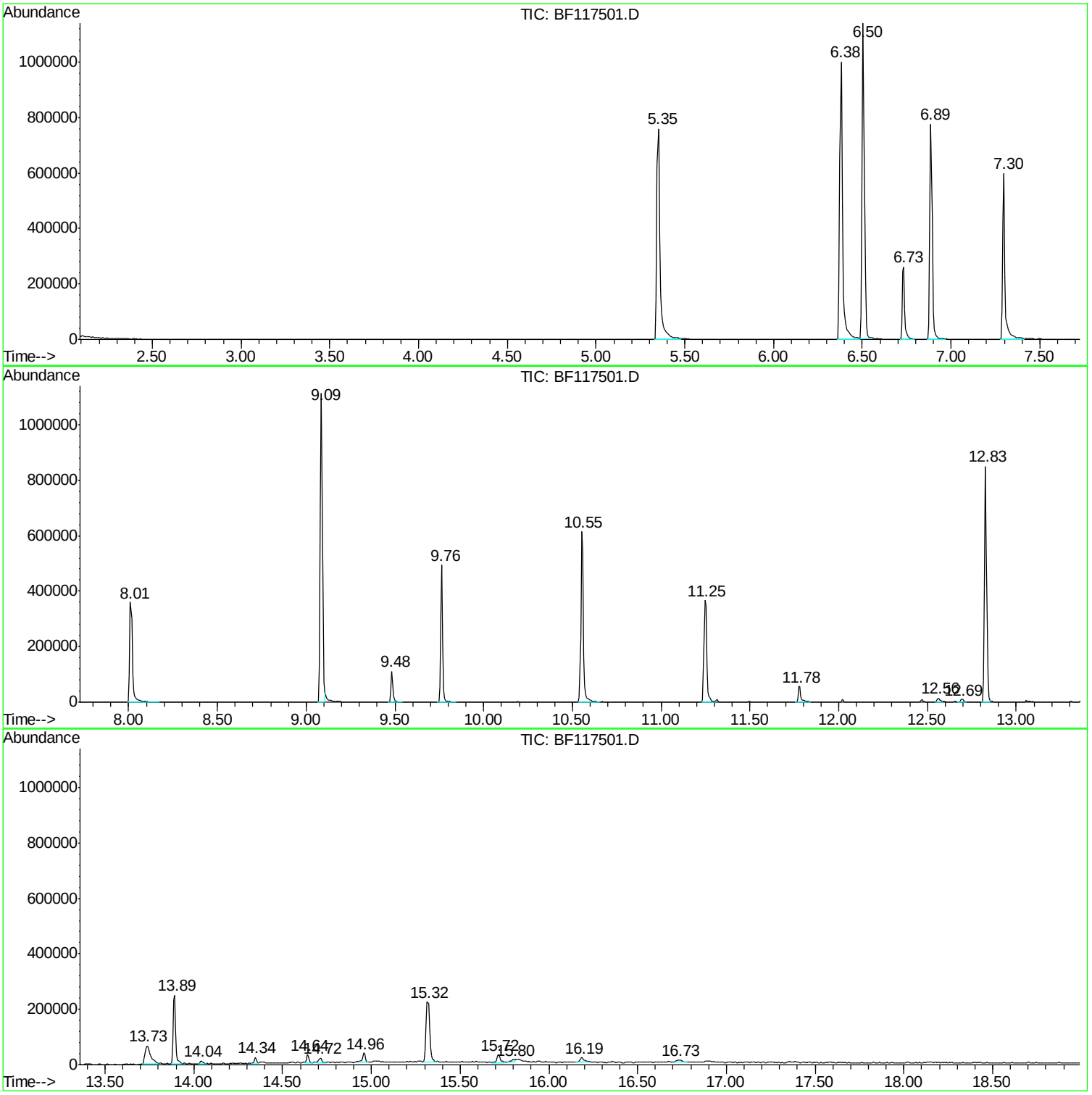
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
169-90-(0-1.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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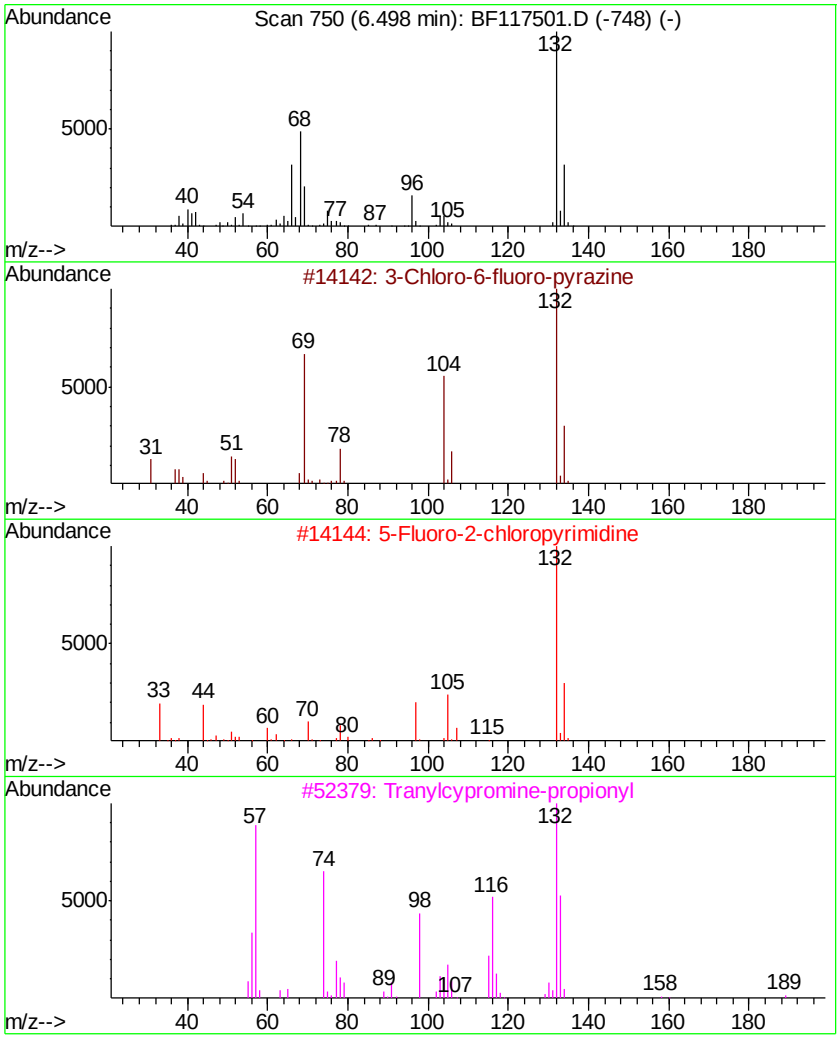
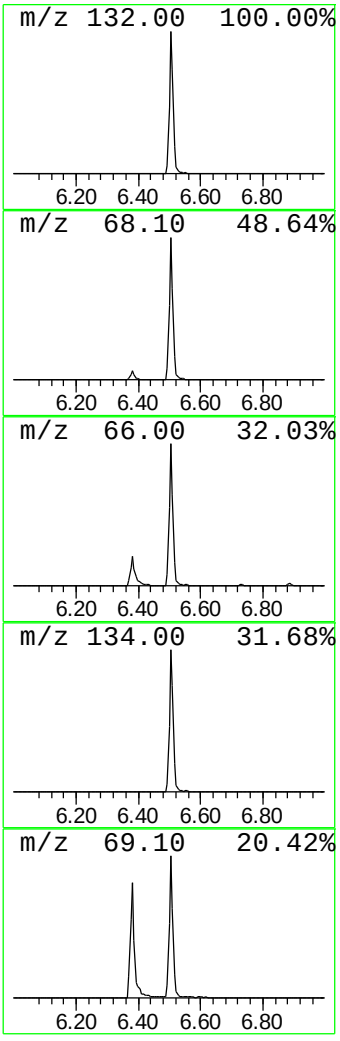
Peak Number 1 unknown6.50 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.50 | 76.35 ng | 1009170 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



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Misc :
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**Instrument :** BNA_F
**ClientSampleId :** 169-90-(0-1.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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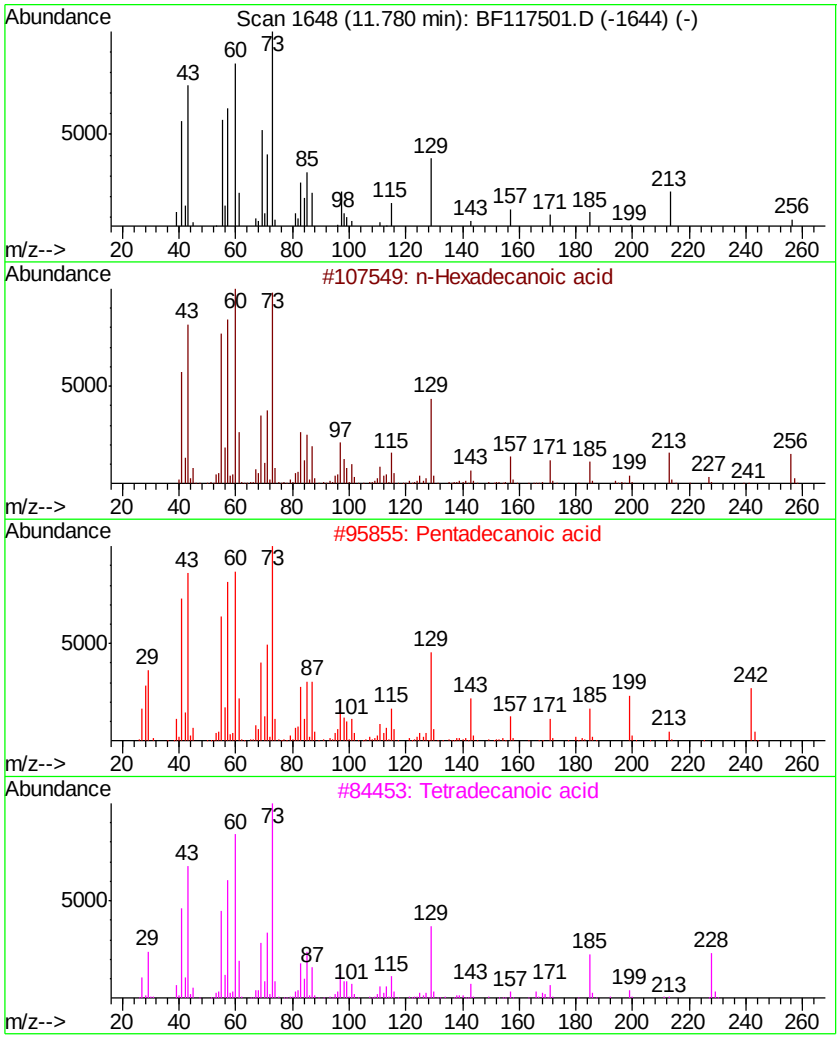
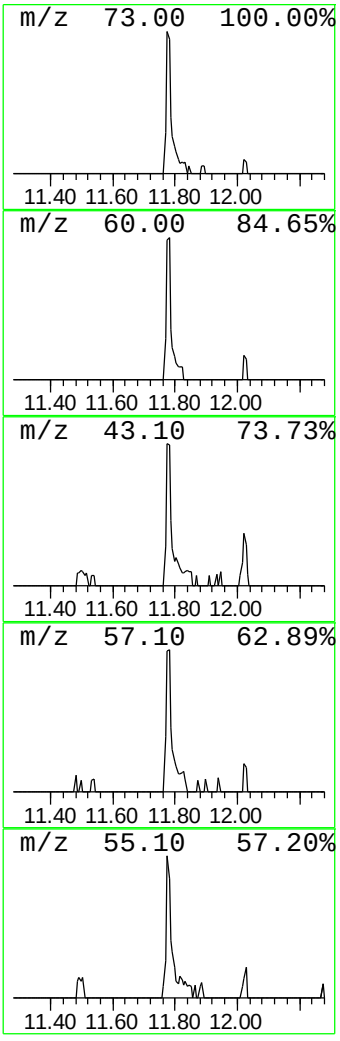
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.78 | 3.50 ng | 66327 | Phenanthrene-d10 | 11.24 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 59 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 53 |



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**Instrument :** BNA_F
**ClientSampleId :** 169-90-(0-1.2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
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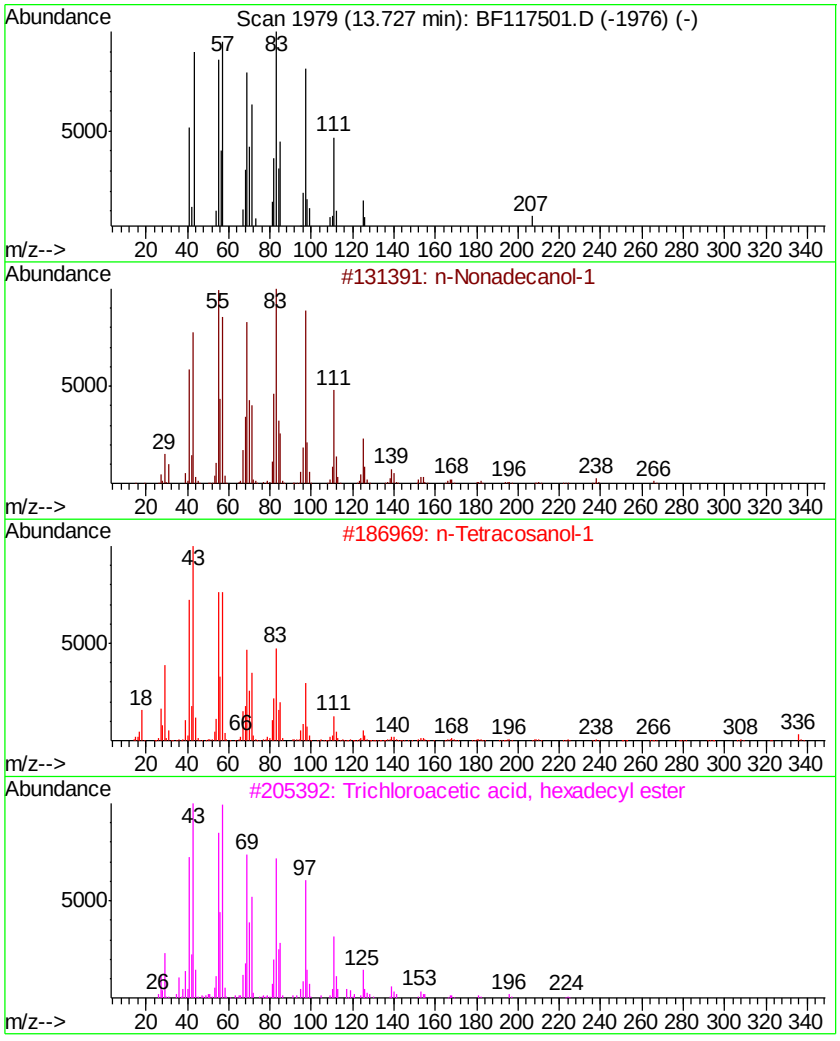
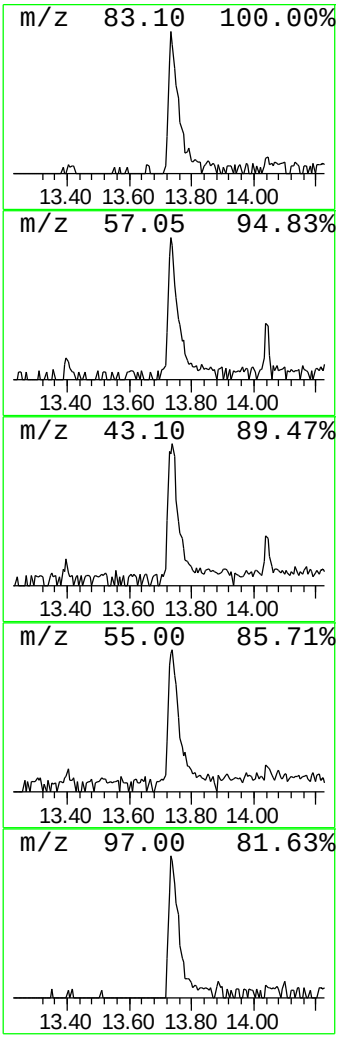
Peak Number 4 n-Nonadecanol-1 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.73 | 11.11 ng | 146198 | Chrysene-d12 | 13.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 93 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 90 |
| 4 | Trichloroacetic acid, tetradecyl... | 358 | C16H29Cl3O2 | 074339-52-9 | 90 |
| 5 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 90 |



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ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
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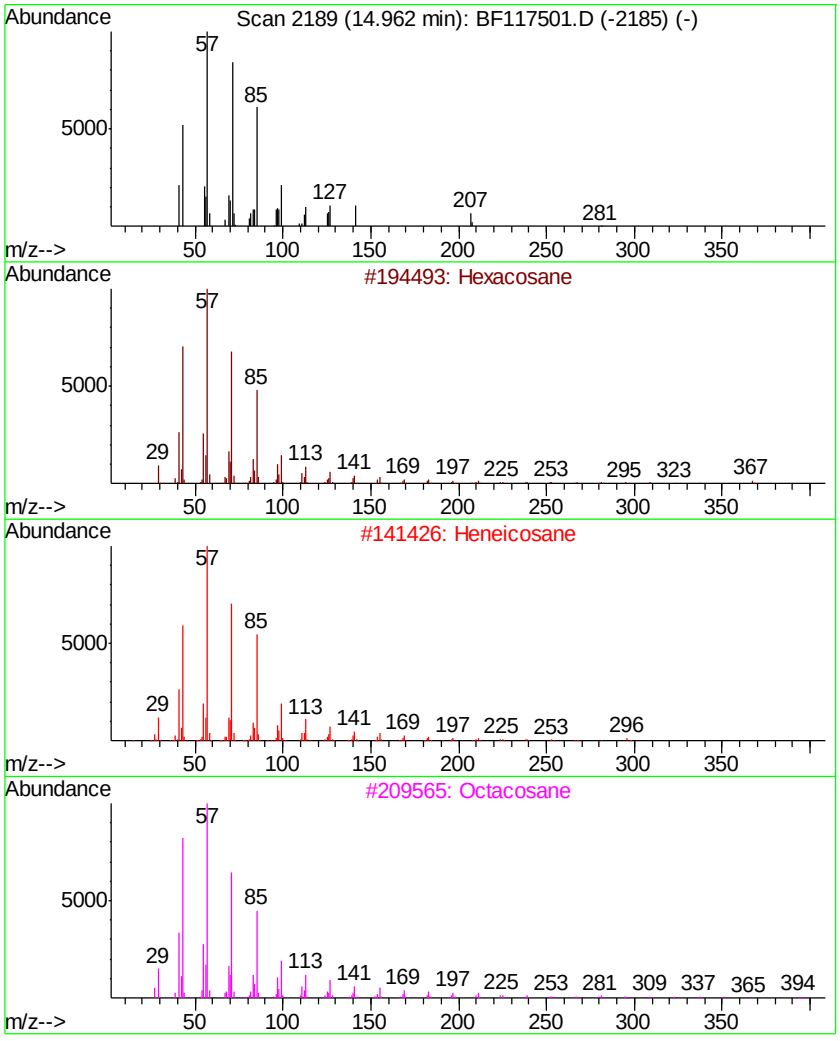
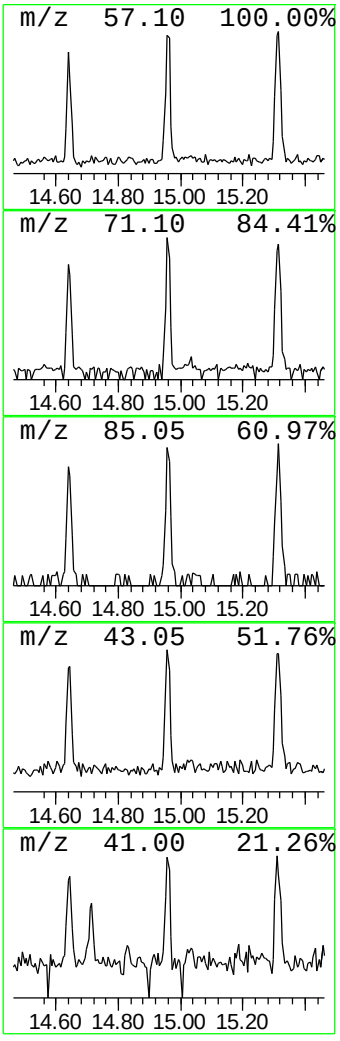
Peak Number 5 Hexacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.96 | 2.52 ng | 36724 | Perylene-d12 | 15.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 90 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 5 | 10-Methylnonadecane | 282 | C20H42 | 056862-62-5 | 86 |



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ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 169-90-(0-1.2)

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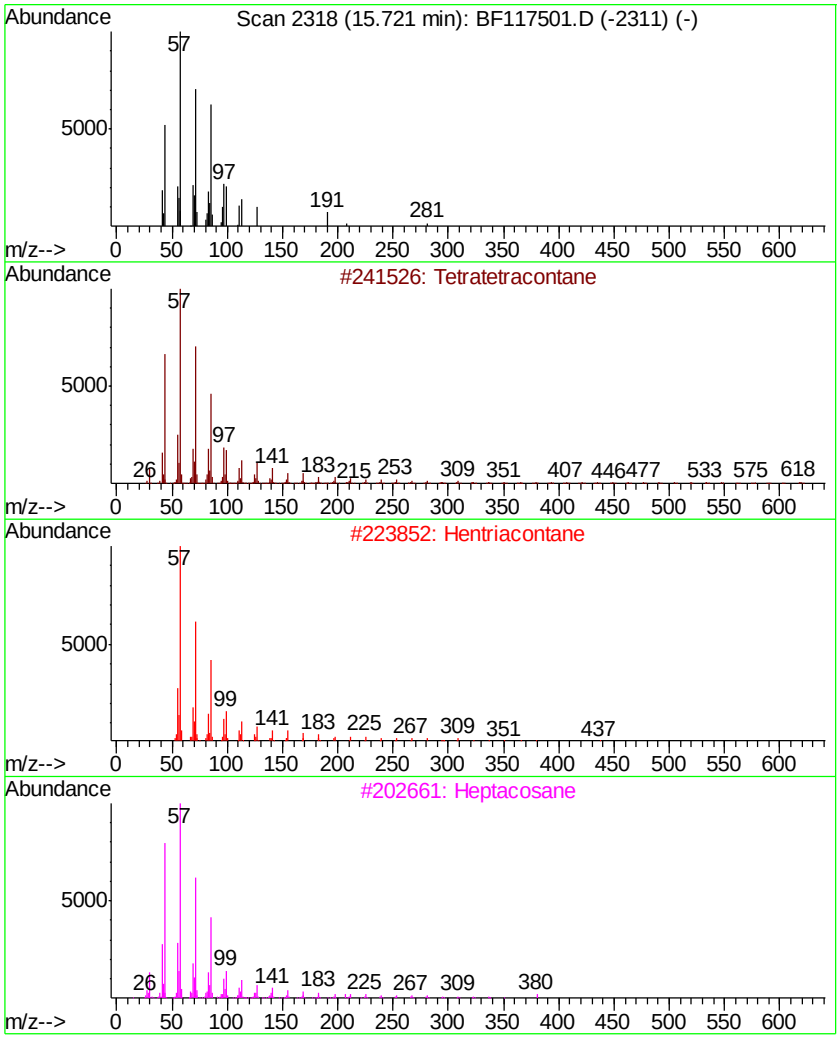
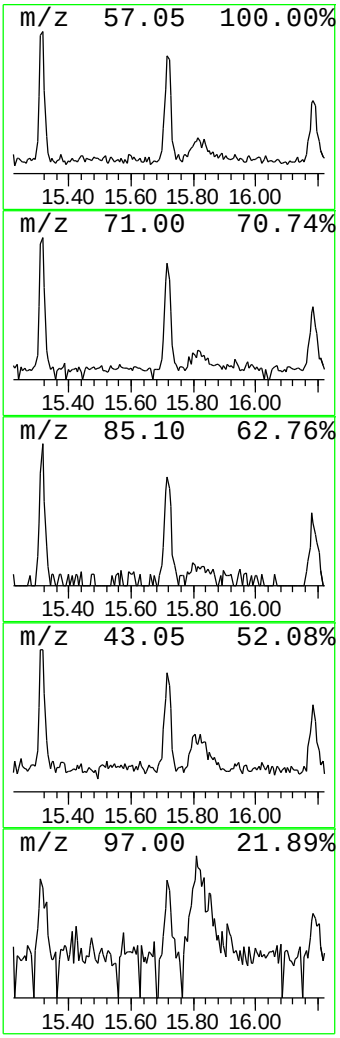
Peak Number 6 Tetratetracontane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.72 | 2.87 ng | 41849 | Perylene-d12 | 15.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |
| 2 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 86 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 83 |
| 4 | Tetrapentacontane | 759 | C54H110 | 005856-66-6 | 80 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 80 |



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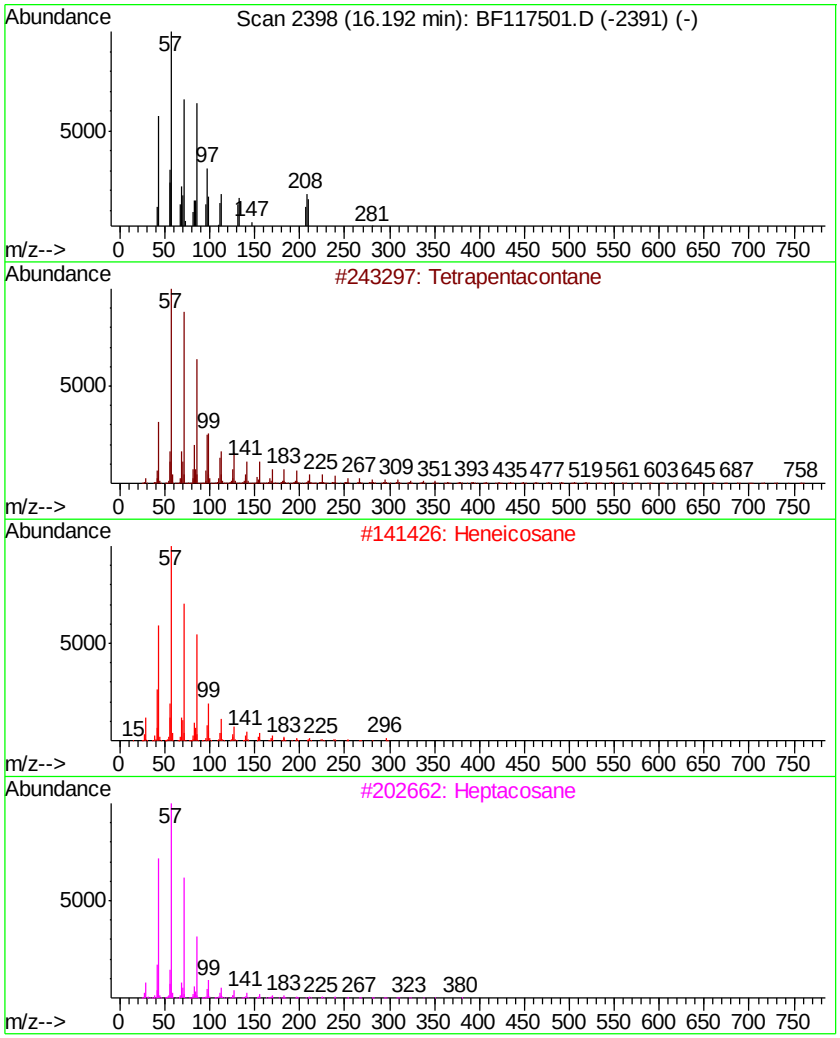
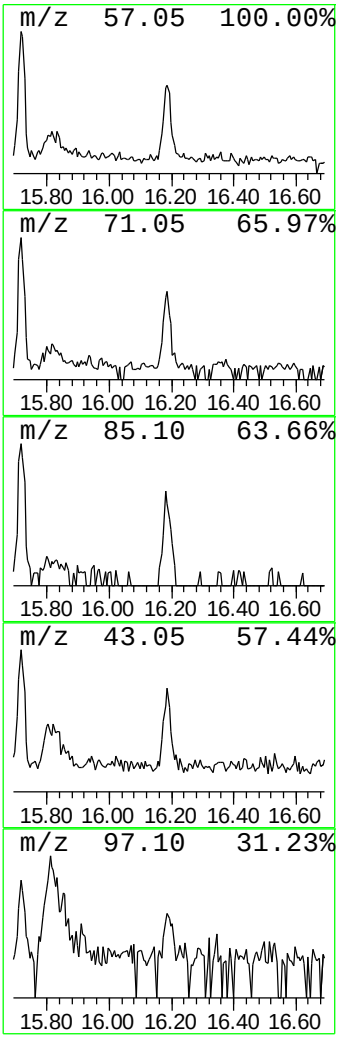
Peak Number 7 Tetrapentacontane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.19 | 2.25 ng | 32756 | Perylene-d12 | 15.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetrapentacontane | 759 | C54H110 | 005856-66-6 | 72 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 64 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 64 |
| 4 | 2-Bromotetradecane | 276 | C14H29Br | 074036-95-6 | 59 |
| 5 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 59 |



Tentatively Identified Compound (LSC) summary

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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown6.50 | 6.50 | 76.3 | ng | 1009170 | 1 | 6.73 | 264349 | 20.0 |
| n-Hexadecanoic acid | 11.78 | 3.5 | ng | 66327 | 4 | 11.24 | 378797 | 20.0 |
| n-Nonadecanol-1 | 13.73 | 11.1 | ng | 146198 | 5 | 13.89 | 263292 | 20.0 |
| Hexacosane | 14.96 | 2.5 | ng | 36724 | 6 | 15.32 | 291373 | 20.0 |
| Tetratetracontane | 15.72 | 2.9 | ng | 41849 | 6 | 15.32 | 291373 | 20.0 |
| Tetrapentacontane | 16.19 | 2.3 | ng | 32756 | 6 | 15.32 | 291373 | 20.0 |