LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060619\
Data File : BF114879.D
Acq On : 6 Jun 2019 22:55
Operator : HP/JU
Sample : K3211-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-20002

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-BF060419.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	5.287	538	544	547	rBV	7955549	10420860	94.90%	10.197%
2	6.316	712	719	722	rBV	7544557	10731422	97.73%	10.501%
3	6.445	735	741	744	rBV	9277094	10933450	99.57%	10.699%
4	6.669	775	779	782	rBV	3270325	2636836	24.01%	2.580%
5	6.828	801	806	809	rBV	8634732	8634336	78.63%	8.449%
6	7.233	868	875	878	rBV	6200146	7326068	66.72%	7.169%
7	7.951	992	997	1000	rBV	3755702	3305929	30.11%	3.235%
8	9.027	1174	1180	1183	rBV	10079456	10981026	100.00%	10.745%
9	9.422	1238	1247	1250	rBV	2436914	2266042	20.64%	2.217%
10	9.698	1288	1294	1298	rBV	3979808	3656639	33.30%	3.578%
11	10.480	1419	1427	1431	rBV	6433607	7163819	65.24%	7.010%
12	10.704	1462	1465	1468	rVV2	117771	116874	1.06%	0.114%
13	11.169	1540	1544	1547	rBV	4031150	3432069	31.25%	3.358%
14	11.716	1631	1637	1645	rBV	1390324	1519212	13.83%	1.487%
15	12.498	1766	1770	1783	rBV	477535	638893	5.82%	0.625%
16	12.633	1790	1793	1797	rBV2	122094	163284	1.49%	0.160%
17	12.757	1809	1814	1817	rBV	8648418	8843028	80.53%	8.653%
18	13.339	1911	1913	1919	rVB	138017	130159	1.19%	0.127%
19	13.657	1963	1967	1977	rBV2	841531	1014250	9.24%	0.992%
20	13.792	1985	1990	1993	rBV	2756325	2602985	23.70%	2.547%
21	13.980	2019	2022	2026	rBV	305582	300626	2.74%	0.294%
22	14.286	2071	2074	2083	rVB	504899	512352	4.67%	0.501%
23	14.580	2120	2124	2128	rBV	566893	570247	5.19%	0.558%
24	14.886	2172	2176	2184	rBV	504643	589524	5.37%	0.577%
25	15.174	2220	2225	2230	rVV	2087658	2390688	21.77%	2.339%
26	15.233	2231	2235	2245	rVB	462240	613517	5.59%	0.600%
27	15.621	2297	2301	2305	rBV	302820	428031	3.90%	0.419%
28	16.074	2374	2378	2383	rBV	184617	272211	2.48%	0.266%

Sum of corrected areas: 102194377

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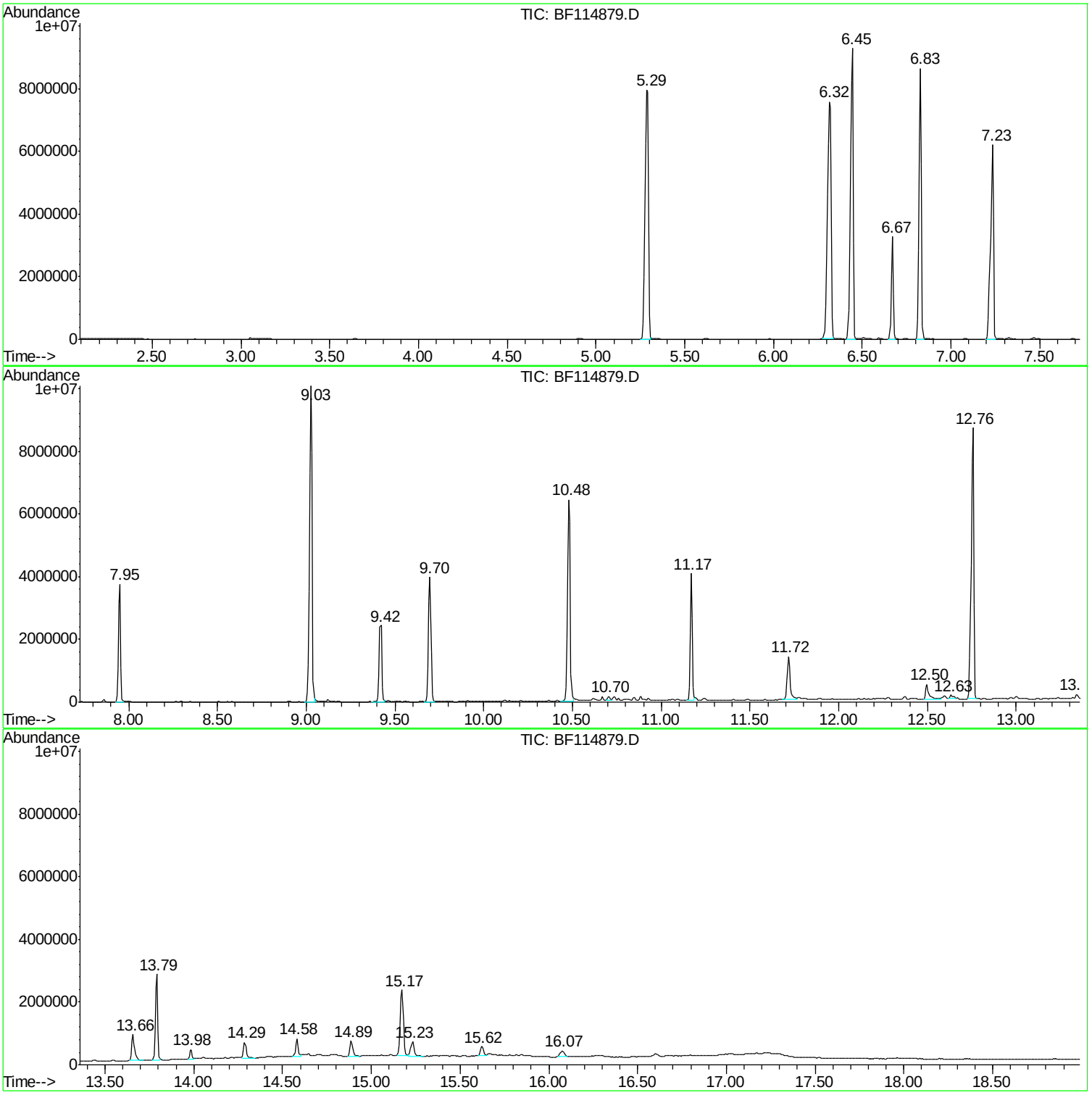
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-20002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060419.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

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Data File : BF114879.D
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Misc :
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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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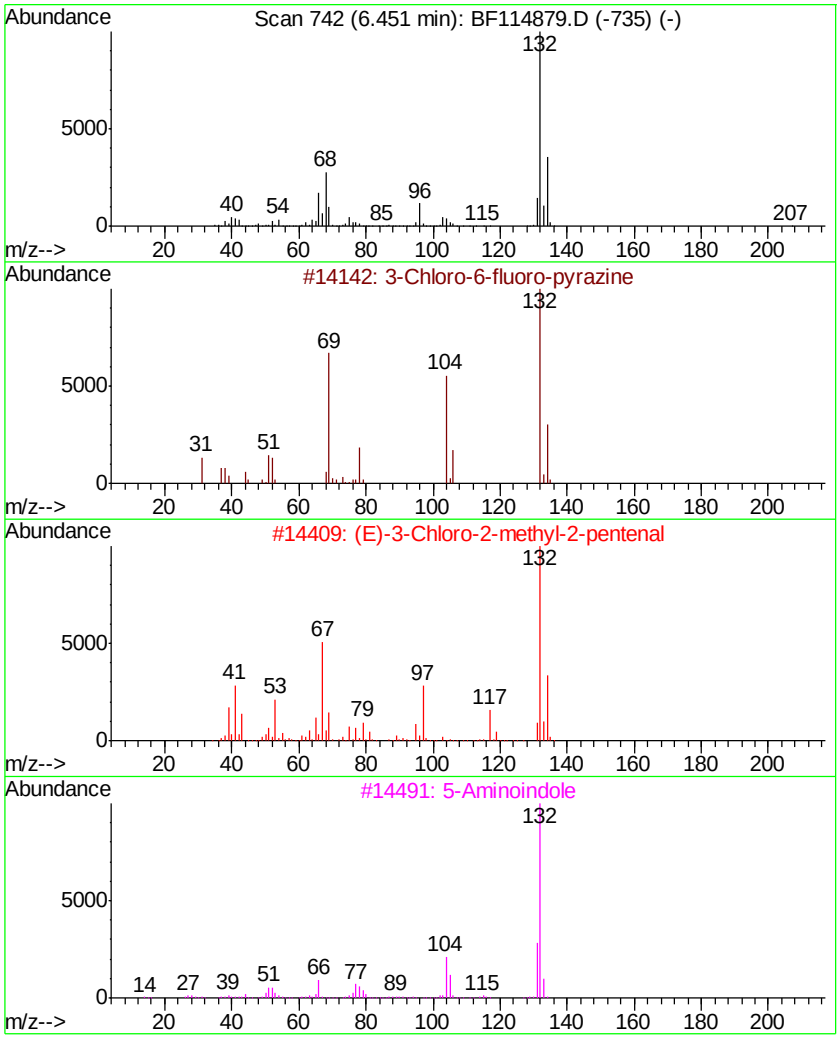
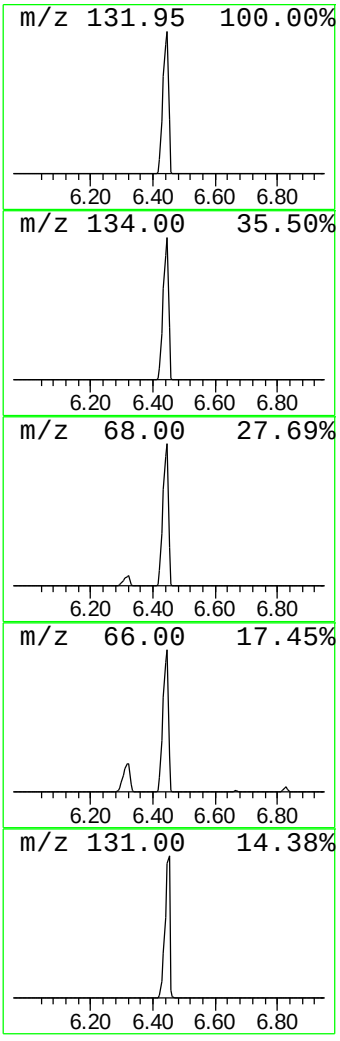
Peak Number 1 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	82.93 ng	10933500	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Sample : K3211-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-20002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060419.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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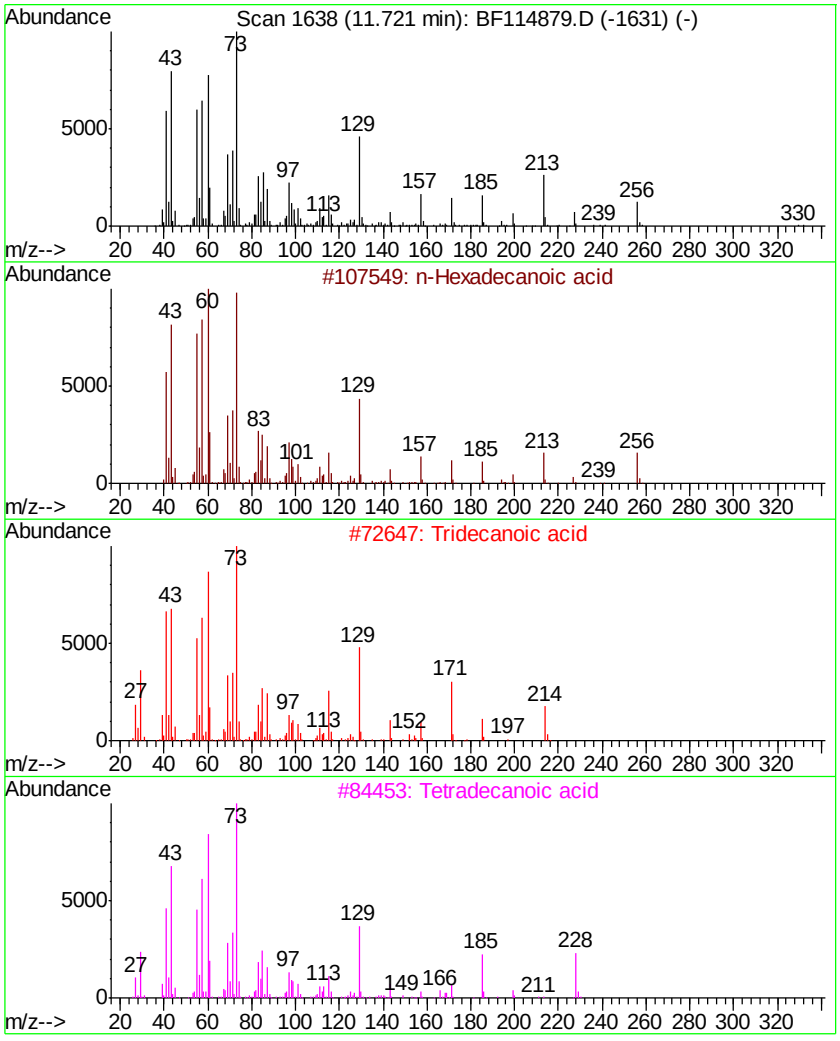
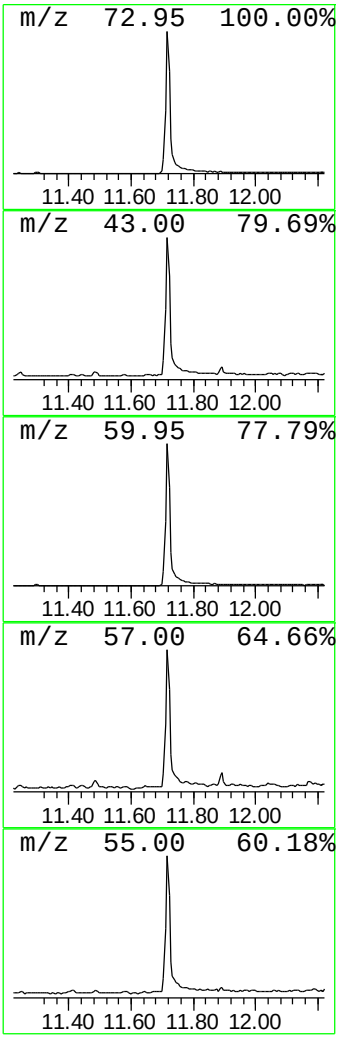
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	8.85 ng	1519210	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF060619\
Data File : BF114879.D
Acq On : 6 Jun 2019 22:55
Operator : HP/JU
Sample : K3211-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-20002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060419.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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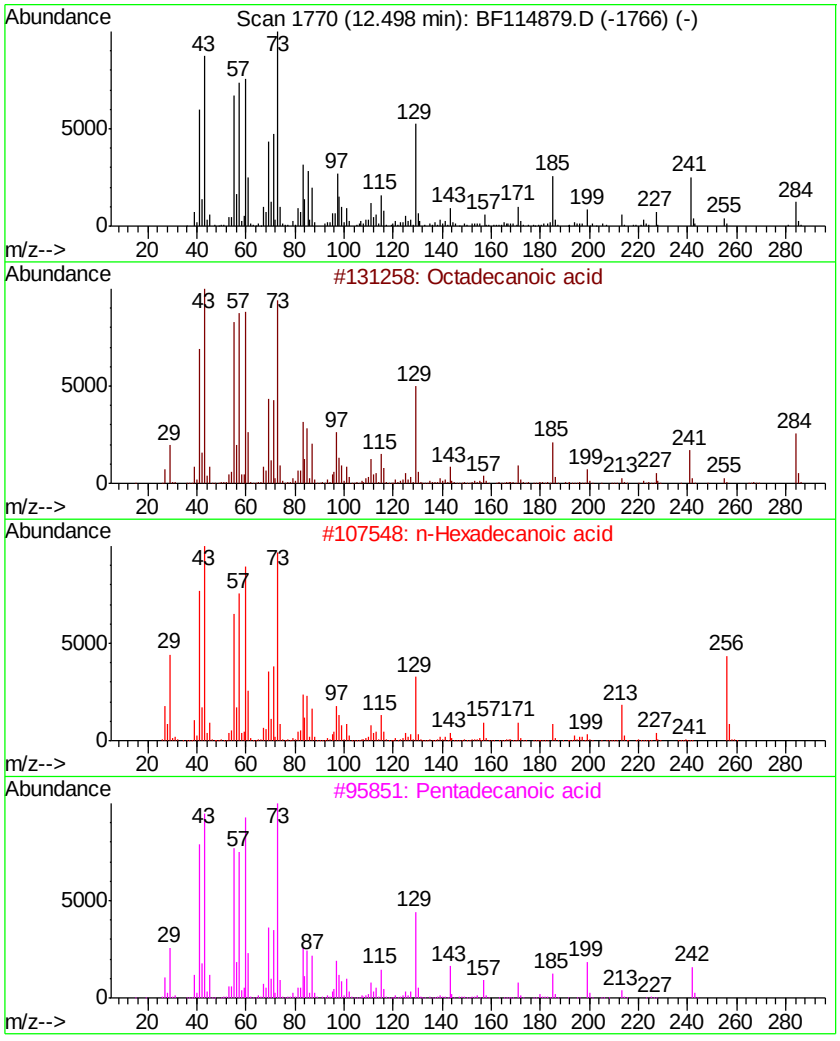
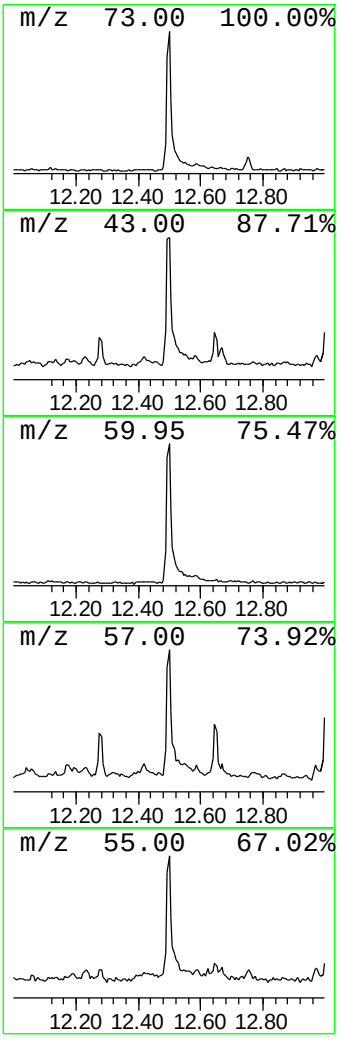
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	4.91 ng	638893	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





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Instrument : BNA_F
ClientSampleId : RBR-20002

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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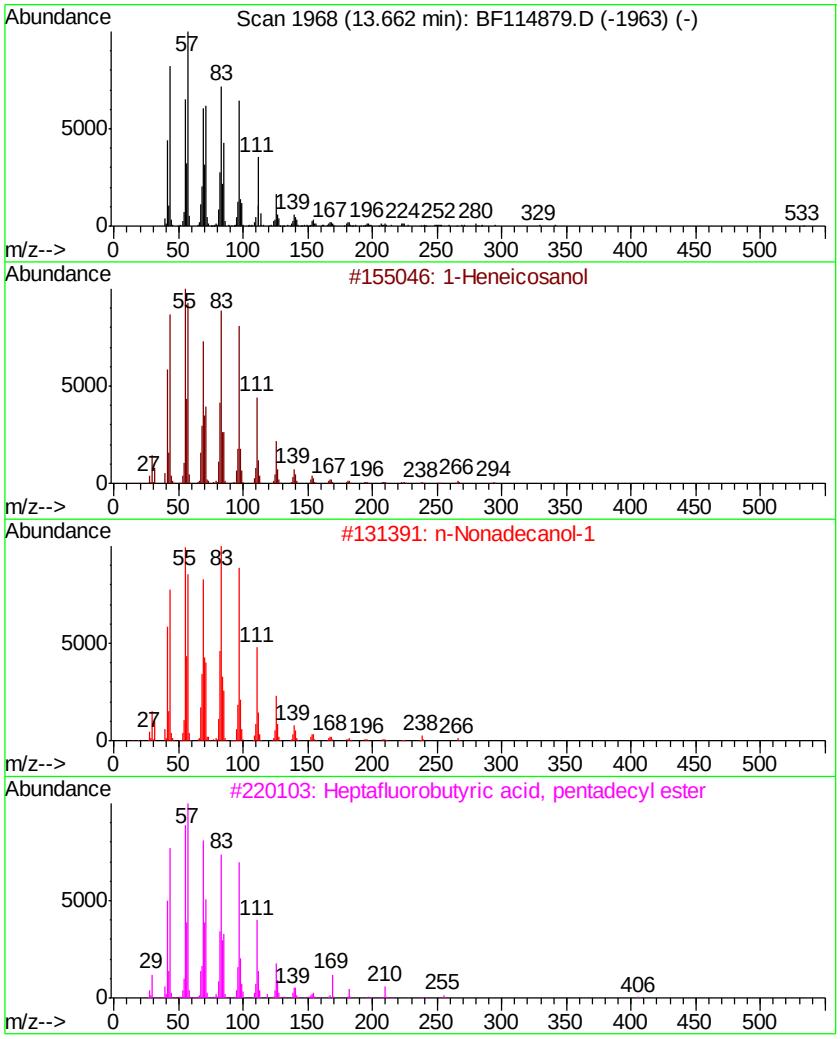
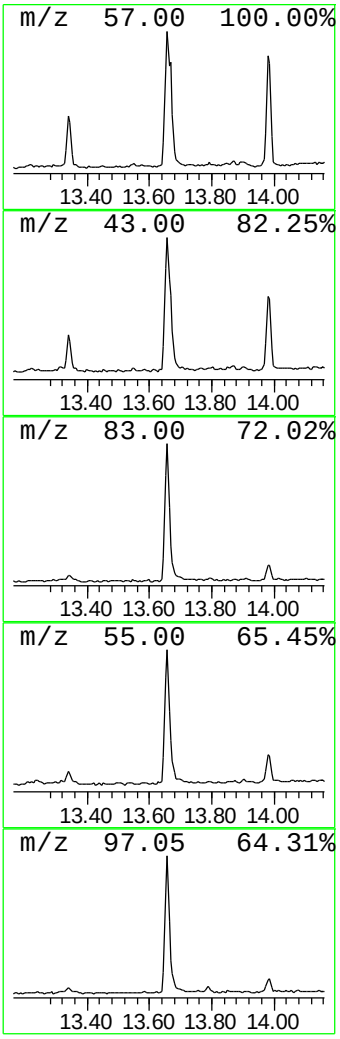
Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	7.79 ng	1014250	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93





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TIC Library : C:\DATABASE\NIST11.L
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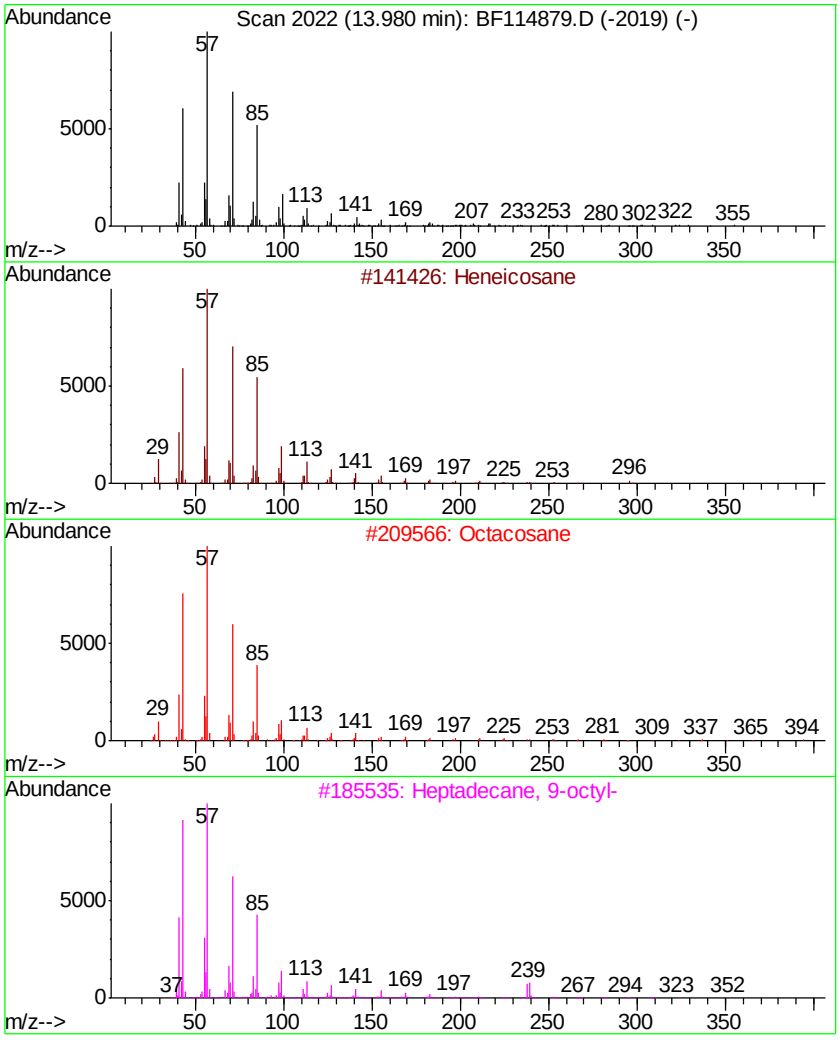
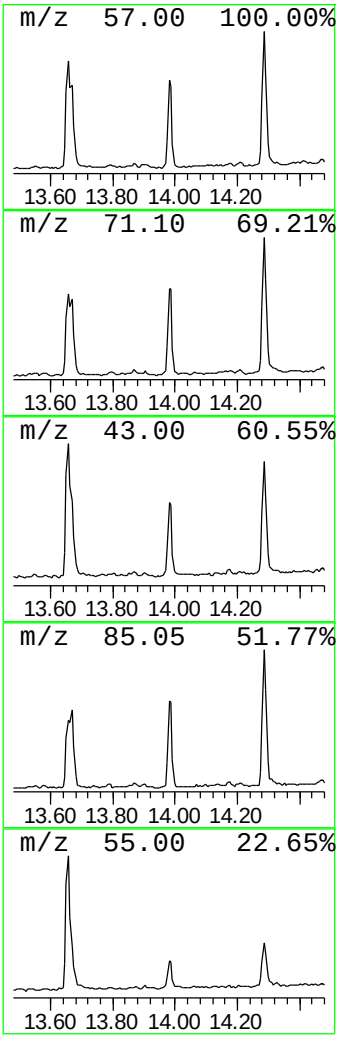
Peak Number 6 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	2.31 ng	300626	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Hexacosane	366	C26H54	000630-01-3	90





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Instrument : BNA_F
ClientSampleId : RBR-20002

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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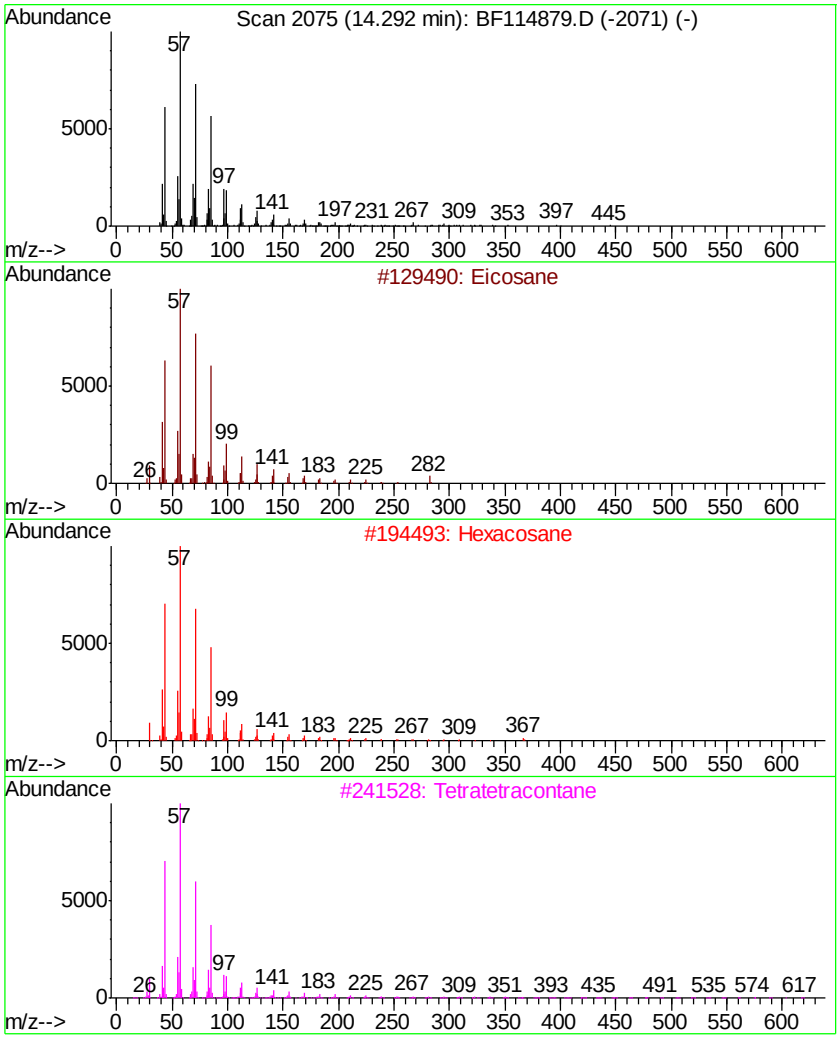
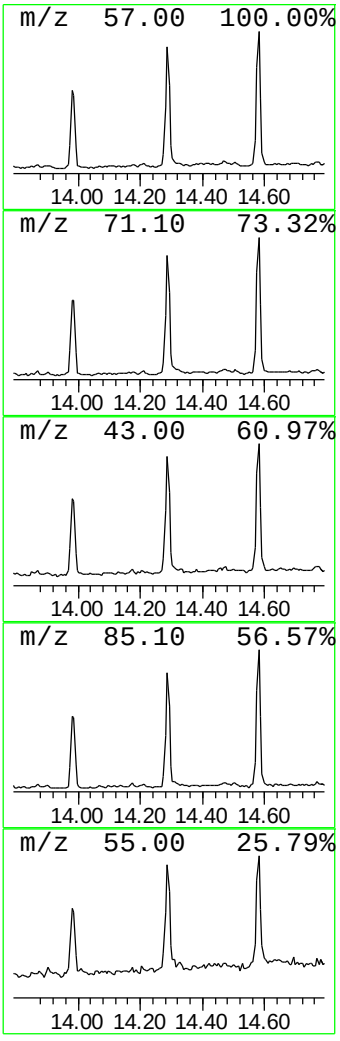
Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	3.94 ng	512352	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexatriacontane	507	C36H74	000630-06-8	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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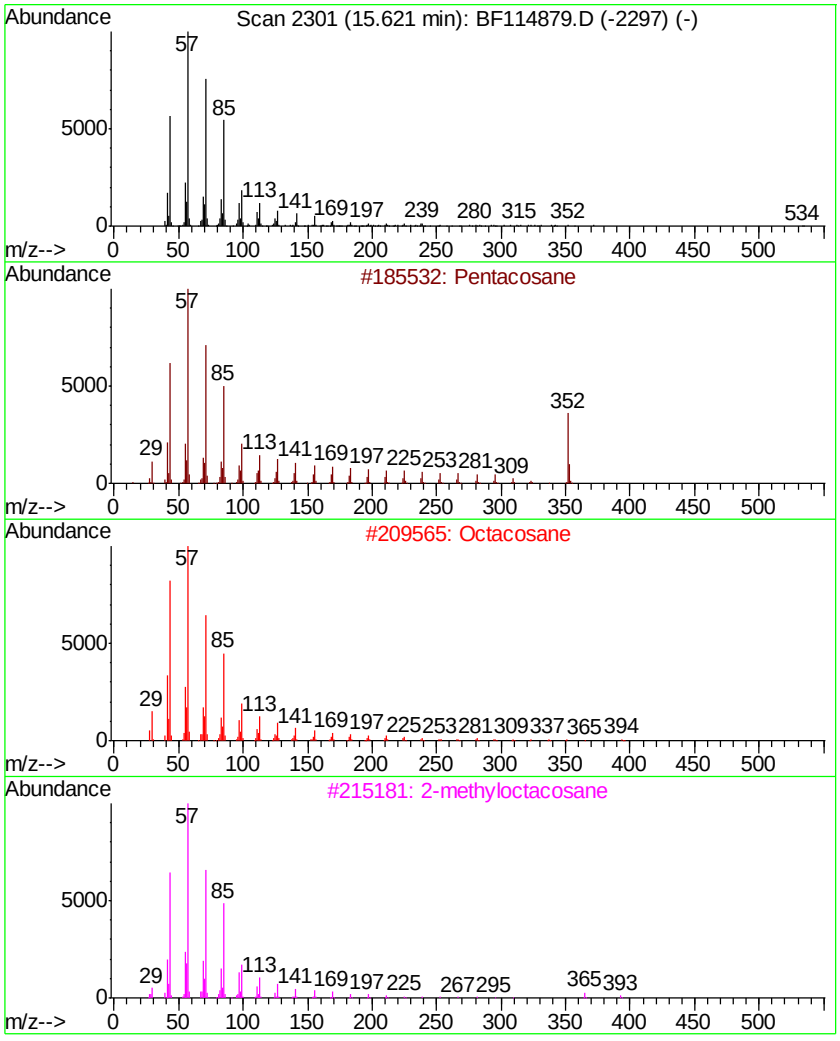
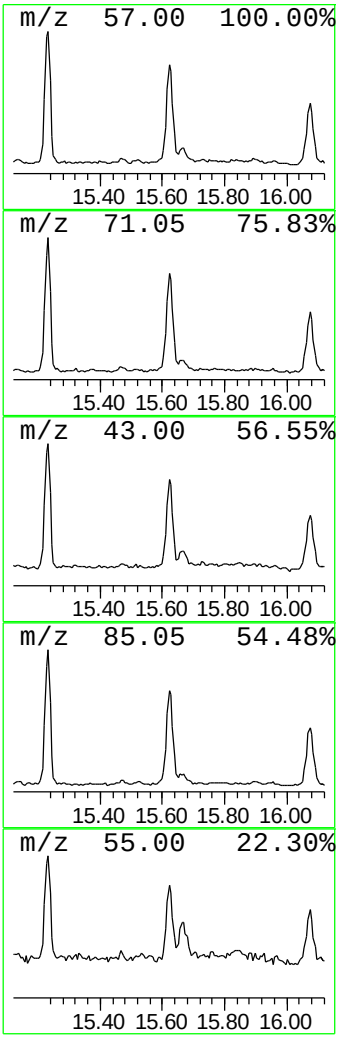
Peak Number 11 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	3.58 ng	428031	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





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
unknown6.45	6.45	82.9	ng	10933500	1	6.67	2636840	20.0
n-Hexadecanoic acid	11.72	8.8	ng	1519210	4	11.17	3432070	20.0
Octadecanoic acid	12.50	4.9	ng	638893	5	13.79	2602990	20.0
1-Heneicosanol	13.66	7.8	ng	1014250	5	13.79	2602990	20.0
Heneicosane	13.98	2.3	ng	300626	5	13.79	2602990	20.0
Eicosane	14.29	3.9	ng	512352	5	13.79	2602990	20.0
Pentacosane	15.62	3.6	ng	428031	6	15.17	2390690	20.0