LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

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-BF042716.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	2.224	10	12	27	rVB	52227	155335	3.94%	0.372%
2	4.967	250	252	257	rBV	69338	109653	2.78%	0.263%
3	5.379	285	288	290	rBV	3329778	3943720	100.00%	9.442%
4	6.419	376	379	381	rBV	3524692	3877705	98.33%	9.284%
5	6.544	387	390	392	rBV	3793328	3699087	93.80%	8.857%
6	6.613	394	396	402	rVB2	42551	69140	1.75%	0.166%
7	6.773	408	410	413	rBV	1714743	1810443	45.91%	4.335%
8	6.933	421	424	426	rBV	3140557	2863202	72.60%	6.855%
9	7.345	457	460	462	rBV	2405072	2519721	63.89%	6.033%
10	7.447	466	469	476	rVB	52755	122782	3.11%	0.294%
11	8.065	520	523	525	rBV	2616943	2421385	61.40%	5.797%
12	8.179	532	533	541	rVB5	21770	41922	1.06%	0.100%
13	9.139	615	617	620	rBV	2914783	3417076	86.65%	8.181%
14	9.539	650	652	654	rBV	387731	353823	8.97%	0.847%
15	9.756	669	671	674	rBV	85325	76763	1.95%	0.184%
16	9.813	674	676	679	rBV2	2102304	2343617	59.43%	5.611%
17	10.259	711	715	716	rBV	127607	161501	4.10%	0.387%
18	10.476	731	734	735	rBV	51361	72705	1.84%	0.174%
19	10.602	742	745	752	rBV	2030005	2067559	52.43%	4.950%
20	10.728	754	756	763	rVB	188896	233505	5.92%	0.559%
21	10.922	771	773	777	rBV2	24549	48728	1.24%	0.117%
22	11.174	793	795	796	rBV	119393	95220	2.41%	0.228%
23	11.299	803	806	808	rBV	1971579	2038190	51.68%	4.880%
24	11.528	824	826	831	rBV	75795	92075	2.33%	0.220%
25	11.596	831	832	839	rVB	44637	47984	1.22%	0.115%
26	12.499	909	911	914	rBV	45806	49356	1.25%	0.118%
27	12.705	927	929	933	rBV2	137363	220341	5.59%	0.528%
28	12.785	935	936	942	rVB	72113	56727	1.44%	0.136%
29	12.877	942	944	947	rBV	1949791	2359066	59.82%	5.648%
30	13.117	961	965	967	rBV	64498	87113	2.21%	0.209%
31	13.414	989	991	993	rBV	154953	141321	3.58%	0.338%
32	13.459	993	995	996	rBV	142809	120131	3.05%	0.288%
33	13.779	1020	1023	1033	rBV	571435	849950	21.55%	2.035%
34	13.928	1033	1036	1043	rBV	1518700	1826521	46.31%	4.373%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

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-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.031	1043	1045	1049	rVB	49467	65703	1.67%	0.157%
36	14.100	1049	1051	1054	rBV	275722	328541	8.33%	0.787%
37	14.408	1076	1078	1084	rBV	416758	428464	10.86%	1.026%
38	14.705	1101	1104	1106	rBV	278753	309923	7.86%	0.742%
39	14.774	1107	1110	1113	rBV3	25806	51459	1.30%	0.123%
40	14.934	1122	1124	1129	rVB	35418	64822	1.64%	0.155%
41	15.014	1129	1131	1135	rBV	184898	224740	5.70%	0.538%
42	15.323	1156	1158	1161	rBV	890481	1383887	35.09%	3.313%
43	15.368	1161	1162	1165	rVB	120525	123458	3.13%	0.296%
44	15.768	1194	1197	1199	rBV	64623	111150	2.82%	0.266%
45	15.814	1199	1201	1206	rVB2	44578	94993	2.41%	0.227%
46	16.225	1234	1237	1239	rBV	38719	70270	1.78%	0.168%
47	16.705	1276	1279	1282	rVB3	36396	70958	1.80%	0.170%
48	17.197	1320	1322	1327	rVB6	20792	44429	1.13%	0.106%

Sum of corrected areas: 41766164

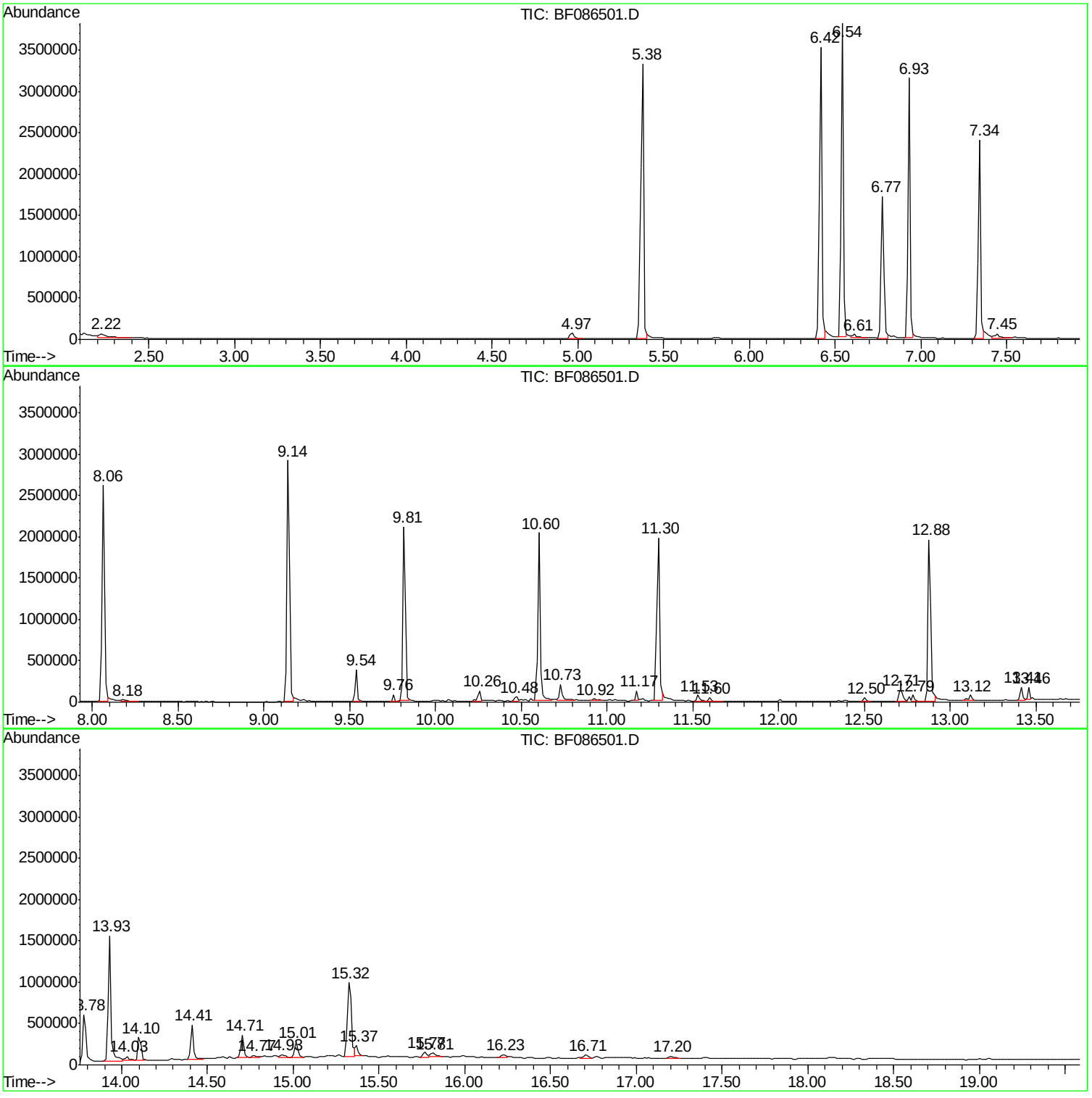
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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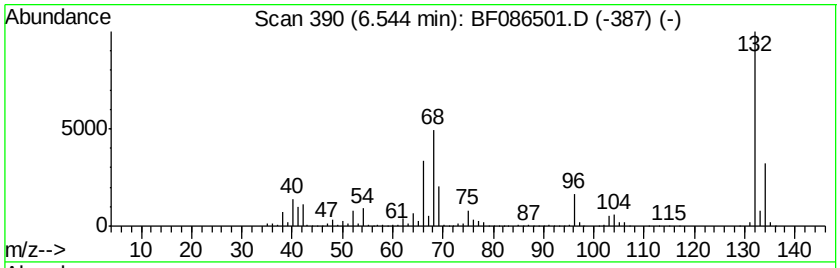
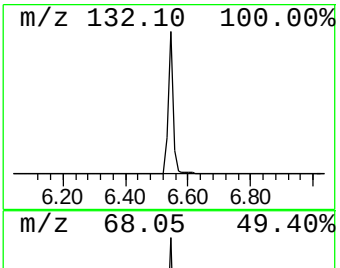
Peak Number 1 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	40.86 ng	3699090	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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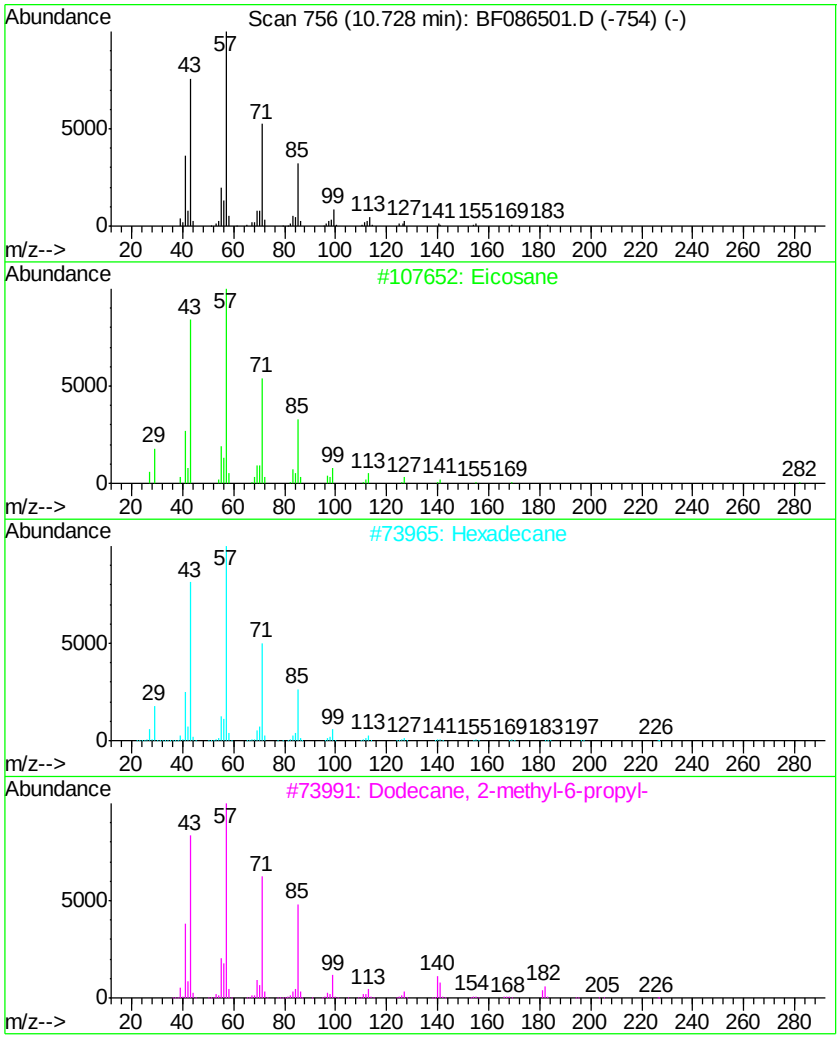
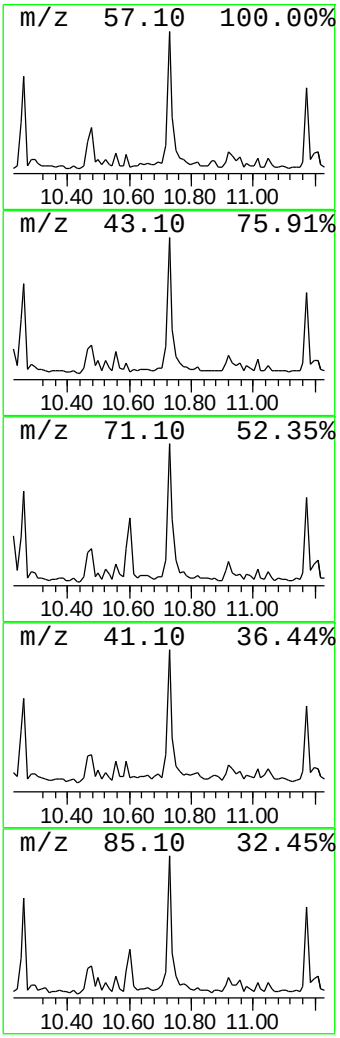
Peak Number 3 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.29 ng	233505	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	90
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
5	Pentadecane	212	C15H32	000629-62-9	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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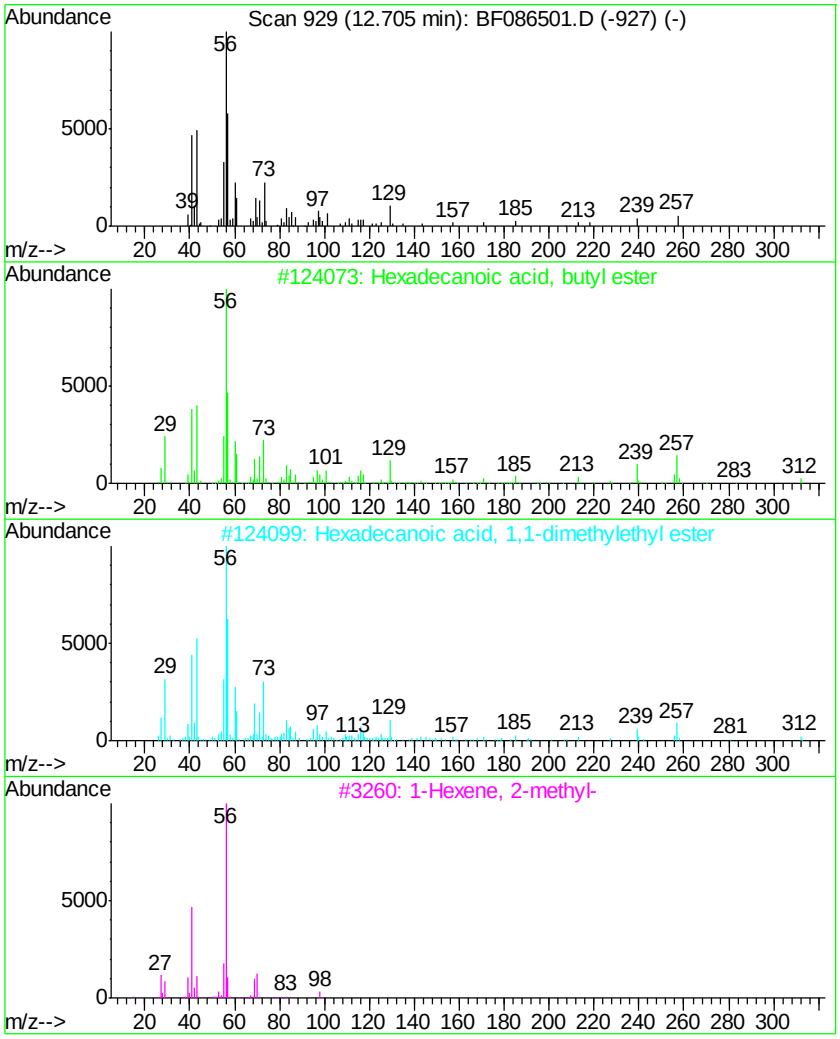
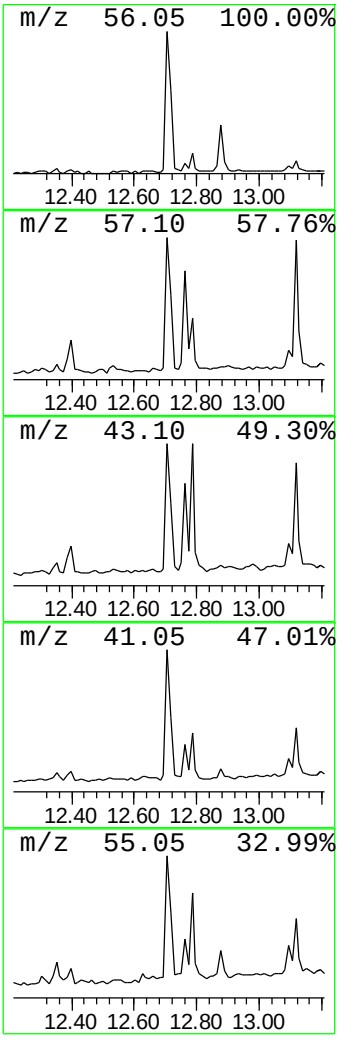
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.41 ng	220341	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
4	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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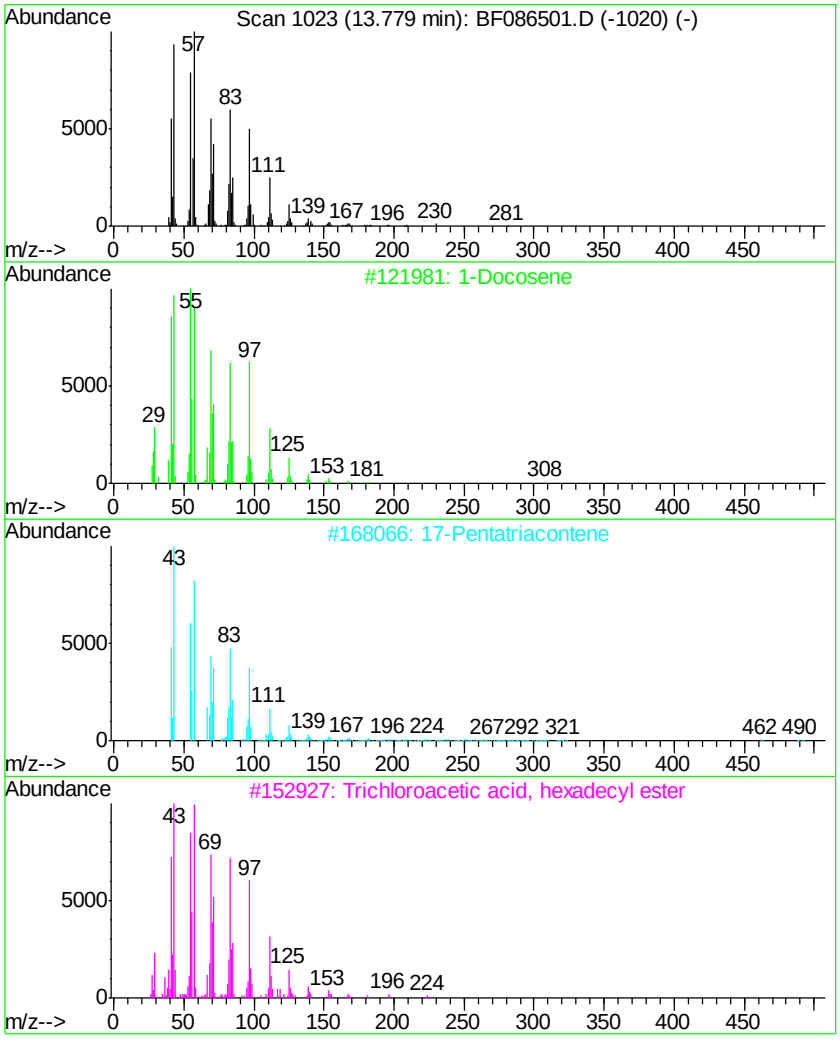
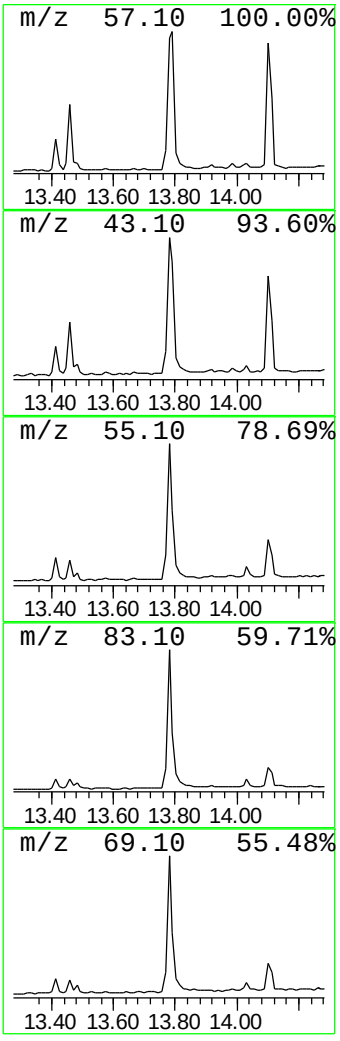
Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	9.31 ng	849950	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	87
5	1-Octadecanol	270	C18H38O	000112-92-5	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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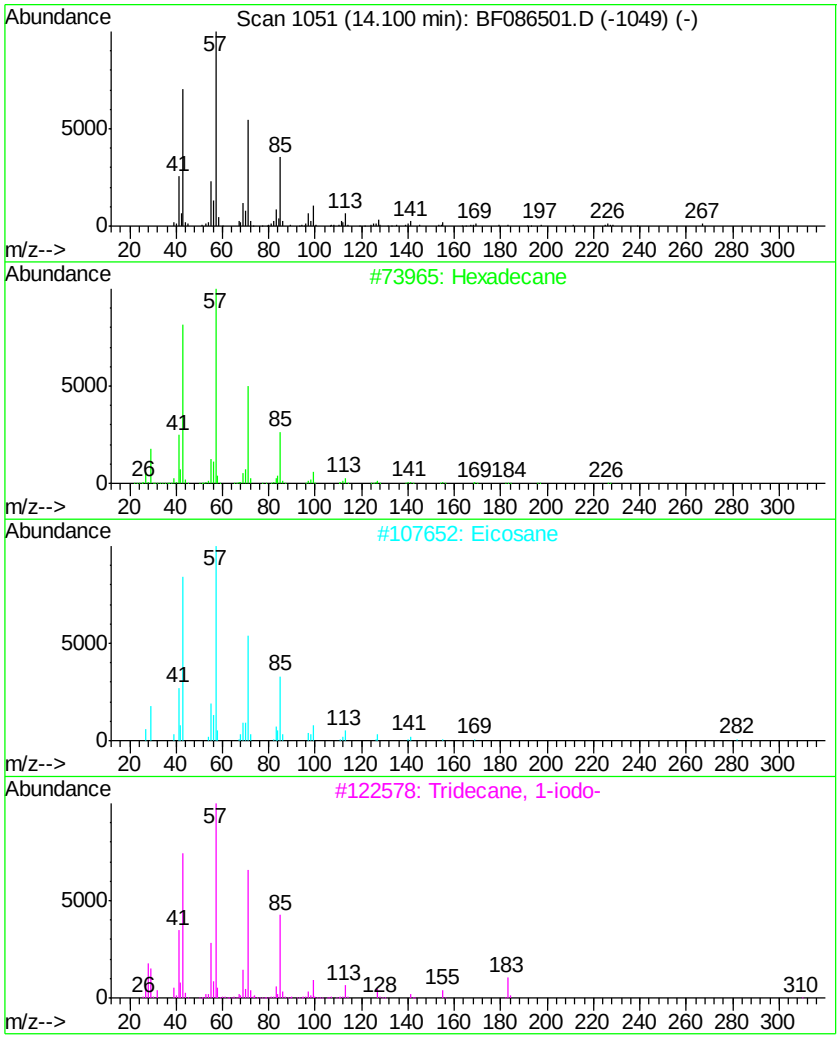
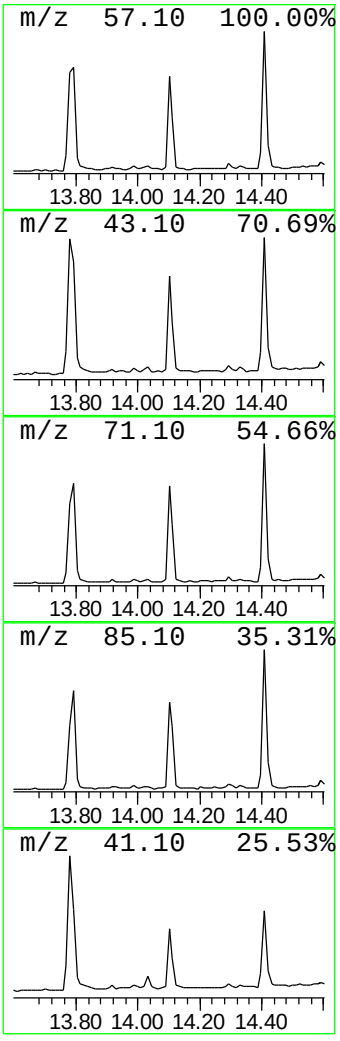
Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	3.60 ng	328541	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Octacosane	394	C28H58	000630-02-4	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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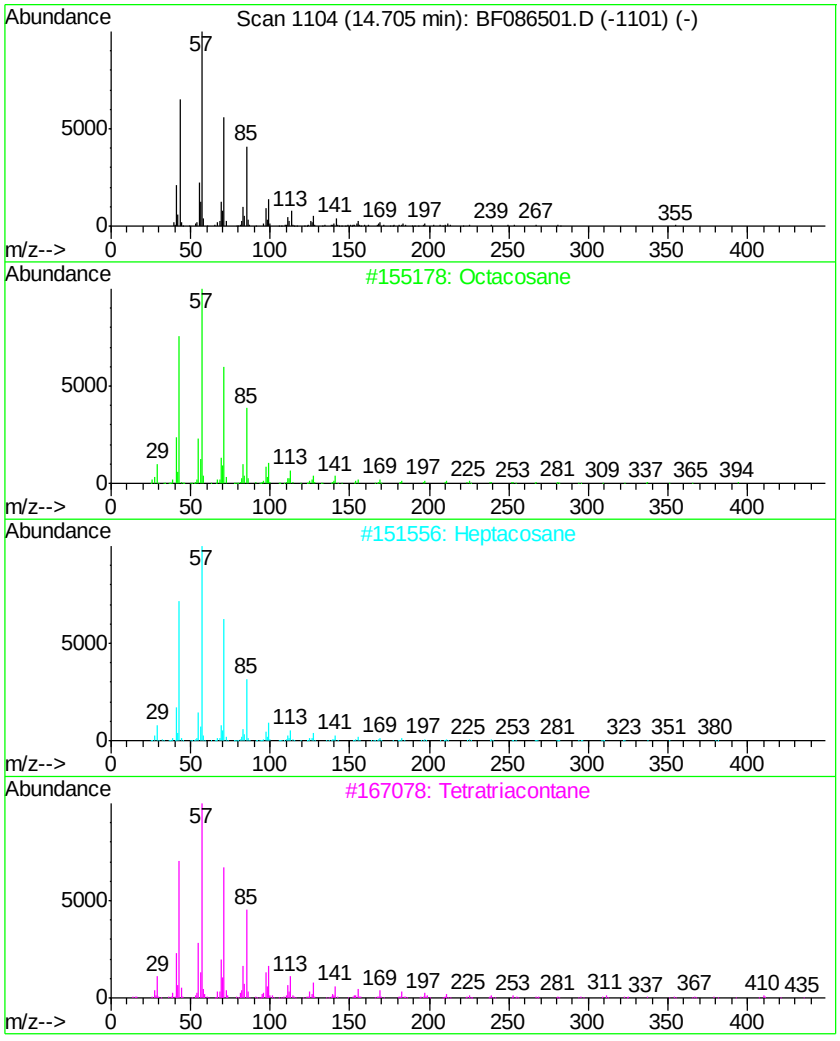
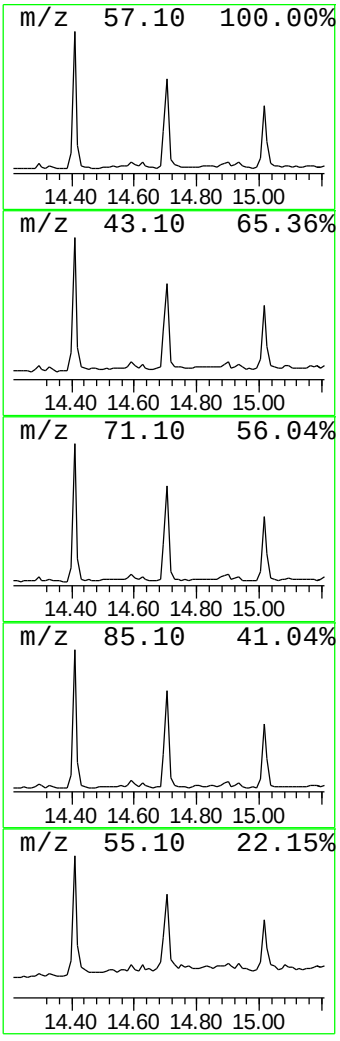
Peak Number 8 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	4.48 ng	309923	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetratriacontane	479	C34H70	014167-59-0	91
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
5	Hexatriacontane	507	C36H74	000630-06-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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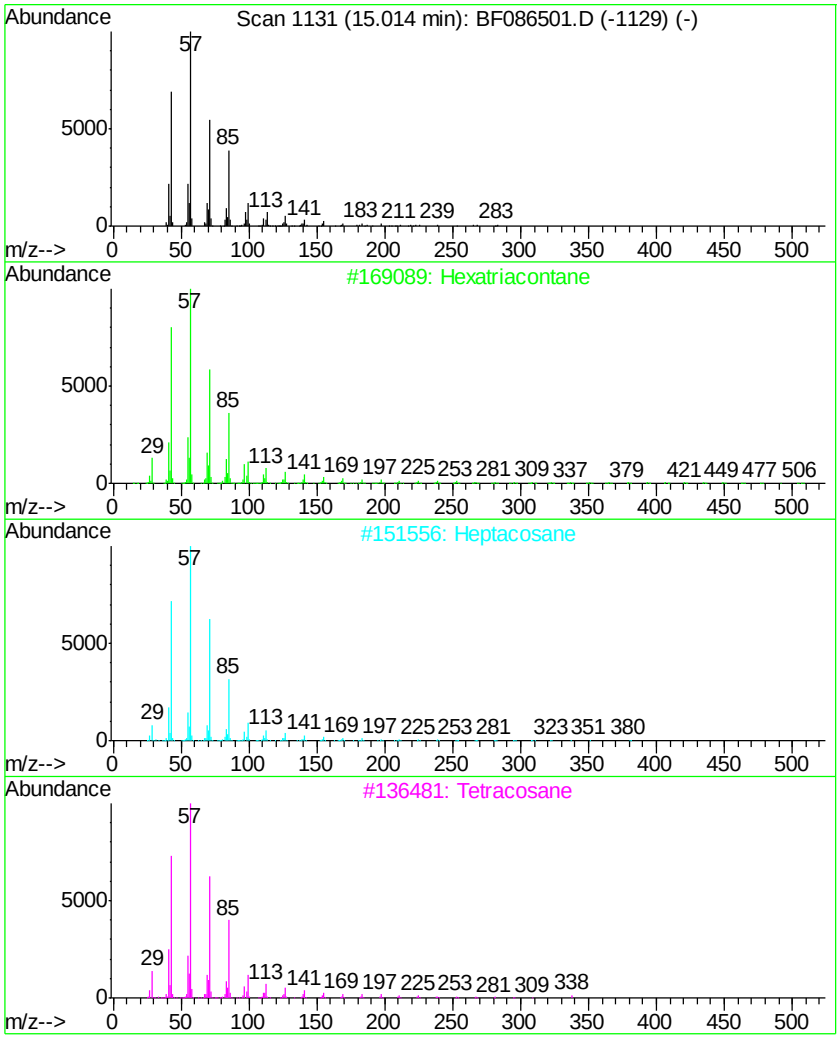
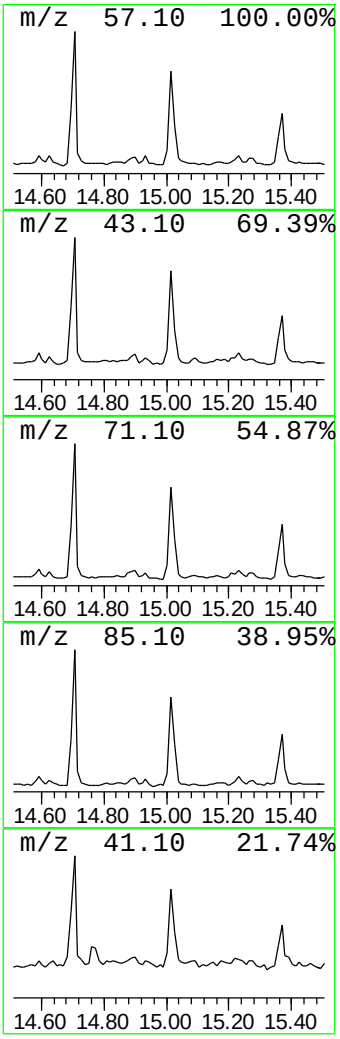
Peak Number 9 Hexatriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	3.25 ng	224740	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042916\
Data File : BF086501.D
Acq On : 29 Apr 2016 19:29
Operator : UM/SJ
Sample : H2654-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-13(6-17FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.54	6.54	40.9	ng	3699090	1	6.77	1810440	20.0
Eicosane	10.73	2.3	ng	233505	4	11.30	2038190	20.0
Hexadecanoic acid...	12.71	2.4	ng	220341	5	13.93	1826520	20.0
1-Docosene	13.78	9.3	ng	849950	5	13.93	1826520	20.0
Hexadecane	14.10	3.6	ng	328541	5	13.93	1826520	20.0
Octacosane	14.71	4.5	ng	309923	6	15.32	1383890	20.0
Hexatriacontane	15.01	3.3	ng	224740	6	15.32	1383890	20.0