LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090254.D
Acq On : 27 Sep 2016 16:22
Operator : UM/SJ
Sample : H4933-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5-15-15.5

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-BF092016.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	1.644	4	5	55	rVB	3290693	9893001	100.00%	22.625%
2	4.559	257	260	270	rBV	392505	682786	6.90%	1.561%
3	5.027	298	301	304	rBV	2066822	3210345	32.45%	7.342%
4	6.136	394	398	400	rBV	2423868	3522760	35.61%	8.056%
5	6.239	404	407	409	rBV	3143681	3191719	32.26%	7.299%
6	6.467	425	427	430	rBV	787576	755706	7.64%	1.728%
7	6.627	438	441	443	rBV	2739100	2534308	25.62%	5.796%
8	7.039	475	477	480	rBV	1458429	2040352	20.62%	4.666%
9	7.187	487	490	495	rVB	90863	152800	1.54%	0.349%
10	7.759	538	540	542	rBV	1136037	1046674	10.58%	2.394%
11	8.845	632	635	637	rBV	3355797	3861116	39.03%	8.830%
12	9.245	667	670	672	rBV	1508360	1465426	14.81%	3.351%
13	9.496	690	692	695	rVB	1120167	1184342	11.97%	2.709%
14	10.285	758	761	764	rBV	2095538	2390390	24.16%	5.467%
15	10.433	770	774	778	rBV2	120269	173051	1.75%	0.396%
16	10.971	818	821	823	rBV	1282913	1271703	12.85%	2.908%
17	11.233	841	844	848	rBV	92387	115911	1.17%	0.265%
18	12.559	957	960	962	rBV	3281010	3644992	36.84%	8.336%
19	13.474	1037	1040	1047	rBV	134539	200234	2.02%	0.458%
20	13.577	1047	1049	1052	rBV	1086205	1225918	12.39%	2.804%
21	14.445	1123	1125	1128	rVB	112361	129290	1.31%	0.296%
22	14.902	1162	1165	1168	rBV	931835	1033977	10.45%	2.365%

Sum of corrected areas: 43726801

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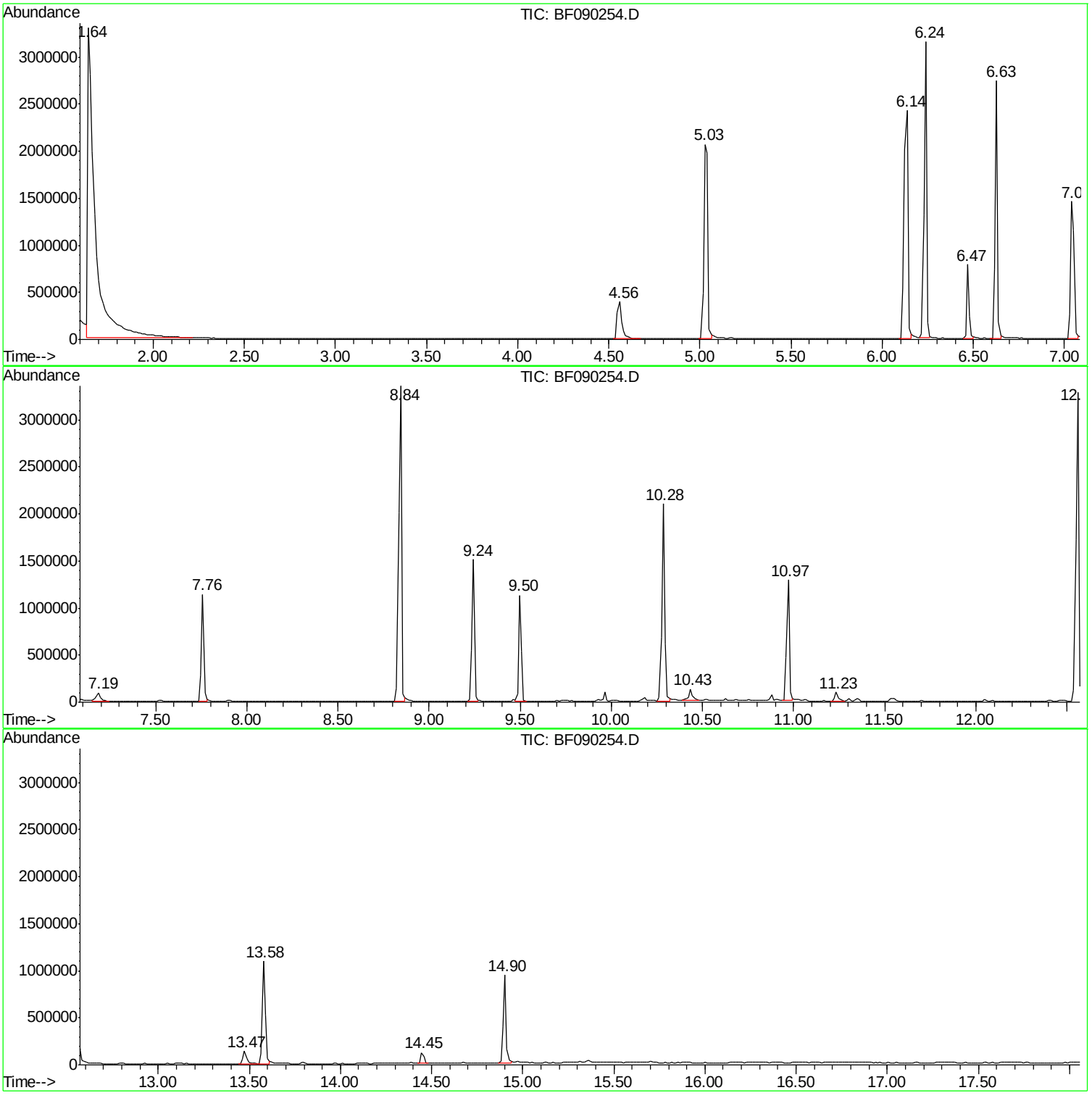
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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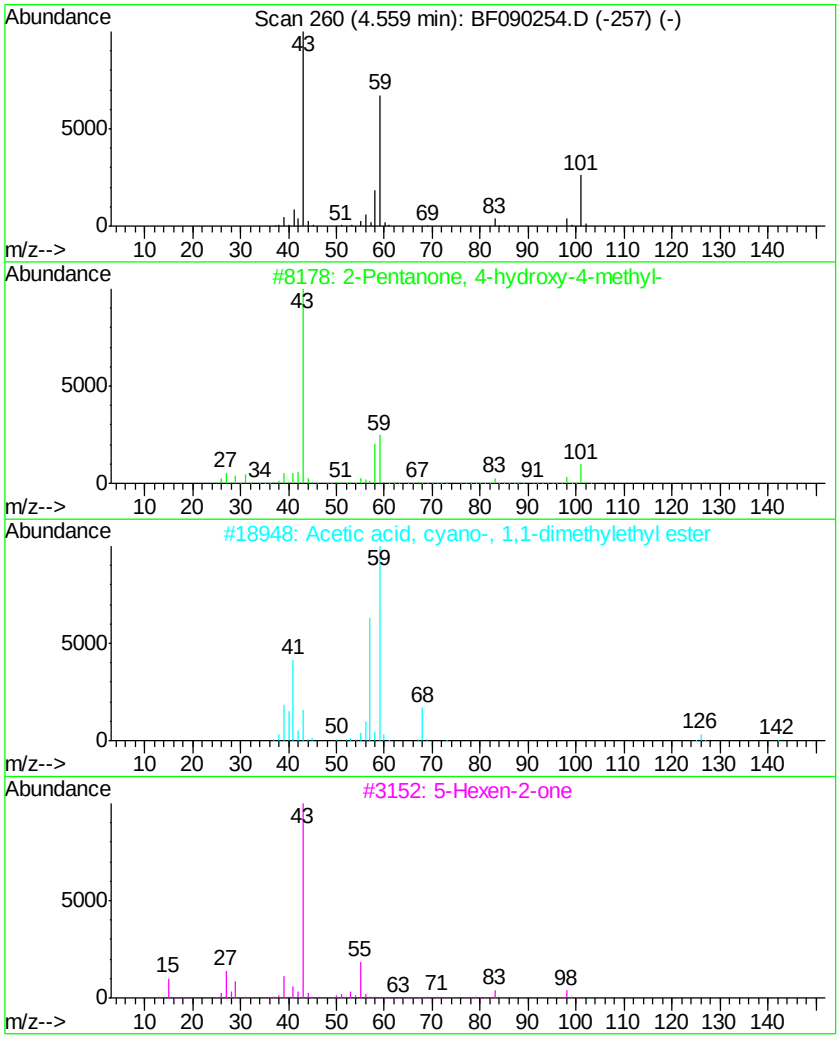
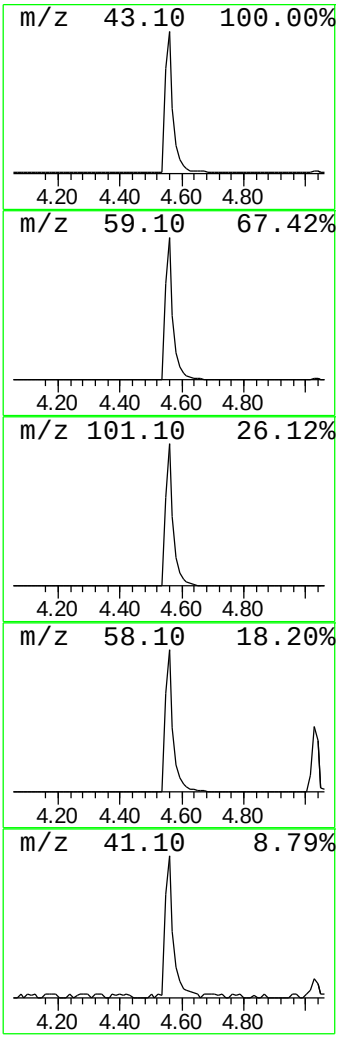
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	18.07 ng	682786	1,4-Dichlorobenzene-d4	6.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Guanidine	59	CH5N3	000113-00-8	9





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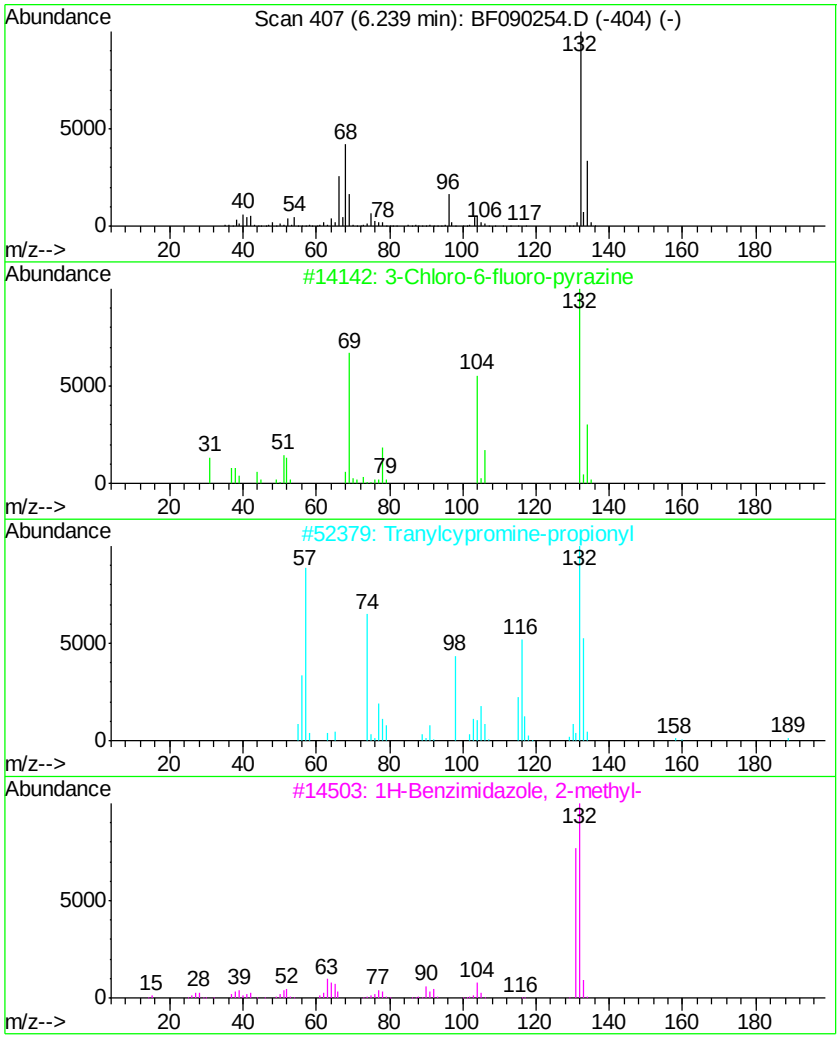
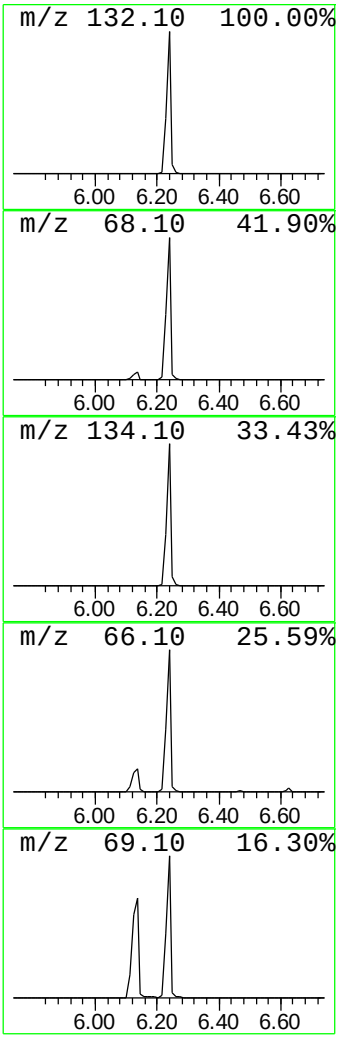
Peak Number 2 unknown6.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	84.47 ng	3191720	1,4-Dichlorobenzene-d4	6.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : B5-15-15.5

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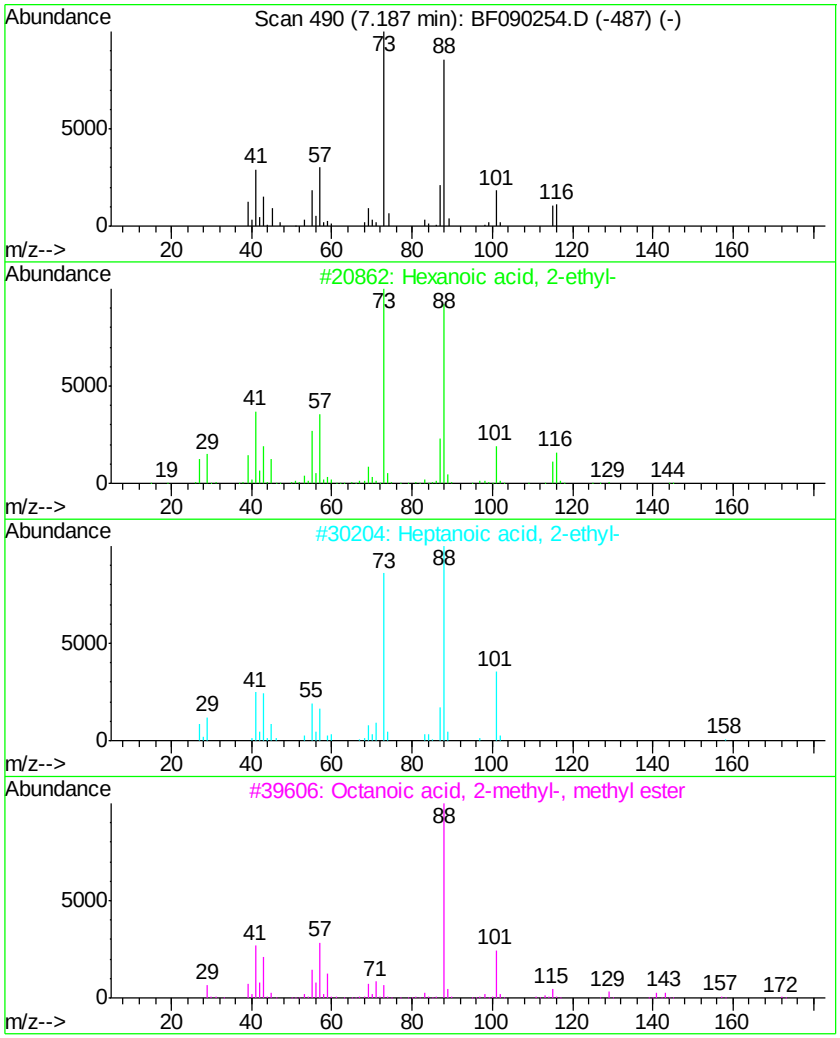
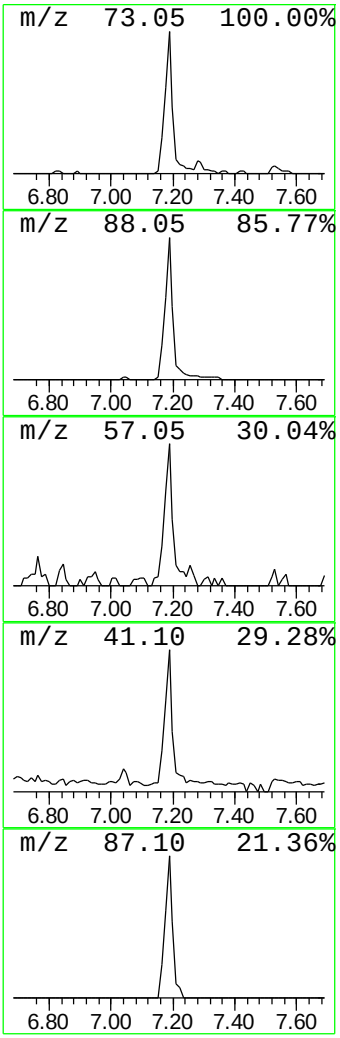
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	2.92 ng	152800	Naphthalene-d8	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45
3	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	38
4	1,4-Dioxane	88	C4H8O2	000123-91-1	37
5	Hydroxypivalic acid	118	C5H10O3	004835-90-9	36





Library Search Compound Report

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ClientSampleId : B5-15-15.5

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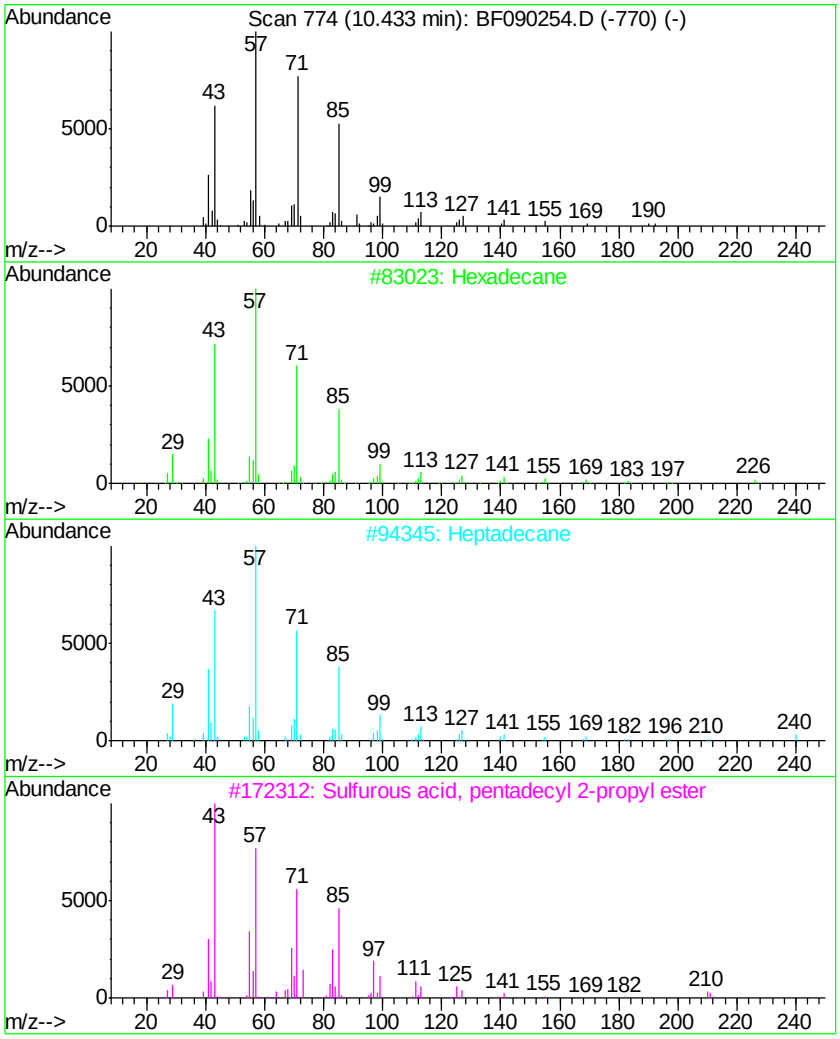
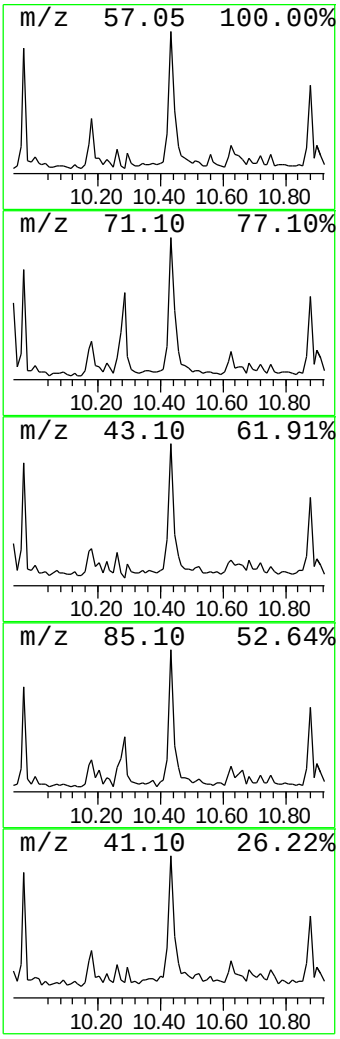
Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.72 ng	173051	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	83
4	Heptacosane	380	C27H56	000593-49-7	80
5	Pentadecane	212	C15H32	000629-62-9	72





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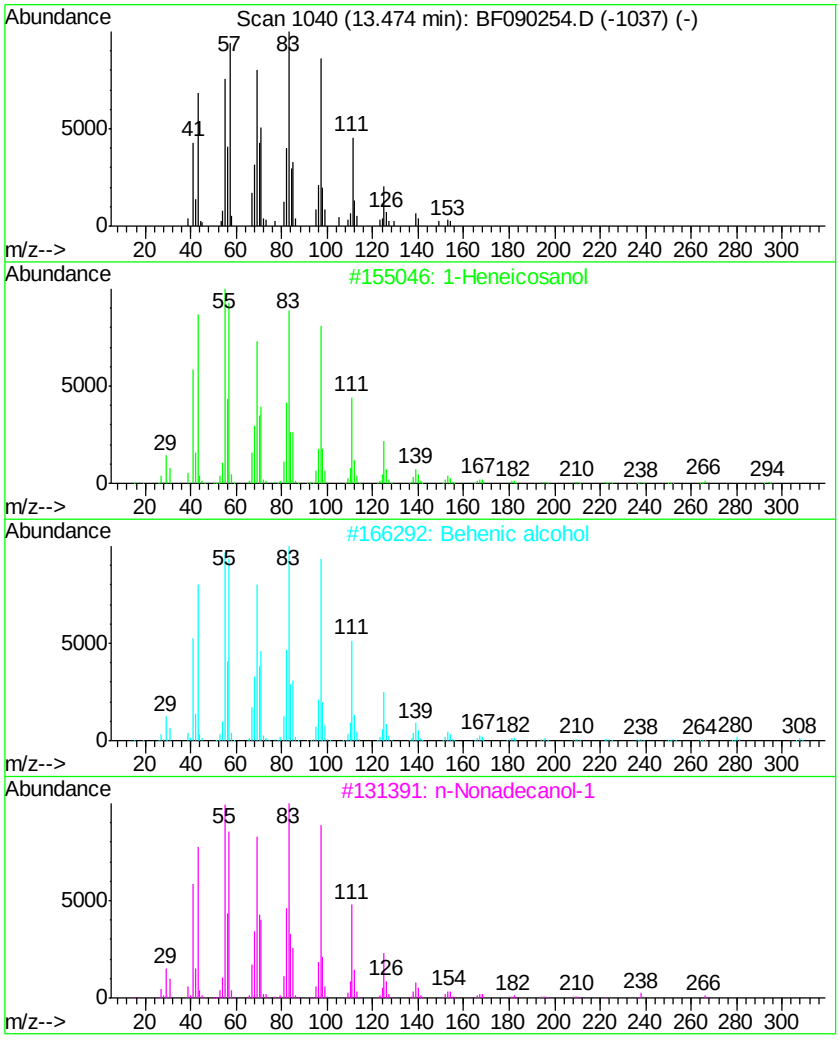
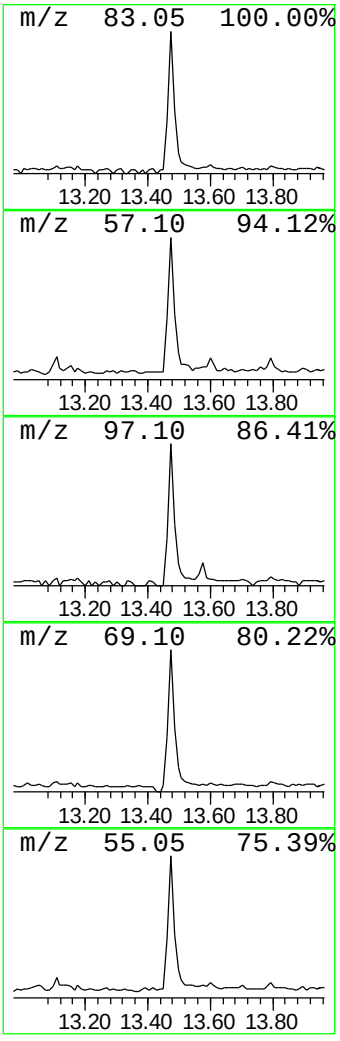
Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	3.27 ng	200234	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91





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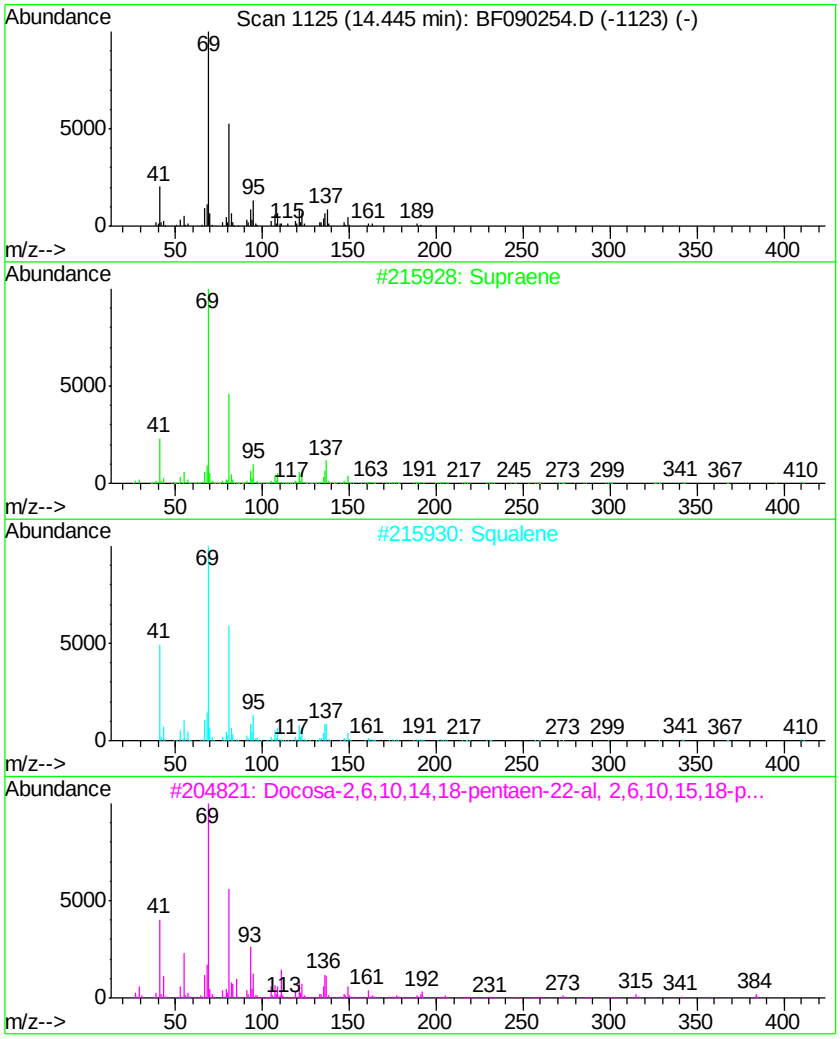
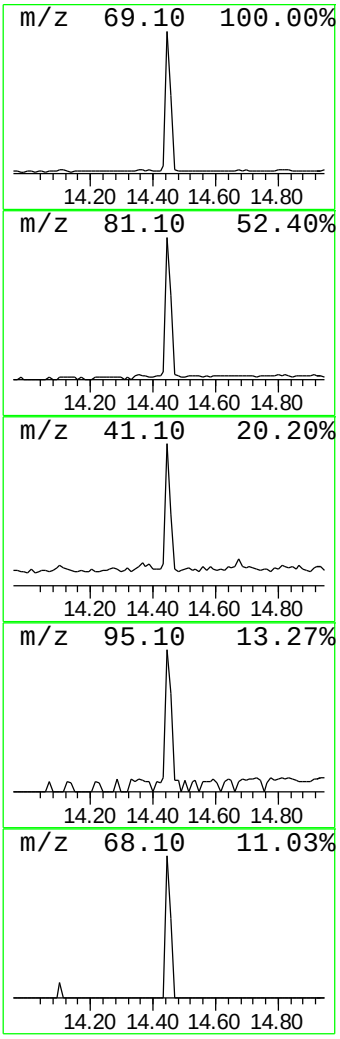
Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.50 ng	129290	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	74
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	Farnesol isomer a	222	C15H26O	1000108-92-4	56





Tentatively Identified Compound (LSC) summary

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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...	4.56	18.1	ng	682786	1	6.47	755706	20.0
unknown6.24	6.24	84.5	ng	3191720	1	6.47	755706	20.0
Hexanoic acid, 2-...	7.19	2.9	ng	152800	2	7.76	1046670	20.0
Hexadecane	10.43	2.7	ng	173051	4	10.97	1271700	20.0
1-Heneicosanol	13.47	3.3	ng	200234	5	13.58	1225920	20.0
Supraene	14.45	2.5	ng	129290	6	14.90	1033980	20.0