LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103633.D
Acq On : 14 Mar 2018 6:22
Operator : SJ/JU
Sample : J1895-02
Misc :
ALS Vial : 36 Sample Multiplier: 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-BF022218.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	5.087	507	510	520	rBV2	21941	55688	1.37%	0.226%
2	5.510	577	582	609	rBV2	127231	760274	18.66%	3.082%
3	6.528	750	755	769	rBV3	139460	539829	13.25%	2.188%
4	6.628	769	772	808	rVV	1028006	2418893	59.38%	9.804%
5	6.857	808	811	833	rVV	379050	799725	19.63%	3.241%
6	7.010	833	837	862	rVV	2123111	2912028	71.48%	11.803%
7	7.428	905	908	932	rBV	1398885	2632924	64.63%	10.672%
8	7.575	932	933	942	rVB	45374	61068	1.50%	0.248%
9	8.139	1026	1029	1056	rBV	479544	1119547	27.48%	4.538%
10	9.210	1208	1211	1229	rBV	3103900	4073882	100.00%	16.512%
11	9.622	1278	1281	1285	rBV	39886	47164	1.16%	0.191%
12	9.810	1309	1313	1316	rBV	72746	72240	1.77%	0.293%
13	9.898	1325	1328	1341	rVV	871976	1097567	26.94%	4.449%
14	10.304	1394	1397	1400	rBV	113150	91522	2.25%	0.371%
15	10.522	1429	1434	1437	rBV	36074	47897	1.18%	0.194%
16	10.692	1460	1463	1475	rBV	935202	1581600	38.82%	6.411%
17	10.780	1475	1478	1488	rVB	127007	188915	4.64%	0.766%
18	11.398	1579	1583	1598	rBV	695574	1152302	28.29%	4.671%
19	12.774	1814	1817	1821	rBV	156691	131401	3.23%	0.533%
20	12.980	1847	1852	1869	rBV	2527708	3028698	74.34%	12.276%
21	13.480	1933	1937	1941	rBV	112416	95095	2.33%	0.385%
22	13.857	1997	2001	2009	rBV	56745	81923	2.01%	0.332%
23	14.057	2031	2035	2051	rBV	552256	764501	18.77%	3.099%
24	14.263	2062	2070	2075	rBV7	19708	49766	1.22%	0.202%
25	14.863	2168	2172	2179	rBV	125700	122665	3.01%	0.497%
26	15.504	2277	2281	2286	rBV	30284	41909	1.03%	0.170%
27	15.562	2286	2291	2307	rVV2	308758	649301	15.94%	2.632%
28	15.945	2352	2356	2361	rBV2	29148	53589	1.32%	0.217%

Sum of corrected areas: 24671913

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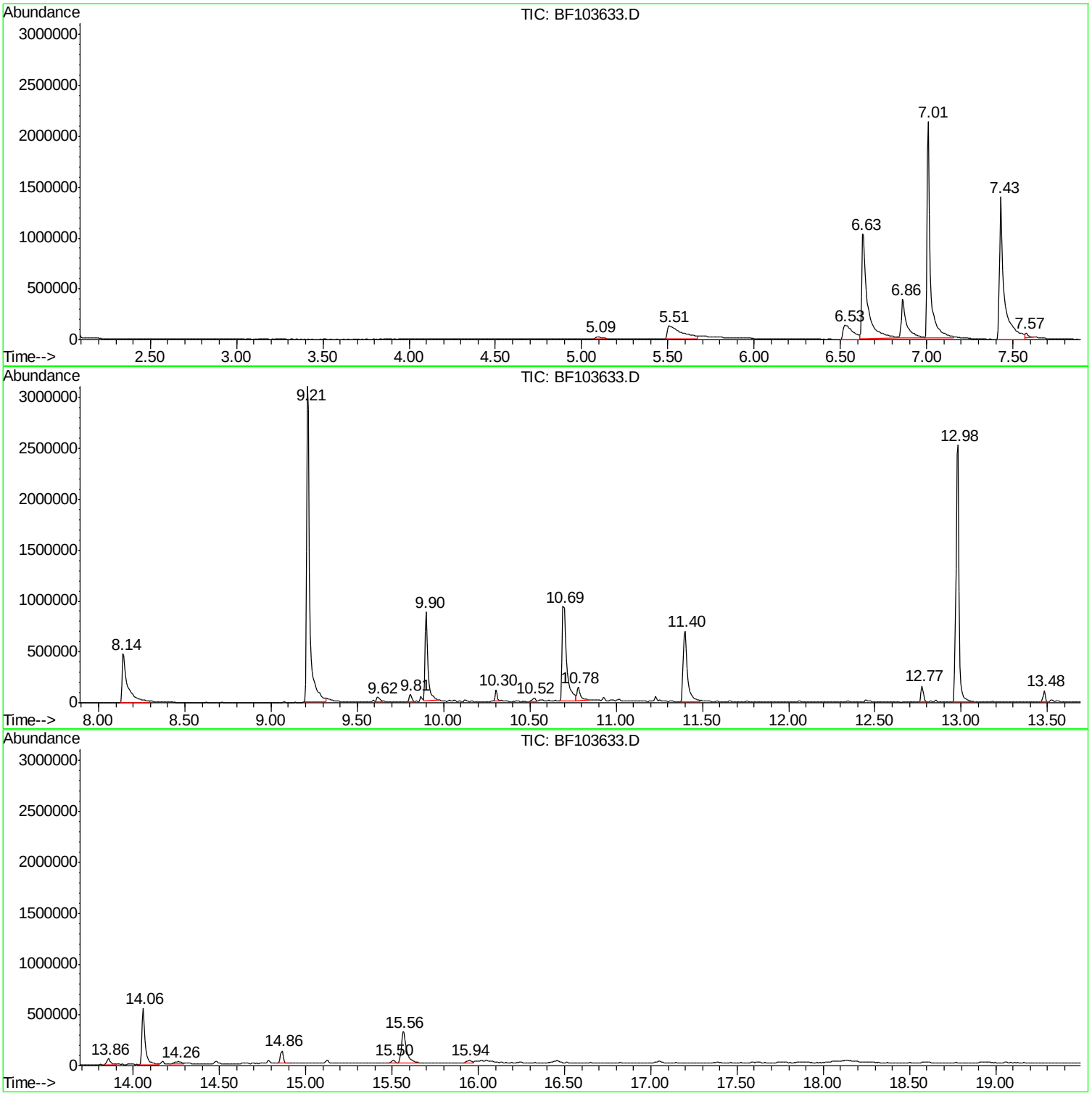
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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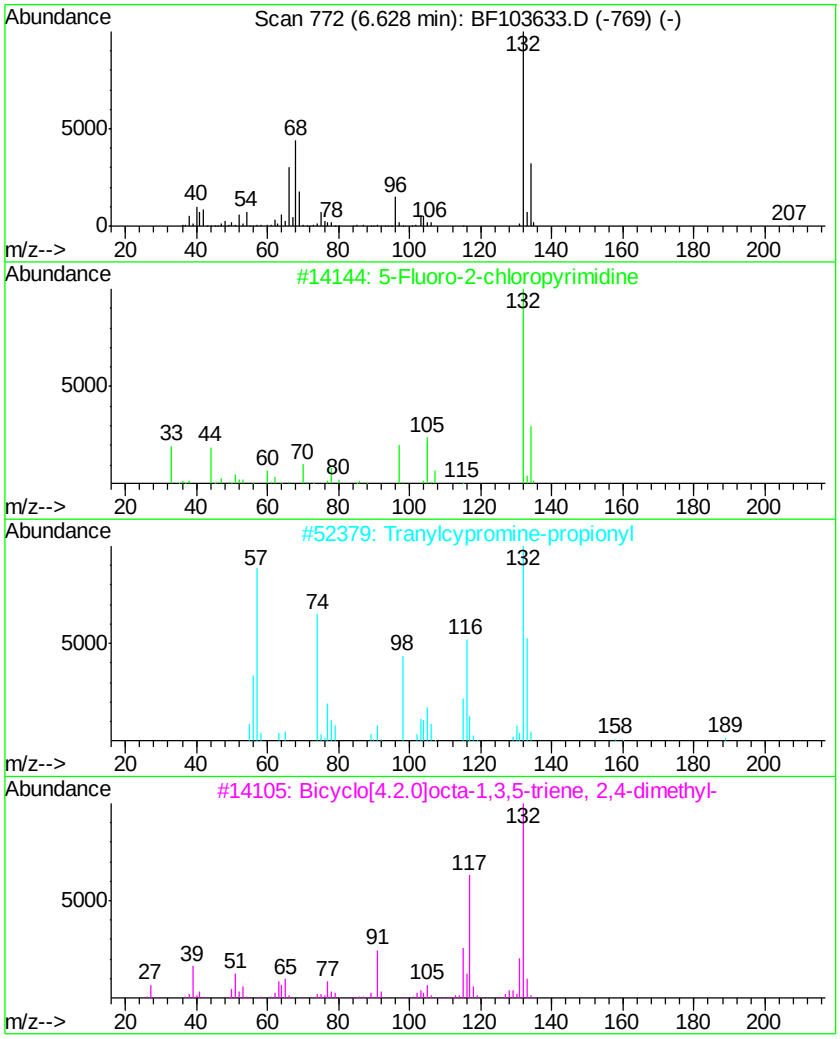
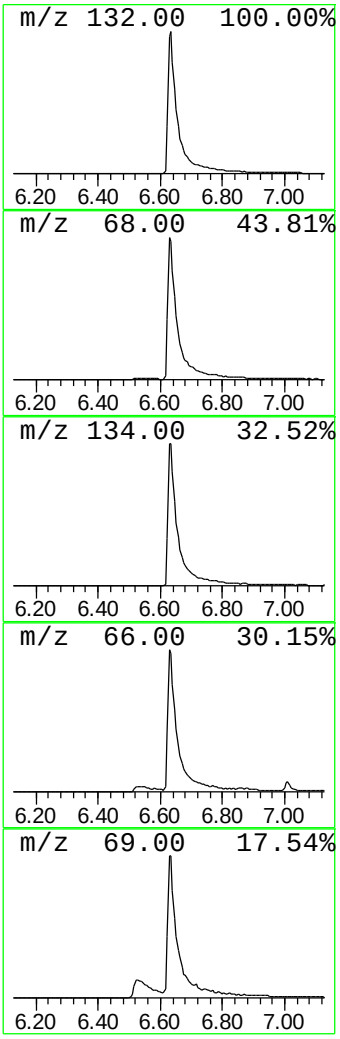
Peak Number 1 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	60.49 ng	2418890	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





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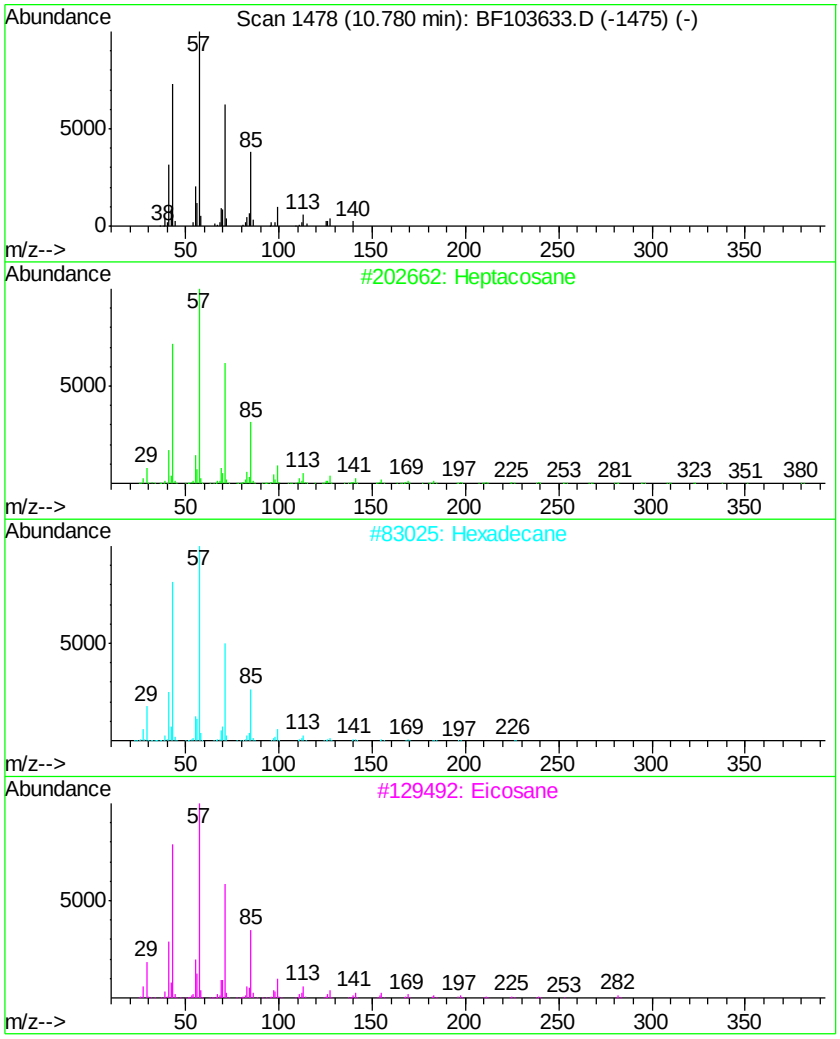
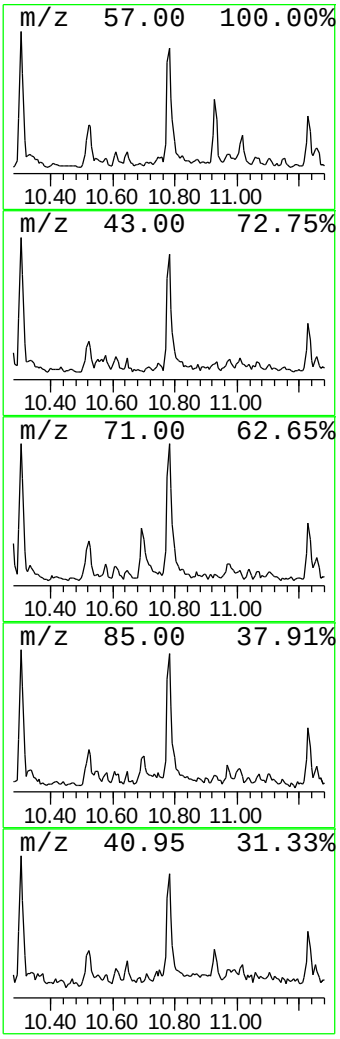
Peak Number 3 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	3.28 ng	188915	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Pentadecane	212	C15H32	000629-62-9	80
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72





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Misc :
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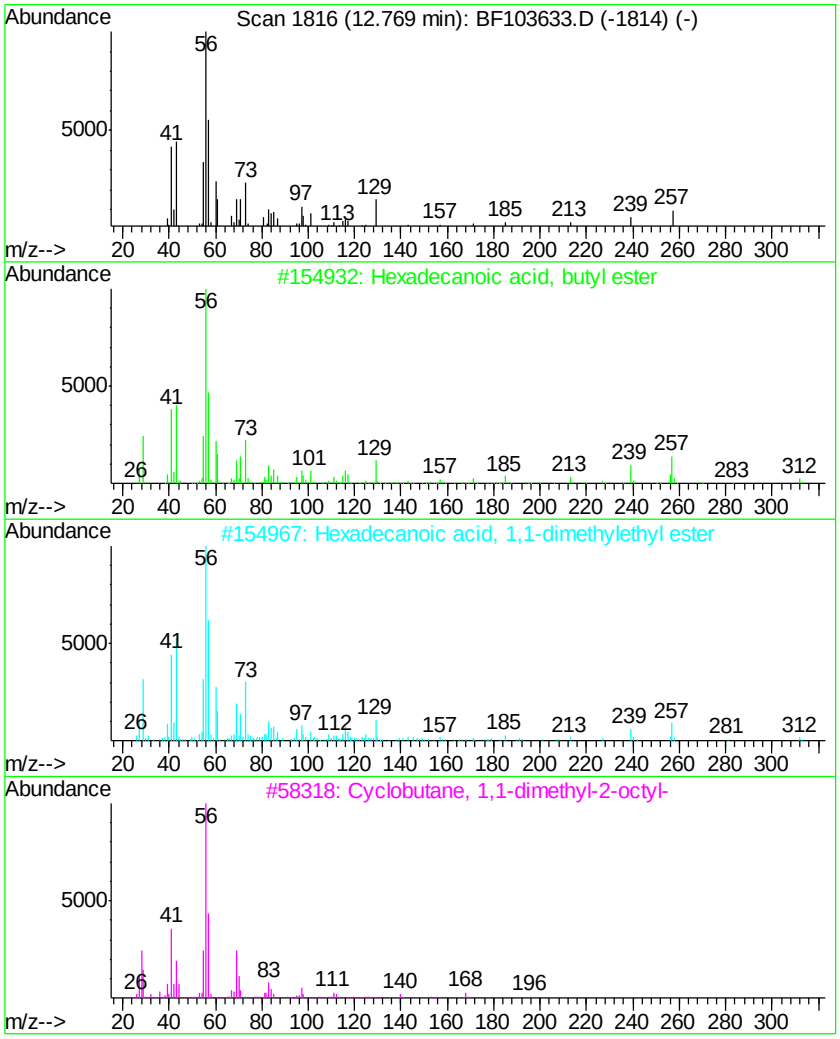
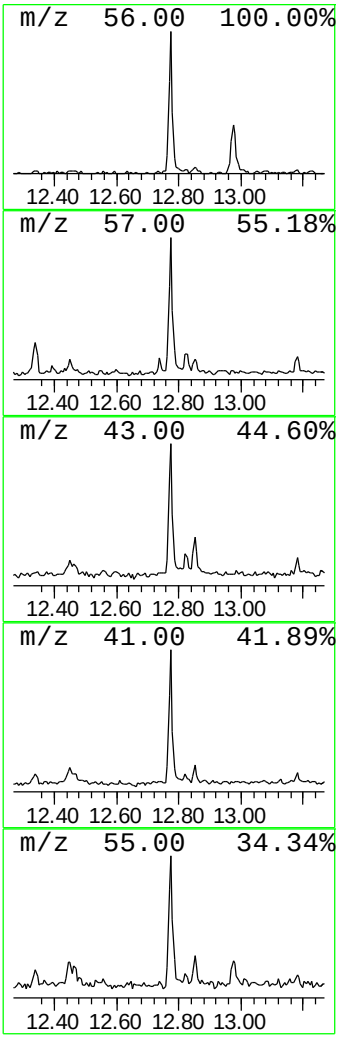
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.44 ng	131401	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	43
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5	Acetic acid, 2,4,4-trimethylpent...	172	C10H20O2	1000368-95-3	37





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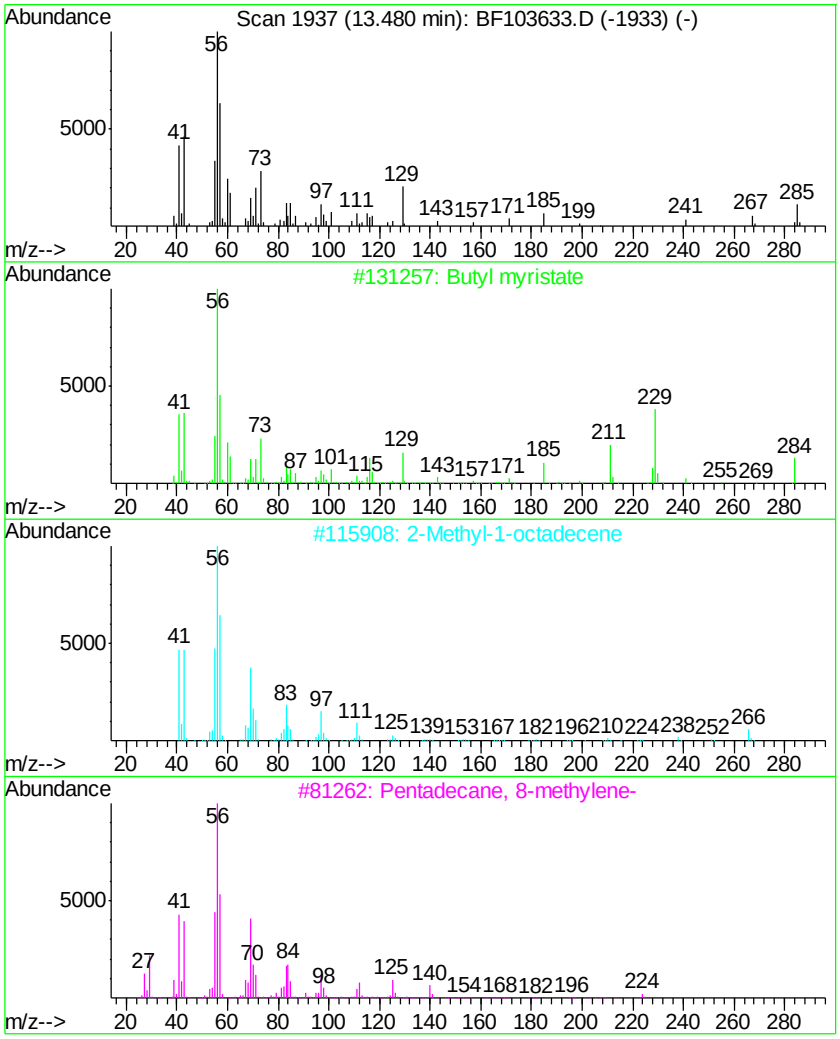
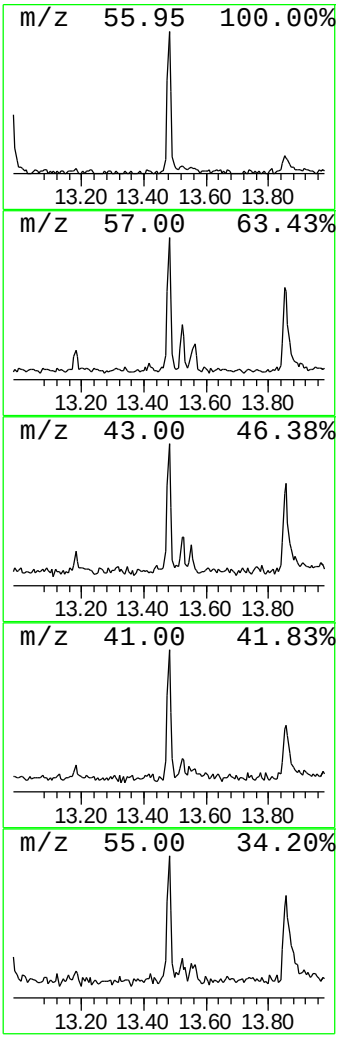
Peak Number 5 Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.49 ng	95095	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	64
2	2-Methyl-1-octadecene	266	C19H38	061868-20-0	38
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	37
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35





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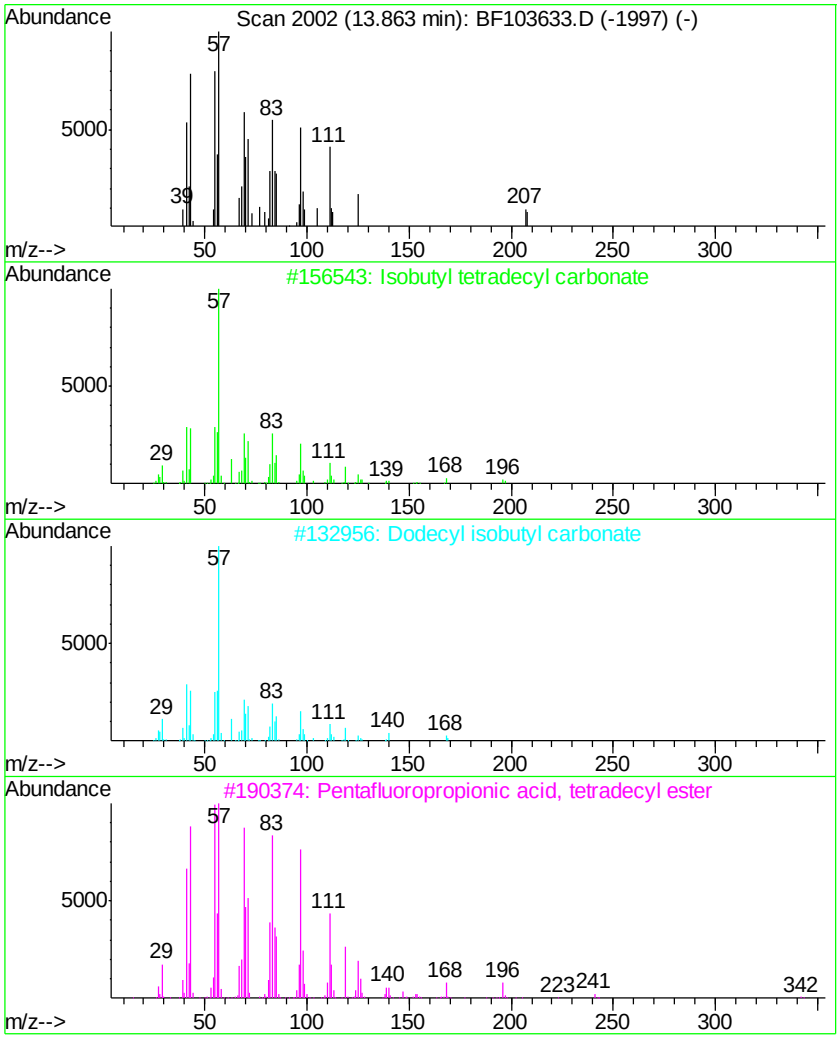
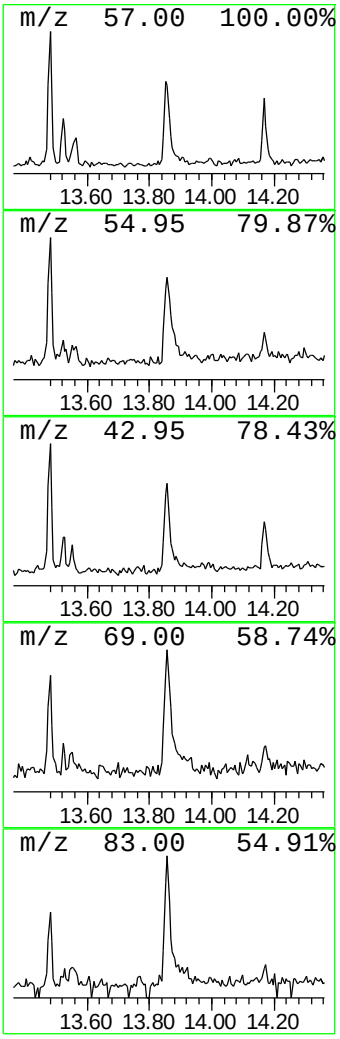
Peak Number 6 Isobutyl tetradecyl carbonate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.14 ng	81923	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	87
2	Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	83
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	81
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	81
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	81





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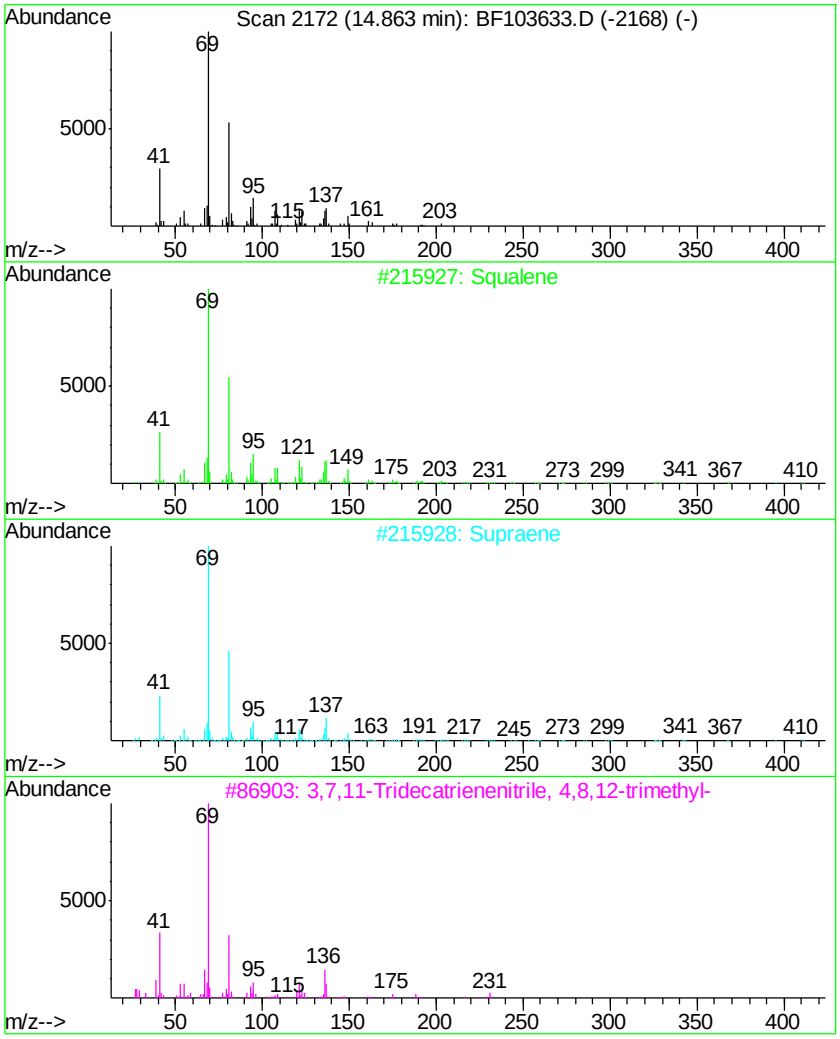
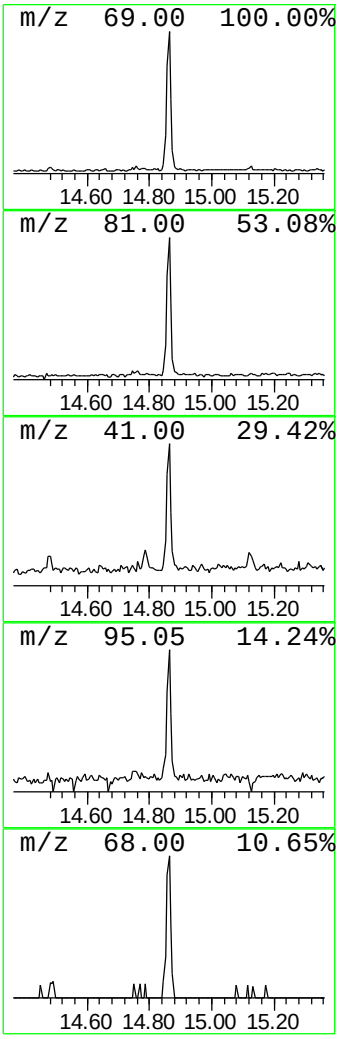
Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	3.78 ng	122665	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.63	6.63	60.5	ng	2418890	1	6.86	799725	20.0
Heptacosane	10.78	3.3	ng	188915	4	11.40	1152300	20.0
Hexadecanoic acid...	12.77	3.4	ng	131401	5	14.06	764501	20.0
Butyl myristate	13.48	2.5	ng	95095	5	14.06	764501	20.0
Isobutyl tetradec...	13.86	2.1	ng	81923	5	14.06	764501	20.0
Squalene	14.86	3.8	ng	122665	6	15.56	649301	20.0