LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102016\
Data File : BF090690.D
Acq On : 20 Oct 2016 18:53
Operator : UM/SJ
Sample : H5343-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RMAB-SB01-19.5-20.0

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-BF101316.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	5.068	236	239	251	rBV	702235	1048612	22.93%	2.738%
2	5.491	273	276	278	rBV	3987705	4573728	100.00%	11.942%
3	6.520	363	366	368	rBV	4220947	4444250	97.17%	11.604%
4	6.646	375	377	380	rBV	3880264	4284474	93.68%	11.186%
5	6.874	395	397	400	rBV	769743	993845	21.73%	2.595%
6	6.943	402	403	409	rVB	44722	47229	1.03%	0.123%
7	7.034	409	411	414	rBV	3564643	3181494	69.56%	8.307%
8	7.446	444	447	449	rBV	2688881	2708238	59.21%	7.071%
9	7.537	453	455	462	rVB	89076	173897	3.80%	0.454%
10	8.166	507	510	512	rBV	1631300	1424613	31.15%	3.720%
11	9.240	602	604	607	rBV	3917994	4023793	87.98%	10.506%
12	9.515	626	628	632	rBV	57066	51994	1.14%	0.136%
13	9.640	636	639	641	rBV	1535732	1367887	29.91%	3.571%
14	9.926	661	664	666	rBV	889858	1256061	27.46%	3.279%
15	10.349	697	701	703	rBV3	57268	93676	2.05%	0.245%
16	10.578	718	721	724	rBV	30743	55607	1.22%	0.145%
17	10.715	730	733	735	rBV2	1770397	2275372	49.75%	5.941%
18	10.829	741	743	747	rVB	115563	132578	2.90%	0.346%
19	11.275	780	782	784	rBV	72875	66830	1.46%	0.174%
20	11.412	791	794	796	rBV	730684	979915	21.42%	2.558%
21	12.989	930	932	935	rBV	2252623	3095968	67.69%	8.083%
22	13.892	1009	1011	1017	rBV	151462	192089	4.20%	0.502%
23	14.041	1022	1024	1027	rBV	645819	937212	20.49%	2.447%
24	14.898	1097	1099	1101	rBV	59826	67848	1.48%	0.177%
25	15.492	1148	1151	1159	rBV	596068	823386	18.00%	2.150%

Sum of corrected areas: 38300596

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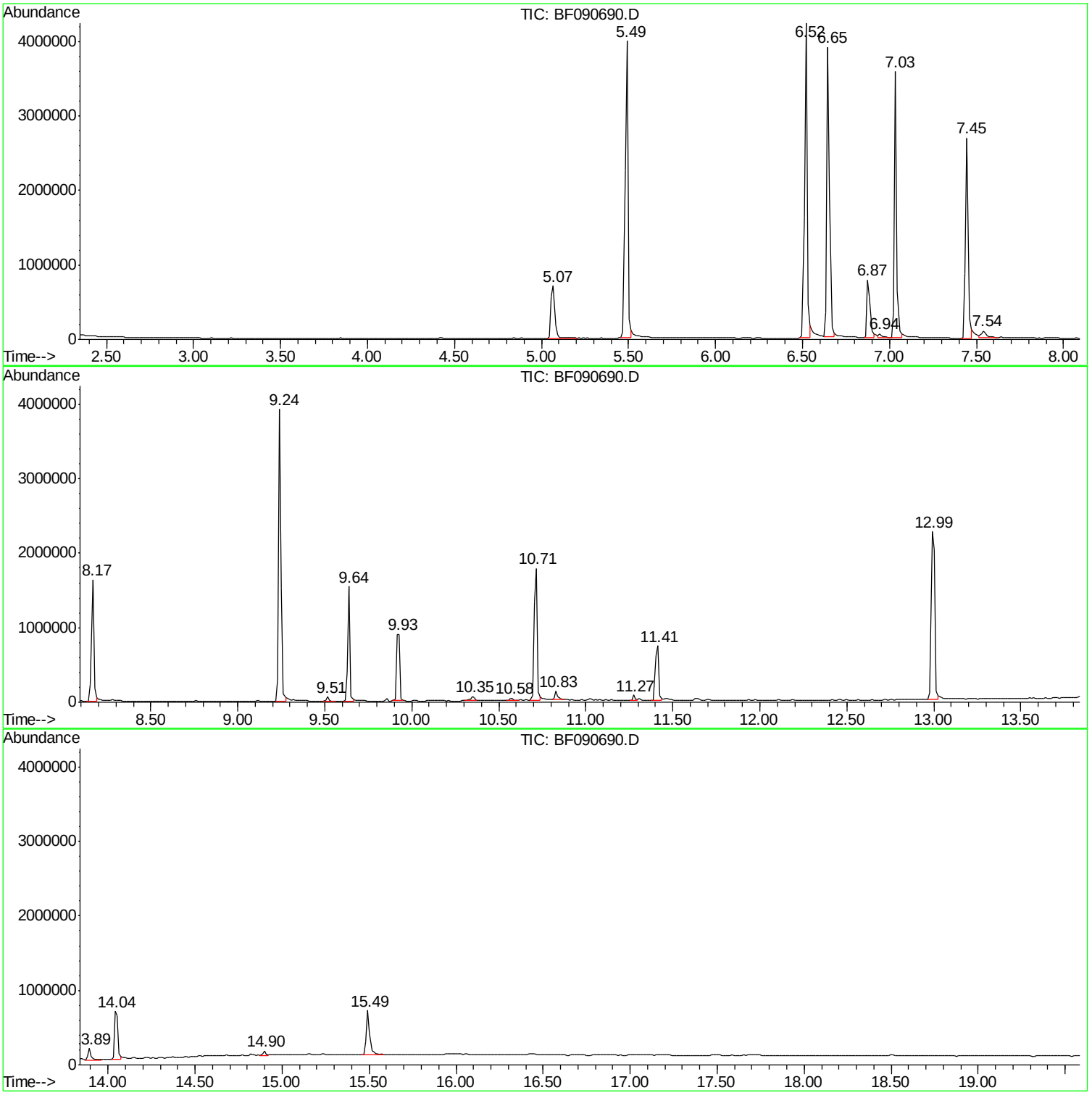
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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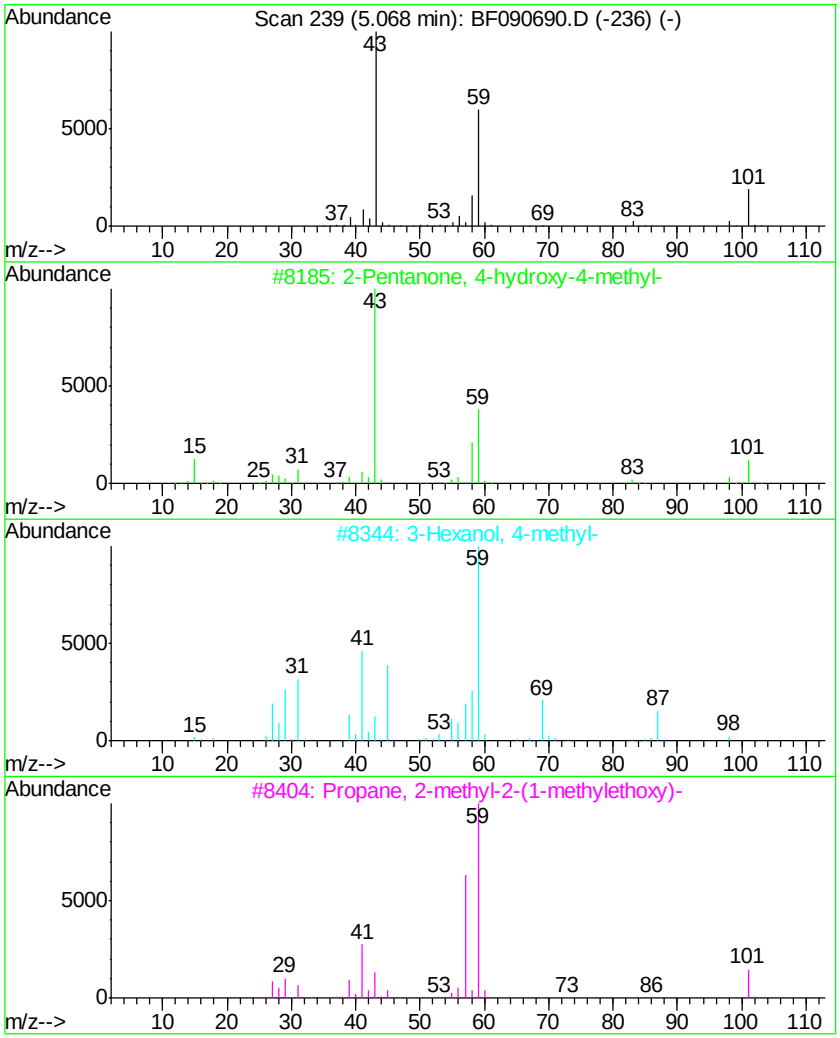
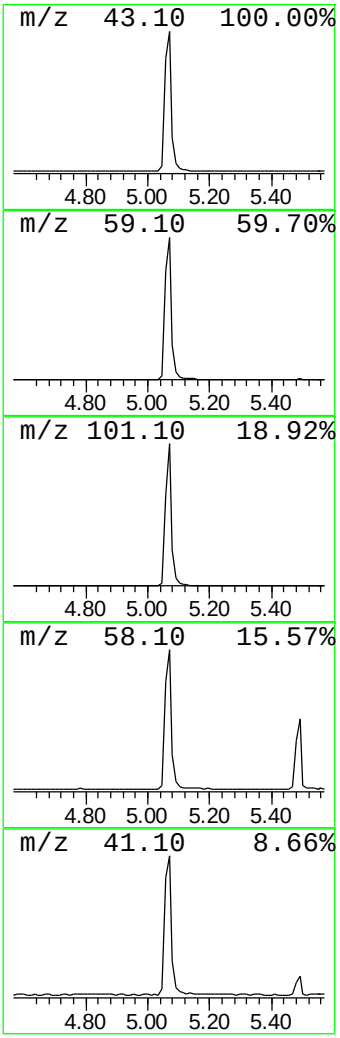
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	21.10 ng	1048610	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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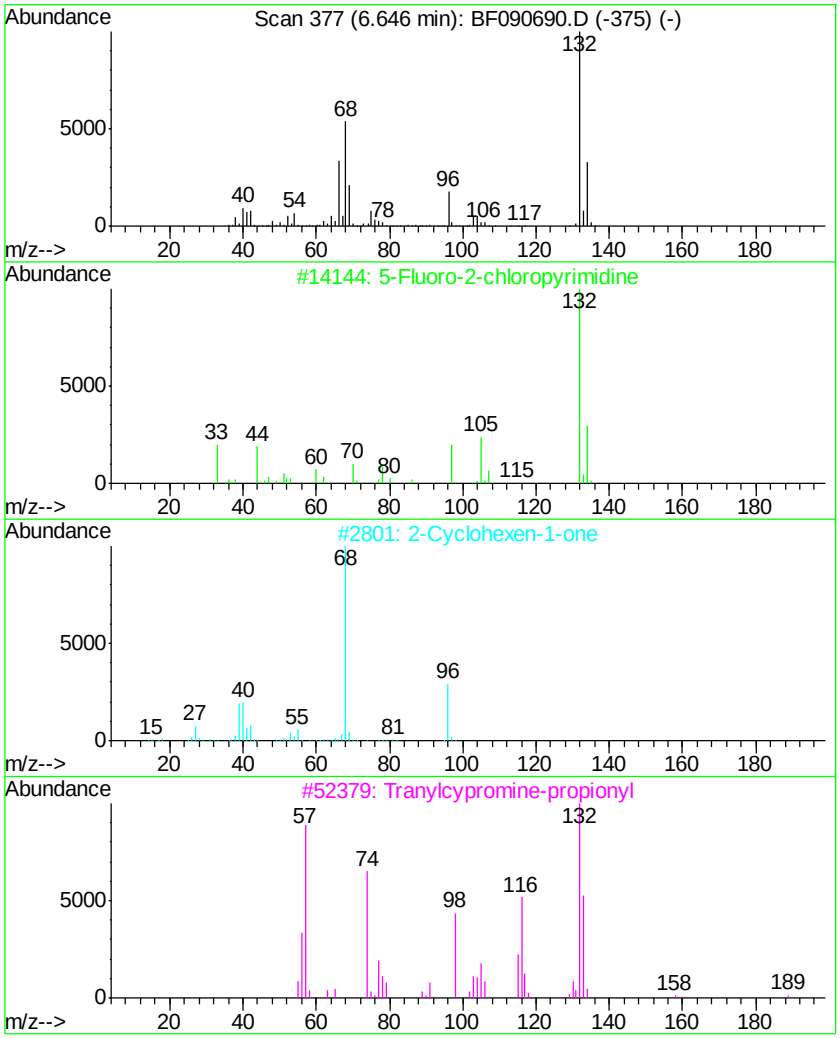
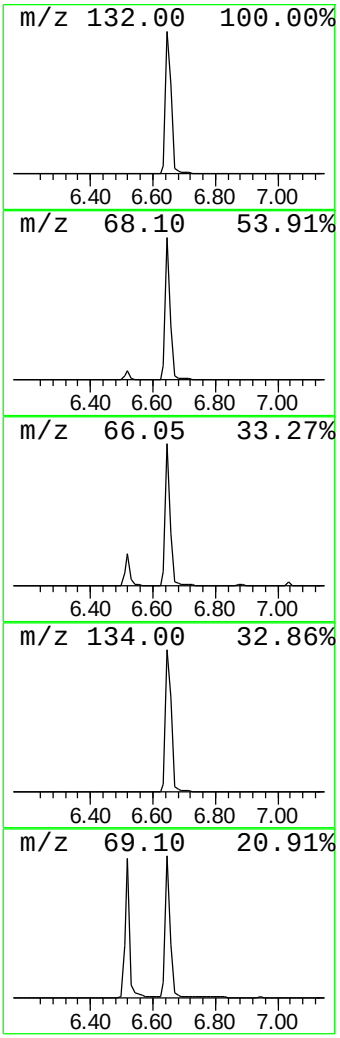
Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	86.22 ng	4284470	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

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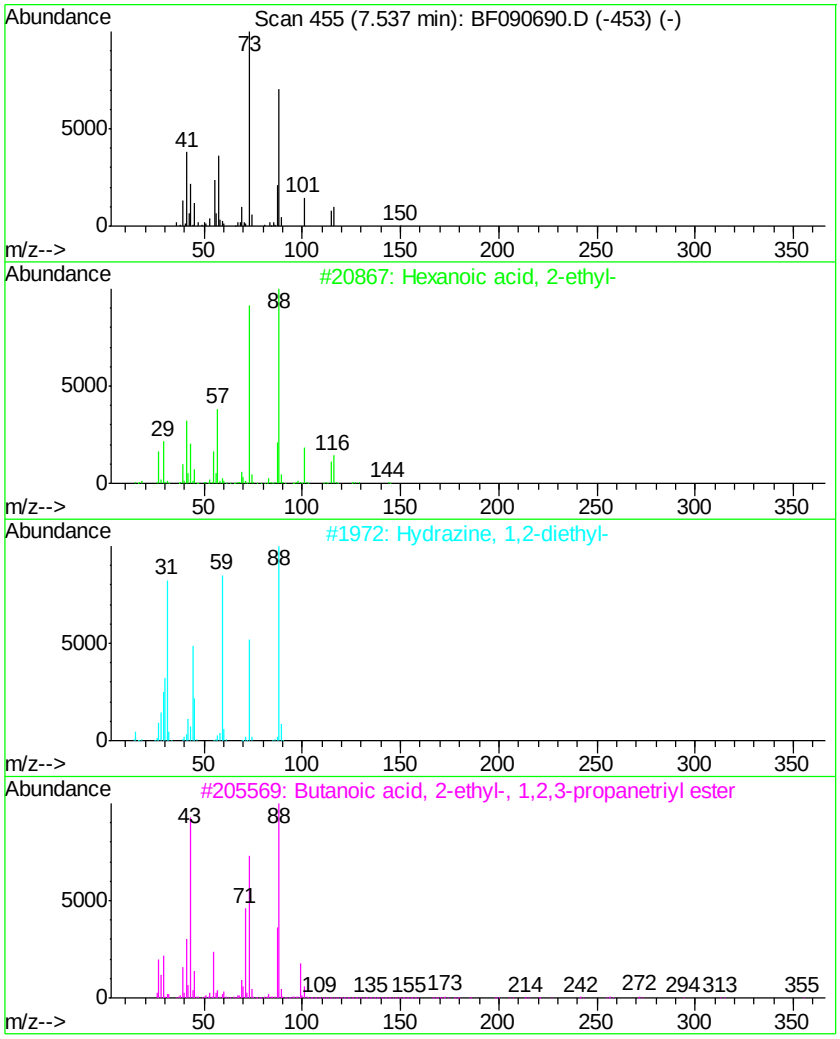
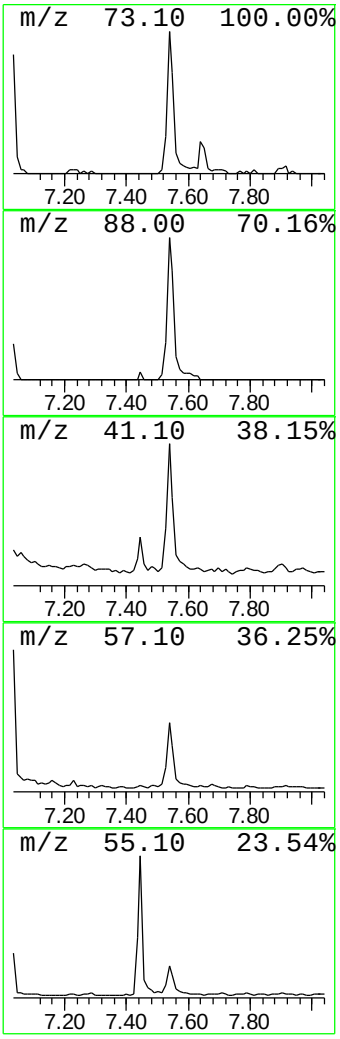
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	2.44 ng	173897	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	64
2	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	43
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38
4	1,4-Dioxane	88	C4H8O2	000123-91-1	35
5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	27





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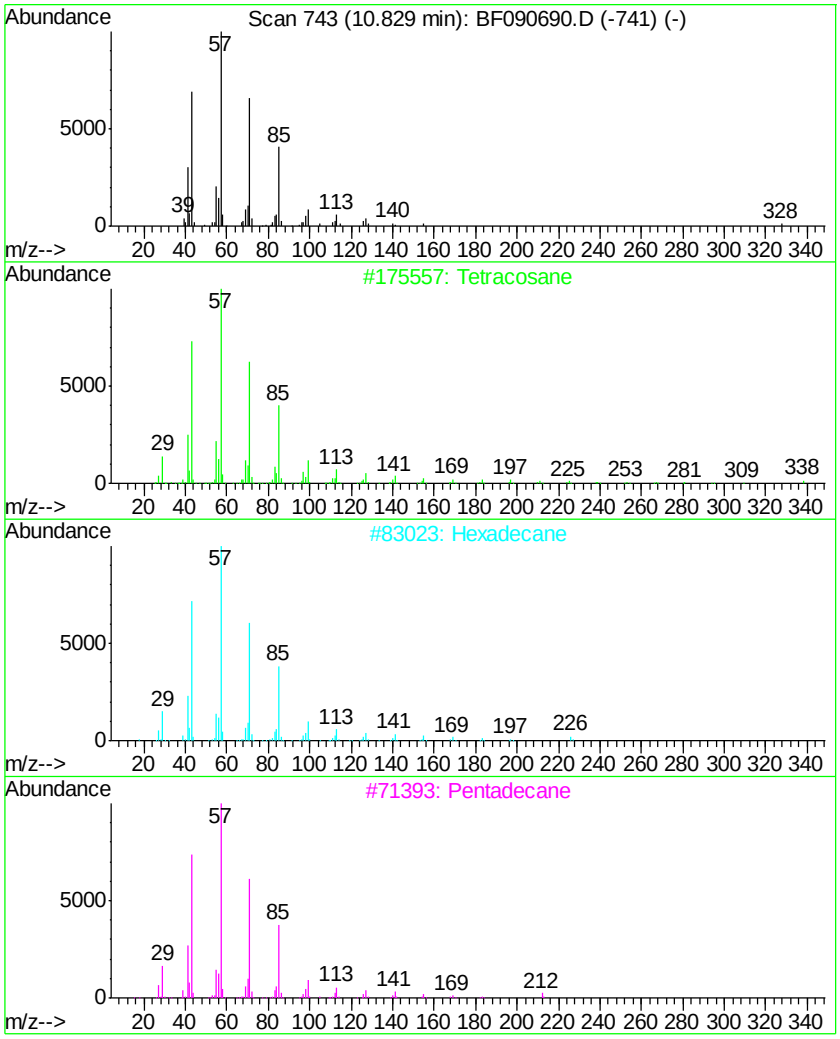
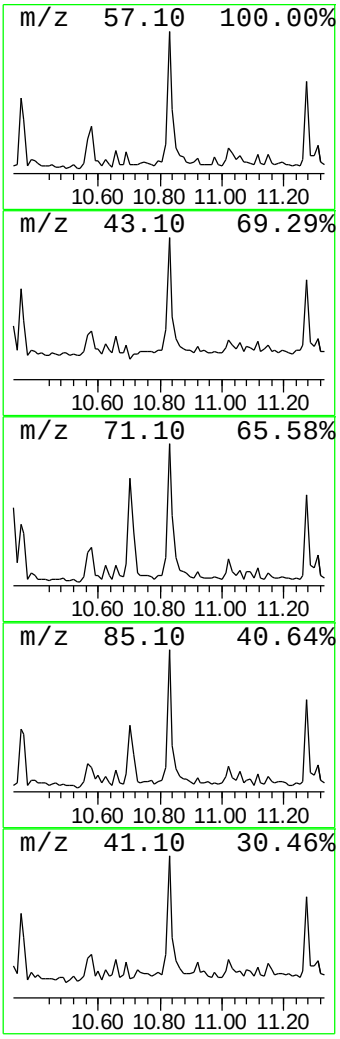
Peak Number 5 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	2.71 ng	132578	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Nonadecane	268	C19H40	000629-92-5	90
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86





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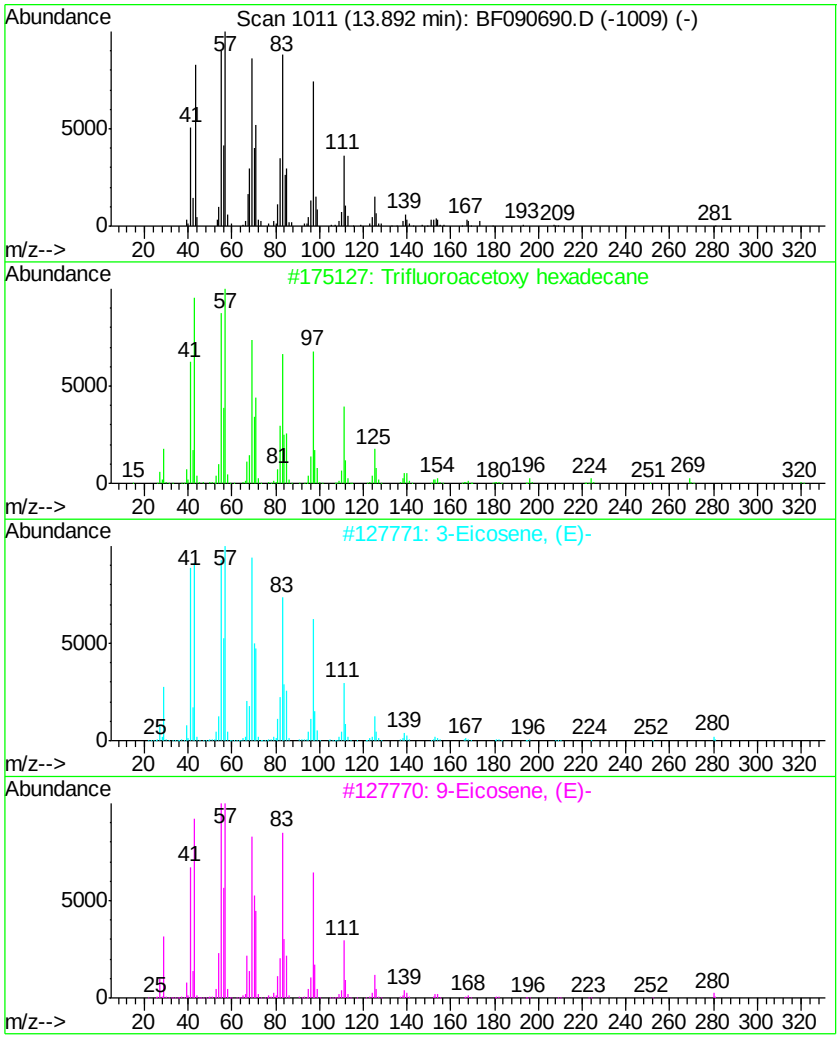
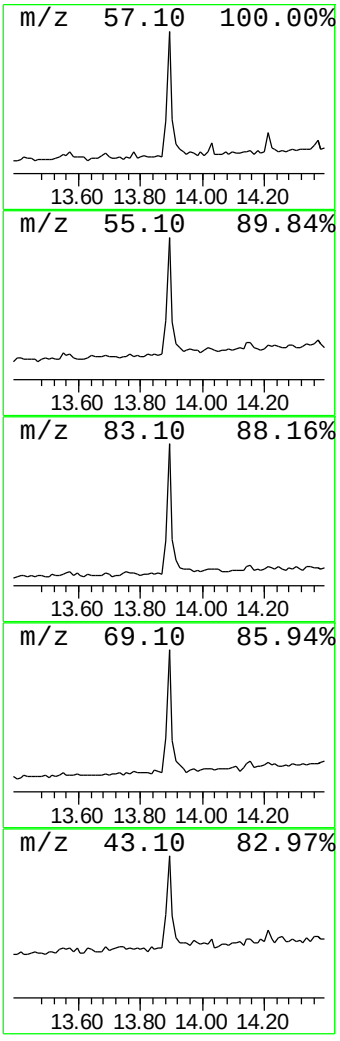
Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	4.10 ng	192089	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





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...	5.07	21.1	ng	1048610	1	6.87	993845	20.0
unknown6.65	6.65	86.2	ng	4284470	1	6.87	993845	20.0
Hexanoic acid, 2-...	7.54	2.4	ng	173897	2	8.17	1424610	20.0
Tetracosane	10.83	2.7	ng	132578	4	11.41	979915	20.0
Trifluoroacetoxy ...	13.89	4.1	ng	192089	5	14.05	937212	20.0