

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096698.D
 Acq On : 12 Jul 2017 18:15
 Operator : SJ/JU
 Sample : I4126-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PP-SW-2

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-BF070117.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	4.857	467	471	484	rBV	371735	607759	17.40%	2.251%
2	5.287	538	544	547	rBV	3027739	3492136	100.00%	12.937%
3	6.316	713	719	722	rBV	2917912	3350540	95.95%	12.412%
4	6.440	735	740	743	rBV	3318050	3452664	98.87%	12.790%
5	6.669	775	779	782	rBV	649761	604313	17.30%	2.239%
6	6.828	801	806	809	rBV	2327530	2311700	66.20%	8.564%
7	7.234	869	875	878	rBV	2054415	2272030	65.06%	8.417%
8	7.945	992	996	1000	rBV	874836	791563	22.67%	2.932%
9	9.028	1174	1180	1183	rBV	3159799	3167745	90.71%	11.735%
10	9.416	1243	1246	1250	rBV	282537	245861	7.04%	0.911%
11	9.698	1290	1294	1298	rBV	1069204	896112	25.66%	3.320%
12	10.145	1367	1370	1373	rVB	46546	37284	1.07%	0.138%
13	10.486	1423	1428	1431	rBV	1709219	1641029	46.99%	6.079%
14	10.616	1447	1450	1457	rBV	74321	81269	2.33%	0.301%
15	11.175	1541	1545	1549	rVB	846272	714575	20.46%	2.647%
16	12.763	1810	1815	1818	rBV	2104929	1999436	57.26%	7.407%
17	13.668	1965	1969	1979	rBV	190850	238602	6.83%	0.884%
18	13.804	1988	1992	1996	rBV	664245	572996	16.41%	2.123%
19	15.198	2224	2229	2235	rBV	394907	469330	13.44%	1.739%
20	15.692	2309	2313	2321	rBV8	28136	47057	1.35%	0.174%

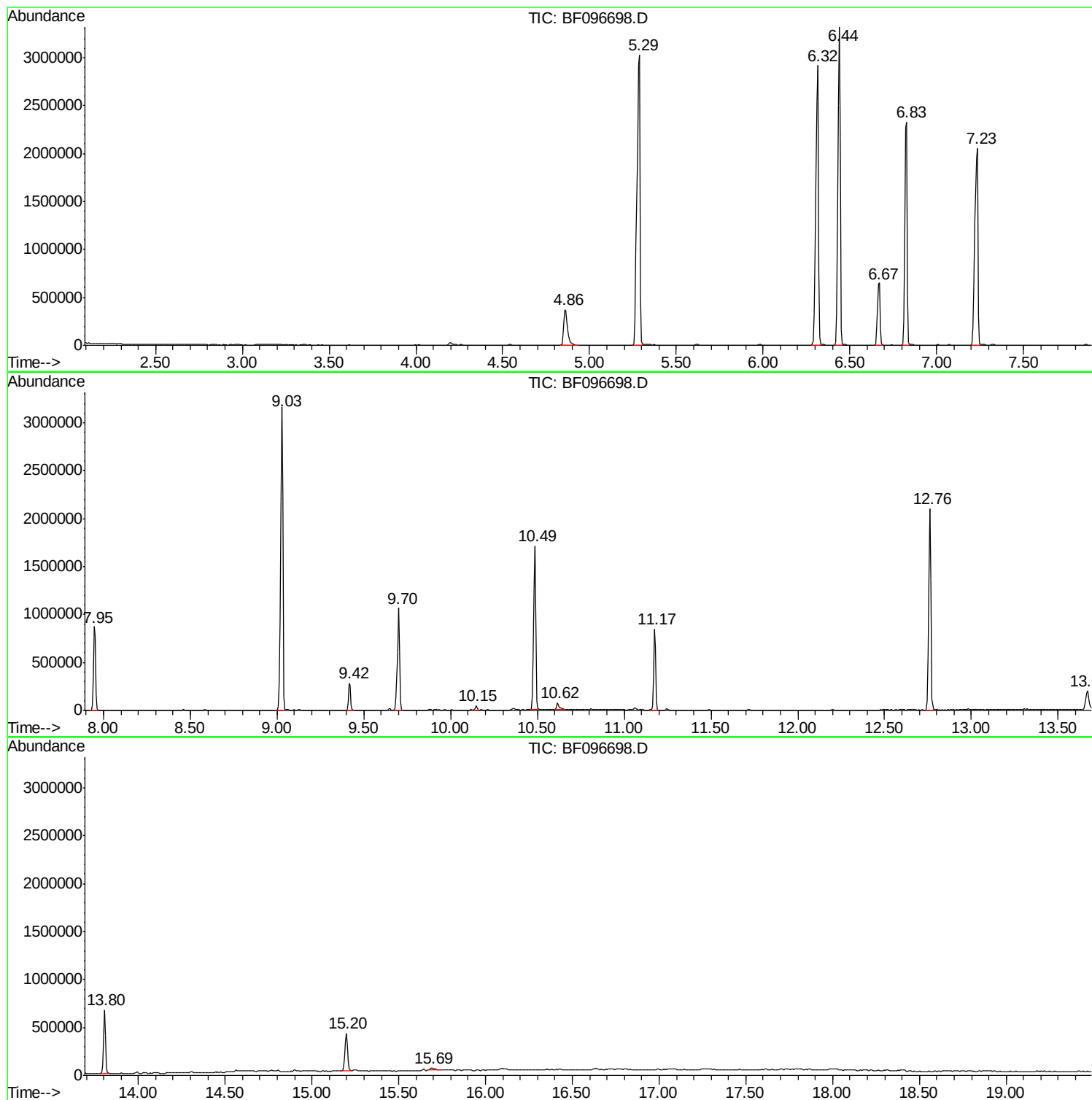
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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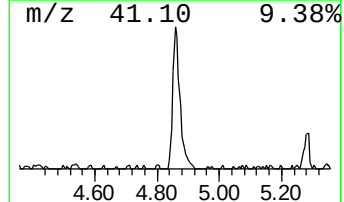
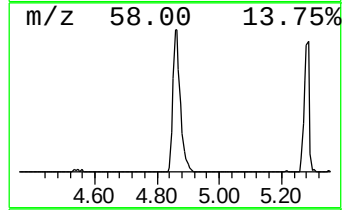
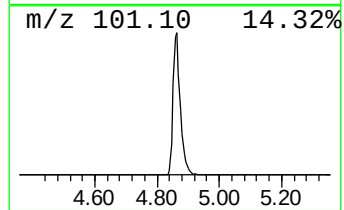
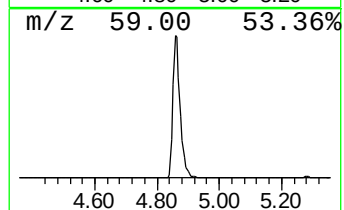
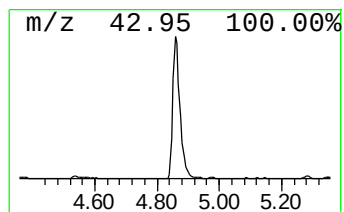
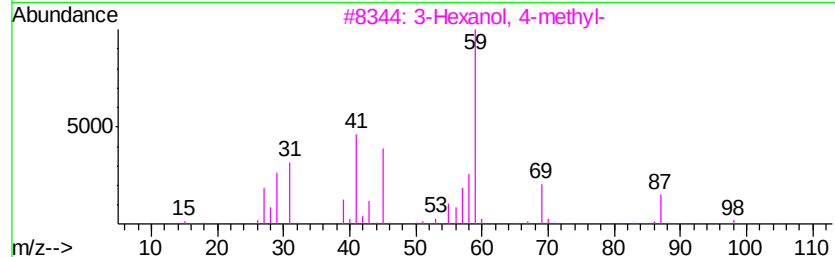
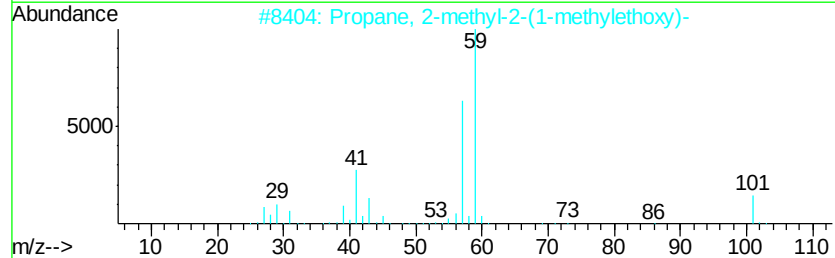
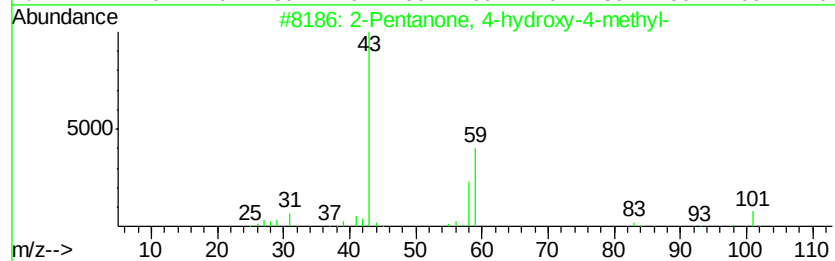
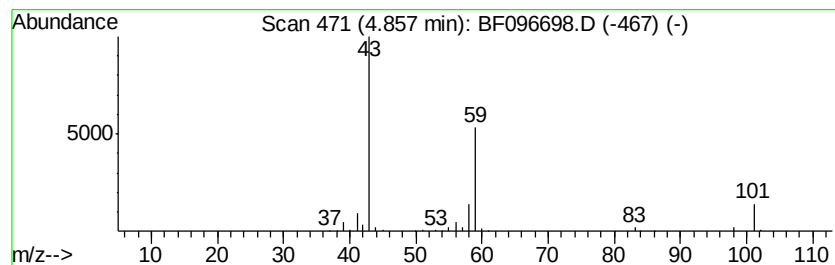
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	20.11 ng	607759	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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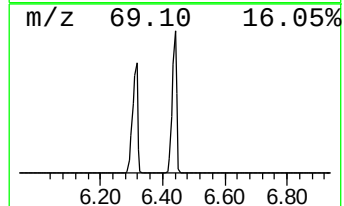
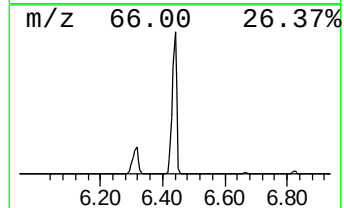
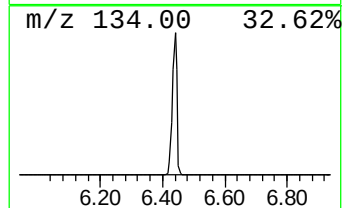
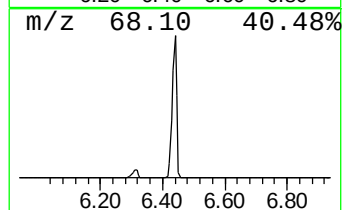
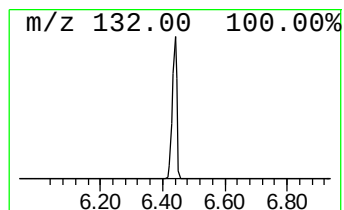
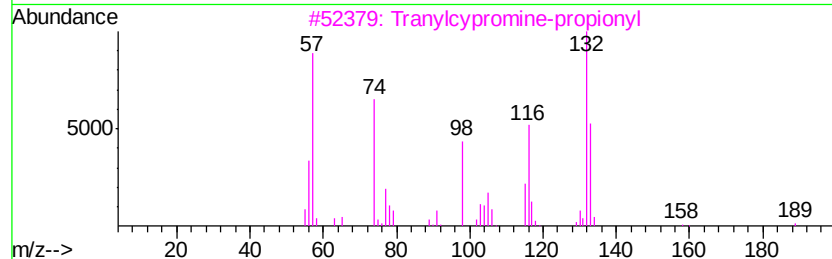
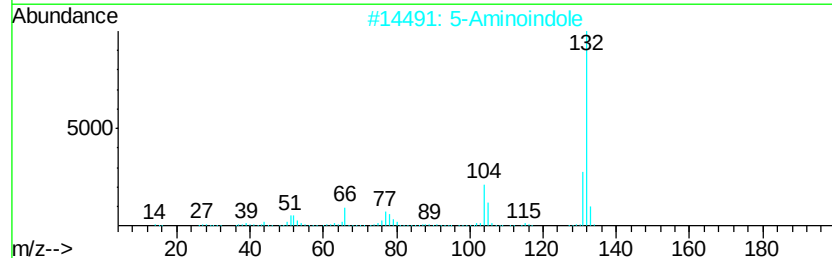
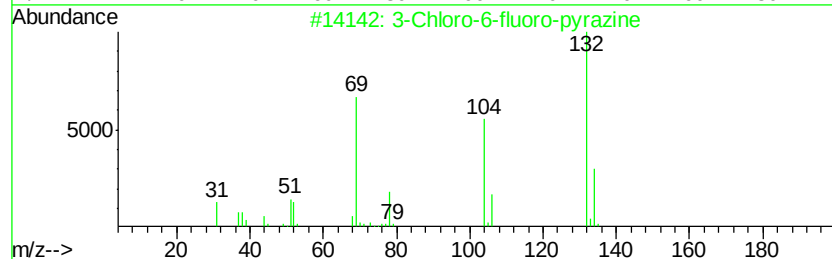
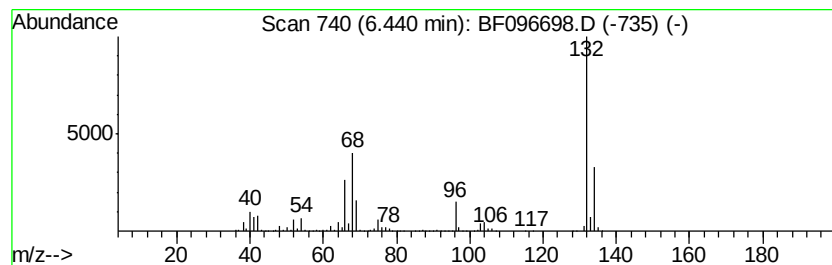
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Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	114.27 ng	3452660	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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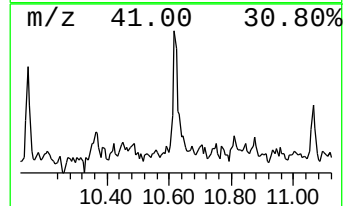
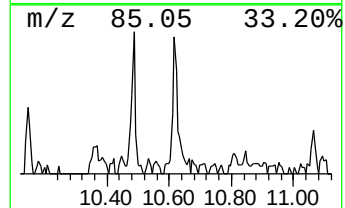
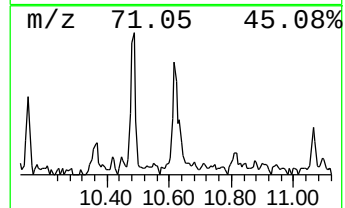
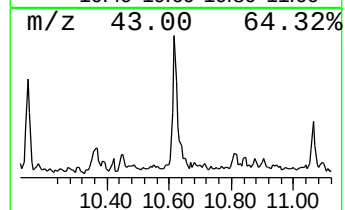
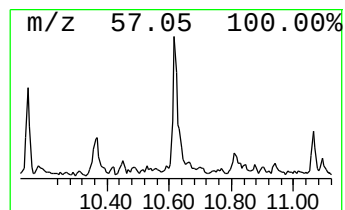
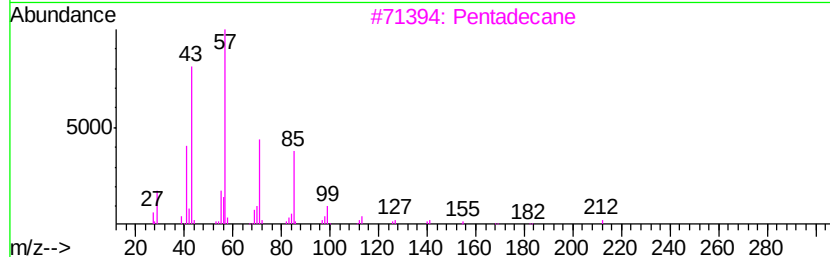
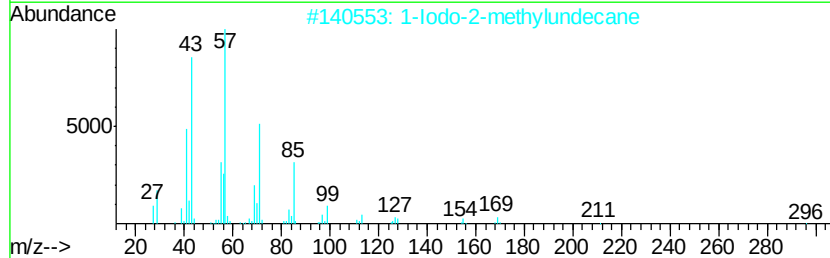
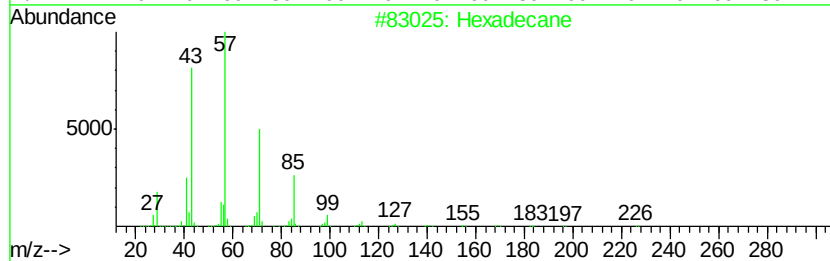
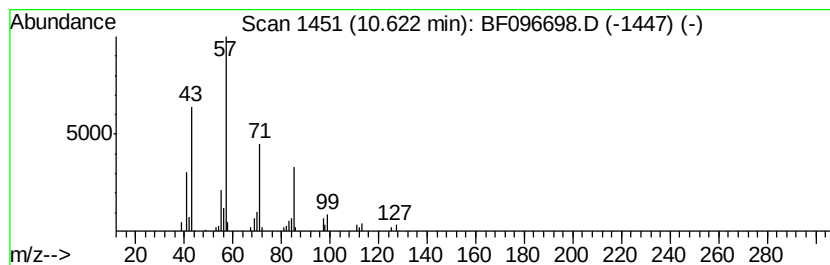
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.62	2.27 ng	81269	Phenanthrene-d10	11.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
3	Pentadecane	212	C15H32	000629-62-9	83
4	Tetradecane	198	C14H30	000629-59-4	80
5	Tridecane	184	C13H28	000629-50-5	78



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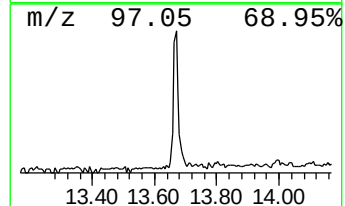
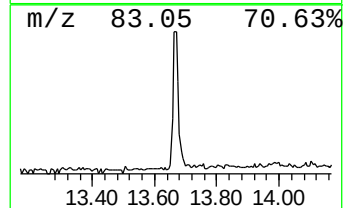
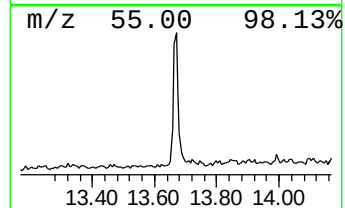
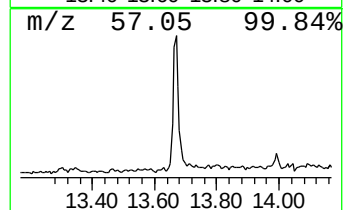
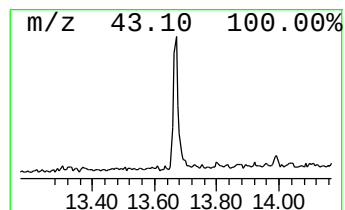
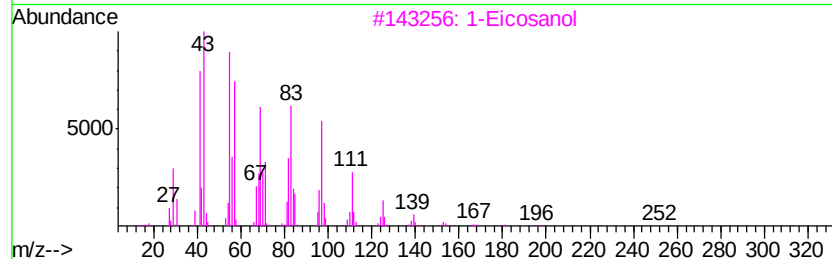
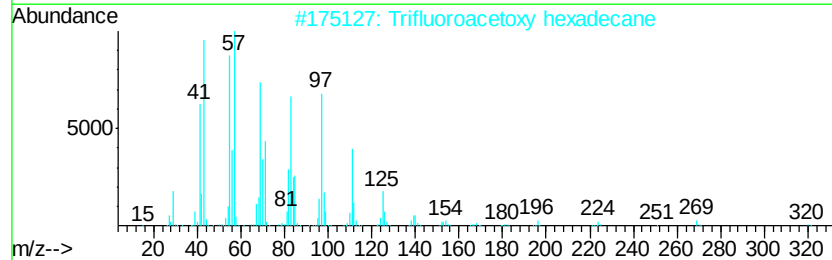
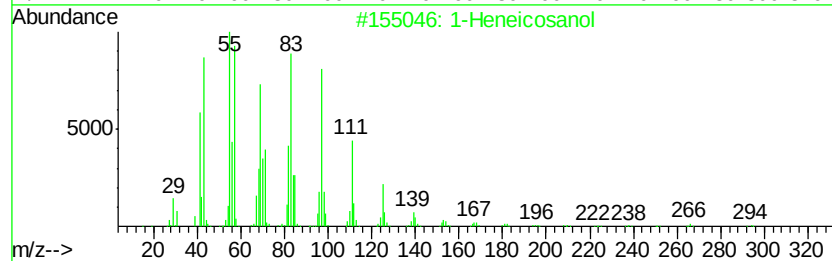
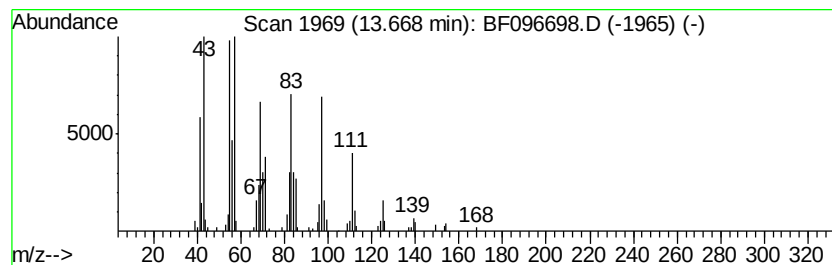
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.67	8.33 ng	238602	Chrysene-d12		13.80		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			1-Eicosanol	298	C20H42O	000629-96-9	91
4			1-Docosene	308	C22H44	001599-67-3	90
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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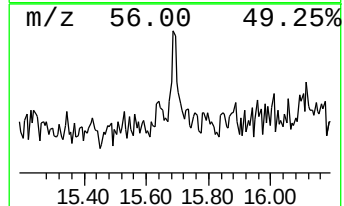
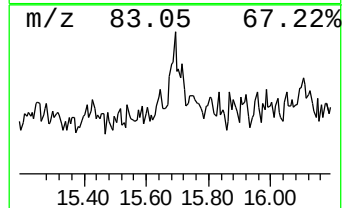
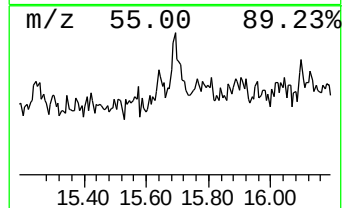
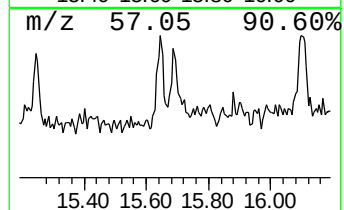
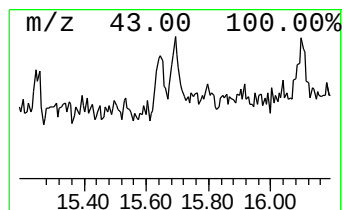
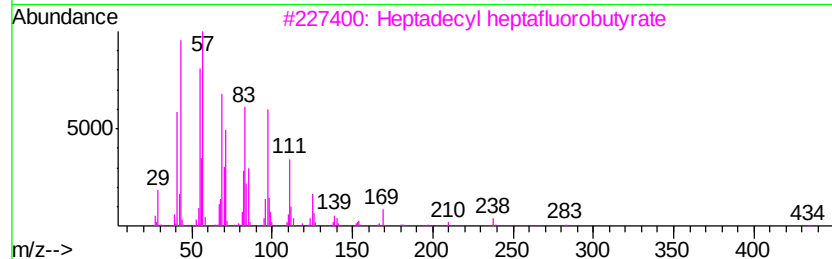
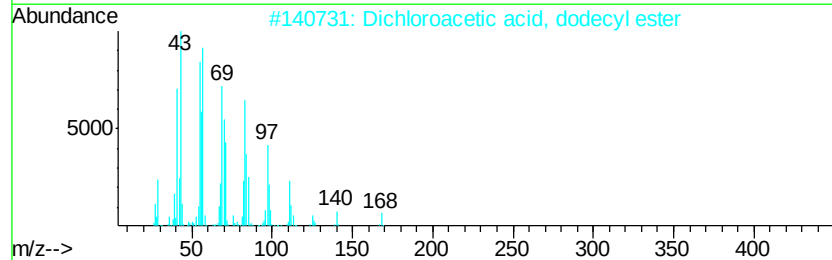
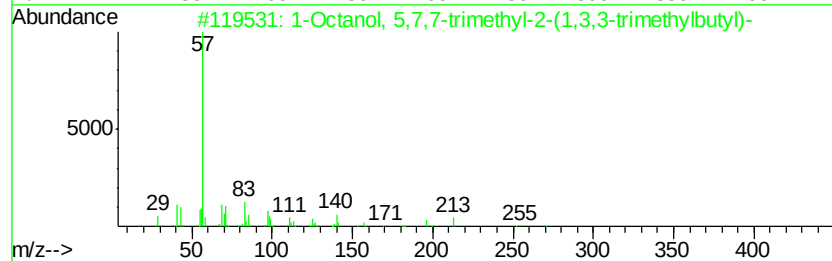
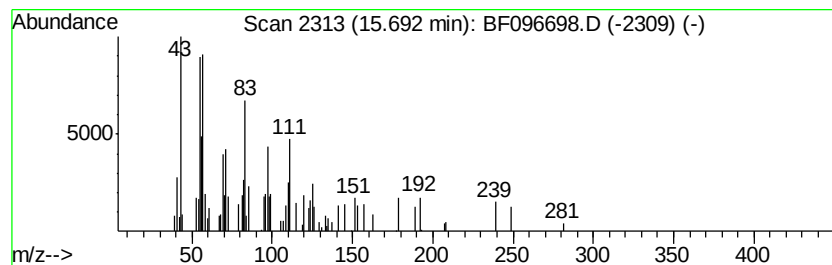
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Peak Number 6 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.69	2.01 ng	47057	Perylene-d12	15.20		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	50	
2	Dichloroacetic acid, dodecyl ester	296	C14H26Cl2O2	083005-01-0	38	
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	38	
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	38	
5	Fumaric acid, decyl 2-methylally...	310	C18H30O4	1000330-55-0	38	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.86	20.1	ng	607759	1	6.67	604313	20.0
unknown6.44	6.44	114.3	ng	3452660	1	6.67	604313	20.0
Hexadecane	10.62	2.3	ng	81269	4	11.17	714575	20.0
1-Heneicosanol	13.67	8.3	ng	238602	5	13.80	572996	20.0
1-Octanol, 5,7,7-...	15.69	2.0	ng	47057	6	15.20	469330	20.0