

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096707.D
 Acq On : 12 Jul 2017 22:27
 Operator : SJ/JU
 Sample : I4127-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-7(7.5-8.0)

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-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	2.987	150	153	165	rBV	35325	86539	3.54%	0.412%
2	4.851	466	470	480	rBV	400888	549916	22.52%	2.618%
3	5.281	538	543	546	rBV	2414539	2355248	96.45%	11.214%
4	6.310	708	718	721	rBV	2277574	2441825	100.00%	11.626%
5	6.439	735	740	743	rBV	2446557	2357923	96.56%	11.226%
6	6.663	775	778	782	rBV	746099	698428	28.60%	3.325%
7	6.822	801	805	809	rBV	1958408	1782621	73.00%	8.487%
8	7.227	869	874	877	rBV	1570588	1515010	62.04%	7.213%
9	7.339	887	893	896	rBV	40277	44089	1.81%	0.210%
10	7.857	977	981	989	rBV	42805	41294	1.69%	0.197%
11	7.951	992	997	1000	rBV	989054	937022	38.37%	4.461%
12	9.027	1174	1180	1183	rBV	2538706	2293642	93.93%	10.920%
13	9.421	1242	1247	1250	rBV	620608	512237	20.98%	2.439%
14	9.698	1289	1294	1298	rBV2	1046742	886584	36.31%	4.221%
15	10.480	1423	1427	1431	rBV	1131719	1116880	45.74%	5.318%
16	10.615	1447	1450	1456	rBV	38909	42084	1.72%	0.200%
17	11.174	1541	1545	1549	rBV	776540	657665	26.93%	3.131%
18	12.762	1810	1815	1818	rBV	1444233	1387508	56.82%	6.606%
19	13.662	1964	1968	1976	rVB	127323	145988	5.98%	0.695%
20	13.804	1988	1992	1999	rVB	651388	558832	22.89%	2.661%
21	14.298	2072	2076	2079	rBV3	29314	38547	1.58%	0.184%
22	15.198	2224	2229	2235	rBV	423654	489997	20.07%	2.333%
23	15.545	2283	2288	2293	rVB3	16303	29601	1.21%	0.141%
24	15.880	2341	2345	2350	rVB5	20329	33961	1.39%	0.162%

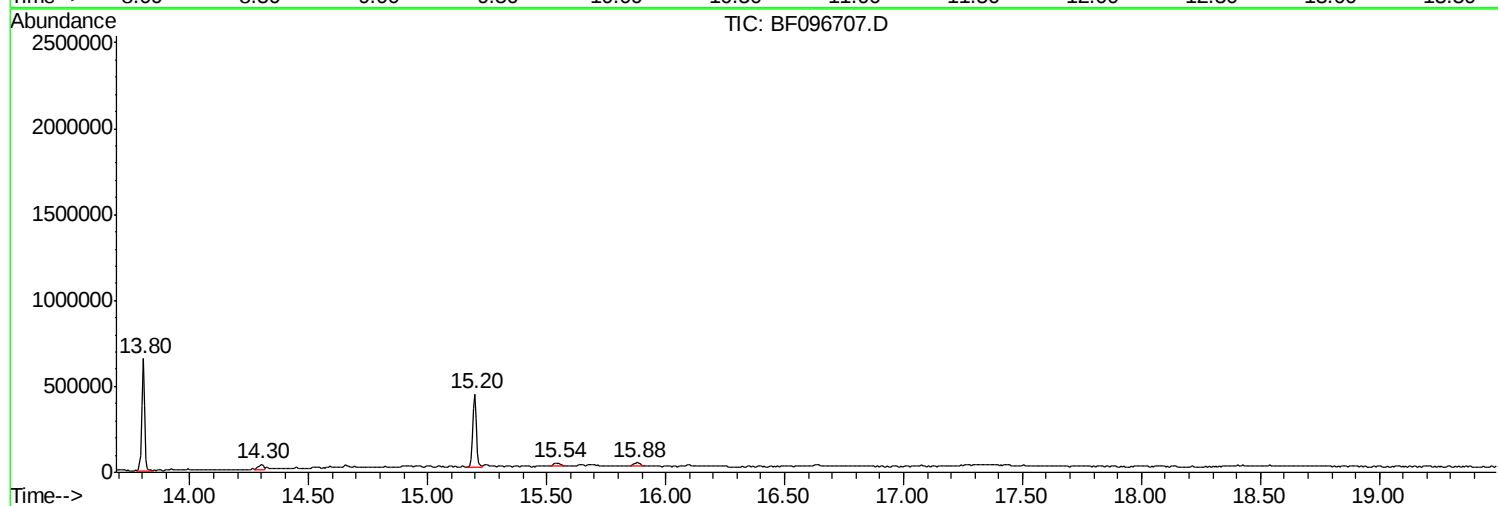
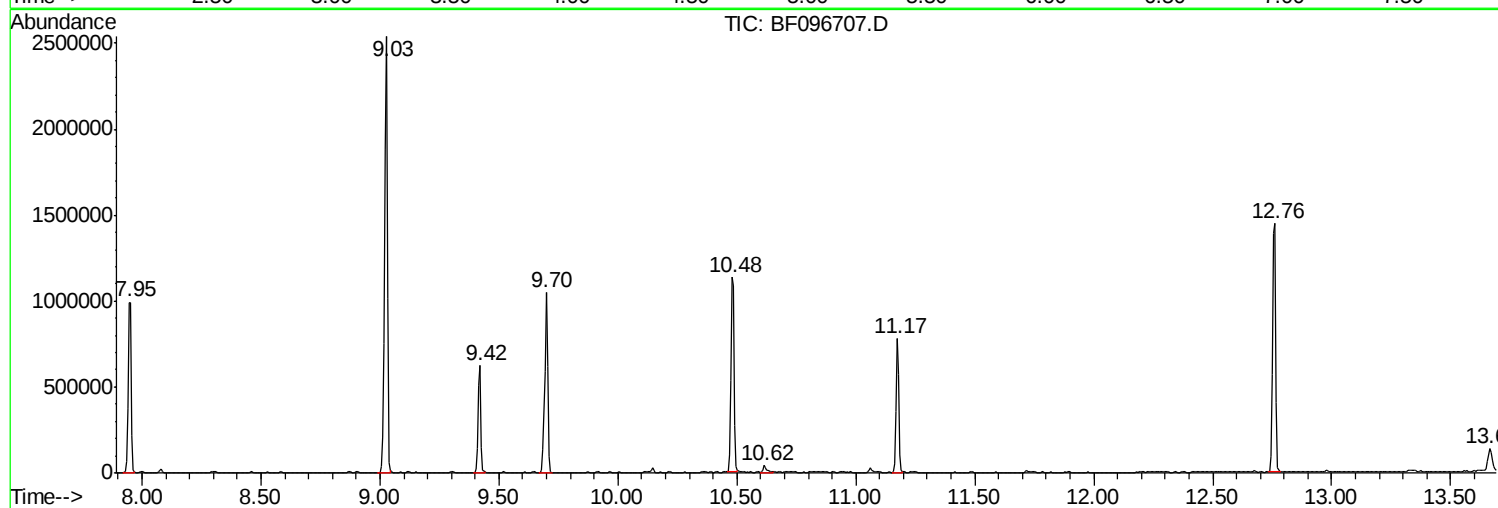
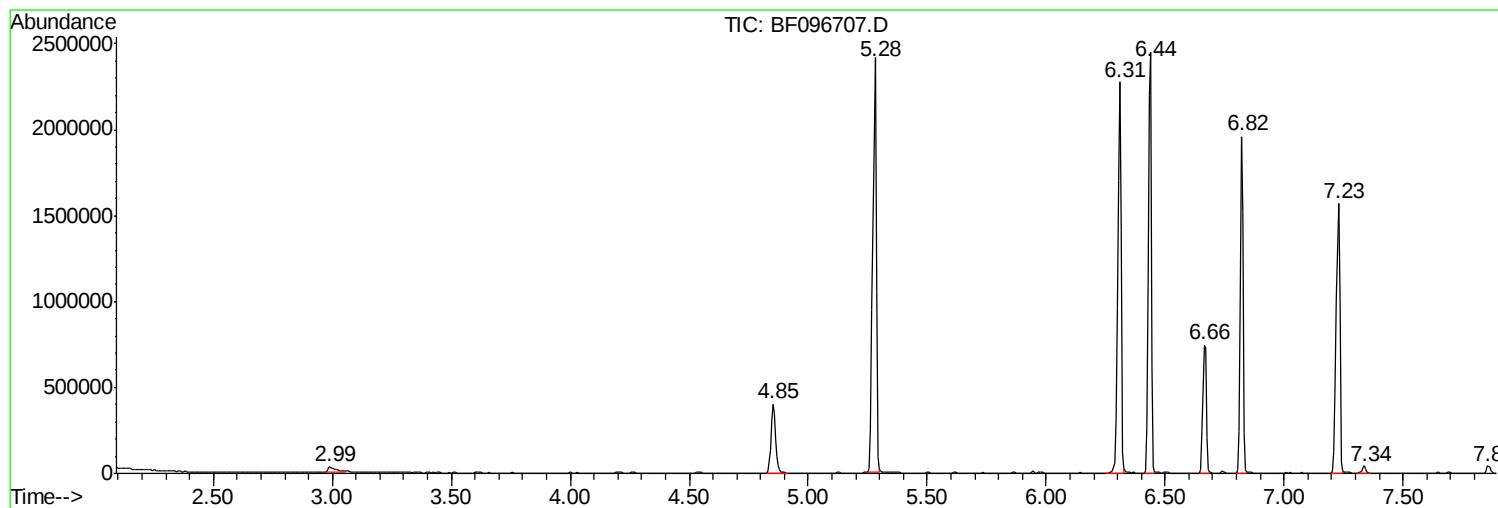
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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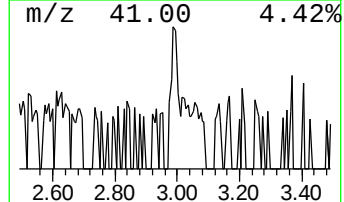
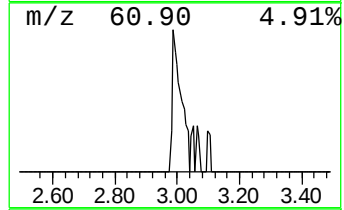
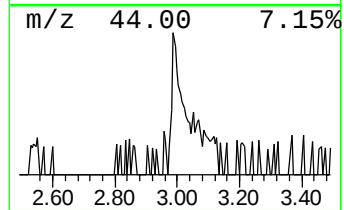
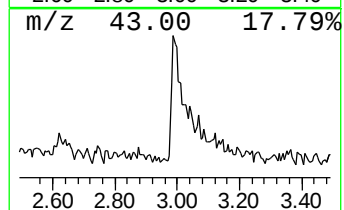
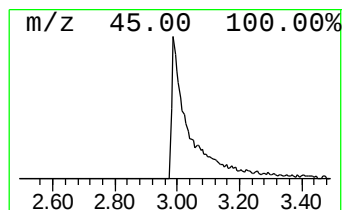
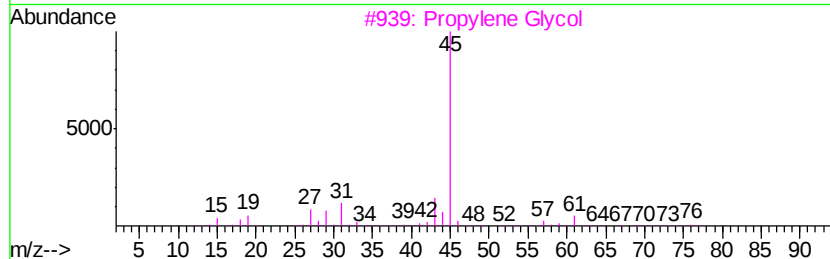
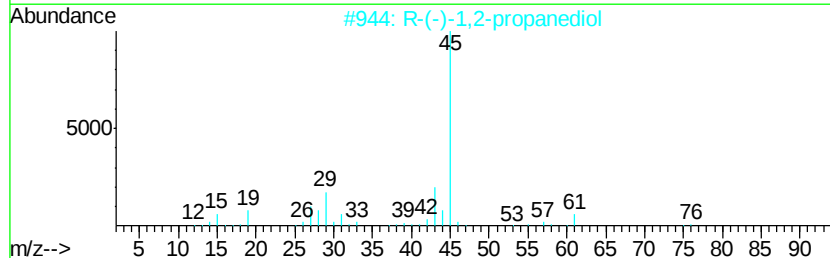
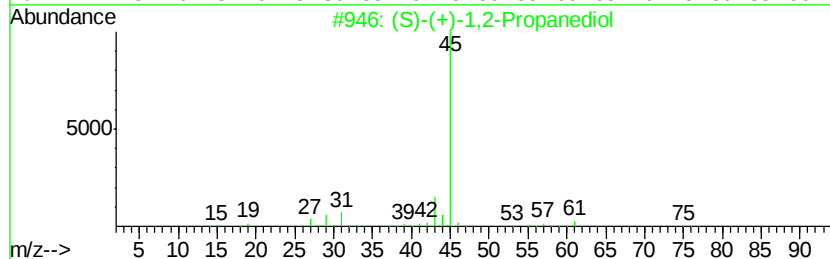
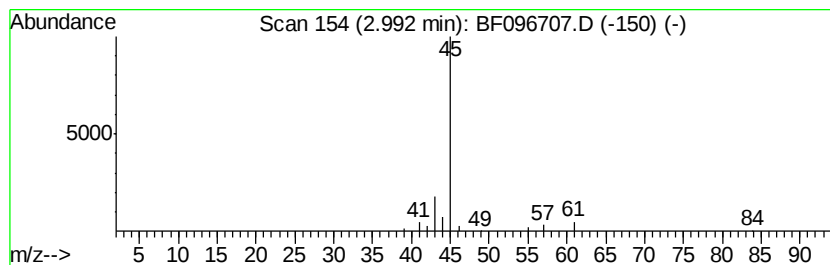
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.99 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	2.48 ng	86539	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	43
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
3	Propylene Glycol			76	C3H8O2	000057-55-6	9
4	2-Heptanol			116	C7H16O	000543-49-7	9
5	Butanenitrile, 2-(methoxymethoxy)			129	C6H11NO2	1000196-86-5	9



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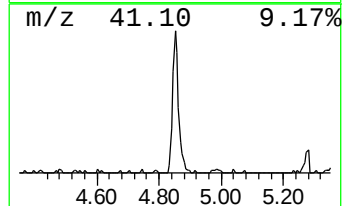
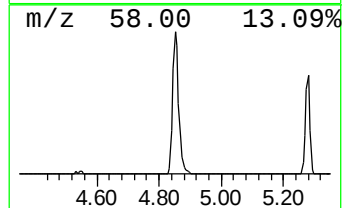
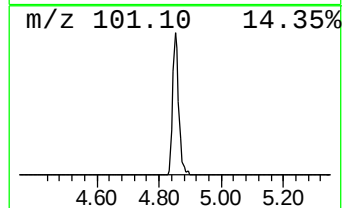
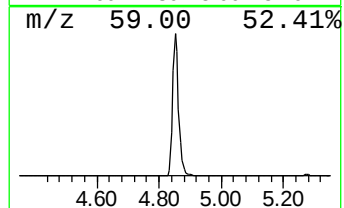
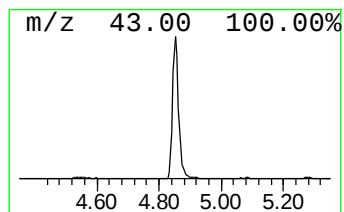
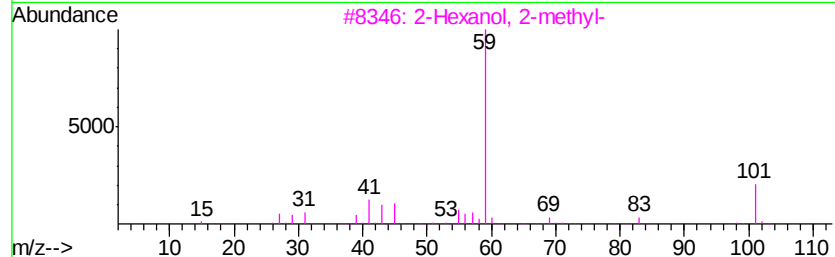
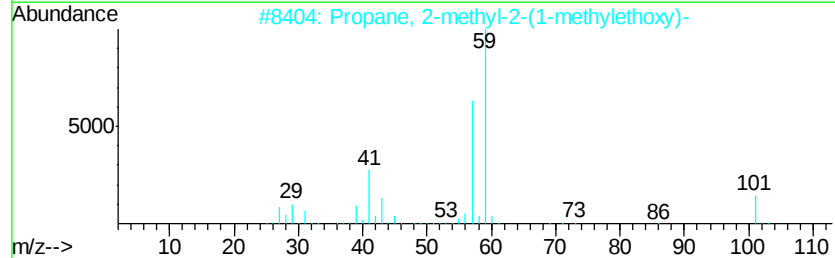
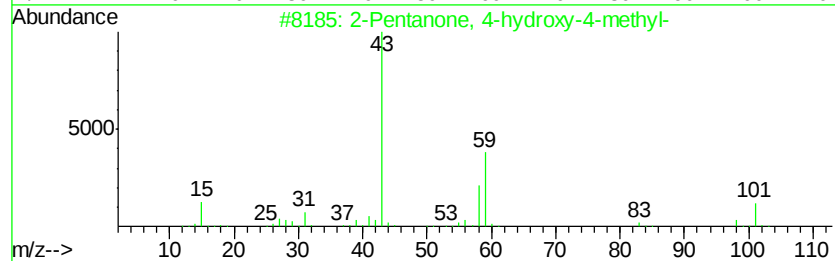
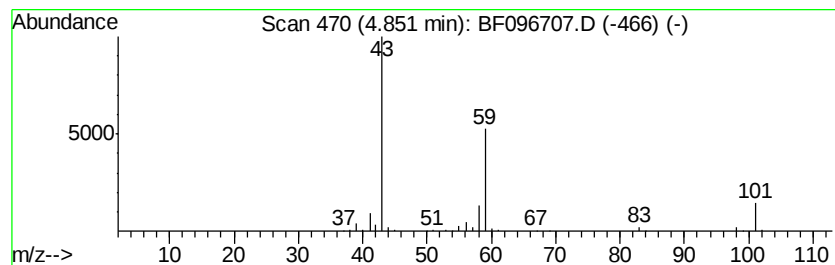
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	15.75 ng	549916	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	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	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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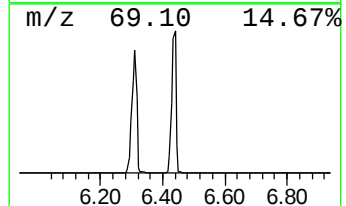
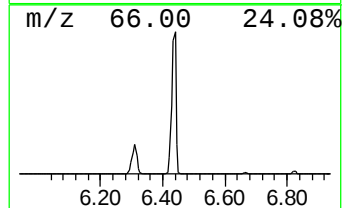
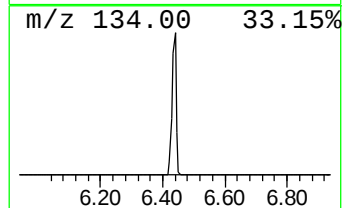
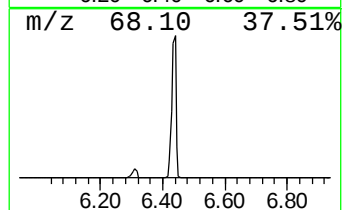
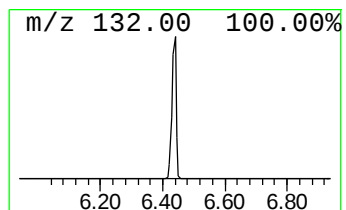
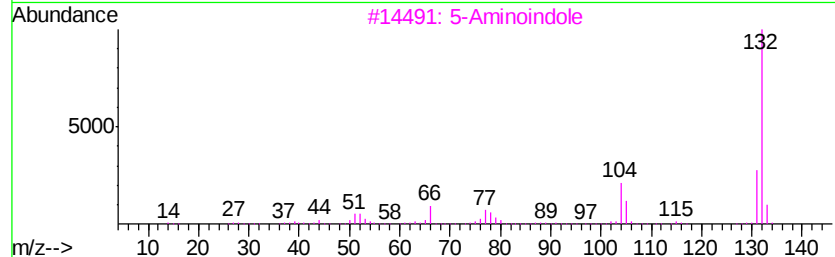
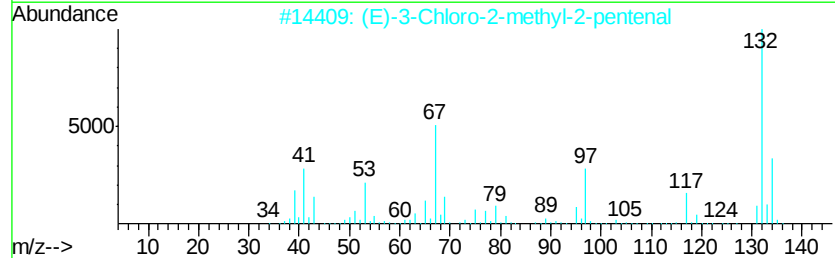
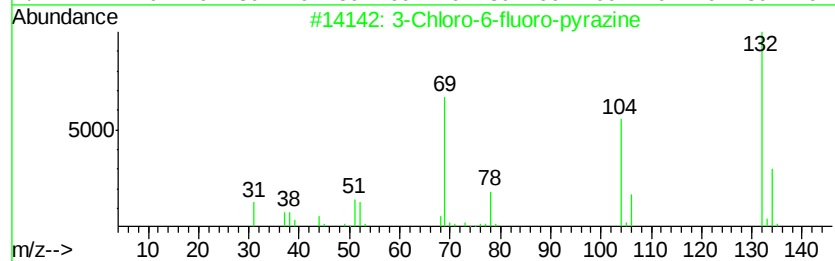
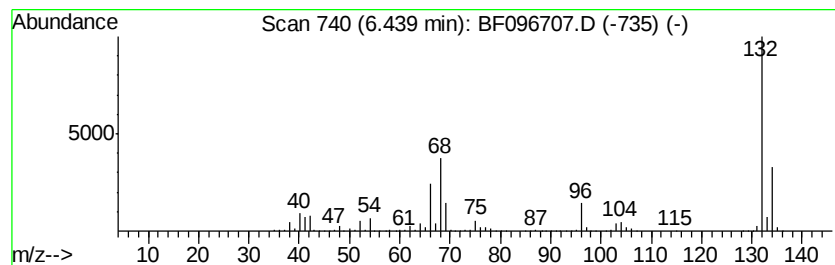
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Peak Number 3 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	67.52 ng	2357920	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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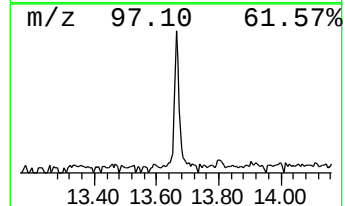
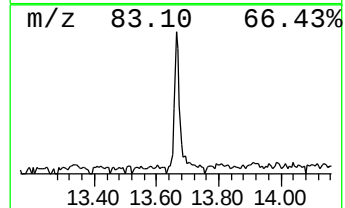
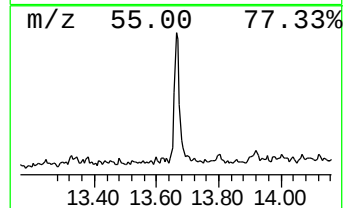
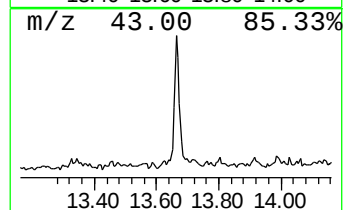
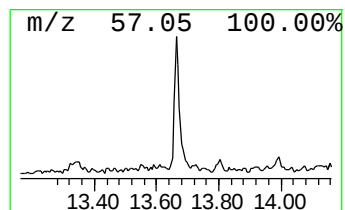
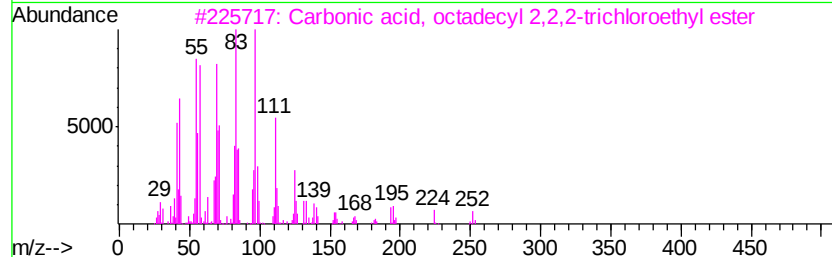
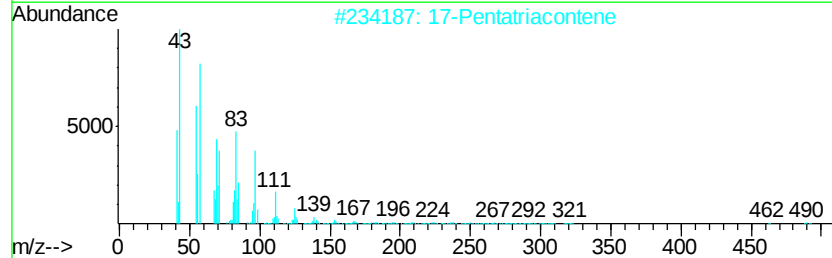
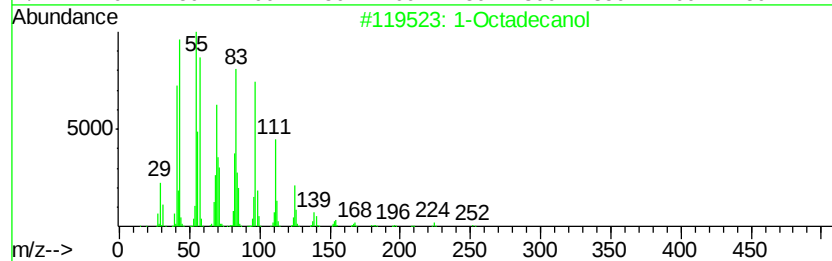
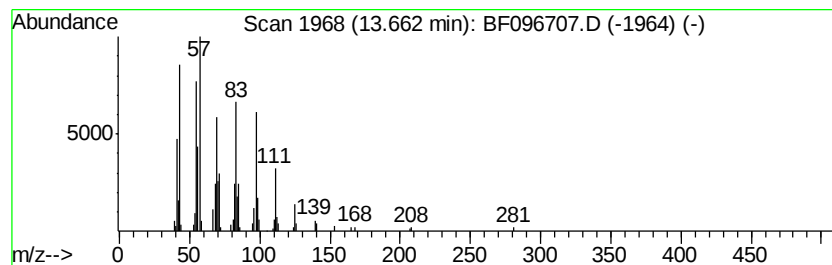
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Peak Number 5 1-Octadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	5.22 ng	145988	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol		270	C18H38O	000112-92-5	91
2	17-Pentatriacontene		491	C35H70	006971-40-0	91
3	Carbonic acid, octadecyl 2,2,2-t...		444	C21H39Cl3O3	1000314-56-3	90
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	90
5	Heptadecyl trifluoroacetate		352	C19H35F3O2	1000351-87-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.99	2.99	2.5	ng	86539	1	6.67	698428	20.0
2-Pentanone, 4-hy...	4.85	15.8	ng	549916	1	6.67	698428	20.0
unknown6.44	6.44	67.5	ng	2357920	1	6.67	698428	20.0
1-Octadecanol	13.66	5.2	ng	145988	5	13.80	558832	20.0