

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090217\
 Data File : BF098254.D
 Acq On : 2 Sep 2017 19:08
 Operator : SJ/JU
 Sample : I5074-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-5-6-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	4.904	476	479	498	rVB	208172	305139	9.92%	1.216%
2	5.322	545	550	554	rBV	2646109	2953613	96.05%	11.771%
3	6.357	720	726	729	rBV	2718043	3074969	100.00%	12.254%
4	6.481	742	747	750	rBV	2800743	2889427	93.97%	11.515%
5	6.710	782	786	789	rBV	853240	649187	21.11%	2.587%
6	6.869	808	813	816	rBV	2272077	2104873	68.45%	8.388%
7	7.281	877	883	886	rBV	1710238	1841732	59.89%	7.340%
8	7.992	1000	1004	1007	rBV	959118	791729	25.75%	3.155%
9	9.069	1182	1187	1190	rBV	3003027	2772562	90.17%	11.049%
10	9.463	1250	1254	1259	rBV	302193	247151	8.04%	0.985%
11	9.745	1297	1302	1310	rBB	734802	694946	22.60%	2.770%
12	10.533	1431	1436	1439	rBV	1383937	1285263	41.80%	5.122%
13	10.651	1453	1456	1465	rBV	29433	37970	1.23%	0.151%
14	11.227	1550	1554	1557	rBV	694604	599124	19.48%	2.388%
15	12.433	1756	1759	1763	rVB	54998	45595	1.48%	0.182%
16	12.663	1792	1798	1801	rBV	56318	52660	1.71%	0.210%
17	12.816	1819	1824	1827	rBV	2272339	2199282	71.52%	8.765%
18	13.710	1972	1976	1984	rBV	215771	255906	8.32%	1.020%
19	13.857	1995	2001	2004	rBV	739436	739129	24.04%	2.946%
20	14.033	2028	2031	2037	rBV7	22840	37764	1.23%	0.150%
21	14.345	2080	2084	2090	rBV	296771	355333	11.56%	1.416%
22	14.768	2153	2156	2160	rVB	51697	46514	1.51%	0.185%
23	14.868	2170	2173	2182	rBV	34697	64361	2.09%	0.256%
24	14.951	2183	2187	2188	rBV3	28017	32236	1.05%	0.128%
25	14.974	2188	2191	2198	rVB	72371	101059	3.29%	0.403%
26	15.274	2237	2242	2252	rVB	566152	700380	22.78%	2.791%
27	15.710	2312	2316	2321	rVB	27545	37788	1.23%	0.151%
28	15.762	2321	2325	2331	rBV9	19771	36996	1.20%	0.147%
29	16.439	2438	2440	2445	rVB4	24236	32001	1.04%	0.128%
30	19.080	2881	2889	2897	rBV8	39741	108137	3.52%	0.431%

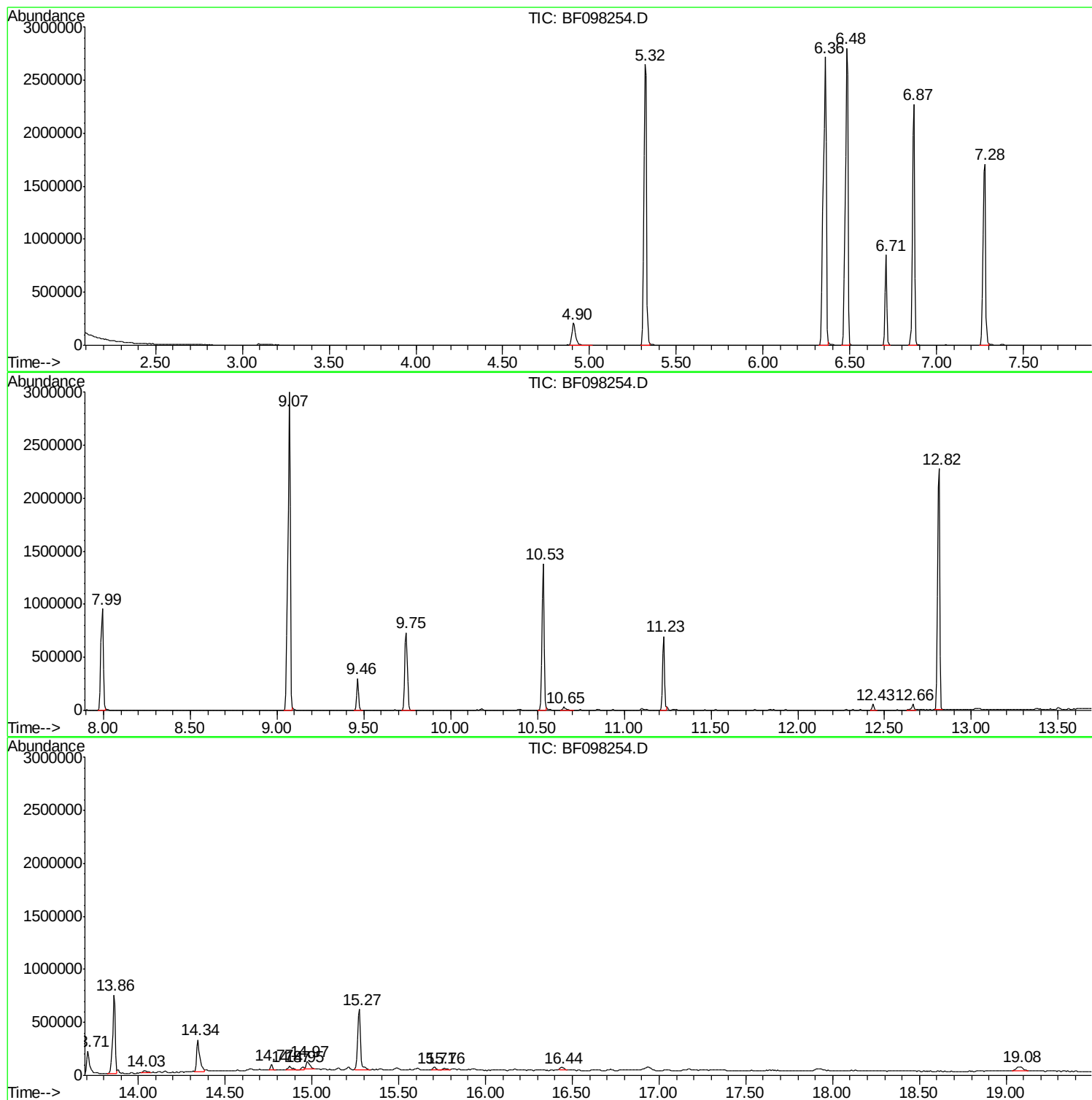
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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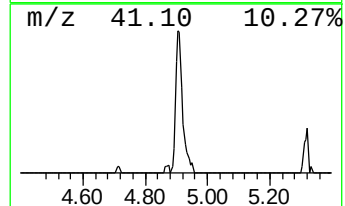
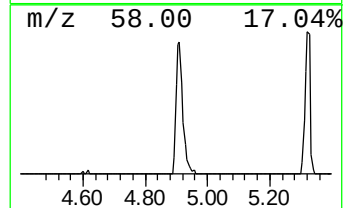
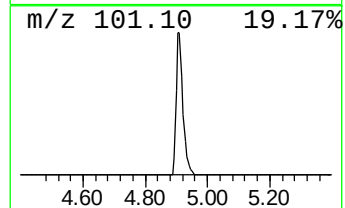
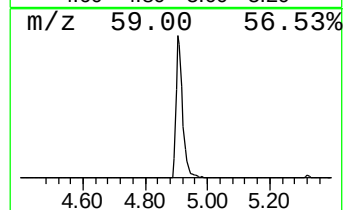
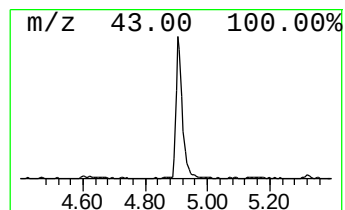
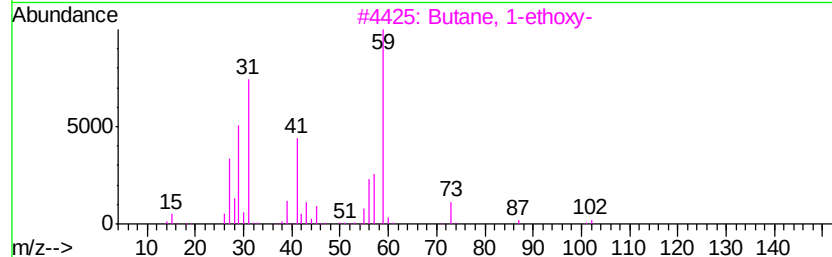
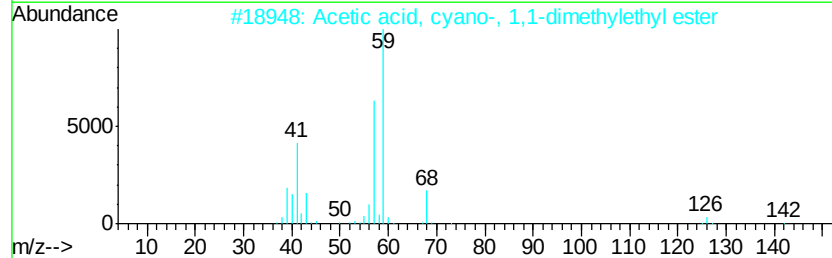
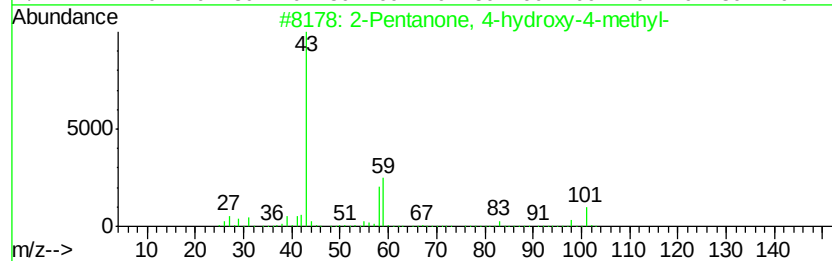
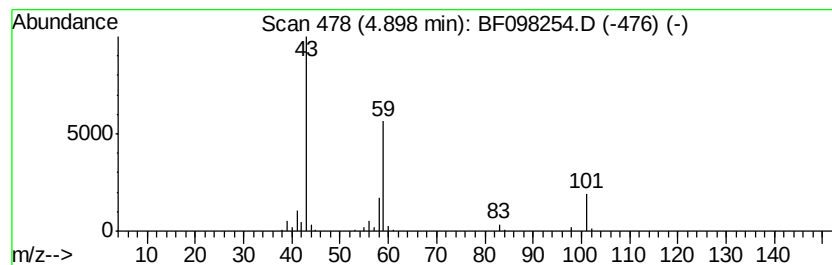
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	9.40 ng	305139	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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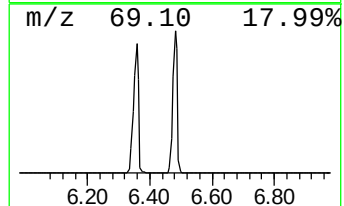
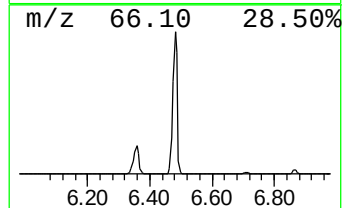
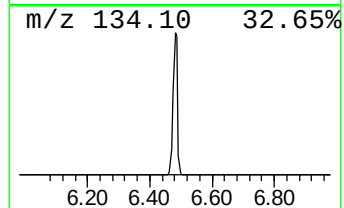
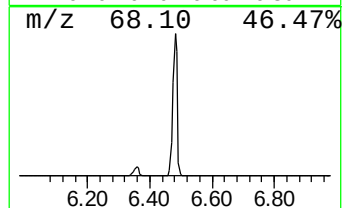
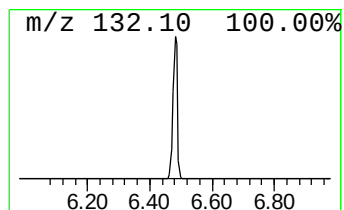
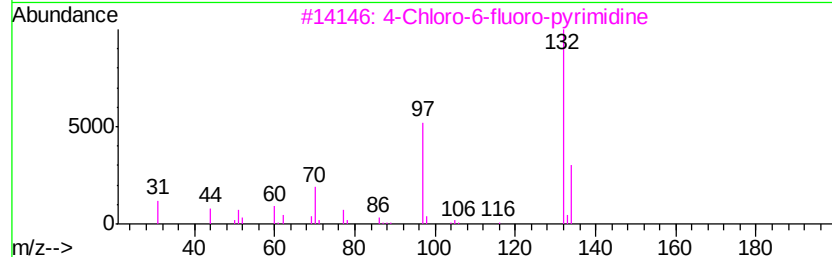
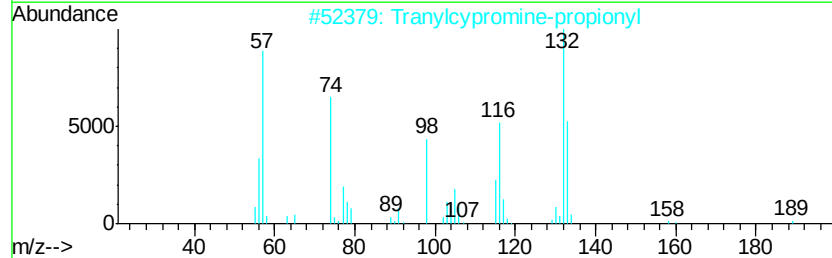
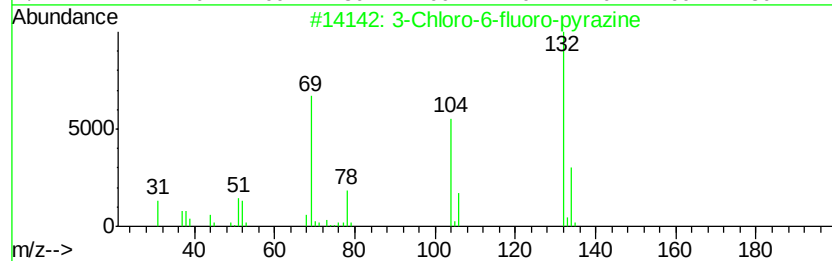
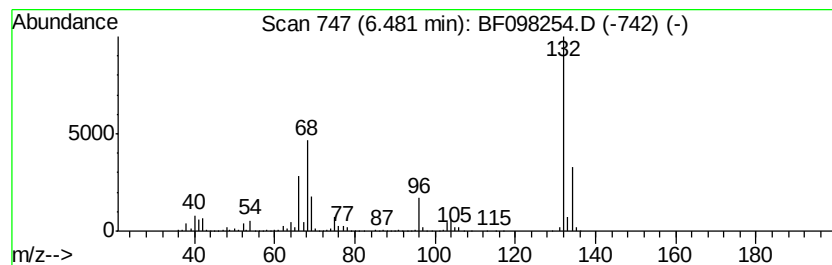
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	89.02 ng	2889430	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5		Xenon	132	Xe	007440-63-3	9



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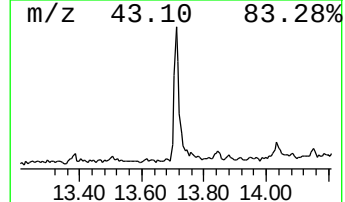
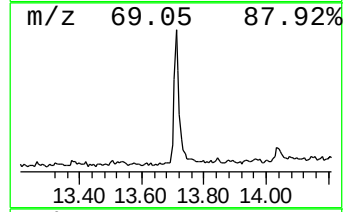
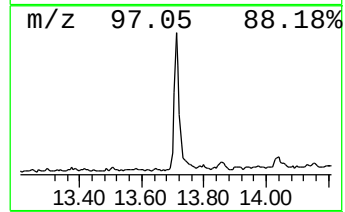
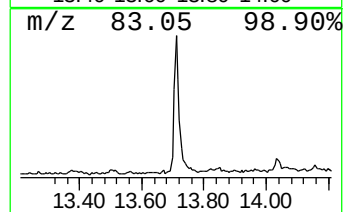
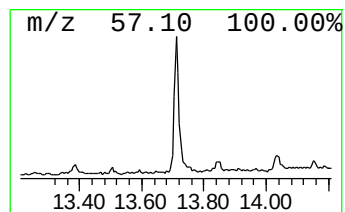
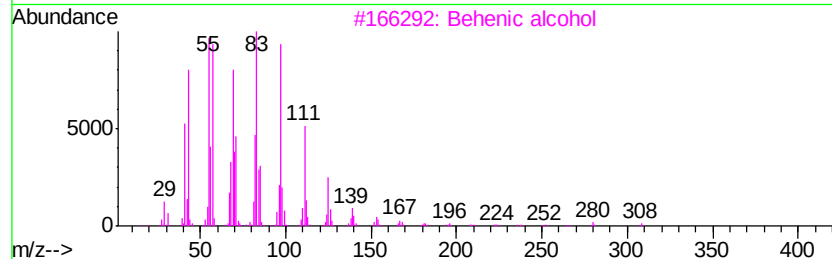
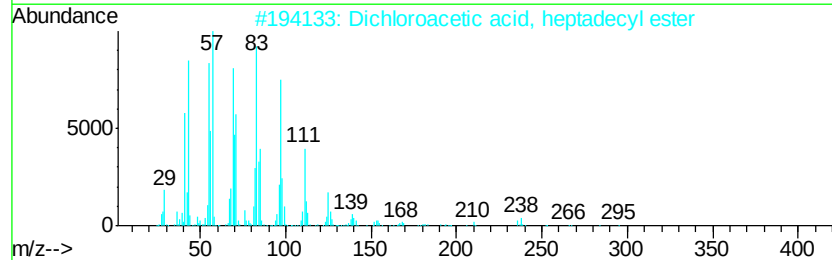
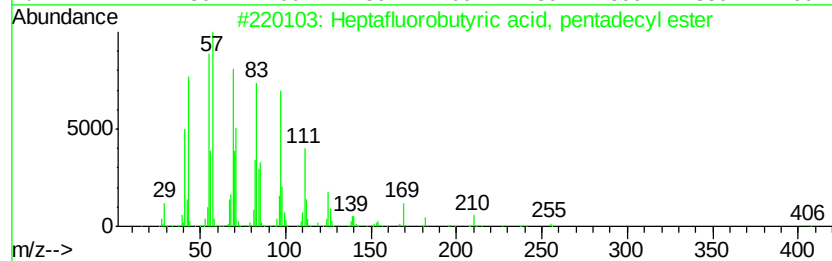
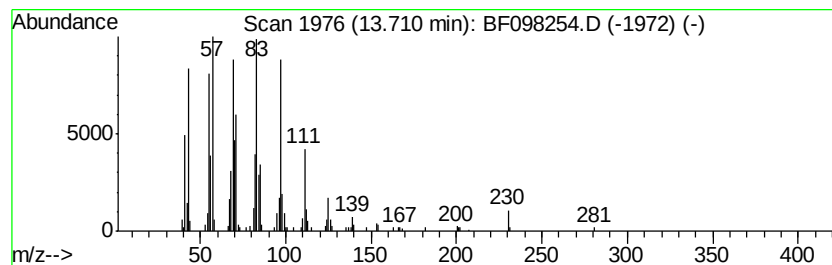
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Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	6.92 ng	255906	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	90



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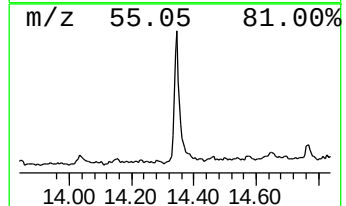
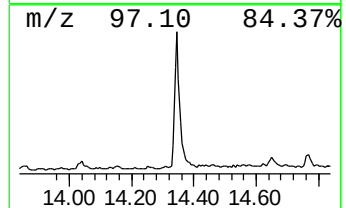
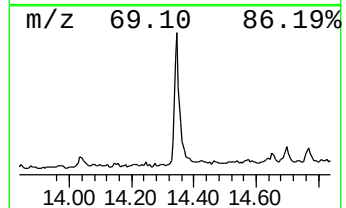
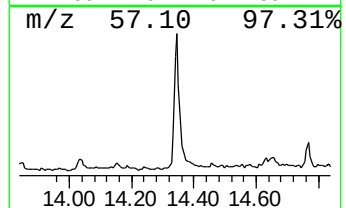
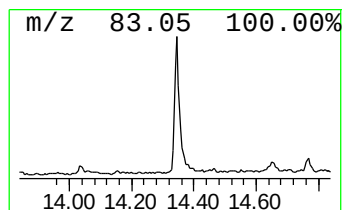
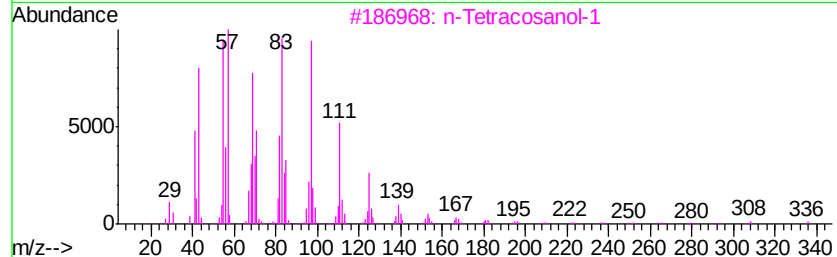
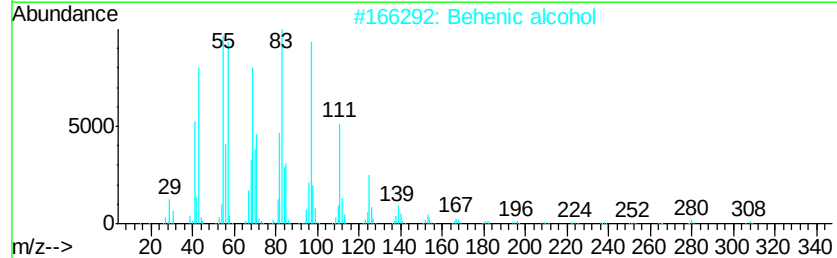
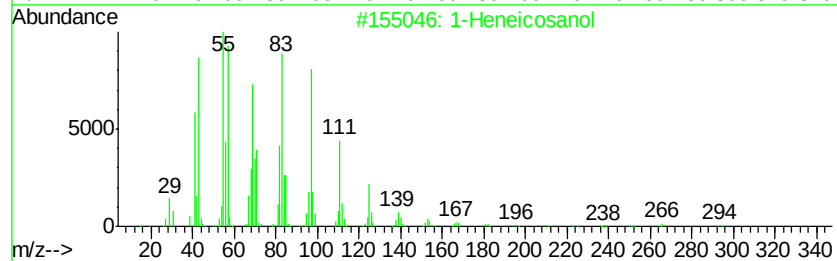
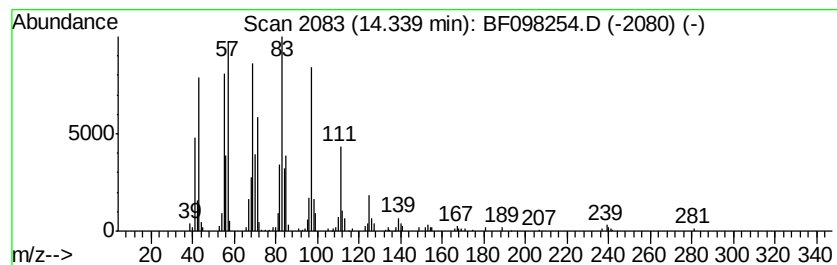
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Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.34	9.61 ng	355333	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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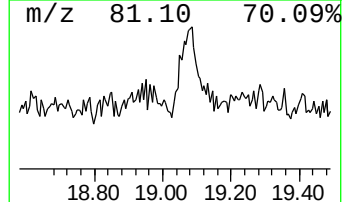
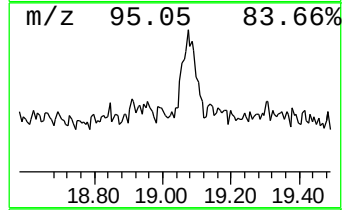
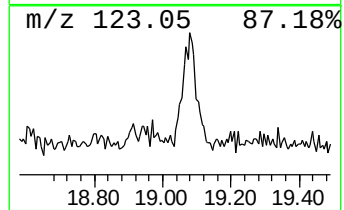
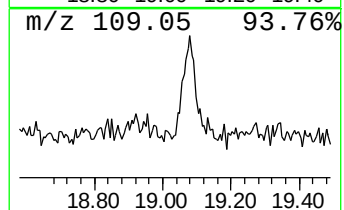
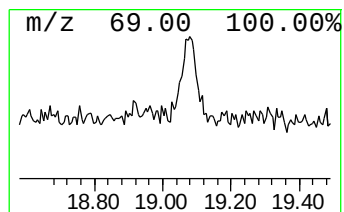
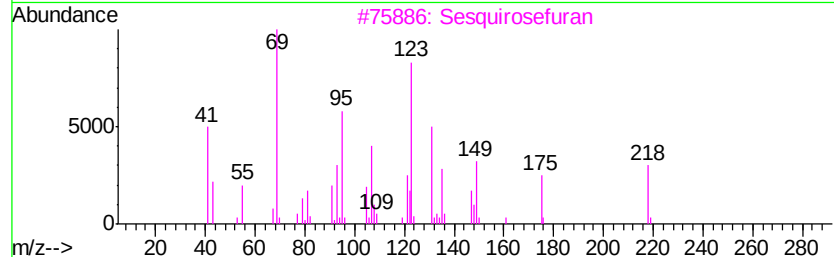
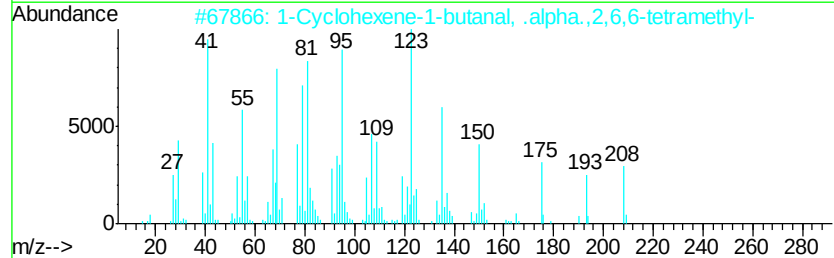
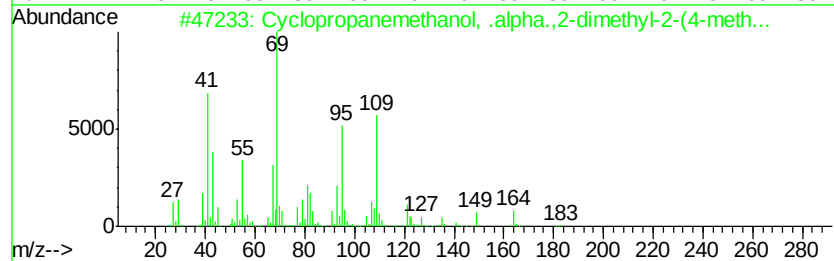
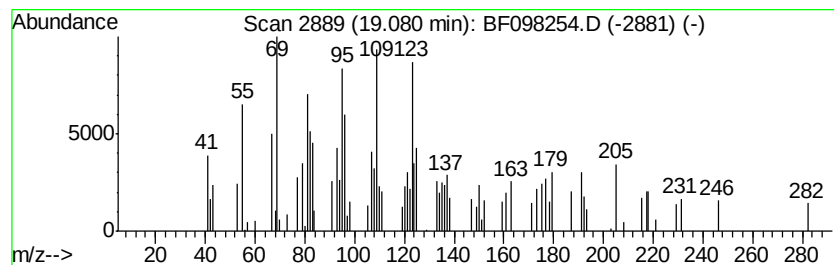
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Peak Number 7 unknown19.08 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.08	3.09 ng	108137	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	43
2		1-Cyclohexene-1-butanal, .alpha....	208	C14H24O	021632-06-4	41
3		Sesquirosefuran	218	C15H22O	039007-93-7	38
4		d-Norandrostane (5.alpha.,14.alp...	246	C18H30	1000281-13-8	35
5		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	9.4	ng	305139	1	6.71	649187	20.0
unknown6.48	6.48	89.0	ng	2889430	1	6.71	649187	20.0
Heptafluorobutyri...	13.71	6.9	ng	255906	5	13.86	739129	20.0
1-Heneicosanol	14.34	9.6	ng	355333	5	13.86	739129	20.0
unknown19.08	19.08	3.1	ng	108137	6	15.27	700380	20.0