

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
 Data File : BF088682.D
 Acq On : 4 Jul 2016 8:44
 Operator : UM/SJ
 Sample : H3849-03
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 F12-B1(0-5)C

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-BF063016.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	1.724	10	12	21	rVV	82709	127519	5.48%	0.588%
2	1.850	21	23	34	rVV	656811	964208	41.42%	4.447%
3	1.998	34	36	39	rVB	54074	66826	2.87%	0.308%
4	4.947	292	294	298	rBV	166391	234563	10.08%	1.082%
5	5.382	329	332	334	rBV	2297288	2294032	98.54%	10.580%
6	6.422	420	423	425	rBV	2272050	2327965	100.00%	10.737%
7	6.547	432	434	437	rBV	1723626	2325487	99.89%	10.725%
8	6.787	452	455	457	rBV	724223	634840	27.27%	2.928%
9	6.947	466	469	471	rVB	1352342	1796235	77.16%	8.284%
10	7.347	501	504	506	rBV	1552152	1417108	60.87%	6.536%
11	7.645	528	530	533	rVB	63399	51535	2.21%	0.238%
12	8.068	565	567	570	rVB	945549	799248	34.33%	3.686%
13	9.142	659	661	664	rBV	1923804	2156831	92.65%	9.947%
14	9.542	694	696	698	rBV	158748	162189	6.97%	0.748%
15	9.816	718	720	722	rBV	859594	775704	33.32%	3.578%
16	10.605	786	789	791	rBV	1309471	1302656	55.96%	6.008%
17	11.176	837	839	841	rBV	64764	62355	2.68%	0.288%
18	11.291	847	849	853	rVB2	568692	703659	30.23%	3.245%
19	12.502	953	955	957	rBV	108137	102284	4.39%	0.472%
20	12.719	971	974	977	rBV2	141814	224099	9.63%	1.034%
21	12.879	986	988	990	rBV	1798217	1580187	67.88%	7.288%
22	13.417	1033	1035	1037	rBV	86046	72516	3.11%	0.334%
23	13.805	1066	1069	1074	rBV2	58922	122205	5.25%	0.564%
24	13.920	1076	1079	1086	rVB	724451	761429	32.71%	3.512%
25	14.925	1165	1167	1173	rBV	51029	136860	5.88%	0.631%
26	15.314	1198	1201	1204	rBV	421074	479753	20.61%	2.213%

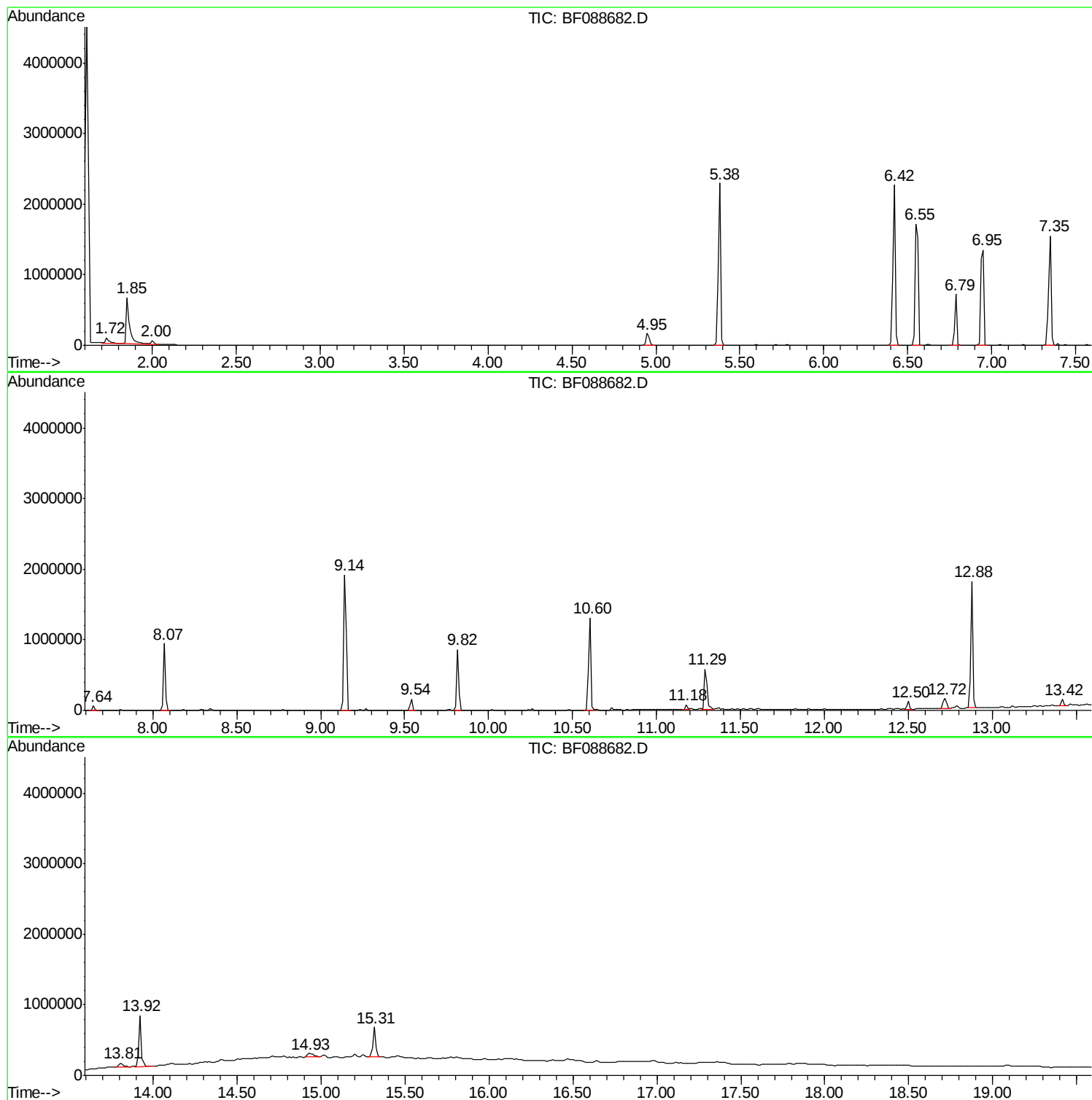
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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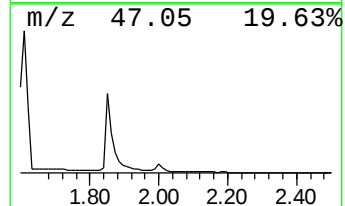
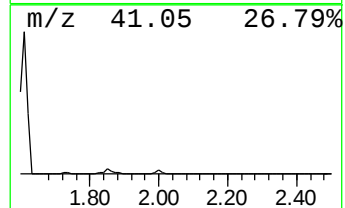
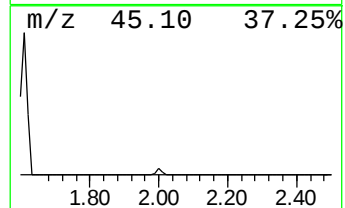
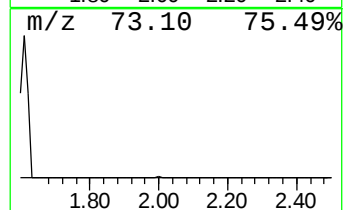
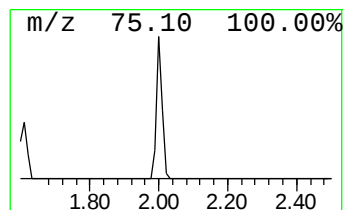
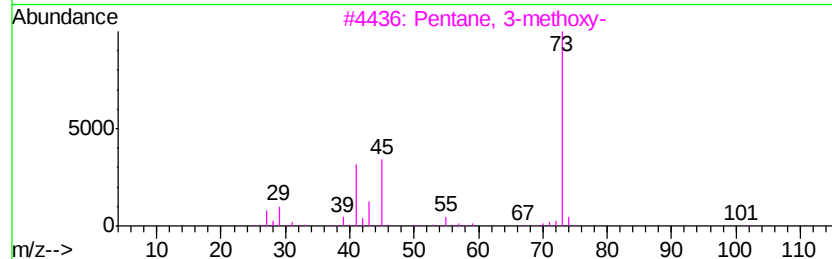
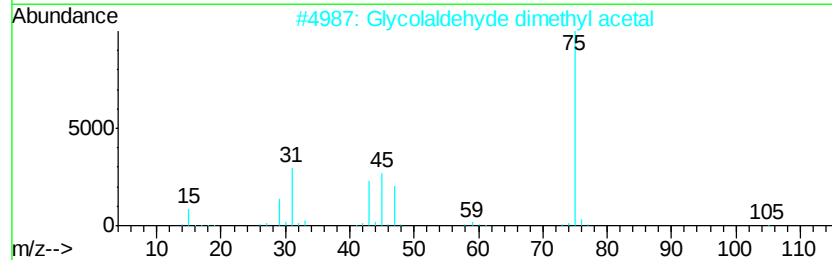
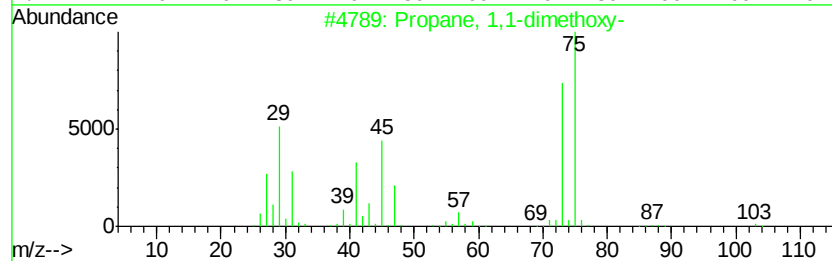
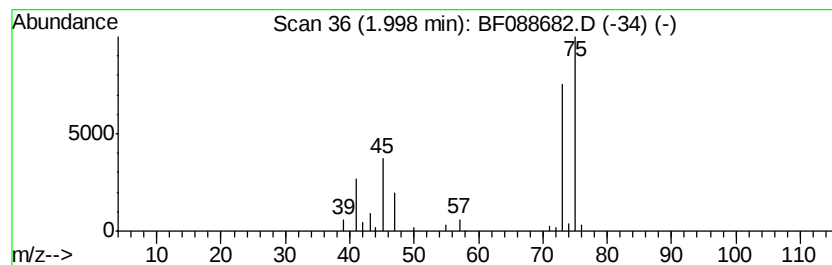
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	2.11 ng	66826	1,4-Dichlorobenzene-d4	6.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	38
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
4		Glycine	75	C2H5NO2	000056-40-6	9
5		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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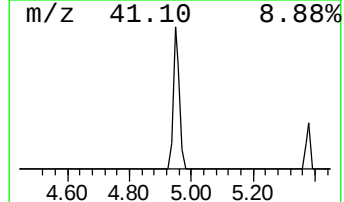
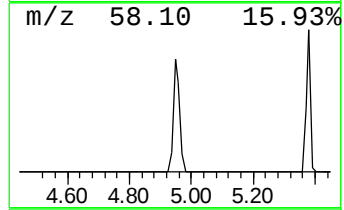
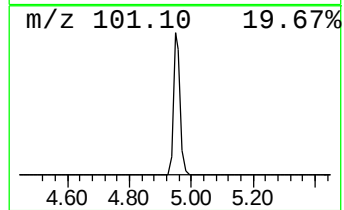
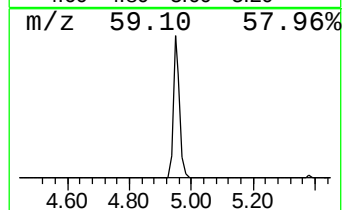
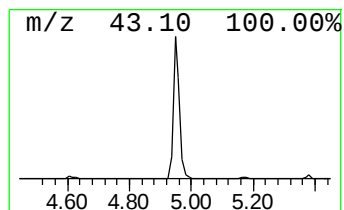
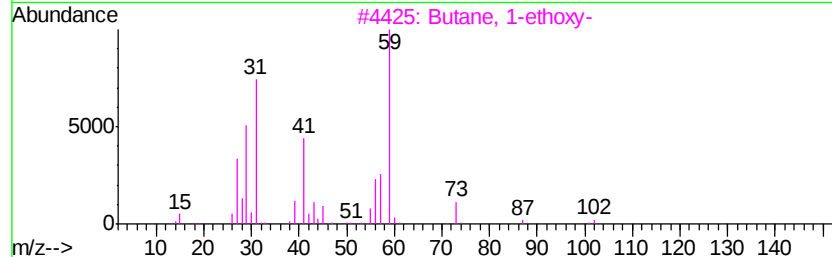
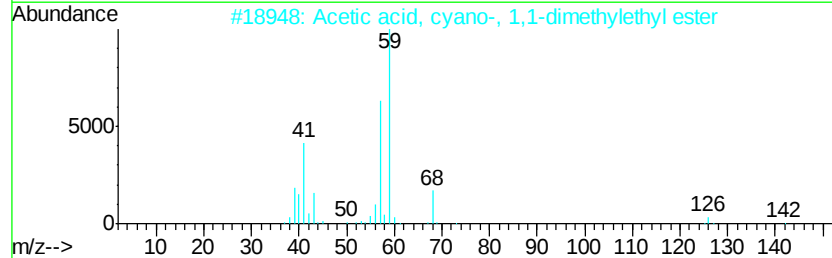
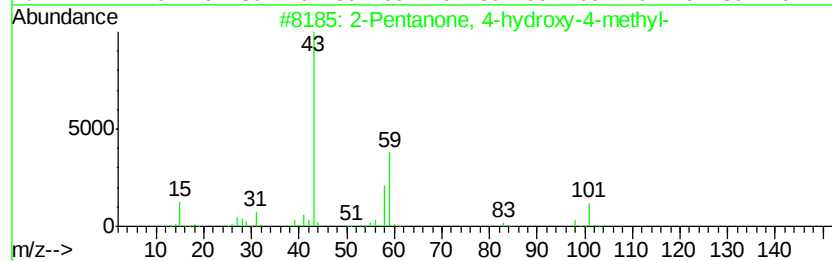
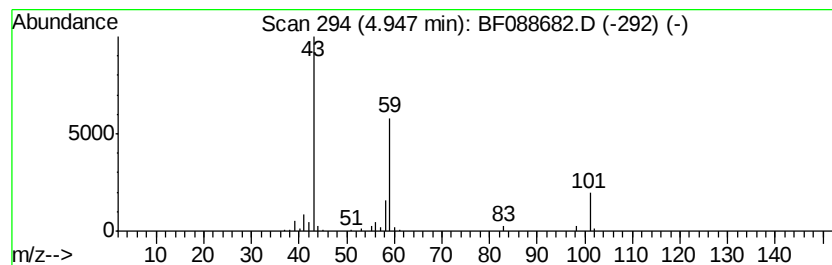
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	7.39 ng	234563	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
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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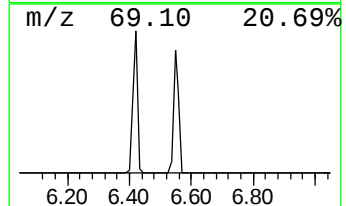
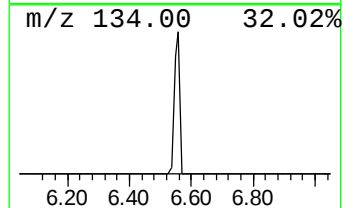
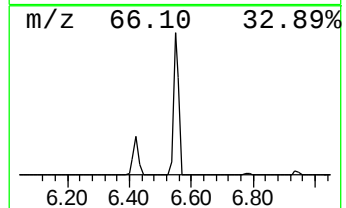
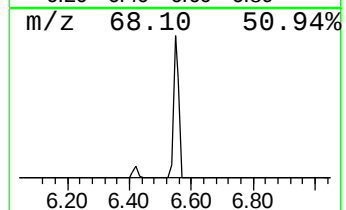
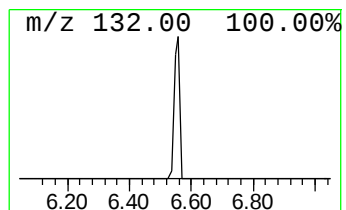
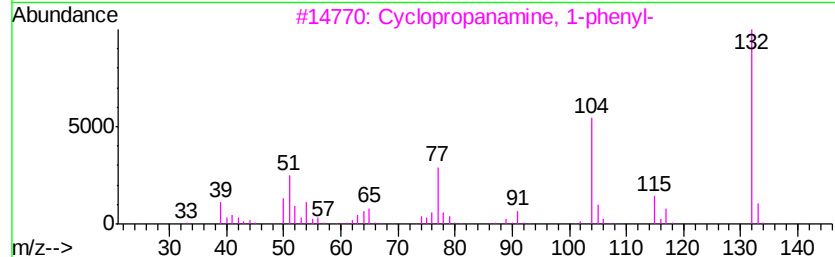
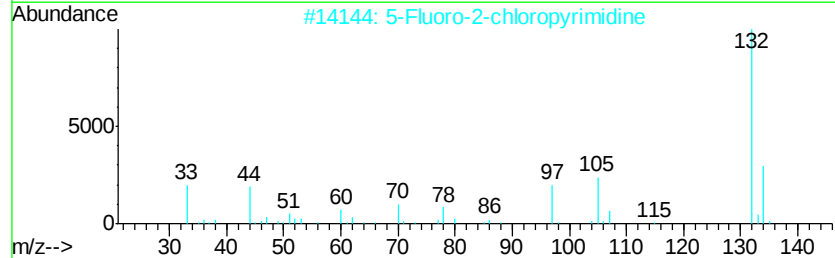
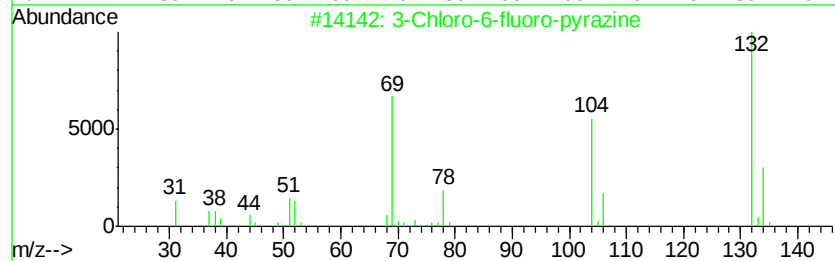
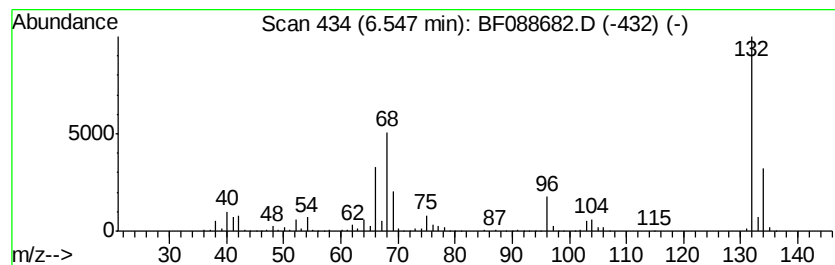
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Peak Number 5 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	73.26 ng	2325490	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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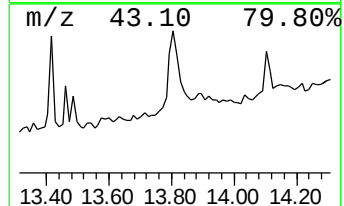
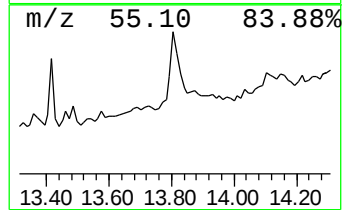
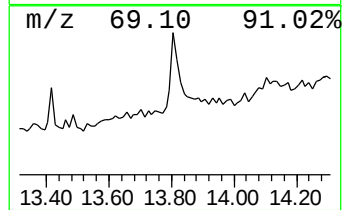
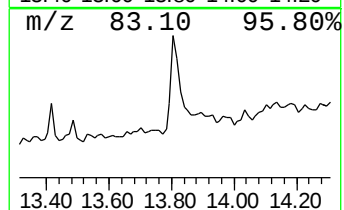
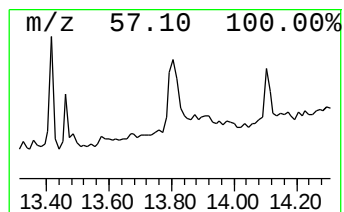
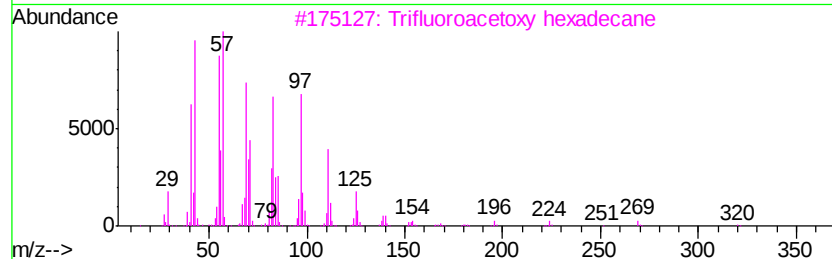
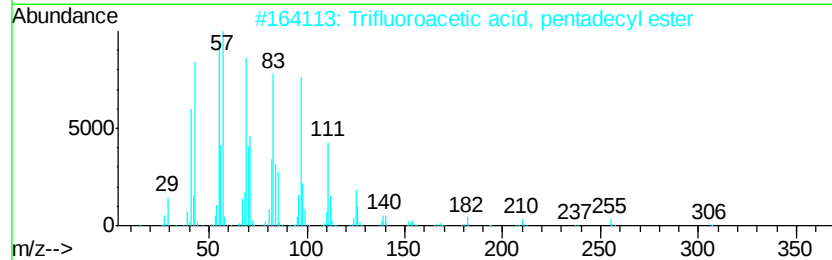
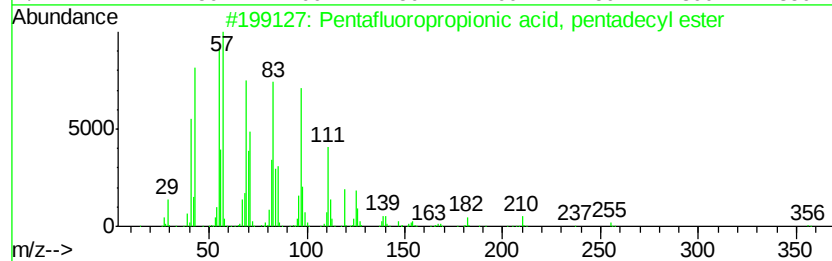
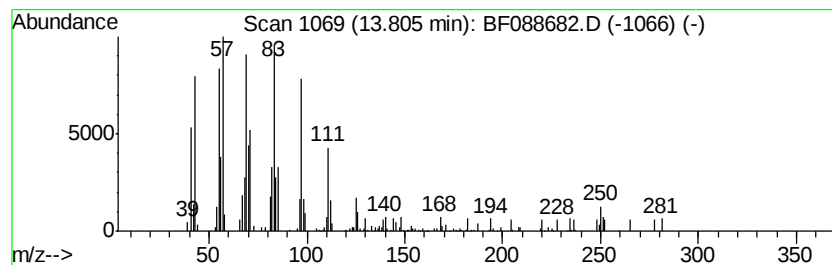
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Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.21 ng	122205	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	93
4		E-7-Octadecene	252	C18H36	1000130-92-0	92
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.00	2.1	ng	66826	1	6.79	634840	20.0
2-Pentanone, 4-hy...	4.95	7.4	ng	234563	1	6.79	634840	20.0
unknown6.55	6.55	73.3	ng	2325490	1	6.79	634840	20.0
Pentafluoropropio...	13.81	3.2	ng	122205	5	13.92	761429	20.0