

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
 Data File : BF099082.D
 Acq On : 4 Oct 2017 22:24
 Operator : SJ/JU
 Sample : I5644-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-10-11-COMP

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-BF092317.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	2.151	6	11	17	rVB	92137	120871	3.69%	0.471%
2	5.087	506	510	526	rVB	394894	486948	14.87%	1.896%
3	5.481	573	577	581	rBV	2033727	2045618	62.47%	7.963%
4	6.492	744	749	752	rBV	2309297	2526402	77.15%	9.835%
5	6.633	768	773	776	rBV	2527740	2324581	70.99%	9.049%
6	6.863	808	812	816	rBV	950447	760596	23.23%	2.961%
7	7.022	834	839	842	rBV	1786111	1608566	49.12%	6.262%
8	7.428	903	908	911	rBV	1719934	1656634	50.59%	6.449%
9	8.145	1026	1030	1033	rBV	1262123	1039152	31.73%	4.045%
10	9.222	1208	1213	1216	rBV	3556171	3274477	100.00%	12.747%
11	9.610	1275	1279	1282	rBV	570897	452930	13.83%	1.763%
12	9.898	1324	1328	1332	rBV	1218240	1132838	34.60%	4.410%
13	10.692	1458	1463	1466	rBV	2082242	2159392	65.95%	8.406%
14	10.792	1477	1480	1487	rBV	54296	54726	1.67%	0.213%
15	11.386	1577	1581	1584	rBV	1310079	1112166	33.96%	4.329%
16	12.598	1783	1787	1790	rBV	83334	65935	2.01%	0.257%
17	12.827	1821	1826	1829	rBV	58836	55412	1.69%	0.216%
18	12.974	1846	1851	1854	rBV	3219669	3229671	98.63%	12.572%
19	13.857	1997	2001	2013	rBV2	72601	93586	2.86%	0.364%
20	14.027	2025	2030	2033	rBV	873437	844275	25.78%	3.287%
21	15.498	2274	2280	2290	rBV	506816	643684	19.66%	2.506%

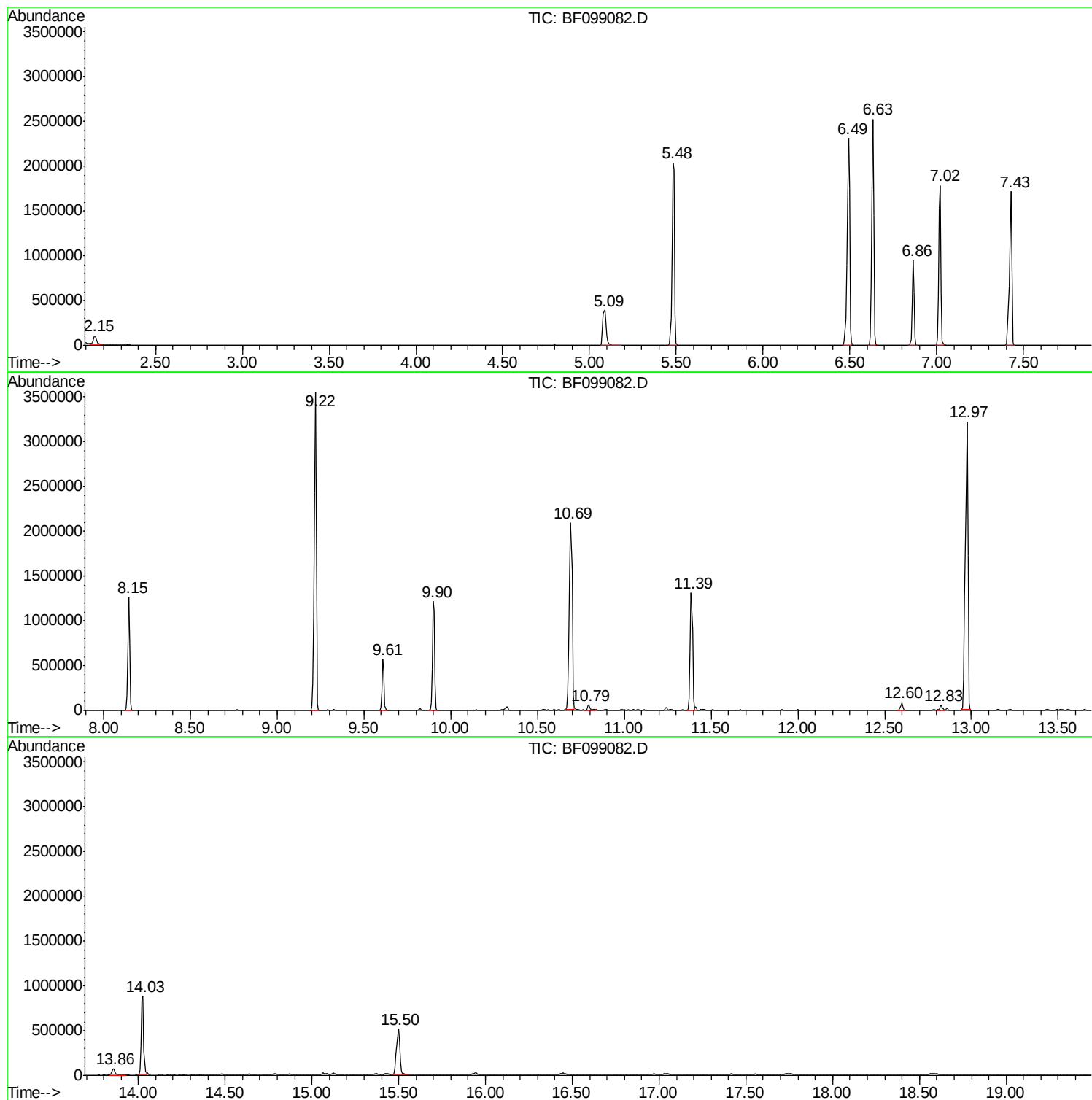
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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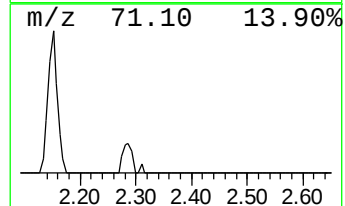
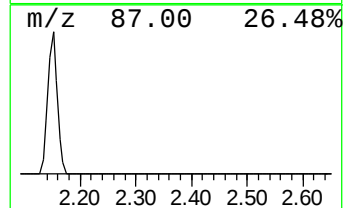
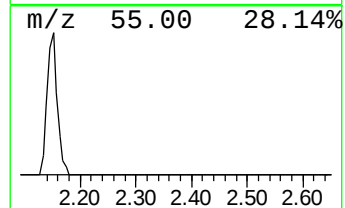
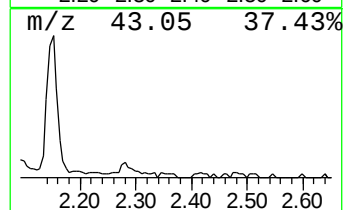
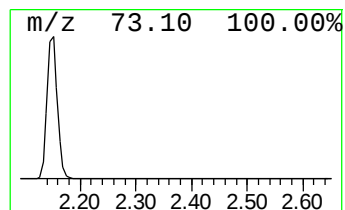
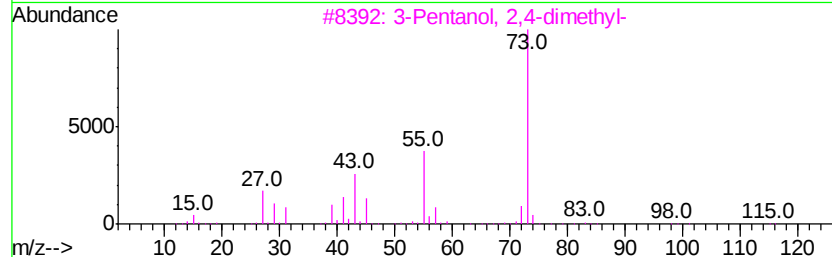
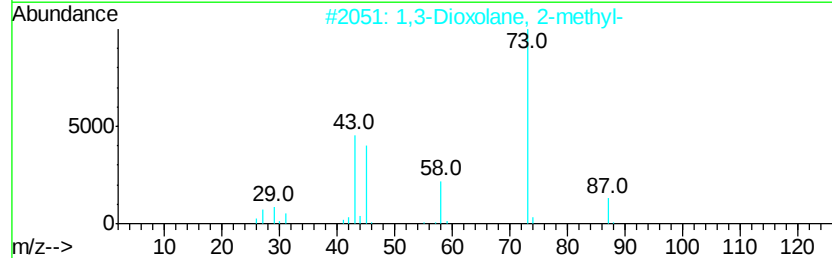
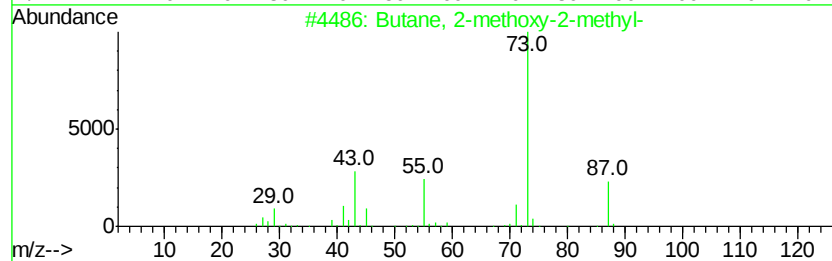
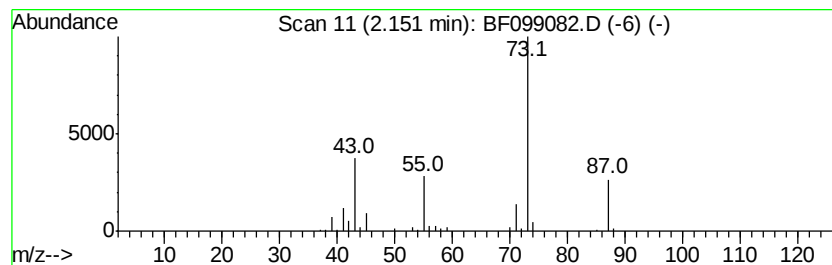
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	3.18 ng	120871	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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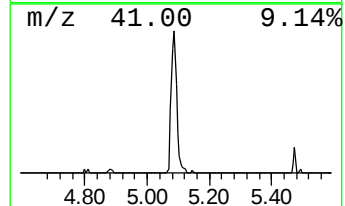
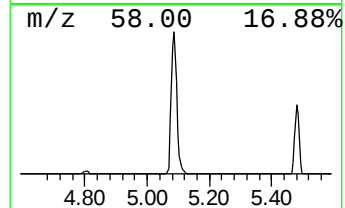
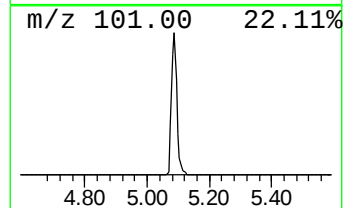
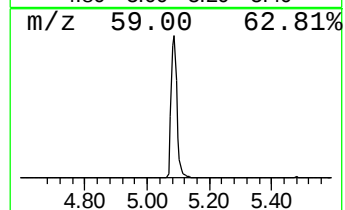
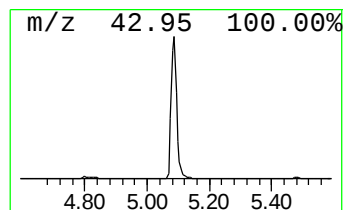
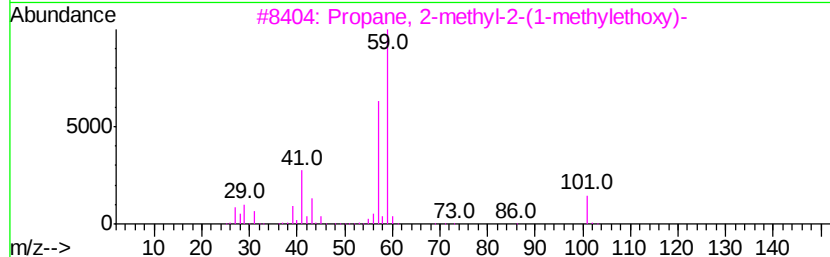
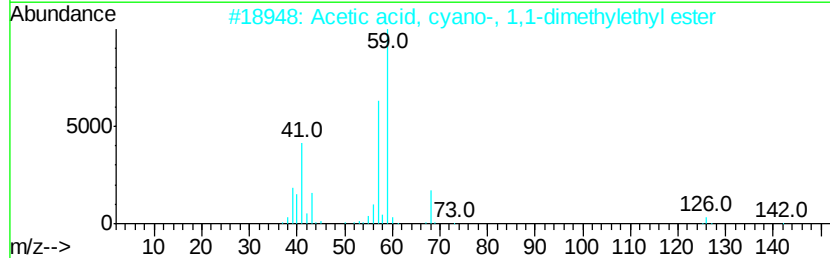
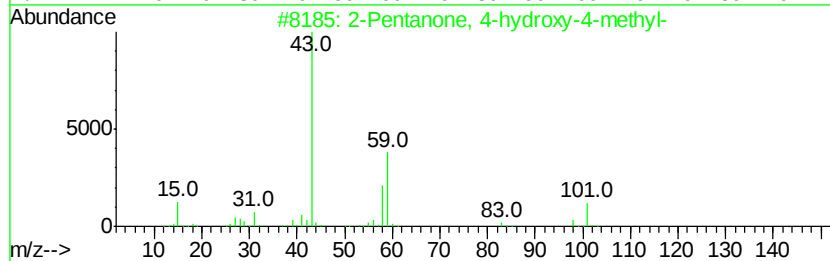
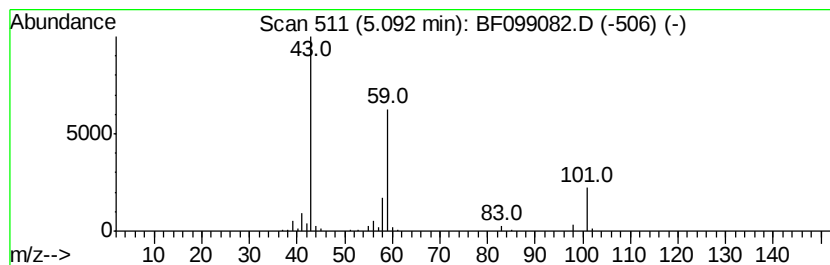
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	12.80 ng	486948	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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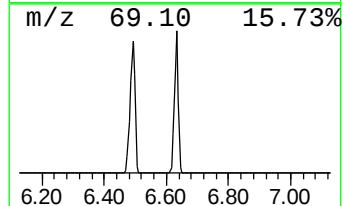
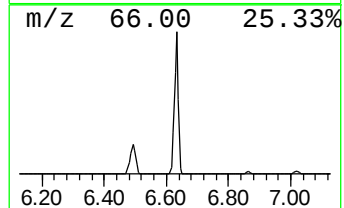
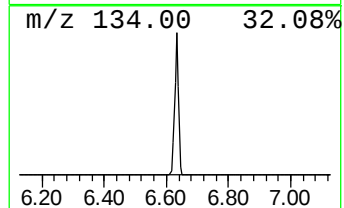
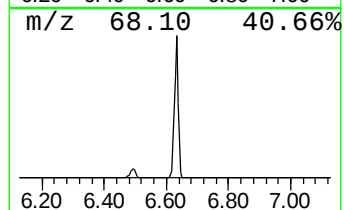
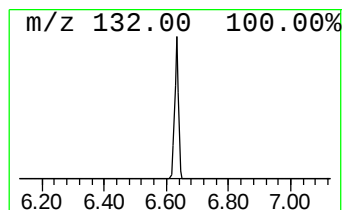
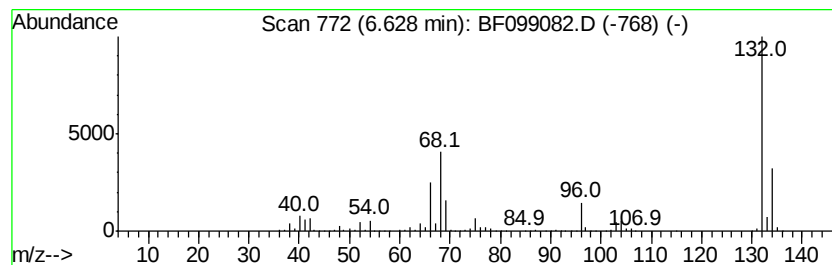
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Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	61.13 ng	2324580	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3	Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5	Aminoindole	132	C8H8N2	005192-03-0	12
4	4	Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4	Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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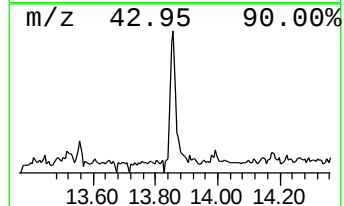
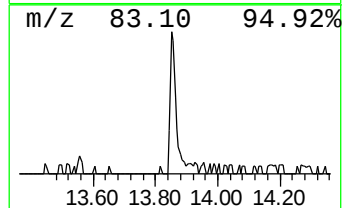
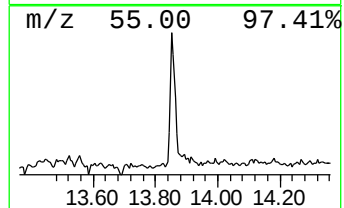
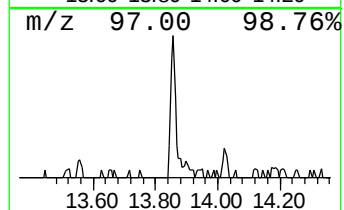
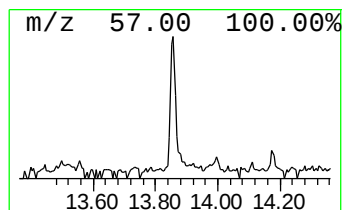
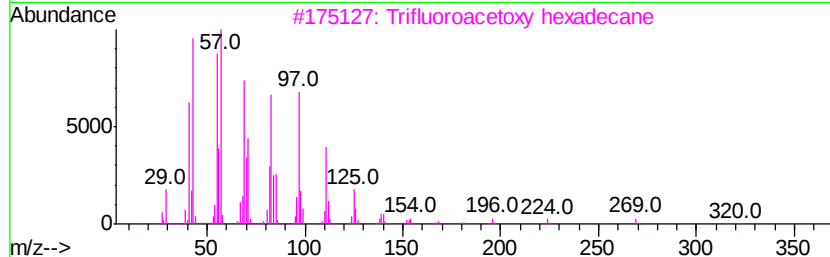
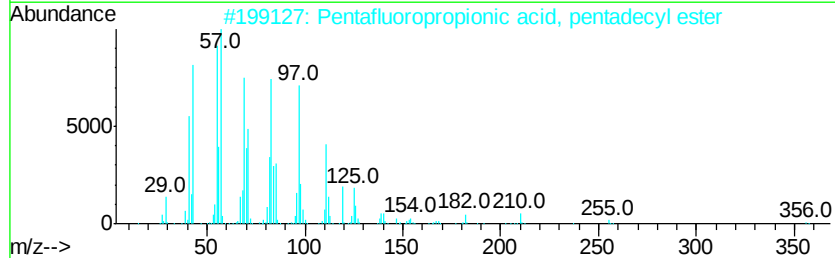
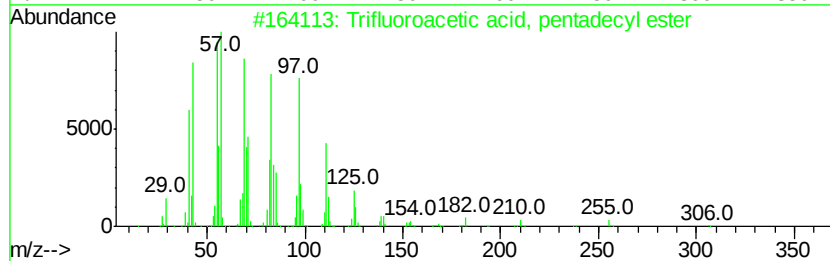
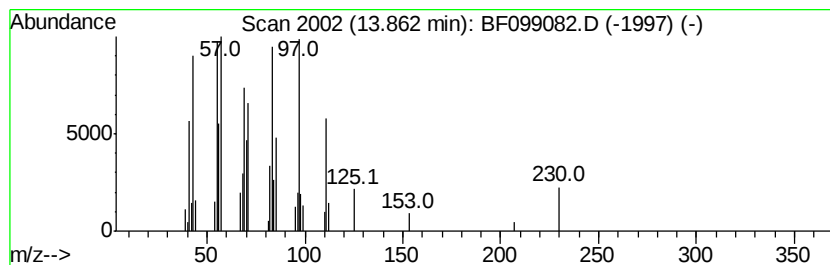
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Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.22 ng	93586	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.15	3.2	ng	120871	1	6.86	760596	20.0
2-Pentanone, 4-hy...	5.09	12.8	ng	486948	1	6.86	760596	20.0
unknown6.63	6.63	61.1	ng	2324580	1	6.86	760596	20.0
Trifluoroacetic a...	13.86	2.2	ng	93586	5	14.03	844275	20.0