

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102517\
 Data File : BF099845.D
 Acq On : 26 Oct 2017 7:03
 Operator : SJ/JU
 Sample : I6057-04
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101917-TIDO-F-U-S

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-BF102317.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	4.993	492	494	510	rBV	71134	96864	4.72%	0.753%
2	5.410	562	565	589	rBV	409088	524174	25.57%	4.077%
3	6.434	736	739	755	rBV	271670	363389	17.72%	2.826%
4	6.563	758	761	772	rVB	1111039	988461	48.21%	7.687%
5	6.792	797	800	810	rBV	440682	368922	17.99%	2.869%
6	6.945	823	826	844	rBV	1550053	1399893	68.28%	10.887%
7	7.363	893	897	921	rBV	1161894	1026790	50.08%	7.986%
8	8.075	1015	1018	1036	rBV	604451	513816	25.06%	3.996%
9	8.639	1111	1114	1121	rBV	66617	61976	3.02%	0.482%
10	9.157	1198	1202	1205	rBV	2322731	2050257	100.00%	15.945%
11	9.551	1267	1269	1278	rBB	60886	54109	2.64%	0.421%
12	9.833	1311	1317	1328	rVB	628793	585048	28.54%	4.550%
13	10.510	1429	1432	1436	rBV	35473	26438	1.29%	0.206%
14	10.551	1436	1439	1449	rVB	353557	264601	12.91%	2.058%
15	10.633	1449	1453	1464	rBV	762436	715803	34.91%	5.567%
16	10.886	1493	1496	1500	rBV	41752	33095	1.61%	0.257%
17	10.933	1500	1504	1507	rBV	135614	143632	7.01%	1.117%
18	10.980	1507	1512	1514	rVB	25354	36550	1.78%	0.284%
19	11.327	1568	1571	1580	rBV	633512	562464	27.43%	4.374%
20	12.916	1837	1841	1845	rBV	2011015	1961268	95.66%	15.253%
21	13.798	1988	1991	1997	rBV	20663	28099	1.37%	0.219%
22	13.980	2019	2022	2030	rVB	558531	524978	25.61%	4.083%
23	15.451	2264	2272	2280	rBV	360858	475327	23.18%	3.697%
24	15.851	2333	2340	2347	rBV3	14003	28168	1.37%	0.219%
25	16.339	2419	2423	2430	rVB4	13557	24037	1.17%	0.187%

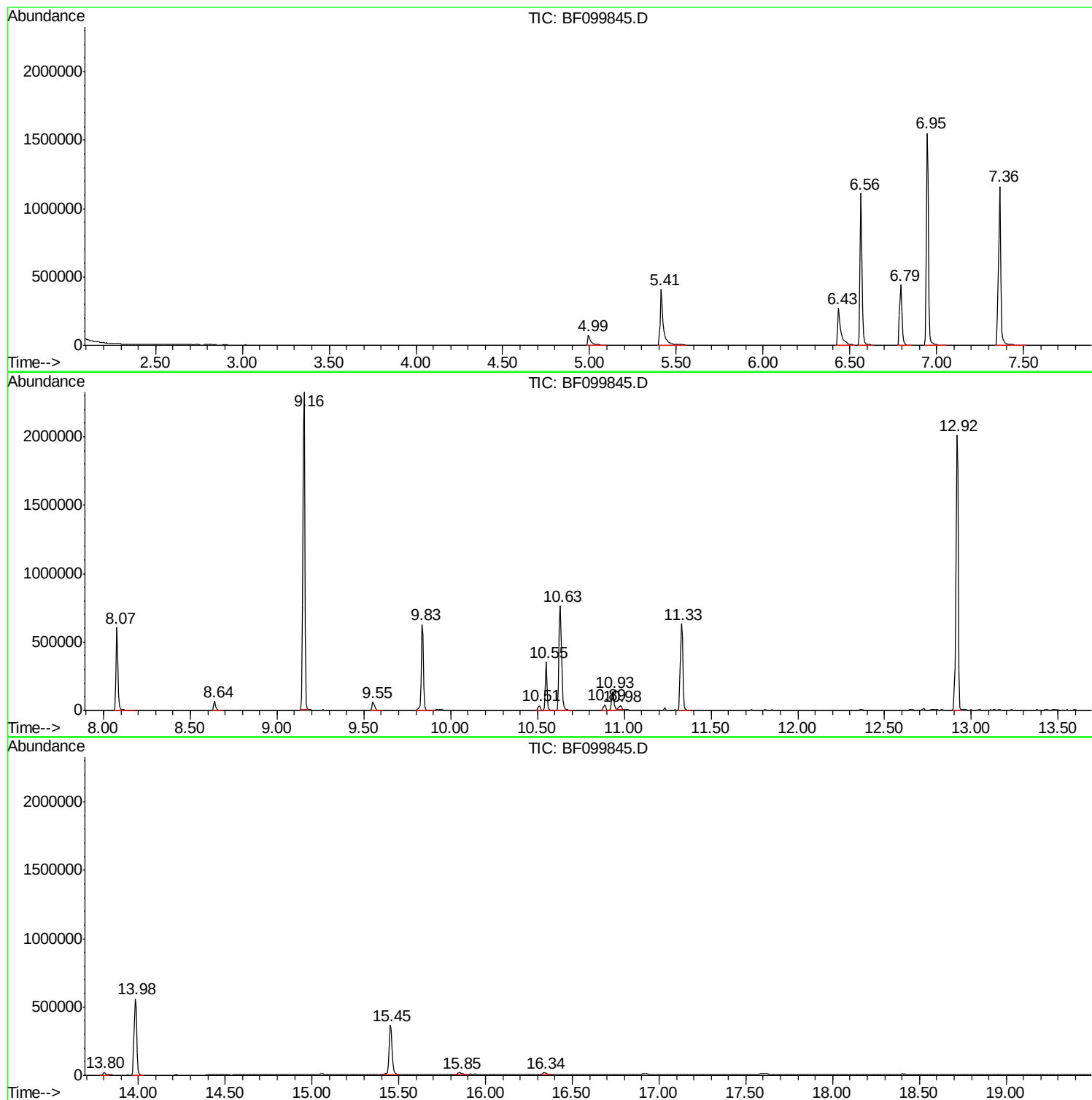
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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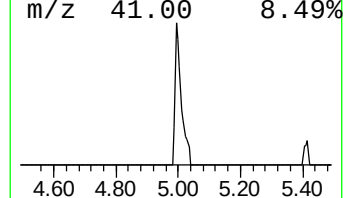
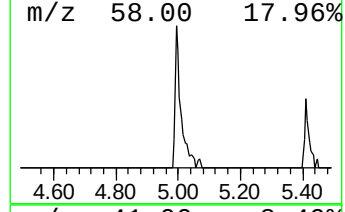
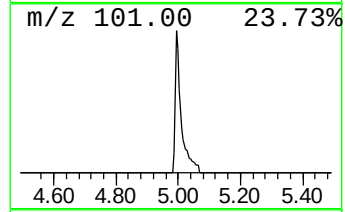
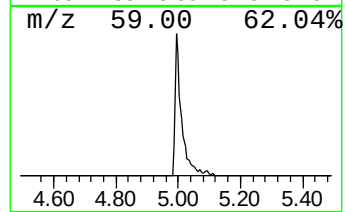
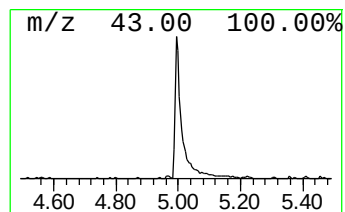
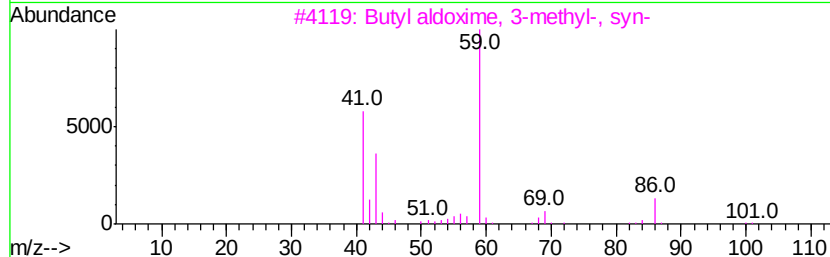
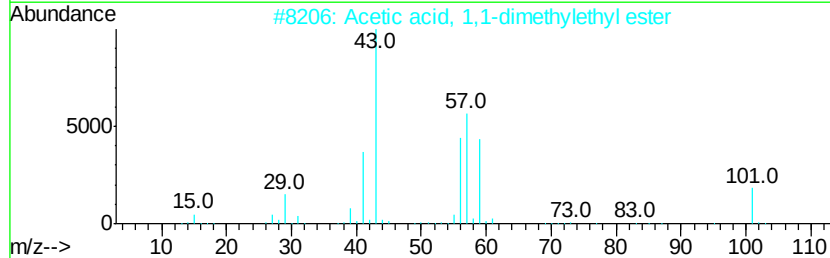
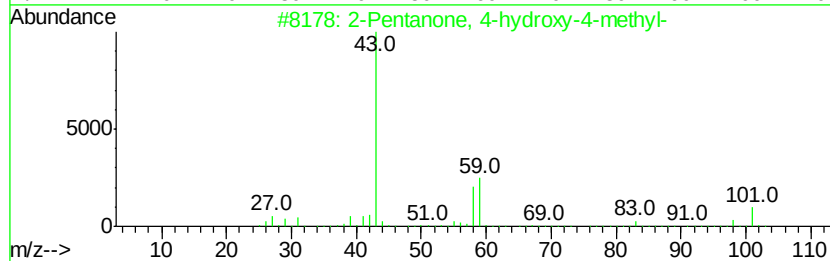
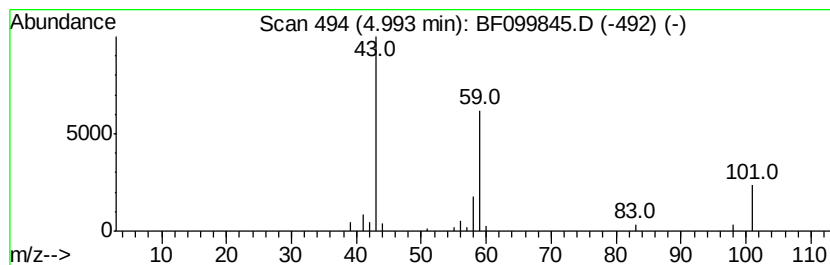
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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.
4.99	5.25 ng	96864	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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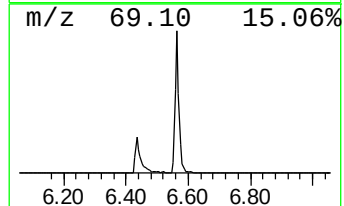
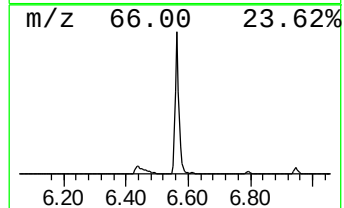
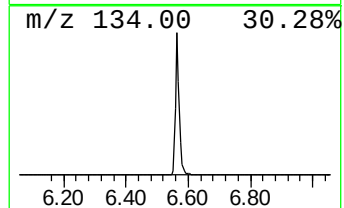
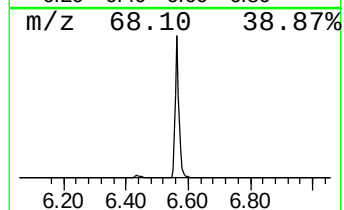
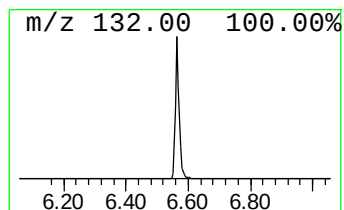
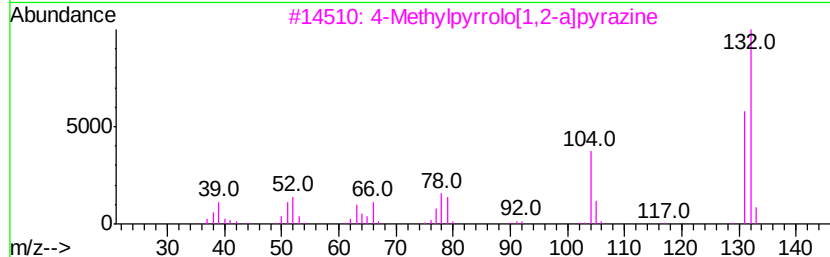
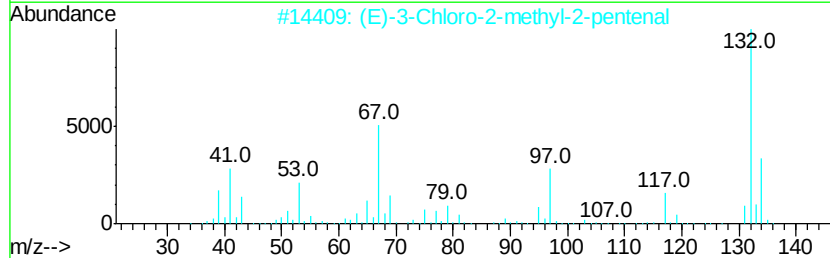
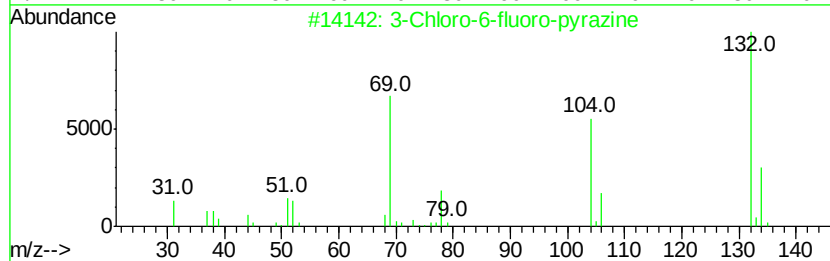
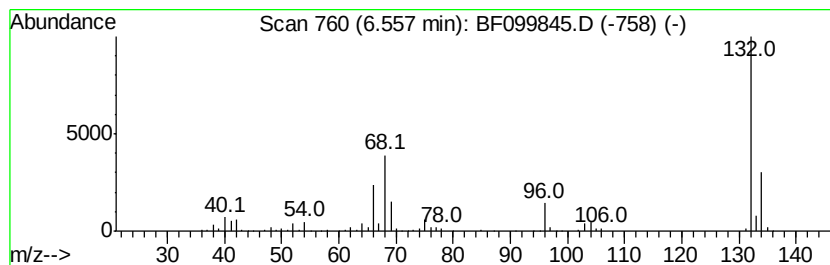
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	53.59 ng	988461	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	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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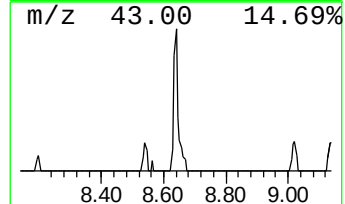
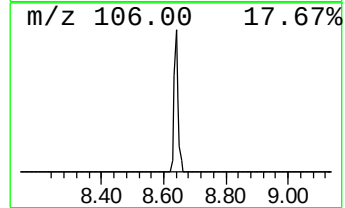
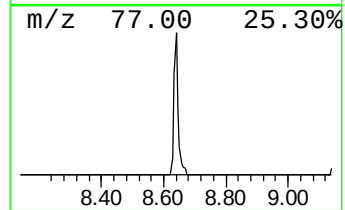
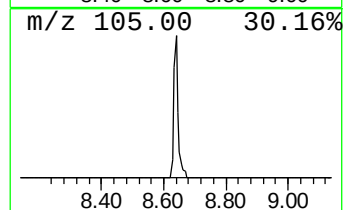
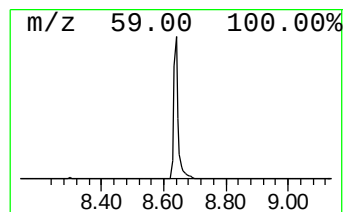
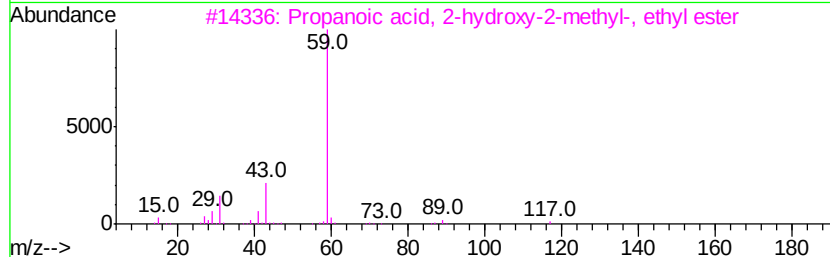
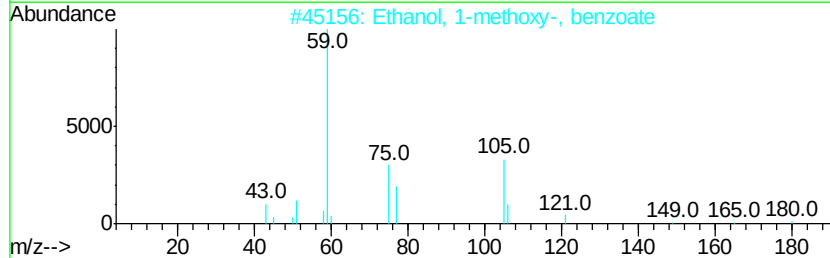
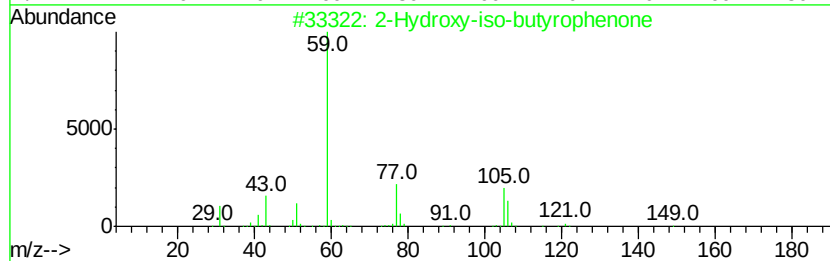
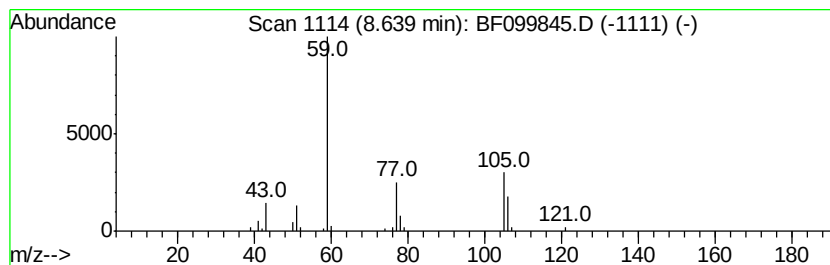
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TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.64	2.41 ng	61976	Napthalene-d8	8.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3		Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
4		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5		Acetamide	59	C2H5NO	000060-35-5	5



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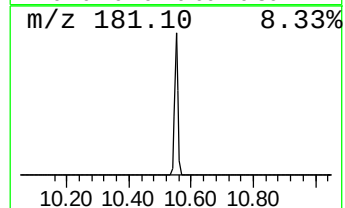
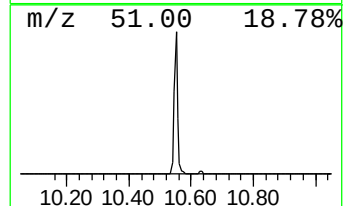
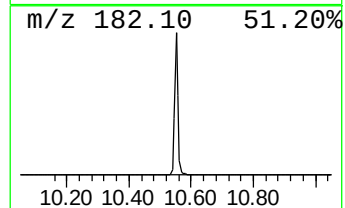
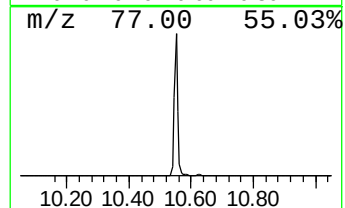
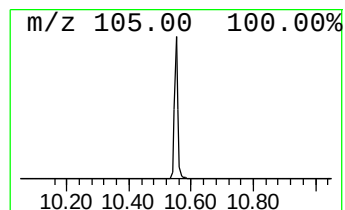
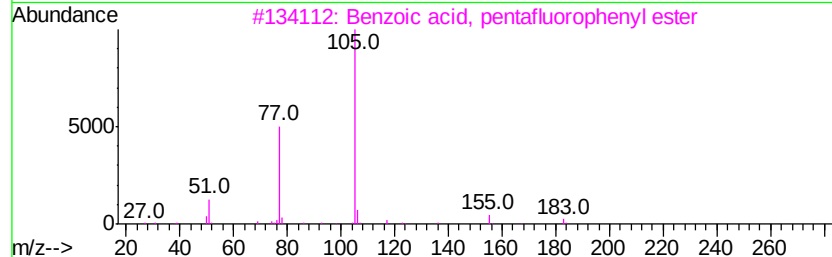
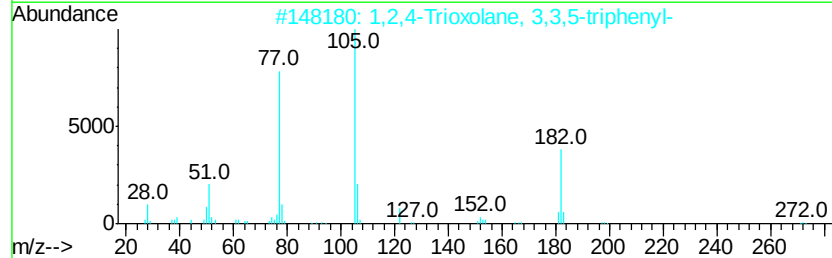
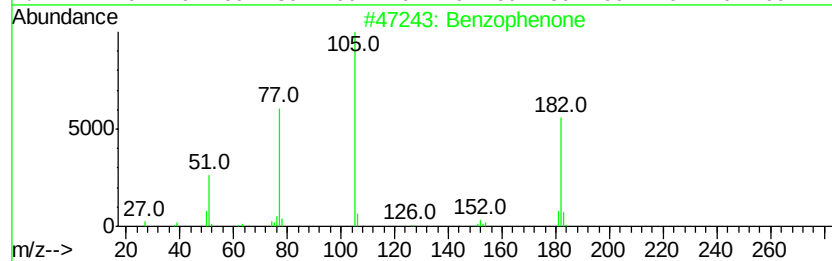
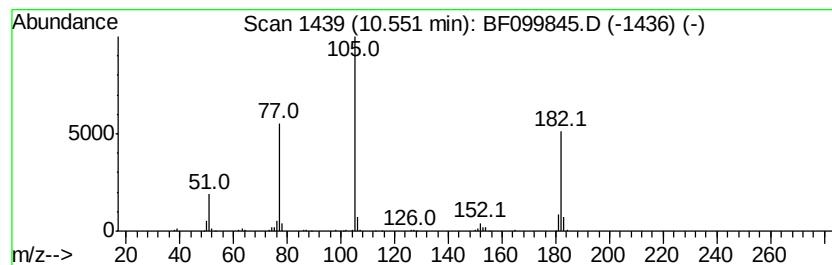
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	9.05 ng	264601	Acenaphthene-d10	9.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		1,2,4-Trioxolane, 3,3,5-triphenyl-	304 C20H16O3	023246-12-0 64
3		Benzoic acid, pentafluorophenyl ...	288 C13H5F5O2	1000360-67-9 47
4		Phenyl 4-pyridyl ketone	183 C12H9NO	014548-46-0 47
5		Vinyl benzoate	148 C9H8O2	000769-78-8 43



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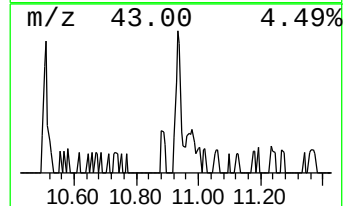
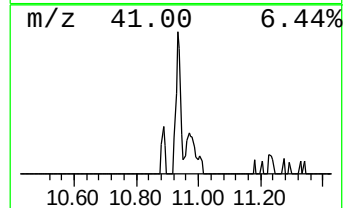
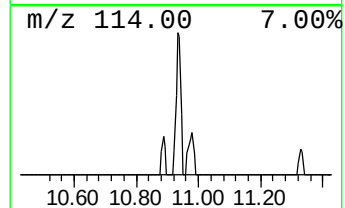
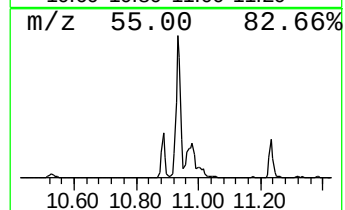
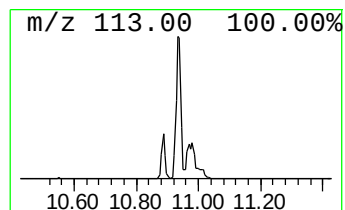
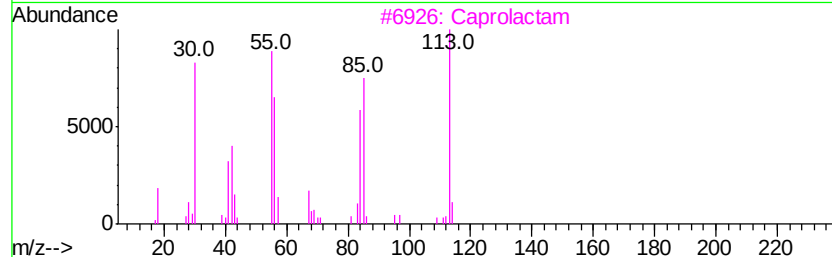
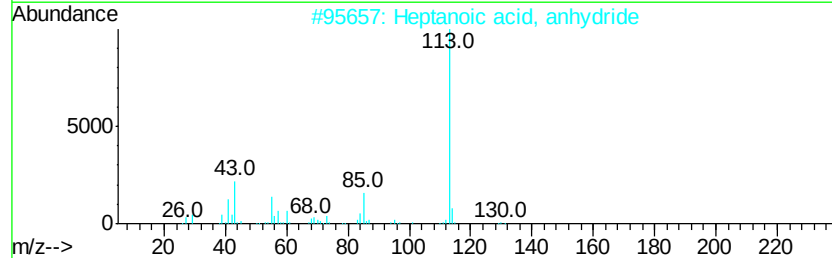
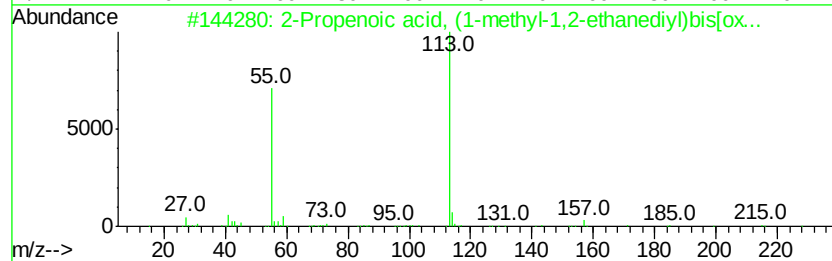
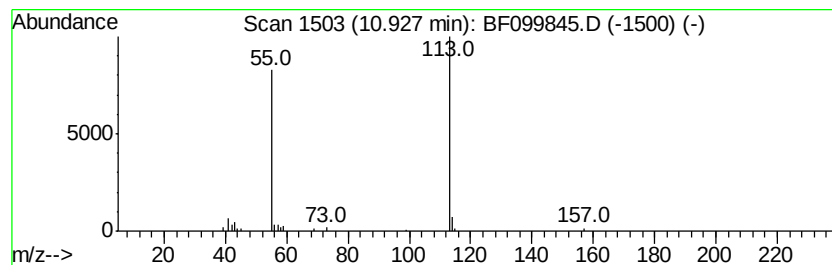
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 2-Propenoic acid, (1-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	5.11 ng	143632	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenoic acid, (1-methyl-1,2-...	300	C15H24O6	042978-66-5	78
2		Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	38
3		Caprolactam	113	C6H11NO	000105-60-2	9
4		Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	9
5		Ethosuximide	141	C7H11NO2	000077-67-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	5.3	ng	96864	1	6.79	368922	20.0
unknown6.56	6.56	53.6	ng	988461	1	6.79	368922	20.0
2-Hydroxy-iso-but...	8.64	2.4	ng	61976	2	8.07	513816	20.0
Benzophenone	10.55	9.1	ng	264601	3	9.83	585048	20.0
2-Propenoic acid,...	10.93	5.1	ng	143632	4	11.33	562464	20.0