

Data Path : Z:\HPCHEM1\BNA G\DATA\BG102817\
 Data File : BG030533.D
 Acq On : 28 Oct 2017 18:42
 Operator : SJ/JU
 Sample : I6029-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-108-2(80-82)

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_G\METHODS\8270-BG101617.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	5.241	326	332	346	rVB	203955	318304	6.88%	1.270%
2	5.717	406	413	425	rBV	1153571	1861936	40.23%	7.430%
3	7.321	678	686	700	rBV	1129493	2052526	44.35%	8.190%
4	7.697	742	750	765	rBV	1139252	1956672	42.28%	7.808%
5	8.167	823	830	843	rVB	220055	374600	8.09%	1.495%
6	8.490	878	885	895	rVB	830294	1429357	30.89%	5.704%
7	9.330	1018	1028	1037	rBV	650352	1171783	25.32%	4.676%
8	10.981	1302	1309	1319	rVB	309383	538072	11.63%	2.147%
9	12.274	1523	1529	1538	rBV	39099	62980	1.36%	0.251%
10	13.408	1715	1722	1733	rBV	1911555	2998316	64.79%	11.964%
11	14.224	1854	1861	1867	rBV	224277	322363	6.97%	1.286%
12	14.782	1949	1956	1967	rVB2	513291	831236	17.96%	3.317%
13	16.128	2178	2185	2191	rBV	172385	248018	5.36%	0.990%
14	16.263	2201	2208	2219	rBV	1681062	2634334	56.93%	10.512%
15	17.520	2415	2422	2432	rBV2	735755	1099061	23.75%	4.386%
16	20.111	2857	2863	2869	rBV	3681383	4627702	100.00%	18.466%
17	21.792	3142	3149	3159	rVB2	760836	1278060	27.62%	5.100%
18	25.106	3701	3713	3730	rVB2	434719	1255389	27.13%	5.009%

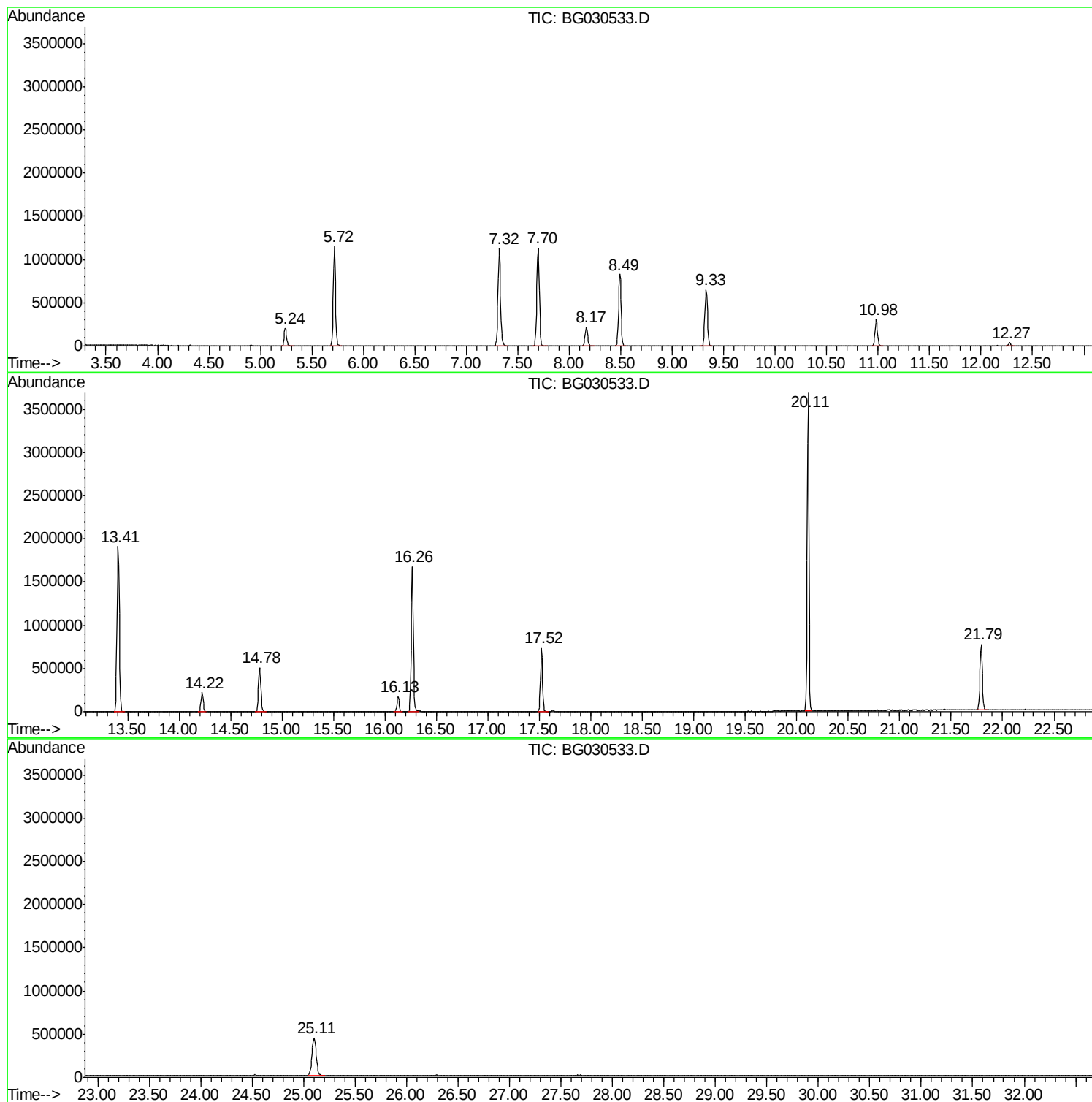
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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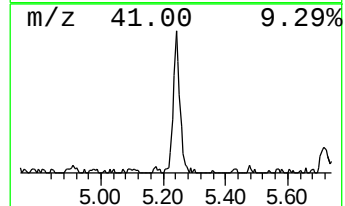
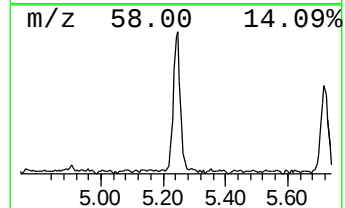
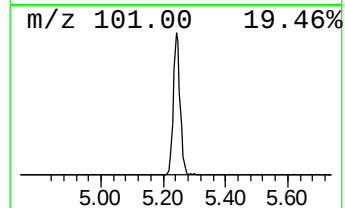
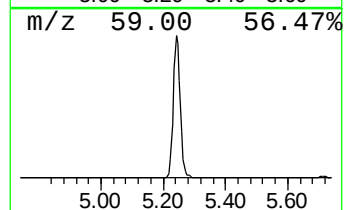
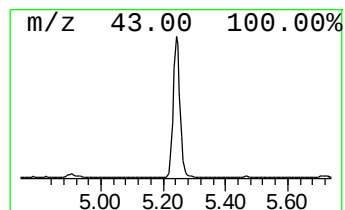
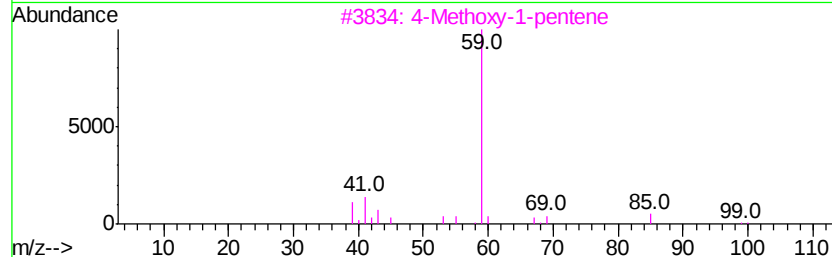
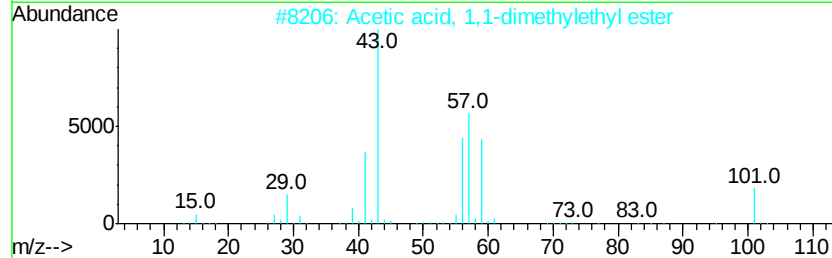
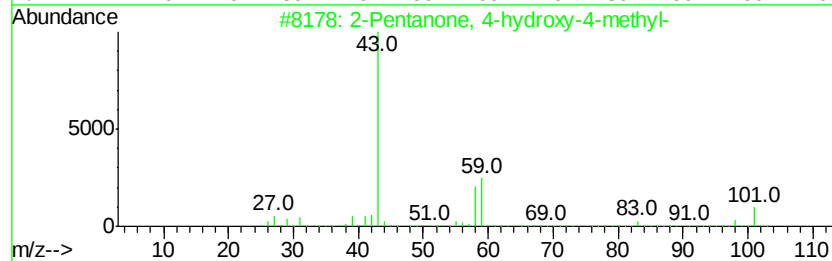
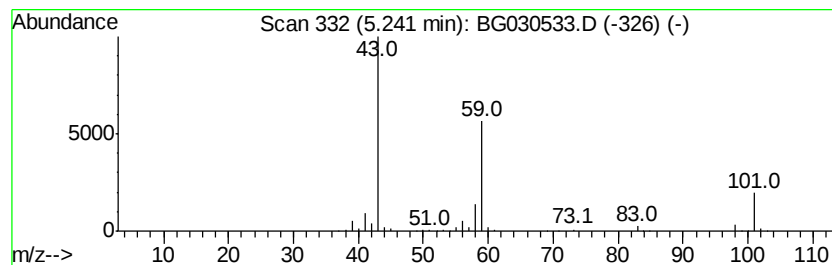
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	16.99 ng	318304	1,4-Dichlorobenzene-d4	8.17

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3			4-Methoxy-1-pentene	100	C6H12O	098386-09-5	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	12



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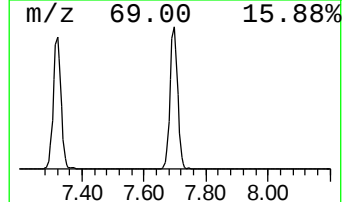
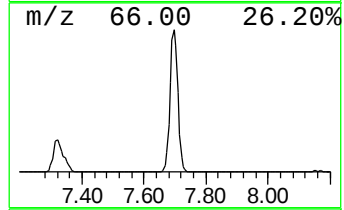
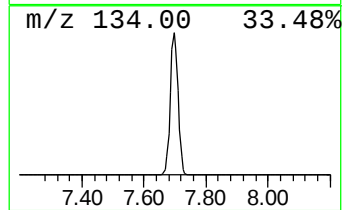
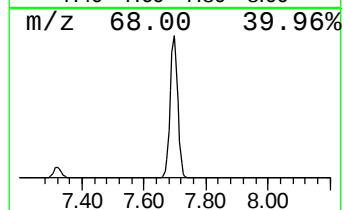
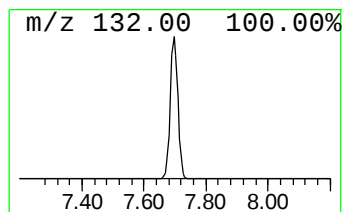
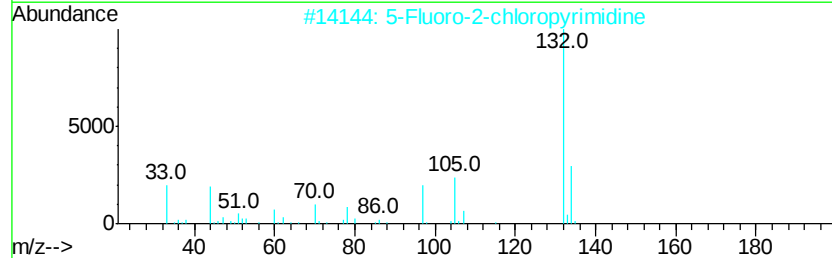
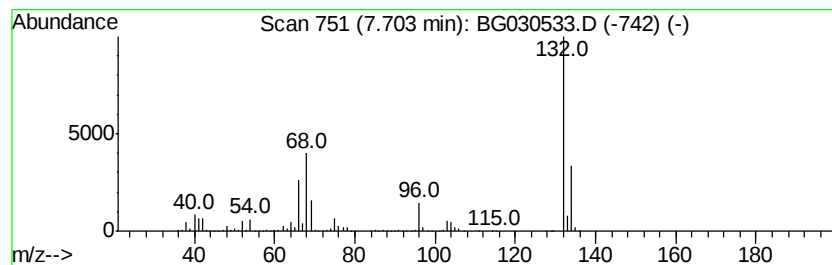
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	104.47 ng	1956670	1,4-Dichlorobenzene-d4	8.17

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	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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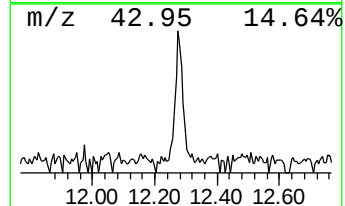
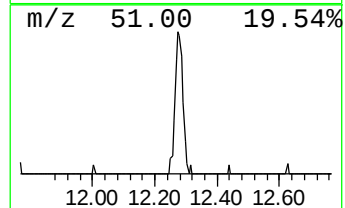
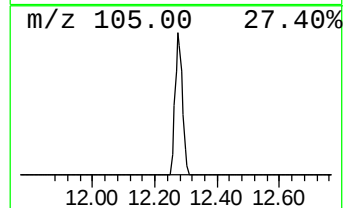
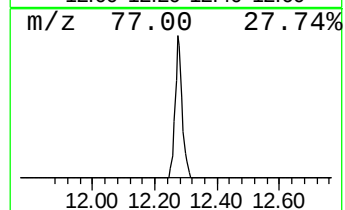
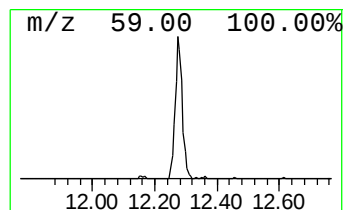
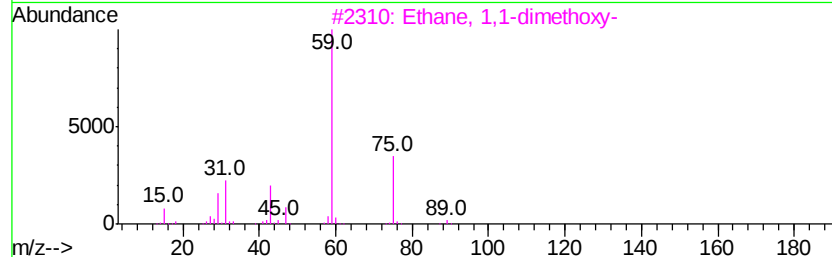
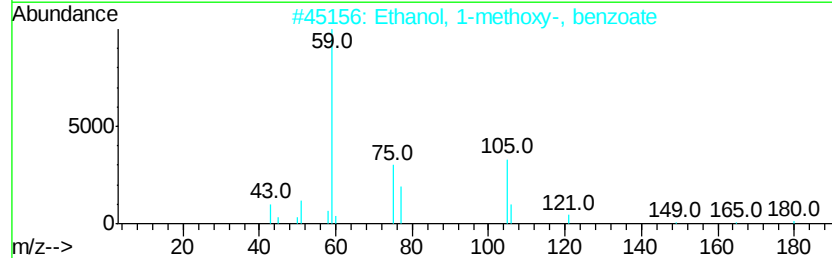
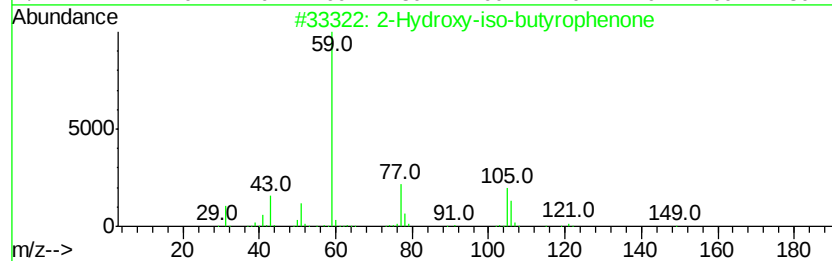
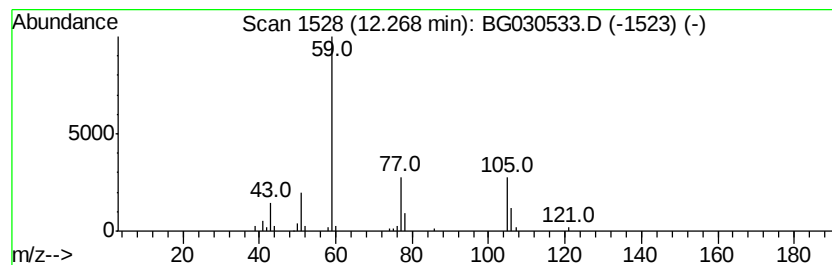
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	2.34 ng	62980	Napthalene-d8	10.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Hydroxy-iso-butyrophenone	164 C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-, benzoate	180 C10H12O3	051835-44-0	50
3	Ethane, 1,1-dimethoxy-	90 C4H10O2	000534-15-6	23
4	Guanidine	59 CH5N3	000113-00-8	9
5	1-Propanol, 2-methoxy-	90 C4H10O2	001589-47-5	9



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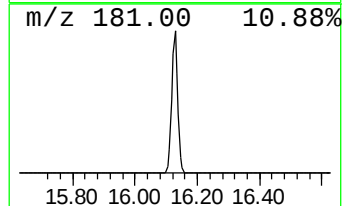
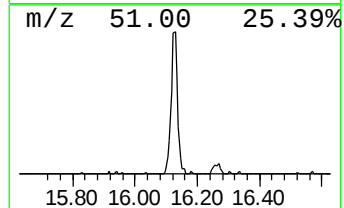
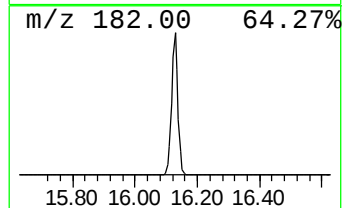
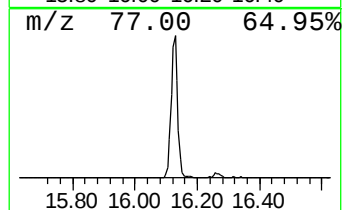
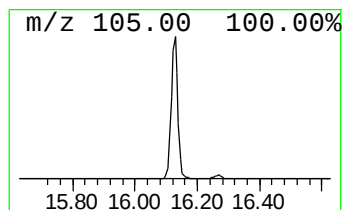
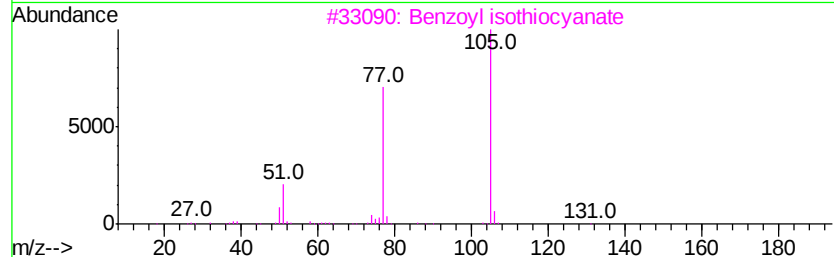
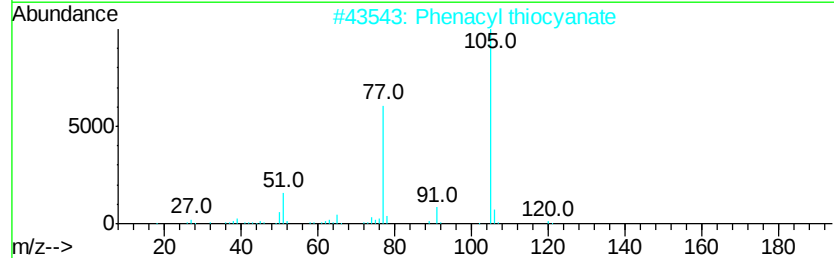
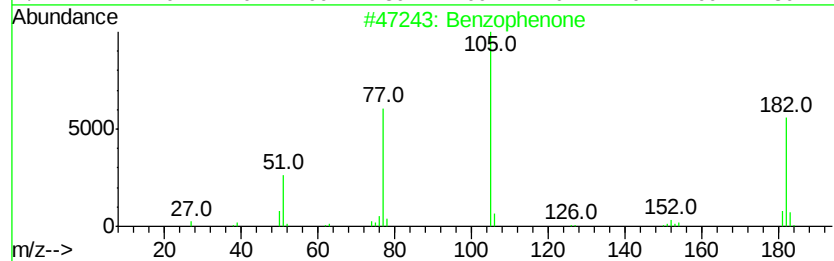
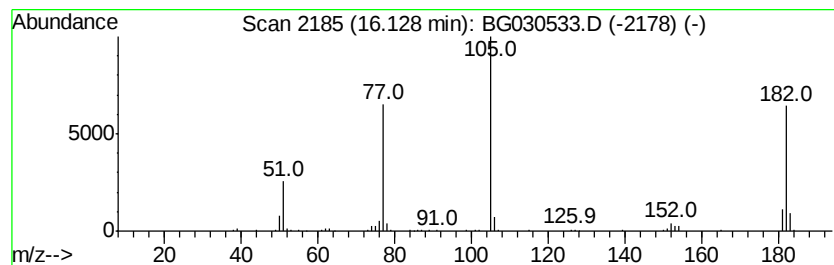
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	5.97 ng	248018	Acenaphthene-d10	14.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	43
3		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
4		Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43
5		1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	17.0	ng	318304	1	8.17	374600	20.0
unknown7.70	7.70	104.5	ng	1956670	1	8.17	374600	20.0
2-Hydroxy-iso-but...	12.27	2.3	ng	62980	2	10.98	538072	20.0
Benzophenone	16.13	6.0	ng	248018	3	14.78	831236	20.0