

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060917\
 Data File : BG027358.D
 Acq On : 9 Jun 2017 22:05
 Operator : SJ/MA
 Sample : I3560-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FILTER-MEDIA

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_G\METHODS\8270-BG060517.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	5.128	238	245	254	rBV	38831	65145	1.34%	0.301%
2	5.704	336	343	353	rBV	262731	419882	8.66%	1.942%
3	6.144	410	418	428	rBV	956829	1631852	33.64%	7.546%
4	6.256	432	437	445	rVB	38792	66026	1.36%	0.305%
5	7.690	668	681	691	rBV	872214	1622828	33.45%	7.505%
6	8.089	740	749	761	rBV	950860	1754641	36.17%	8.114%
7	8.553	820	828	836	rBV	152069	275745	5.68%	1.275%
8	8.882	875	884	894	rVB	656223	1202052	24.78%	5.559%
9	9.717	1017	1026	1038	rBV	564012	1082361	22.31%	5.005%
10	11.373	1300	1308	1324	rBV	225718	430537	8.88%	1.991%
11	13.759	1706	1714	1723	rBV	1627376	2635076	54.32%	12.186%
12	15.134	1939	1948	1958	rVB2	341262	593218	12.23%	2.743%
13	16.620	2193	2201	2214	rBV	1401762	2268433	46.76%	10.490%
14	17.883	2410	2416	2424	rBV	487109	792069	16.33%	3.663%
15	19.981	2769	2773	2781	rBV2	30335	52488	1.08%	0.243%
16	20.463	2848	2855	2864	rBV	3551774	4850809	100.00%	22.432%
17	22.267	3155	3162	3171	rVB	522733	996501	20.54%	4.608%
18	25.950	3778	3789	3808	rVB3	257538	884389	18.23%	4.090%

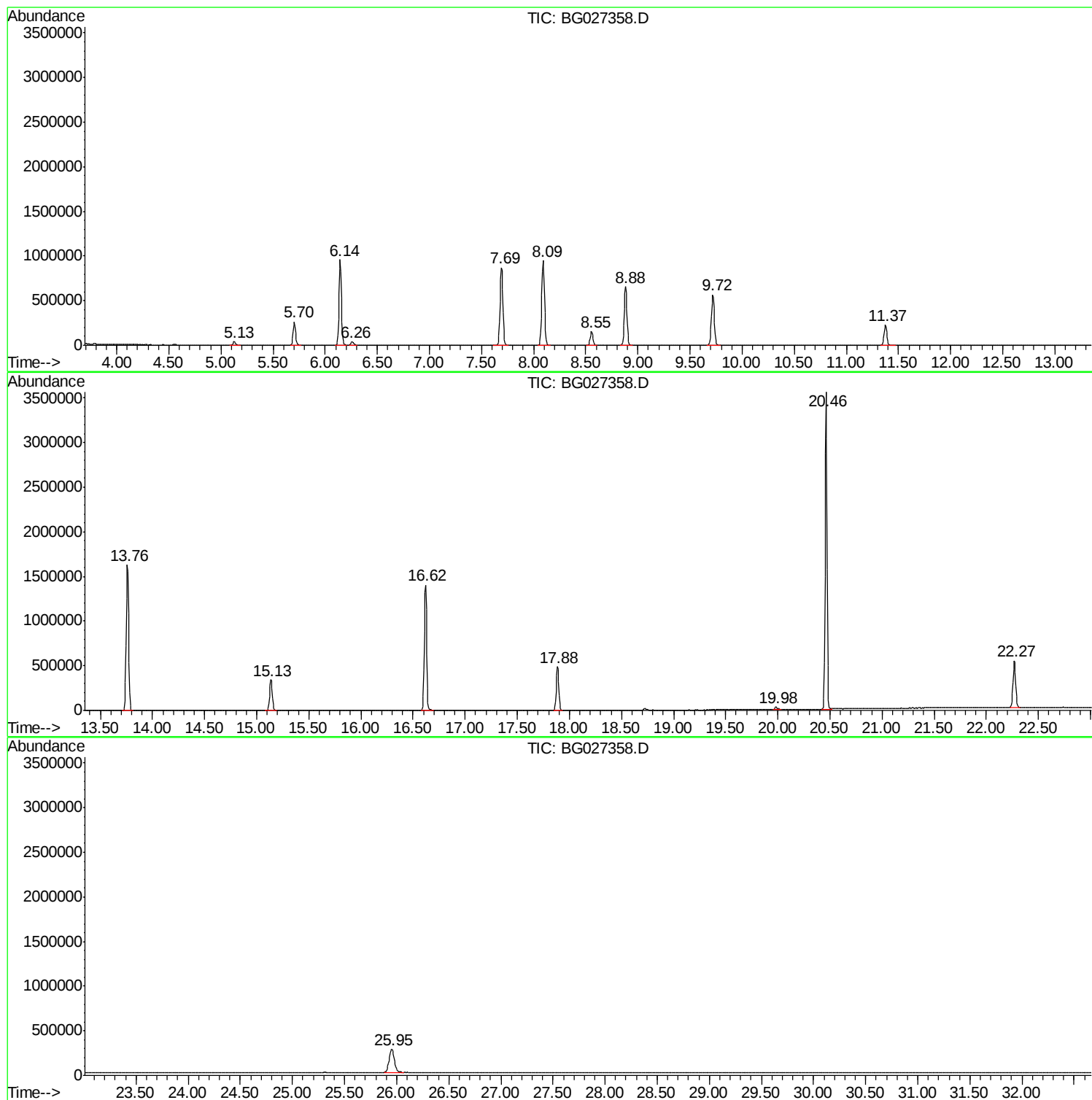
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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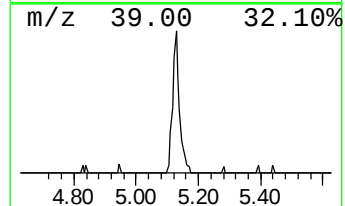
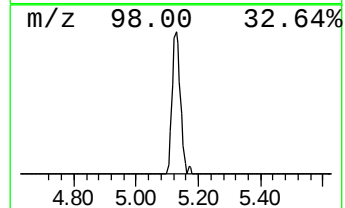
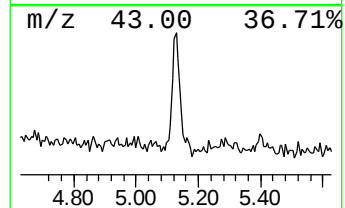
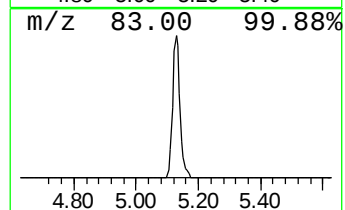
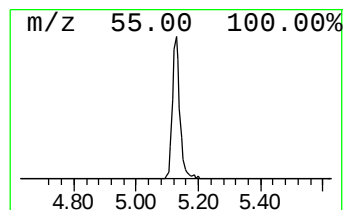
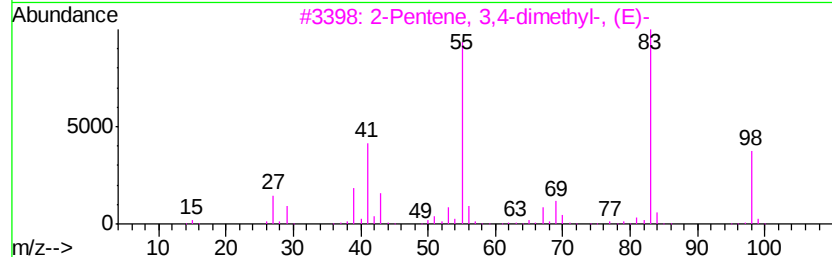
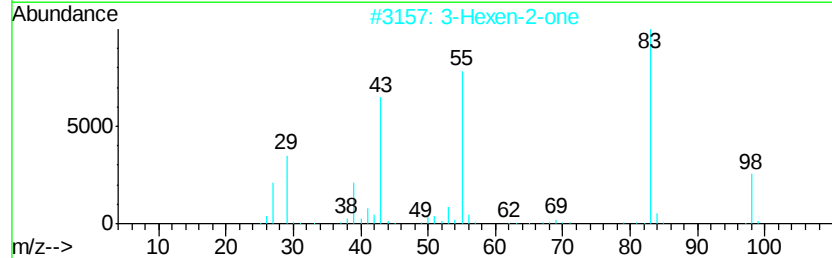
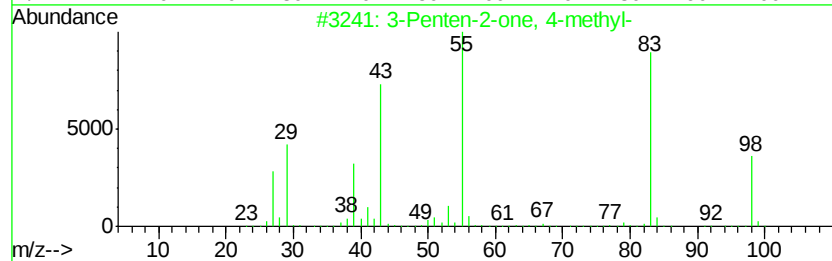
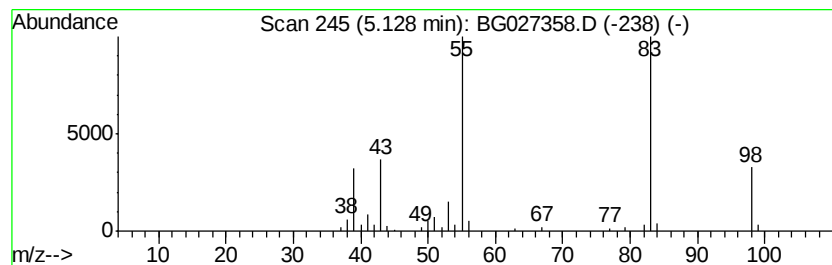
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.73 ng	65145	1,4-Dichlorobenzene-d4	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72



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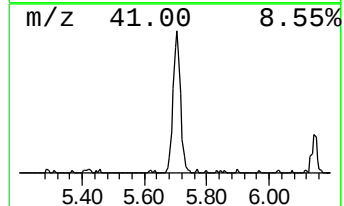
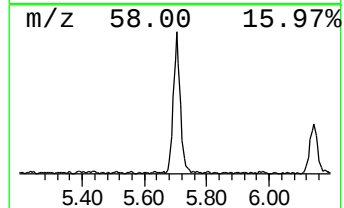
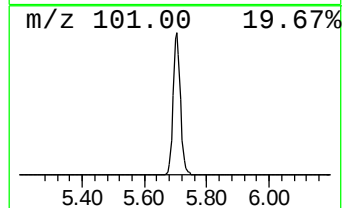
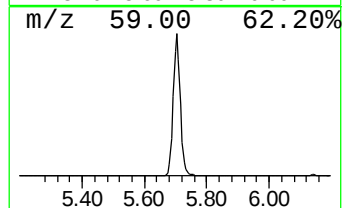
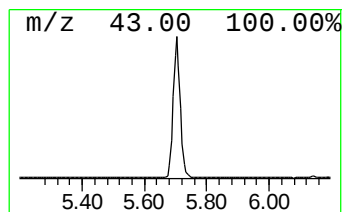
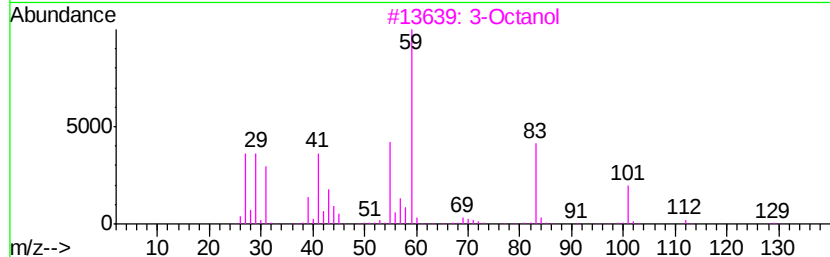
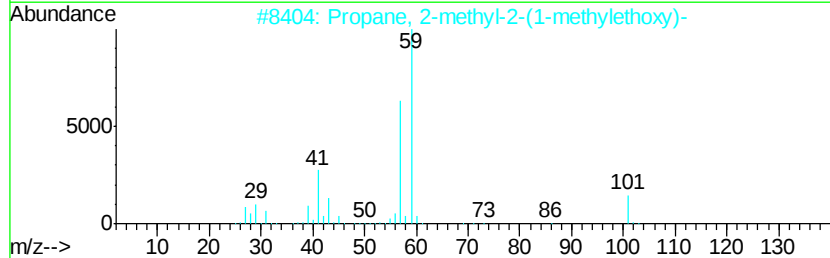
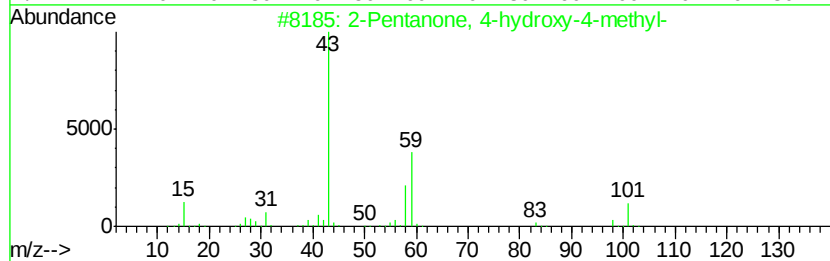
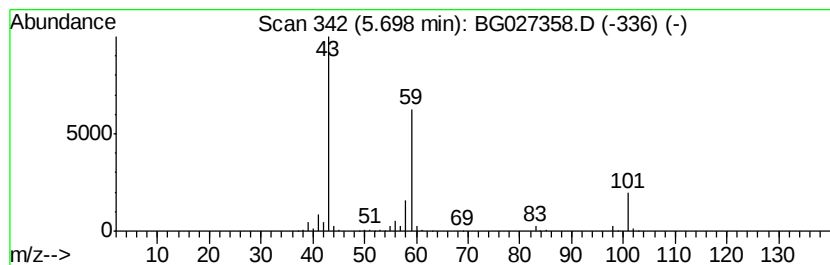
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	30.45 ng	419882	1,4-Dichlorobenzene-d4	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Octanol	130	C8H18O	000589-98-0	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		Acetone	58	C3H6O	000067-64-1	9



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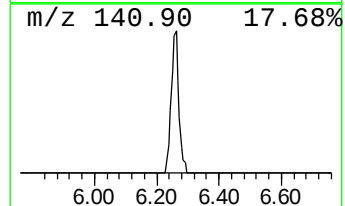
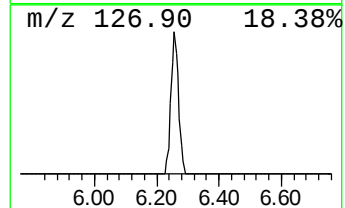
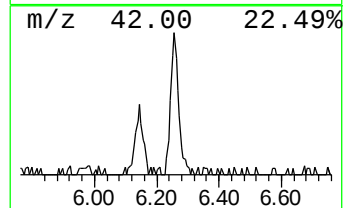
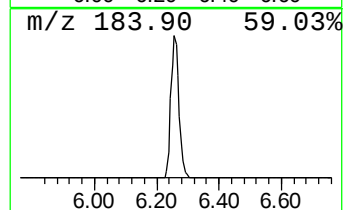
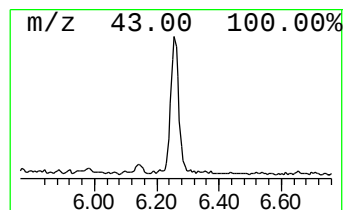
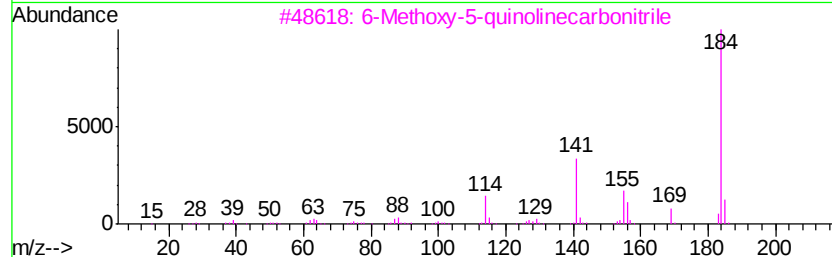
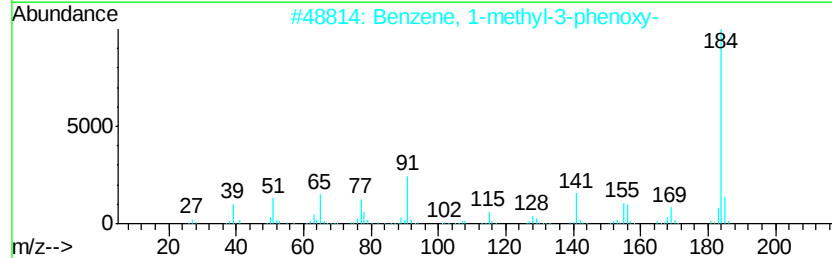
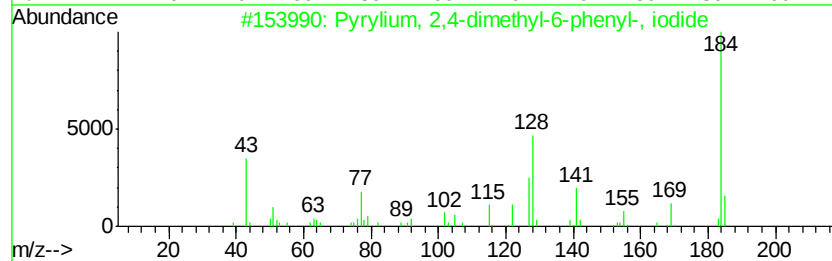
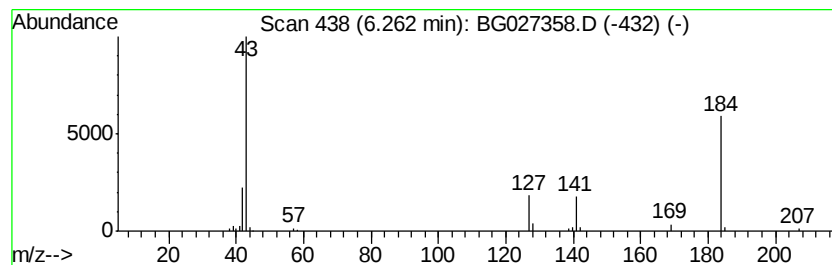
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Peak Number 3 unknown6.26 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	4.79 ng	66026	1,4-Dichlorobenzene-d4	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrylium, 2,4-dimethyl-6-phenyl-...	312	C13H13IO	032339-28-9	25
2		Benzene, 1-methyl-3-phenoxy-	184	C13H12O	003586-14-9	12
3		6-Methoxy-5-quinolinecarbonitrile	184	C11H8N2O	087299-97-6	9
4		4,6(1H)-Pyrimidinedione, 3,4,5,6...	127	C4H5N3O2	004425-67-6	9
5		Cis-1-(2-furyl)-2-phenylcyclopro...	184	C13H12O	039763-89-8	9



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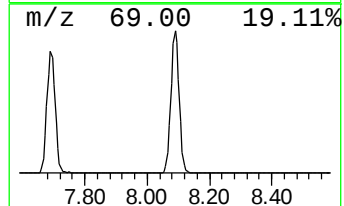
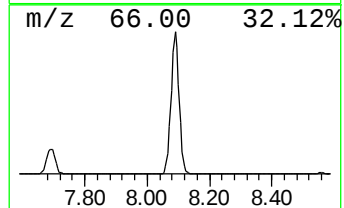
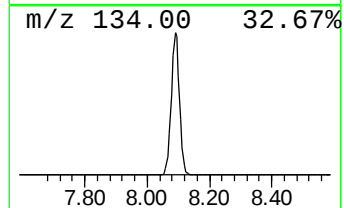
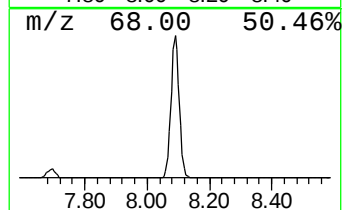
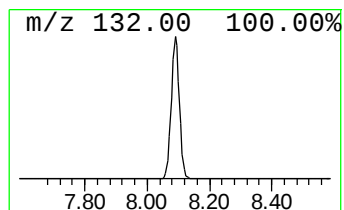
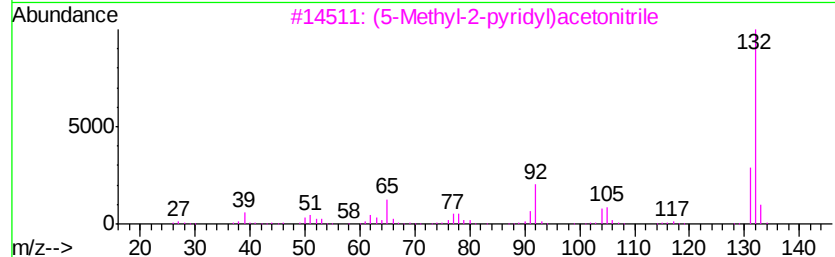
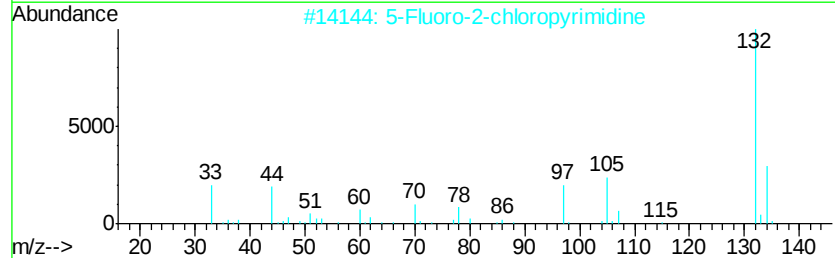
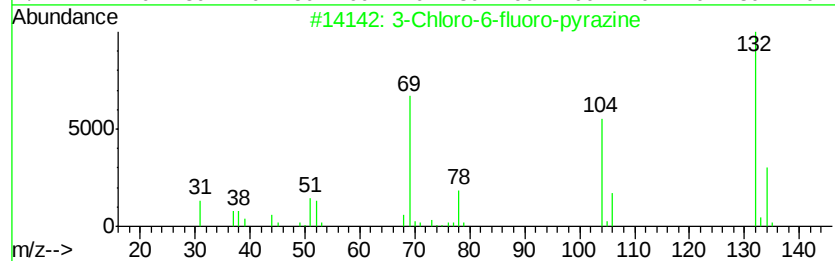
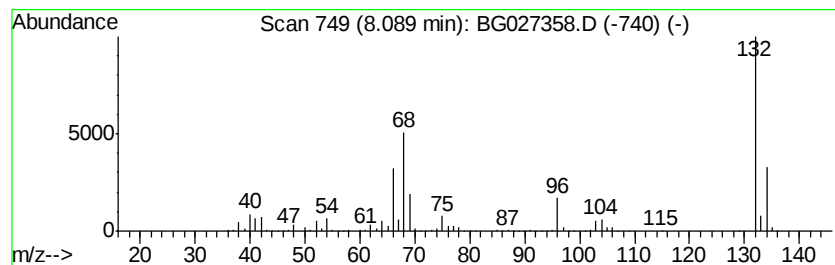
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Peak Number 4 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	127.27 ng	1754640	1,4-Dichlorobenzene-d4	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	5.13	4.7	ng	65145	1	8.55	275745	20.0
2-Pentanone, 4-hy...	5.70	30.4	ng	419882	1	8.55	275745	20.0
unknown6.26	6.26	4.8	ng	66026	1	8.55	275745	20.0
unknown8.09	8.09	127.3	ng	1754640	1	8.55	275745	20.0