

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032818\
 Data File : BG033392.D
 Acq On : 28 Mar 2018 18:58
 Operator : SJ/JU
 Sample : J2072-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0AB3

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-BG031918.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	3.482	25	33	43	rBV	128208	271839	8.19%	1.466%
2	3.570	43	48	58	rVB	97115	148442	4.47%	0.800%
3	5.779	418	424	431	rBV2	35185	62333	1.88%	0.336%
4	6.314	507	515	529	rBV	684587	1265056	38.14%	6.822%
5	8.000	792	802	827	rBV	606786	1318338	39.74%	7.109%
6	8.388	860	868	880	rBV	765907	1483277	44.71%	7.999%
7	8.864	942	949	967	rBV2	135867	284130	8.57%	1.532%
8	9.199	997	1006	1020	rBV	528465	1016960	30.66%	5.484%
9	10.068	1144	1154	1169	rBV	419471	906042	27.31%	4.886%
10	11.748	1432	1440	1450	rBV	215788	409845	12.35%	2.210%
11	14.110	1835	1842	1854	rBV	1403072	2324226	70.06%	12.534%
12	15.485	2069	2076	2088	rBV2	386210	679787	20.49%	3.666%
13	15.750	2114	2121	2129	rBV2	51732	108751	3.28%	0.586%
14	16.167	2186	2192	2203	rBV	67155	167900	5.06%	0.905%
15	16.960	2320	2327	2340	rBV	1231701	1973520	59.49%	10.642%
16	18.217	2534	2541	2551	rVB2	481114	802782	24.20%	4.329%
17	18.823	2640	2644	2649	rVB6	51679	83214	2.51%	0.449%
18	20.250	2884	2887	2890	rBV4	22409	34746	1.05%	0.187%
19	20.738	2964	2970	2977	rVB	2425251	3317299	100.00%	17.889%
20	22.559	3274	3280	3292	rVB	483725	940395	28.35%	5.071%
21	26.337	3912	3923	3939	rVB2	281884	945021	28.49%	5.096%

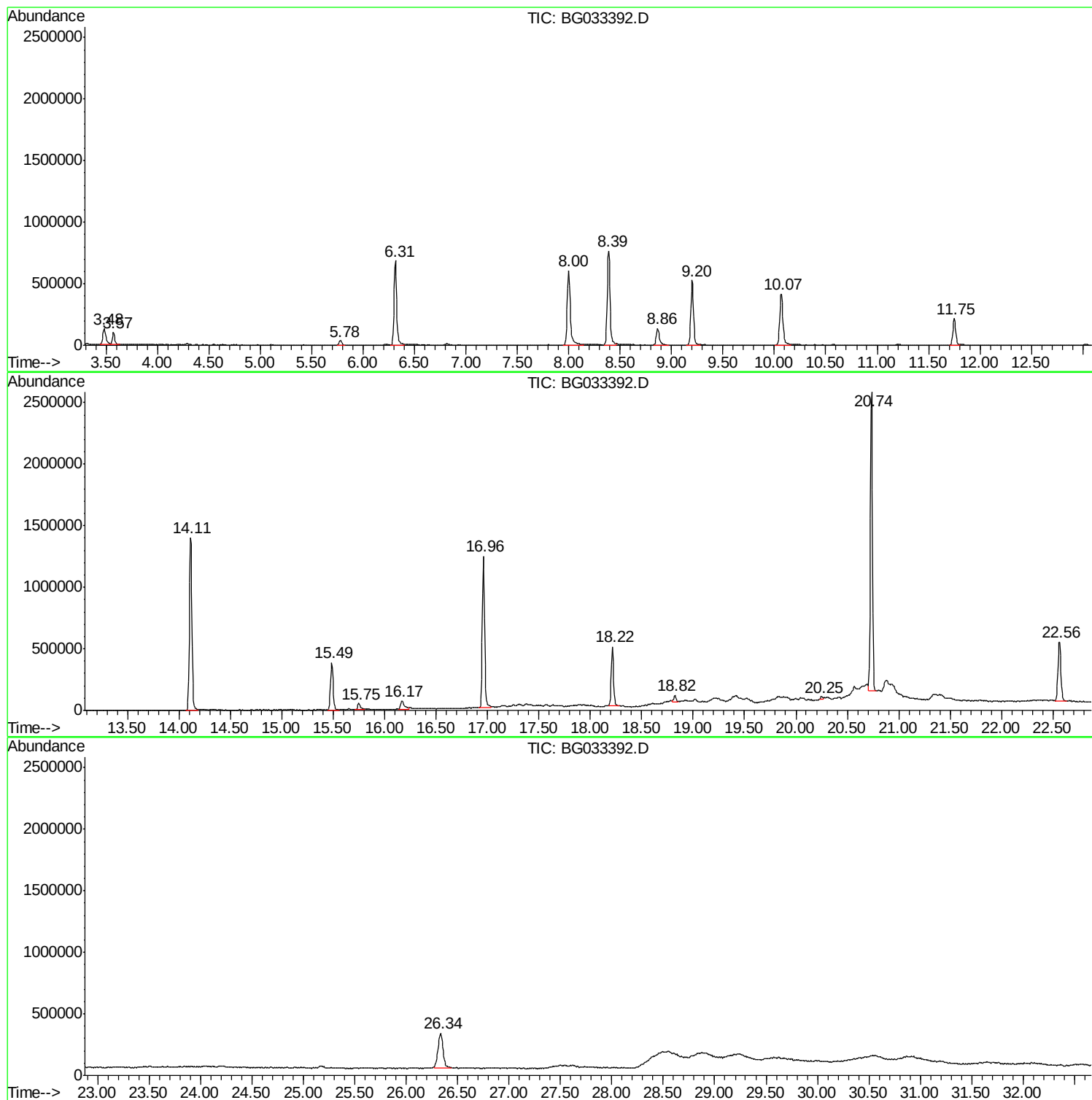
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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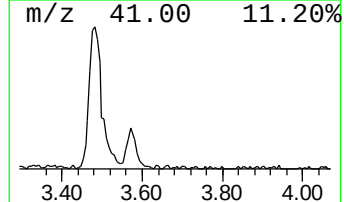
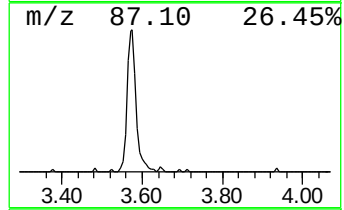
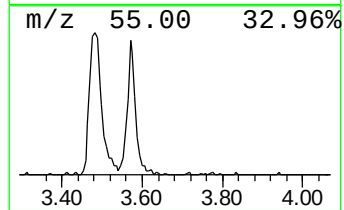
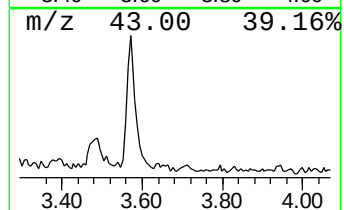
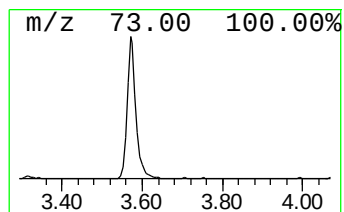
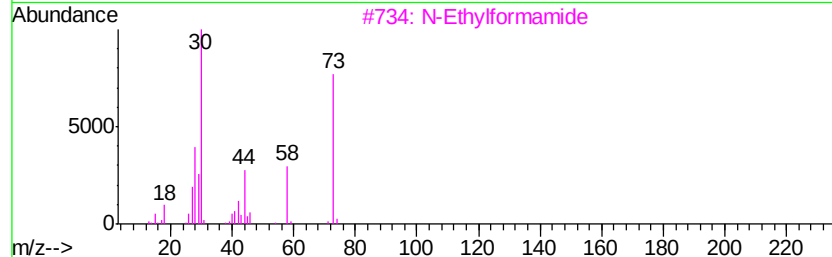
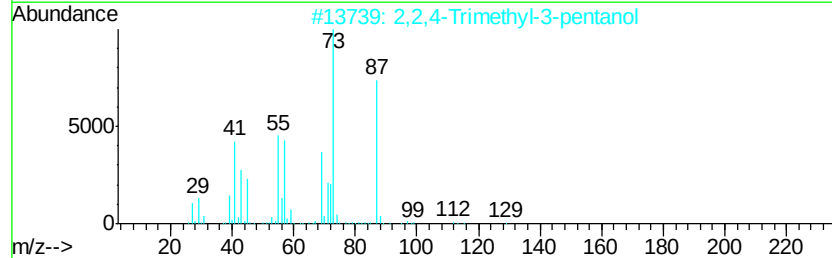
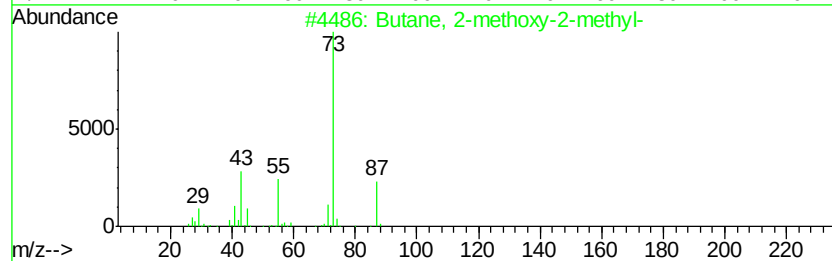
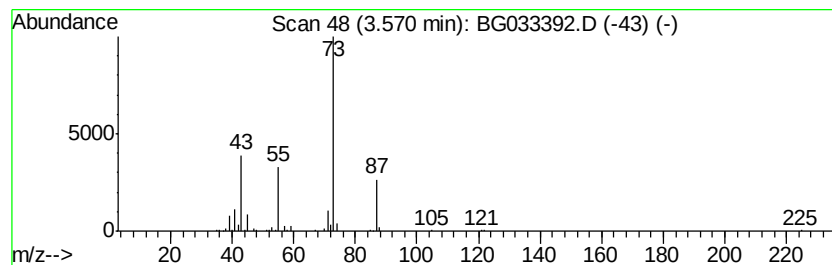
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	10.45 ng	148442	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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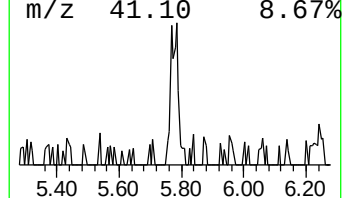
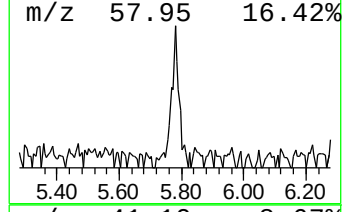
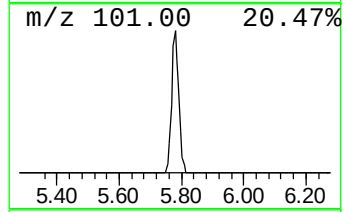
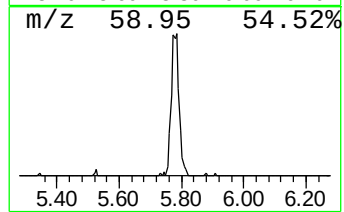
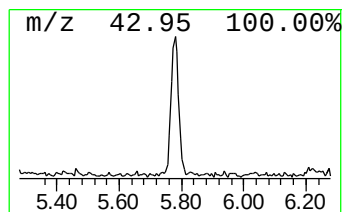
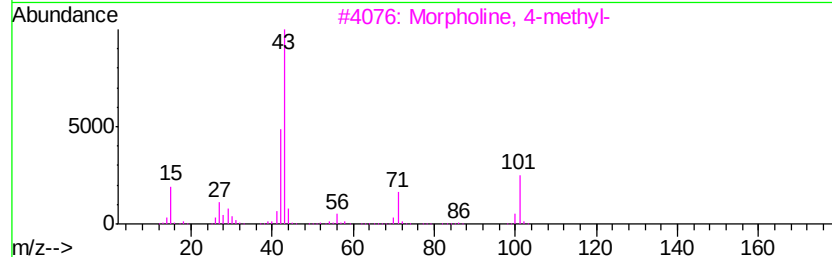
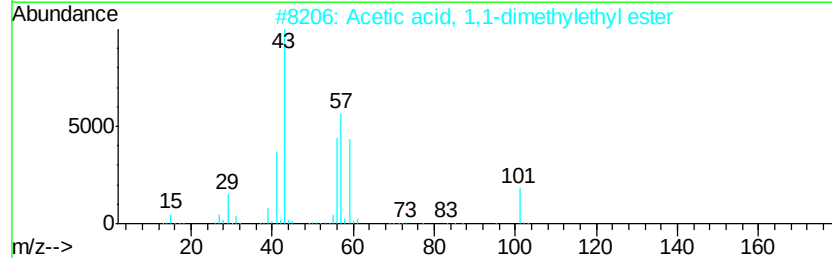
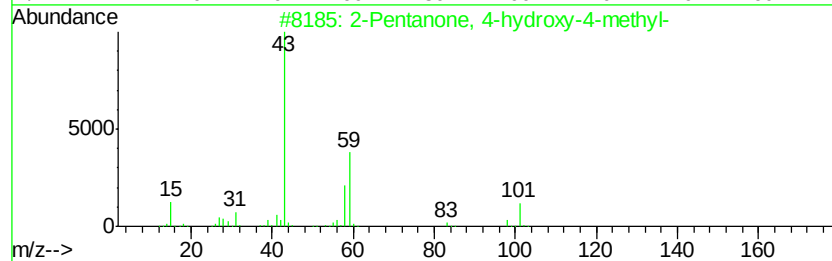
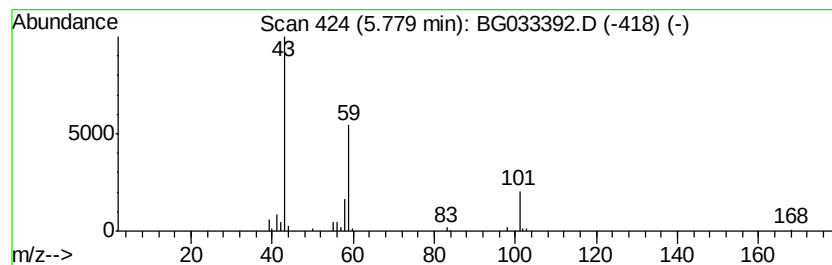
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	4.39 ng	62333	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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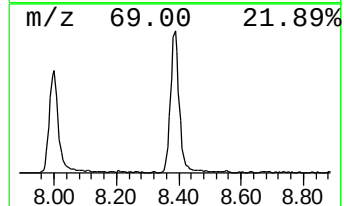
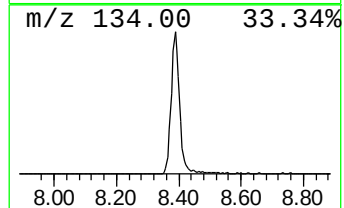
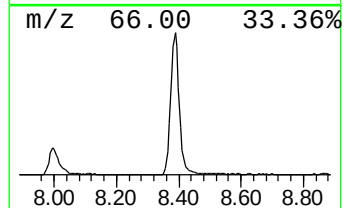
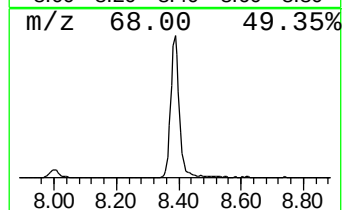
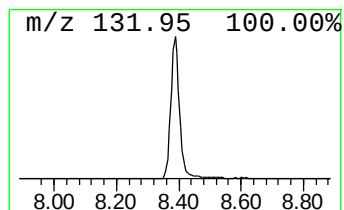
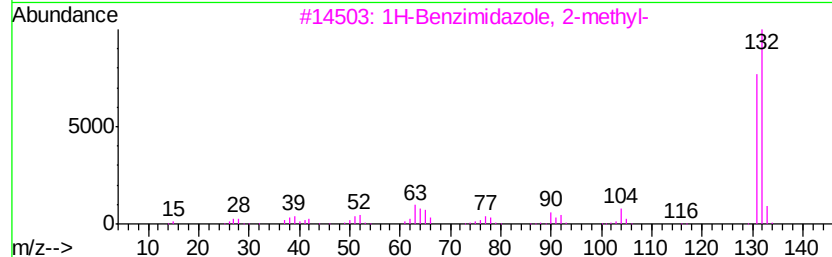
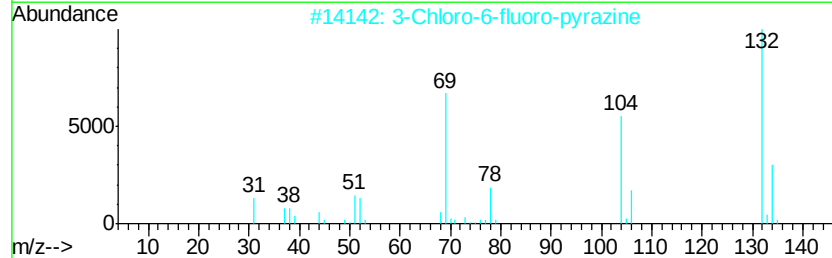
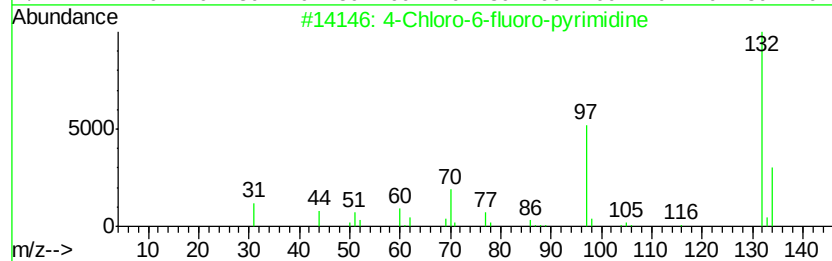
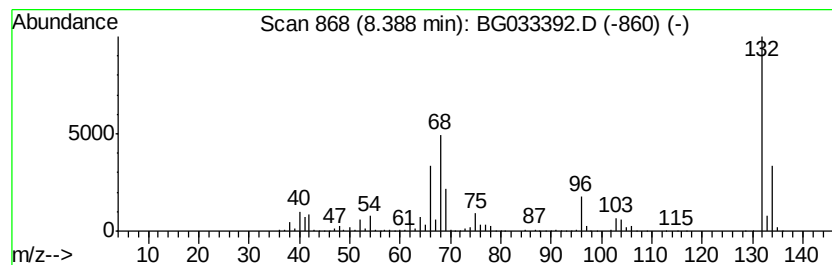
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Peak Number 4 unknown8.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.39	104.41 ng	1483280	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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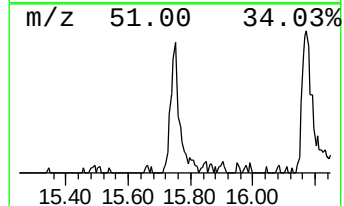
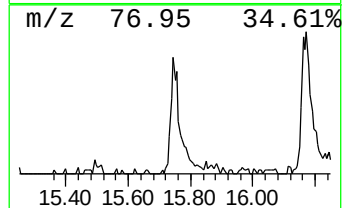
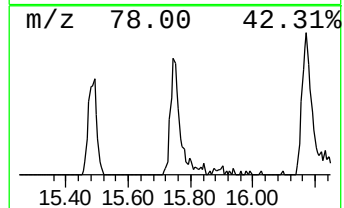
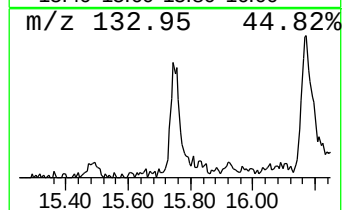
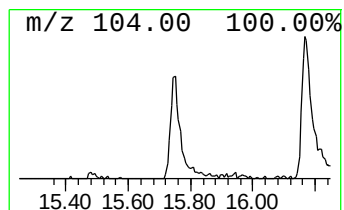
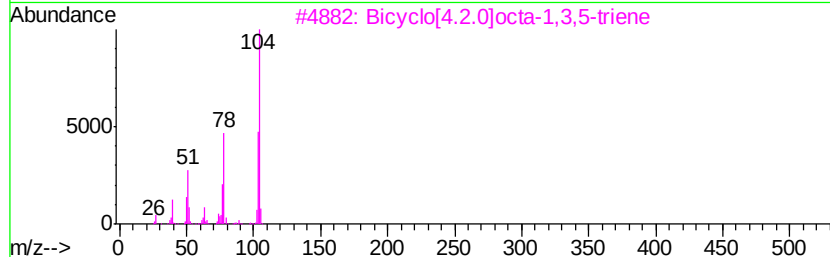
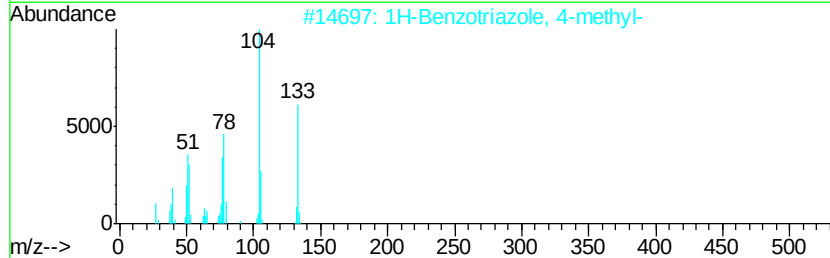
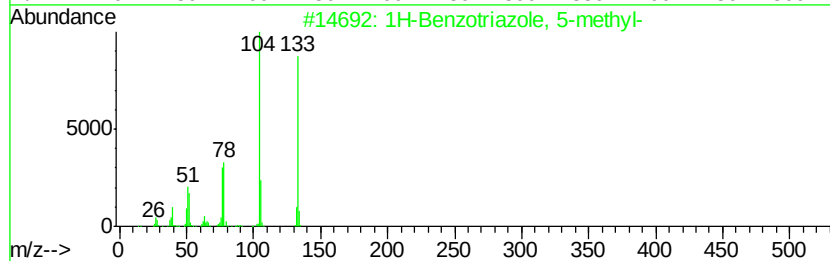
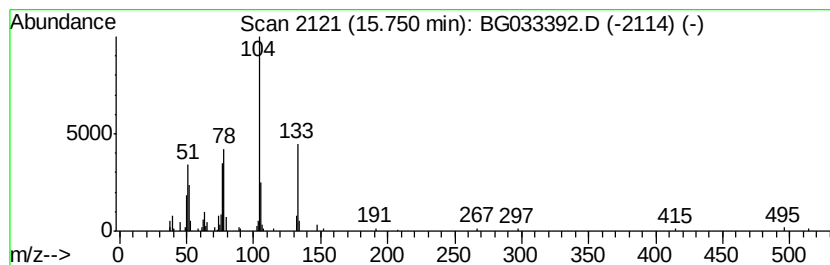
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Peak Number 6 1H-Benzotriazole, 5-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.75	3.20 ng	108751	Acenaphthene-d10	15.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	94
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	81
3	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	45
4	Styrene	104	C8H8	000100-42-5	45
5	4-Ethylbenzoic acid, 2-phenyleth...	254	C17H18O2	1000293-50-1	43



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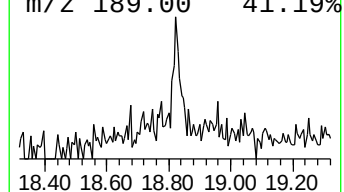
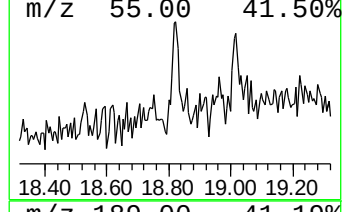
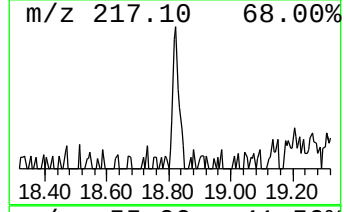
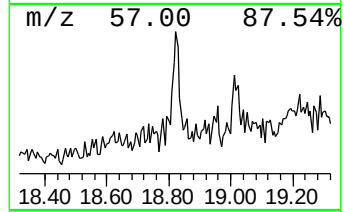
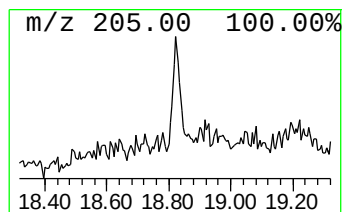
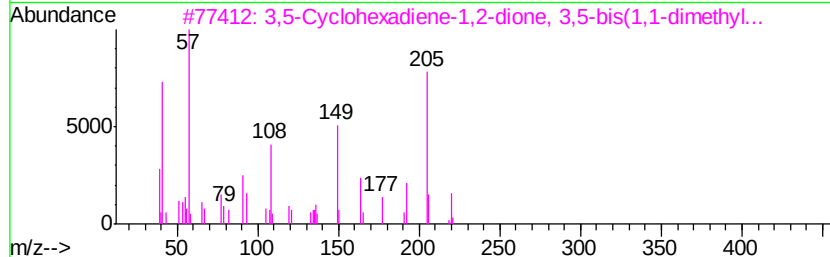
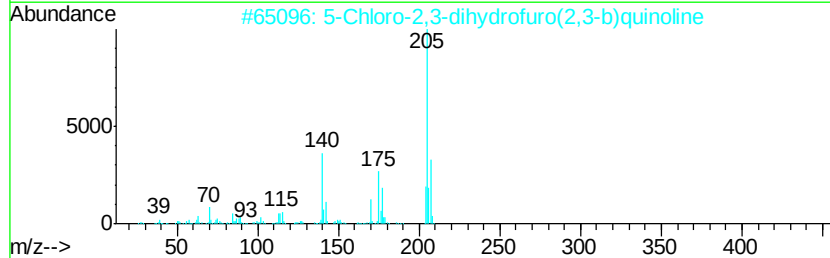
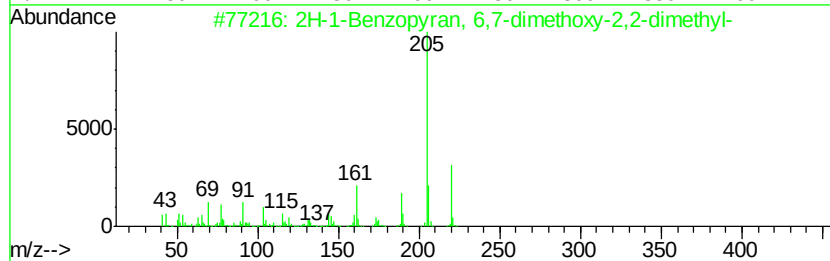
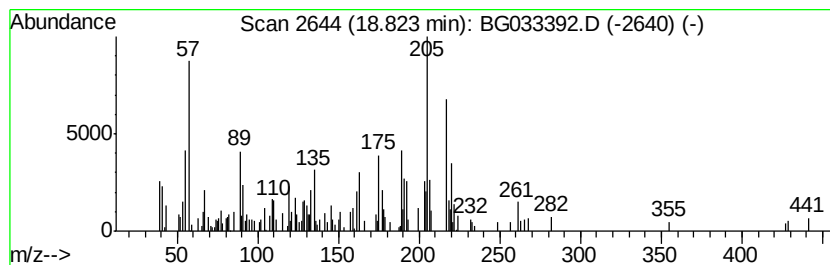
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Peak Number 8 unknown18.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.82	2.07 ng	83214	Phenanthrene-d10	18.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	42
2	5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	38
3	3,5-Cyclohexadiene-1,2-dione, 3...	220	C14H2O2	003383-21-9	35
4	7-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-91-0	27
5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	10.4	ng	148442	1	8.86	284130	20.0
2-Pentanone, 4-hy...	5.78	4.4	ng	62333	1	8.86	284130	20.0
unknown8.39	8.39	104.4	ng	1483280	1	8.86	284130	20.0
1H-Benzotriazole, ...	15.75	3.2	ng	108751	3	15.49	679787	20.0
unknown18.82	18.82	2.1	ng	83214	4	18.22	802782	20.0