

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
 Data File : BF080477.D
 Acq On : 15 Jul 2015 6:26
 Operator : TP/UM
 Sample : PB84447BL
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84447BL

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_F\METHODS\8270-BF071415.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	2.156	4	6	16	rBV	108786	214044	28.70%	3.690%
2	2.281	16	17	22	rVB2	8462	13686	1.84%	0.236%
3	4.739	229	232	235	rBV	9135	14621	1.96%	0.252%
4	5.333	282	284	300	rBV	267670	293280	39.33%	5.055%
5	5.756	319	321	335	rBB	535514	507940	68.11%	8.755%
6	6.144	353	355	360	rBV	15722	20280	2.72%	0.350%
7	6.762	407	409	419	rBV	545142	528333	70.85%	9.107%
8	6.899	419	421	424	rBV	682987	557714	74.79%	9.613%
9	7.127	439	441	443	rBV	110604	120270	16.13%	2.073%
10	7.276	453	454	457	rBV	296379	395678	53.06%	6.820%
11	7.687	488	490	492	rBV	399336	319682	42.87%	5.510%
12	8.408	551	553	556	rBV	188412	174157	23.35%	3.002%
13	9.482	645	647	650	rBV	806259	657808	88.21%	11.339%
14	10.168	705	707	710	rBB	194253	193926	26.00%	3.343%
15	10.956	774	776	779	rBV2	296144	350939	47.06%	6.049%
16	11.665	836	838	840	rBV	234453	211367	28.34%	3.643%
17	13.265	976	978	981	rBV	610435	745746	100.00%	12.855%
18	14.454	1079	1082	1084	rBV	176063	228452	30.63%	3.938%
19	16.145	1227	1230	1233	rBV	197976	253478	33.99%	4.369%

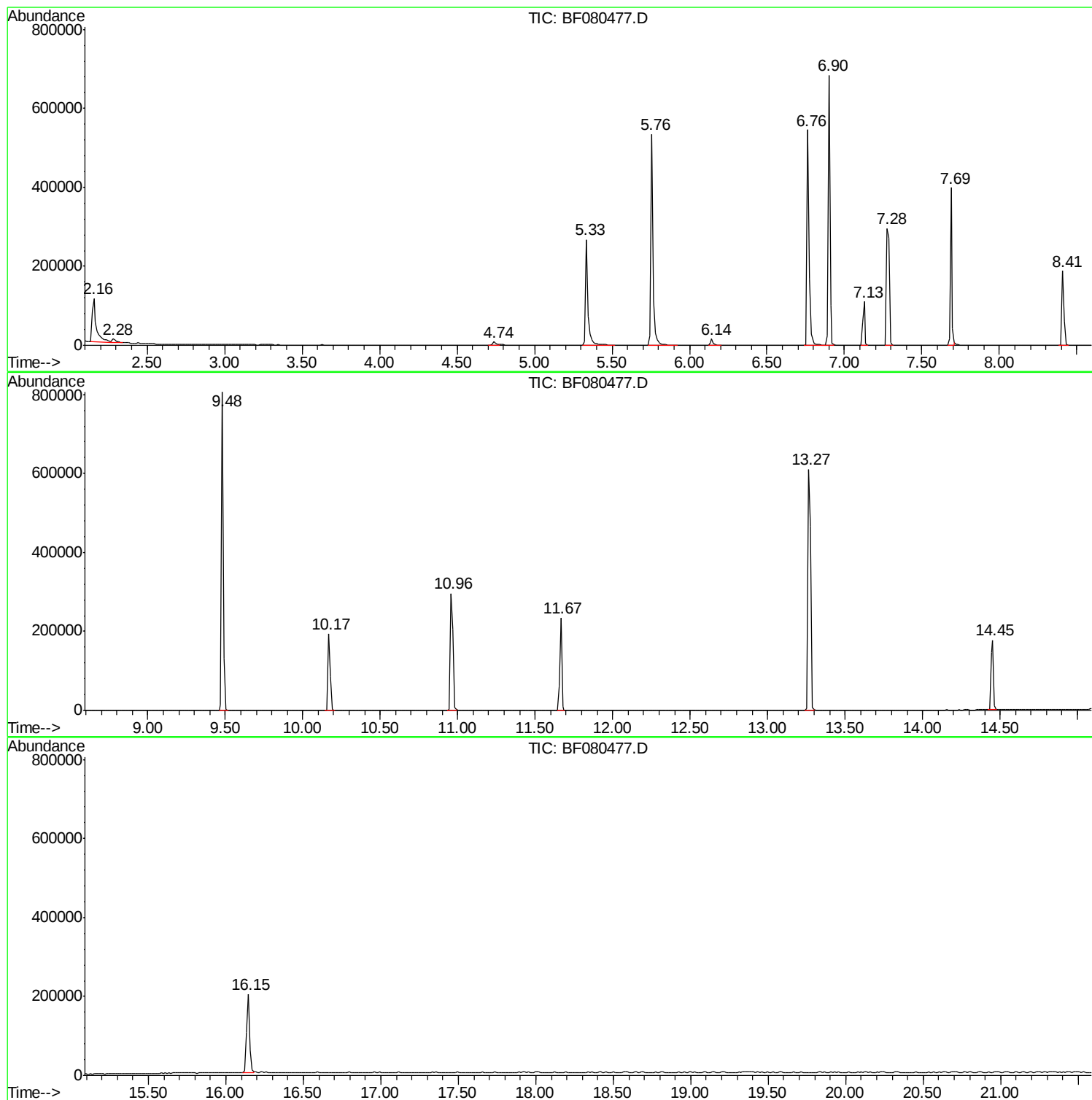
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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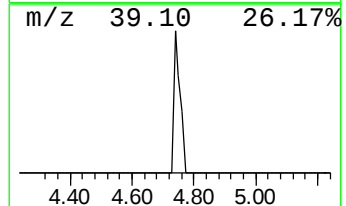
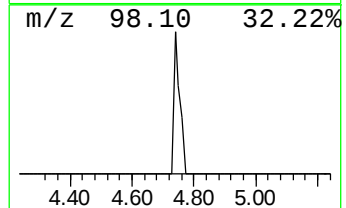
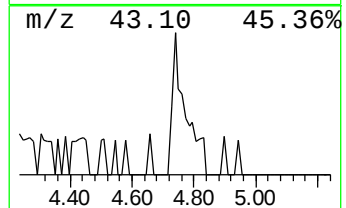
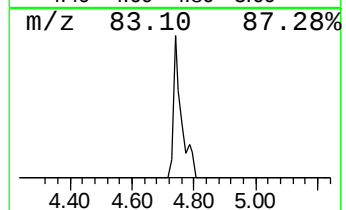
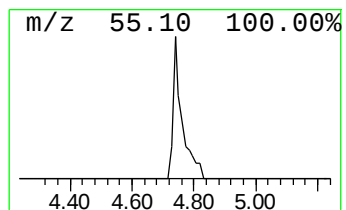
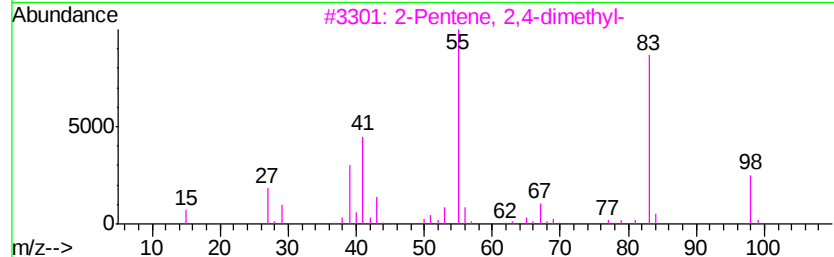
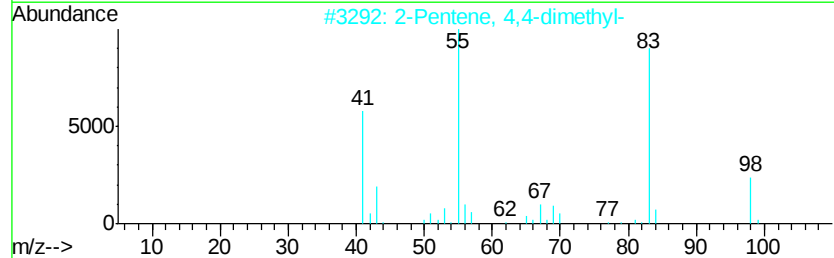
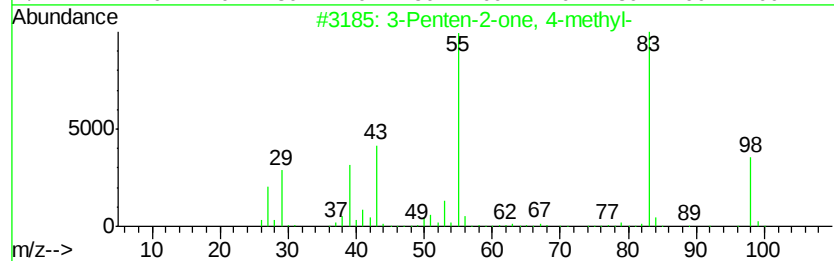
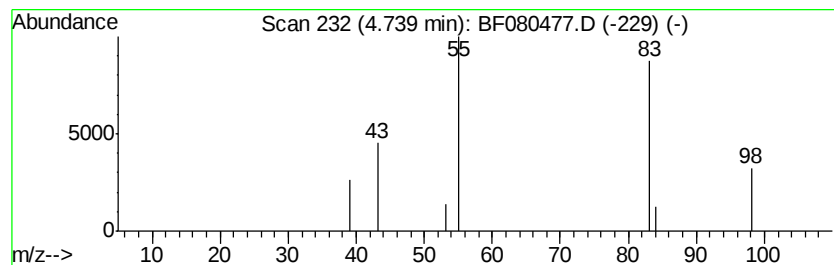
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	2.43 ng	14621	1,4-Dichlorobenzene-d4	7.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	83
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	74
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	74
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	74



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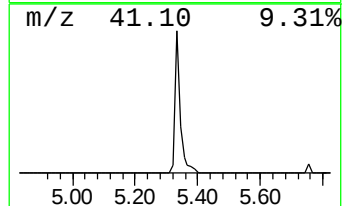
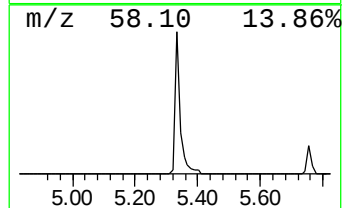
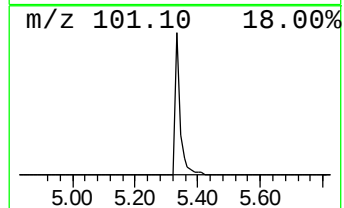
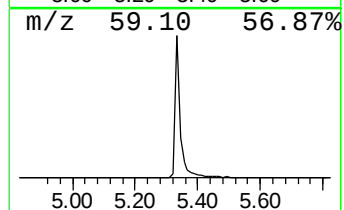
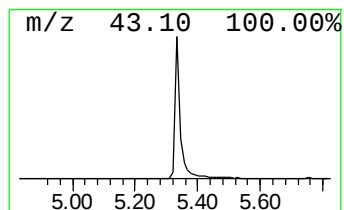
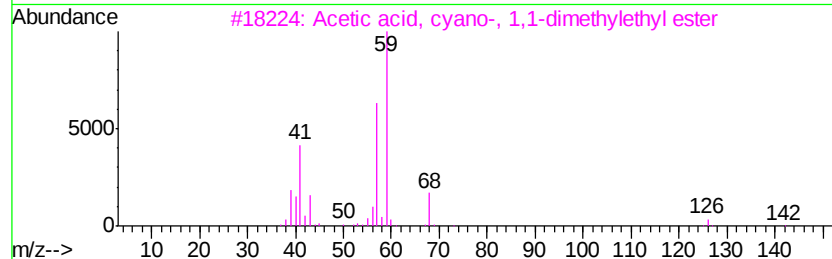
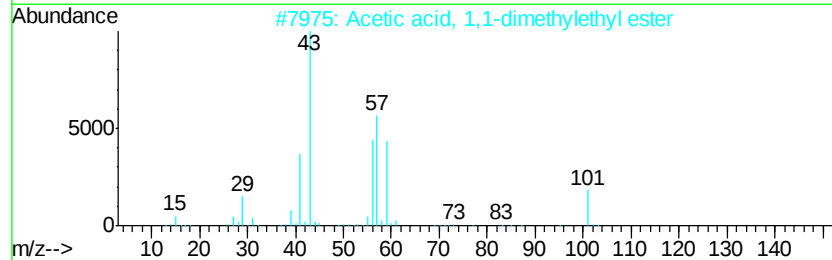
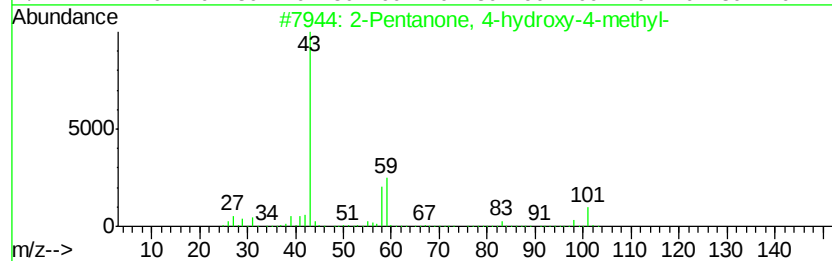
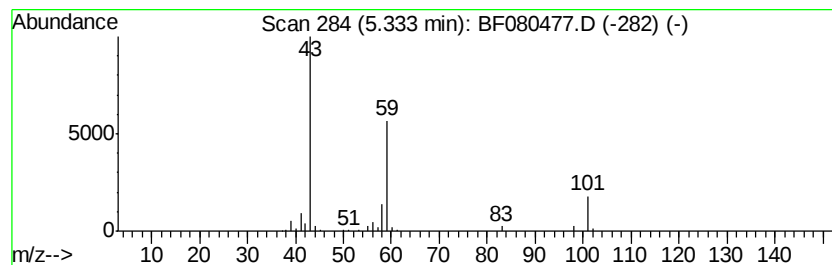
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	48.77 ng	293280	1,4-Dichlorobenzene-d4	7.13

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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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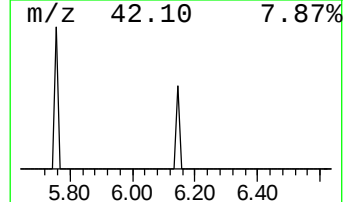
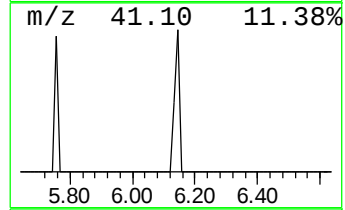
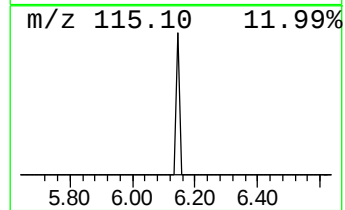
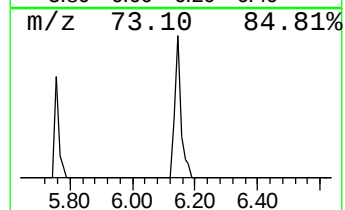
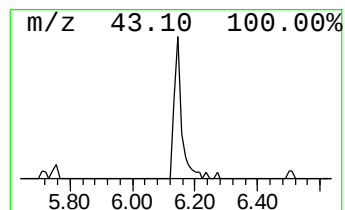
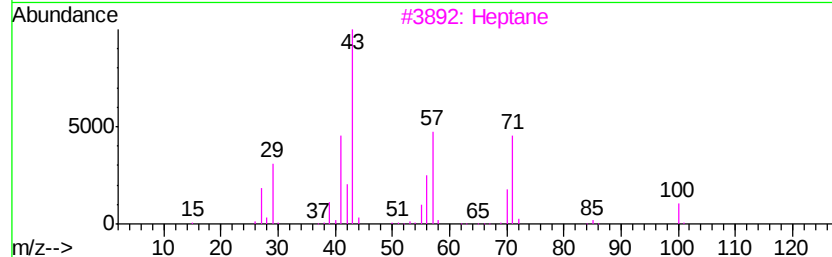
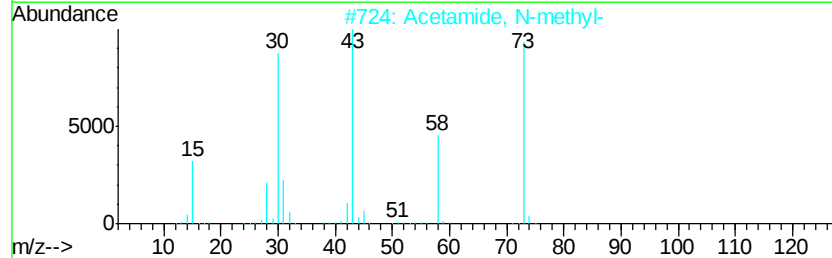
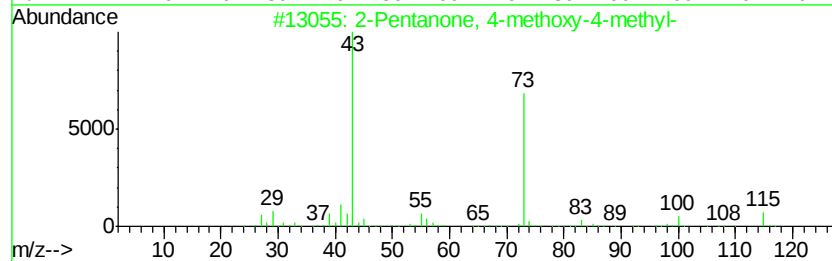
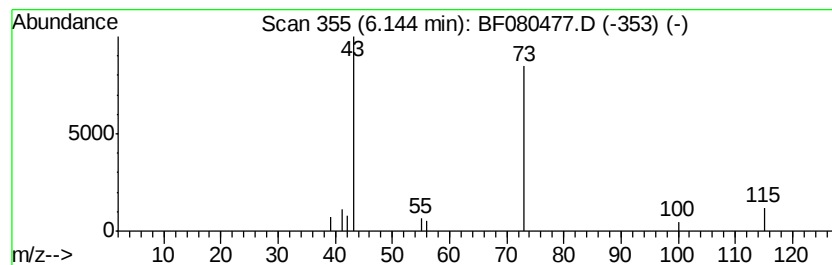
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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	3.37 ng	20280	1,4-Dichlorobenzene-d4	7.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	74
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
3		Heptane	100	C7H16	000142-82-5	4
4		Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	4
5		N-trimethylsilylaziridine	115	C5H13NSi	002116-90-7	4



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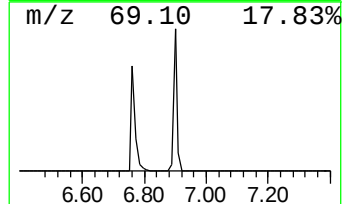
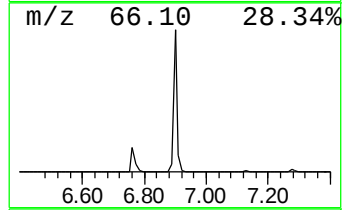
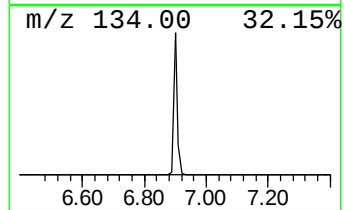
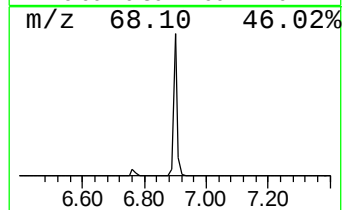
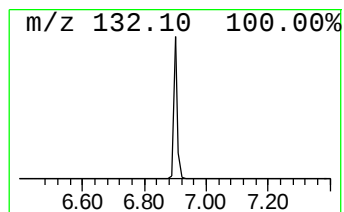
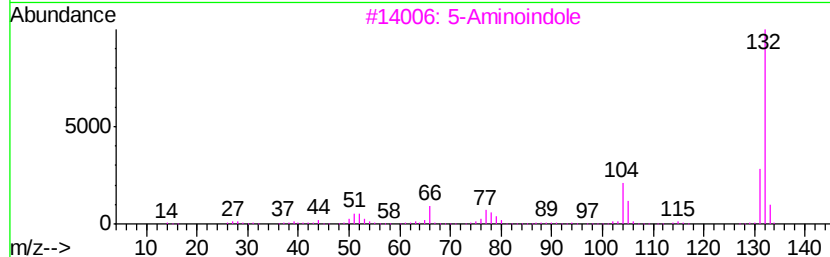
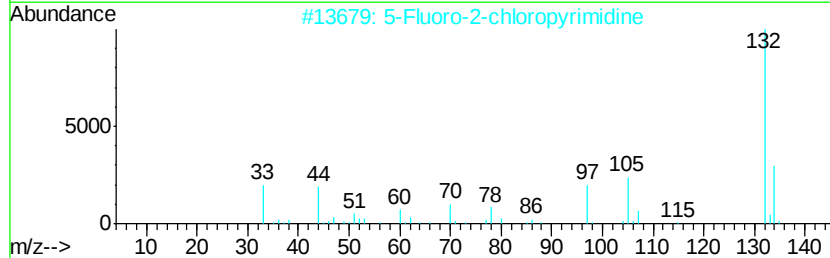
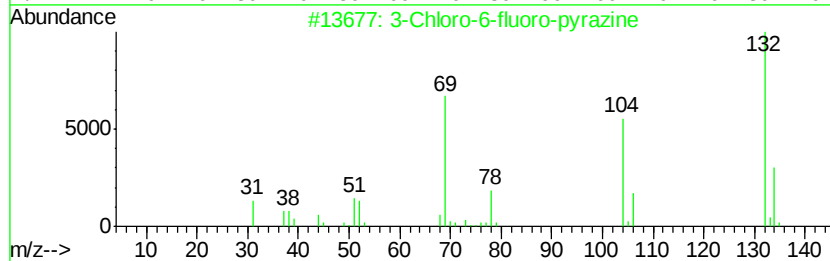
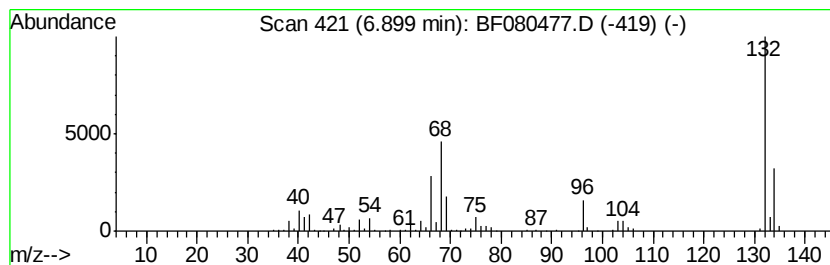
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Peak Number 6 unknown6.90 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	92.74 ng	557714	1,4-Dichlorobenzene-d4	7.13

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.74	2.4	ng	14621	1	7.13	120270	20.0
2-Pentanone, 4-hy...	5.33	48.8	ng	293280	1	7.13	120270	20.0
2-Pentanone, 4-me...	6.14	3.4	ng	20280	1	7.13	120270	20.0
unknown6.90	6.90	92.7	ng	557714	1	7.13	120270	20.0