

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062016\
 Data File : BF088182.D
 Acq On : 20 Jun 2016 20:24
 Operator : UM/SJ
 Sample : PB91363BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91363BL

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-BF060716.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	1.655	4	6	14	rVV	324231	683852	27.23%	3.136%
2	1.770	14	16	24	rVV	1026919	1717985	68.41%	7.879%
3	1.873	24	25	54	rVB2	83597	351737	14.01%	1.613%
4	4.113	219	221	235	rBV	340920	500516	19.93%	2.295%
5	4.833	279	284	286	rBV	1026549	1696072	67.54%	7.778%
6	5.267	320	322	338	rBV	1317704	1256494	50.03%	5.762%
7	5.667	355	357	360	rBV	99624	92062	3.67%	0.422%
8	6.319	412	414	416	rBV	1358278	1266409	50.43%	5.808%
9	6.433	422	424	427	rBV	1391608	1264068	50.33%	5.797%
10	6.662	443	444	447	rBV	557646	566862	22.57%	2.600%
11	6.822	455	458	460	rBV	1761207	1552108	61.80%	7.118%
12	7.233	492	494	497	rBV	1131191	1129000	44.96%	5.177%
13	7.953	555	557	559	rBV	750047	791888	31.53%	3.632%
14	9.028	648	651	654	rBV	2168694	2252993	89.71%	10.332%
15	9.702	707	710	712	rBV	804757	906948	36.11%	4.159%
16	10.479	776	778	781	rBV2	606780	756357	30.12%	3.469%
17	11.176	837	839	841	rBV	1059865	936710	37.30%	4.296%
18	12.765	975	978	980	rBV	1865323	2511341	100.00%	11.517%
19	13.805	1066	1069	1071	rBV	910569	891712	35.51%	4.089%
20	15.177	1186	1189	1197	rBV	582778	680867	27.11%	3.122%

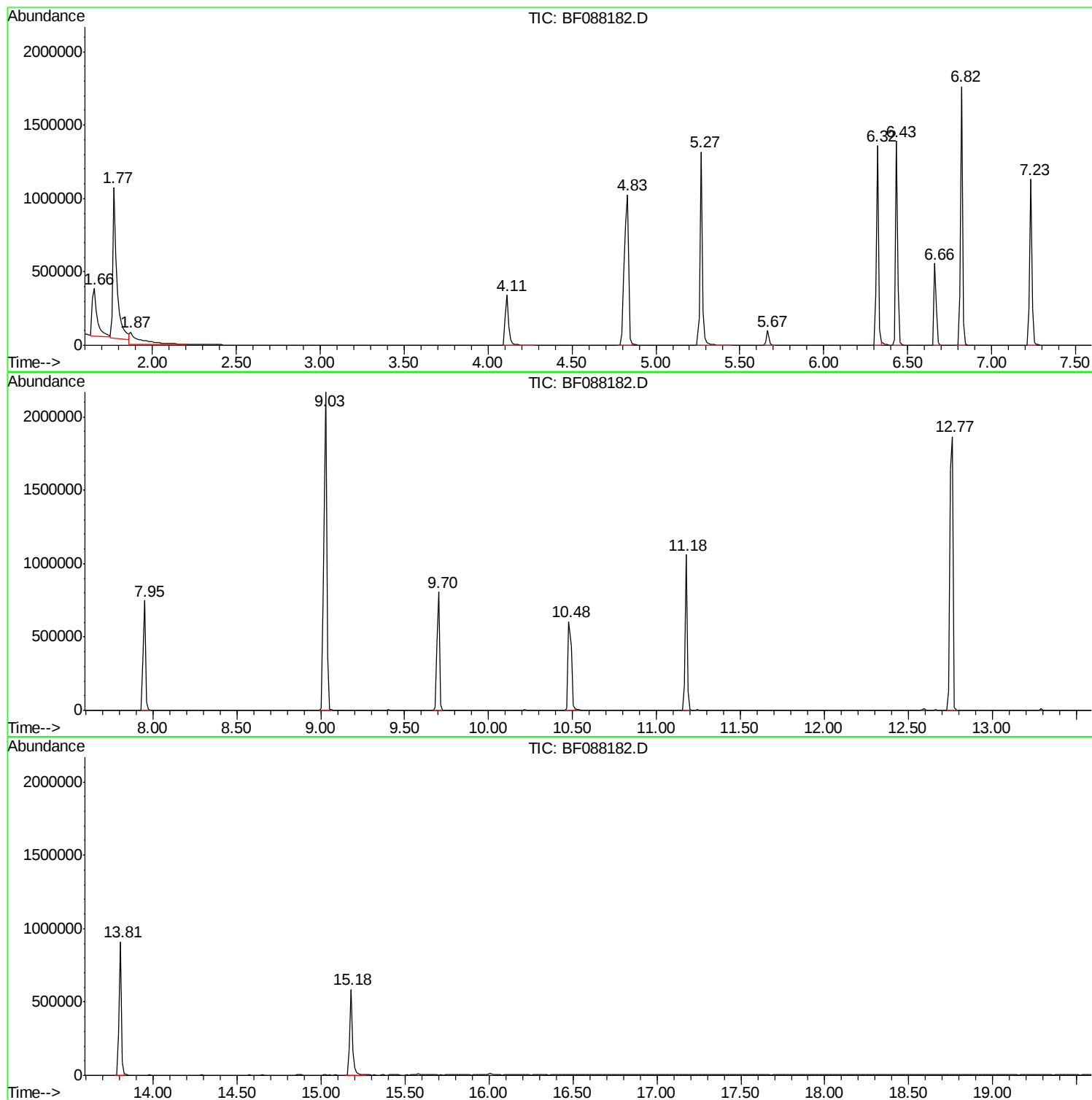
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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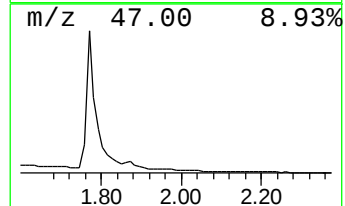
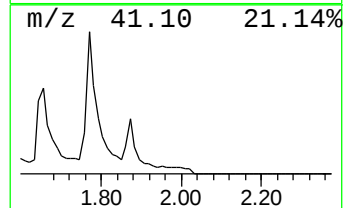
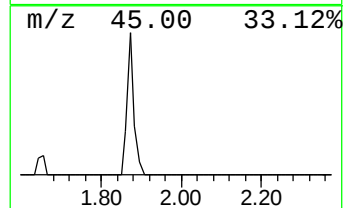
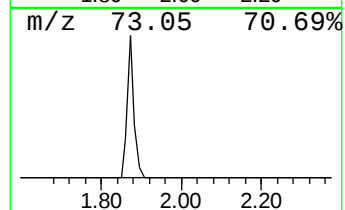
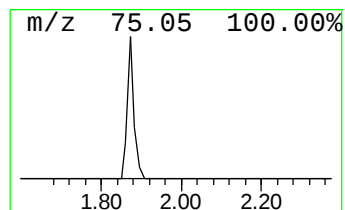
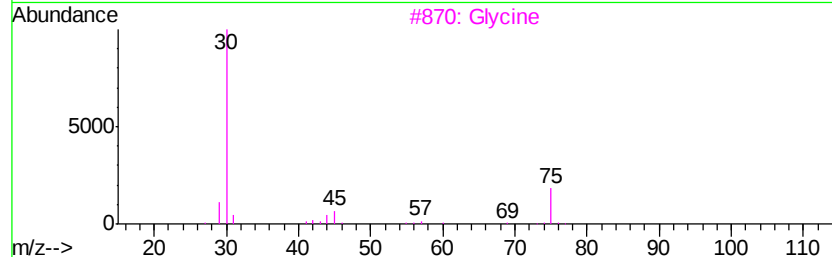
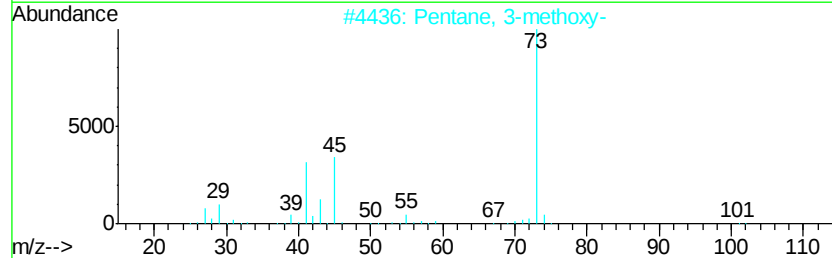
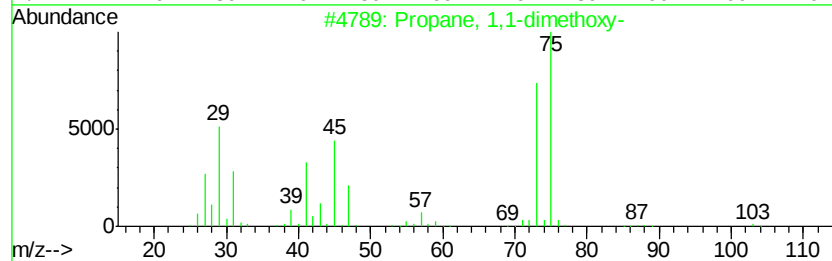
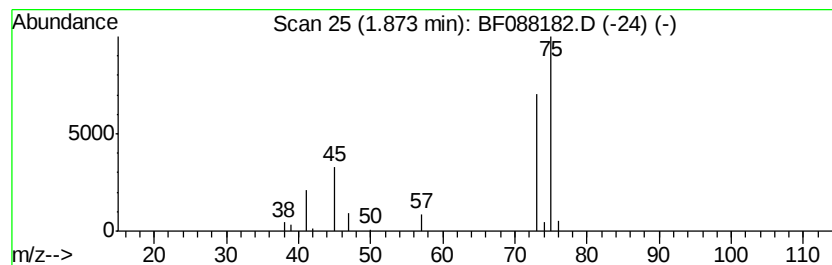
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.87	12.41 ng	351737	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3		Glycine	75	C2H5NO2	000056-40-6	7
4		Methanamine, N,N-dimethyl-, N-oxide	75	C3H9NO	001184-78-7	4
5		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	4



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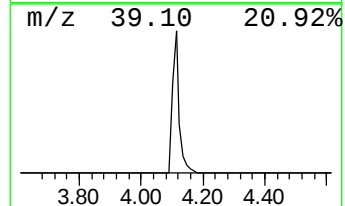
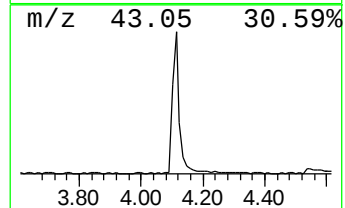
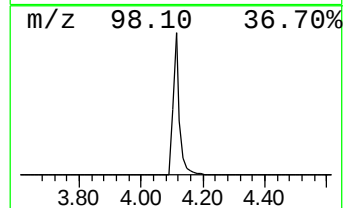
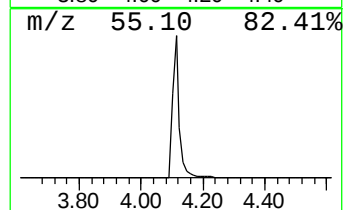
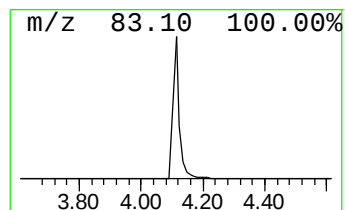
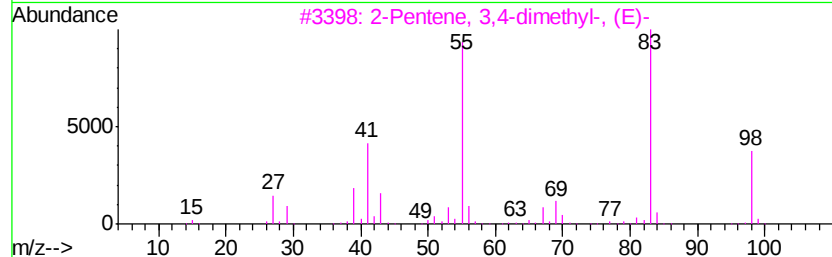
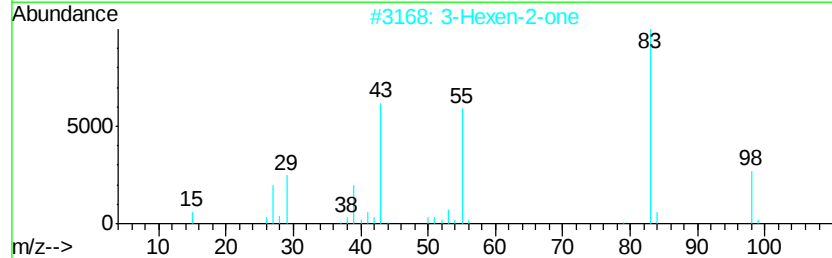
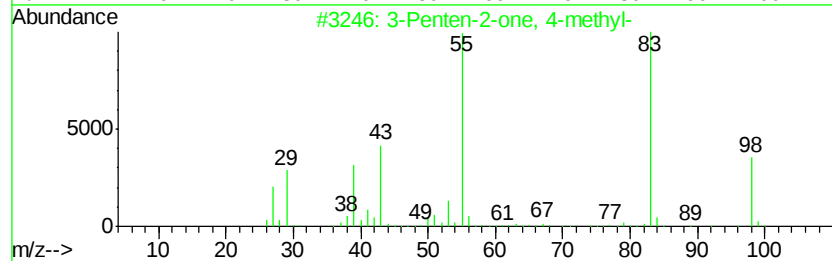
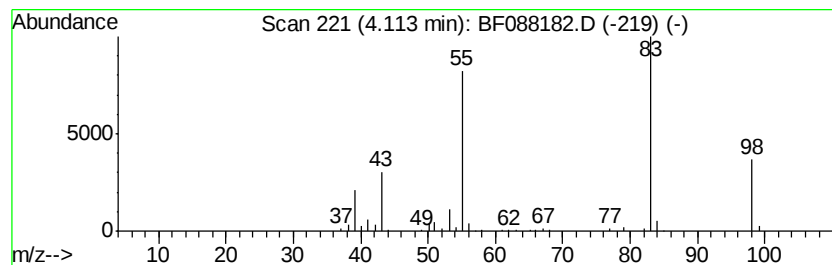
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Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	17.66 ng	500516	1,4-Dichlorobenzene-d4	6.66

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	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N2O2	042282-85-9	78



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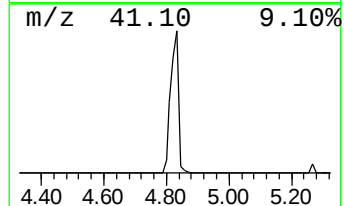
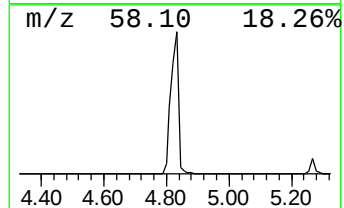
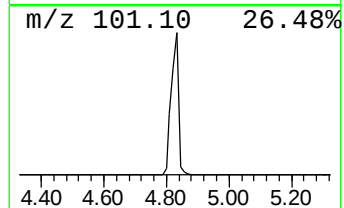
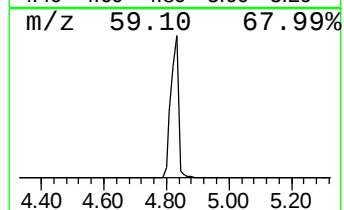
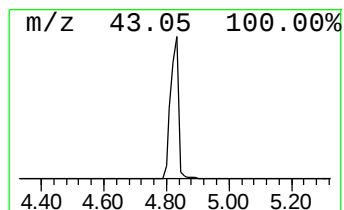
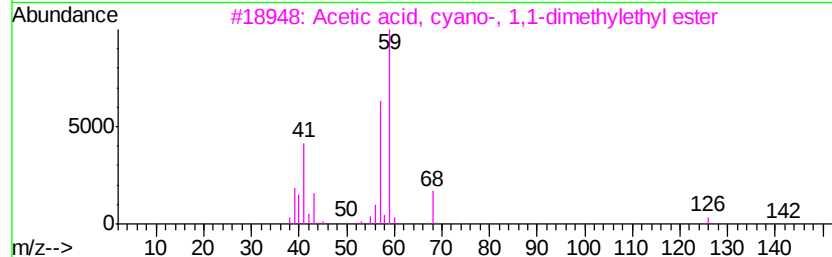
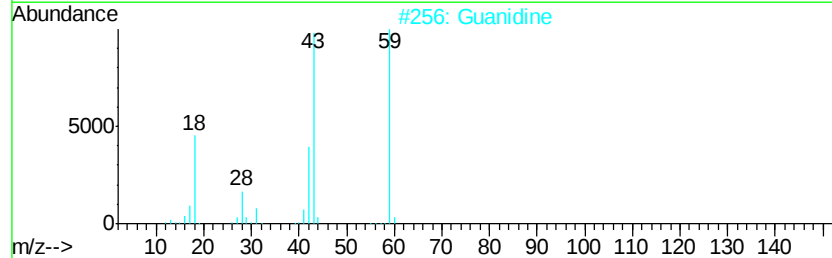
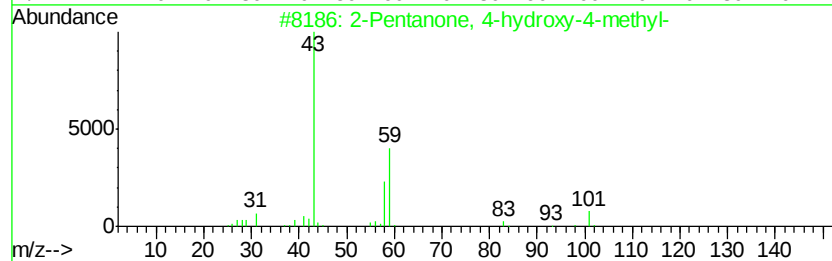
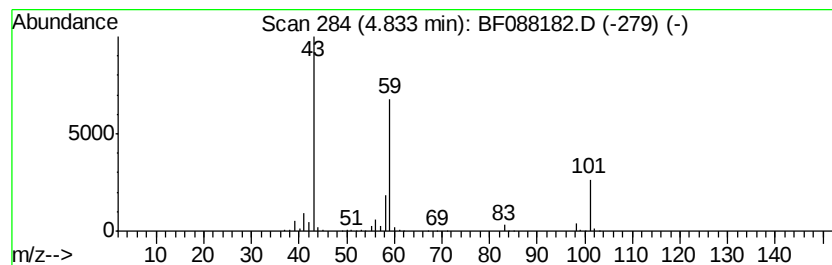
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	59.84 ng	1696070	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Guanidine	59	CH5N3	000113-00-8	43
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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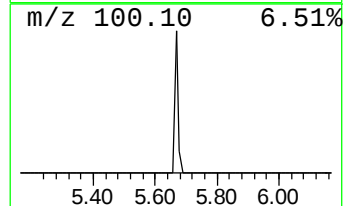
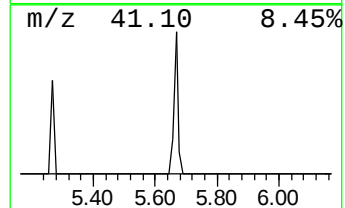
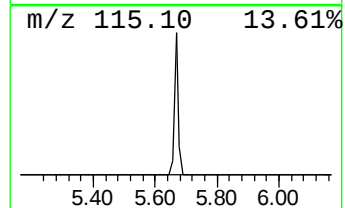
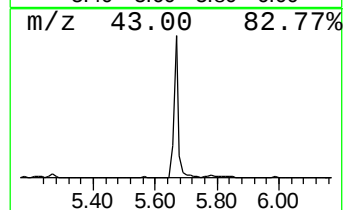
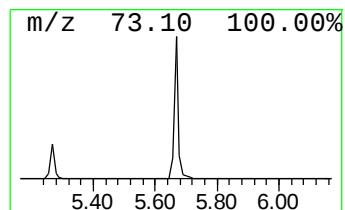
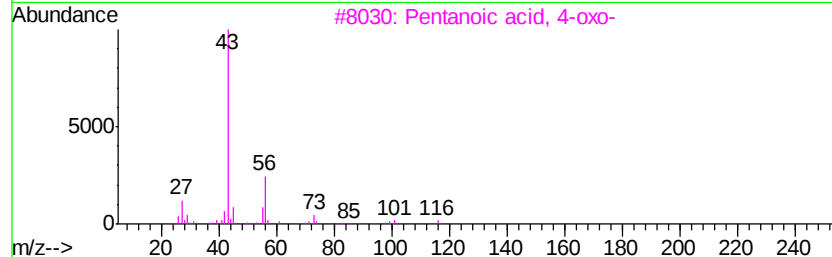
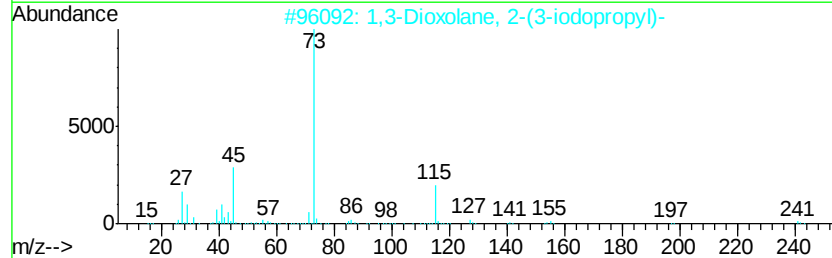
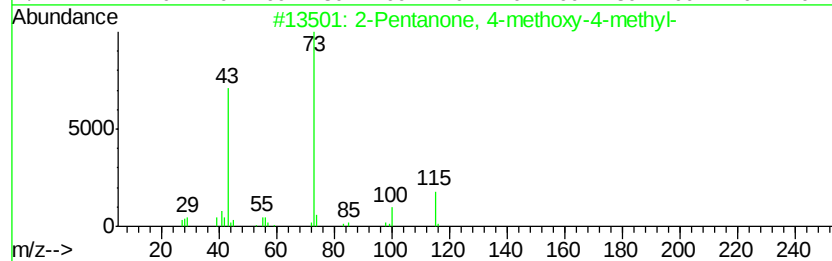
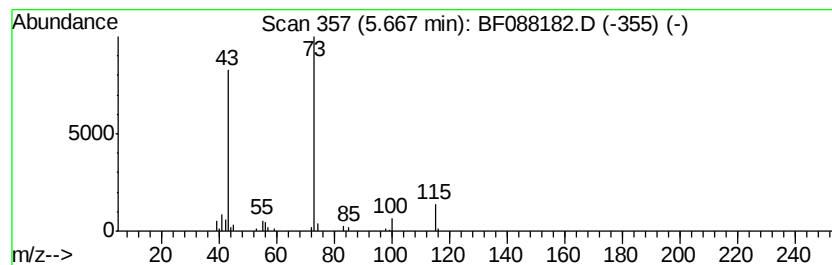
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Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	3.25 ng	92062	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1,3-Dioxolane, 2-(3-iodopropyl)-	242	C6H11IO2	058135-25-4	28
3		Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	12
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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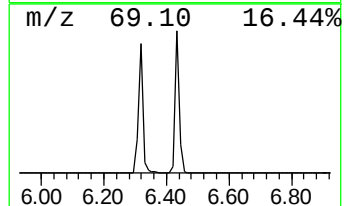
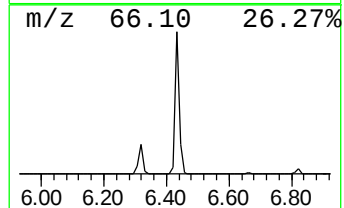
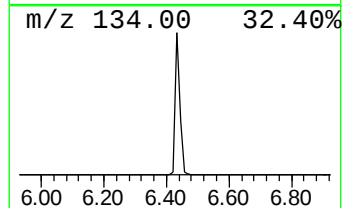
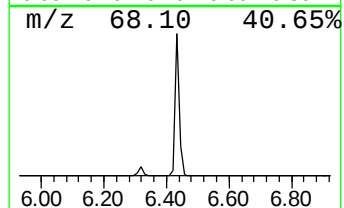
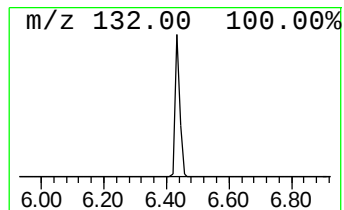
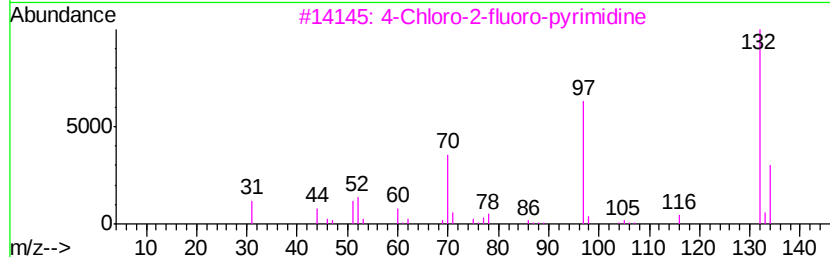
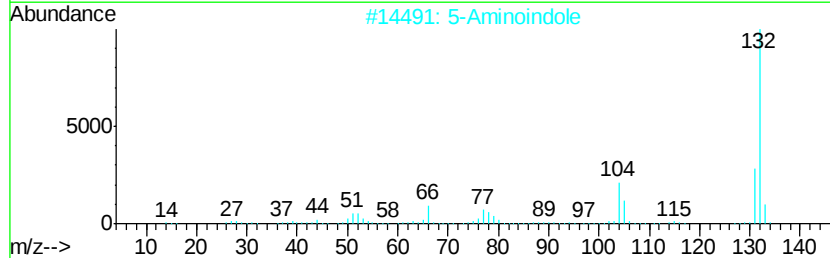
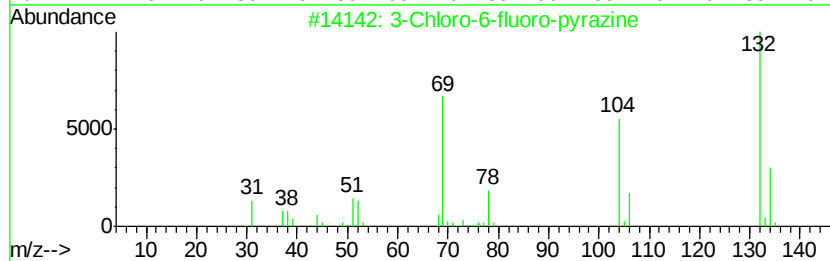
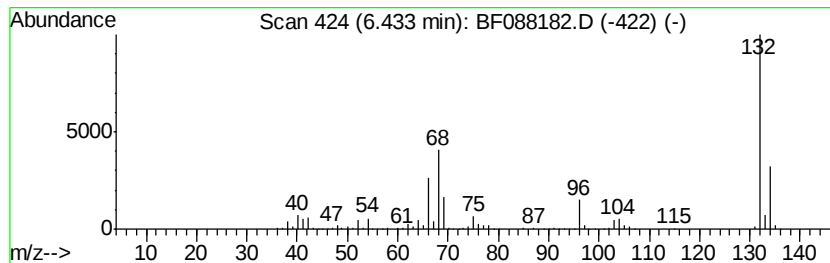
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Peak Number 7 unknown6.43 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	44.60 ng	1264070	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.87	12.4	ng	351737	1	6.66	566862	20.0
3-Penten-2-one, 4...	4.11	17.7	ng	500516	1	6.66	566862	20.0
2-Pentanone, 4-hy...	4.83	59.8	ng	1696070	1	6.66	566862	20.0
2-Pentanone, 4-me...	5.67	3.3	ng	92062	1	6.66	566862	20.0
unknown6.43	6.43	44.6	ng	1264070	1	6.66	566862	20.0