

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061716\
 Data File : BF088101.D
 Acq On : 17 Jun 2016 19:06
 Operator : UM/SJ
 Sample : PB91310BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91310BL

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	1.667	5	7	16	rVB	451933	672096	26.14%	2.869%
2	1.781	16	17	28	rVV	1011264	2017379	78.45%	8.611%
3	1.918	28	29	65	rVB2	78536	368657	14.34%	1.574%
4	4.159	223	225	235	rVB	406275	540524	21.02%	2.307%
5	4.867	282	287	289	rBV	1141907	1798254	69.93%	7.676%
6	5.290	321	324	327	rBV	1418111	1321636	51.40%	5.641%
7	5.690	357	359	362	rBV	86850	102201	3.97%	0.436%
8	6.342	413	416	418	rBV	1184815	1431575	55.67%	6.111%
9	6.456	424	426	429	rBV	1128100	1383942	53.82%	5.907%
10	6.696	445	447	449	rBV	664690	598729	23.28%	2.556%
11	6.845	458	460	463	rBV	1209181	1633944	63.54%	6.974%
12	7.267	494	497	499	rBV	1097099	1371671	53.34%	5.855%
13	7.976	557	559	562	rBV	749311	800778	31.14%	3.418%
14	9.062	651	654	656	rBV	2428851	2571426	100.00%	10.976%
15	9.725	710	712	715	rBV	748607	960252	37.34%	4.099%
16	10.514	779	781	784	rBV	951774	989587	38.48%	4.224%
17	11.211	839	842	844	rBV	1157353	1007767	39.19%	4.302%
18	12.799	978	981	983	rBV	2133467	2477198	96.34%	10.574%
19	13.840	1069	1072	1074	rBV	850932	783543	30.47%	3.344%
20	15.223	1190	1193	1200	rBV	508950	596823	23.21%	2.547%

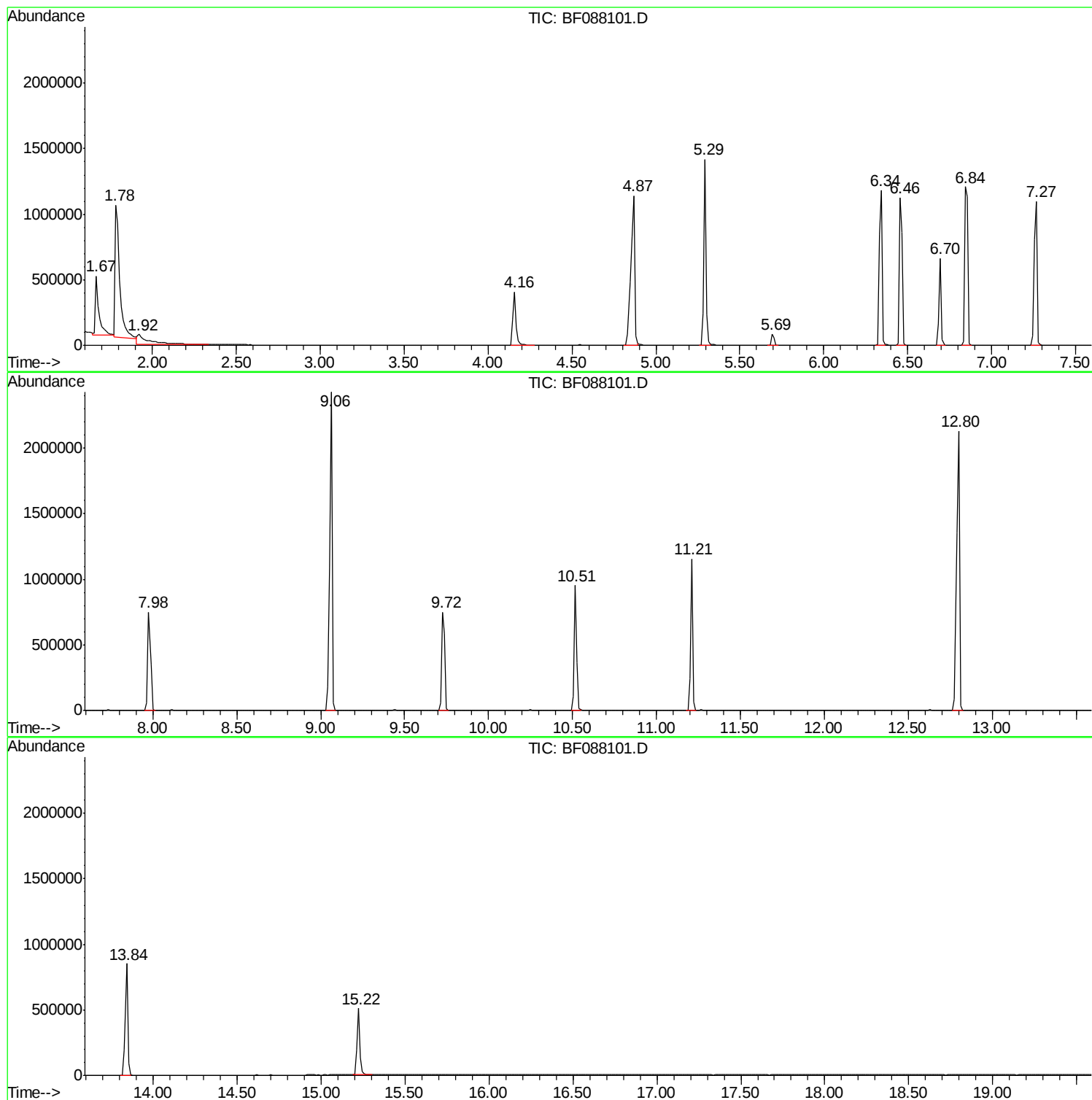
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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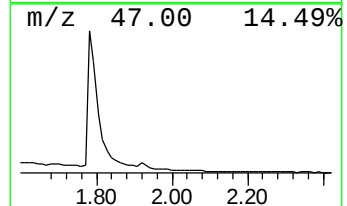
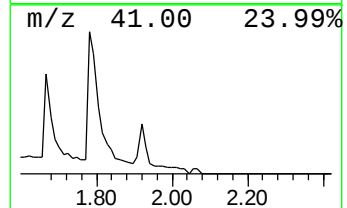
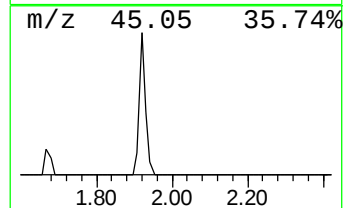
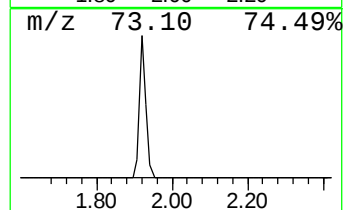
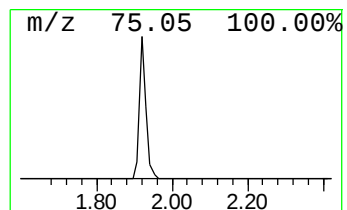
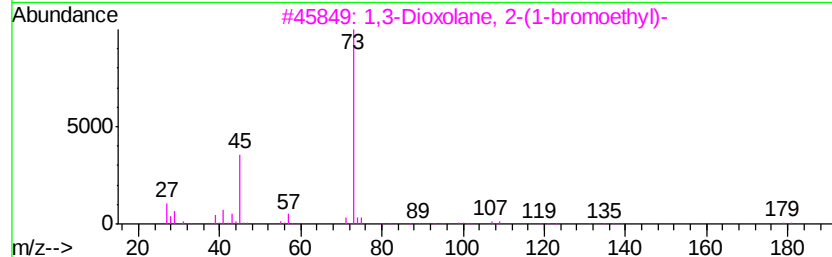
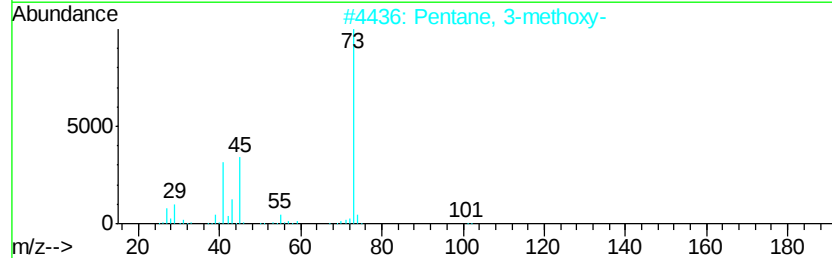
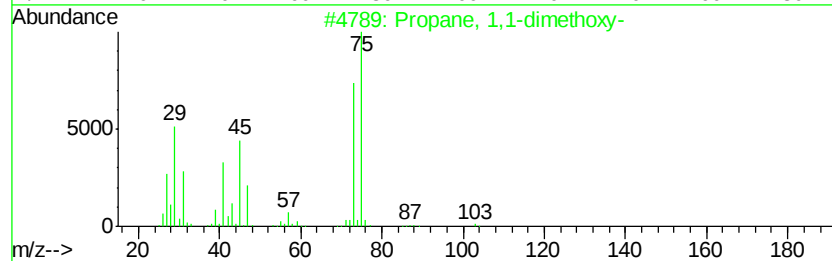
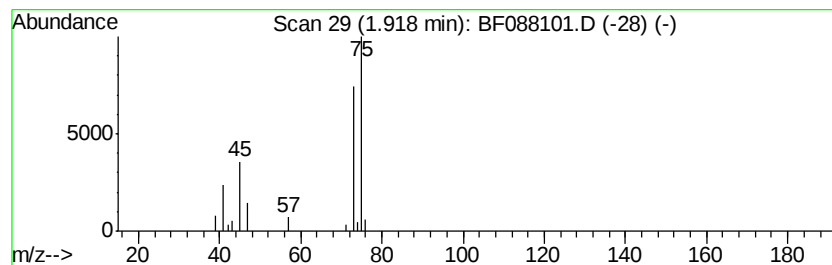
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.92	12.31 ng	368657	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5		Glycine	75	C2H5NO2	000056-40-6	7



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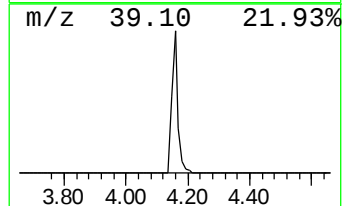
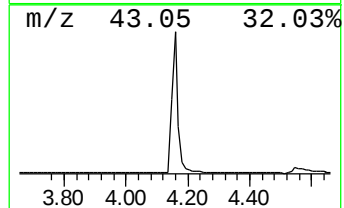
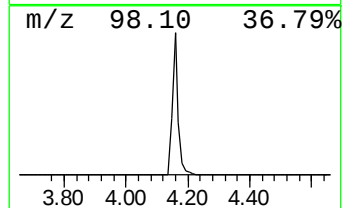
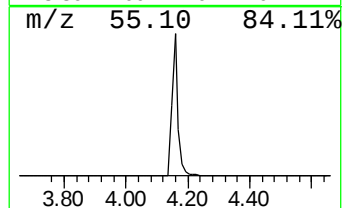
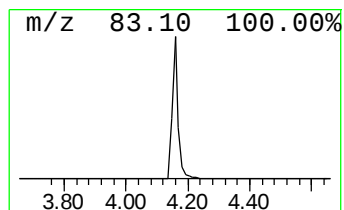
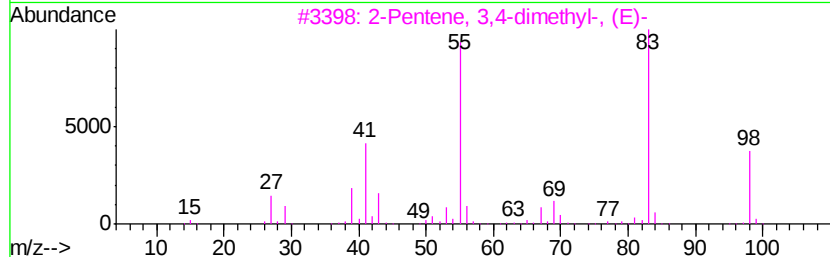
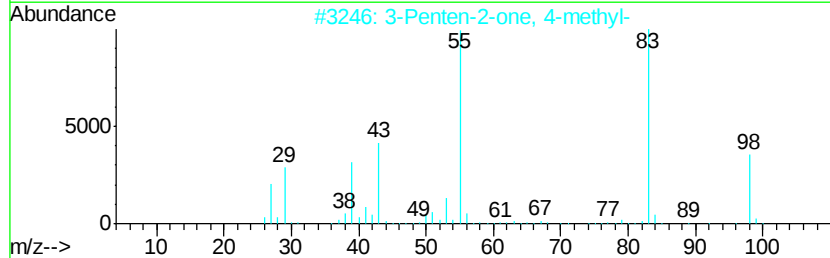
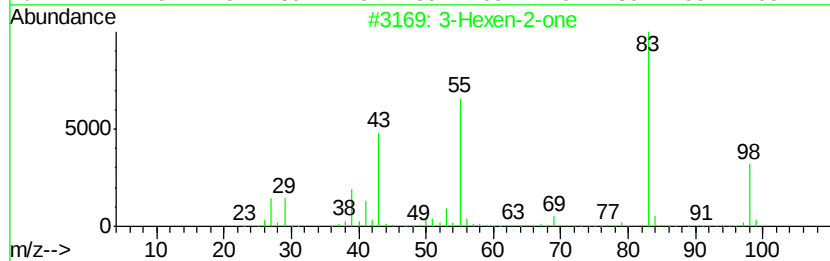
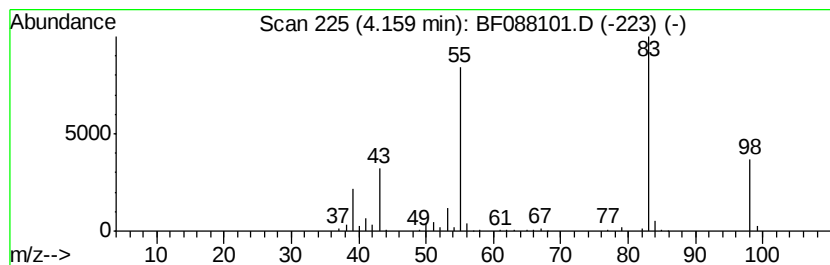
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Peak Number 4 3-Hexen-2-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	18.06 ng	540524	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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	78
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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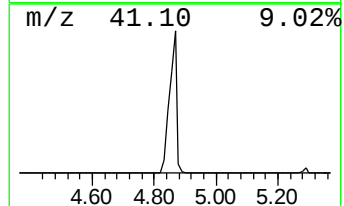
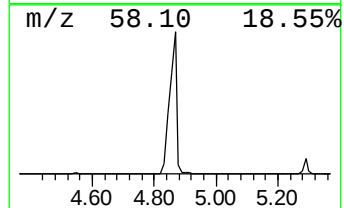
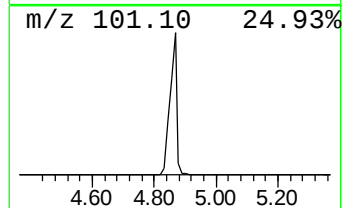
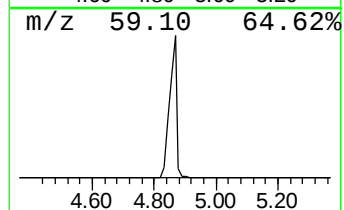
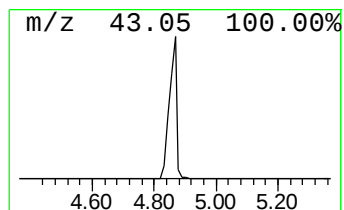
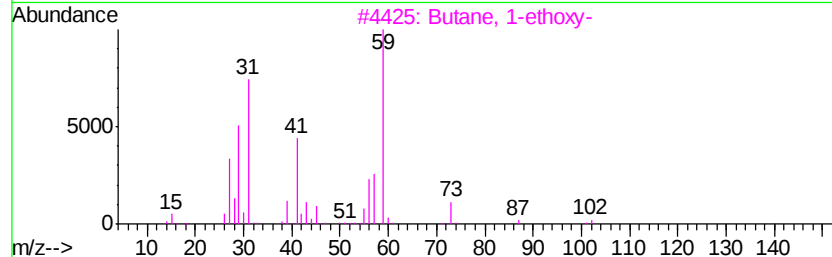
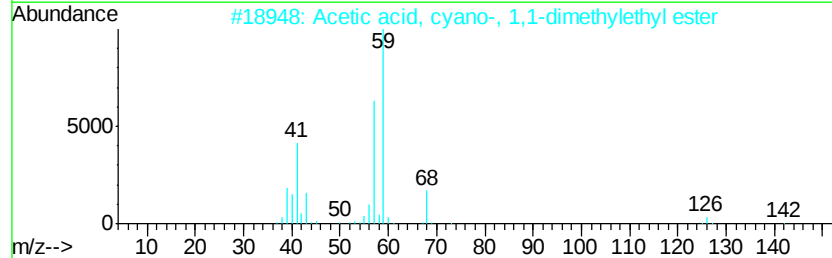
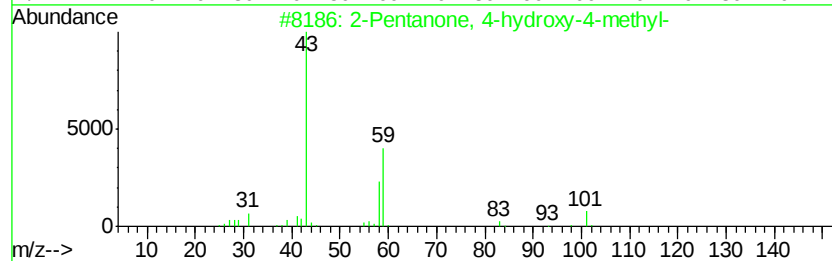
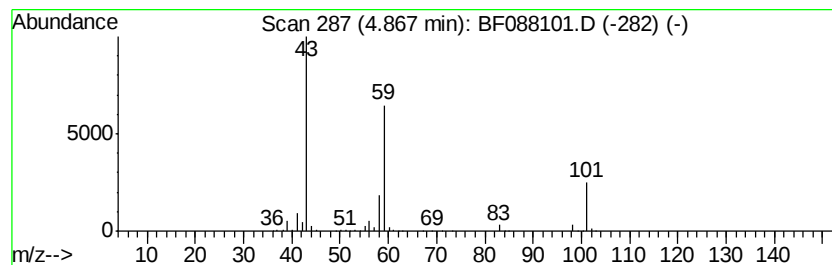
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	60.07 ng	1798250	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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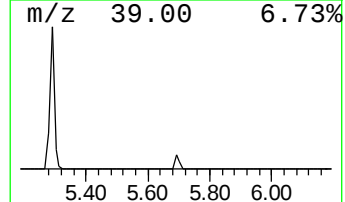
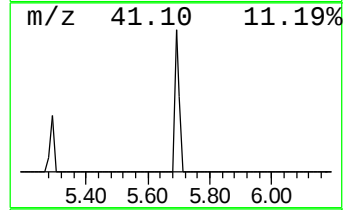
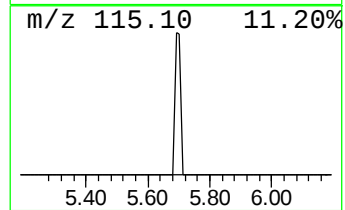
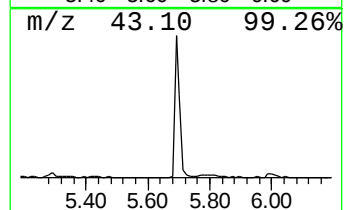
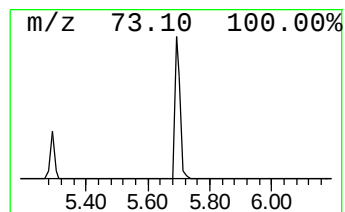
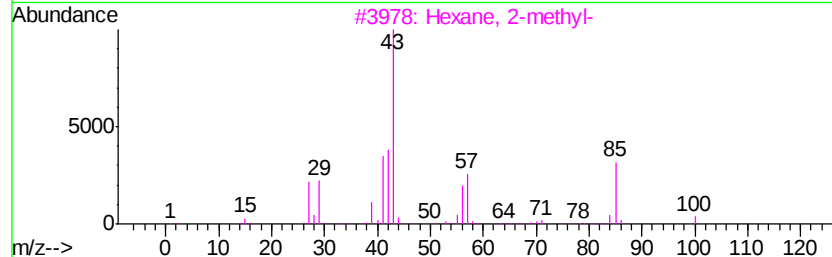
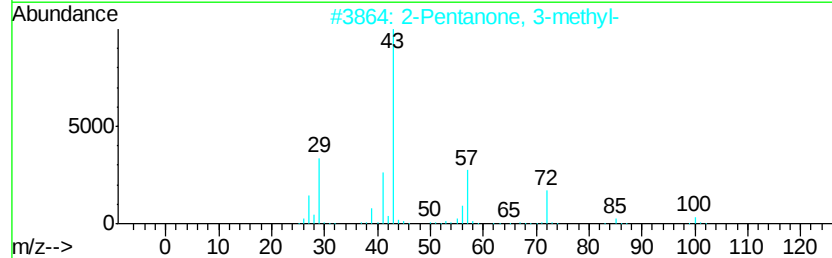
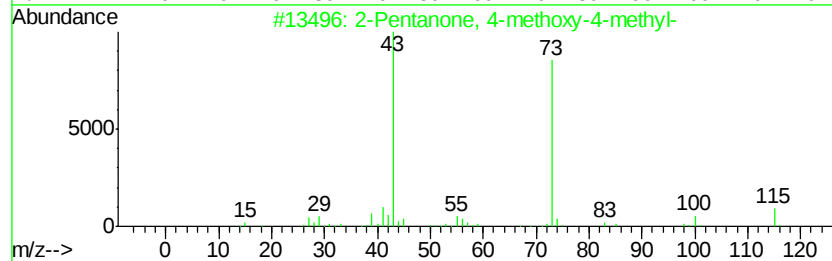
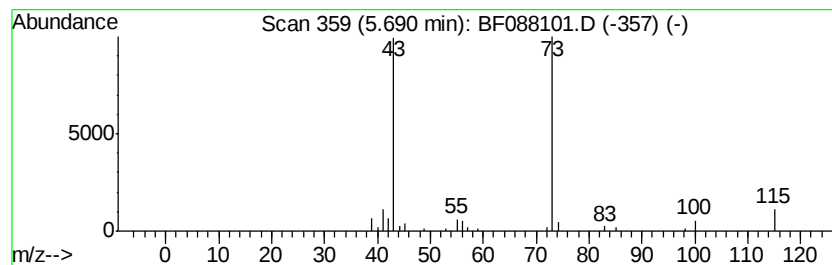
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Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	3.41 ng	102201	1,4-Dichlorobenzene-d4	6.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
3		Hexane, 2-methyl-	100	C7H16	000591-76-4	9
4		Heptane	100	C7H16	000142-82-5	9
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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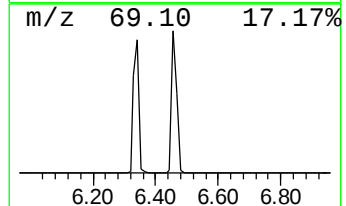
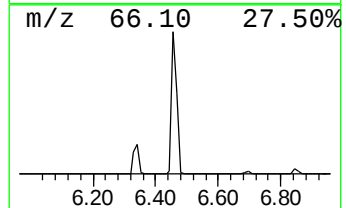
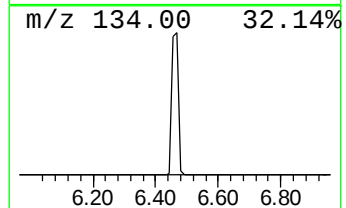
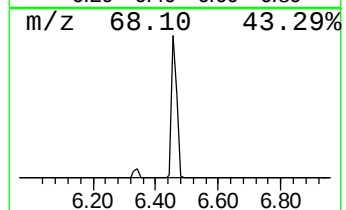
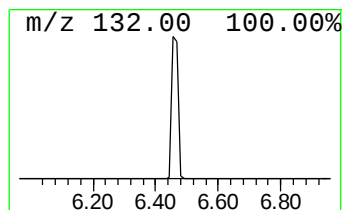
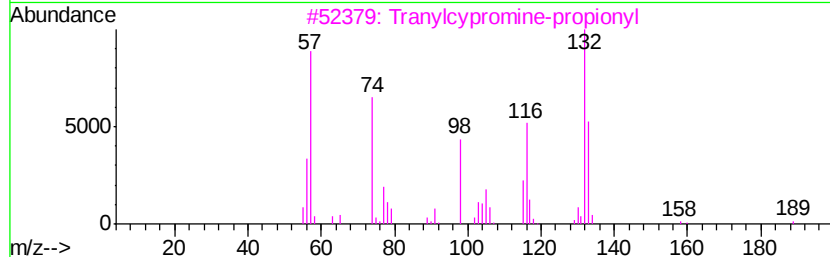
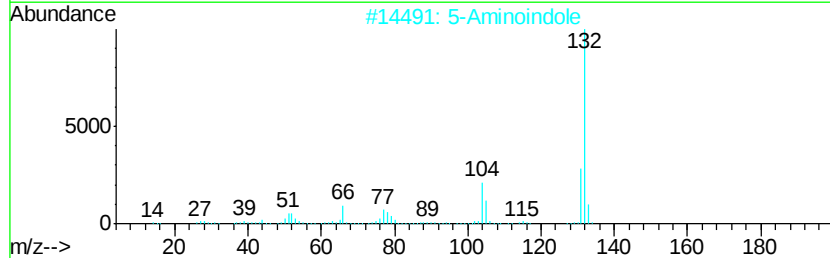
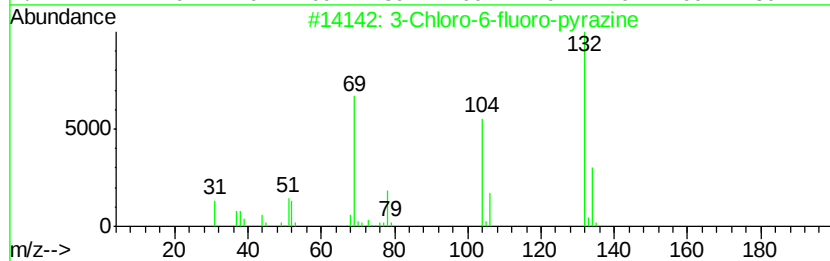
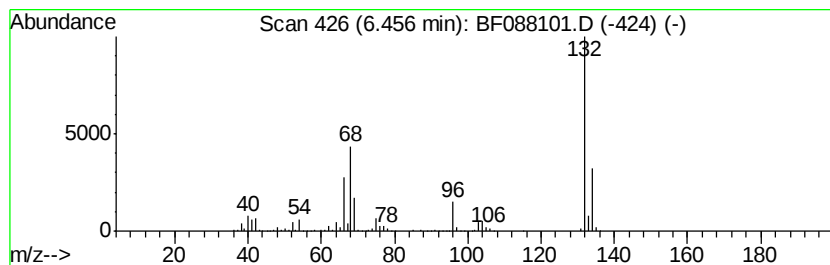
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Peak Number 7 unknown6.46 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	46.23 ng	1383940	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.92	12.3	ng	368657	1	6.70	598729	20.0
3-Hexen-2-one	4.16	18.1	ng	540524	1	6.70	598729	20.0
2-Pentanone, 4-hy...	4.87	60.1	ng	1798250	1	6.70	598729	20.0
2-Pentanone, 4-me...	5.69	3.4	ng	102201	1	6.70	598729	20.0
unknown6.46	6.46	46.2	ng	1383940	1	6.70	598729	20.0