

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032816\
 Data File : BF085831.D
 Acq On : 29 Mar 2016 5:13
 Operator : UM/SJ
 Sample : H1942-09
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-927ANCOMP

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-BF032416.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	2.367	4	7	19	rVB2	11317	48526	1.45%	0.175%
2	2.618	27	29	37	rVB	115081	170402	5.10%	0.616%
3	4.356	177	181	186	rBV2	34327	67878	2.03%	0.245%
4	4.561	197	199	204	rBV	27744	37898	1.13%	0.137%
5	5.007	235	238	248	rBV	919407	1408213	42.11%	5.089%
6	5.430	272	275	277	rBV	2414125	2797776	83.66%	10.111%
7	5.830	307	310	314	rBV	98592	136015	4.07%	0.492%
8	6.459	362	365	367	rBV	2317400	2631880	78.70%	9.512%
9	6.584	373	376	379	rBV	2695172	2679413	80.12%	9.684%
10	6.813	394	396	399	rBV	730193	680409	20.35%	2.459%
11	6.973	408	410	412	rBV	2722318	2463242	73.65%	8.902%
12	7.384	443	446	448	rBV	2037784	2055424	61.46%	7.429%
13	8.104	506	509	513	rBV2	725176	1253977	37.50%	4.532%
14	8.813	570	571	574	rVB	61911	52768	1.58%	0.191%
15	8.916	575	580	583	rBV	28087	46836	1.40%	0.169%
16	9.179	600	603	605	rBV	3550936	3344343	100.00%	12.087%
17	9.853	660	662	664	rBV	1020132	887764	26.55%	3.208%
18	10.276	695	699	701	rBV	89258	82019	2.45%	0.296%
19	10.585	723	726	728	rBV	60308	64015	1.91%	0.231%
20	10.642	728	731	734	rBV	1643518	1774353	53.06%	6.413%
21	11.008	761	763	767	rVB	35006	64040	1.91%	0.231%
22	11.099	767	771	773	rVB3	61554	108858	3.25%	0.393%
23	11.339	789	792	794	rBV	881497	815335	24.38%	2.947%
24	12.745	913	915	920	rVB2	34589	36169	1.08%	0.131%
25	12.928	928	931	933	rBV	2472431	2896423	86.61%	10.468%
26	13.968	1020	1022	1025	rBV	522005	529514	15.83%	1.914%
27	15.385	1143	1146	1153	rBV	383401	535818	16.02%	1.937%

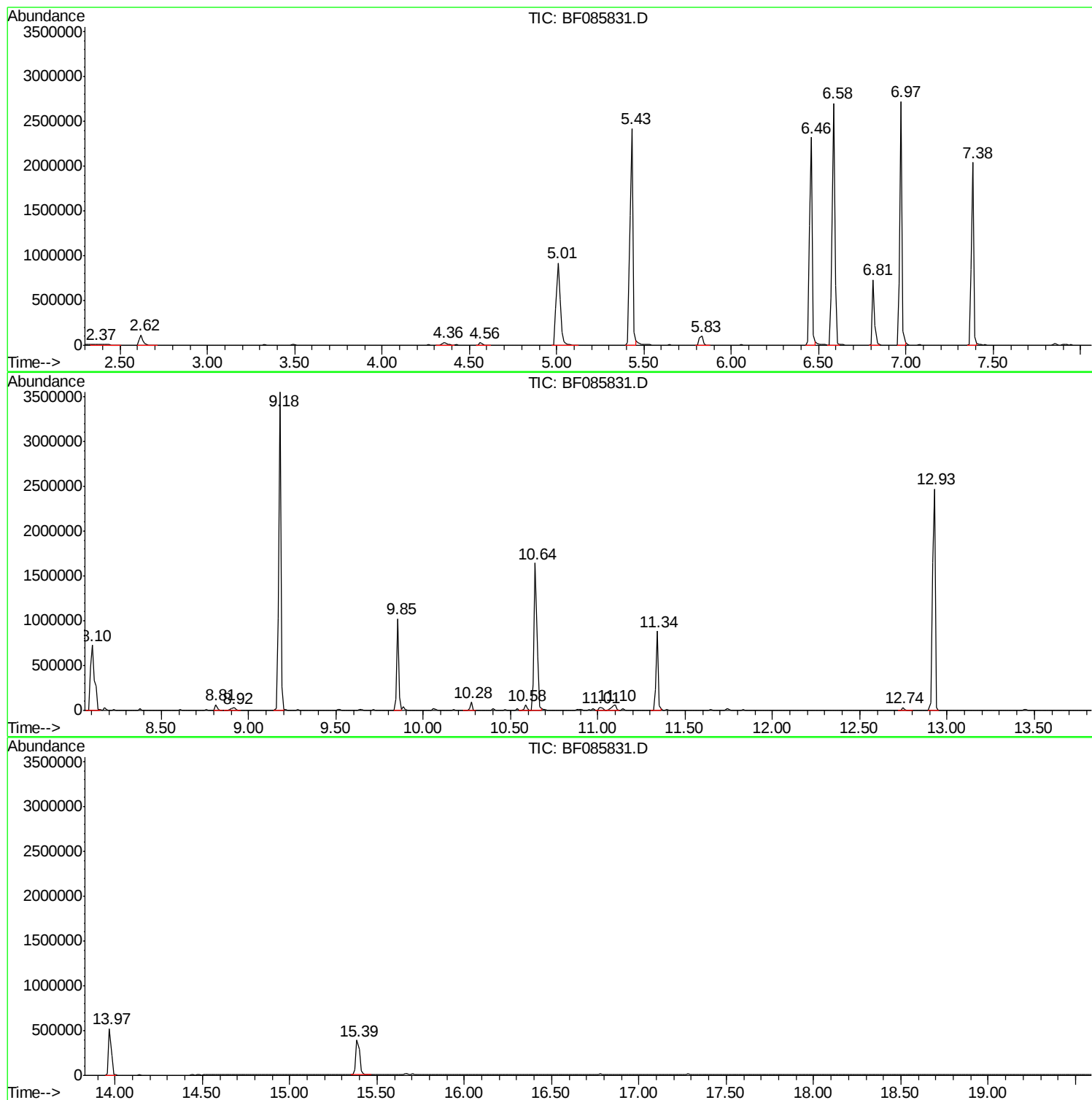
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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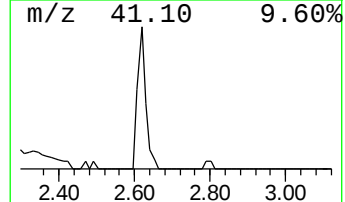
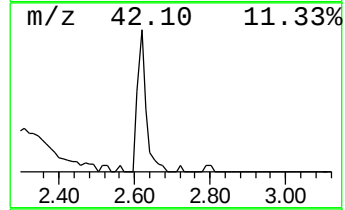
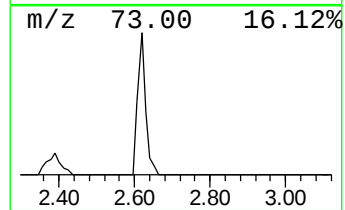
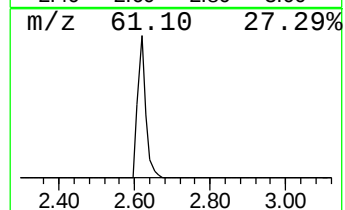
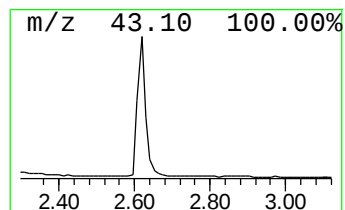
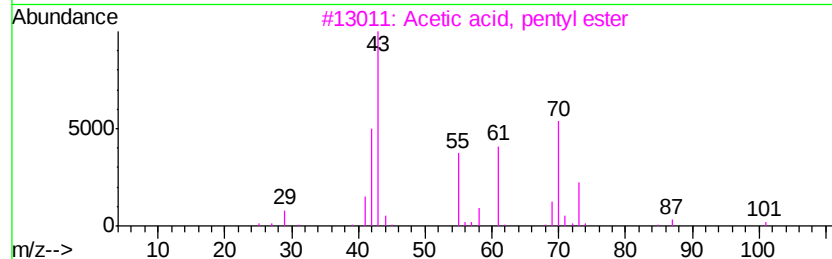
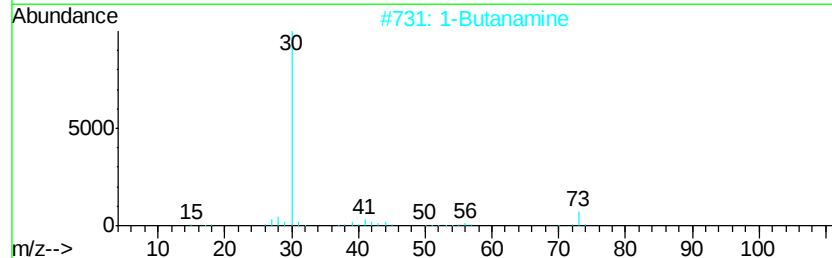
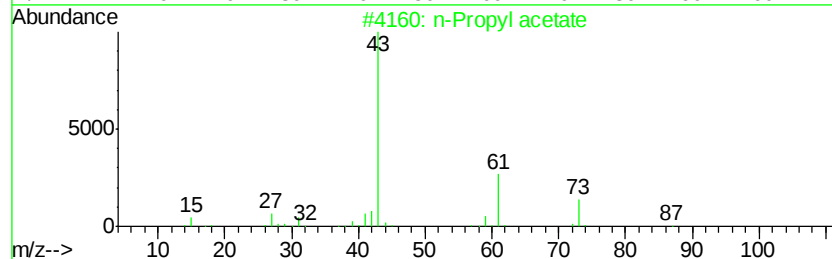
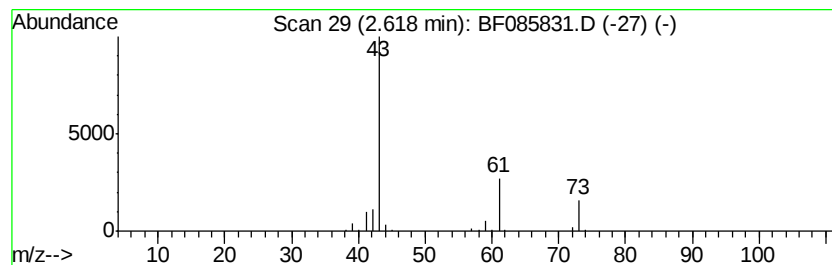
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	5.01 ng	170402	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		1-Butanamine	73	C4H11N	000109-73-9	9
3		Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
4		Isobutylamine	73	C4H11N	000078-81-9	7
5		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7



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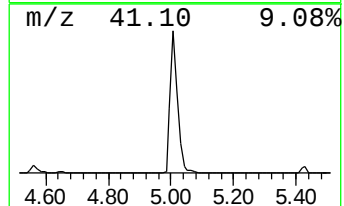
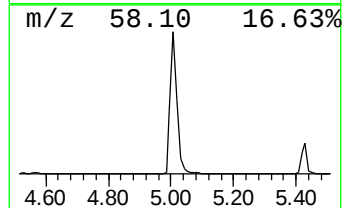
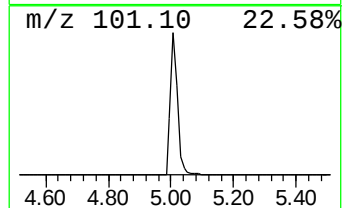
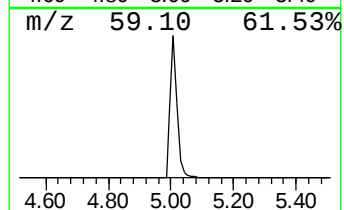
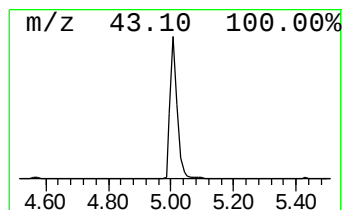
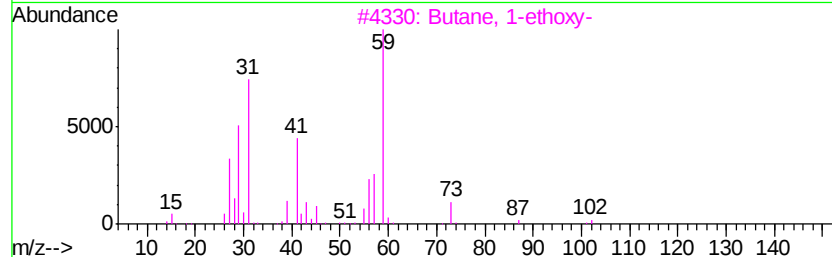
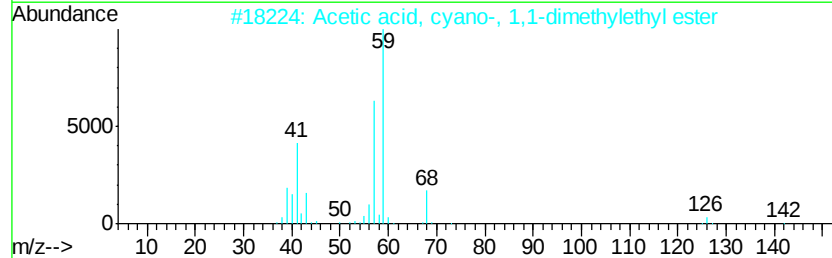
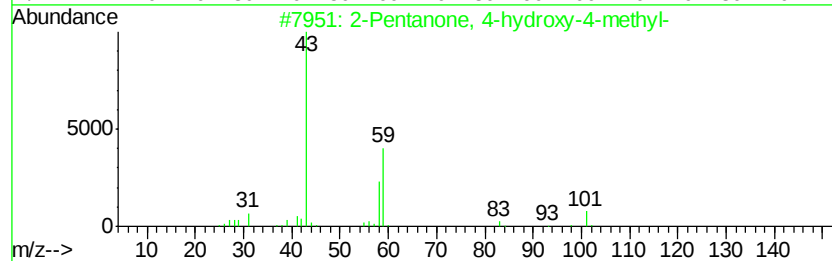
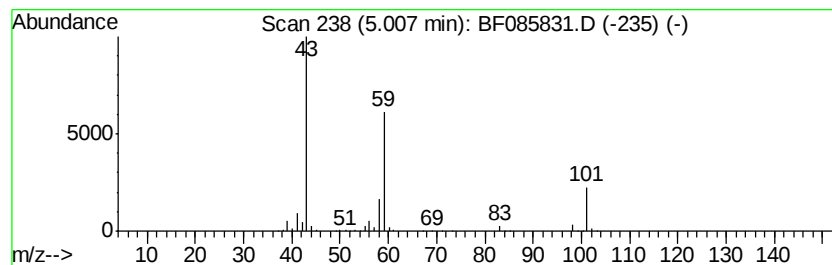
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	41.39 ng	1408210	1,4-Dichlorobenzene-d4	6.81

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-dimethy...	141	C7H11NO2	001116-98-9	25
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
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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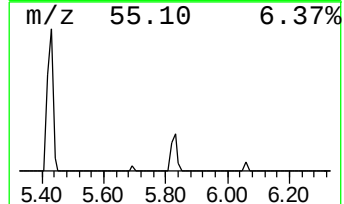
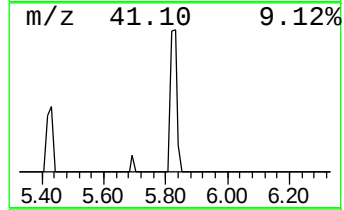
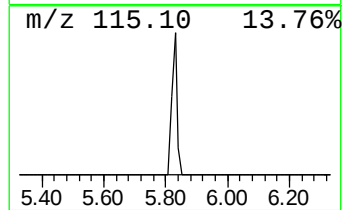
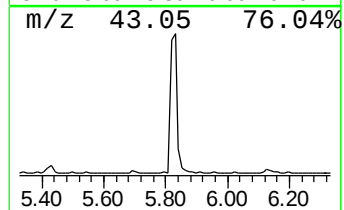
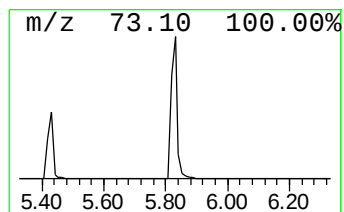
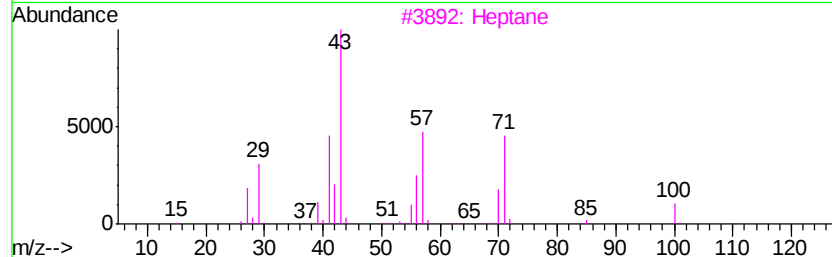
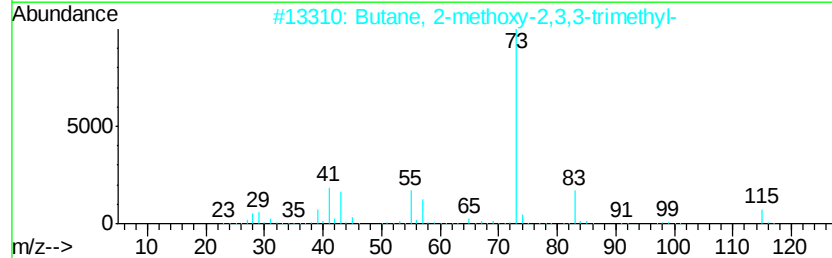
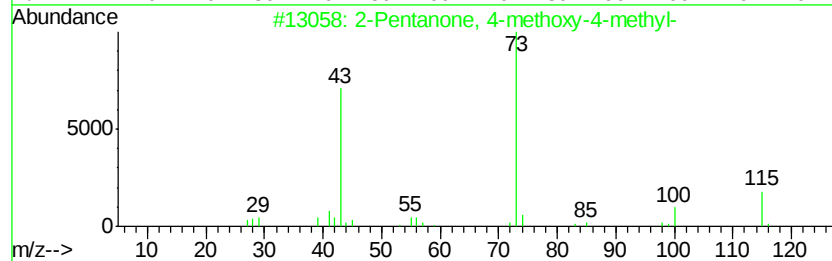
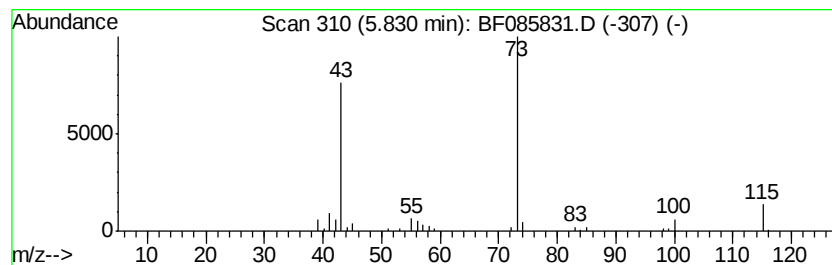
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.83	4.00 ng	136015	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
3		Heptane	100	C7H16	000142-82-5	16
4		6-Hydroxy-4,4,6-trimethyltetrahy...	191	C7H13NO2	016504-29-3	12
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	12



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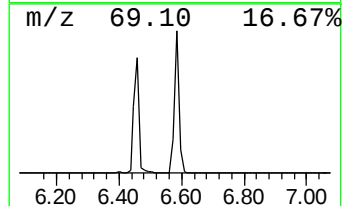
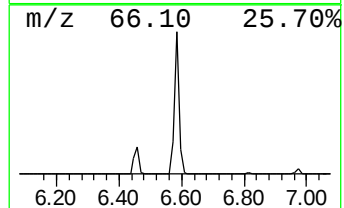
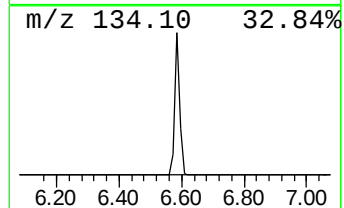
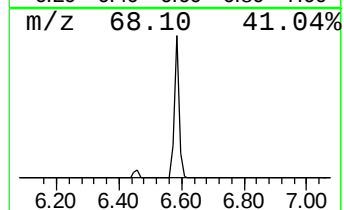
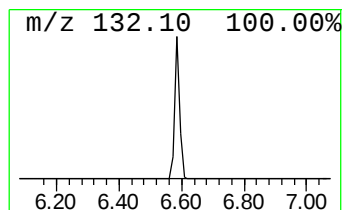
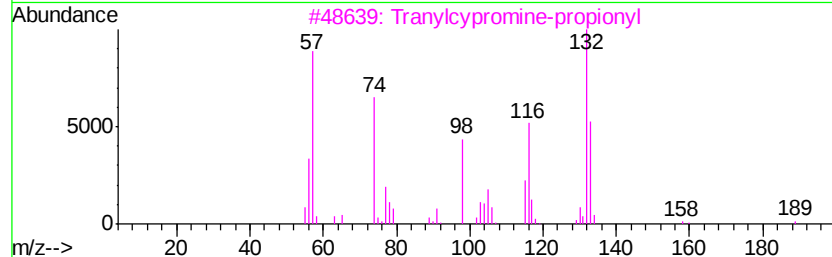
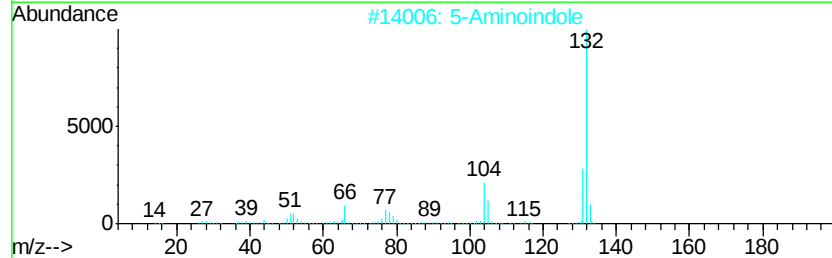
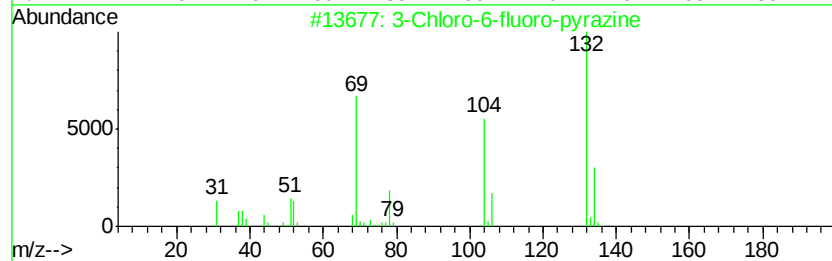
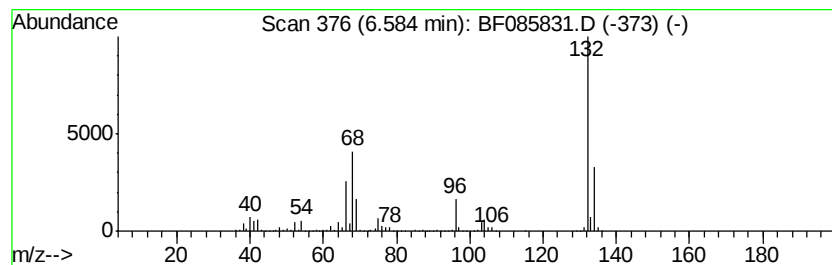
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	78.76 ng	2679410	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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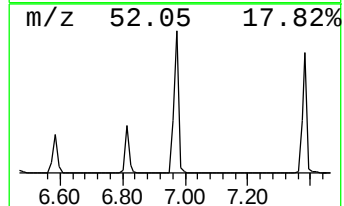
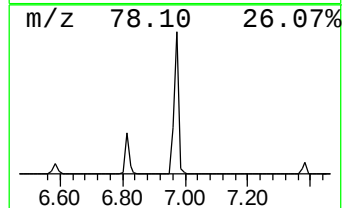
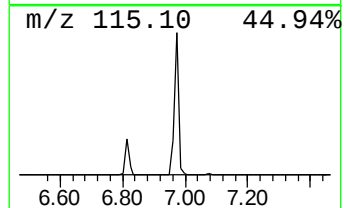
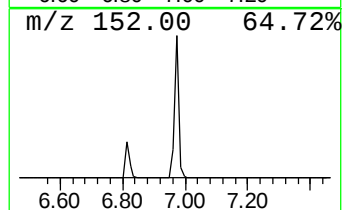
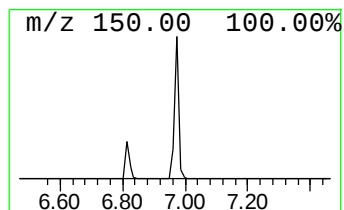
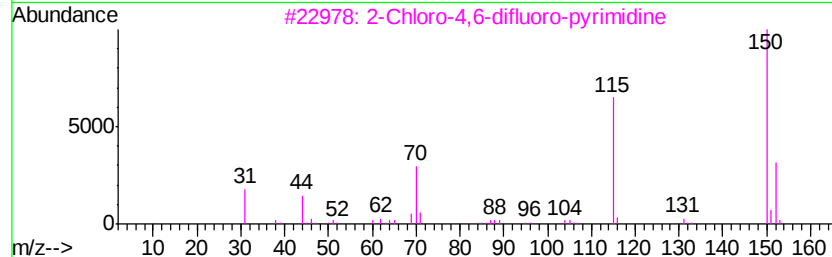
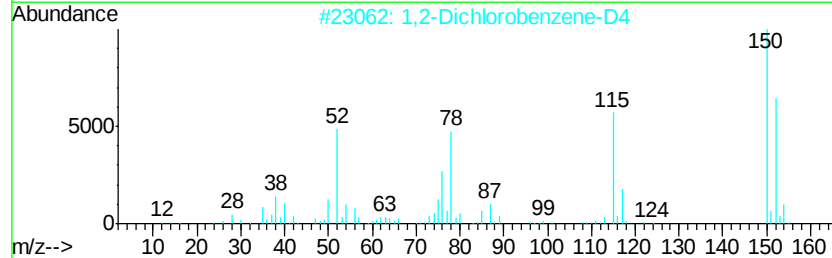
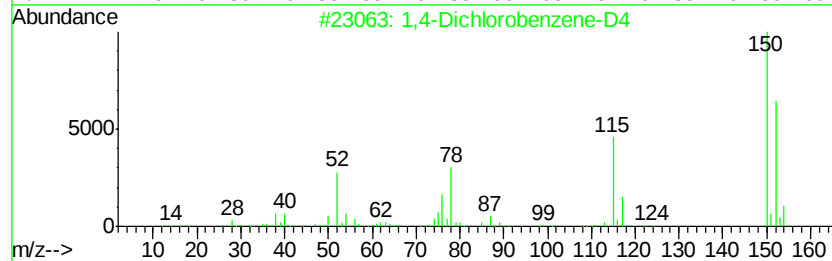
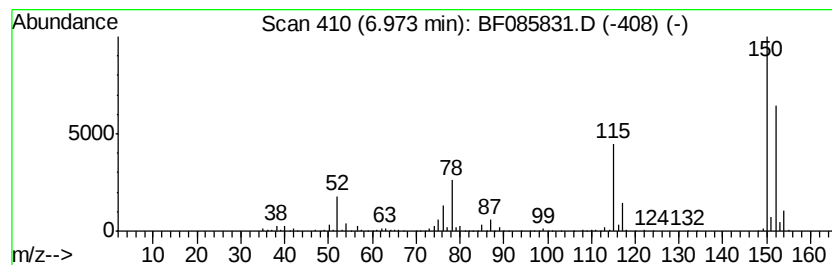
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 2-Chloro-4,6-difluoro-pyrim... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.97	72.40 ng	2463240	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
2		1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	91
3		2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	50
4		9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	22
5		But-2-yne-1,4-diol, o,o'-bis(3-n...	384	C18H12N2O8	055709-58-5	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.62	5.0	ng	170402	1	6.81	680409	20.0
2-Pentanone, 4-hy...	5.01	41.4	ng	1408210	1	6.81	680409	20.0
2-Pentanone, 4-me...	5.83	4.0	ng	136015	1	6.81	680409	20.0
unknown6.58	6.58	78.8	ng	2679410	1	6.81	680409	20.0
2-Chloro-4,6-difl...	6.97	72.4	ng	2463240	1	6.81	680409	20.0