

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020116\
 Data File : BF084730.D
 Acq On : 2 Feb 2016 1:00
 Operator : SJ/IZ
 Sample : H1286-16
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B024(5-7)

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-BF020116.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	4.167	178	182	188	rBV2	186928	300607	7.75%	0.745%
2	4.304	191	194	197	rBV	59661	84250	2.17%	0.209%
3	4.658	223	225	229	rVB	35652	40208	1.04%	0.100%
4	4.864	240	243	246	rBV	1969330	3086641	79.62%	7.650%
5	5.310	279	282	284	rBV	3133133	3637208	93.82%	9.015%
6	5.710	315	317	319	rBV	215483	187104	4.83%	0.464%
7	6.361	371	374	376	rBV	3320797	3868576	99.79%	9.588%
8	6.476	382	384	387	rBV	3571420	3350527	86.43%	8.304%
9	6.704	402	404	407	rBV	953837	979383	25.26%	2.427%
10	6.864	416	418	420	rBV	3276254	2707048	69.83%	6.709%
11	7.276	451	454	456	rBV	2355650	2186897	56.41%	5.420%
12	7.996	515	517	519	rBV	1675078	1409308	36.35%	3.493%
13	9.070	609	611	614	rBV	2797300	3876685	100.00%	9.608%
14	9.470	644	646	648	rBV	553863	518345	13.37%	1.285%
15	9.688	664	665	668	rBV	60374	65163	1.68%	0.162%
16	9.745	668	670	672	rBV	1567683	1456709	37.58%	3.610%
17	10.190	707	709	711	rVB	137532	108637	2.80%	0.269%
18	10.408	725	728	731	rBV	38773	61549	1.59%	0.153%
19	10.533	736	739	741	rBV	2650169	2513696	64.84%	6.230%
20	10.659	749	750	757	rVB	137496	162732	4.20%	0.403%
21	11.105	788	789	794	rVB	70946	98012	2.53%	0.243%
22	11.231	797	800	803	rVV	1139133	1704352	43.96%	4.224%
23	11.299	803	806	808	rVB2	42967	52277	1.35%	0.130%
24	11.756	844	846	849	rVB	52507	51249	1.32%	0.127%
25	11.836	851	853	857	rVB2	48303	66184	1.71%	0.164%
26	12.431	903	905	908	rBV	470663	400681	10.34%	0.993%
27	12.659	922	925	927	rBV	396264	393771	10.16%	0.976%
28	12.808	936	938	941	rVB	2655304	3630673	93.65%	8.999%
29	12.945	948	950	951	rBV	53488	46951	1.21%	0.116%
30	12.991	951	954	956	rVB	33878	46163	1.19%	0.114%
31	13.299	979	981	986	rVB	39515	75258	1.94%	0.187%
32	13.734	1017	1019	1026	rVB2	55156	129476	3.34%	0.321%
33	13.859	1027	1030	1031	rVV	1133248	1429573	36.88%	3.543%
34	13.882	1031	1032	1034	rVB	144868	101939	2.63%	0.253%

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SUP-B024(5-7)

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-BF020116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.854	1115	1117	1121	rBV	134633	241140	6.22%	0.598%
36	15.128	1138	1141	1143	rVB	62604	84021	2.17%	0.208%
37	15.174	1143	1145	1148	rVB	77133	106350	2.74%	0.264%
38	15.231	1148	1150	1153	rBV	622739	912232	23.53%	2.261%
39	16.534	1261	1264	1269	rBV2	43541	92224	2.38%	0.229%
40	16.923	1295	1298	1303	rVB	43493	82864	2.14%	0.205%

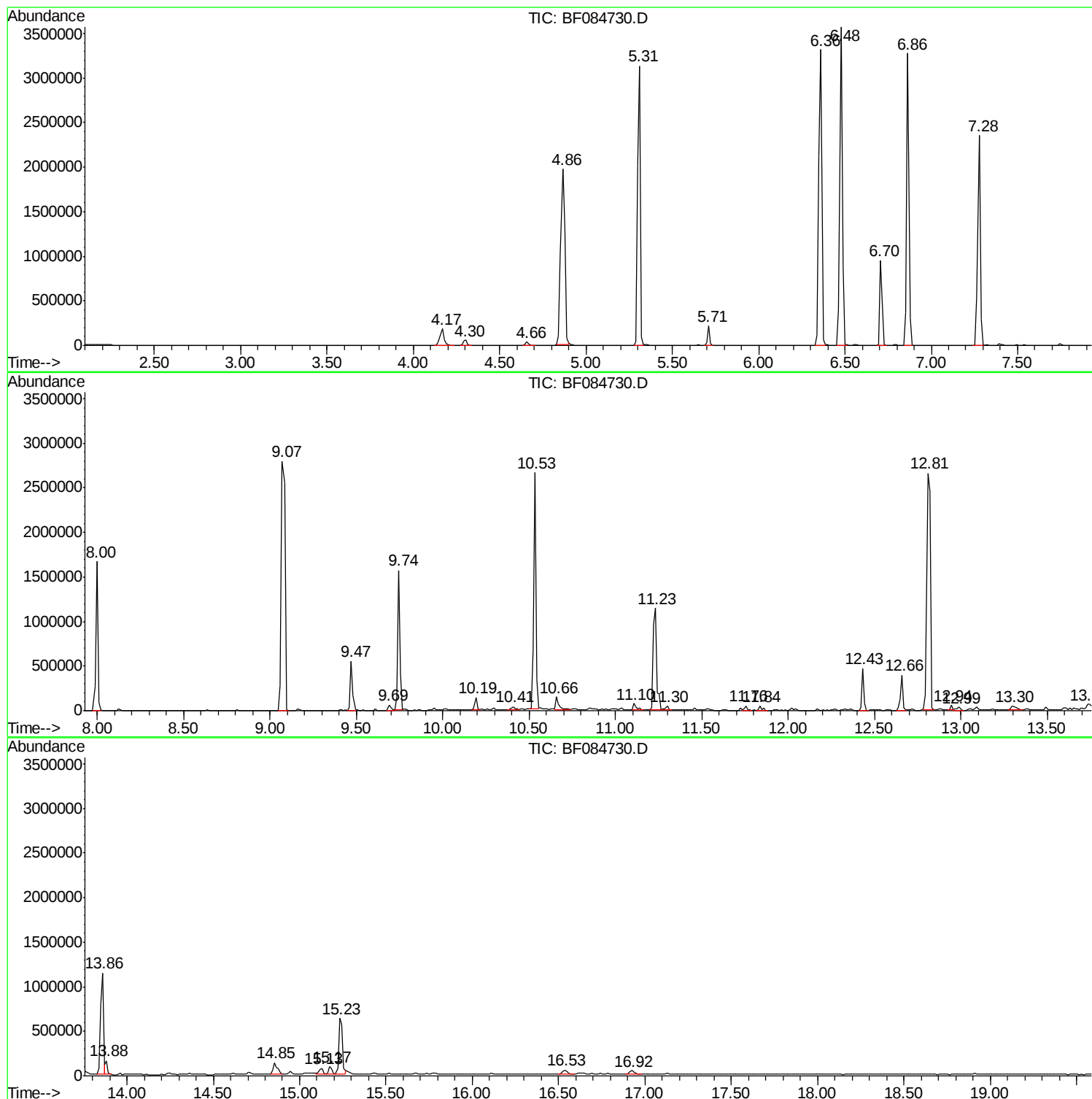
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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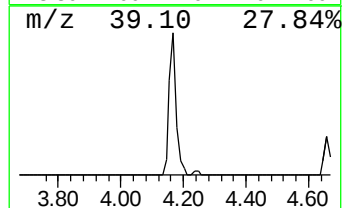
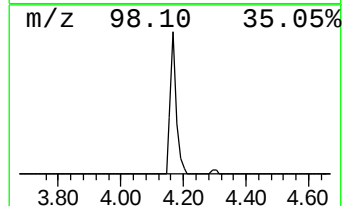
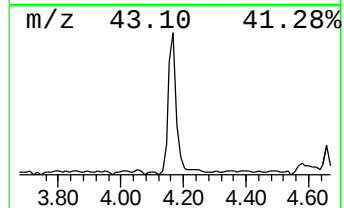
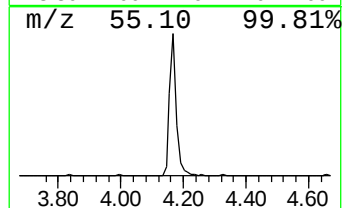
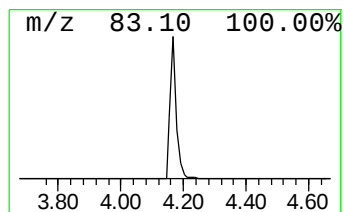
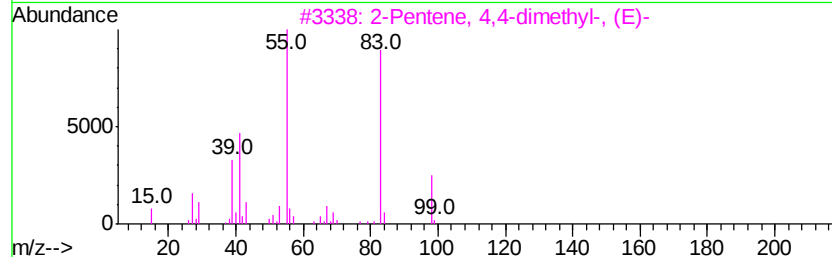
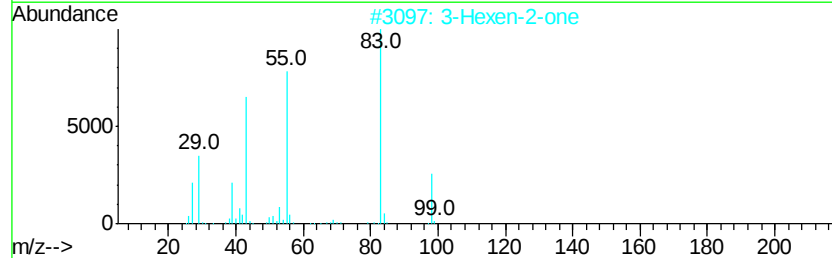
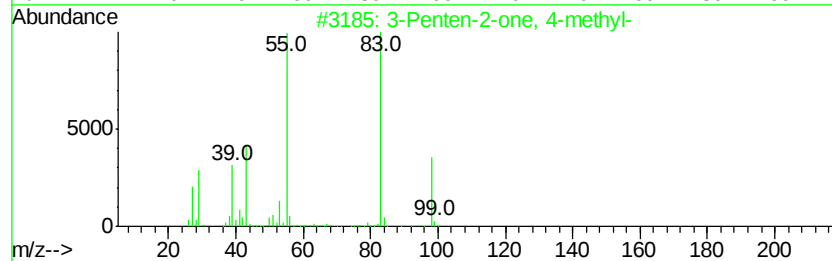
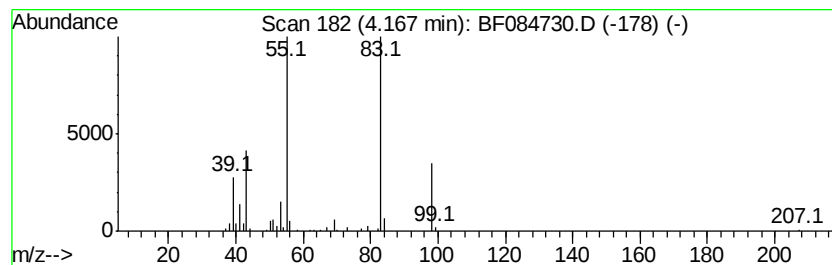
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.17	6.14 ng	300607	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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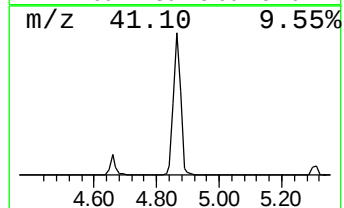
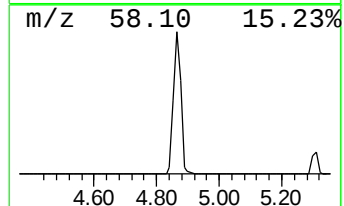
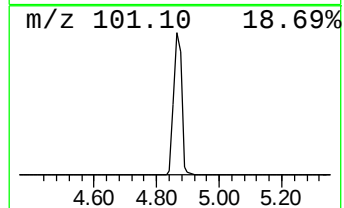
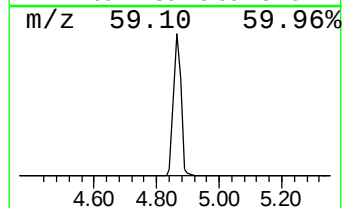
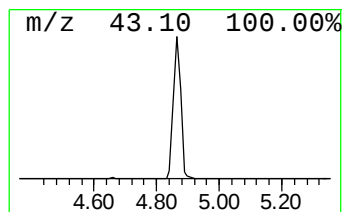
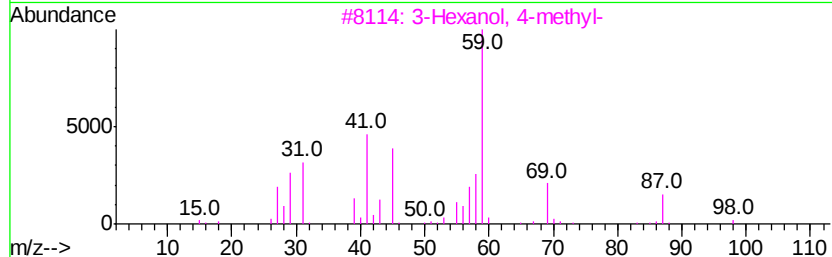
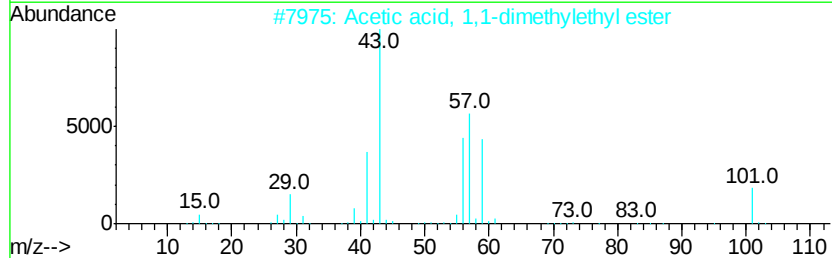
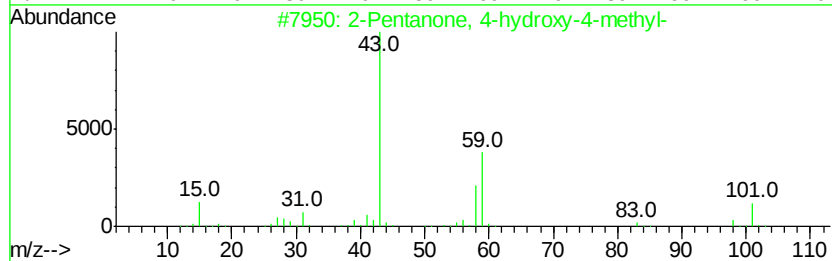
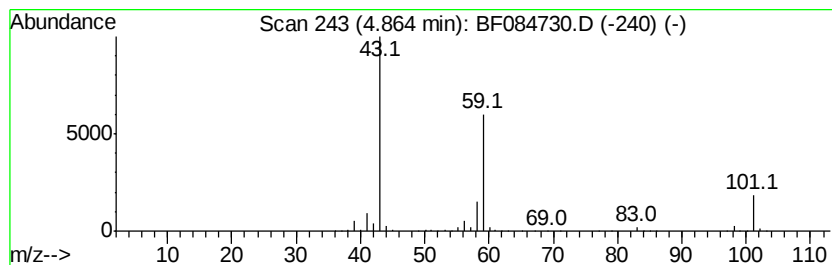
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	63.03 ng	3086640	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	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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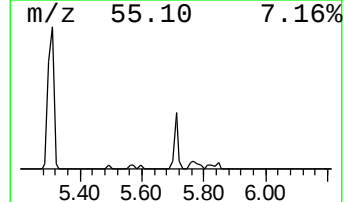
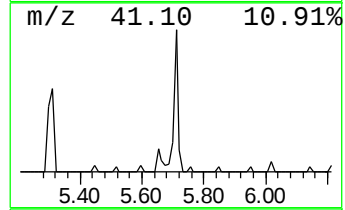
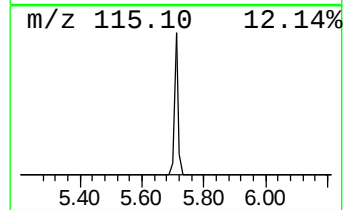
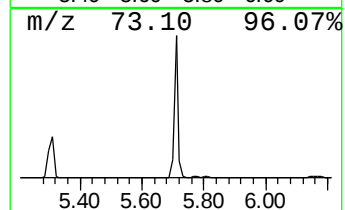
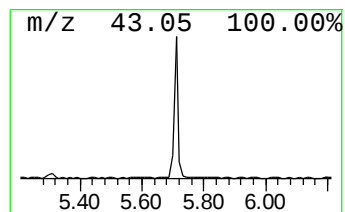
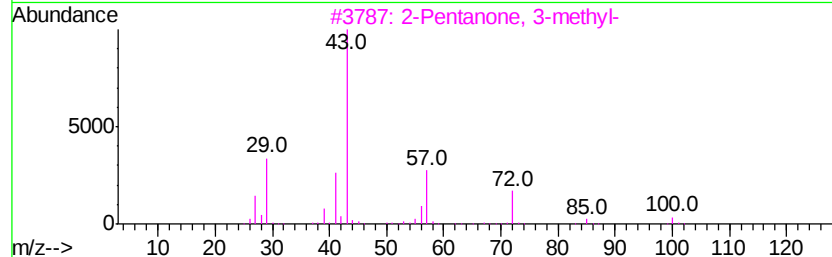
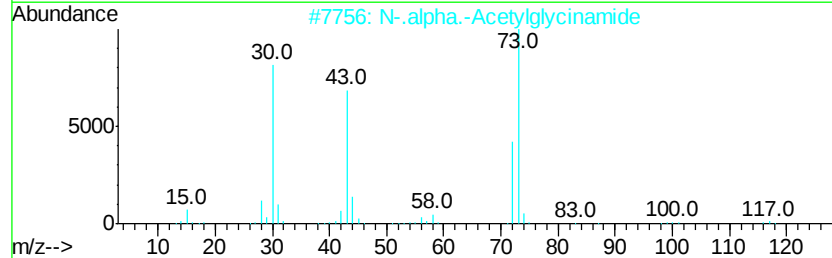
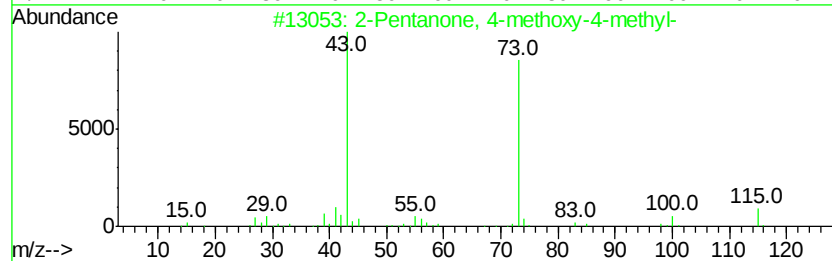
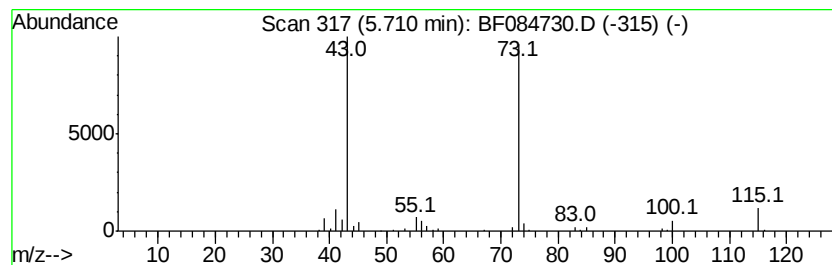
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	3.82 ng	187104	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglucineamide	116	C4H8N2O2	002620-63-5	25
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5		Heptane	100	C7H16	000142-82-5	9



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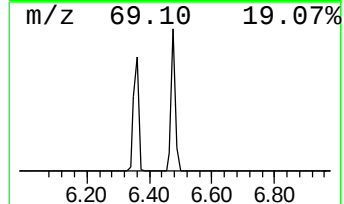
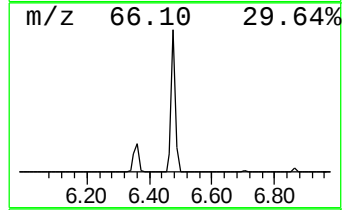
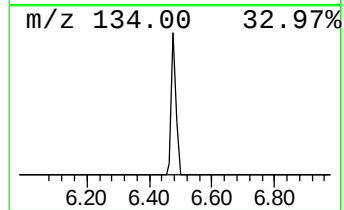
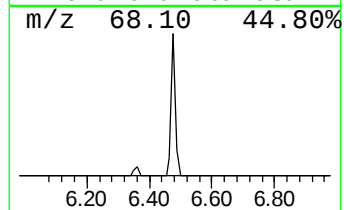
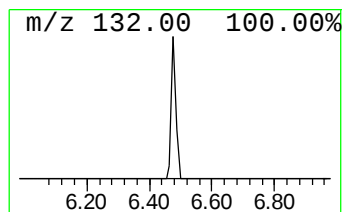
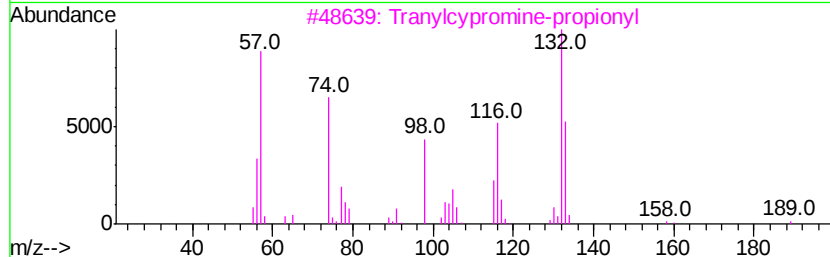
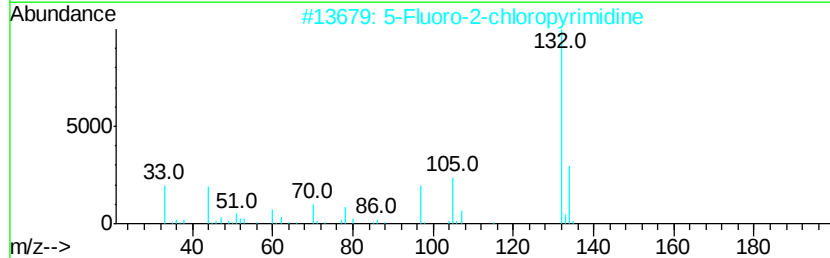
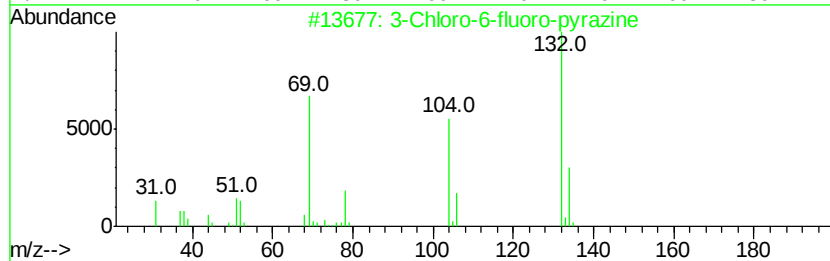
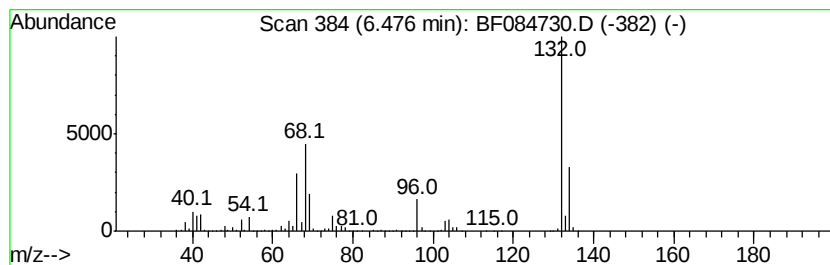
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	68.42 ng	3350530	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.17	6.1	ng	300607	1	6.70	979383	20.0
2-Pentanone, 4-hy...	4.86	63.0	ng	3086640	1	6.70	979383	20.0
2-Pentanone, 4-me...	5.71	3.8	ng	187104	1	6.70	979383	20.0
unknown6.48	6.48	68.4	ng	3350530	1	6.70	979383	20.0