

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011516\
 Data File : BF084520.D
 Acq On : 16 Jan 2016 5:20
 Operator : SJ/UM
 Sample : H1144-07
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-2

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-BF123115.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	4.327	194	196	200	rBV	229842	286825	3.24%	0.496%
2	4.990	251	254	257	rBV	1559722	1765546	19.96%	3.054%
3	5.424	289	292	294	rBV	4100429	3670712	41.50%	6.349%
4	5.824	325	327	329	rBV	392002	332378	3.76%	0.575%
5	6.464	380	383	385	rBV	1690709	2228036	25.19%	3.854%
6	6.590	391	394	396	rBV	6481553	5912082	66.83%	10.226%
7	6.819	412	414	416	rBV	1896055	1538083	17.39%	2.660%
8	6.979	425	428	430	rBV	6689632	5971409	67.50%	10.329%
9	7.390	461	464	466	rBV	5149288	5224747	59.06%	9.037%
10	8.110	524	527	529	rBV	1933475	2010445	22.73%	3.478%
11	9.185	618	621	624	rBV	6362894	8846054	100.00%	15.301%
12	9.859	678	680	683	rBV	2000362	2063781	23.33%	3.570%
13	10.282	715	717	720	rVB2	66143	110118	1.24%	0.190%
14	10.659	747	750	752	rBV2	3648801	5150800	58.23%	8.909%
15	11.345	808	810	813	rBV	2299980	1968121	22.25%	3.404%
16	12.751	931	933	936	rBV2	154431	170004	1.92%	0.294%
17	12.934	946	949	951	rBV	5438079	6800866	76.88%	11.764%
18	12.968	951	952	954	rVB	950658	671541	7.59%	1.162%
19	13.985	1038	1041	1043	rBV	1570458	1625958	18.38%	2.812%
20	15.402	1162	1165	1168	rBV	1194648	1465243	16.56%	2.534%

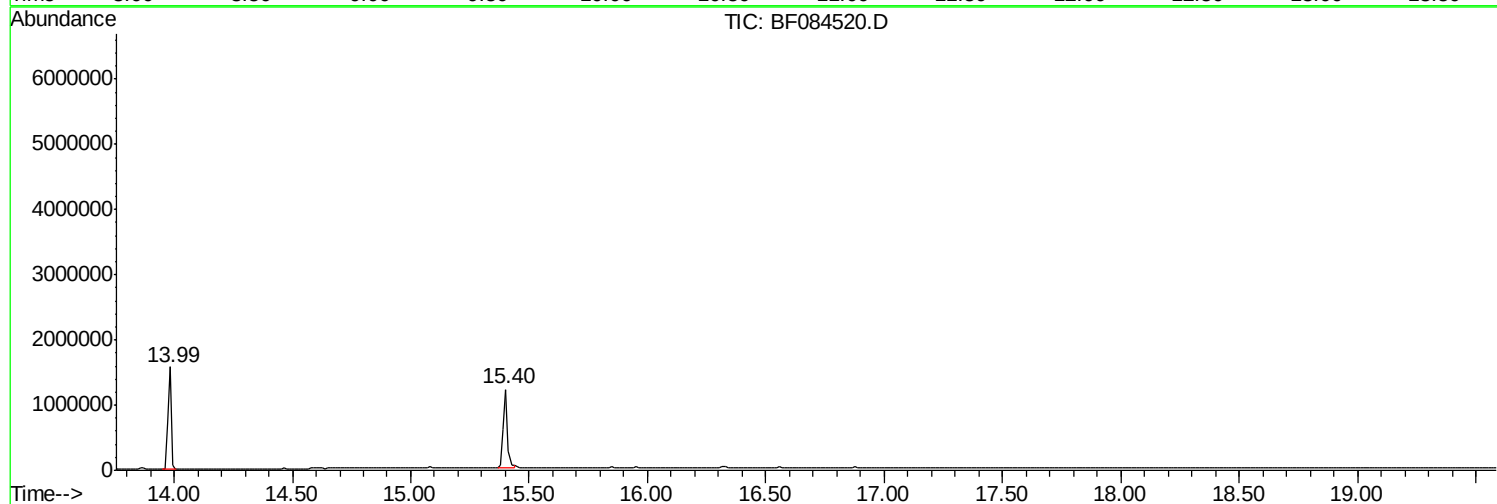
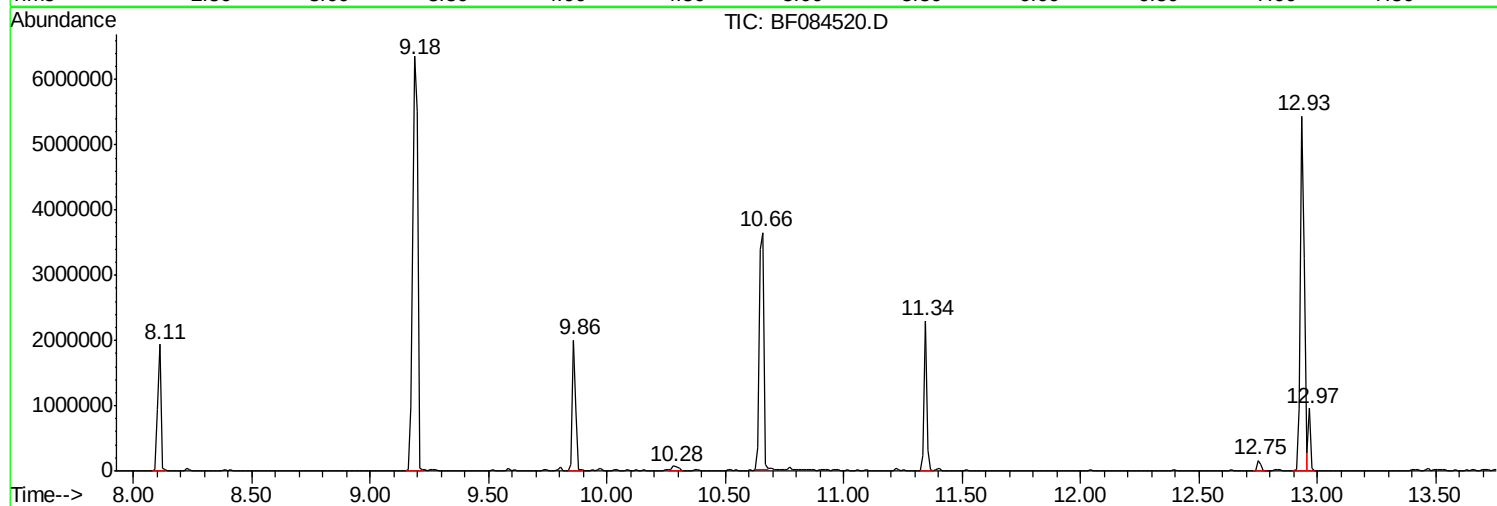
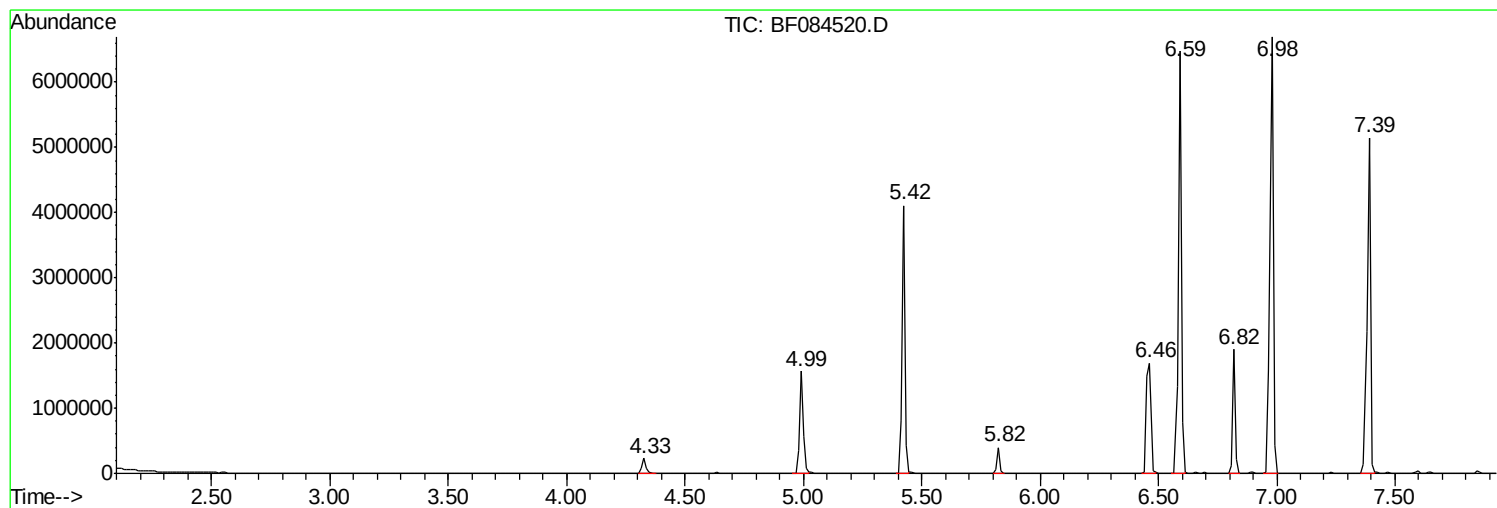
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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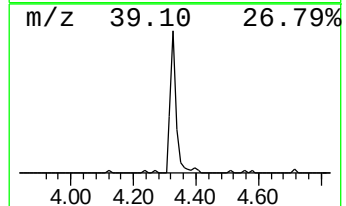
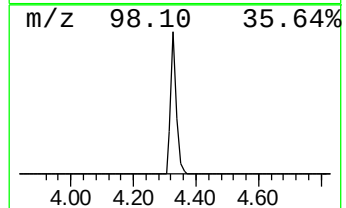
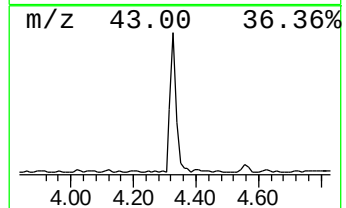
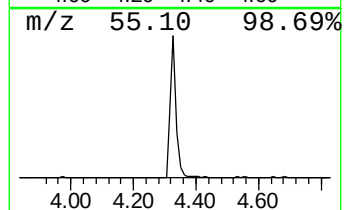
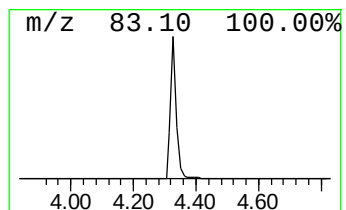
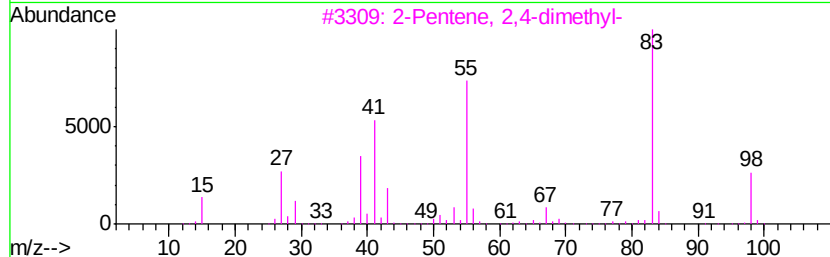
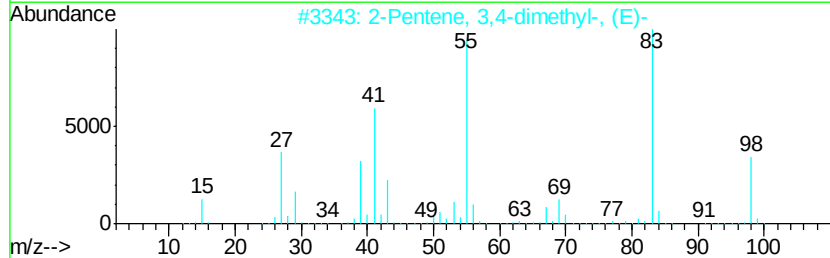
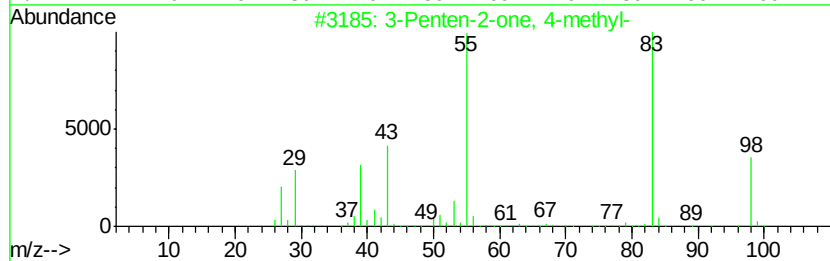
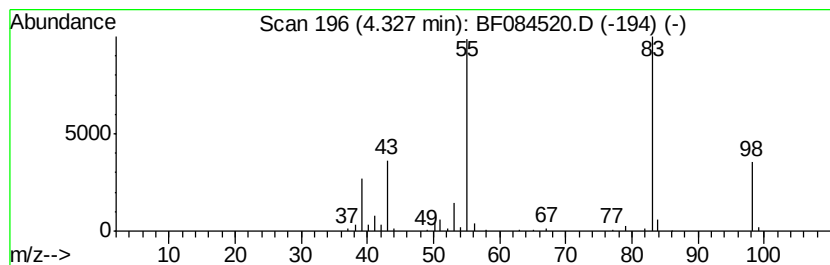
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	3.73 ng	286825	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		3-Hexen-2-one	98	C6H10O	000763-93-9	86



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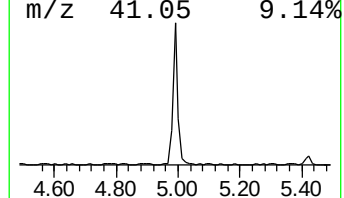
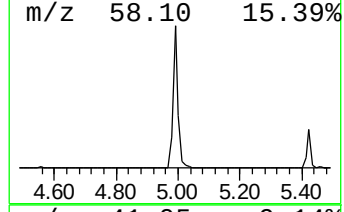
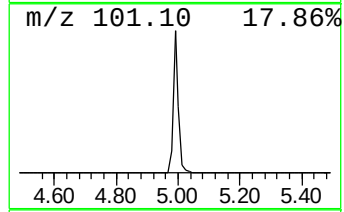
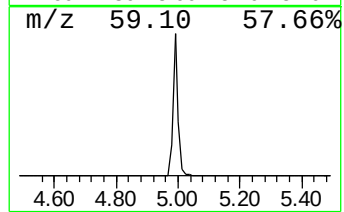
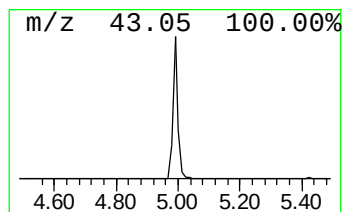
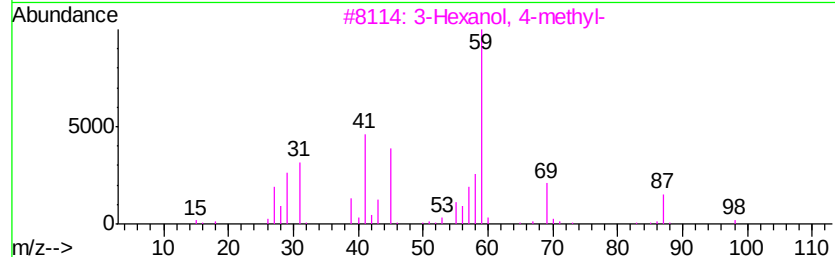
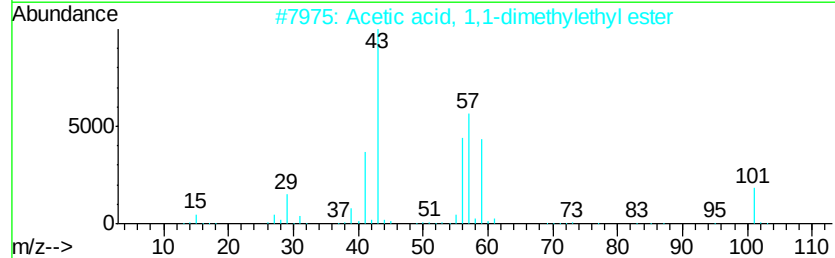
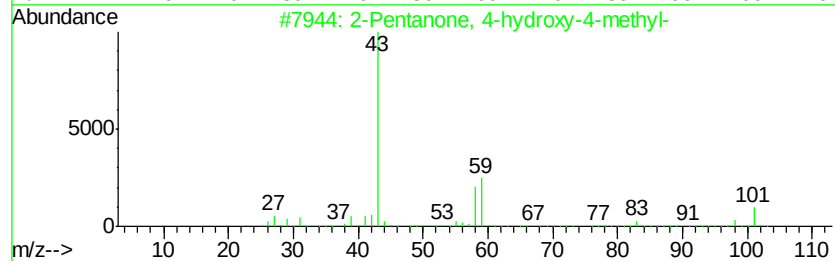
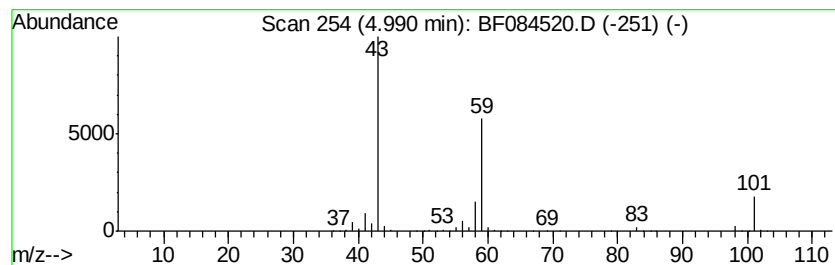
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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.
4.99	22.96 ng	1765550	1,4-Dichlorobenzene-d4	6.82

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	23



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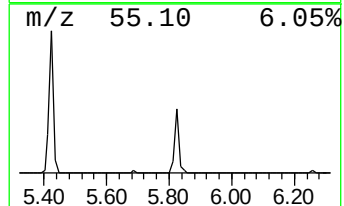
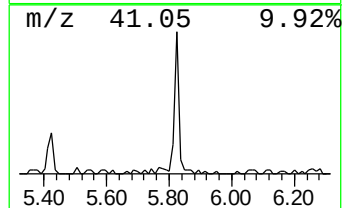
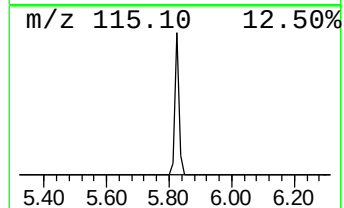
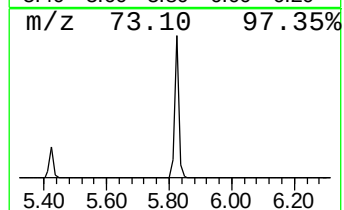
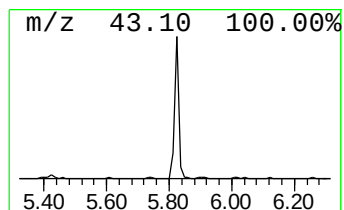
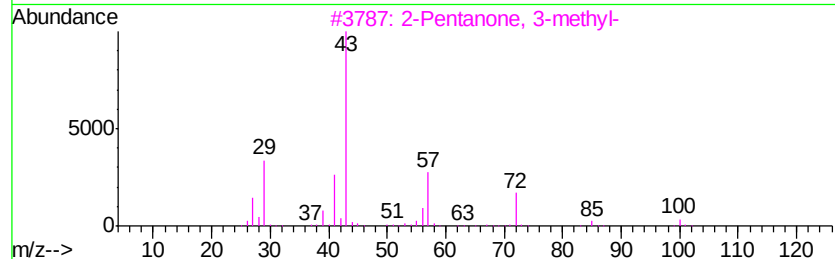
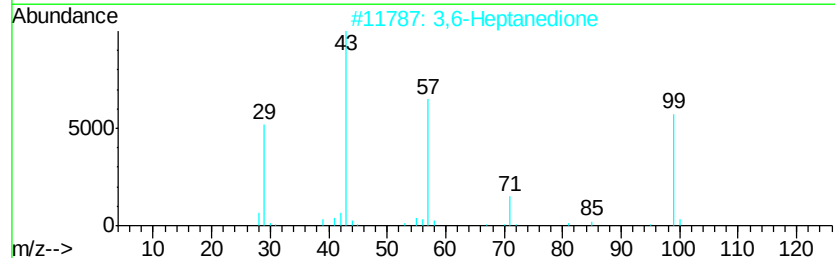
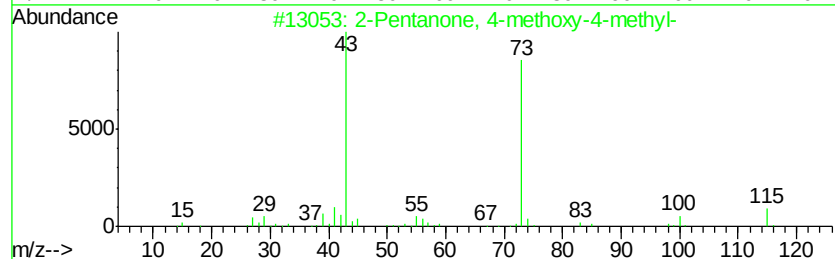
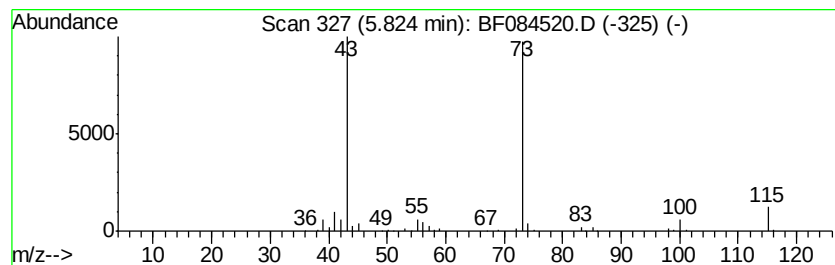
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	4.32 ng	332378	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3,6-Heptanedione	128	C7H12O2	001703-51-1	17
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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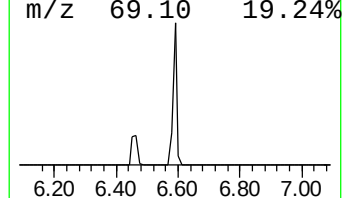
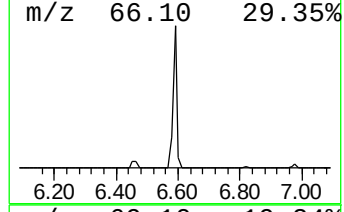
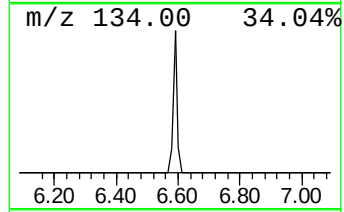
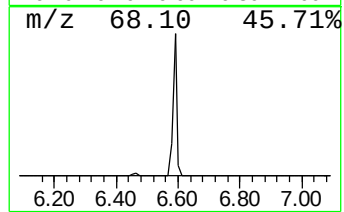
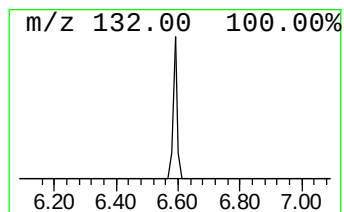
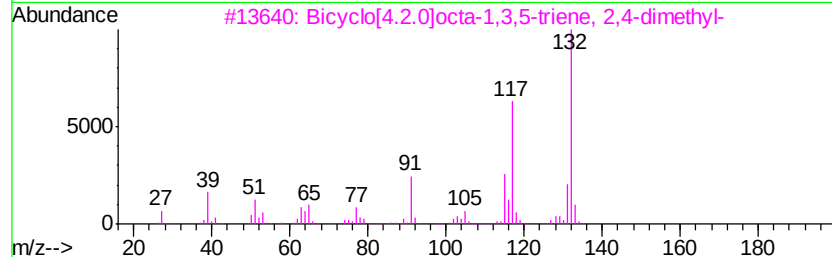
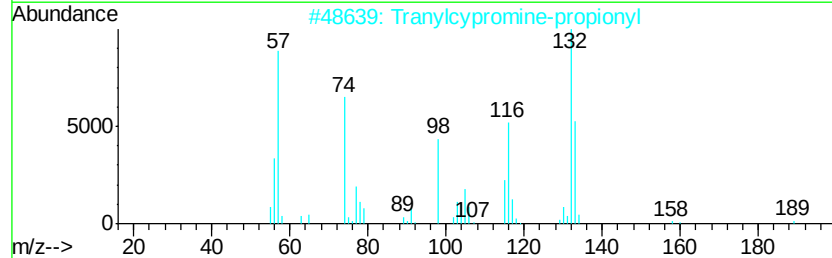
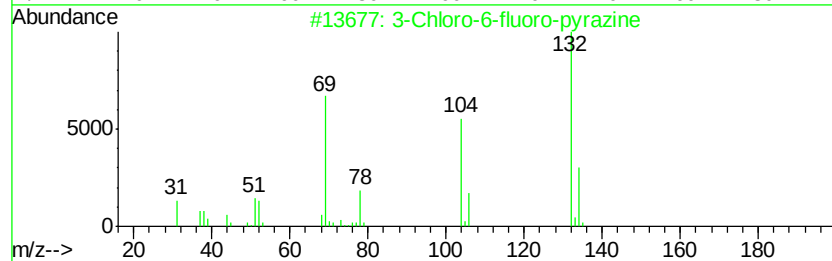
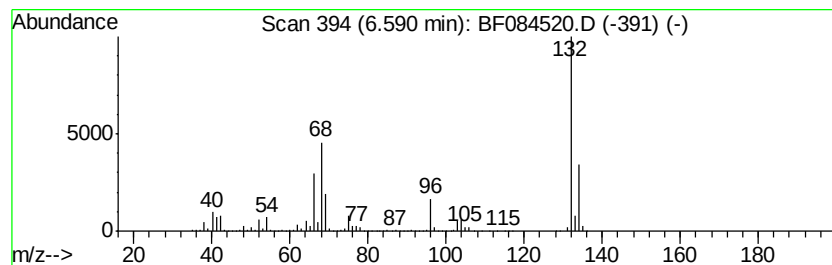
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	76.88 ng	5912080	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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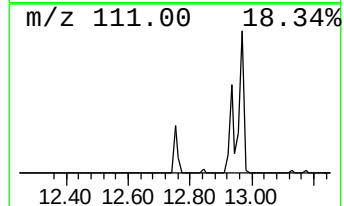
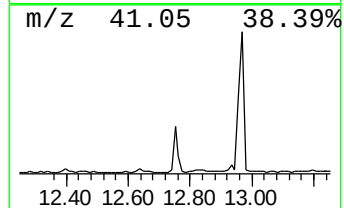
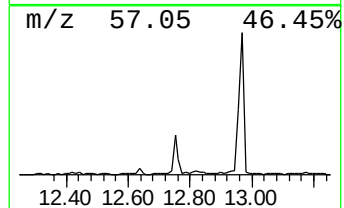
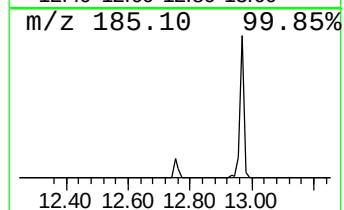
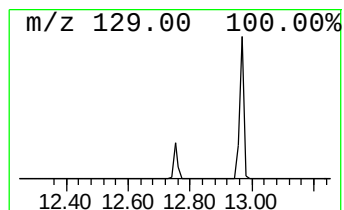
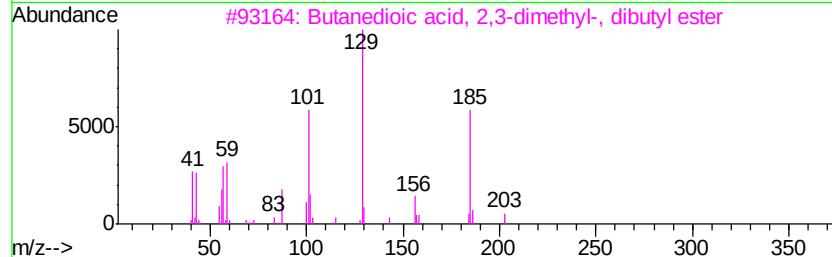
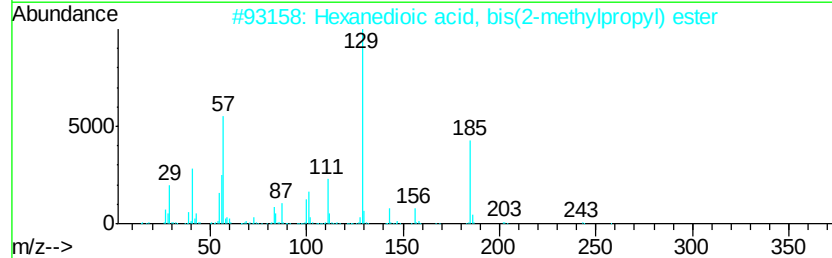
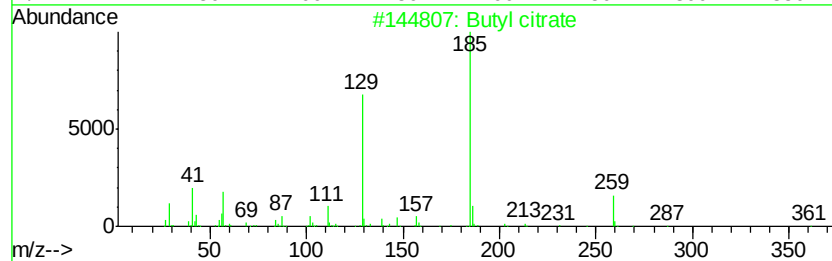
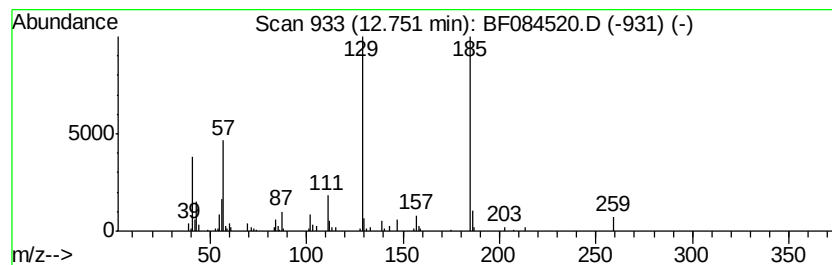
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 Peak Number 6 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	2.09 ng	170004	Chrysene-d12	13.99
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl citrate	360 C18H32O7	000077-94-1 91
2		Hexanedioic acid, bis(2-methylpr...	258 C14H26O4	000141-04-8 78
3		Butanedioic acid, 2,3-dimethyl-,...	258 C14H26O4	056051-57-1 56
4		Hexanedioic acid, bis(1-methylpr...	258 C14H26O4	038447-22-2 43
5		5-Hydroxy-4-nitroguaiacol	185 C7H7NO5	100960-04-1 25



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.33	3.7	ng	286825	1	6.82	1538080	20.0
2-Pentanone, 4-hy...	4.99	23.0	ng	1765550	1	6.82	1538080	20.0
2-Pentanone, 4-me...	5.82	4.3	ng	332378	1	6.82	1538080	20.0
unknown6.59	6.59	76.9	ng	5912080	1	6.82	1538080	20.0
Butyl citrate	12.75	2.1	ng	170004	5	13.99	1625960	20.0