

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011916\
 Data File : BF084550.D
 Acq On : 19 Jan 2016 14:20
 Operator : SJ/UM
 Sample : PB87864BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87864BL

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	4.304	192	194	201	rVB	230629	286592	4.01%	0.484%
2	4.979	250	253	265	rBV	2751529	4032947	56.43%	6.810%
3	5.402	287	290	293	rBV	5312731	5314778	74.37%	8.974%
4	5.802	323	325	327	rBV	188003	191881	2.68%	0.324%
5	6.442	377	381	383	rBV	4815983	6204393	86.82%	10.476%
6	6.567	389	392	394	rBV	4383696	5888424	82.40%	9.942%
7	6.796	409	412	414	rBV	980664	1299194	18.18%	2.194%
8	6.945	423	425	428	rBV	4238516	4235319	59.26%	7.151%
9	7.356	458	461	464	rBV	3402535	3492032	48.86%	5.896%
10	8.076	521	524	527	rBV	1956258	1791757	25.07%	3.025%
11	9.162	615	619	621	rBV	5779254	7084161	99.13%	11.961%
12	9.836	675	678	680	rBV	1598014	2034082	28.46%	3.434%
13	10.625	744	747	749	rBV	3745589	4454285	62.33%	7.521%
14	11.311	805	807	810	rBV	2099531	2028880	28.39%	3.426%
15	12.911	944	947	949	rBV	4908945	7146420	100.00%	12.067%
16	13.951	1035	1038	1040	rBV	2016819	2049620	28.68%	3.461%
17	15.357	1158	1161	1164	rBV	1229578	1438543	20.13%	2.429%
18	15.780	1192	1198	1206	rVB2	67482	251911	3.52%	0.425%

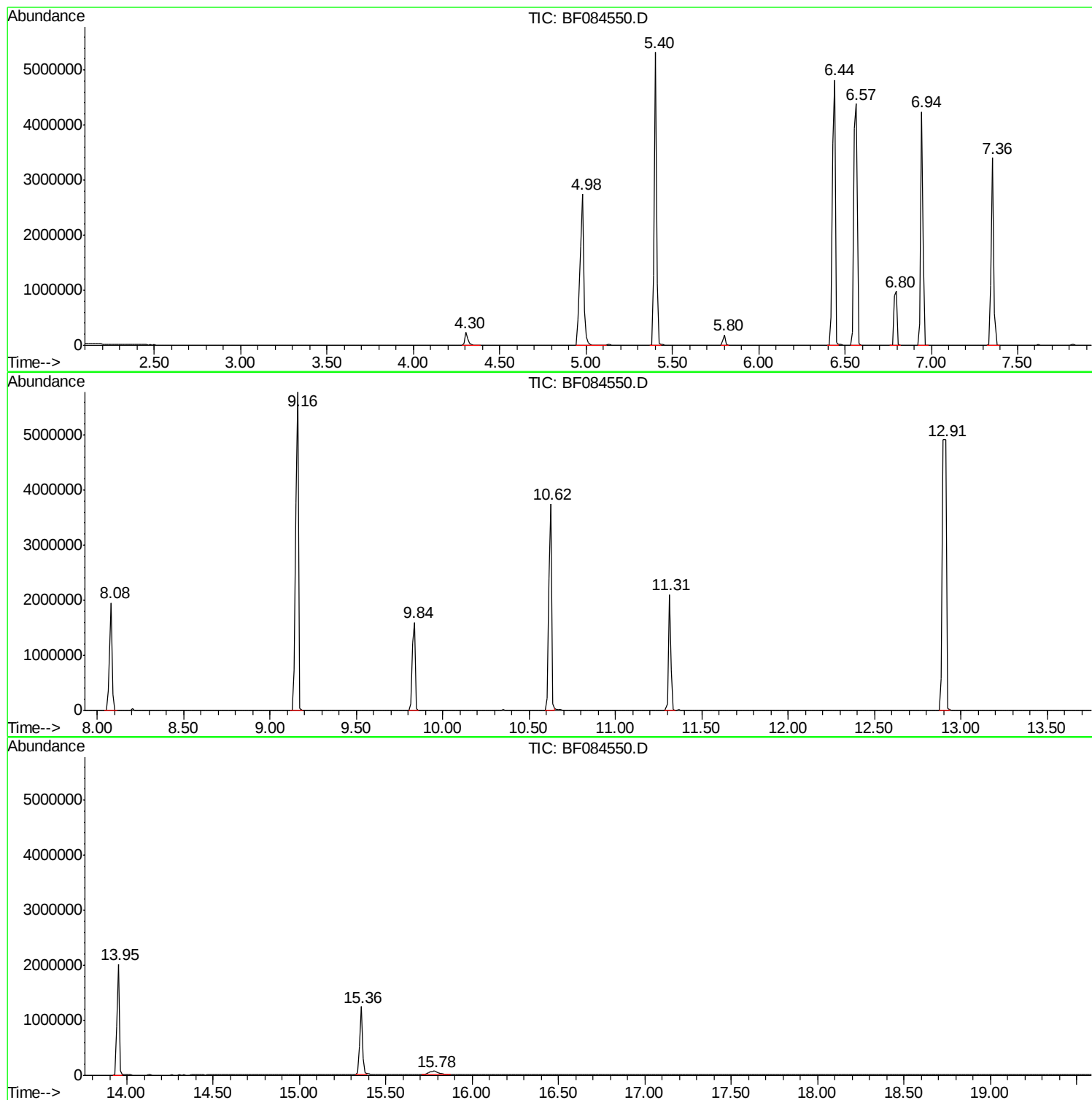
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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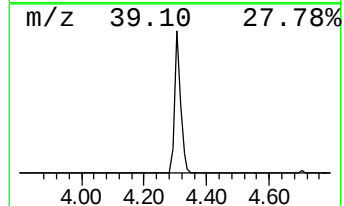
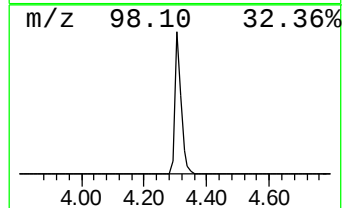
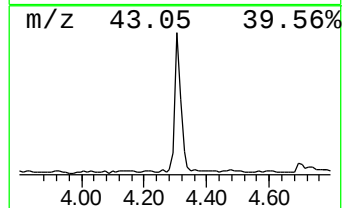
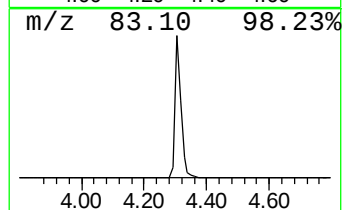
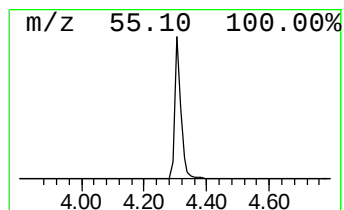
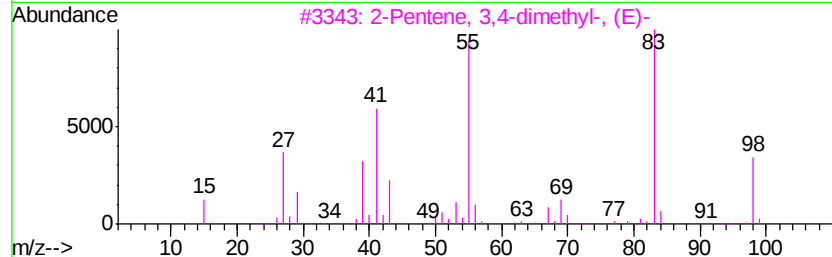
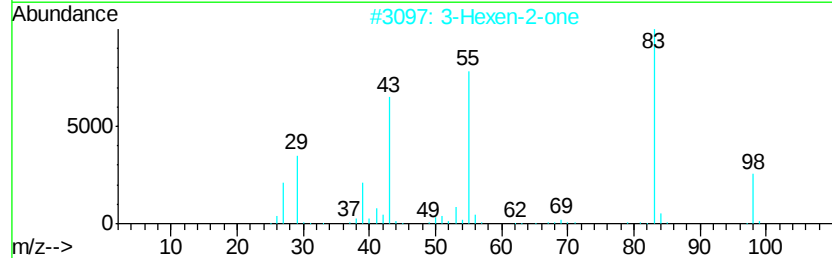
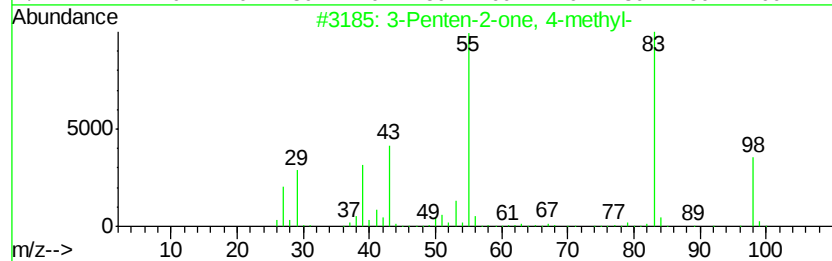
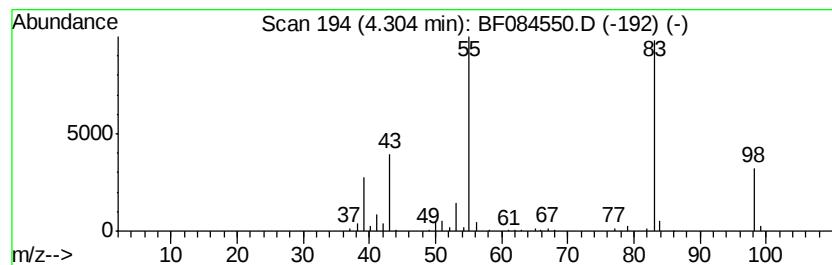
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	4.41 ng	286592	1,4-Dichlorobenzene-d4	6.80

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	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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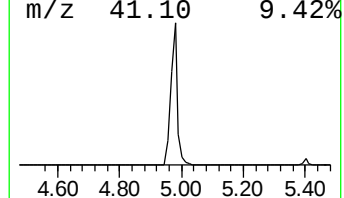
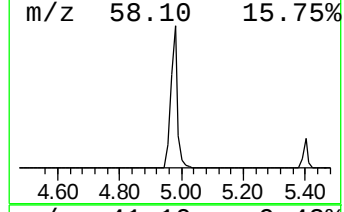
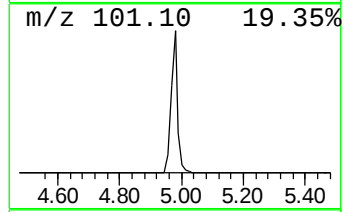
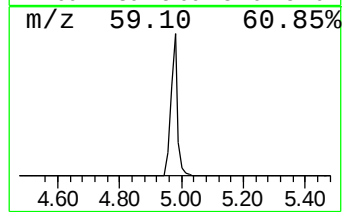
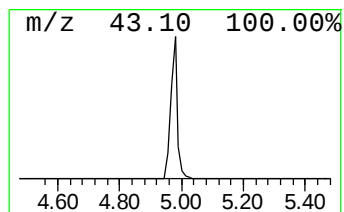
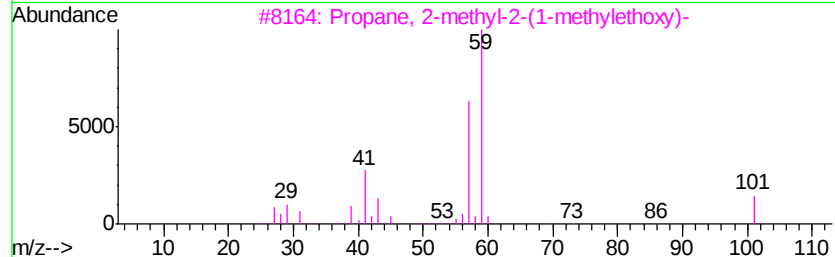
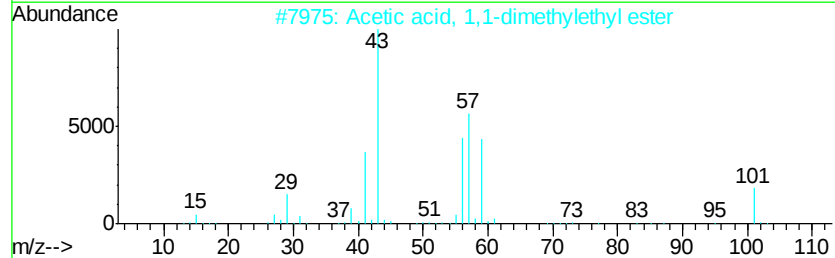
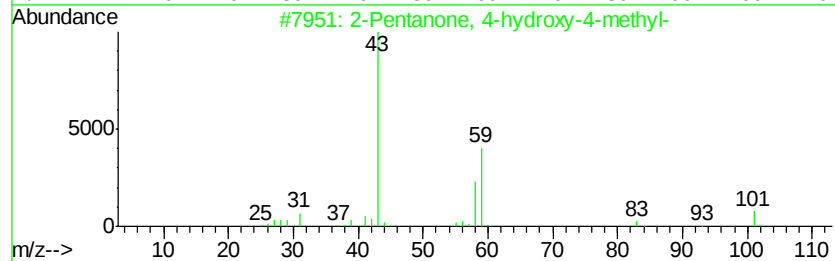
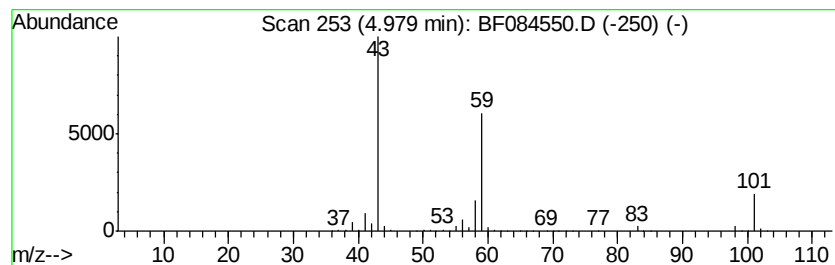
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	62.08 ng	4032950	1,4-Dichlorobenzene-d4	6.80

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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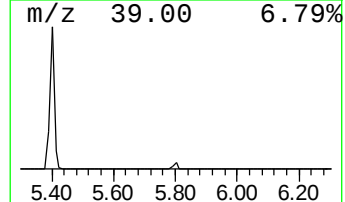
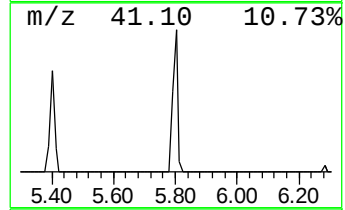
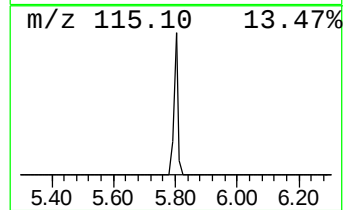
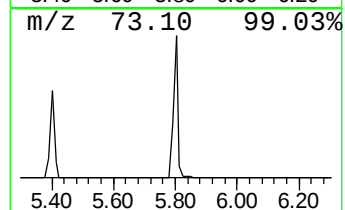
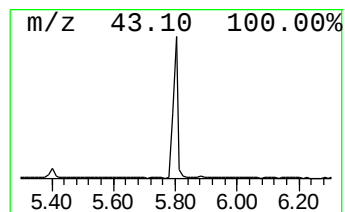
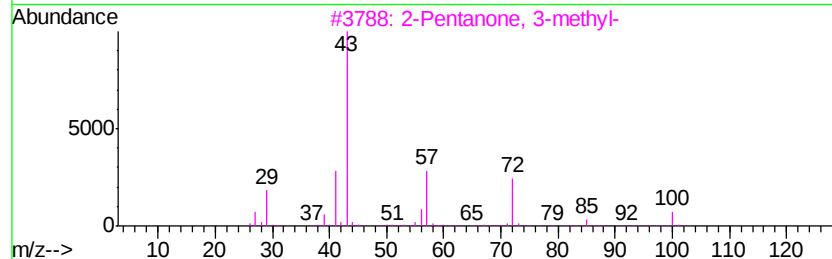
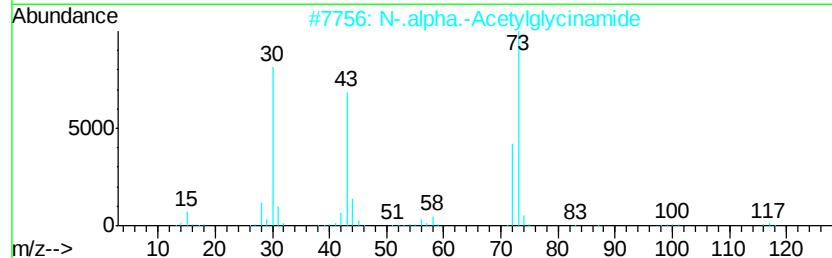
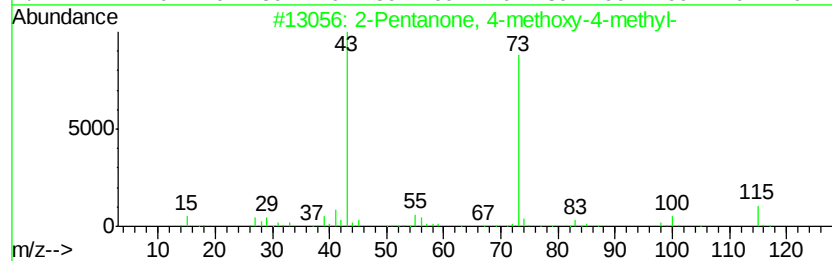
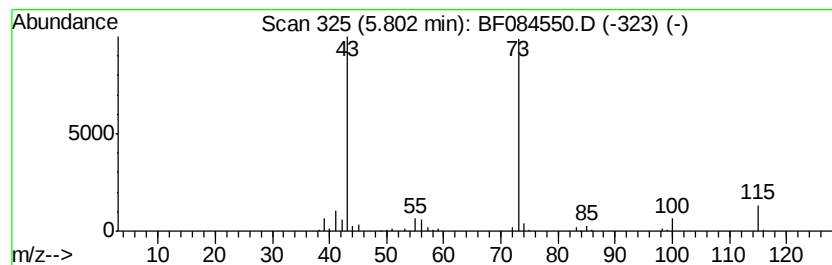
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	2.95 ng	191881	1,4-Dichlorobenzene-d4	6.80

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	16
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
5		3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	12



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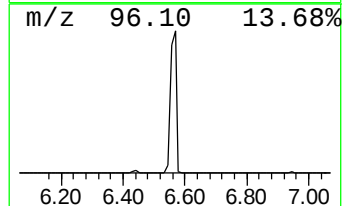
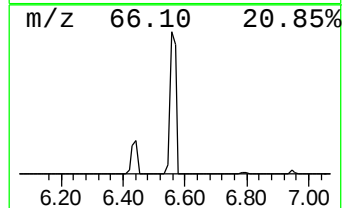
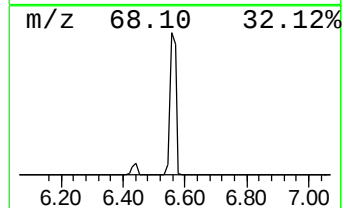
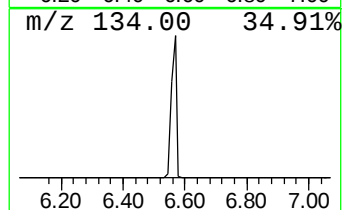
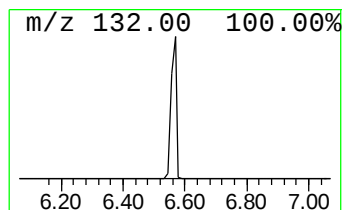
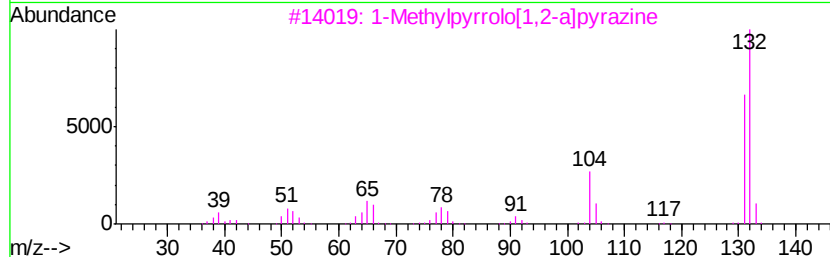
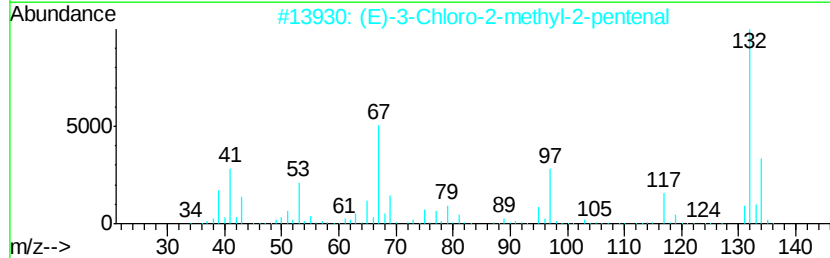
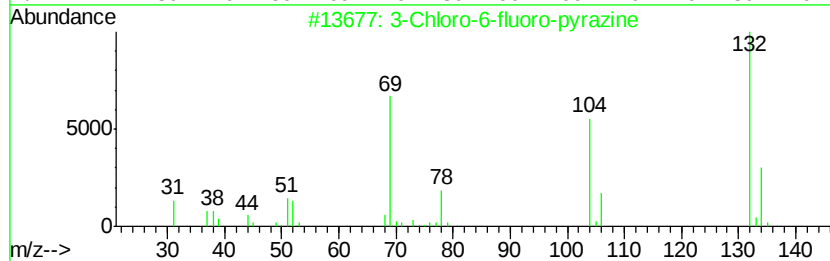
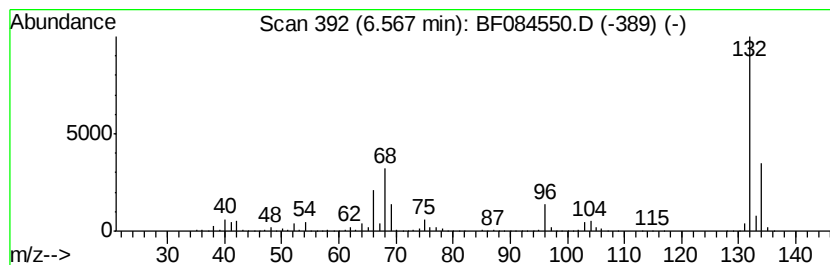
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	90.65 ng	5888420	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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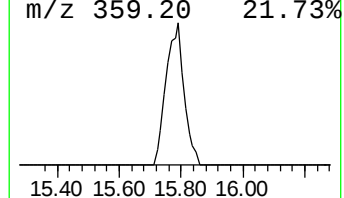
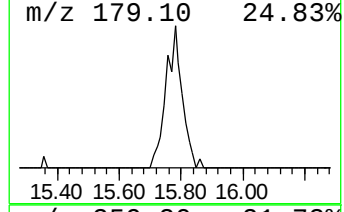
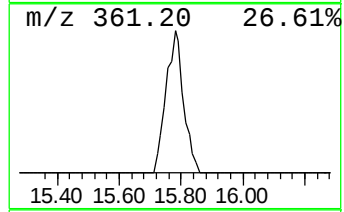
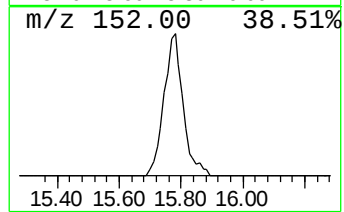
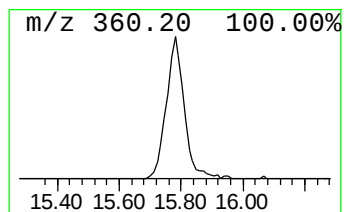
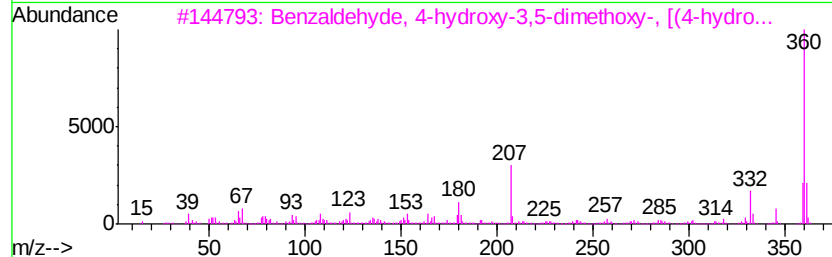
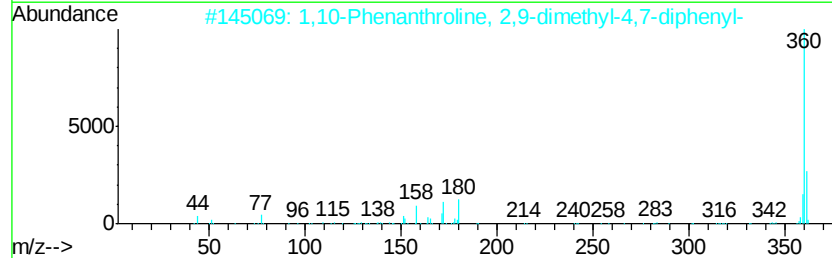
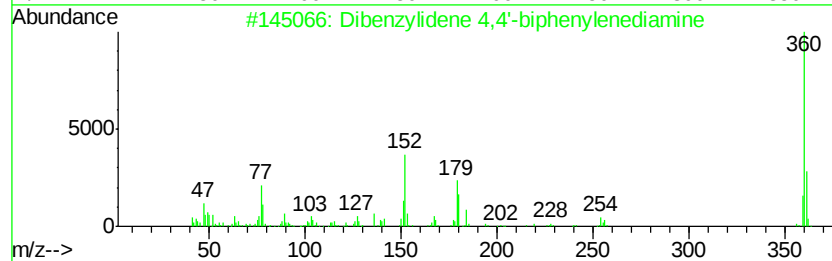
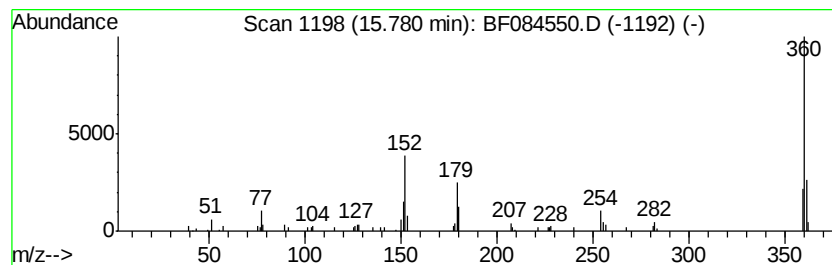
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	3.50 ng	251911	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	93
2		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	50
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4		Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	43
5		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.30	4.4	ng	286592	1	6.80	1299190	20.0
2-Pentanone, 4-hy...	4.98	62.1	ng	4032950	1	6.80	1299190	20.0
2-Pentanone, 4-me...	5.80	3.0	ng	191881	1	6.80	1299190	20.0
unknown6.57	6.57	90.7	ng	5888420	1	6.80	1299190	20.0
Dibenzylidene 4,4...	15.78	3.5	ng	251911	6	15.36	1438540	20.0