

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012716\
 Data File : BF084618.D
 Acq On : 27 Jan 2016 13:47
 Operator : SJ/IZ
 Sample : PB87993BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87993BL

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-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	4.213	184	186	193	rBB	266280	354371	5.35%	0.710%
2	4.921	243	248	250	rBV	2935645	5760633	86.95%	11.542%
3	5.344	282	285	287	rBV	2712272	3638268	54.91%	7.290%
4	5.733	317	319	322	rBV	208786	270280	4.08%	0.542%
5	6.384	373	376	378	rBV	3715519	3958066	59.74%	7.931%
6	6.499	384	386	389	rBV	2851572	3504471	52.89%	7.022%
7	6.739	404	407	409	rVB	949973	1137514	17.17%	2.279%
8	6.887	418	420	423	rBV	3509940	3825060	57.73%	7.664%
9	7.299	453	456	459	rBV	2728988	3109264	46.93%	6.230%
10	8.019	517	519	522	rBV	1649135	1503073	22.69%	3.012%
11	9.105	611	614	616	rBV	5792429	6122362	92.41%	12.267%
12	9.779	670	673	675	rBV	1223870	1692346	25.54%	3.391%
13	10.556	738	741	744	rBV2	2356044	2810322	42.42%	5.631%
14	11.253	799	802	804	rBV	2157373	1875761	28.31%	3.758%
15	12.842	938	941	944	rBV	5259460	6625443	100.00%	13.275%
16	13.882	1030	1032	1035	rBV	1668446	1800020	27.17%	3.607%
17	15.277	1151	1154	1157	rBV	1149292	1380604	20.84%	2.766%
18	15.494	1164	1173	1182	rBV	128137	541489	8.17%	1.085%

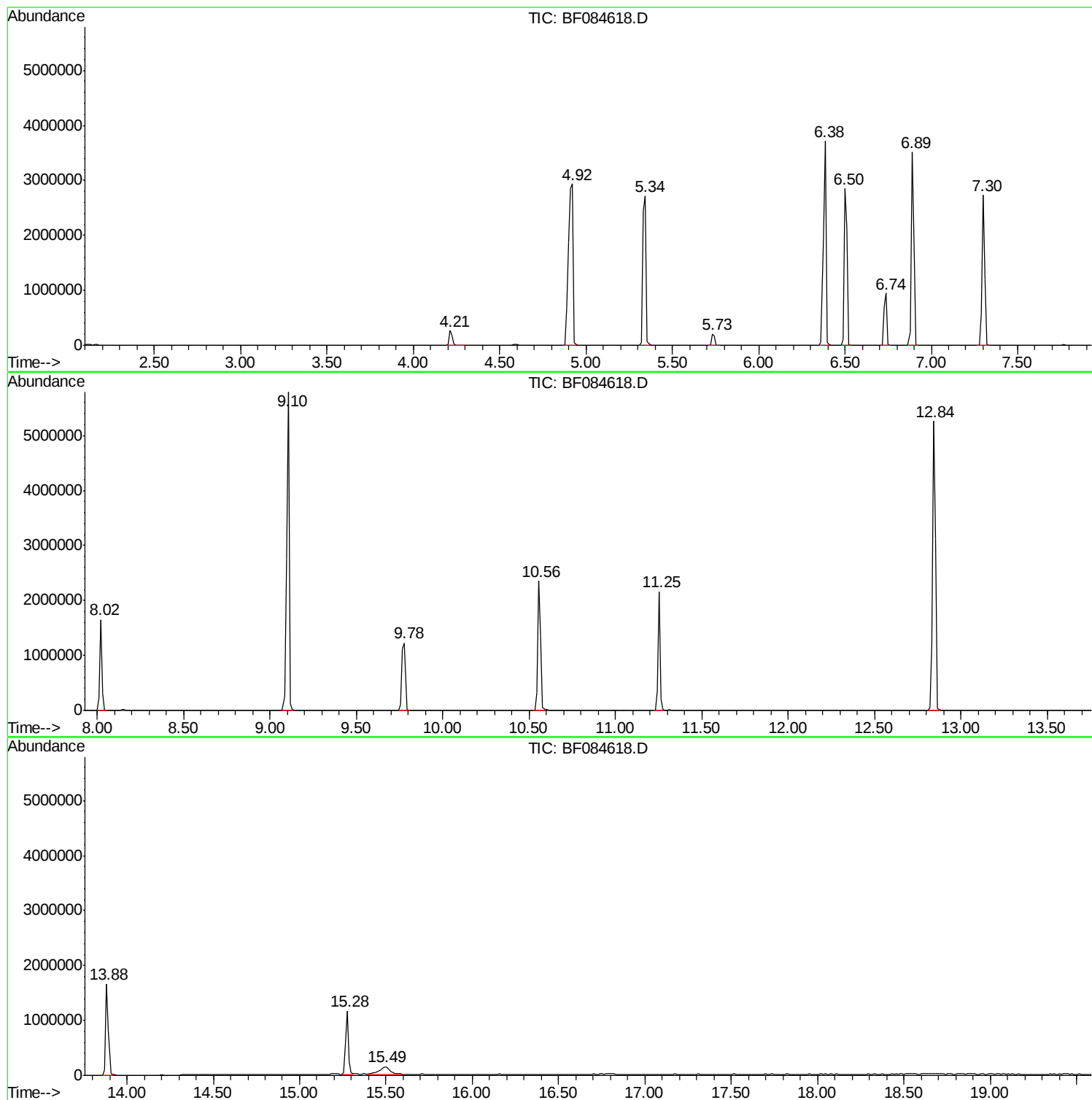
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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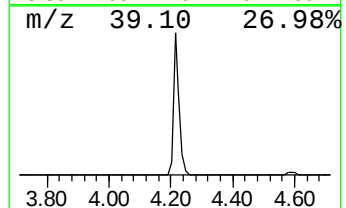
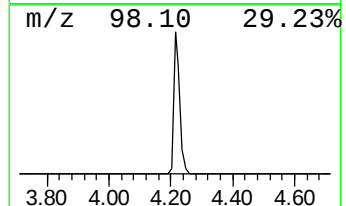
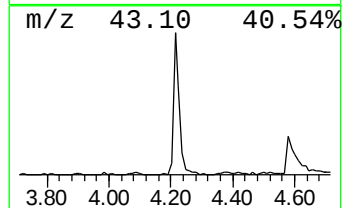
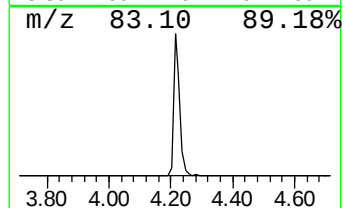
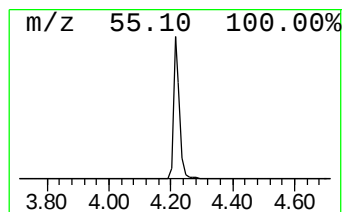
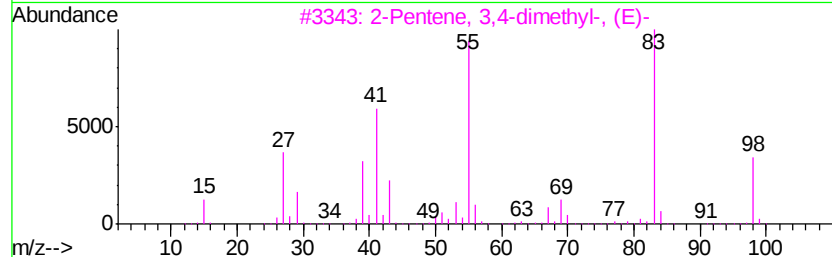
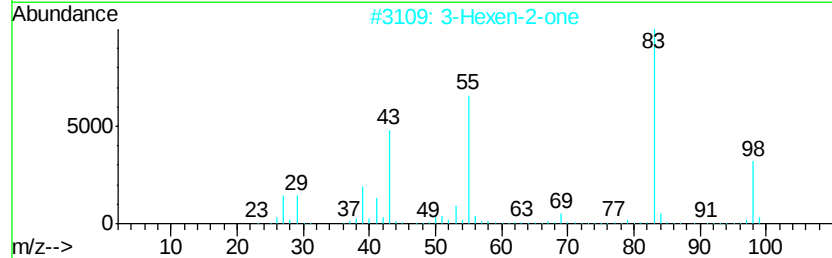
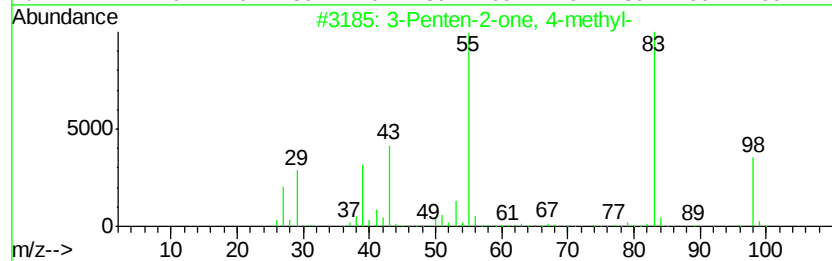
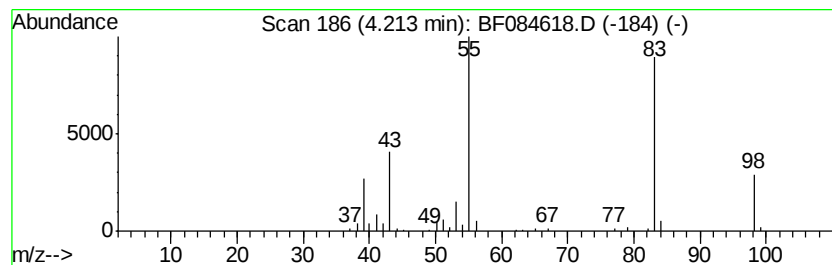
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.21	6.23 ng	354371	1,4-Dichlorobenzene-d4	6.74

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	87
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78
5		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	78



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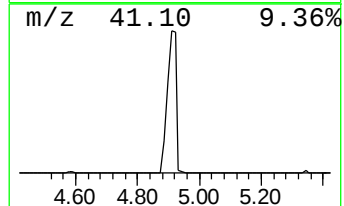
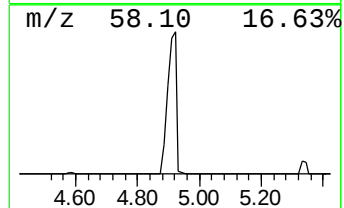
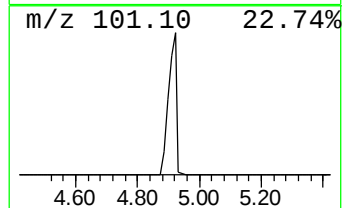
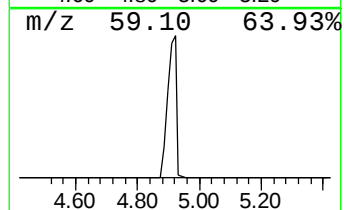
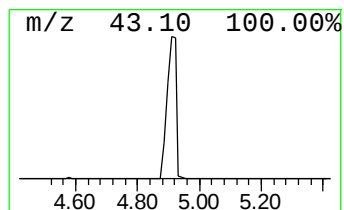
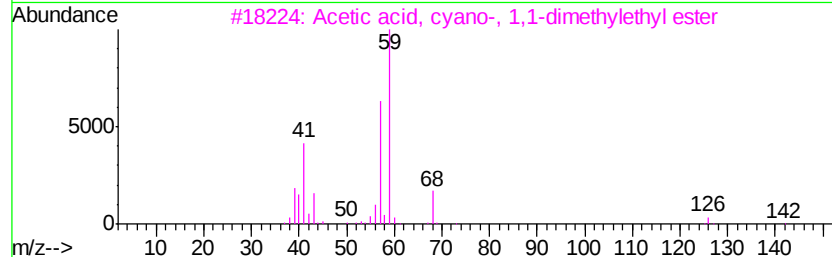
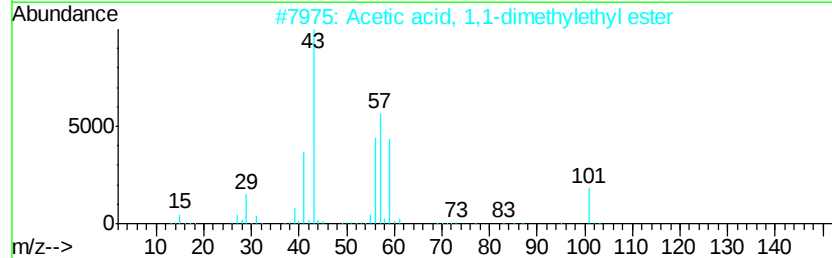
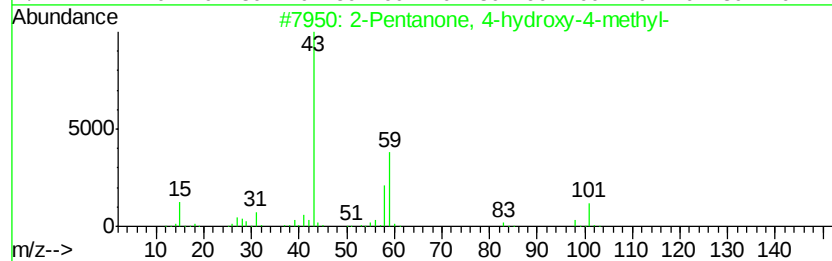
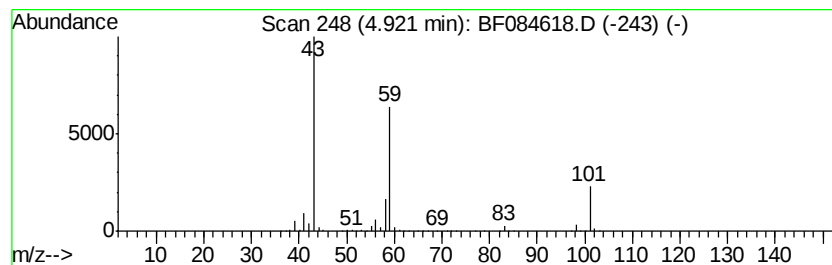
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	101.29 ng	5760630	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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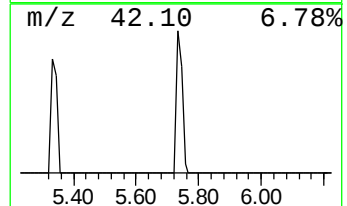
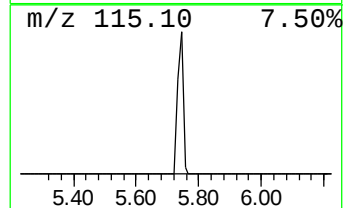
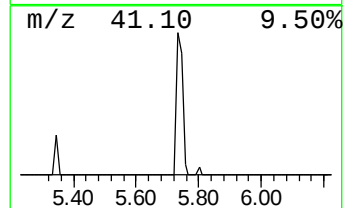
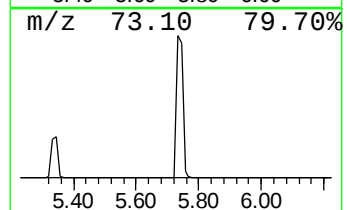
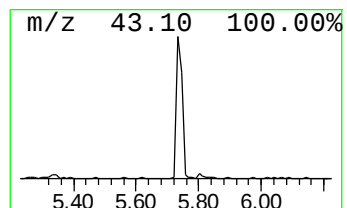
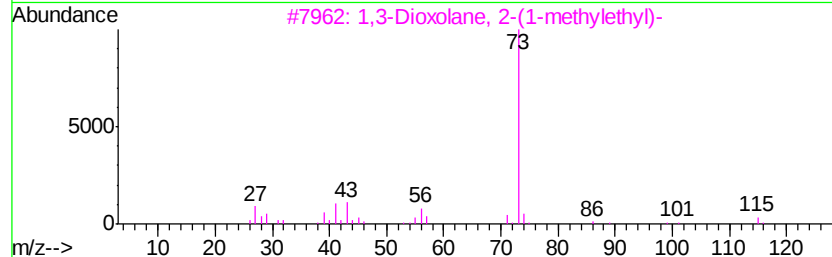
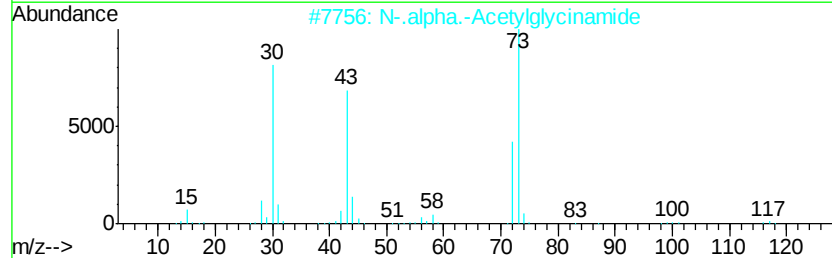
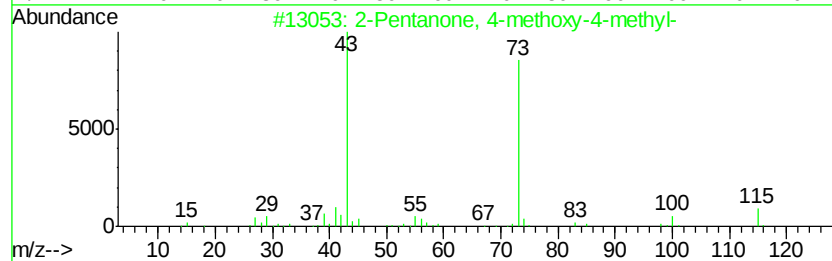
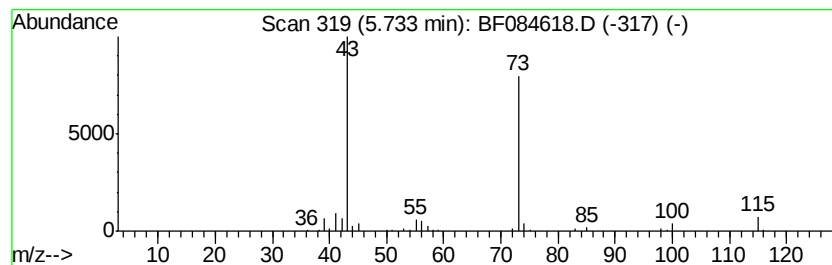
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	4.75 ng	270280	1,4-Dichlorobenzene-d4	6.74

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.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	43
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	35
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
5		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	16



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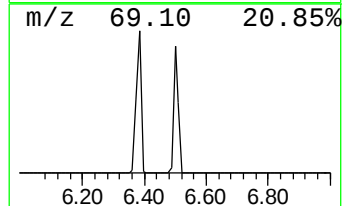
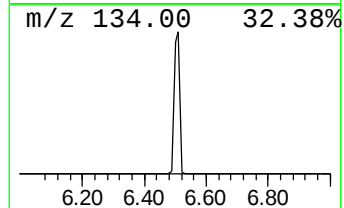
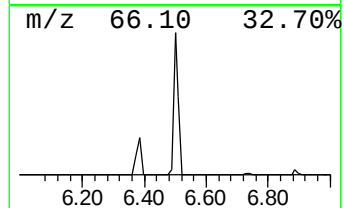
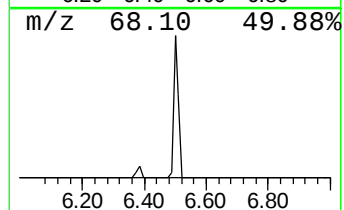
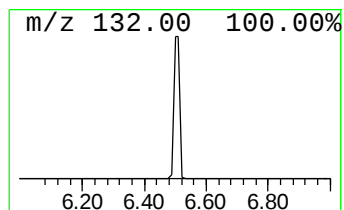
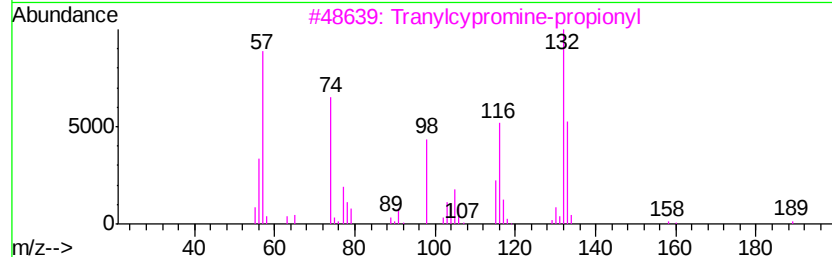
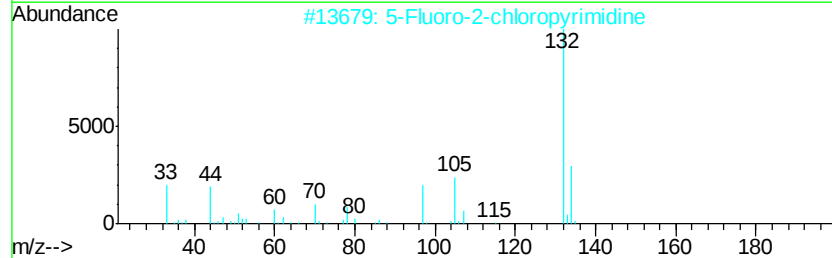
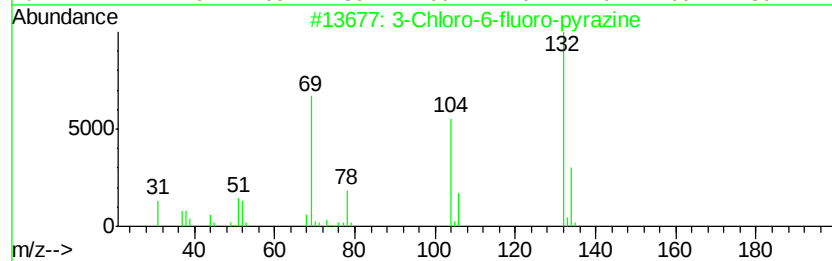
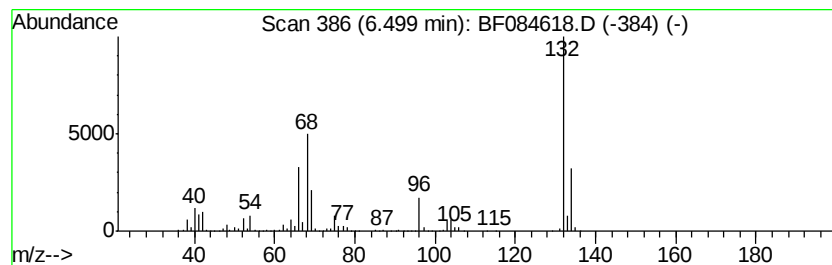
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Peak Number 4 unknown6.50 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	61.62 ng	3504470	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9



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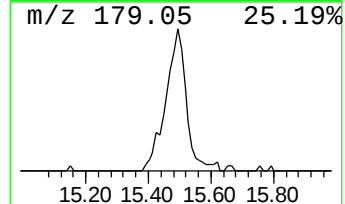
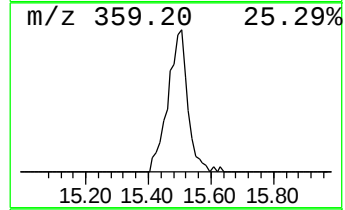
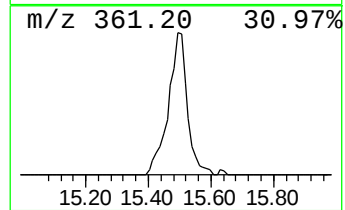
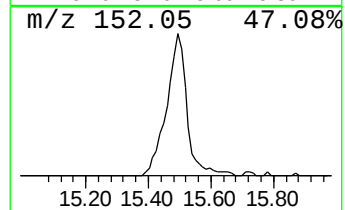
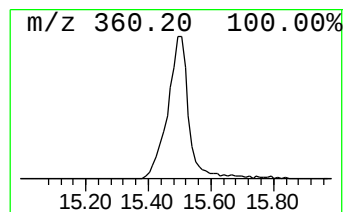
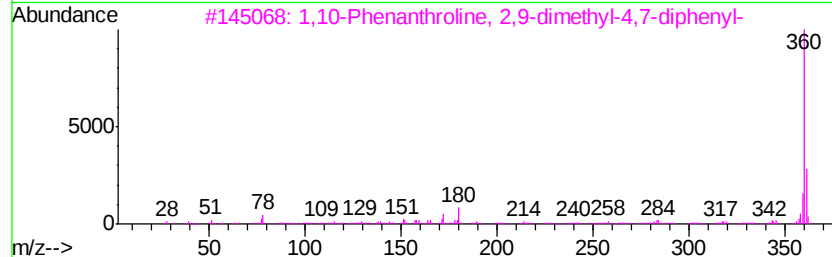
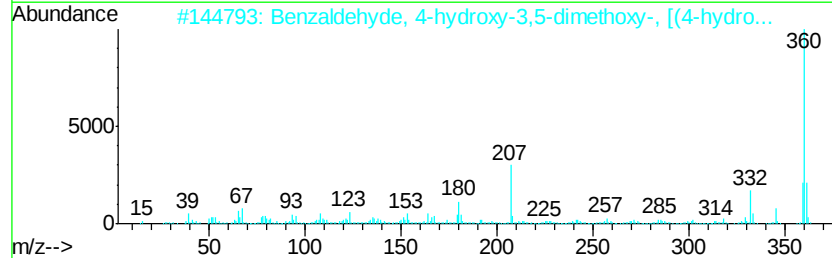
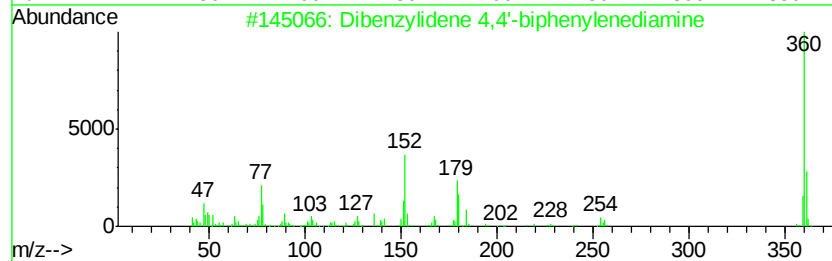
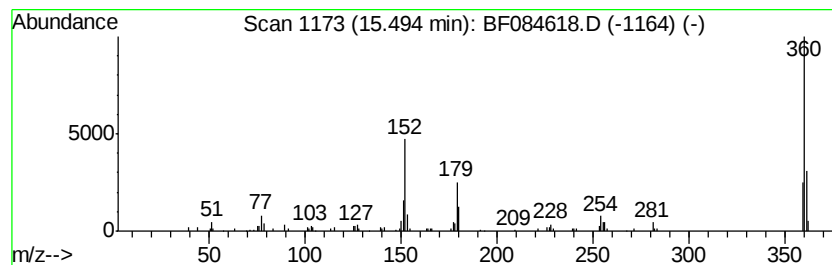
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	7.84 ng	541489	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	87
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
3		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	49
4		Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	47
5		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	46



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.21	6.2	ng	354371	1	6.74	1137510	20.0
2-Pentanone, 4-hy...	4.92	101.3	ng	5760630	1	6.74	1137510	20.0
2-Pentanone, 4-me...	5.73	4.8	ng	270280	1	6.74	1137510	20.0
unknown6.50	6.50	61.6	ng	3504470	1	6.74	1137510	20.0
Dibenzylidene 4,4...	15.49	7.8	ng	541489	6	15.28	1380600	20.0