

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010816\
 Data File : BF084328.D
 Acq On : 8 Jan 2016 15:22
 Operator : SJ/UM
 Sample : PB87668BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87668BL

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	2.155	5	6	20	rVB4	41889	140577	2.01%	0.242%
2	4.396	199	202	206	rBV	194749	229687	3.28%	0.395%
3	5.059	256	260	262	rBV	2861295	4971600	70.98%	8.550%
4	5.470	293	296	298	rBV	4886436	4596611	65.62%	7.905%
5	5.859	328	330	333	rVB	179757	182537	2.61%	0.314%
6	6.499	383	386	388	rBV	4271503	4914788	70.17%	8.452%
7	6.624	394	397	399	rBV	5071893	4501906	64.27%	7.742%
8	6.853	415	417	419	rBV	1963180	1613481	23.04%	2.775%
9	7.013	428	431	433	rBV	5627961	5067296	72.34%	8.714%
10	7.424	464	467	469	rBV	4040862	4654710	66.45%	8.005%
11	8.145	527	530	532	rBV	2098388	2195884	31.35%	3.776%
12	9.219	621	624	627	rBV	6725395	6708442	95.78%	11.537%
13	9.893	681	683	686	rVB	2351578	2320242	33.13%	3.990%
14	10.682	749	752	755	rBV	3107915	2989906	42.69%	5.142%
15	11.379	810	813	816	rBV	2757858	2395944	34.21%	4.120%
16	12.968	949	952	955	rBV	5936664	7004362	100.00%	12.046%
17	14.019	1041	1044	1046	rBV	1823825	2078436	29.67%	3.574%
18	15.448	1165	1169	1171	rBV	965263	1422125	20.30%	2.446%
19	16.122	1222	1228	1234	rVB2	37821	160600	2.29%	0.276%

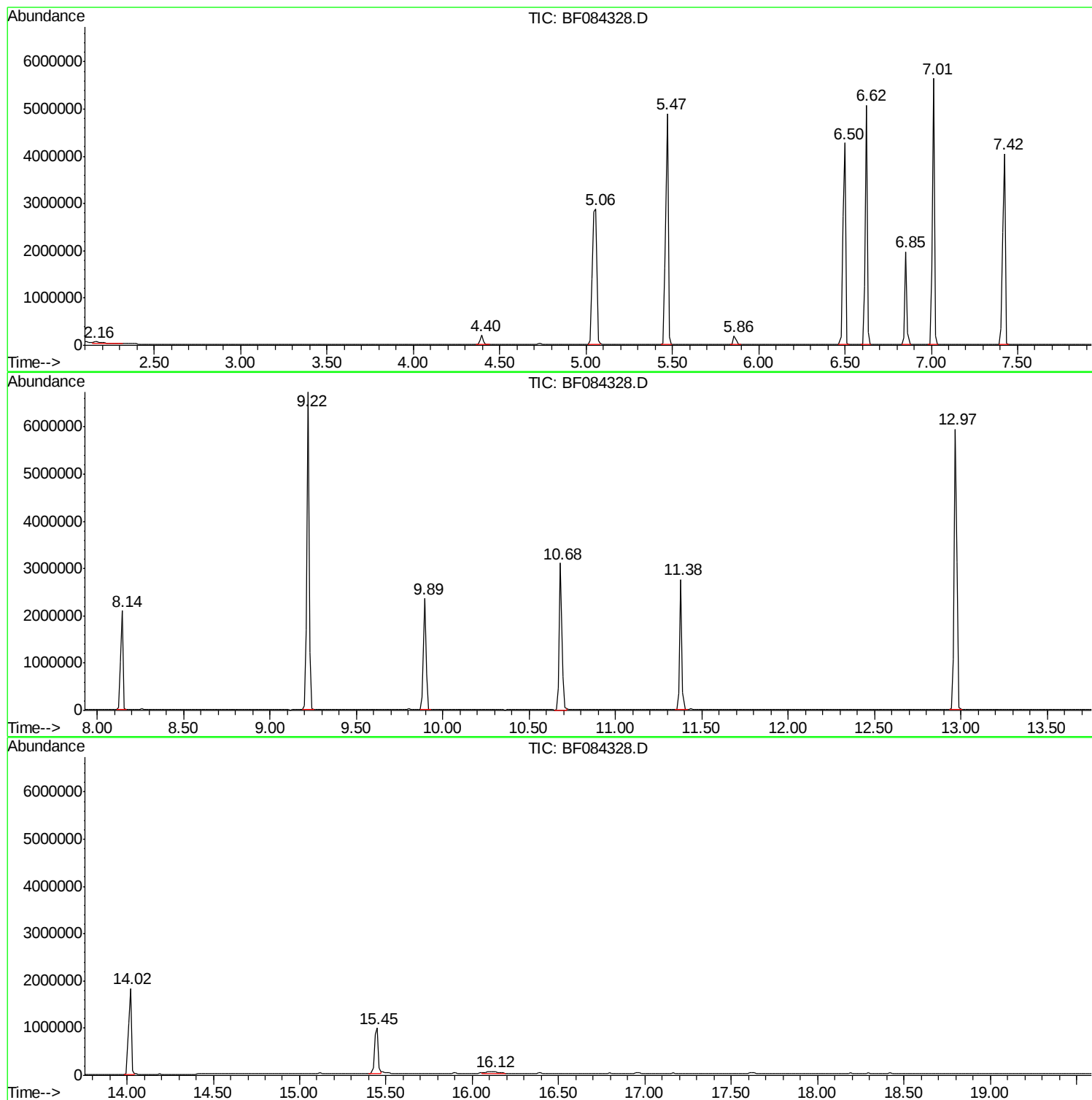
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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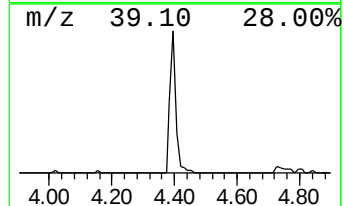
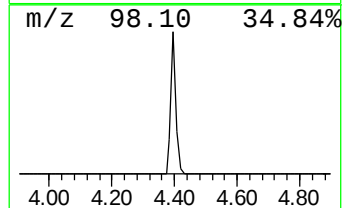
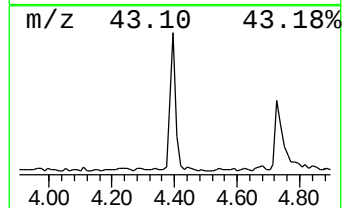
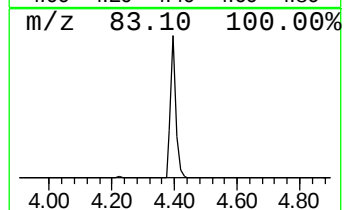
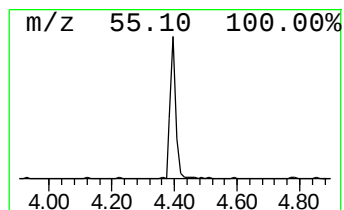
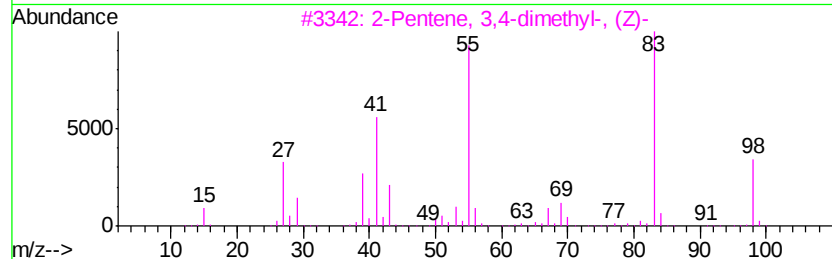
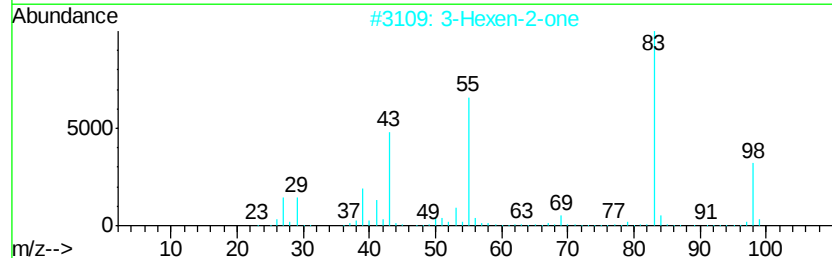
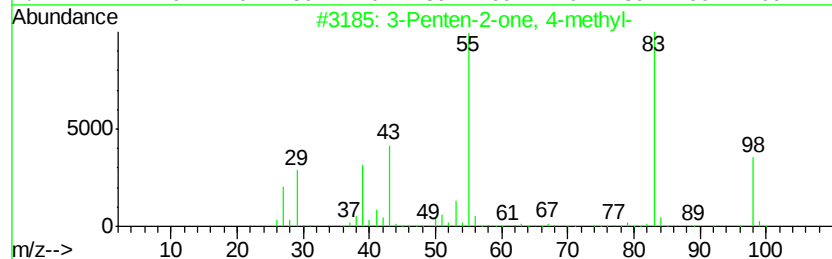
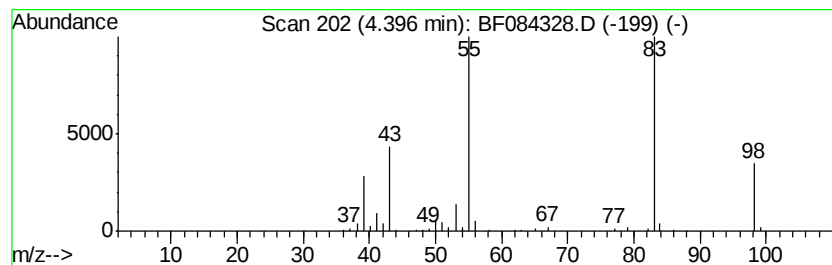
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.40	2.85 ng	229687	1,4-Dichlorobenzene-d4	6.85

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	80
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72



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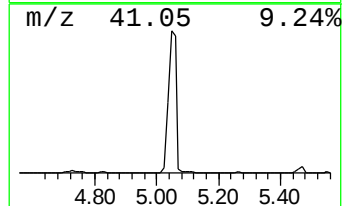
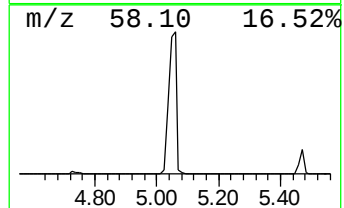
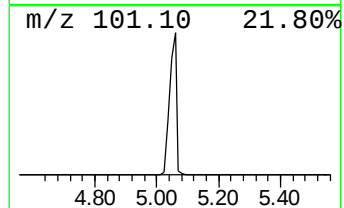
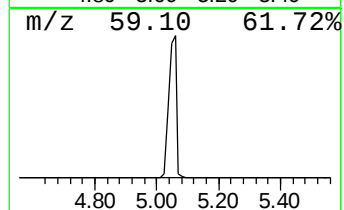
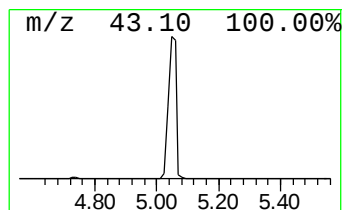
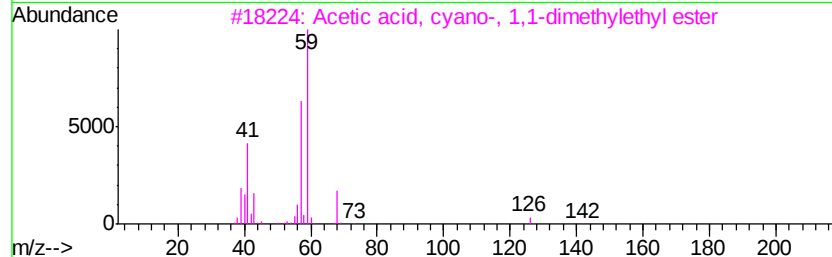
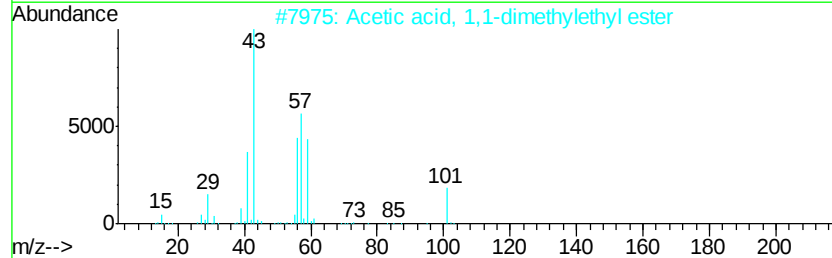
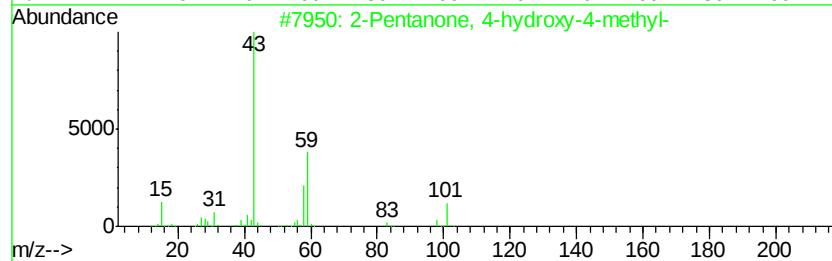
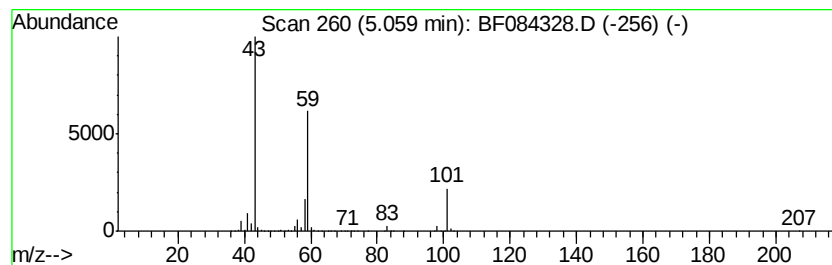
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	61.63 ng	4971600	1,4-Dichlorobenzene-d4	6.85

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		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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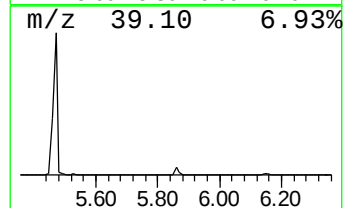
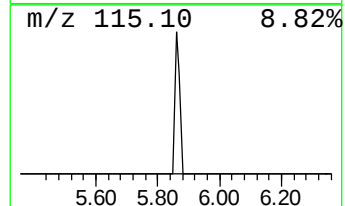
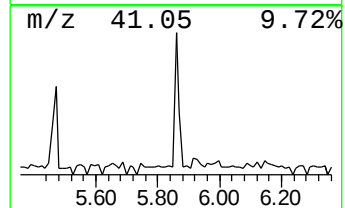
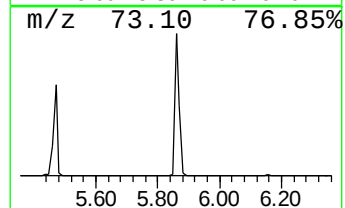
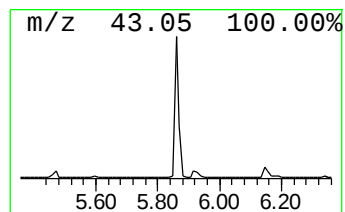
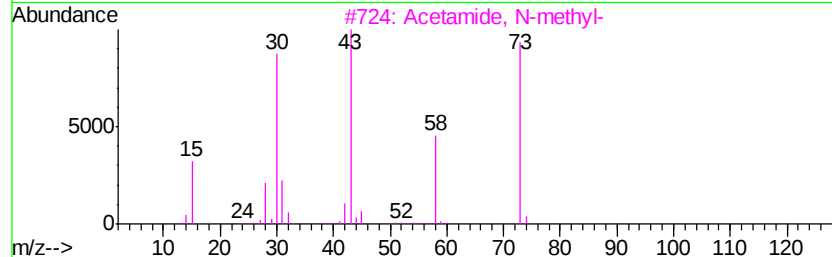
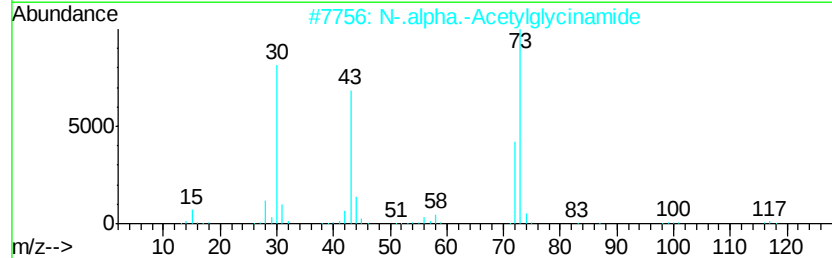
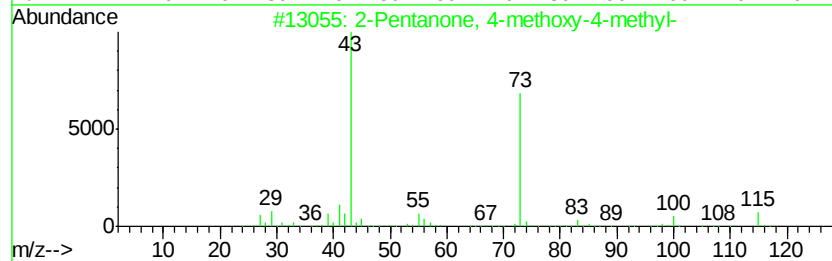
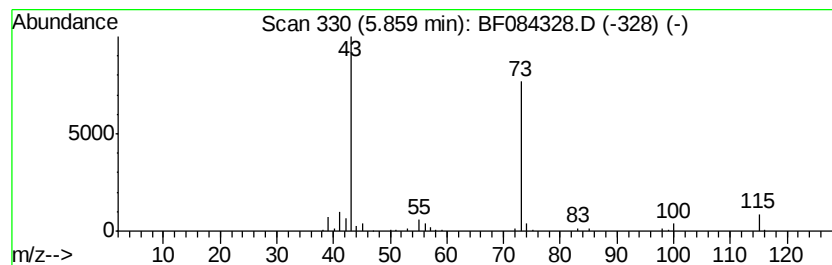
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	2.26 ng	182537	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	43
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
5		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12



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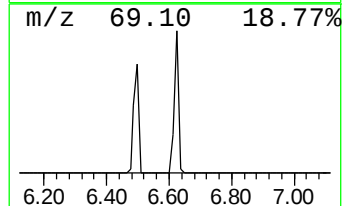
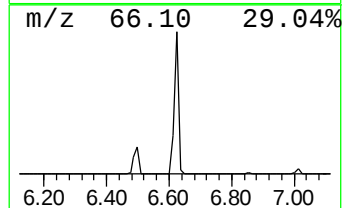
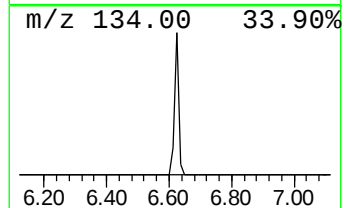
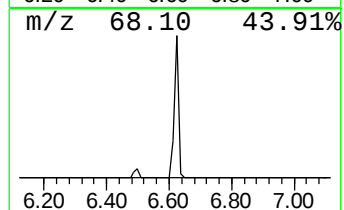
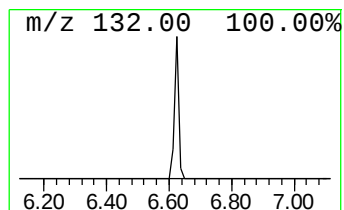
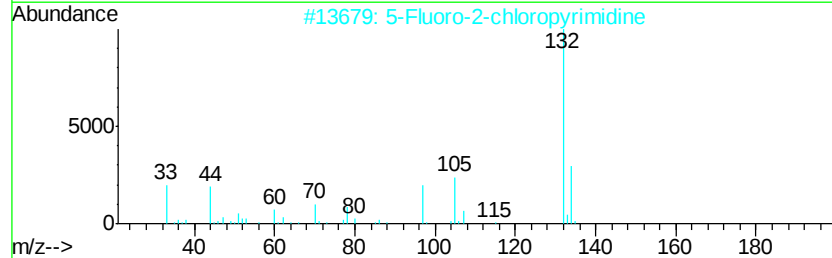
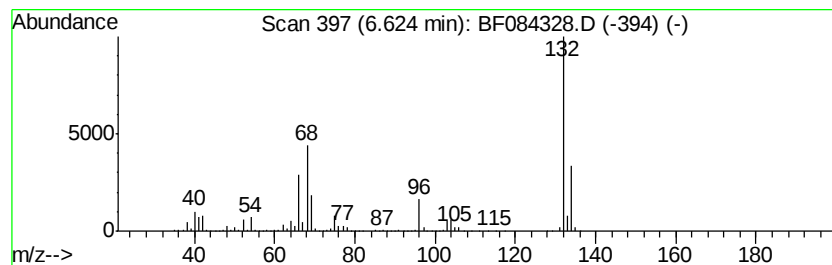
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Peak Number 4 unknown6.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	55.80 ng	4501910	1,4-Dichlorobenzene-d4	6.85

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	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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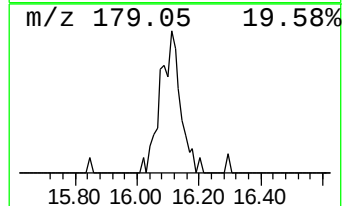
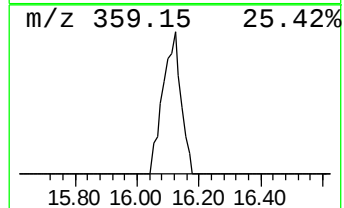
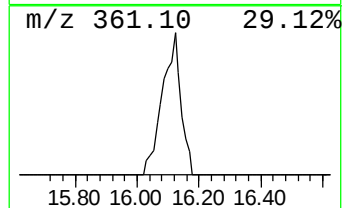
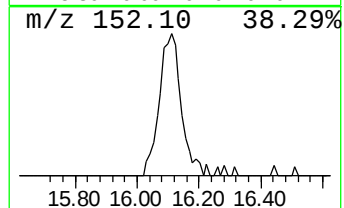
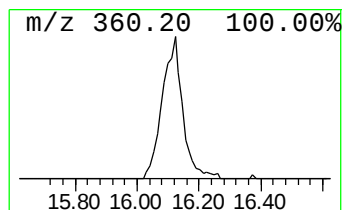
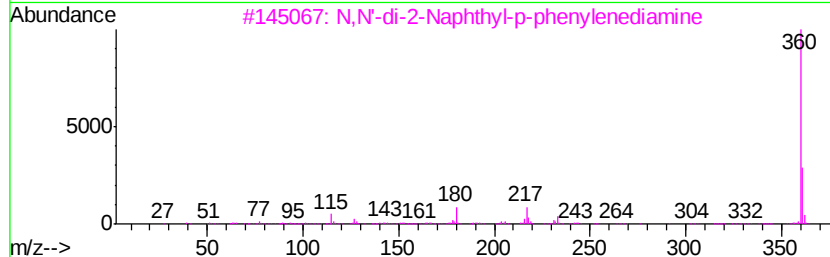
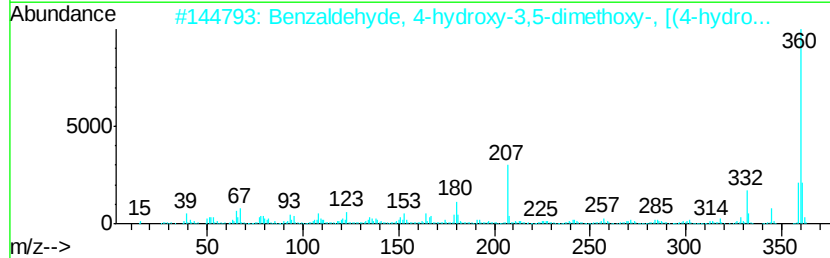
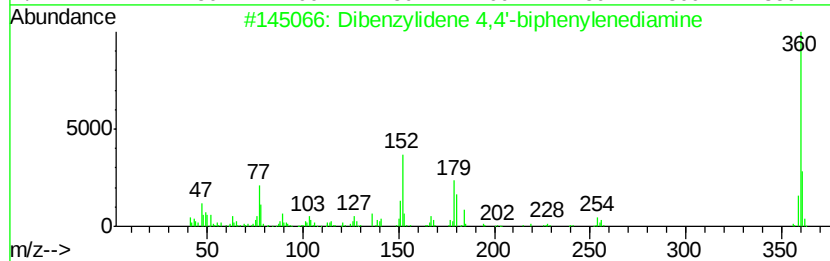
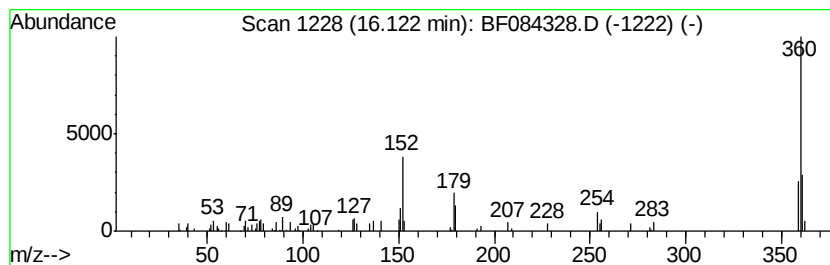
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.26 ng	160600	Perylene-d12	15.45

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



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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...	4.40	2.9	ng	229687	1	6.85	1613480	20.0
2-Pentanone, 4-hy...	5.06	61.6	ng	4971600	1	6.85	1613480	20.0
2-Pentanone, 4-me...	5.86	2.3	ng	182537	1	6.85	1613480	20.0
unknown6.62	6.62	55.8	ng	4501910	1	6.85	1613480	20.0
Dibenzylidene 4,4...	16.12	2.3	ng	160600	6	15.45	1422130	20.0