

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010816\
 Data File : BF084342.D
 Acq On : 8 Jan 2016 23:35
 Operator : SJ/UM
 Sample : H1026-06
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OSSINING-STOCKPILE(0-2)

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	2.715	52	55	60	rVB	161902	223456	2.73%	0.313%
2	4.407	201	203	208	rVB	287017	357225	4.37%	0.500%
3	5.070	257	261	269	rVB	1640551	2627358	32.13%	3.679%
4	5.493	295	298	300	rBV	5909623	7470462	91.36%	10.460%
5	6.510	384	387	389	rBV	5973985	6018839	73.61%	8.427%
6	6.636	395	398	400	rBV	7549079	7877348	96.34%	11.029%
7	6.853	415	417	419	rBV	2163164	1734149	21.21%	2.428%
8	7.013	428	431	433	rVB	6566949	5797729	70.91%	8.118%
9	7.425	464	467	469	rBV	4950307	5532433	67.66%	7.746%
10	8.145	527	530	532	rBV	1854201	2497868	30.55%	3.497%
11	9.219	621	624	627	rBV	7869732	8121144	99.32%	11.371%
12	9.893	680	683	685	rBV	2727144	2606074	31.87%	3.649%
13	10.682	749	752	755	rBV2	3827256	5802090	70.96%	8.124%
14	11.379	810	813	815	rBV	3089118	2711666	33.16%	3.797%
15	12.968	949	952	955	rBV	7101226	8176672	100.00%	11.449%
16	14.008	1041	1043	1046	rBV	1592121	2077991	25.41%	2.909%
17	15.437	1165	1168	1171	rBV	1118136	1483694	18.15%	2.077%
18	16.088	1220	1225	1236	rVB5	39650	200874	2.46%	0.281%
19	16.374	1248	1250	1256	rBV	46548	104018	1.27%	0.146%

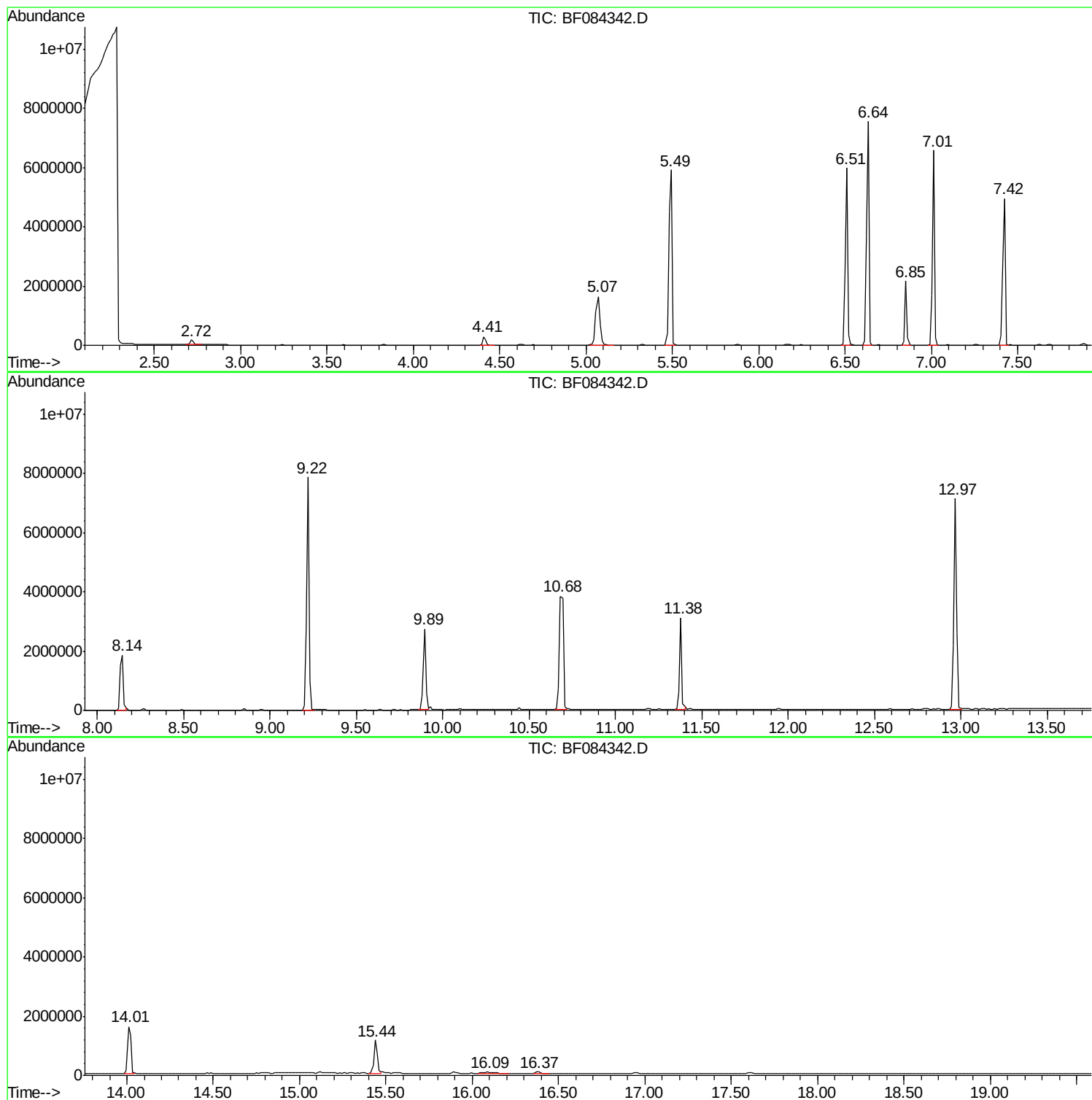
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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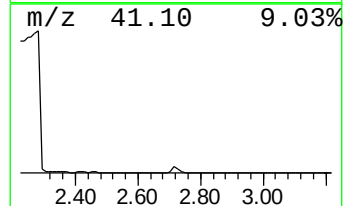
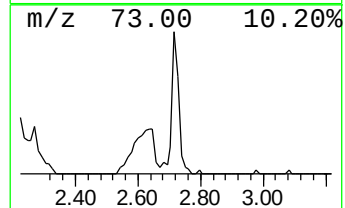
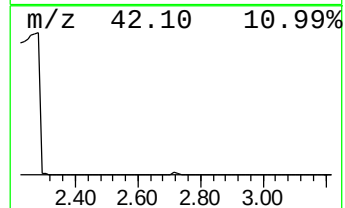
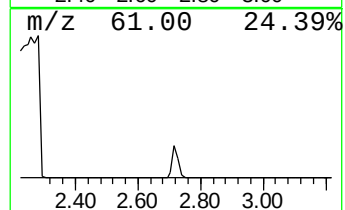
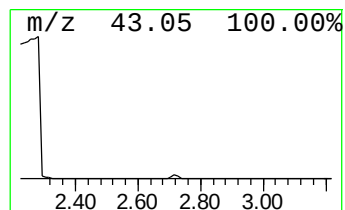
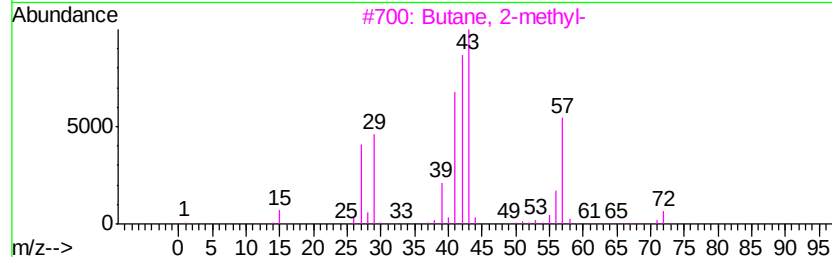
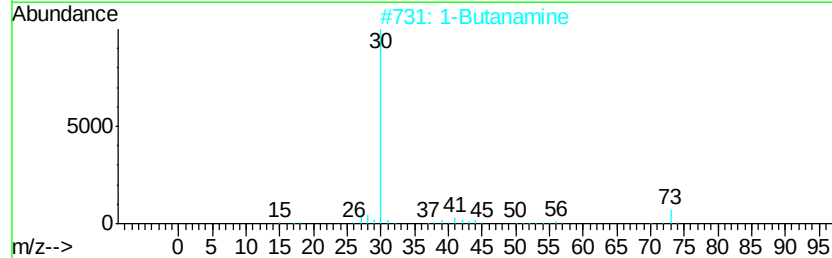
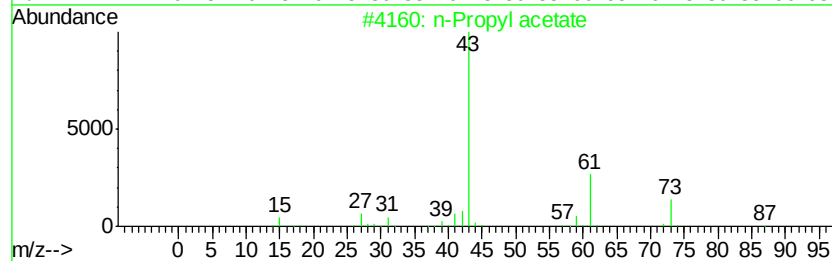
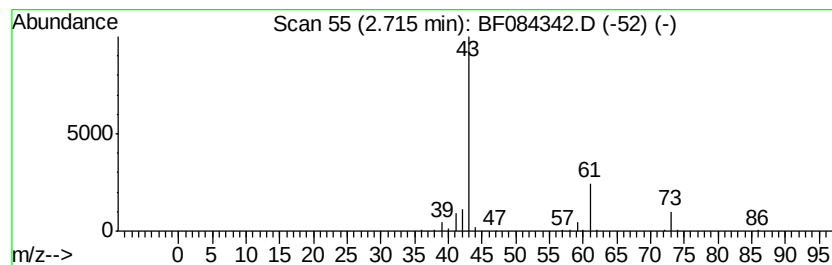
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.72	2.58 ng	223456	1,4-Dichlorobenzene-d4	6.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Butane, 2-methyl-	72	C5H12	000078-78-4	4
4	Isobutylamine	73	C4H11N	000078-81-9	4
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4



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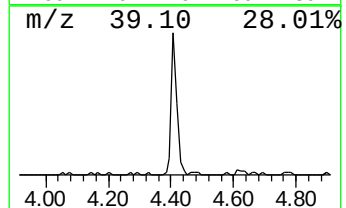
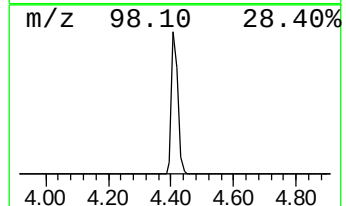
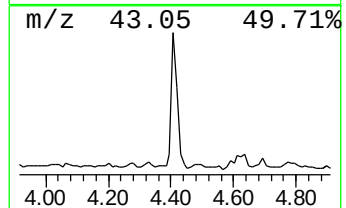
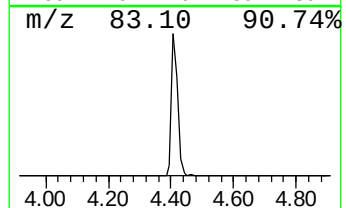
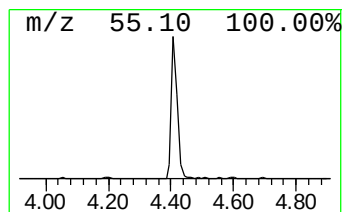
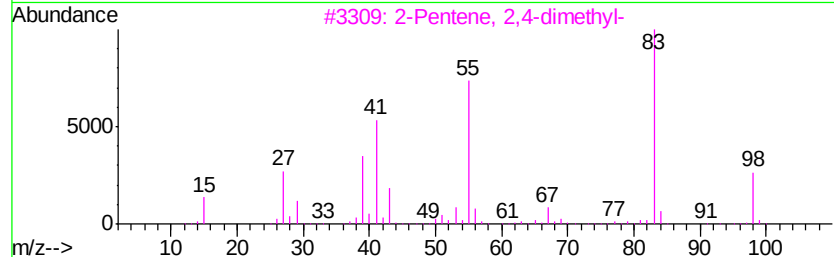
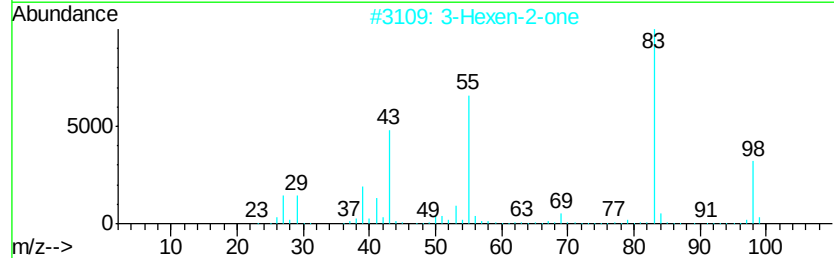
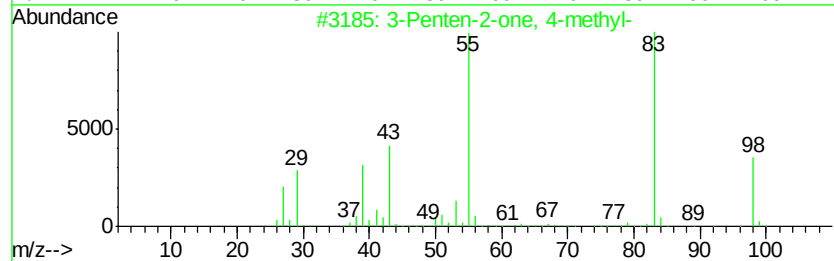
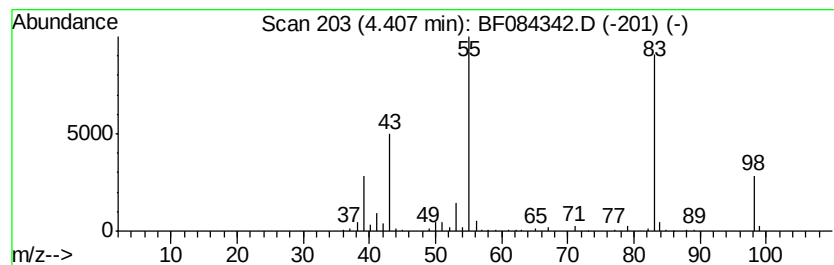
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	4.12 ng	357225	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	87
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72



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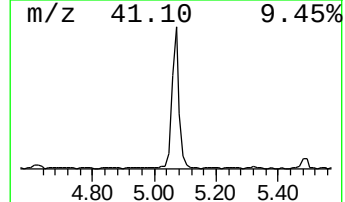
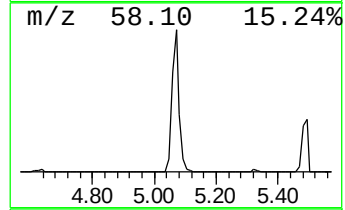
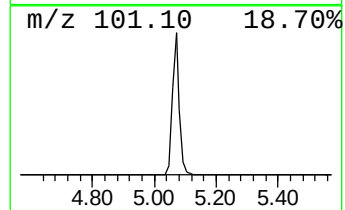
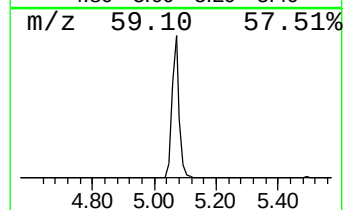
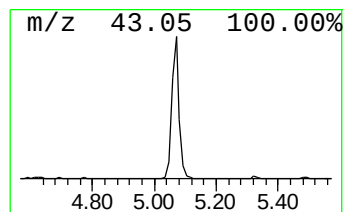
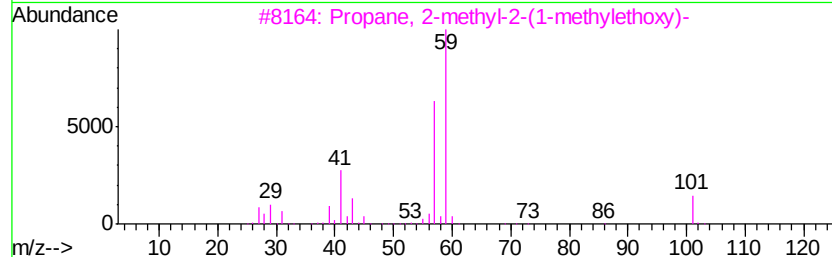
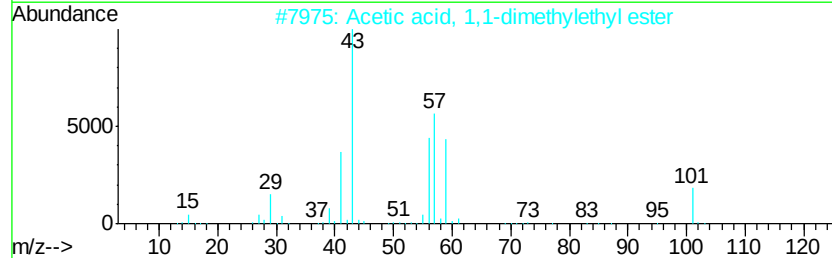
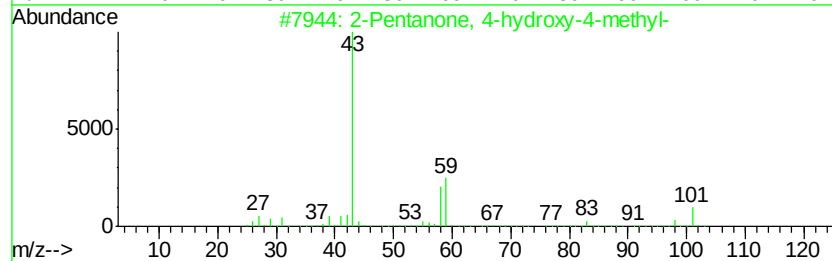
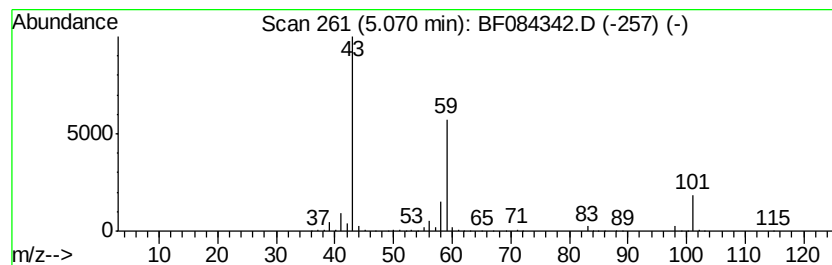
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	30.30 ng	2627360	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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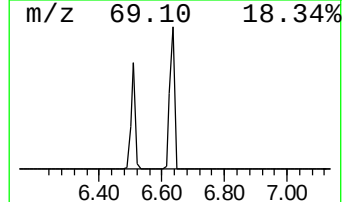
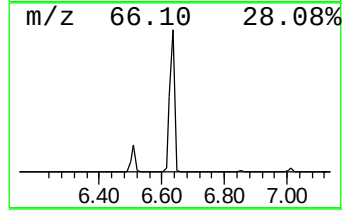
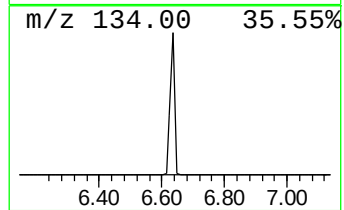
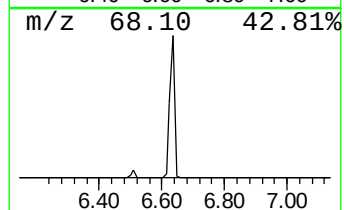
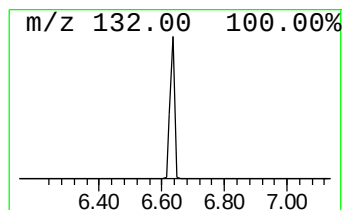
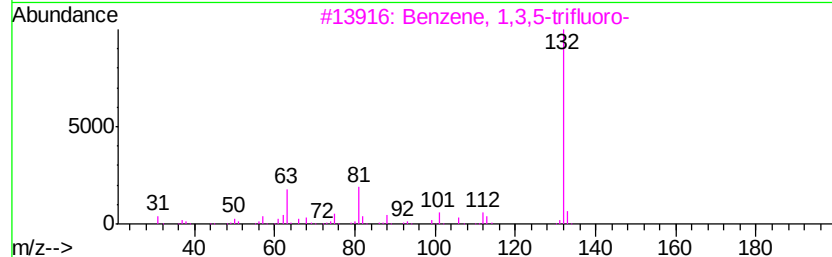
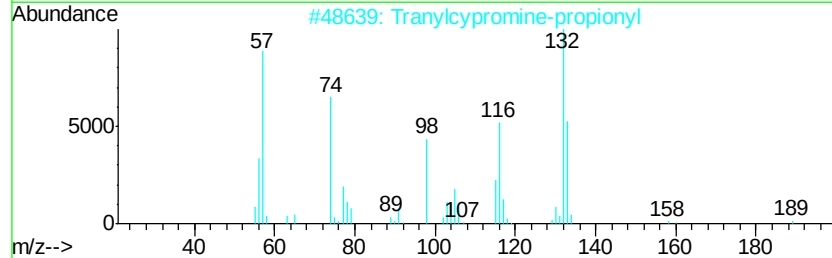
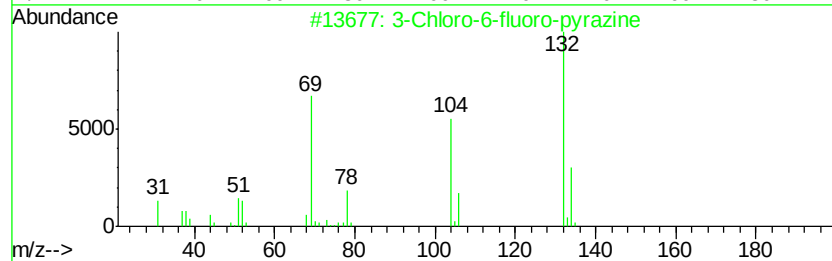
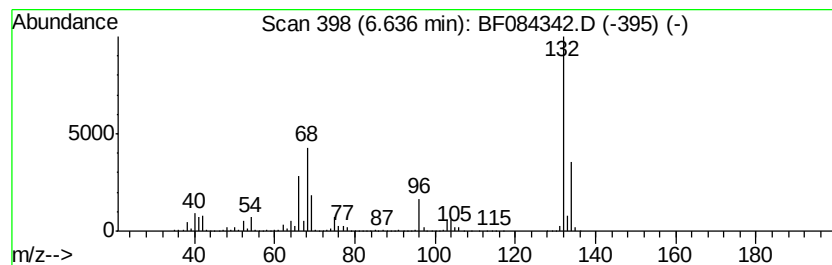
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Peak Number 4 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	90.85 ng	7877350	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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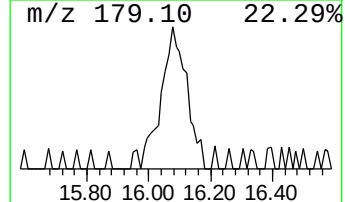
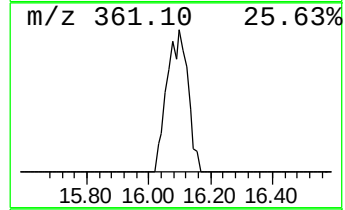
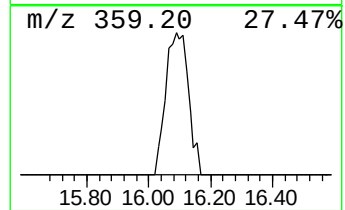
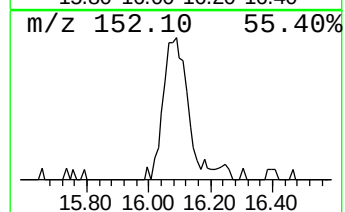
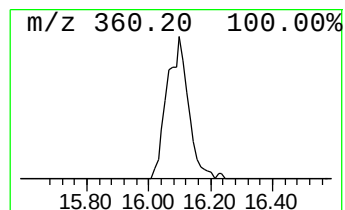
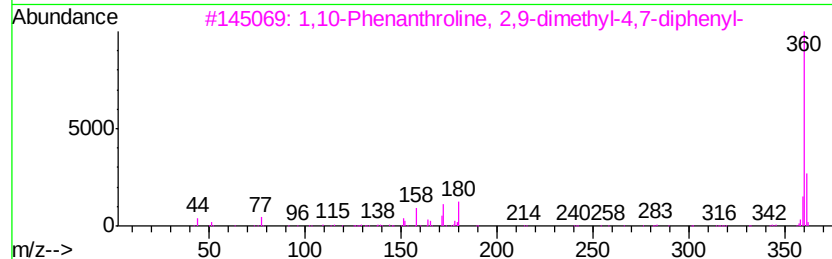
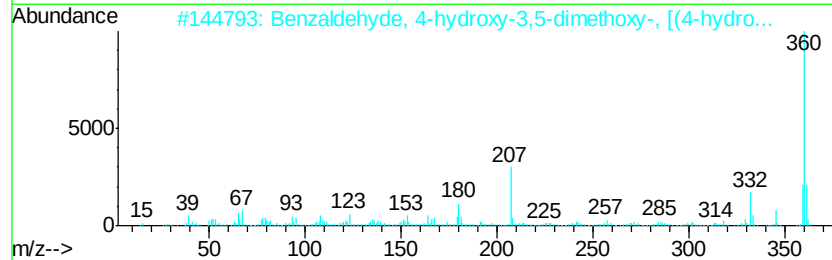
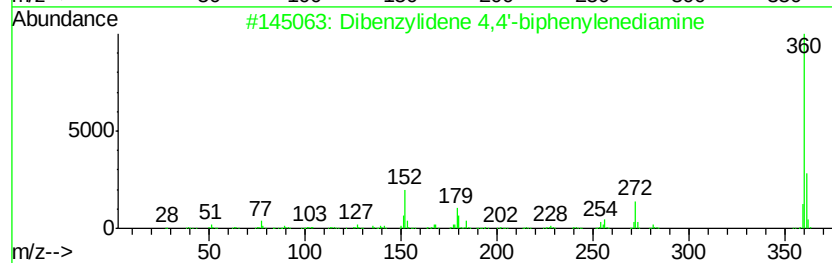
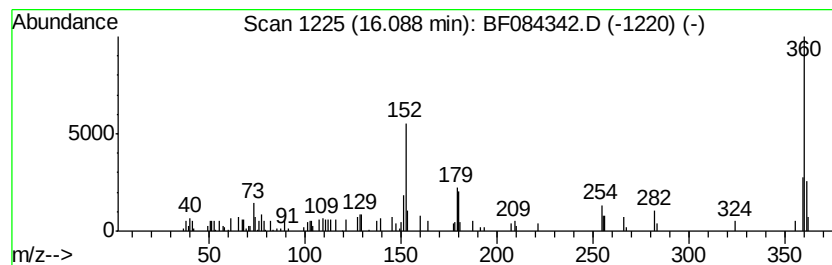
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Peak Number 6 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	2.71 ng	200874	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	81
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
3		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
4		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43
5		Benzoic acid, 4-(3,4-dihydro-2,4...	361	C20H15N3O4	317326-96-8	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.72	2.6	ng	223456	1	6.85	1734150	20.0
3-Penten-2-one, 4...	4.41	4.1	ng	357225	1	6.85	1734150	20.0
2-Pentanone, 4-hy...	5.07	30.3	ng	2627360	1	6.85	1734150	20.0
unknown6.64	6.64	90.8	ng	7877350	1	6.85	1734150	20.0
Dibenzylidene 4,4...	16.09	2.7	ng	200874	6	15.44	1483690	20.0