

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011216\
 Data File : BF084413.D
 Acq On : 12 Jan 2016 16:41
 Operator : SJ/UM
 Sample : PB87765BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB87765BL

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	4.373	197	200	203	rBV	172022	263575	3.16%	0.341%
2	5.036	254	258	265	rBV	2213657	3547690	42.47%	4.592%
3	5.184	268	271	279	rBV	54783	90619	1.08%	0.117%
4	5.459	292	295	297	rBV	7703066	7969176	95.40%	10.316%
5	5.847	327	329	331	rBV	169765	146153	1.75%	0.189%
6	6.487	382	385	387	rBV	7057893	7023867	84.09%	9.092%
7	6.613	393	396	398	rBV	7776365	7156095	85.67%	9.263%
8	6.842	414	416	418	rBV	2851902	2352361	28.16%	3.045%
9	7.002	427	430	432	rBV	5905386	6231343	74.60%	8.066%
10	7.402	462	465	468	rBV	3839047	5025313	60.16%	6.505%
11	8.122	526	528	531	rBV	2380919	2983877	35.72%	3.863%
12	9.208	620	623	625	rBV	8161326	8353238	100.00%	10.813%
13	9.756	662	671	673	rBV	44637	141348	1.69%	0.183%
14	9.802	673	675	679	rVV	58438	137812	1.65%	0.178%
15	9.882	679	682	685	rVB	3640077	3368682	40.33%	4.361%
16	10.671	748	751	754	rBV	4812347	5185988	62.08%	6.713%
17	11.368	809	812	814	rBV	3873052	3382488	40.49%	4.379%
18	12.957	948	951	954	rBV	7719396	7945853	95.12%	10.286%
19	14.008	1040	1043	1045	rBV	2590092	3146489	37.67%	4.073%
20	15.425	1164	1167	1170	rBV	1678784	2280366	27.30%	2.952%
21	16.043	1216	1221	1234	rVB	132598	518722	6.21%	0.671%

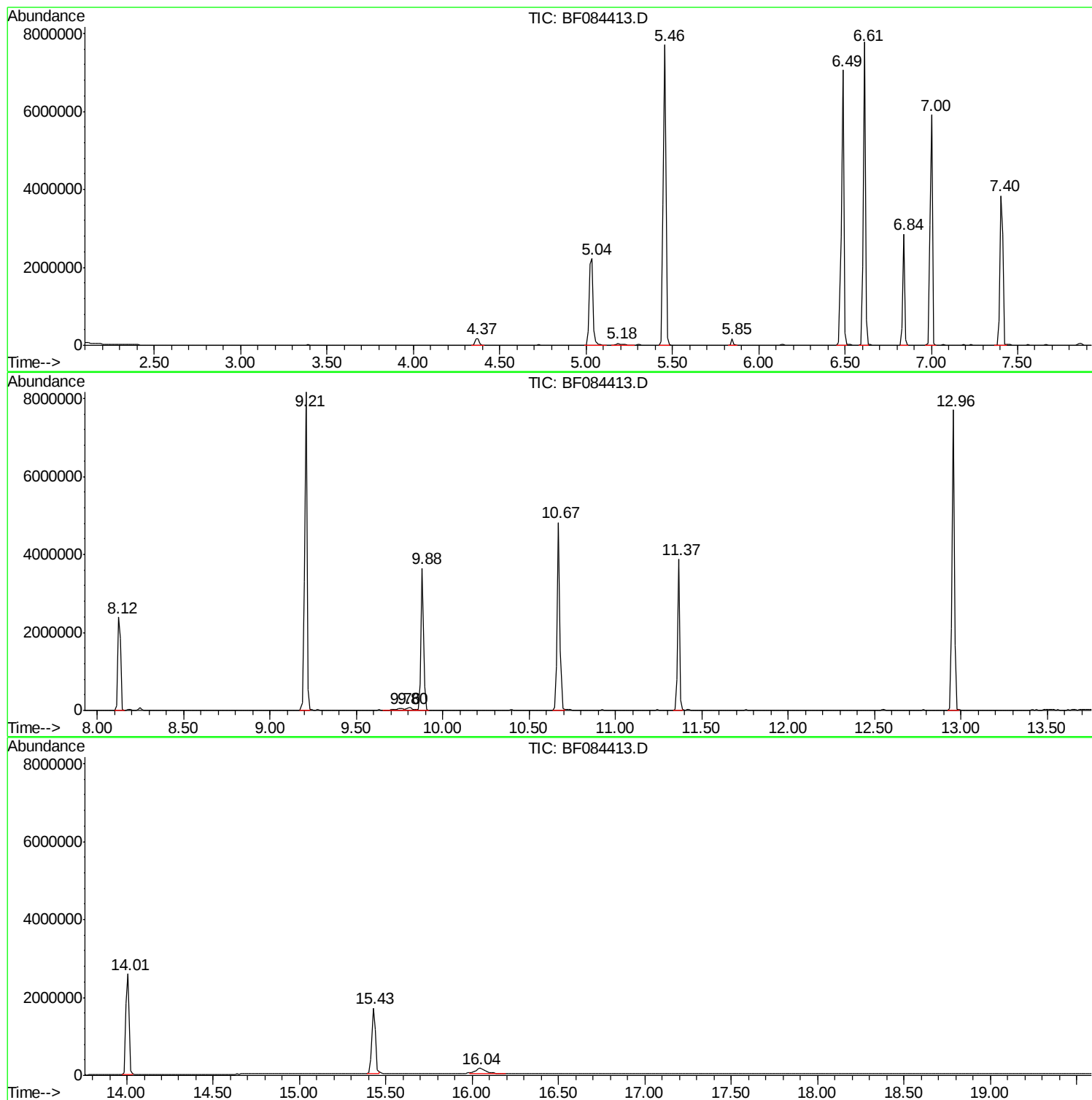
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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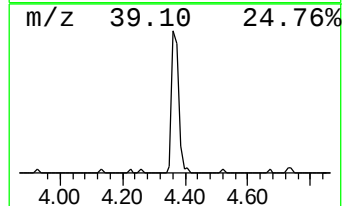
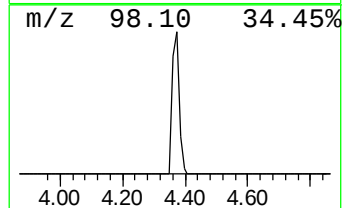
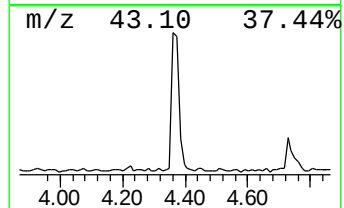
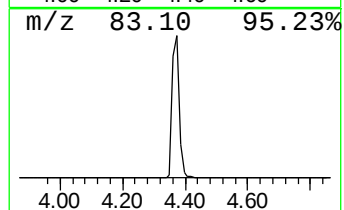
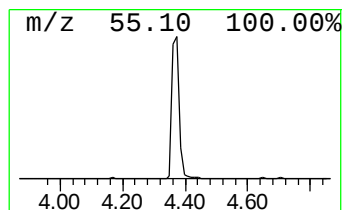
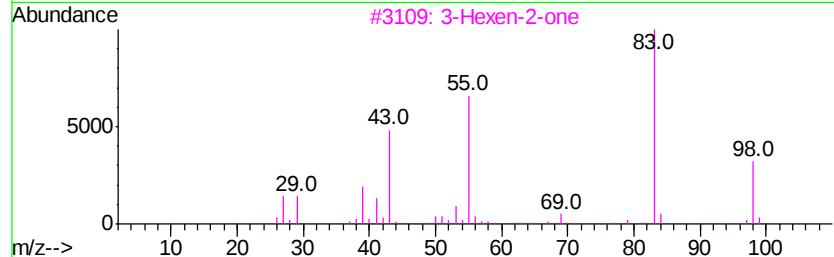
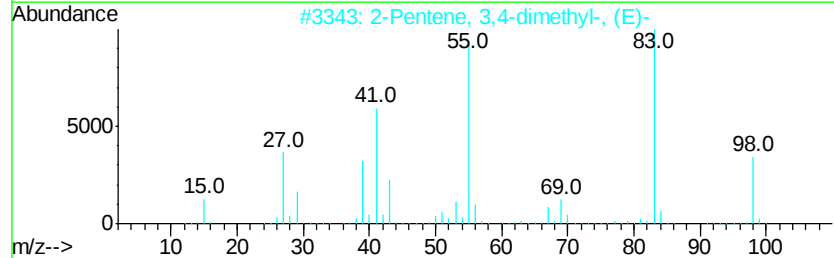
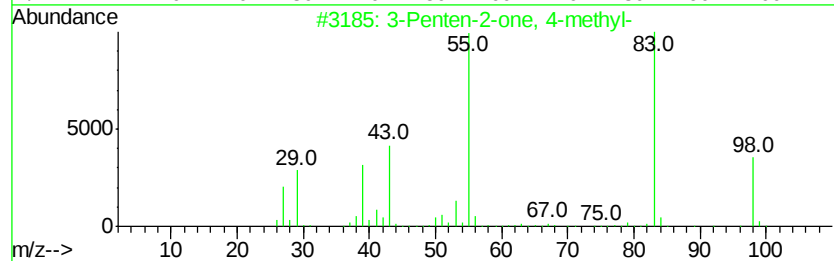
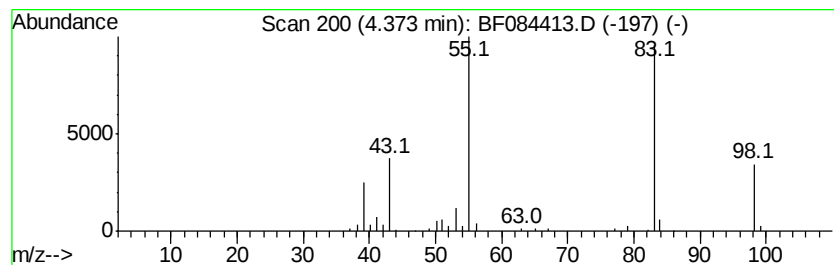
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.37	2.24 ng	263575	1,4-Dichlorobenzene-d4	6.84

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		3-Hexen-2-one	98	C6H10O	000763-93-9	87
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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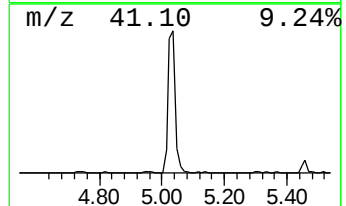
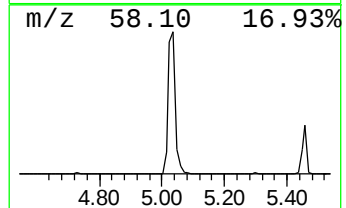
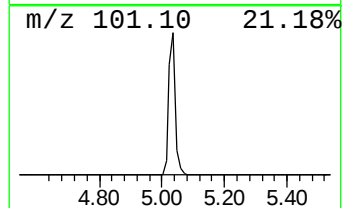
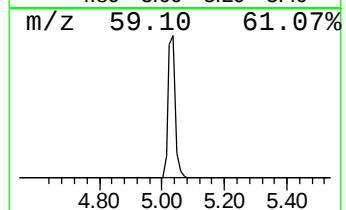
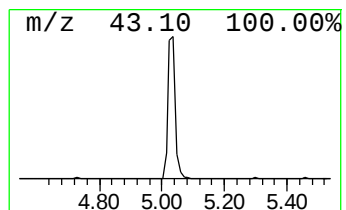
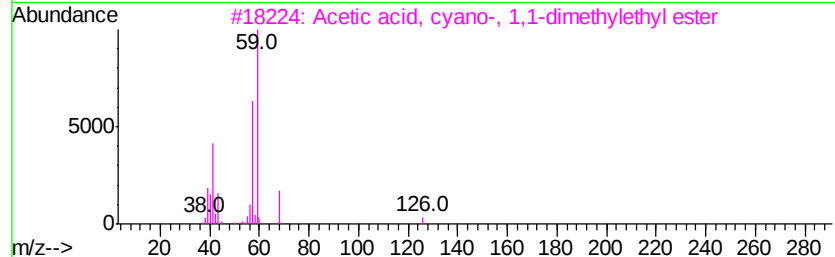
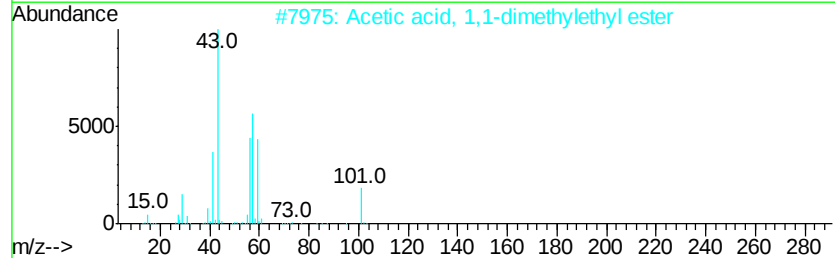
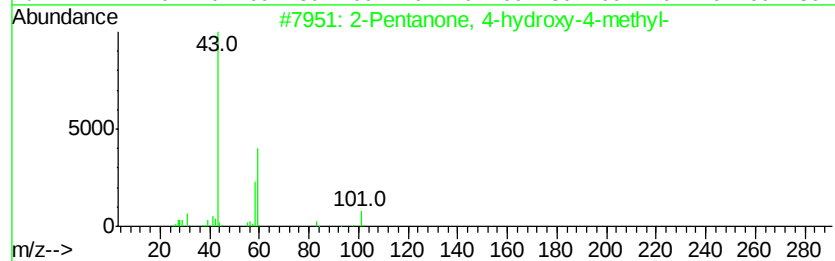
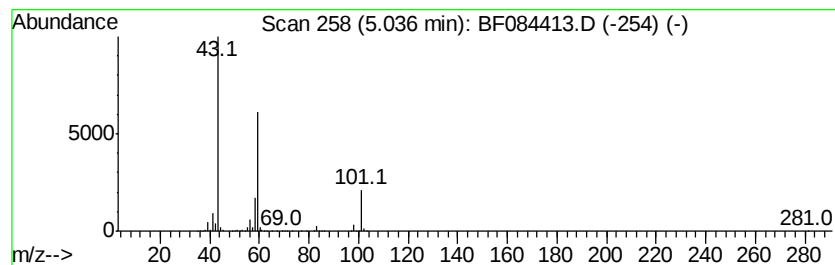
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	30.16 ng	3547690	1,4-Dichlorobenzene-d4	6.84

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		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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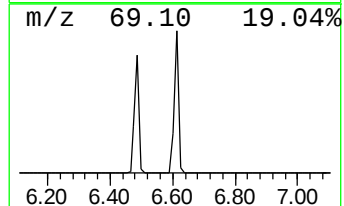
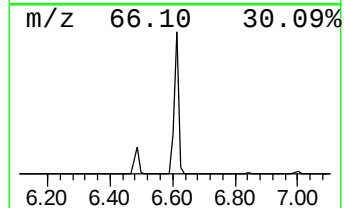
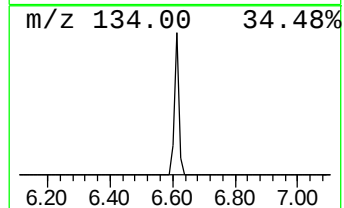
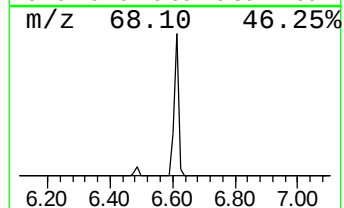
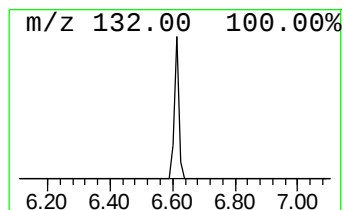
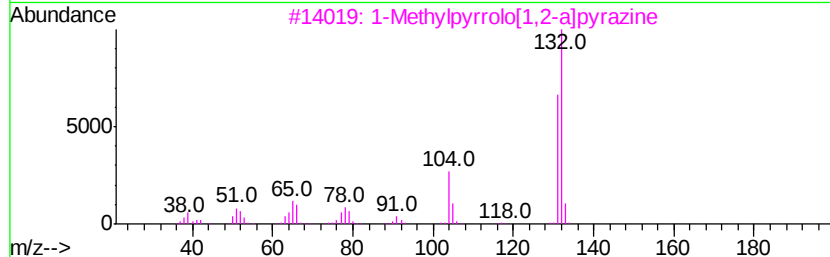
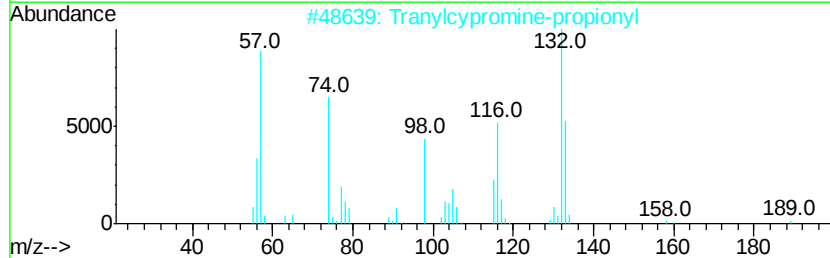
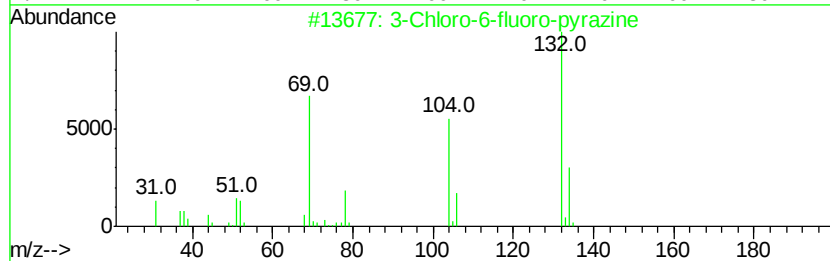
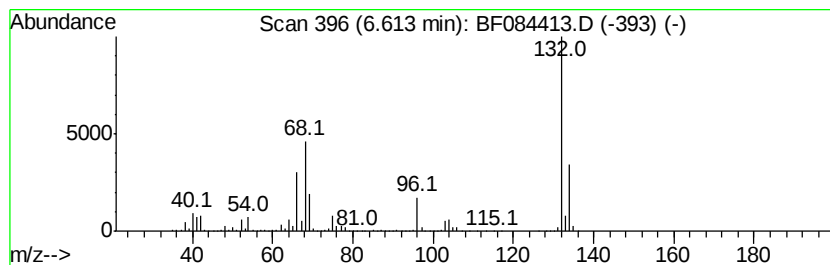
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Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	60.84 ng	7156100	1,4-Dichlorobenzene-d4	6.84

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		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Xenon	132	Xe	007440-63-3	9



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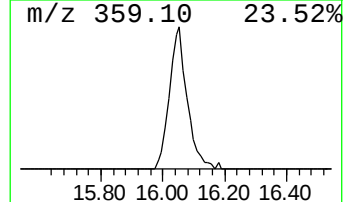
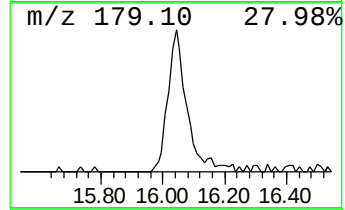
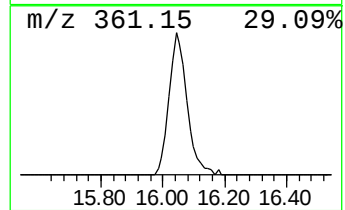
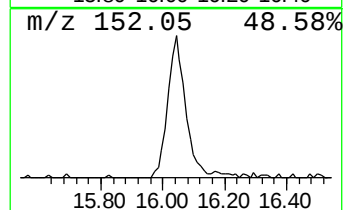
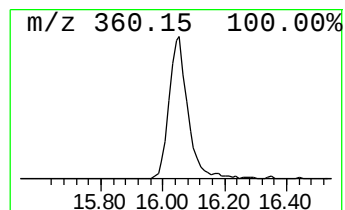
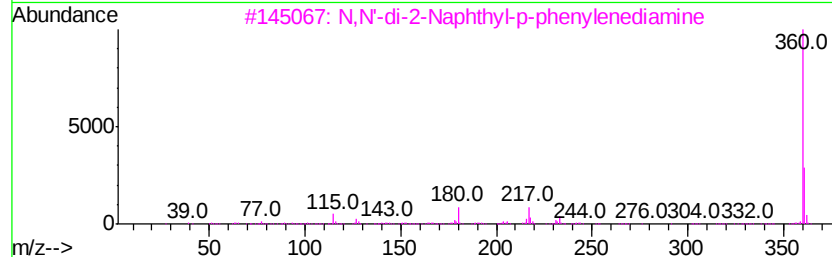
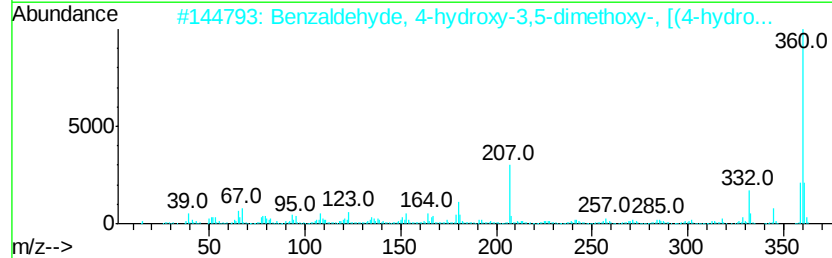
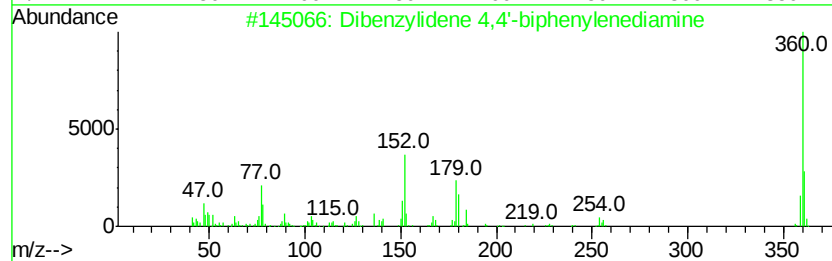
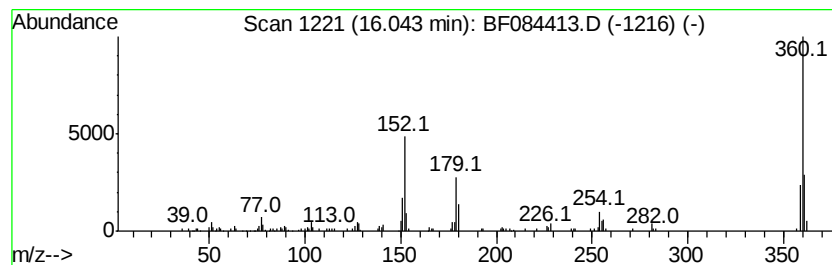
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Peak Number 5 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	4.55 ng	518722	Perylene-d12	15.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	90
2		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
3		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	46
4		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43
5		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.37	2.2	ng	263575	1	6.84	2352360	20.0
2-Pentanone, 4-hy...	5.04	30.2	ng	3547690	1	6.84	2352360	20.0
unknown6.61	6.61	60.8	ng	7156100	1	6.84	2352360	20.0
Dibenzylidene 4,4...	16.04	4.5	ng	518722	6	15.43	2280370	20.0