

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031115\
 Data File : BF077703.D
 Acq On : 11 Mar 2015 23:50
 Operator : TP/IZ
 Sample : PB82075BL
 Misc : W
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB82075BL

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-BF031115.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	1.344	37	40	42	rBV	2728056	3468999	100.00%	19.171%
2	1.458	46	50	54	rVB	25112	54600	1.57%	0.302%
3	1.790	78	79	86	rBV	30270	49894	1.44%	0.276%
4	4.933	352	354	362	rVB	166558	221827	6.39%	1.226%
5	5.459	397	400	402	rBV	976974	1302373	37.54%	7.197%
6	6.727	509	511	514	rBV	941001	1291868	37.24%	7.139%
7	6.876	522	524	527	rBV	1433661	1375266	39.64%	7.600%
8	7.173	547	550	552	rVB	265089	321107	9.26%	1.775%
9	7.356	563	566	568	rBV	1248670	1134038	32.69%	6.267%
10	7.859	608	610	613	rBV	880266	800111	23.06%	4.422%
11	8.739	685	687	690	rBV	354019	438349	12.64%	2.423%
12	10.088	803	805	808	rBV	2006493	1810753	52.20%	10.007%
13	10.911	875	877	880	rVB	557880	536852	15.48%	2.967%
14	11.894	960	963	965	rBV	973474	1063262	30.65%	5.876%
15	12.751	1036	1038	1040	rBV	644319	590643	17.03%	3.264%
16	14.751	1210	1213	1215	rBV	1810408	2218386	63.95%	12.260%
17	16.031	1322	1325	1327	rBV	520182	600765	17.32%	3.320%
18	17.734	1471	1474	1477	rBV	486321	584117	16.84%	3.228%
19	19.094	1585	1593	1601	rBV	53381	231656	6.68%	1.280%

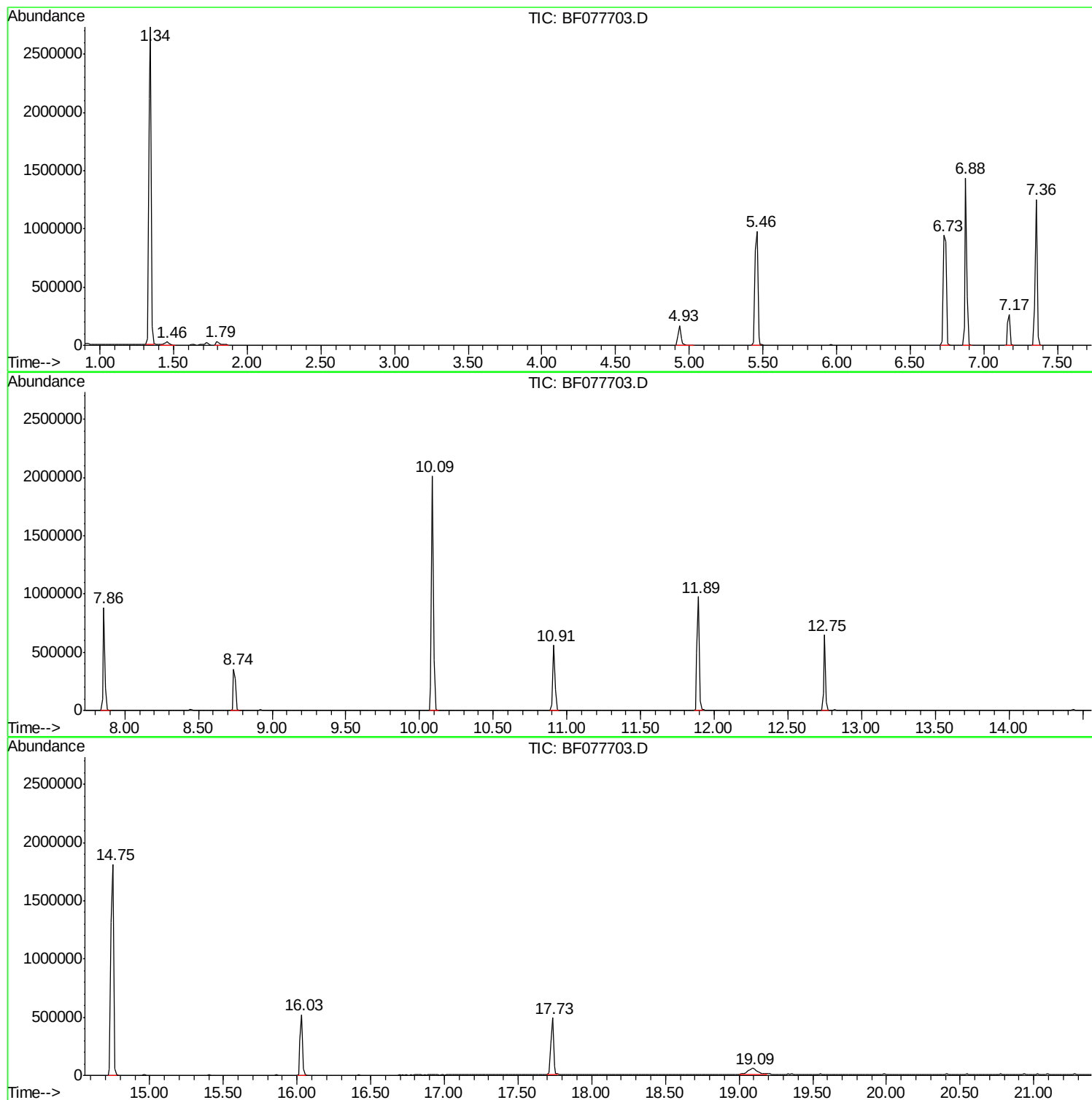
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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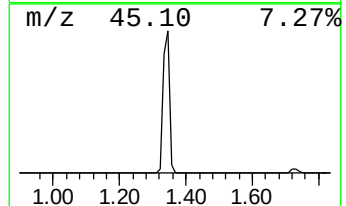
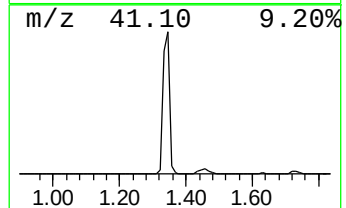
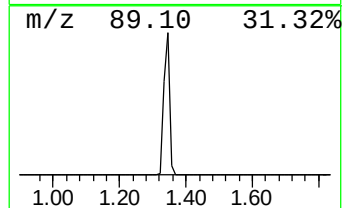
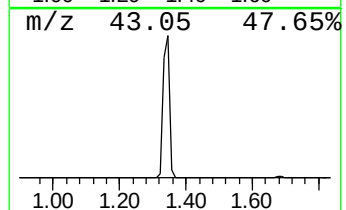
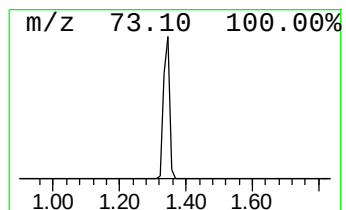
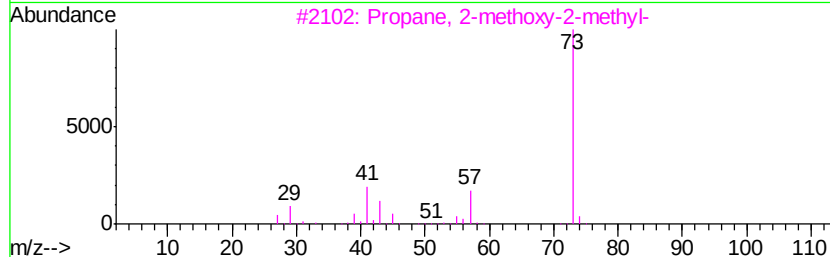
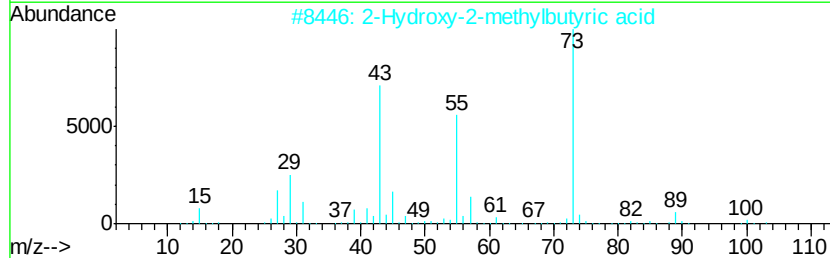
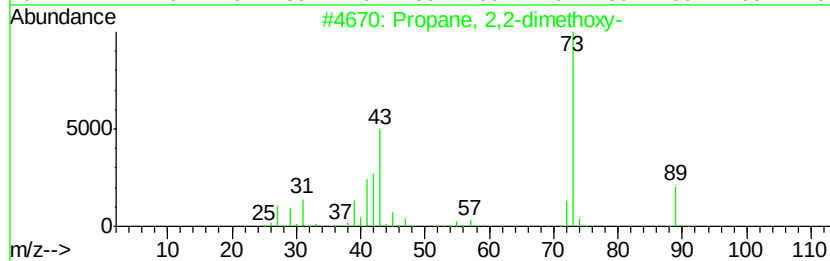
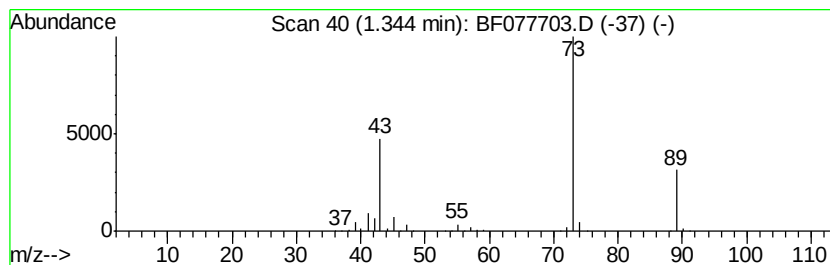
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.34	216.07 ng	3469000	1,4-Dichlorobenzene-d4	7.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



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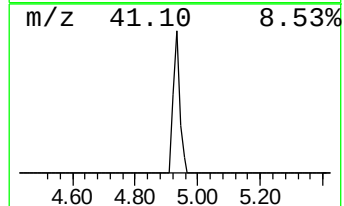
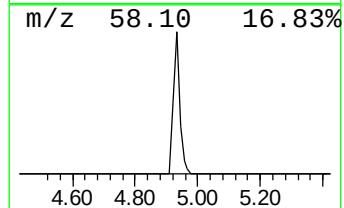
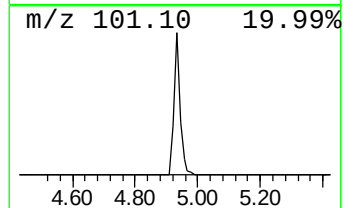
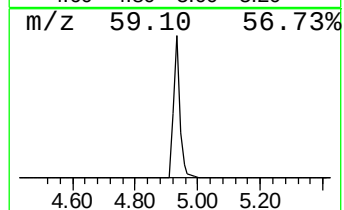
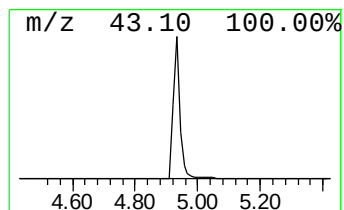
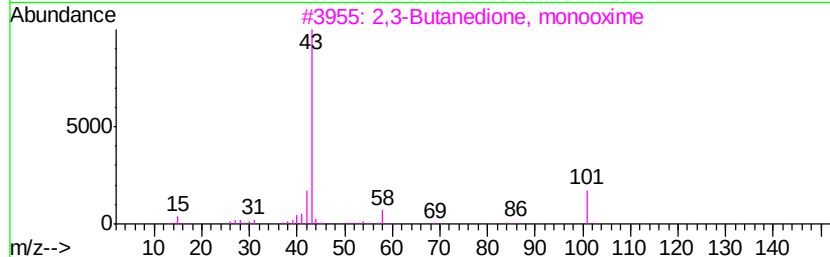
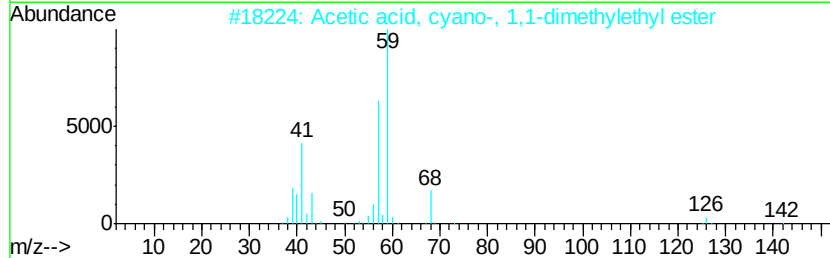
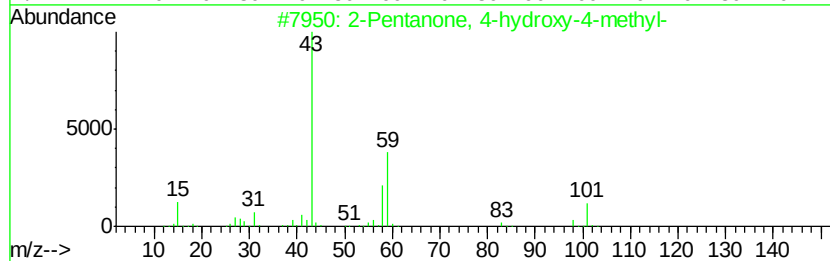
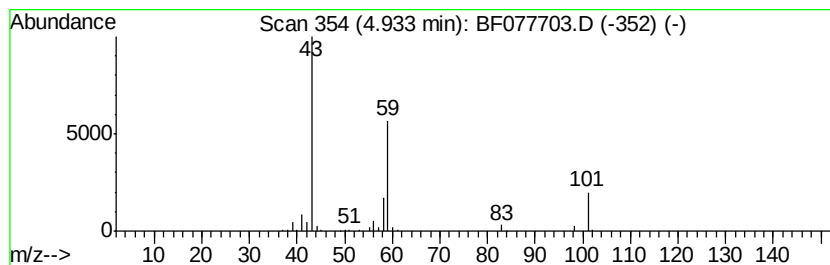
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	13.82 ng	221827	1,4-Dichlorobenzene-d4	7.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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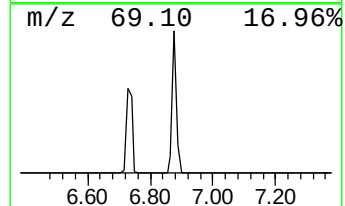
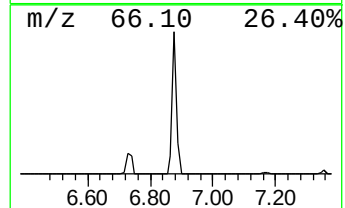
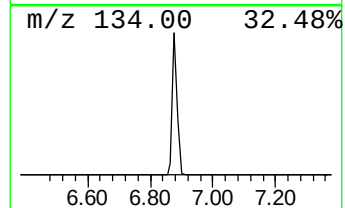
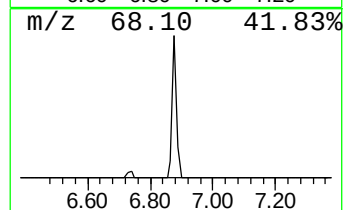
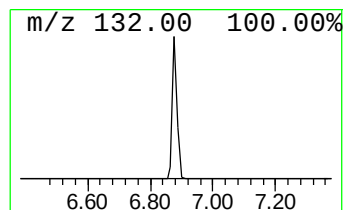
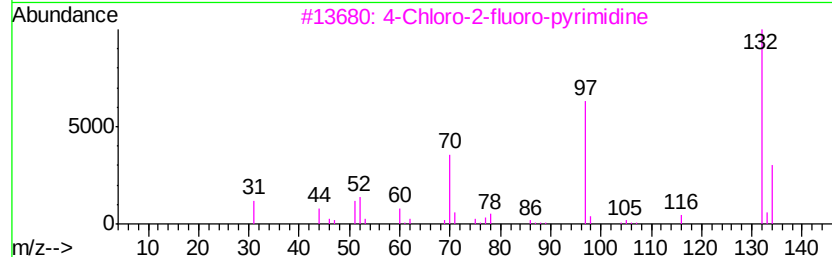
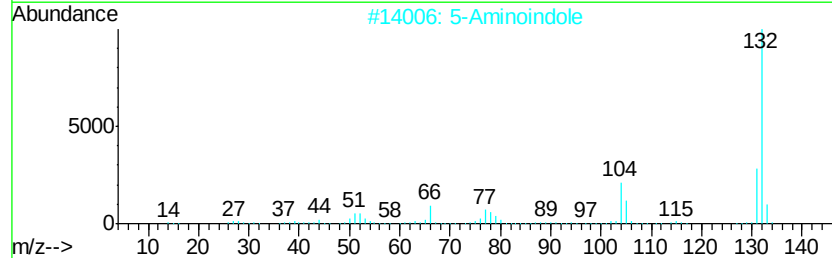
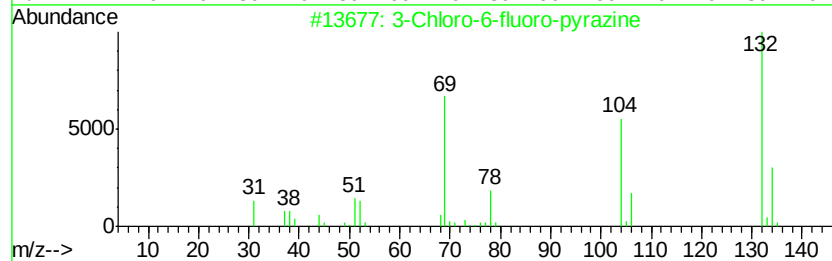
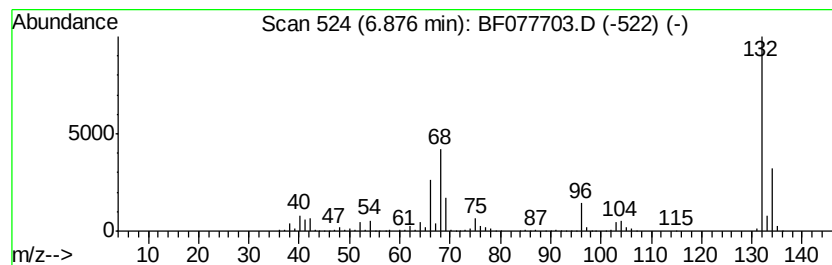
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Peak Number 5 unknown6.88 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	85.66 ng	1375270	1,4-Dichlorobenzene-d4	7.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9
4	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9
5	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9



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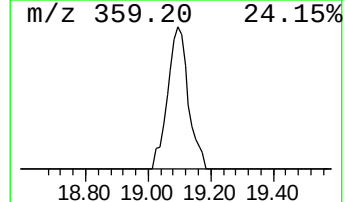
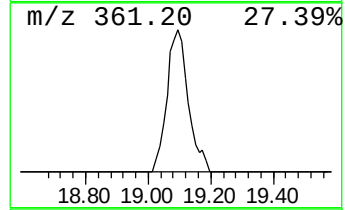
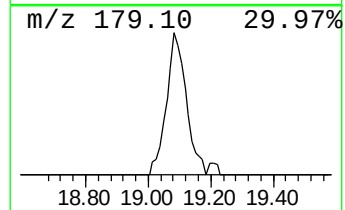
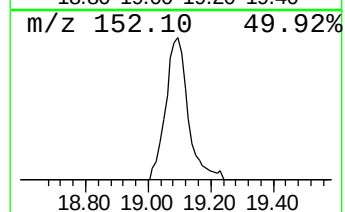
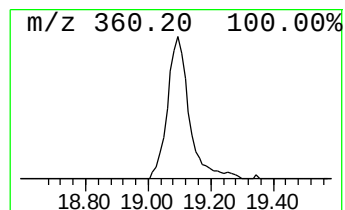
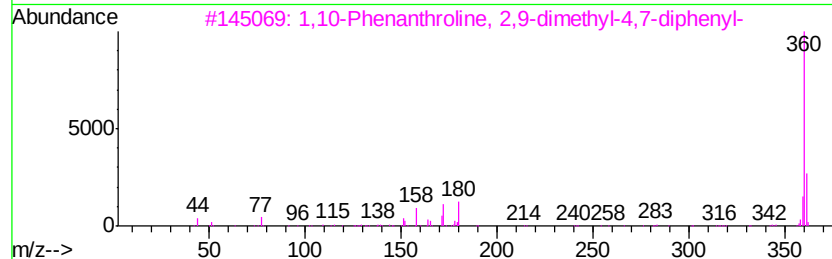
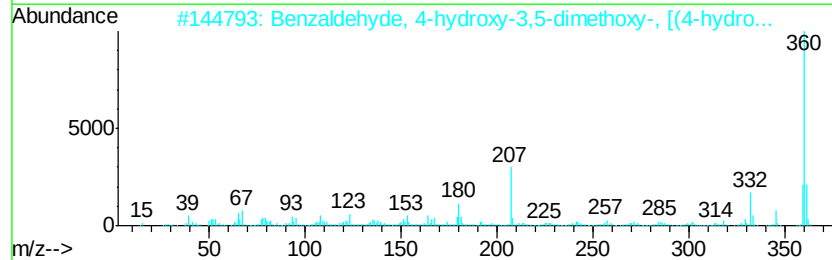
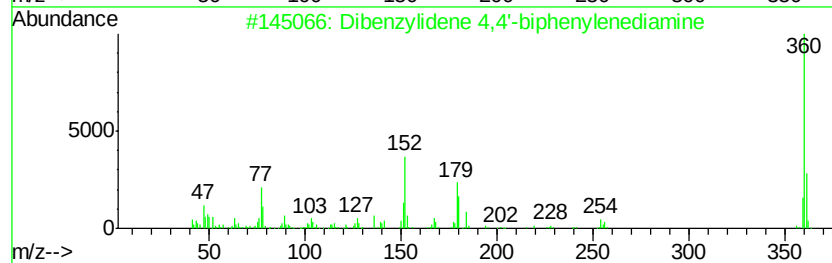
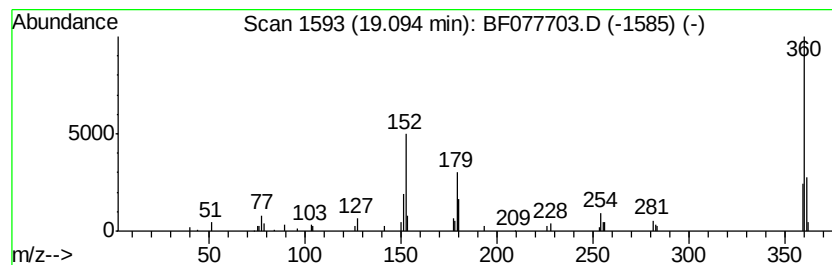
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Peak Number 7 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.09	7.93 ng	231656	Perylene-d12	17.73

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	46
3		1,10-Phenanthroline, 2,9-dimethv...	360	C26H20N2	004733-39-5	43
4		1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
5		N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.34	1.34	216.1	ng	3469000	1	7.17	321107	20.0
2-Pentanone, 4-hy...	4.93	13.8	ng	221827	1	7.17	321107	20.0
unknown6.88	6.88	85.7	ng	1375270	1	7.17	321107	20.0
Dibenzylidene 4,4...	19.09	7.9	ng	231656	6	17.73	584117	20.0