

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062916\
 Data File : BF088507.D
 Acq On : 29 Jun 2016 22:30
 Operator : UM/SJ
 Sample : PB91573BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB91573BL

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-BF062916.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	1.770	8	16	19	rVV	6039277	16809276	100.00%	24.618%
2	1.873	23	25	47	rVB	1487133	2870882	17.08%	4.205%
3	2.147	47	49	73	rVB2	71820	239246	1.42%	0.350%
4	5.027	298	301	307	rBV	260179	444871	2.65%	0.652%
5	5.427	332	336	339	rBV	3633820	5221195	31.06%	7.647%
6	6.456	422	426	428	rBV	3880346	4849906	28.85%	7.103%
7	6.593	434	438	440	rBV	4337435	5245971	31.21%	7.683%
8	6.822	455	458	460	rBV	1565631	1395165	8.30%	2.043%
9	6.982	469	472	474	rVB	3711163	4266611	25.38%	6.249%
10	7.382	504	507	510	rBV	2720149	3310390	19.69%	4.848%
11	8.102	567	570	573	rVB	1755640	1832322	10.90%	2.684%
12	9.188	661	665	667	rBV	4034982	6315421	37.57%	9.249%
13	9.851	720	723	726	rBV	1787975	1987731	11.83%	2.911%
14	10.639	788	792	795	rBV	2644109	3168729	18.85%	4.641%
15	11.336	850	853	855	rVB	1525792	2002908	11.92%	2.933%
16	12.925	988	992	994	rBV	4097320	5180253	30.82%	7.587%
17	13.954	1080	1082	1085	rBV	1540765	1433418	8.53%	2.099%
18	15.360	1202	1205	1208	rBV	1100593	1282497	7.63%	1.878%
19	15.760	1234	1240	1244	rBV	118361	422766	2.52%	0.619%

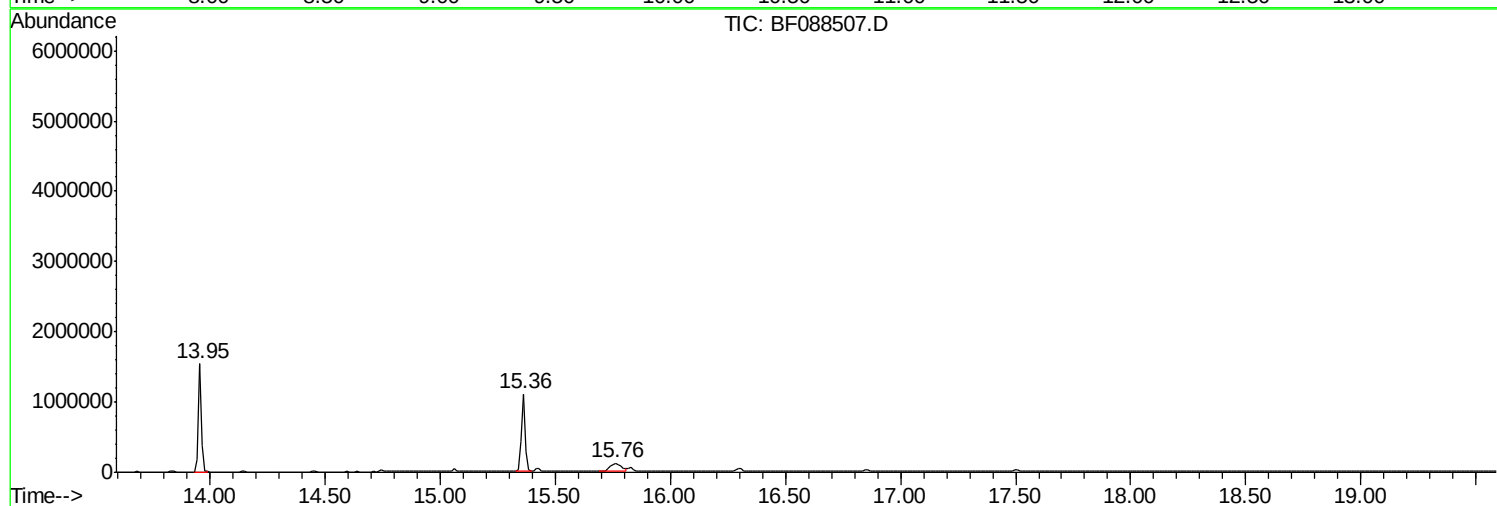
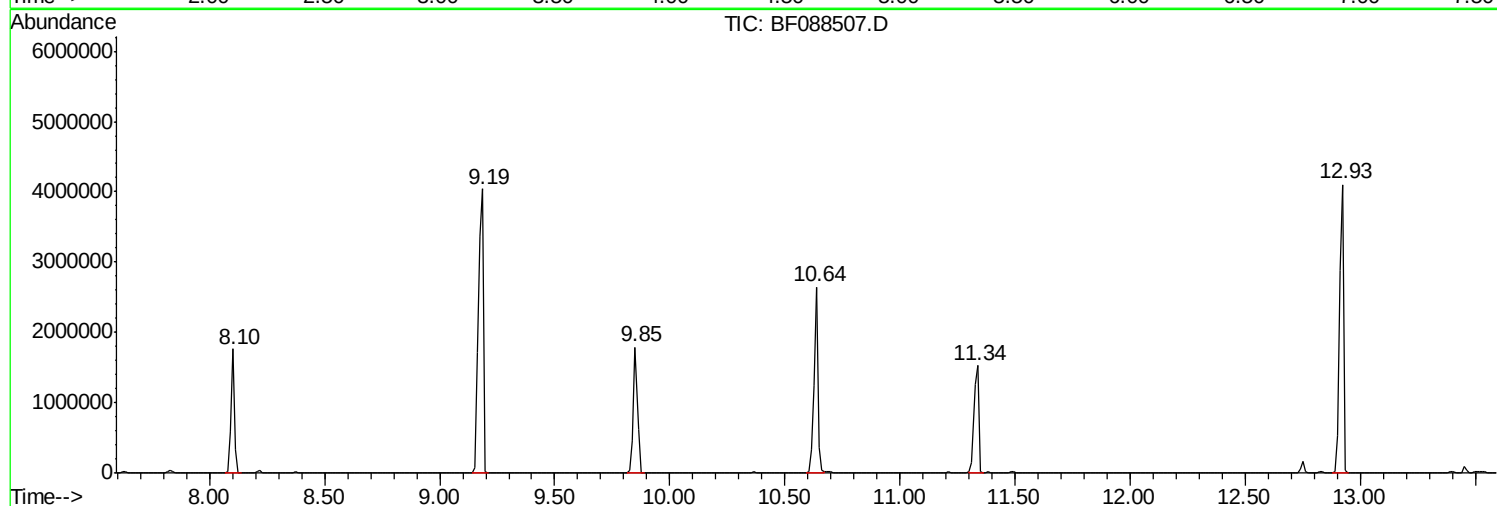
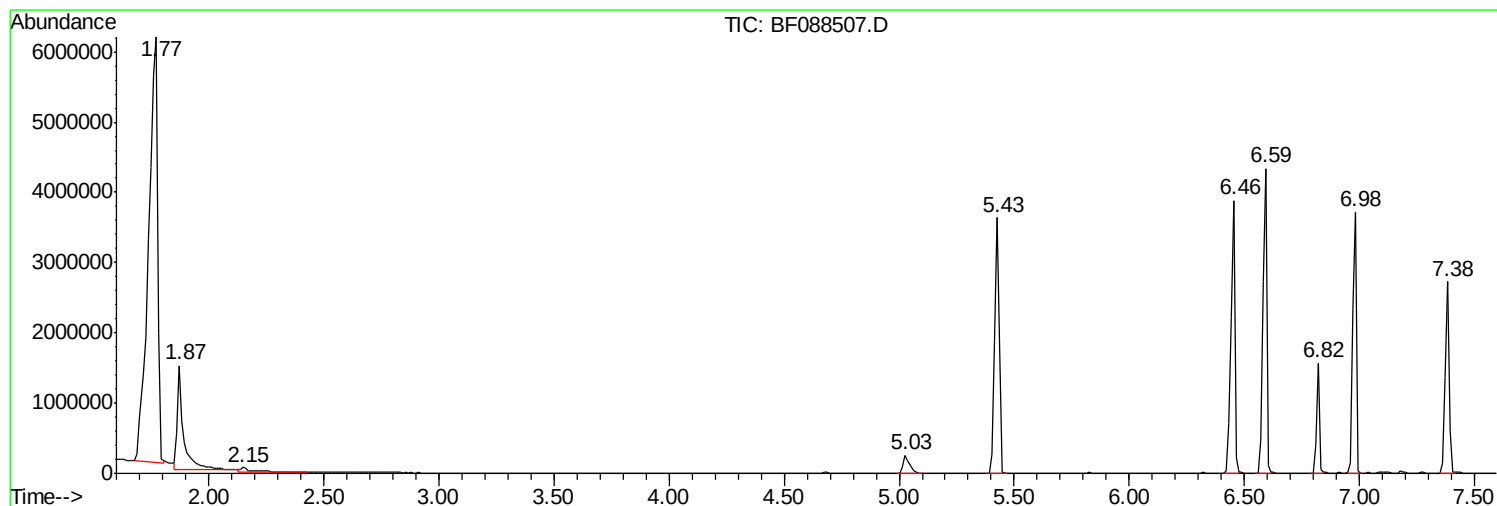
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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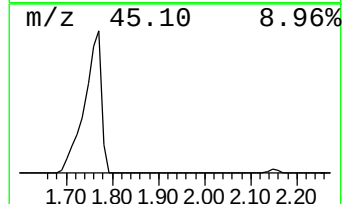
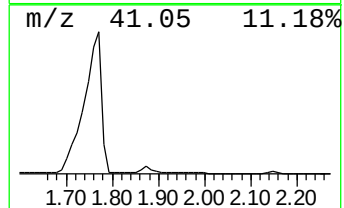
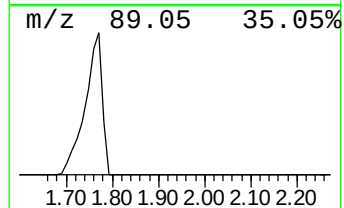
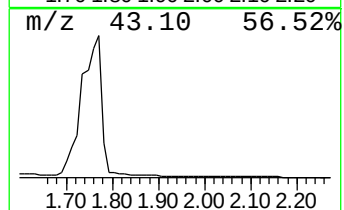
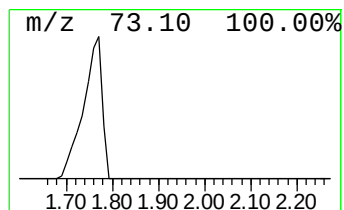
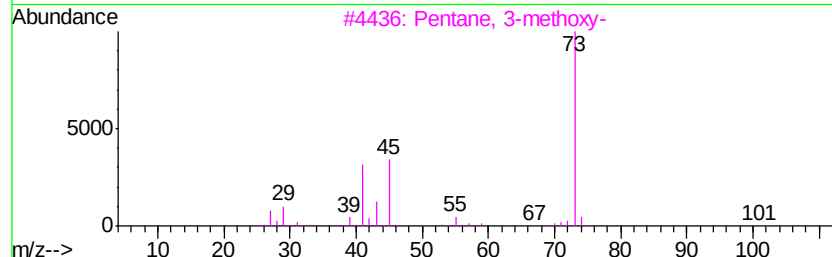
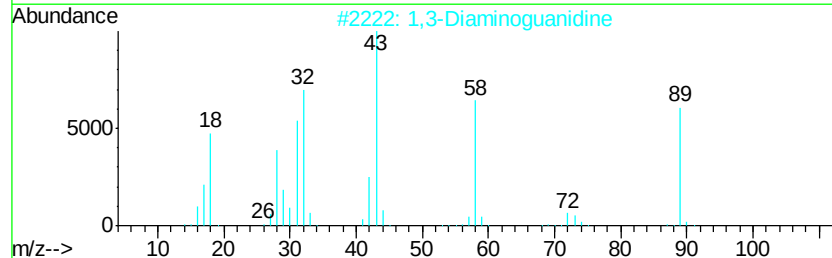
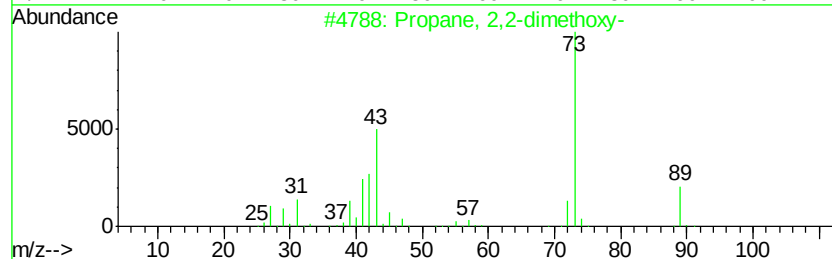
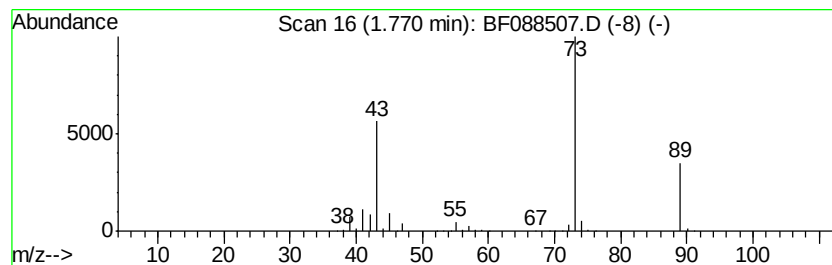
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	240.97 ng	16809300	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2			1,3-Diaminoquinidine	89	CH7N5	004364-78-7	25
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



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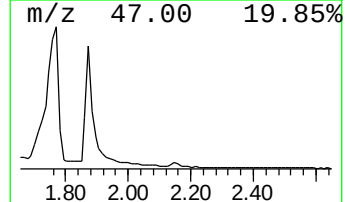
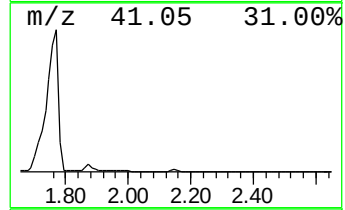
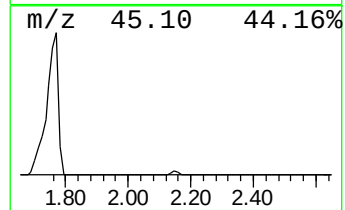
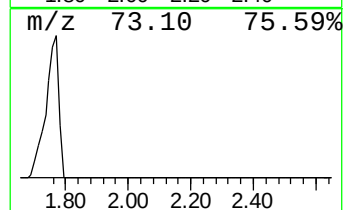
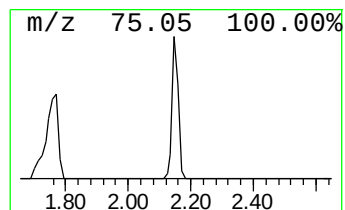
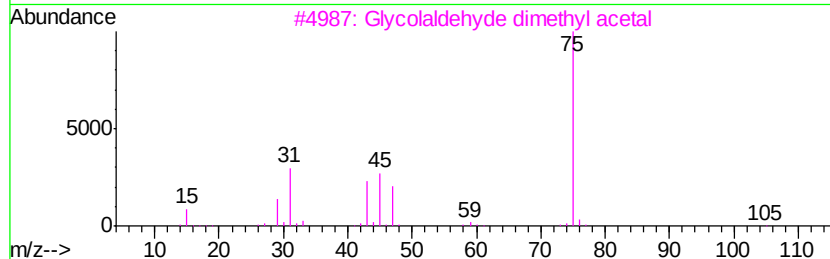
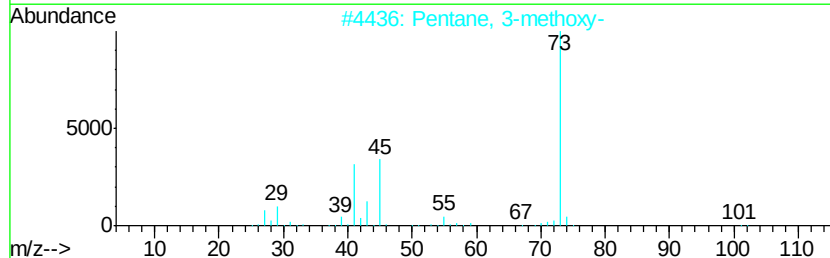
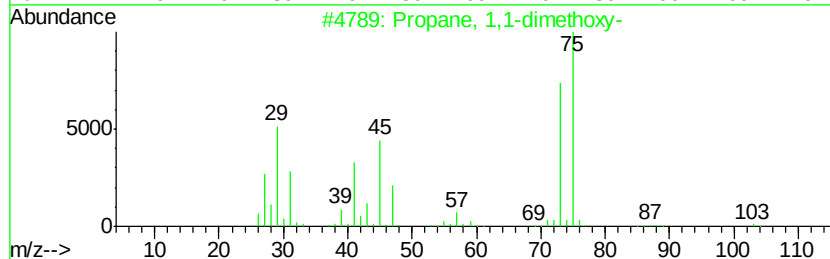
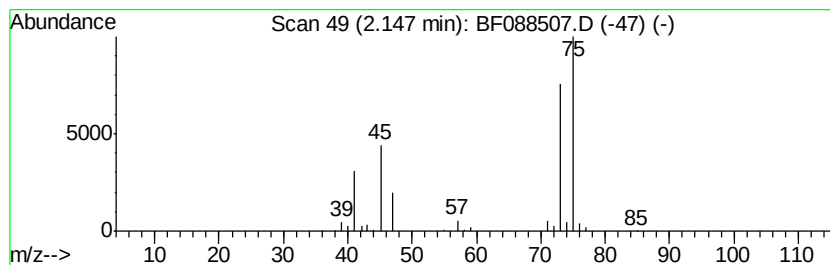
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Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	3.43 ng	239246	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	5
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	5



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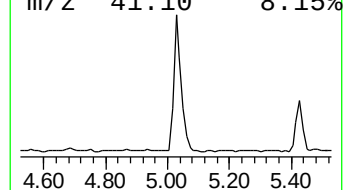
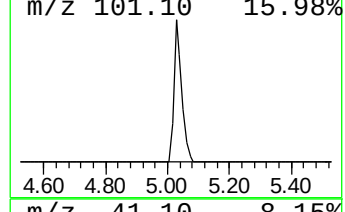
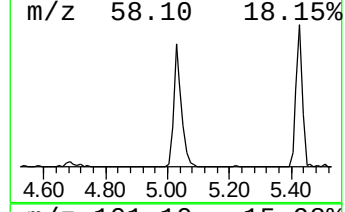
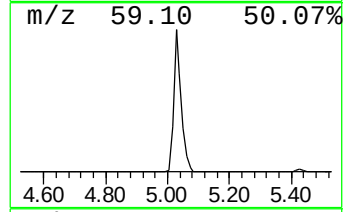
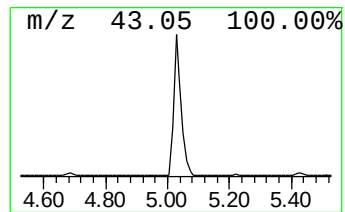
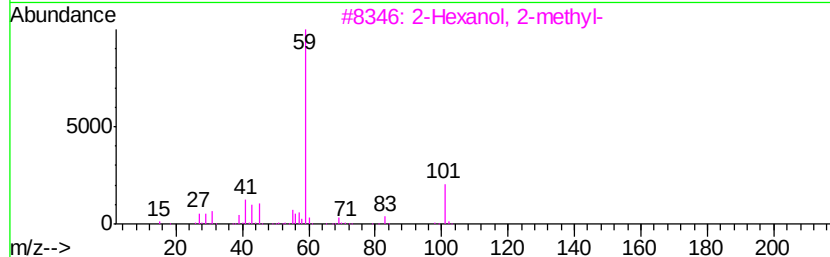
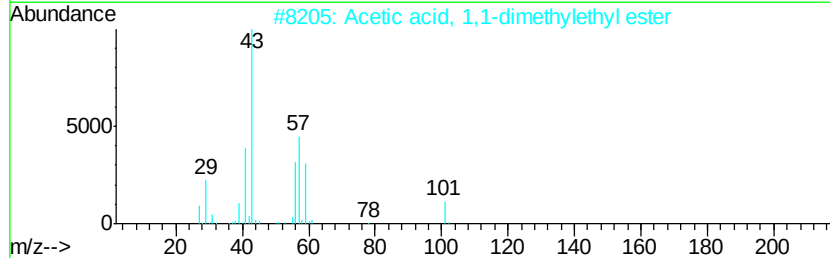
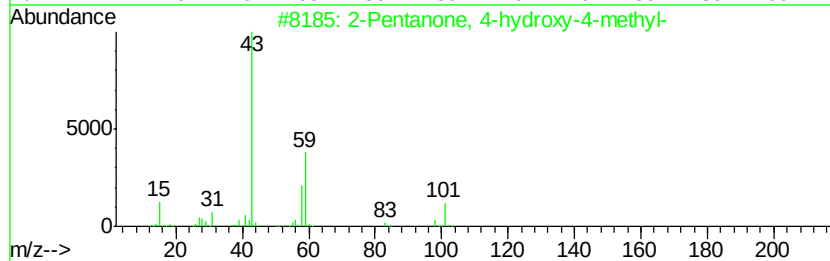
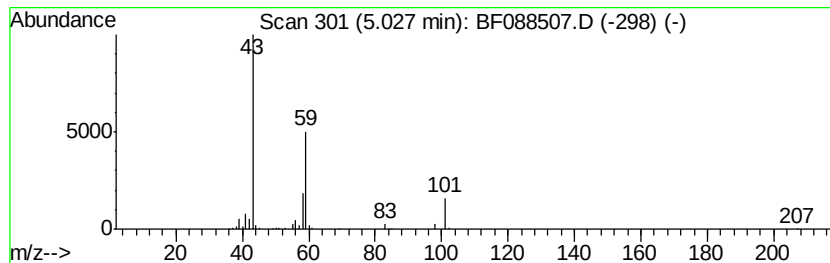
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	6.38 ng	444871	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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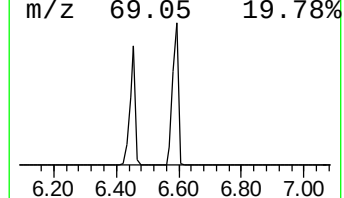
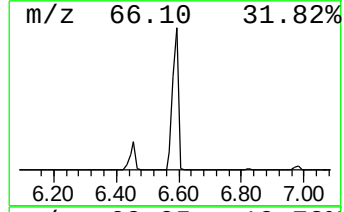
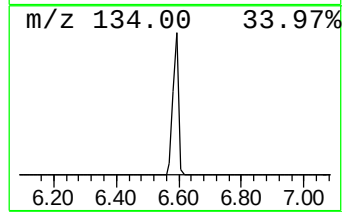
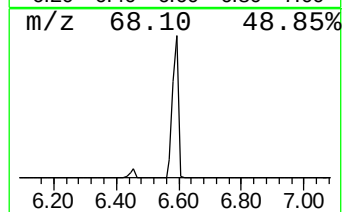
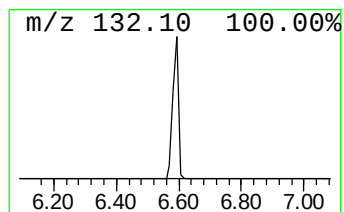
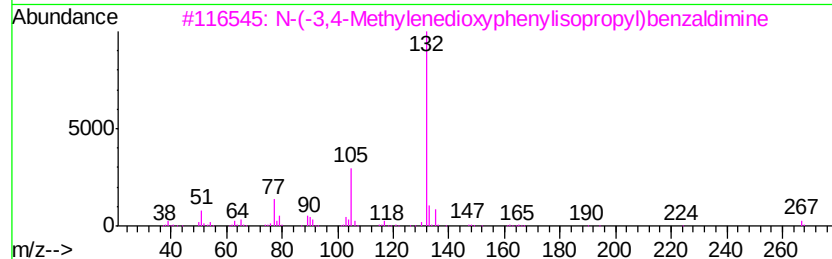
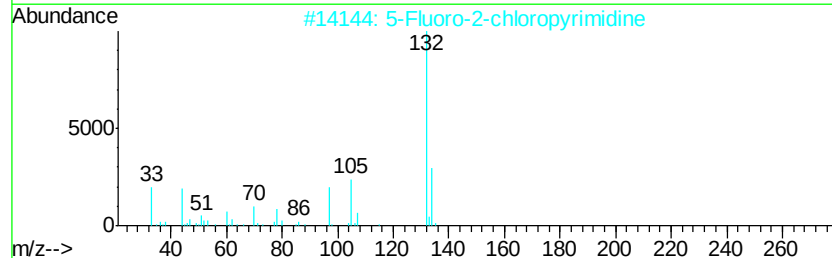
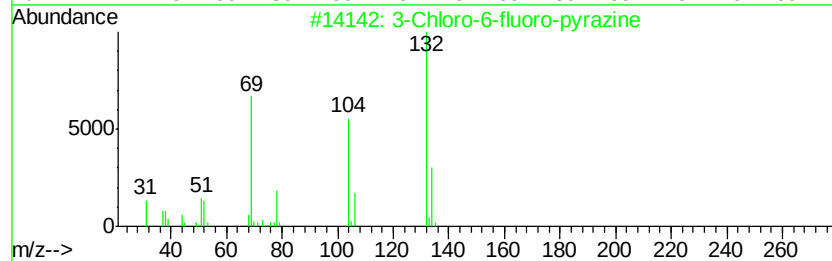
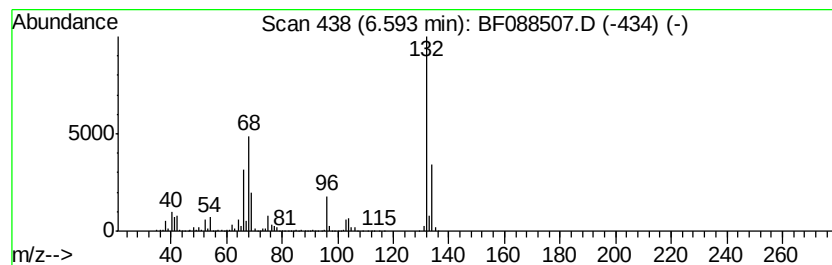
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Peak Number 5 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	75.20 ng	5245970	1,4-Dichlorobenzene-d4	6.82

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		N-(-3,4-Methylenedioxyphenylisopropyl)benzaldimine	267	C17H17NO2	1000378-96-6	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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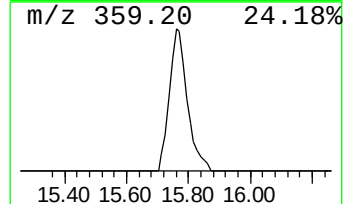
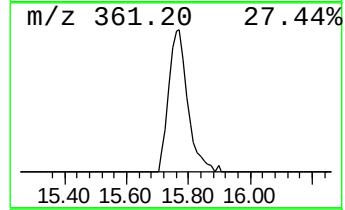
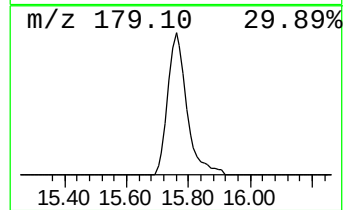
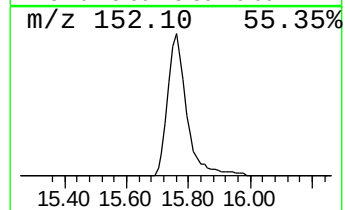
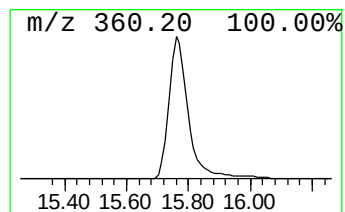
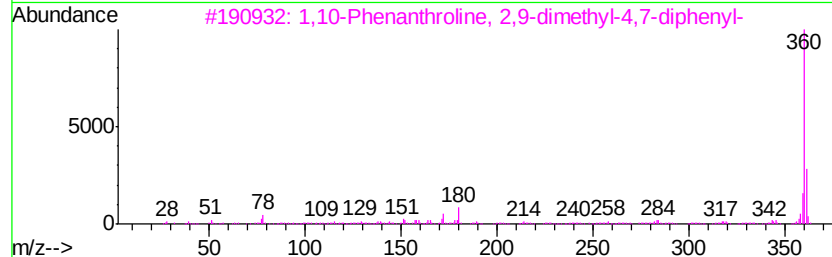
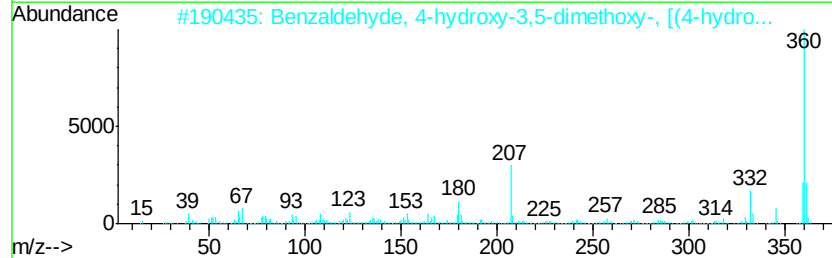
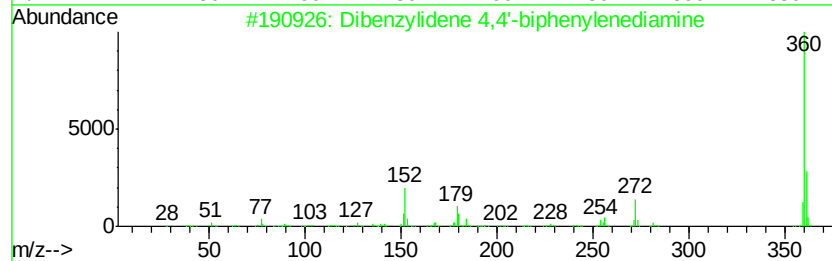
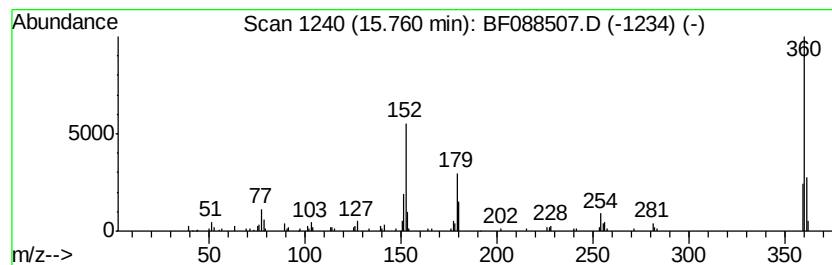
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Peak Number 7 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	6.59 ng	422766	Perylene-d12	15.36

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-dimethv...	360	C26H20N2	004733-39-5	46
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
Propane, 2,2-dime...	1.77	241.0	ng	16809300	1	6.82	1395170	20.0
Propane, 1,1-dime...	2.15	3.4	ng	239246	1	6.82	1395170	20.0
2-Pentanone, 4-hy...	5.03	6.4	ng	444871	1	6.82	1395170	20.0
unknown6.59	6.59	75.2	ng	5245970	1	6.82	1395170	20.0
Dibenzylidene 4,4...	15.76	6.6	ng	422766	6	15.36	1282500	20.0