

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111417\
 Data File : BF100549.D
 Acq On : 14 Nov 2017 18:15
 Operator : SJ/JU
 Sample : I6388-15
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3N-8

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-BF110817.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	2.199	17	19	26	rVB2	21524	30221	1.21%	0.139%
2	5.116	510	515	524	rVB	364721	467835	18.67%	2.150%
3	5.510	576	582	585	rBV	2293884	2440792	97.40%	11.219%
4	6.510	746	752	762	rBV	2405888	2506034	100.00%	11.519%
5	6.651	772	776	780	rBV	2397164	2417641	96.47%	11.113%
6	6.886	812	816	819	rVB	843894	746824	29.80%	3.433%
7	7.039	838	842	846	rBV	2108316	1913211	76.34%	8.794%
8	7.445	906	911	914	rBV	1653202	1494431	59.63%	6.869%
9	8.163	1029	1033	1037	rBV	975952	929874	37.11%	4.274%
10	8.716	1123	1127	1130	rBV	146672	117967	4.71%	0.542%
11	9.239	1211	1216	1219	rBV	2787001	2442011	97.45%	11.225%
12	9.627	1278	1282	1285	rBV	213319	166160	6.63%	0.764%
13	9.922	1328	1332	1335	rBV	995919	831089	33.16%	3.820%
14	10.627	1449	1452	1456	rBV	299021	260125	10.38%	1.196%
15	10.710	1462	1466	1469	rBV	1176305	1089538	43.48%	5.008%
16	11.404	1581	1584	1588	rBV	779201	702668	28.04%	3.230%
17	12.986	1849	1853	1857	rBV	1791662	1771704	70.70%	8.144%
18	13.874	2000	2004	2011	rBV	71271	88230	3.52%	0.406%
19	14.045	2029	2033	2036	rBV	830059	738601	29.47%	3.395%
20	15.151	2218	2221	2224	rVB2	27964	30571	1.22%	0.141%
21	15.521	2279	2284	2291	rVB	404994	532202	21.24%	2.446%
22	15.974	2358	2361	2366	rVB3	27442	37271	1.49%	0.171%

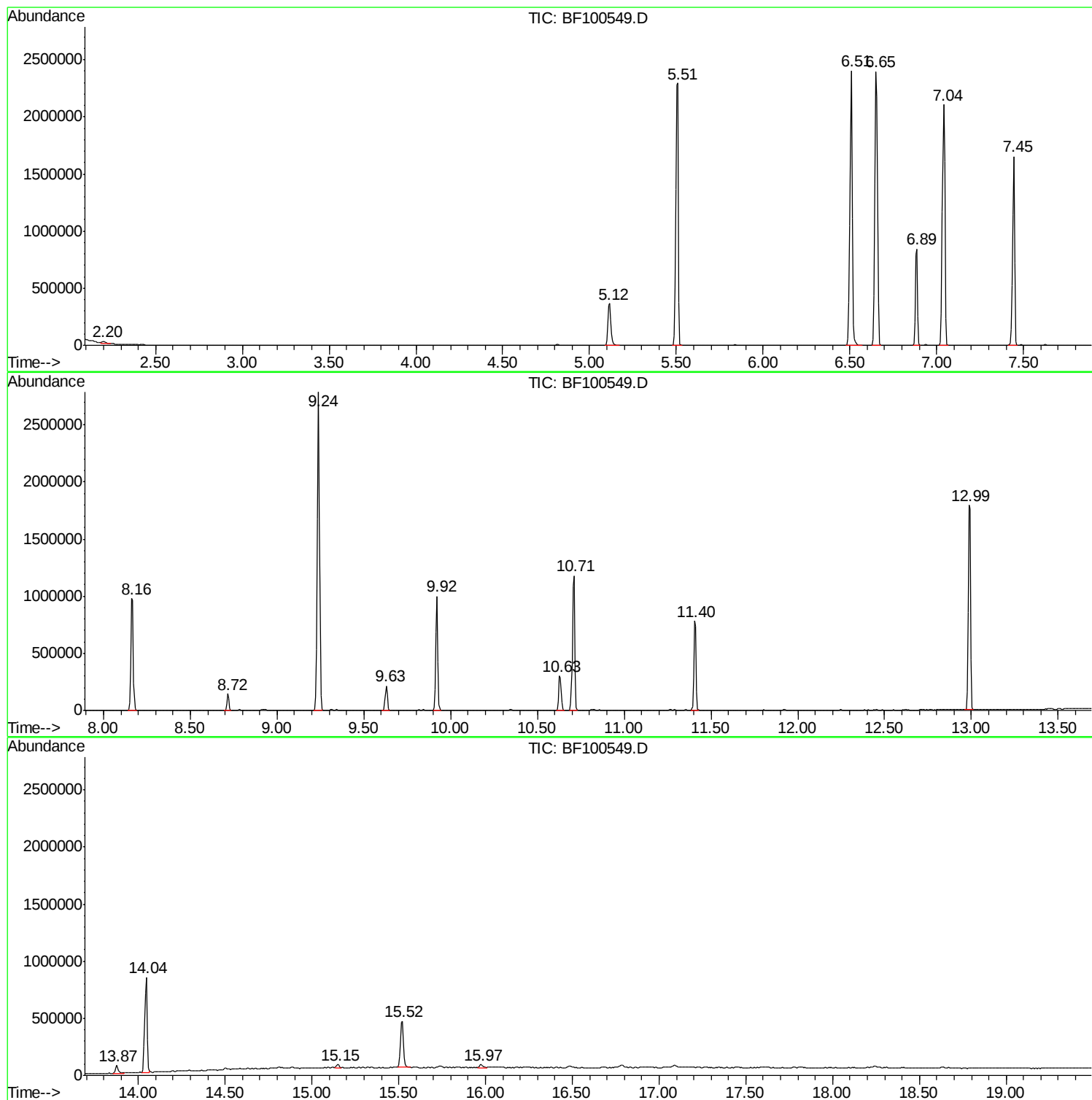
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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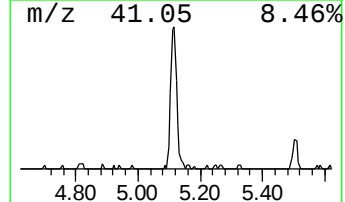
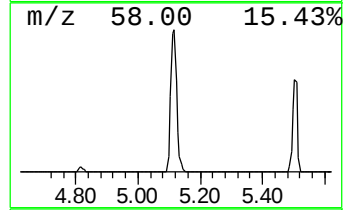
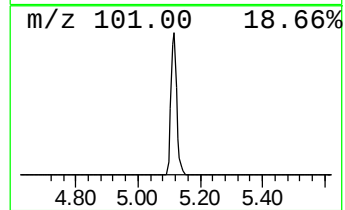
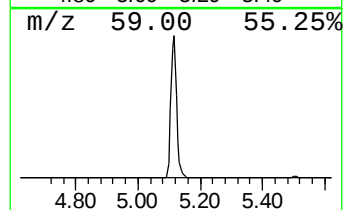
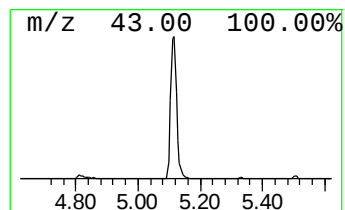
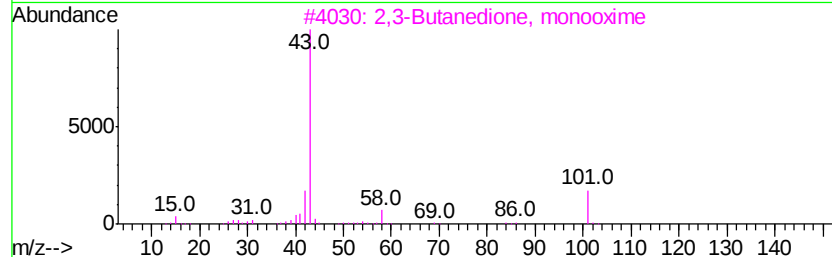
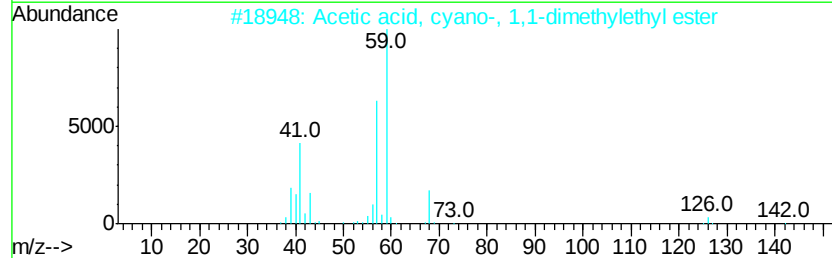
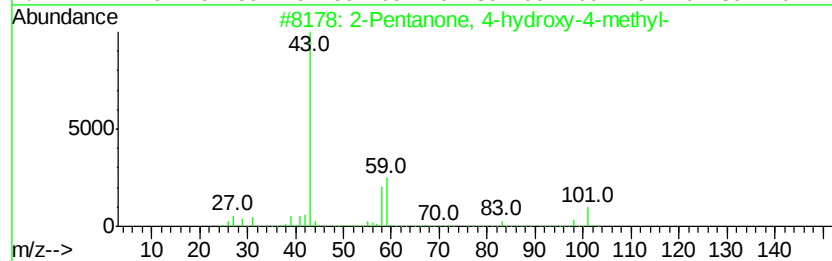
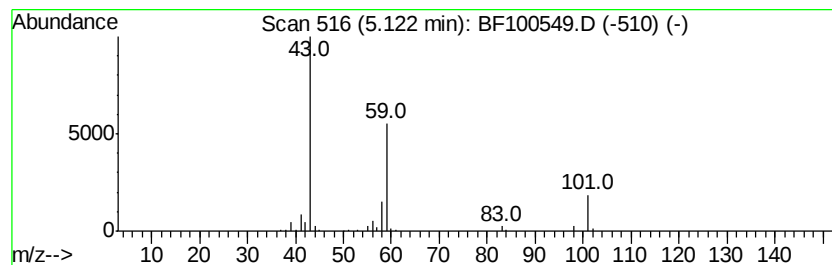
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.53 ng	467835	1,4-Dichlorobenzene-d4	6.89

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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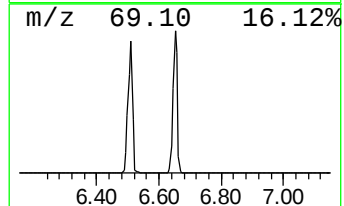
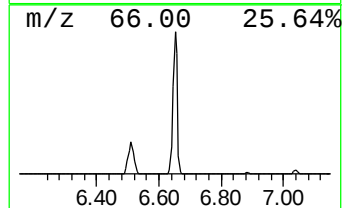
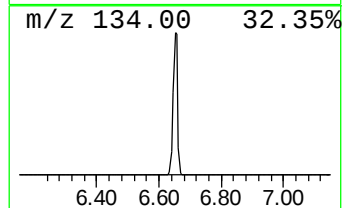
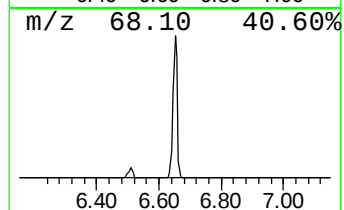
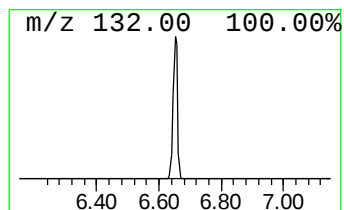
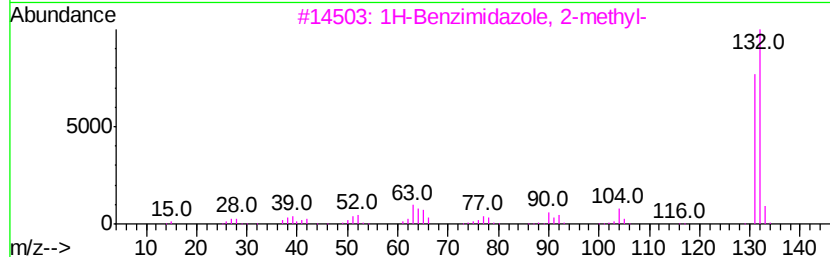
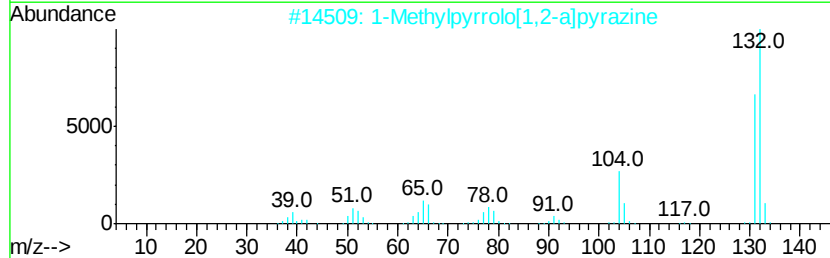
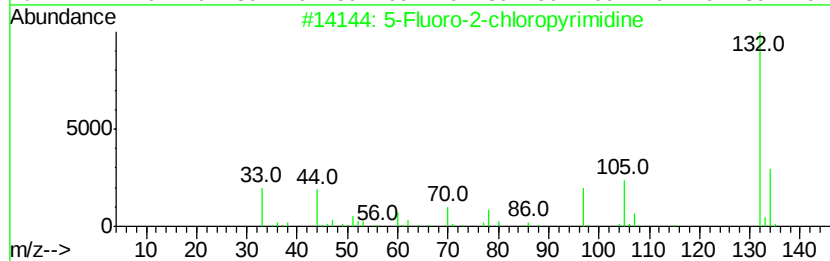
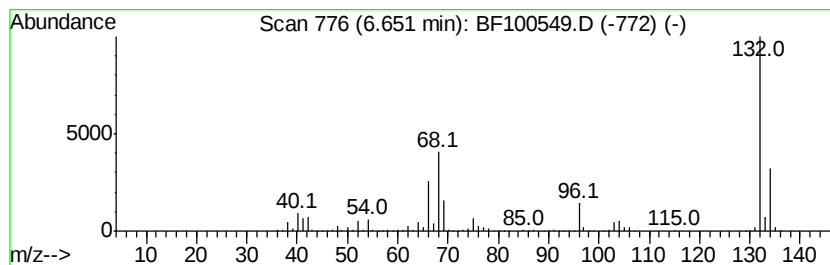
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	64.74 ng	2417640	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
2		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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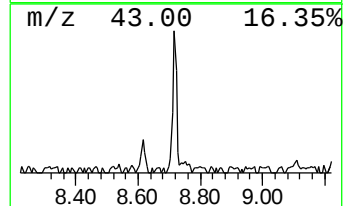
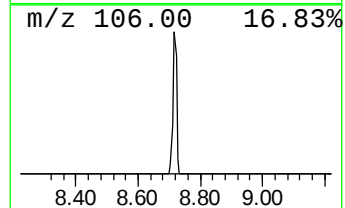
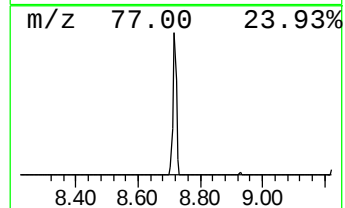
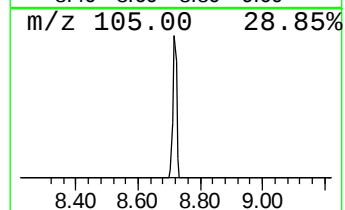
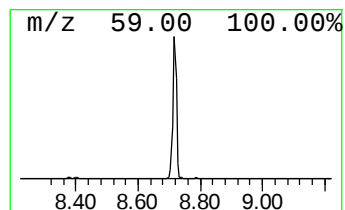
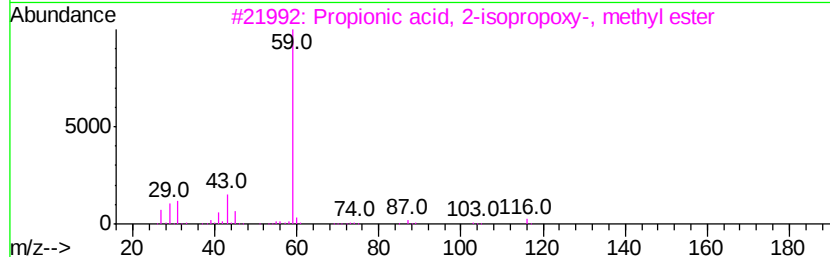
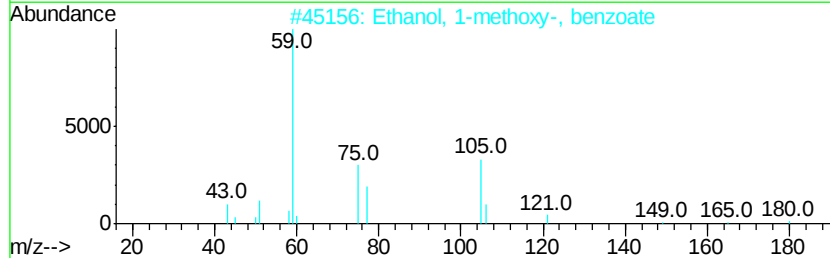
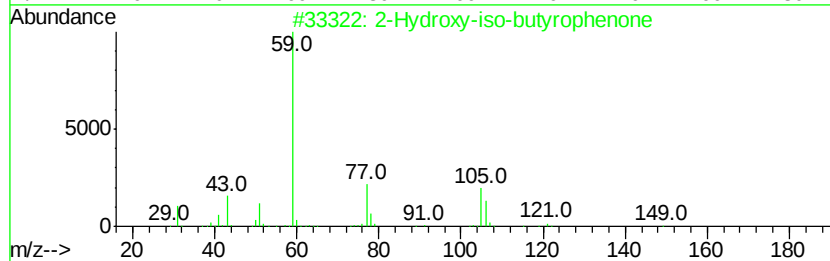
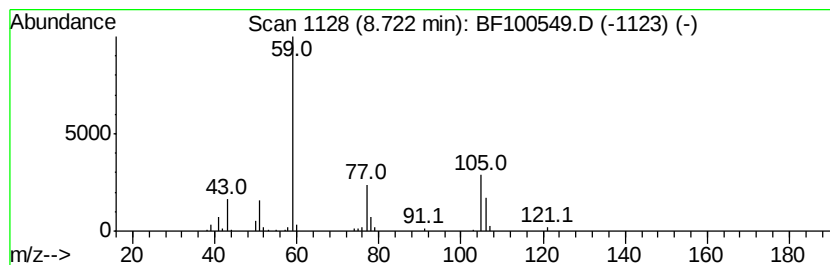
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.54 ng	117967	Napthalene-d8	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	23
4		Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
5		Guanidine	59	CH5N3	000113-00-8	7



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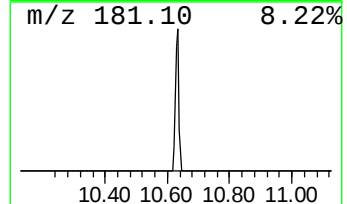
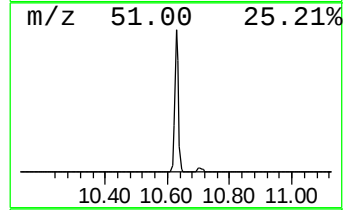
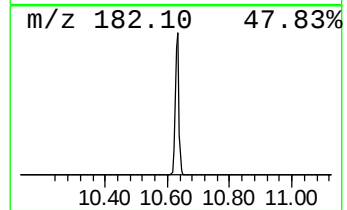
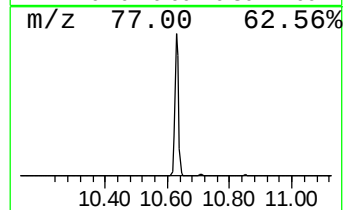
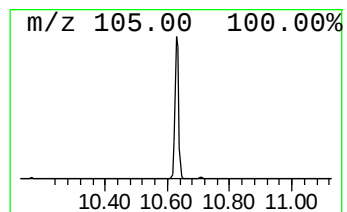
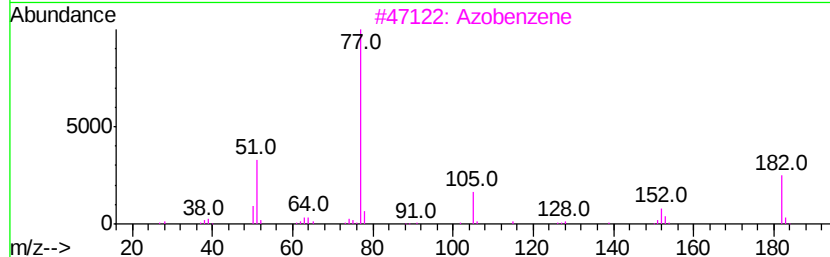
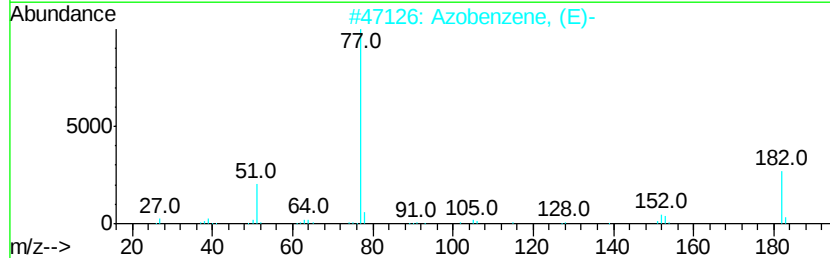
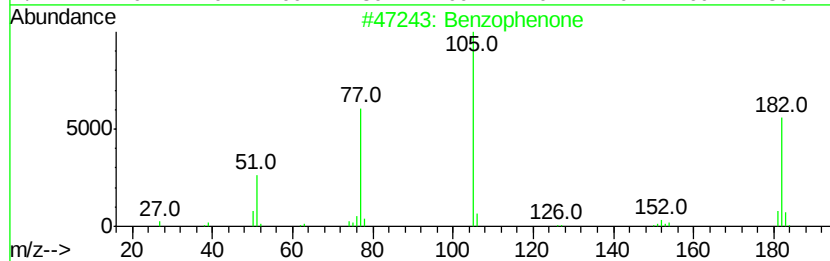
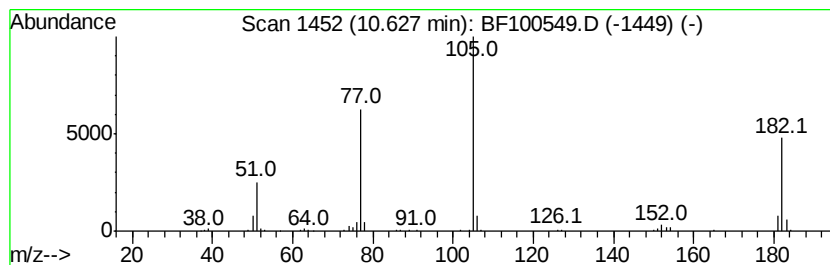
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	6.26 ng	260125	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3		Azobenzene	182	C12H10N2	000103-33-3	59
4		Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5		Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



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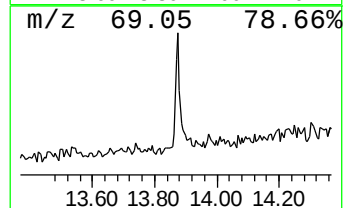
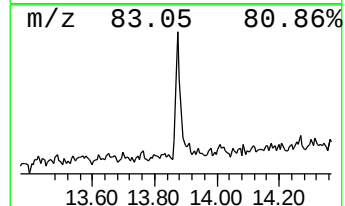
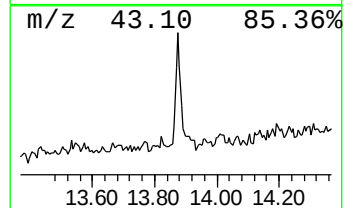
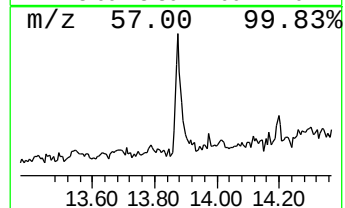
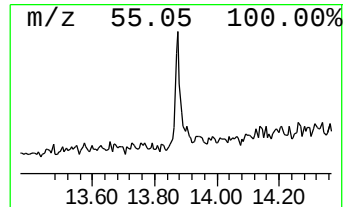
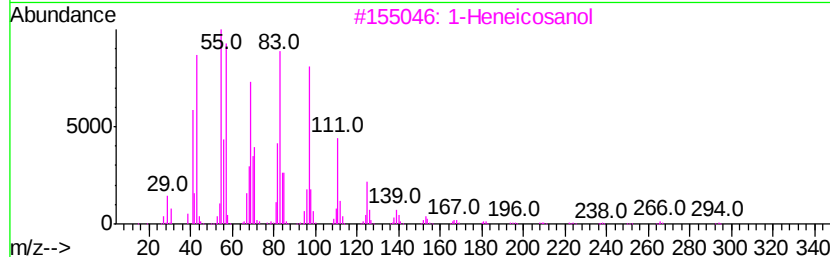
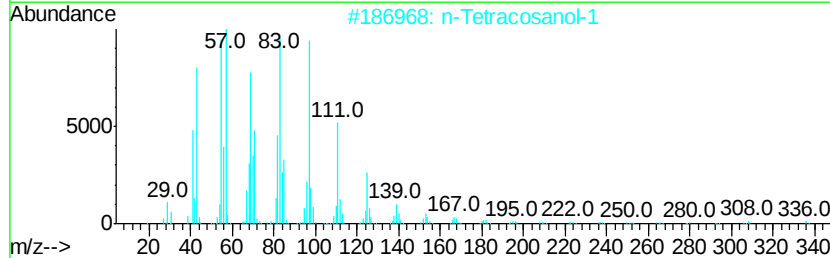
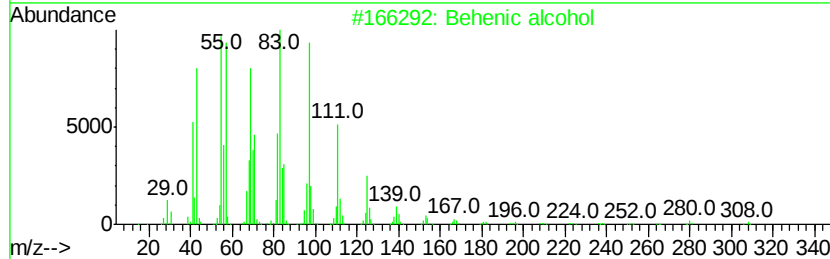
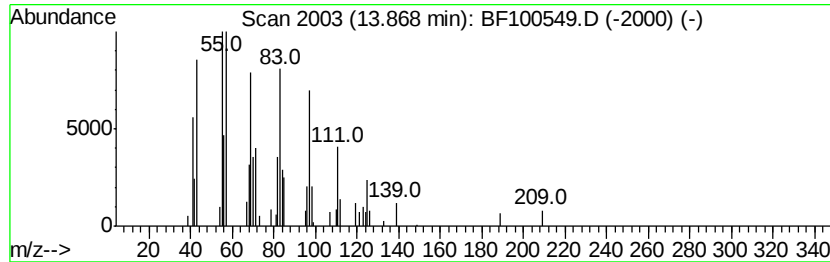
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Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.39 ng	88230	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	12.5	ng	467835	1	6.89	746824	20.0
unknown6.65	6.65	64.7	ng	2417640	1	6.89	746824	20.0
2-Hydroxy-iso-but...	8.72	2.5	ng	117967	2	8.17	929874	20.0
Benzophenone	10.63	6.3	ng	260125	3	9.92	831089	20.0
Behenic alcohol	13.87	2.4	ng	88230	5	14.04	738601	20.0