

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100612.D
 Acq On : 16 Nov 2017 3:00
 Operator : SJ/JU
 Sample : I6426-10
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110917-JETT-F-D-S

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-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	2.175	11	15	21	rVB	40277	54481	1.70%	0.279%
2	5.098	508	512	523	rBV	188683	197164	6.14%	1.011%
3	5.493	575	579	583	rBV	1072005	924887	28.78%	4.740%
4	6.498	746	750	759	rVB	666206	628283	19.55%	3.220%
5	6.645	771	775	779	rBV	1803020	1628614	50.68%	8.347%
6	6.881	811	815	819	rBB	833074	658952	20.51%	3.377%
7	7.040	837	842	845	rBV	2483065	2187288	68.07%	11.210%
8	7.445	905	911	914	rBV	1822648	1791762	55.76%	9.183%
9	8.163	1029	1033	1036	rBV	1048466	862339	26.84%	4.420%
10	8.716	1123	1127	1130	rBV	170737	135683	4.22%	0.695%
11	9.239	1211	1216	1219	rBV	3438823	3213208	100.00%	16.468%
12	9.628	1278	1282	1285	rBV	95717	77028	2.40%	0.395%
13	9.916	1328	1331	1335	rVB2	1075163	923855	28.75%	4.735%
14	10.628	1448	1452	1455	rBV	423052	326908	10.17%	1.675%
15	10.704	1461	1465	1468	rBV	1449823	1254770	39.05%	6.431%
16	11.404	1580	1584	1587	rVB	998577	858603	26.72%	4.401%
17	12.986	1848	1853	1856	rBV	2600614	2488854	77.46%	12.756%
18	13.868	1999	2003	2012	rBV	60006	75332	2.34%	0.386%
19	14.039	2028	2032	2035	rVB	638625	572419	17.81%	2.934%
20	14.721	2144	2148	2151	rBV	34606	38561	1.20%	0.198%
21	15.510	2277	2282	2290	rBV	484602	612263	19.05%	3.138%

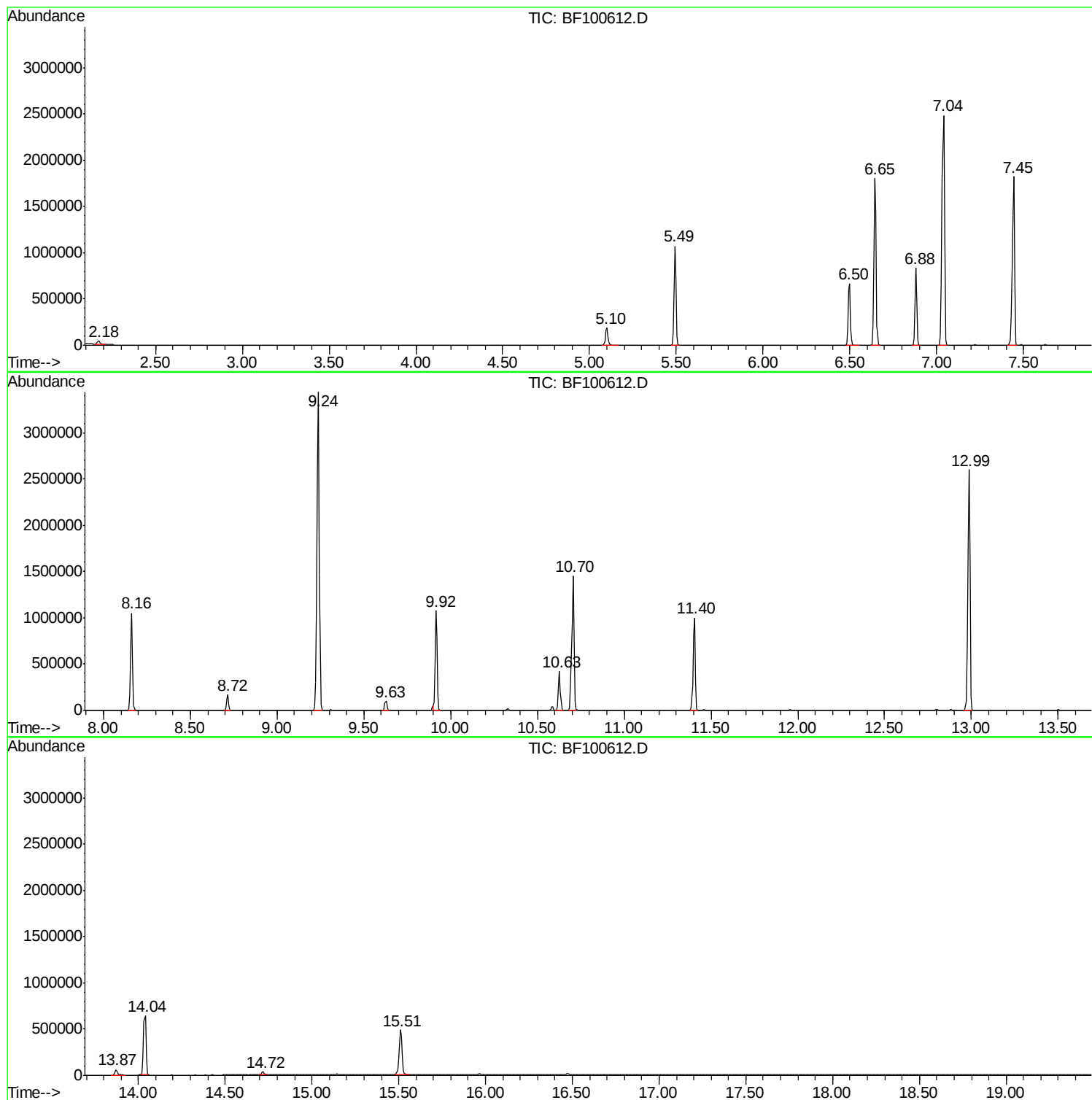
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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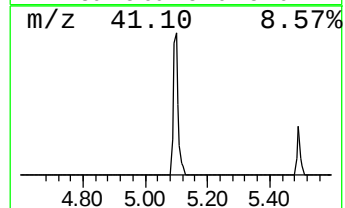
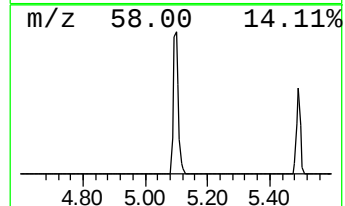
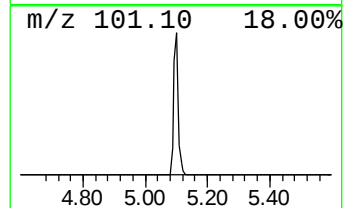
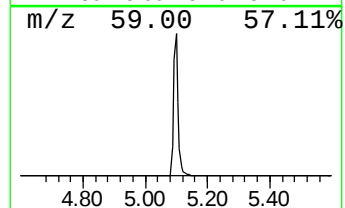
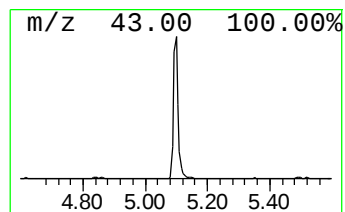
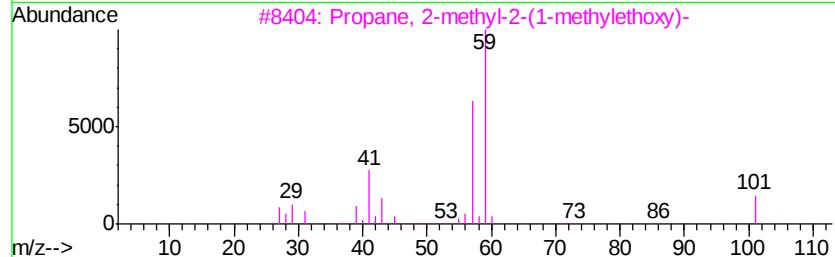
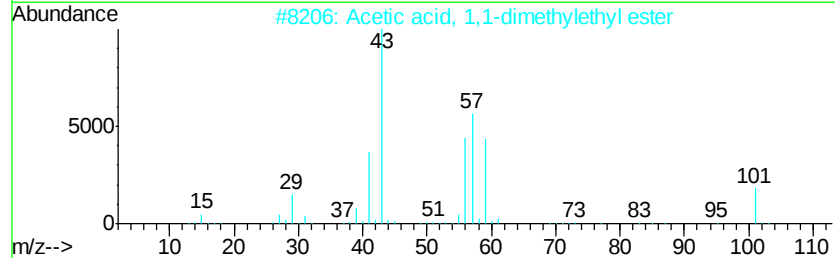
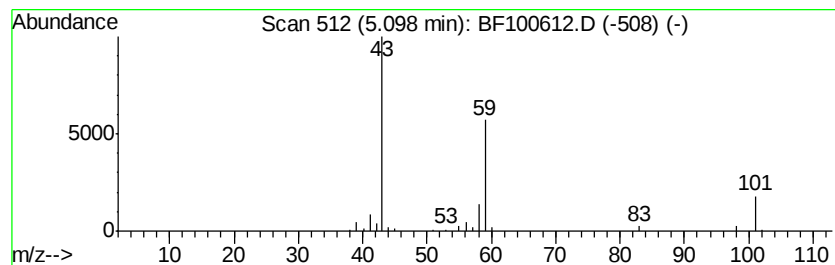
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	5.98 ng	197164	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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	36
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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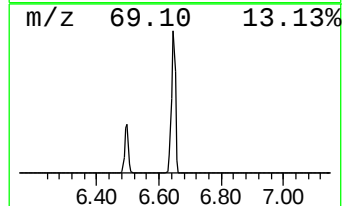
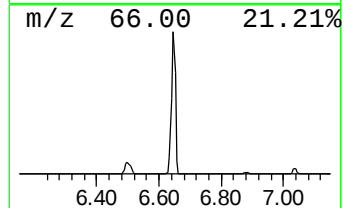
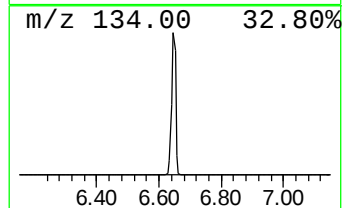
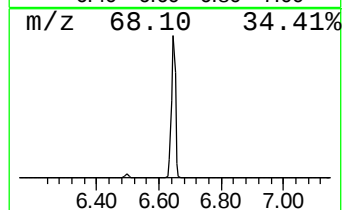
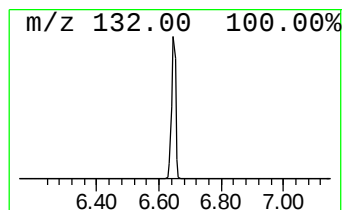
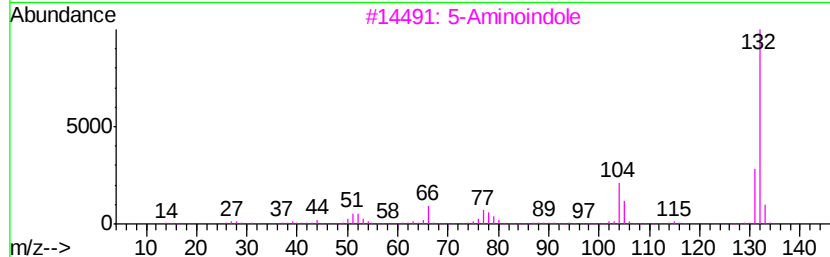
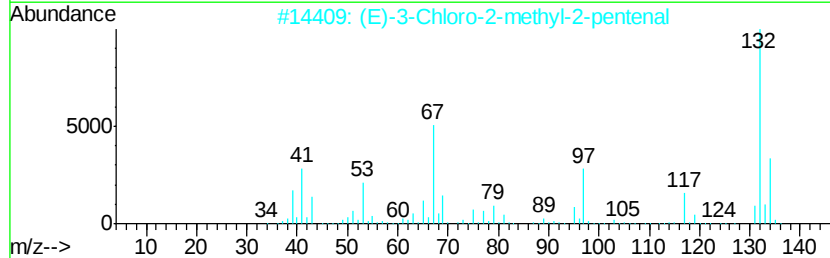
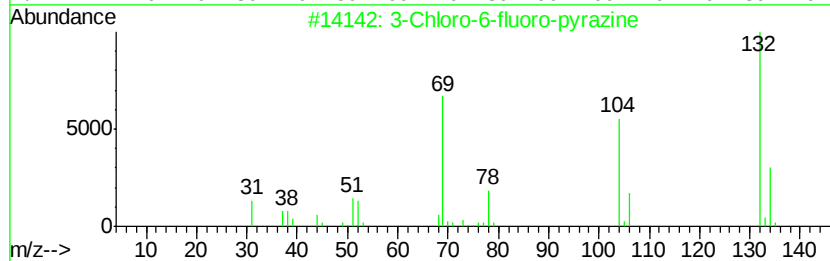
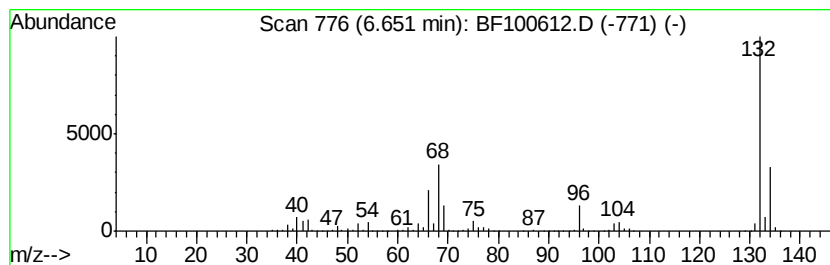
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Peak Number 2 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	49.43 ng	1628610	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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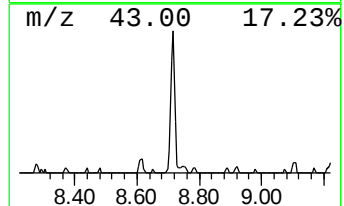
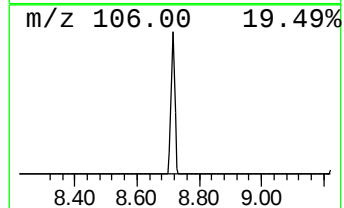
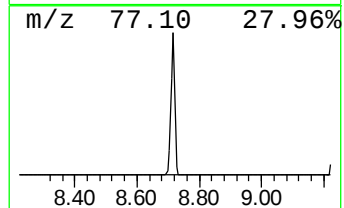
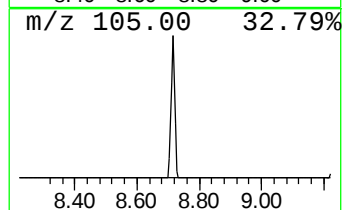
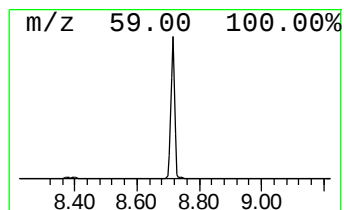
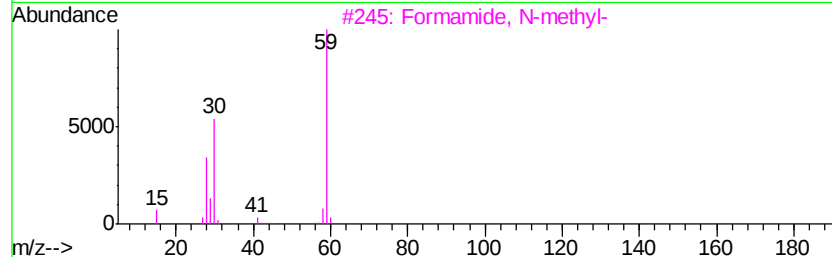
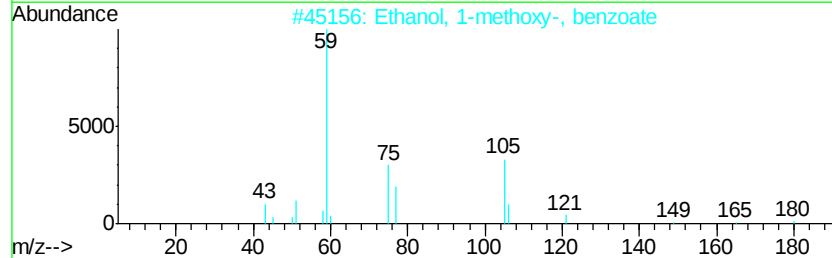
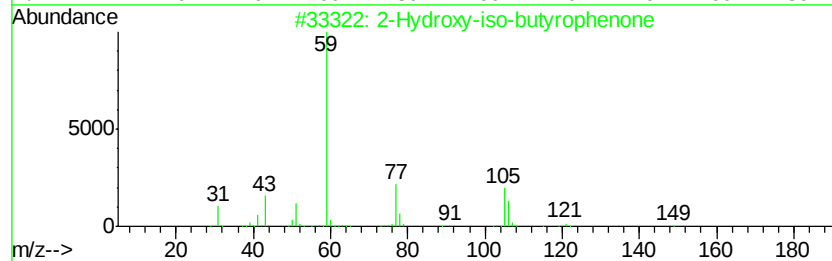
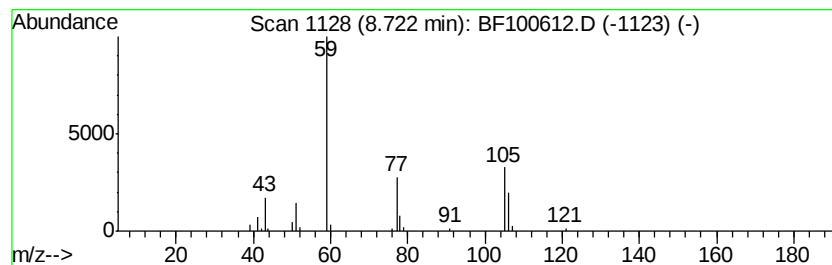
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	3.15 ng	135683	Napthalene-d8	8.16

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	50
3		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
4		2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	5
5		2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	5



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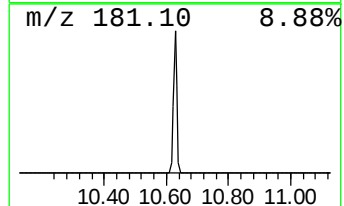
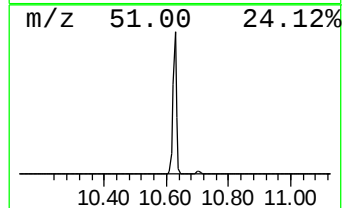
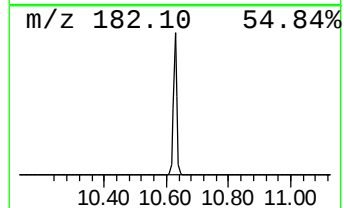
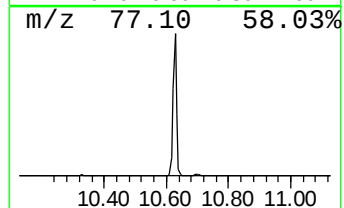
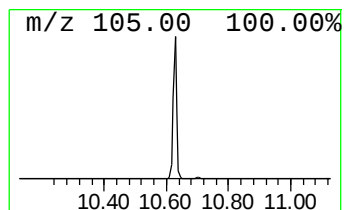
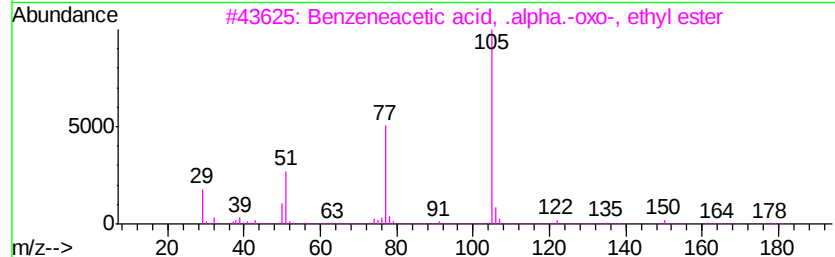
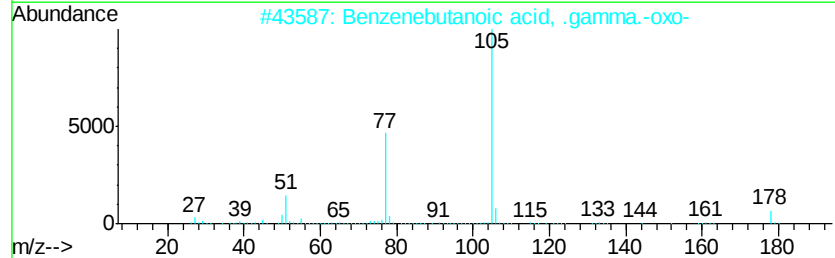
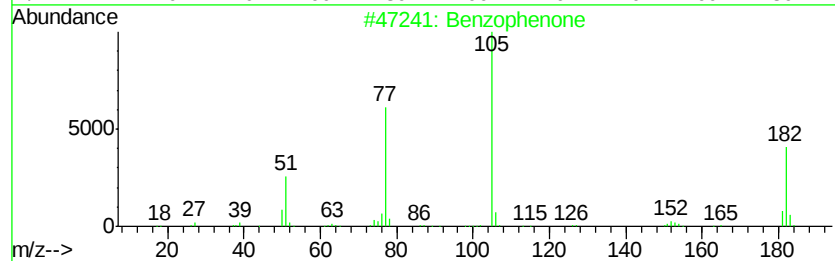
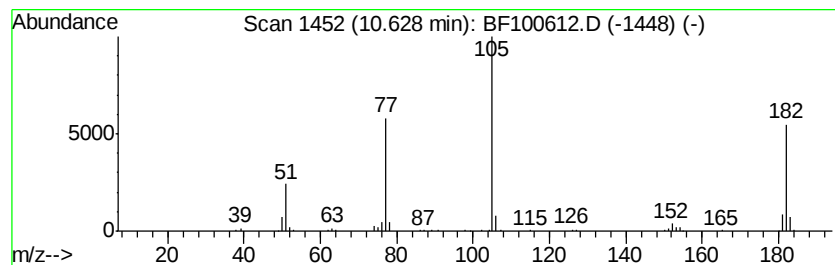
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	7.08 ng	326908	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
3		Benzeneacetic acid, .alpha.-oxo-...	178 C10H10O3	001603-79-8 47
4		Acetophenone, 2-chloro-	154 C8H7ClO	000532-27-4 47
5		1-Butanone, 1-phenyl-	148 C10H12O	000495-40-9 47



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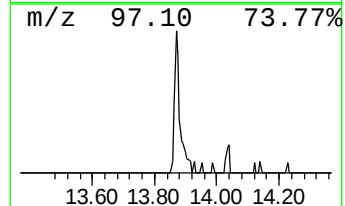
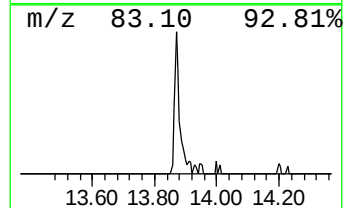
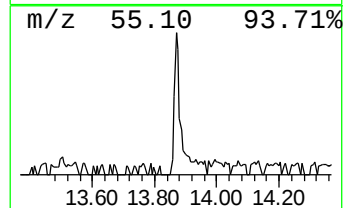
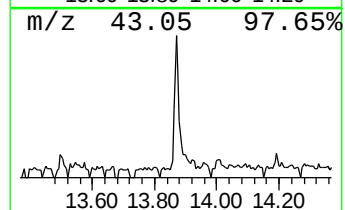
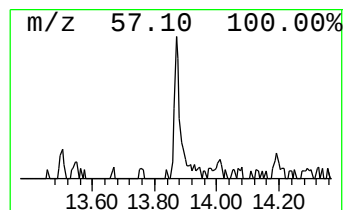
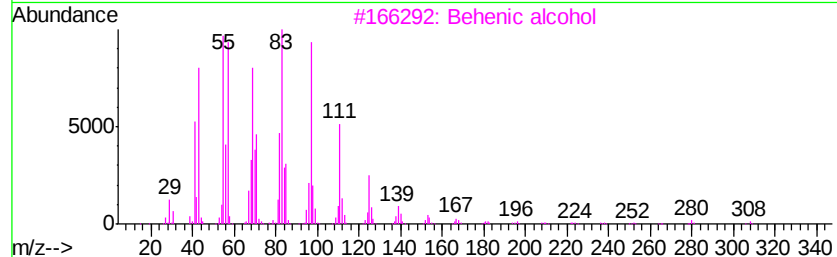
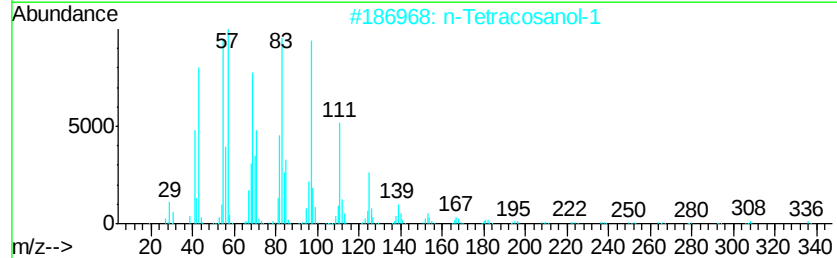
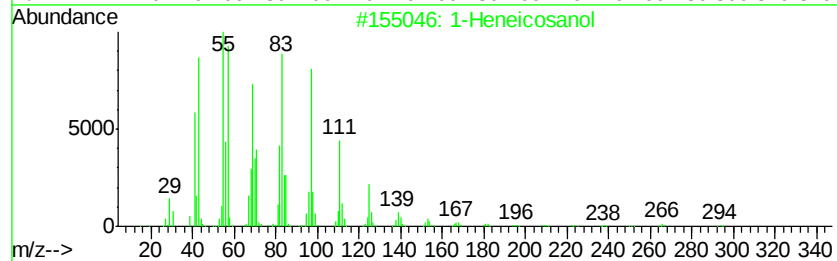
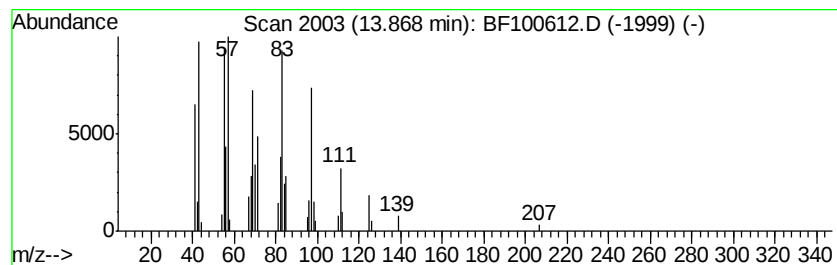
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Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.63 ng	75332	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	6.0	ng	197164	1	6.88	658952	20.0
unknown6.65	6.65	49.4	ng	1628610	1	6.88	658952	20.0
2-Hydroxy-iso-but...	8.72	3.1	ng	135683	2	8.16	862339	20.0
Benzophenone	10.63	7.1	ng	326908	3	9.92	923855	20.0
1-Heneicosanol	13.87	2.6	ng	75332	5	14.04	572419	20.0