

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100817\
 Data File : BF099252.D
 Acq On : 9 Oct 2017 1:09
 Operator : SJ/JU
 Sample : I5646-01
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 100217-TIDO-E-D-M

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-BF092317.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	2.169	9	14	33	rVB	598836	837004	20.66%	3.396%
2	5.092	507	511	521	rVB	193958	221787	5.47%	0.900%
3	5.492	575	579	590	rBV	1340320	1260088	31.10%	5.112%
4	6.492	746	749	764	rVB	920392	790550	19.51%	3.207%
5	6.633	769	773	777	rBV	2261825	2160303	53.31%	8.764%
6	6.863	809	812	816	rBV	892467	699824	17.27%	2.839%
7	7.022	834	839	842	rBV	2931317	2853224	70.41%	11.575%
8	7.433	903	909	912	rBV	2263606	2343782	57.84%	9.508%
9	8.145	1026	1030	1034	rBV	1148902	976005	24.09%	3.959%
10	9.222	1207	1213	1216	rBV	3887027	4052215	100.00%	16.439%
11	9.610	1276	1279	1287	rVB	80850	66196	1.63%	0.269%
12	9.898	1324	1328	1332	rBV	1158094	1056856	26.08%	4.287%
13	10.692	1458	1463	1466	rBV	1625099	1477821	36.47%	5.995%
14	11.386	1577	1581	1585	rBV	1141030	1014482	25.04%	4.116%
15	12.974	1846	1851	1854	rBV	3217770	3309362	81.67%	13.425%
16	14.027	2026	2030	2036	rBV	817955	703980	17.37%	2.856%
17	14.651	2129	2136	2147	rVB5	44091	167470	4.13%	0.679%
18	15.503	2276	2281	2288	rBV	512830	659009	16.26%	2.673%

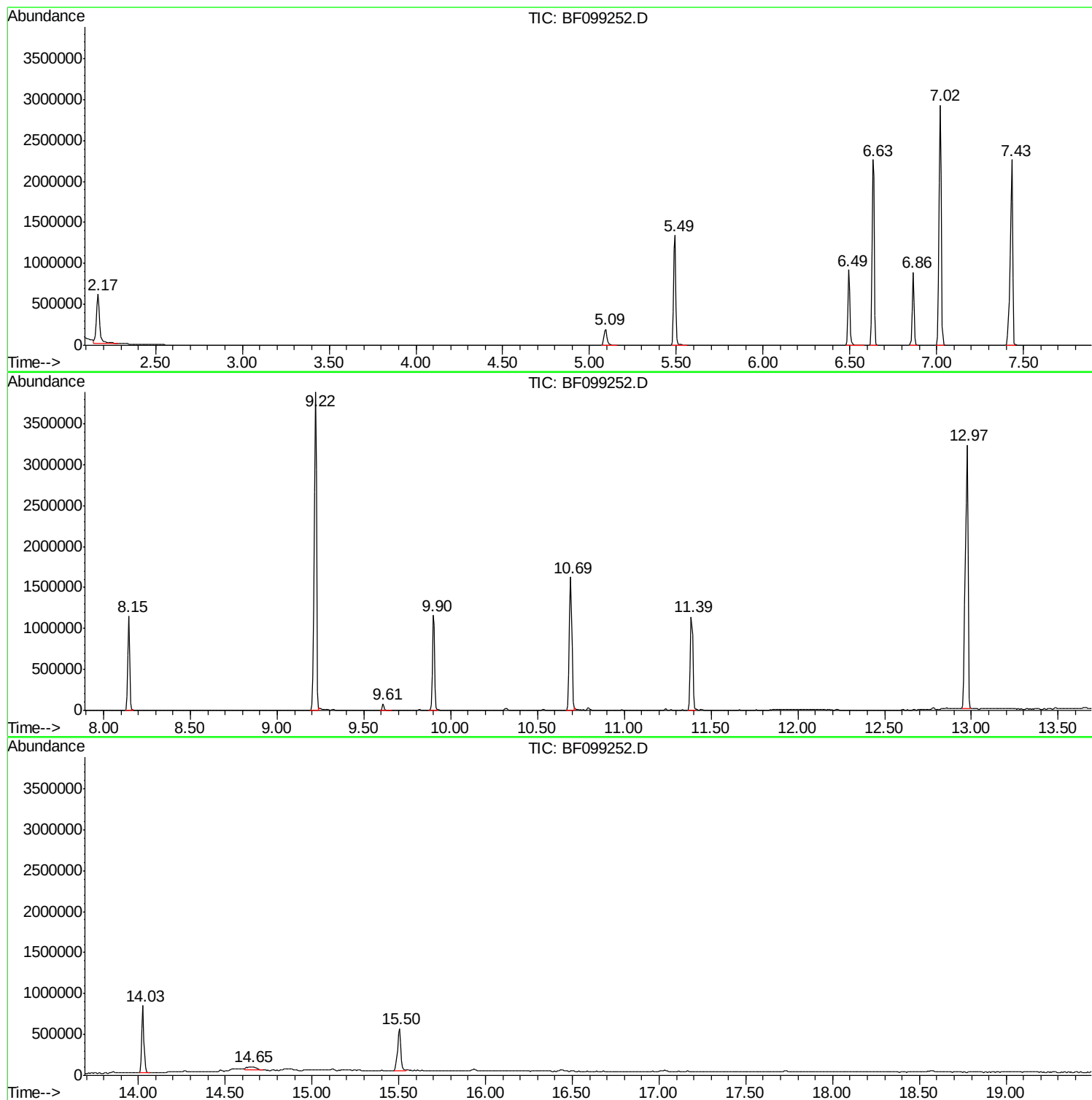
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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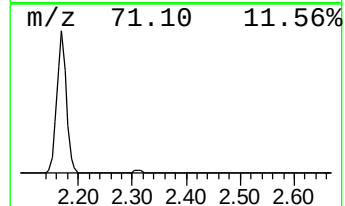
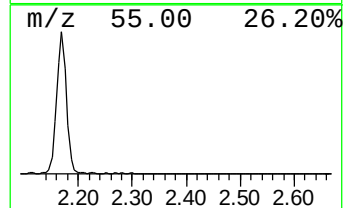
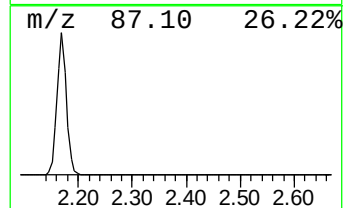
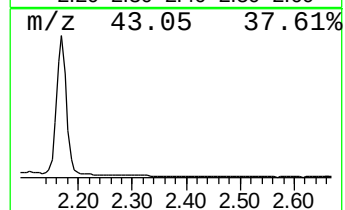
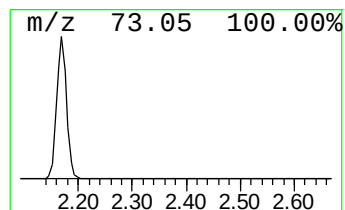
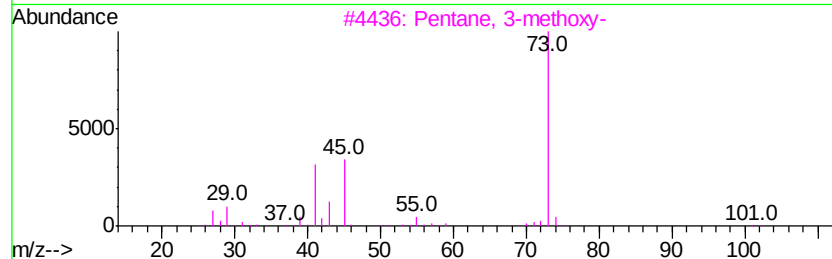
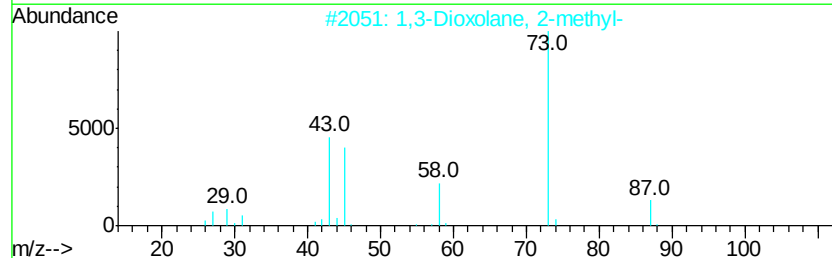
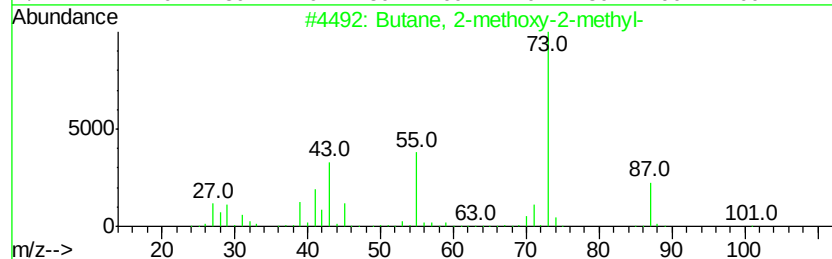
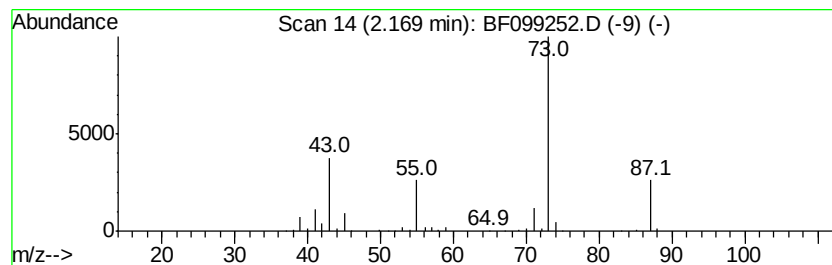
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	23.92 ng	837004	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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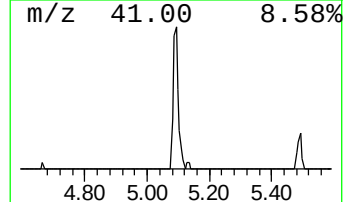
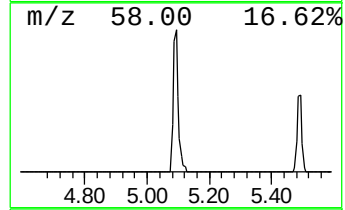
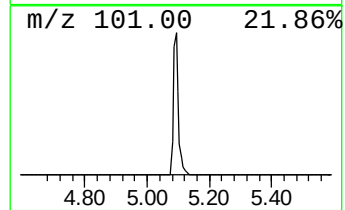
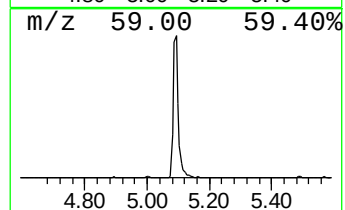
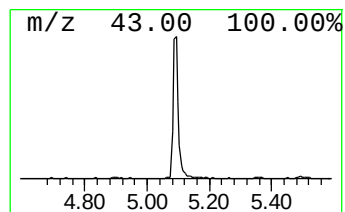
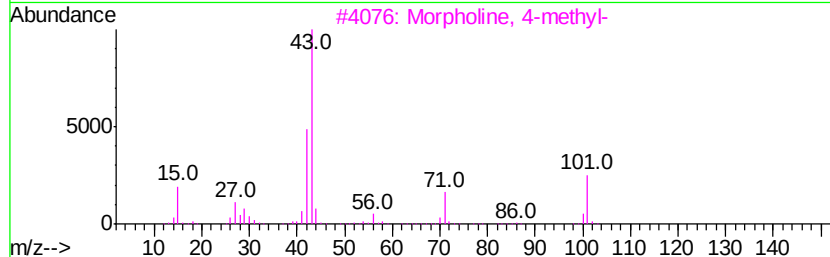
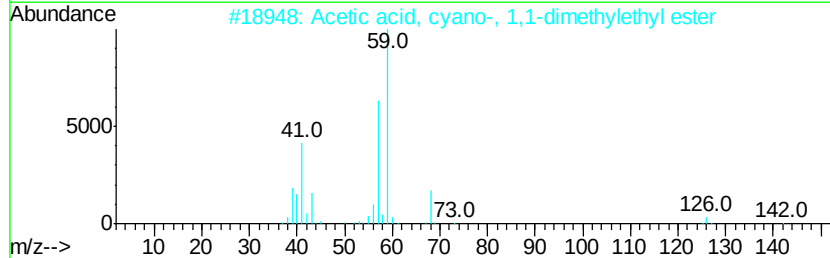
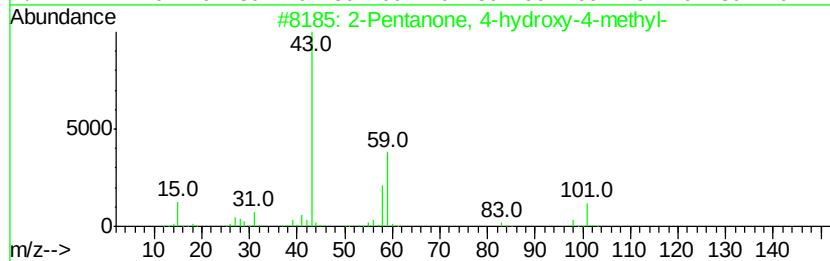
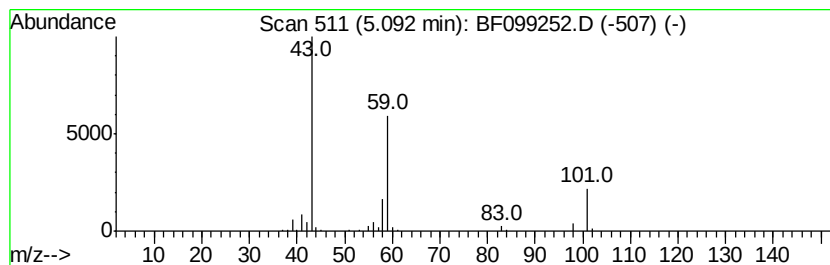
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.34 ng	221787	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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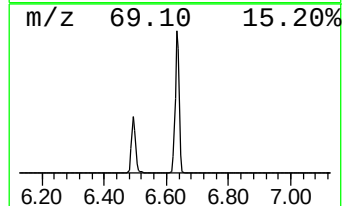
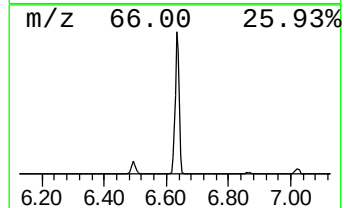
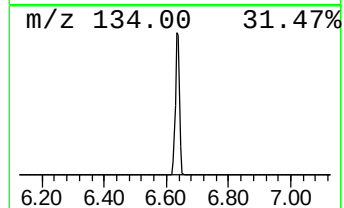
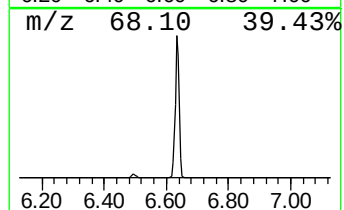
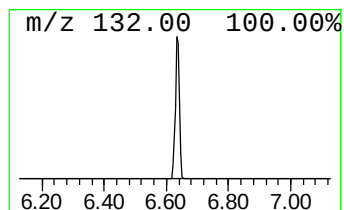
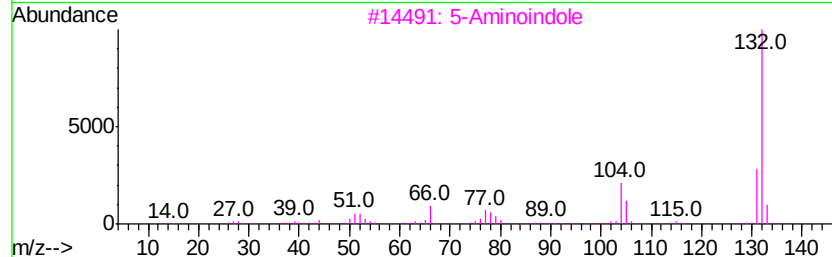
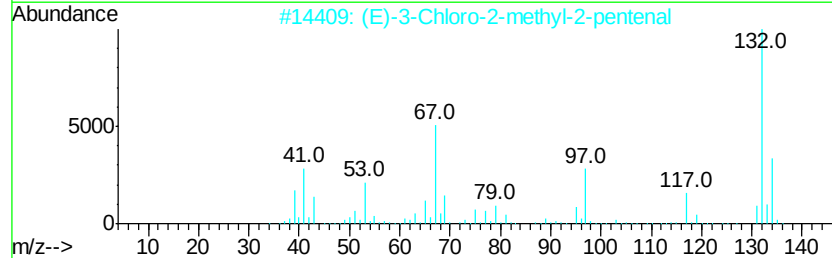
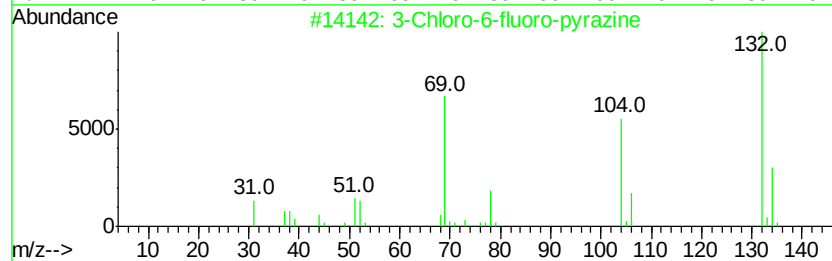
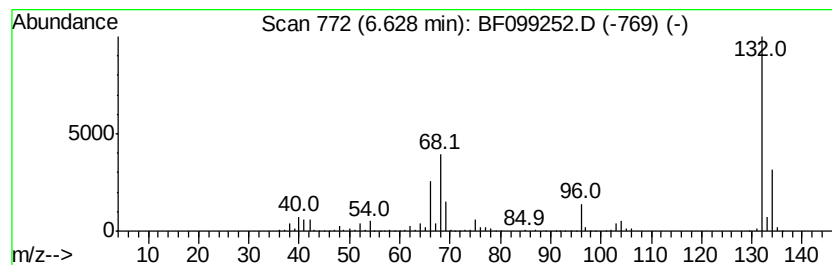
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Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	61.74 ng	2160300	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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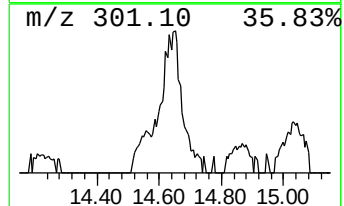
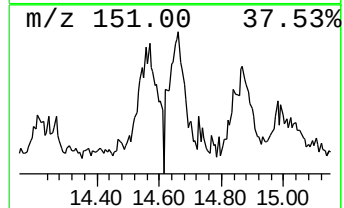
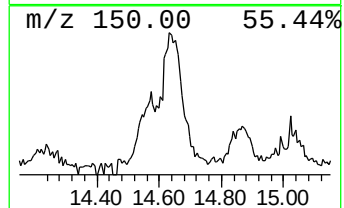
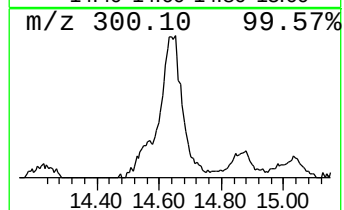
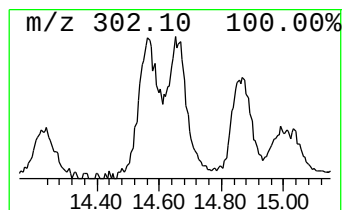
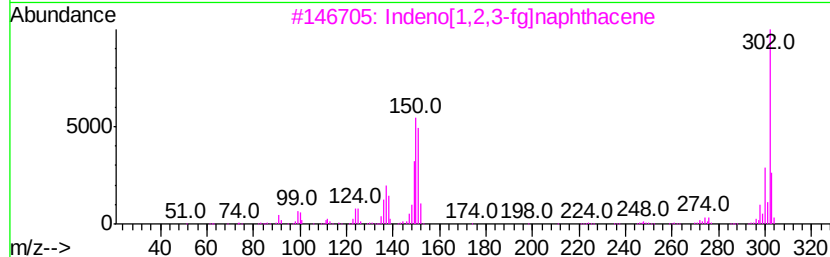
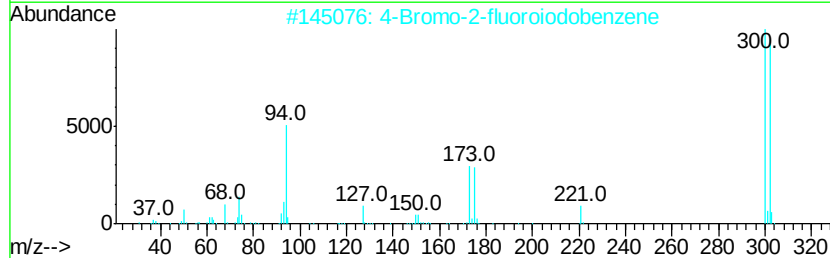
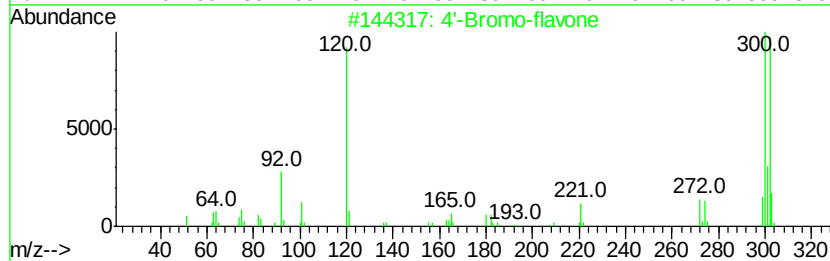
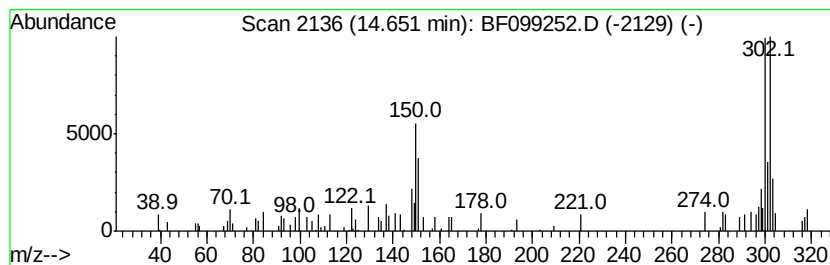
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Peak Number 5 4'-Bromo-flavone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.65	4.76 ng	167470	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4'-Bromo-flavone	300	C15H9BrO2	020525-20-6	52
2	4-Bromo-2-fluoriodobenzene	300	C6H3BrFI	105931-73-5	43
3	Indeno[1,2,3-f]naphthacene	302	C24H14	000203-11-2	38
4	Hesperetin	302	C16H14O6	000520-33-2	38
5	Coronene	300	C24H12	000191-07-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	23.9	ng	837004	1	6.86	699824	20.0
2-Pentanone, 4-hy...	5.09	6.3	ng	221787	1	6.86	699824	20.0
unknown6.63	6.63	61.7	ng	2160300	1	6.86	699824	20.0
4'-Bromo-flavone	14.65	4.8	ng	167470	5	14.03	703980	20.0