

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092217\
 Data File : BF098700.D
 Acq On : 22 Sep 2017 15:19
 Operator : SJ/JU
 Sample : I5333-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SV-30745L

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-BF092117.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	2.245	23	27	46	rVB	261340	437638	9.76%	1.518%
2	5.151	518	521	529	rVB	222612	235009	5.24%	0.815%
3	5.539	583	587	591	rBV	2069979	1981288	44.18%	6.873%
4	6.539	752	757	760	rBV	1494192	1195701	26.66%	4.148%
5	6.698	779	784	787	rBV	3470626	3521645	78.53%	12.216%
6	6.927	819	823	827	rBV	1050564	821708	18.32%	2.850%
7	7.086	845	850	853	rBV	3694050	3345913	74.61%	11.606%
8	7.492	913	919	922	rBV	2620685	2675387	59.66%	9.280%
9	8.210	1037	1041	1044	rVB	1311146	1077738	24.03%	3.738%
10	9.286	1218	1224	1227	rBV	4733388	4484602	100.00%	15.556%
11	9.963	1335	1339	1343	rBV2	1208568	1018471	22.71%	3.533%
12	10.751	1467	1473	1476	rBV	2403836	2189373	48.82%	7.594%
13	11.451	1588	1592	1595	rBV	1003863	814518	18.16%	2.825%
14	11.962	1675	1679	1685	rBV3	57876	63874	1.42%	0.222%
15	12.751	1810	1813	1823	rBV4	72530	109526	2.44%	0.380%
16	13.033	1857	1861	1865	rBV	3172993	3228527	71.99%	11.199%
17	14.086	2037	2040	2044	rVB	956463	813314	18.14%	2.821%
18	15.580	2289	2294	2303	rVB	626402	814251	18.16%	2.824%

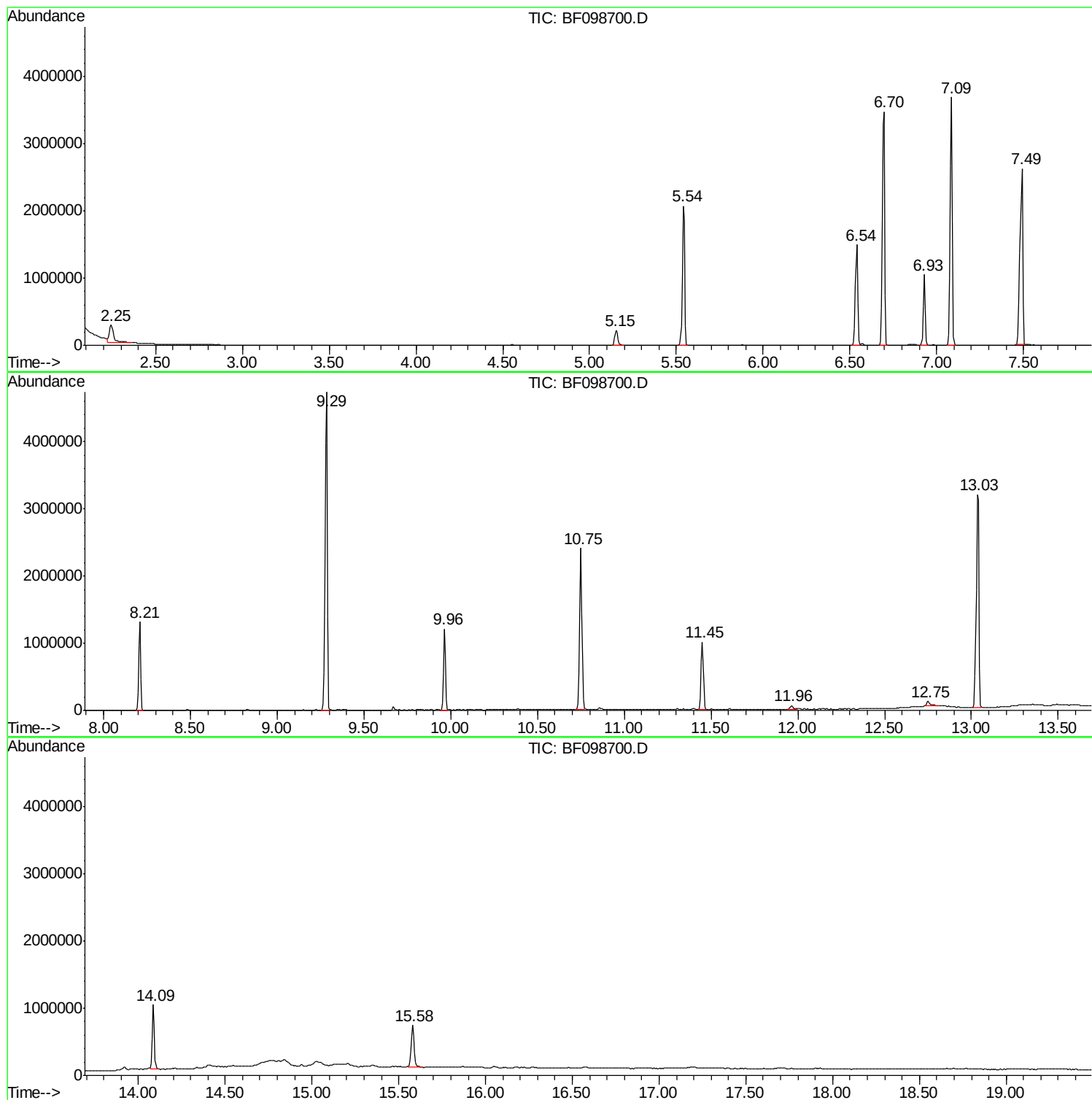
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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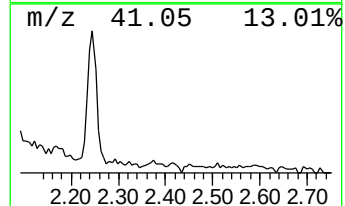
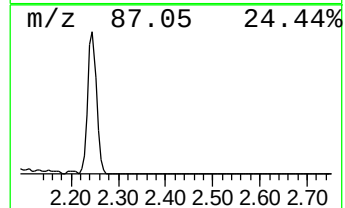
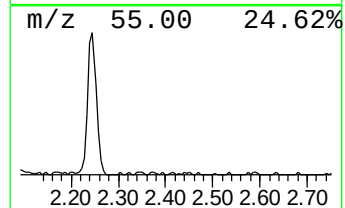
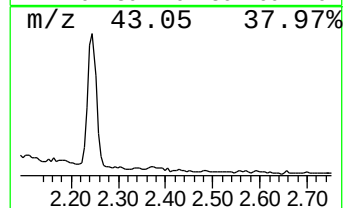
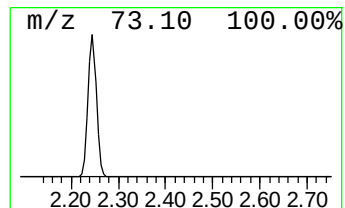
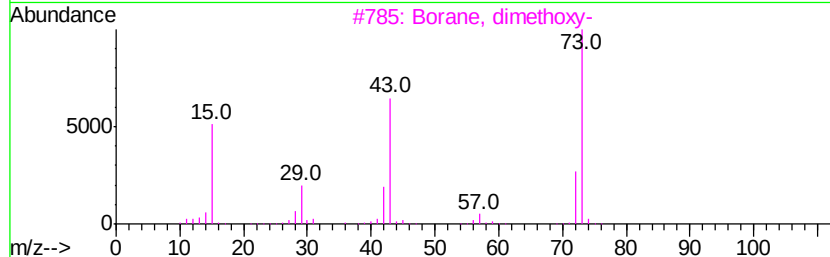
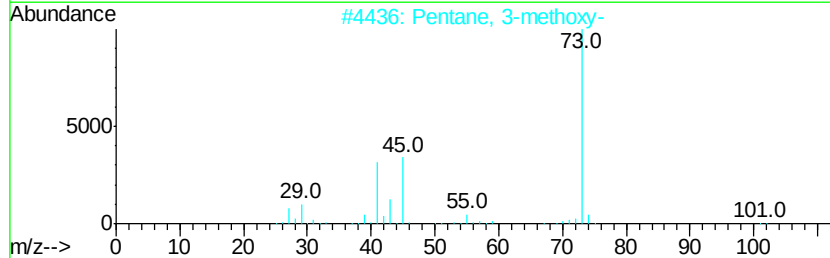
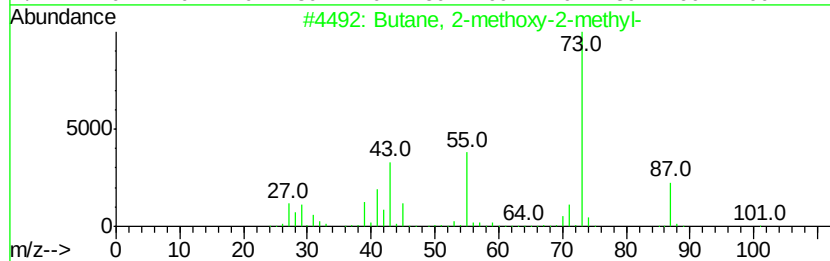
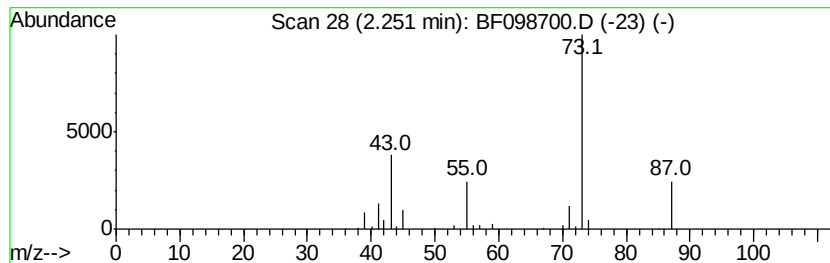
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	10.65 ng	437638	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,4-Butanediamine	88	C4H12N2	000110-60-1	9



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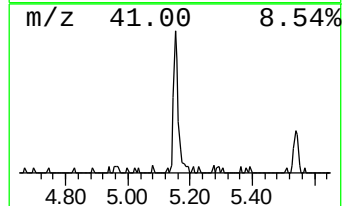
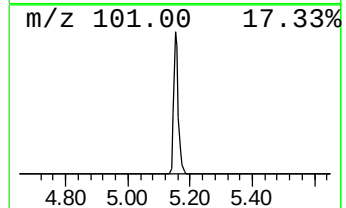
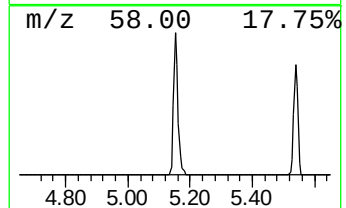
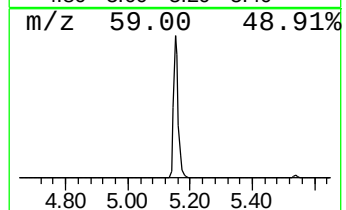
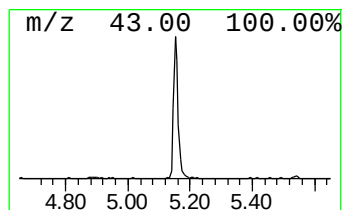
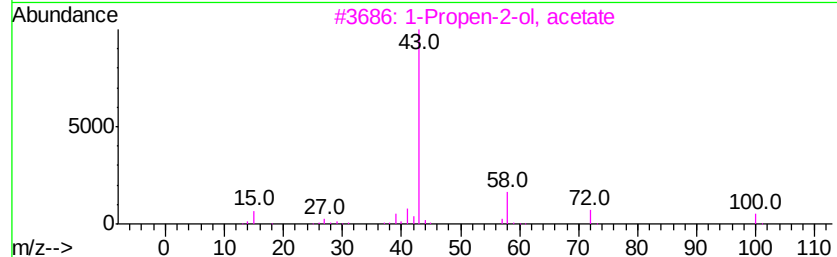
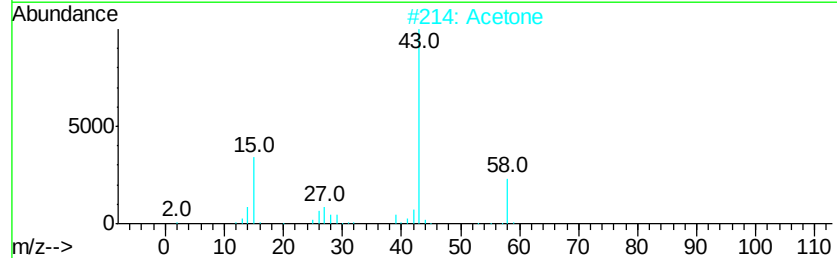
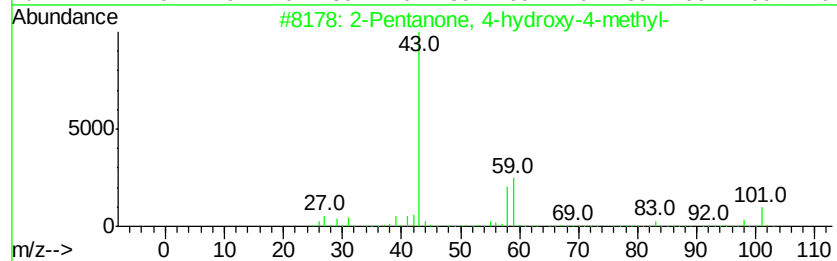
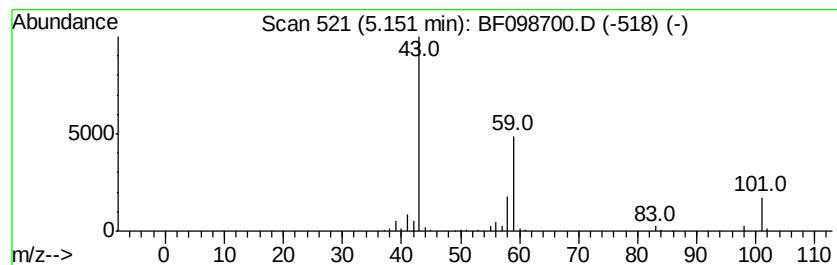
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	5.72 ng	235009	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetone	58	C3H6O	000067-64-1	12
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9



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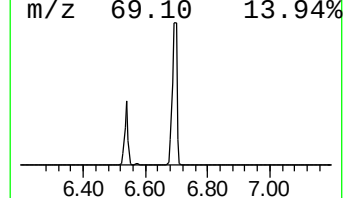
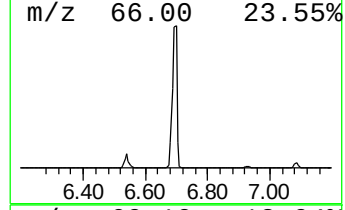
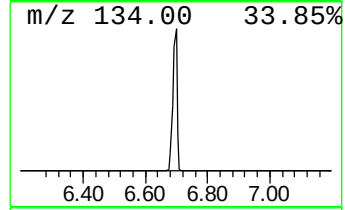
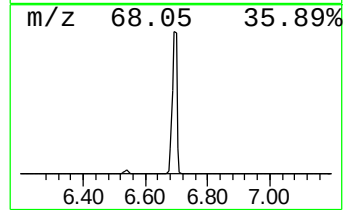
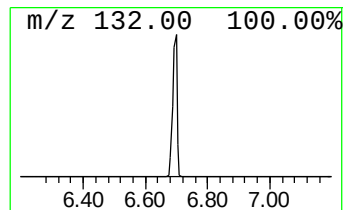
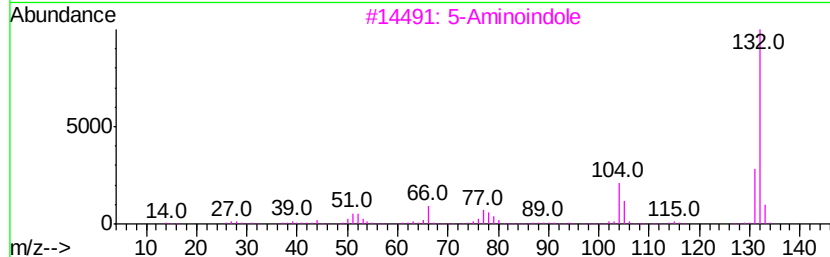
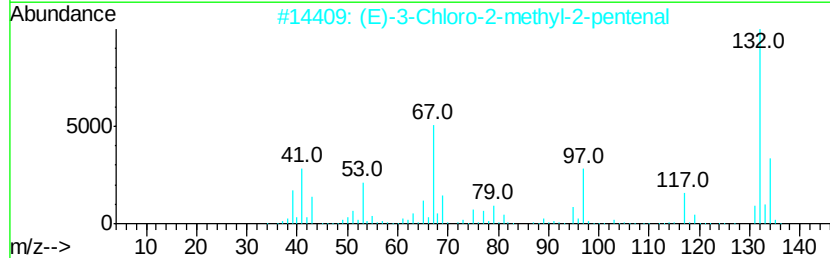
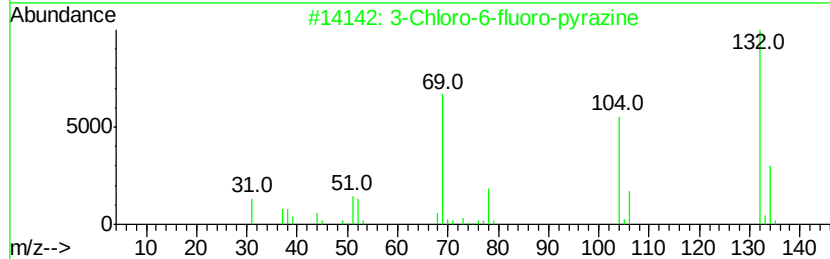
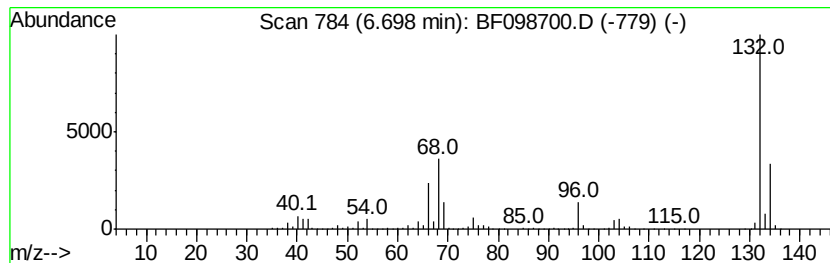
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Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	85.72 ng	3521650	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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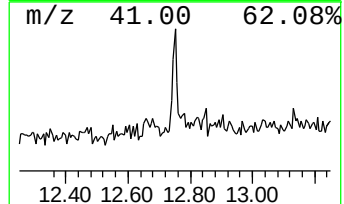
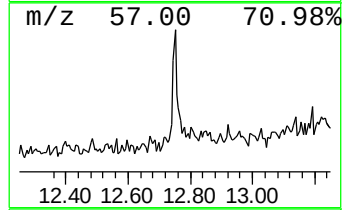
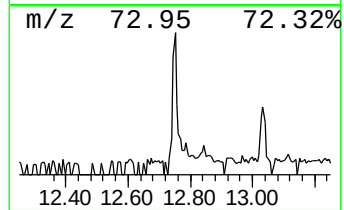
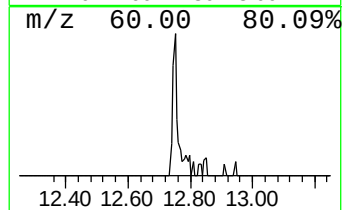
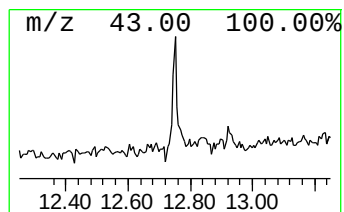
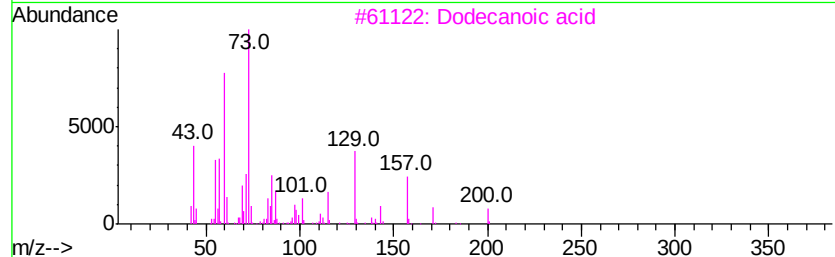
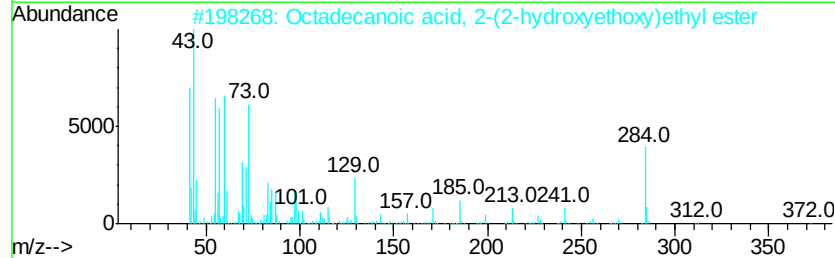
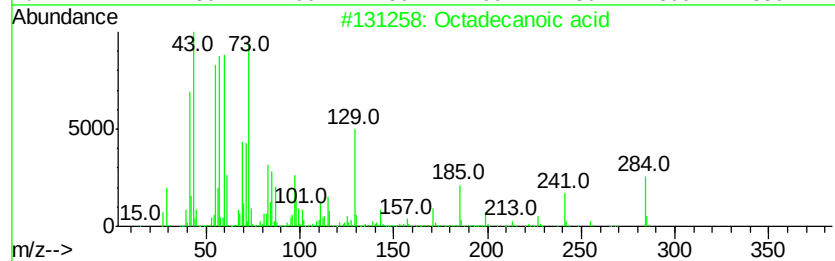
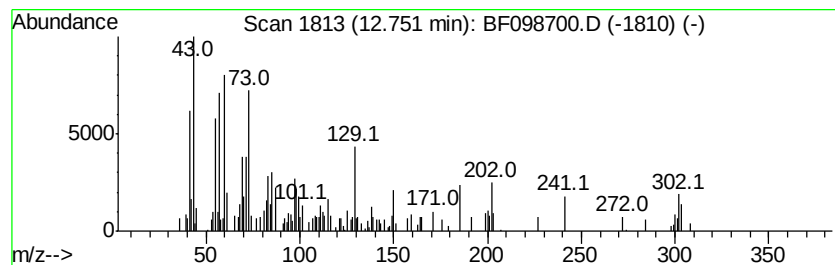
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.75	2.69 ng	109526	Phenanthrene-d10	11.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	70
2	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	58
3	Dodecanoic acid	200	C12H24O2	000143-07-7	55
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.25	10.7	ng	437638	1	6.93	821708	20.0
2-Pentanone, 4-hy...	5.15	5.7	ng	235009	1	6.93	821708	20.0
unknown6.70	6.70	85.7	ng	3521650	1	6.93	821708	20.0
Octadecanoic acid	12.75	2.7	ng	109526	4	11.45	814518	20.0