

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
 Data File : BF093087.D
 Acq On : 22 Feb 2017 20:42
 Operator : SJ/MA
 Sample : I1930-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 14A-9-11

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-BF013017.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	4.338	195	197	207	rBV	189018	254621	7.29%	0.788%
2	5.001	253	255	265	rBV	981679	1248872	35.76%	3.866%
3	5.436	290	293	295	rBV	2701591	3092550	88.55%	9.574%
4	6.476	381	384	386	rBV	2429985	3217702	92.13%	9.961%
5	6.602	393	395	397	rBV	3283904	3117413	89.26%	9.651%
6	6.830	413	415	418	rBV	1060034	890733	25.51%	2.758%
7	6.990	426	429	431	rBV	2450835	2400956	68.75%	7.433%
8	7.402	462	465	467	rBV	1940361	2036167	58.30%	6.304%
9	8.122	525	528	530	rBV	1012847	1163069	33.30%	3.601%
10	9.196	619	622	624	rBV	3549218	3492379	100.00%	10.812%
11	9.585	654	656	659	rBV	486900	568228	16.27%	1.759%
12	9.802	671	675	677	rBV	43764	58568	1.68%	0.181%
13	9.870	678	681	683	rVB	1542371	1353741	38.76%	4.191%
14	10.305	715	719	720	rBV	58765	79831	2.29%	0.247%
15	10.522	734	738	739	rBV	28340	42726	1.22%	0.132%
16	10.659	747	750	752	rBV	1918540	1914477	54.82%	5.927%
17	10.773	758	760	765	rVB	108674	123385	3.53%	0.382%
18	11.219	797	799	800	rBV	65480	58829	1.68%	0.182%
19	11.356	808	811	813	rBV	1223978	1381925	39.57%	4.278%
20	11.585	828	831	834	rBV2	29893	49719	1.42%	0.154%
21	12.934	947	949	952	rBV	2827061	3016555	86.38%	9.339%
22	13.837	1025	1028	1033	rBV	146301	234263	6.71%	0.725%
23	13.985	1039	1041	1044	rVB	1406556	1291914	36.99%	4.000%
24	15.414	1163	1166	1173	rBV	821552	1082255	30.99%	3.350%
25	15.837	1200	1203	1206	rBV	27251	43520	1.25%	0.135%
26	16.305	1241	1244	1250	rBV	24971	47358	1.36%	0.147%
27	16.854	1289	1292	1298	rVB3	16980	39979	1.14%	0.124%

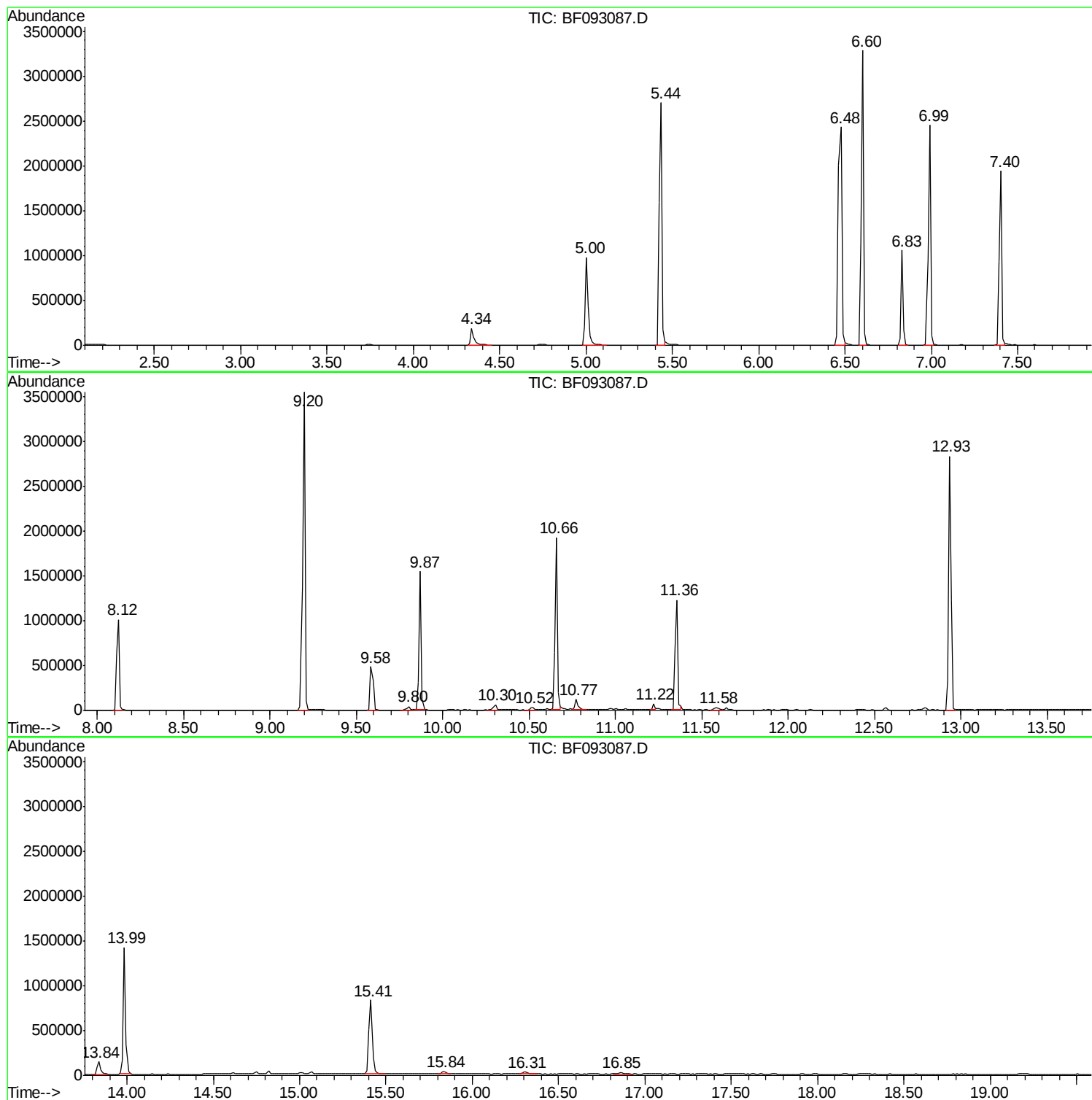
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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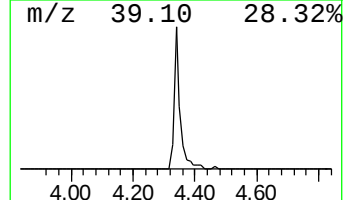
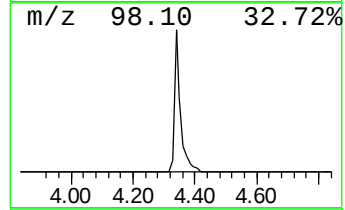
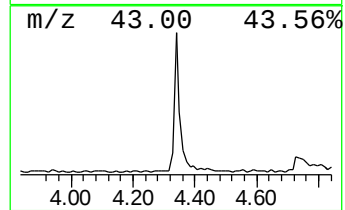
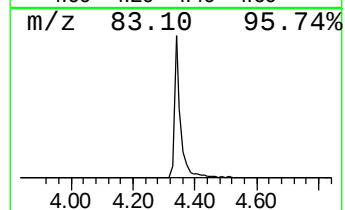
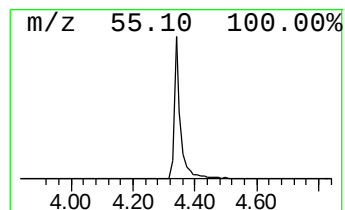
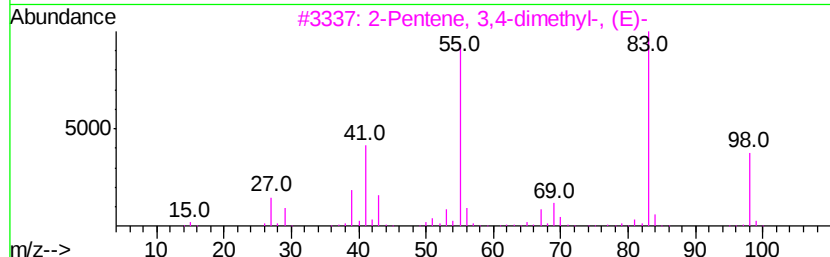
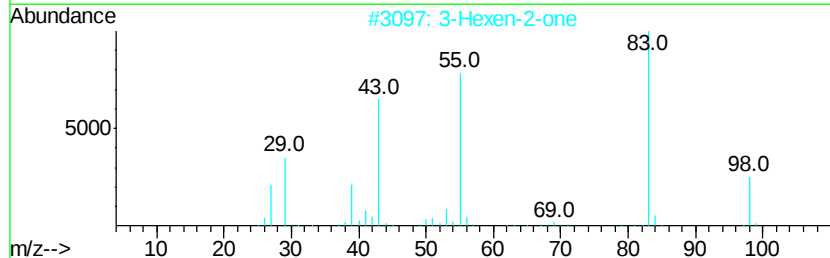
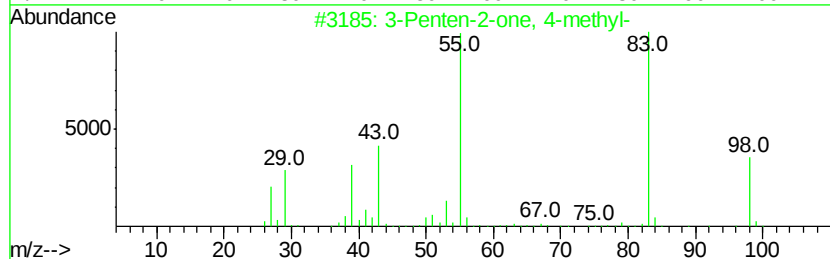
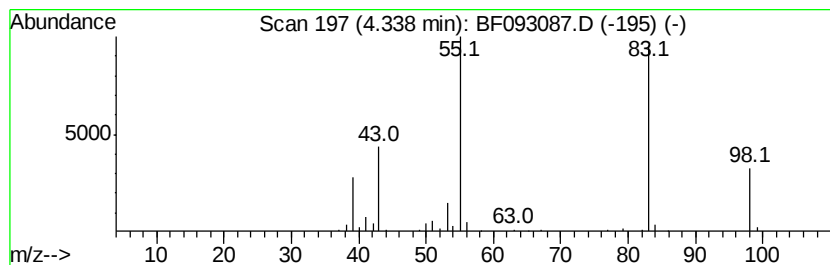
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.34	5.72 ng	254621	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72



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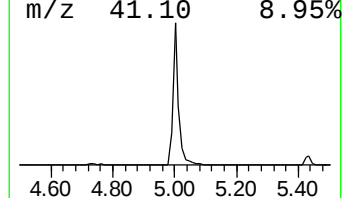
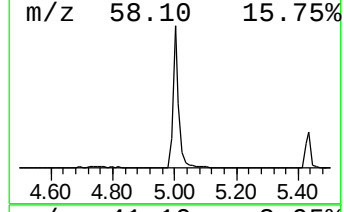
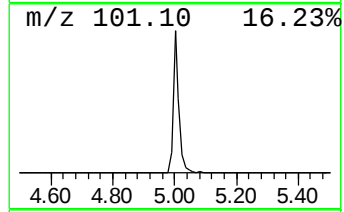
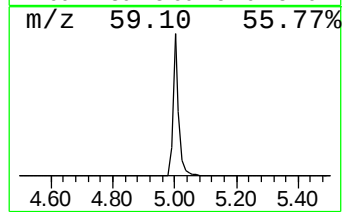
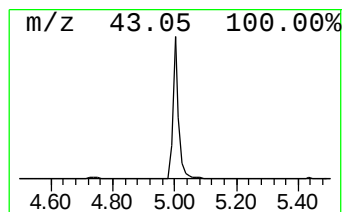
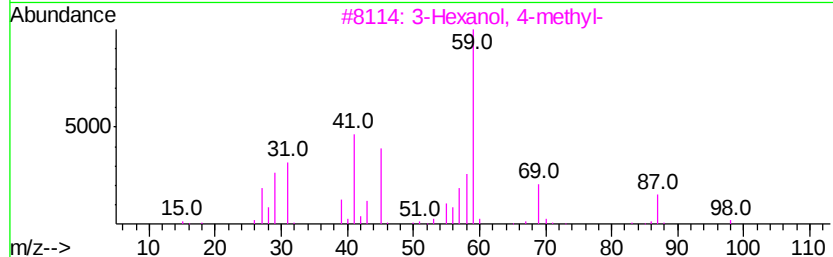
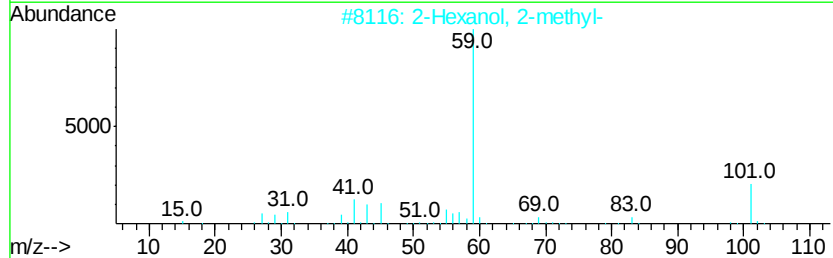
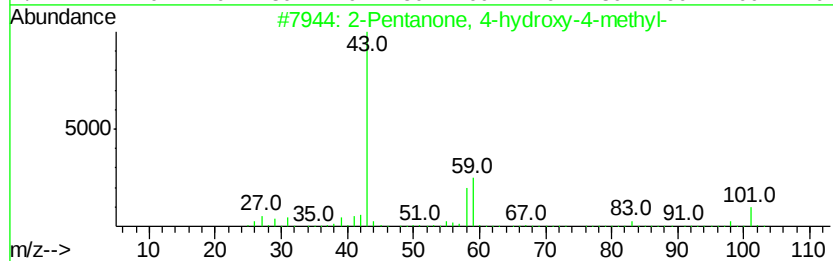
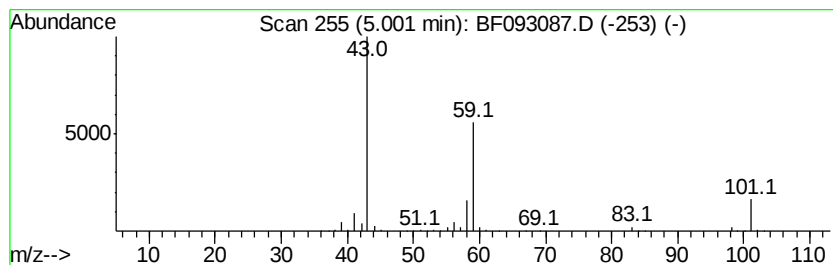
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	28.04 ng	1248870	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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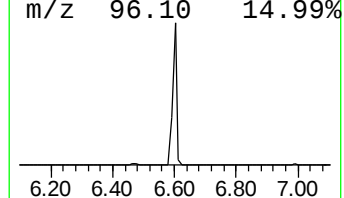
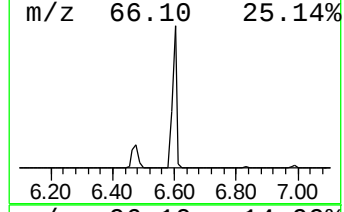
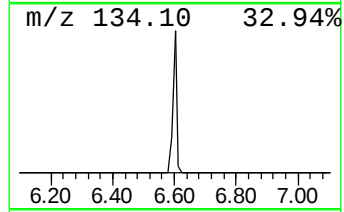
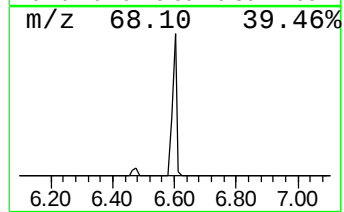
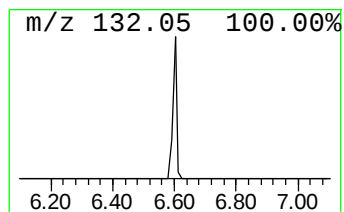
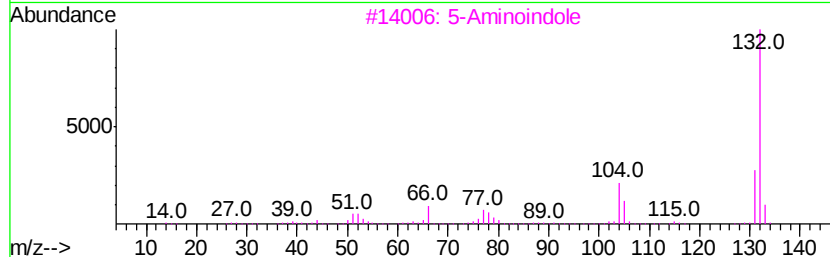
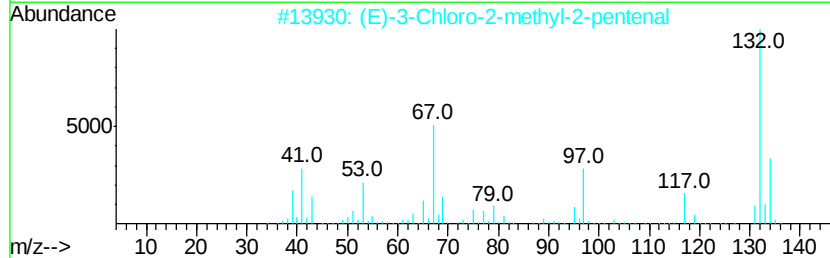
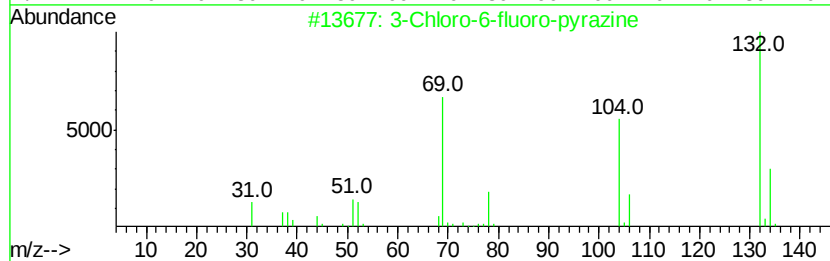
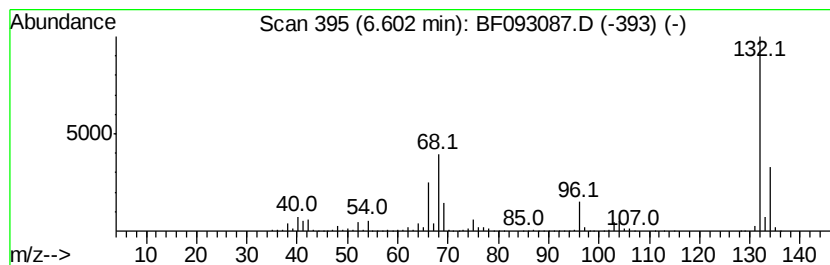
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Peak Number 3 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	70.00 ng	3117410	1,4-Dichlorobenzene-d4	6.83

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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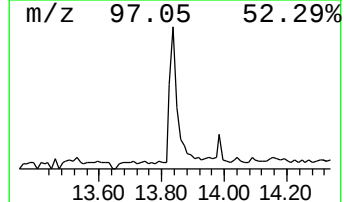
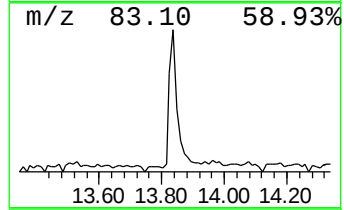
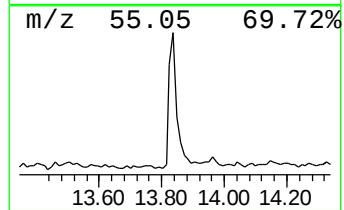
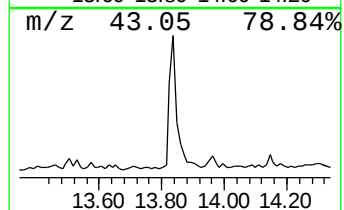
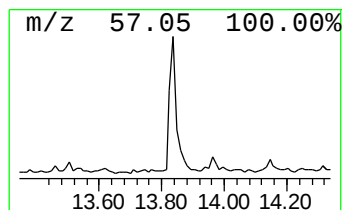
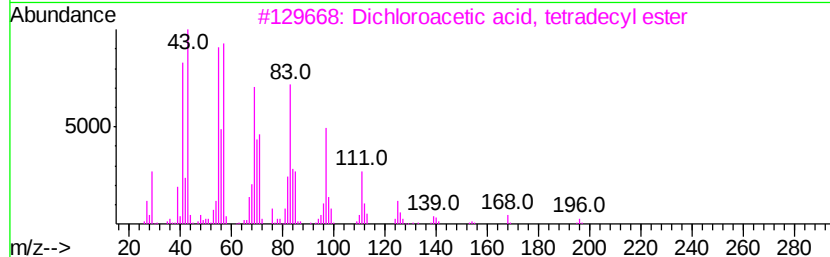
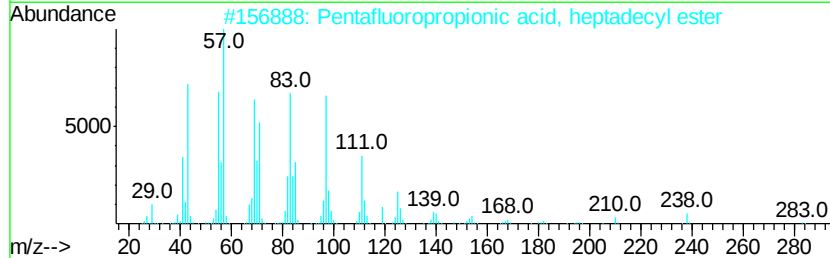
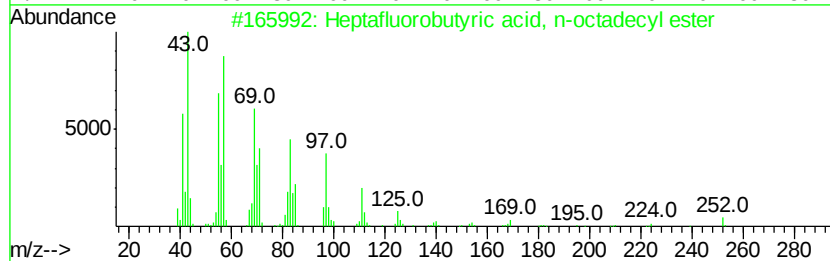
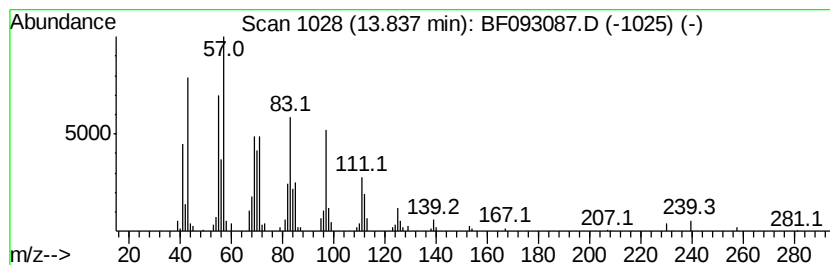
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Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.63 ng	234263	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	90
2		Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	1000283-04-2	87
3		Dichloroacetic acid, tetradecyl ester	324	C16H30Cl2O2	083005-02-1	87
4		Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	87
5		Heptafluorobutanoic acid, heptadecyl ester	452	C21H35F7O2	1000282-97-3	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.34	5.7	ng	254621	1	6.83	890733	20.0
2-Pentanone, 4-hy...	5.00	28.0	ng	1248870	1	6.83	890733	20.0
unknown6.60	6.60	70.0	ng	3117410	1	6.83	890733	20.0
Heptafluorobutyri...	13.84	3.6	ng	234263	5	13.99	1291910	20.0