

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040717\
 Data File : BF094270.D
 Acq On : 7 Apr 2017 13:55
 Operator : SJ/MA
 Sample : I2572-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-3460

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-BF032217.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	1.910	3	4	10	rVB	100295	96449	1.84%	0.219%
2	3.393	233	256	260	rBV2	46669	207704	3.96%	0.472%
3	3.998	354	359	369	rBV	485563	724995	13.81%	1.648%
4	4.387	420	425	428	rBV	3897134	4524240	86.15%	10.285%
5	5.457	601	607	612	rBV2	3438493	5031260	95.81%	11.437%
6	5.592	624	630	633	rBV	4064889	4785456	91.13%	10.879%
7	5.845	668	673	676	rBV	1044021	979326	18.65%	2.226%
8	6.022	698	703	707	rBV	3348381	3670619	69.90%	8.344%
9	6.498	776	784	787	rBV	2504590	3110562	59.23%	7.071%
10	7.345	923	928	932	rBV	1358801	1318532	25.11%	2.997%
11	8.675	1146	1154	1157	rBV	4277409	5251528	100.00%	11.938%
12	9.163	1230	1237	1241	rBV	483598	475028	9.05%	1.080%
13	9.486	1284	1292	1296	rBV	1298232	1465555	27.91%	3.332%
14	10.463	1450	1458	1461	rBV	2455883	2998099	57.09%	6.815%
15	10.663	1487	1492	1502	rVB	76350	108473	2.07%	0.247%
16	11.216	1581	1586	1590	rBV	65378	67968	1.29%	0.155%
17	11.304	1596	1601	1604	rBV	1313023	1410510	26.86%	3.206%
18	11.333	1604	1606	1610	rVB	172642	140607	2.68%	0.320%
19	12.798	1850	1855	1858	rBV	141458	149497	2.85%	0.340%
20	13.068	1897	1901	1906	rVB	156624	158609	3.02%	0.361%
21	13.292	1931	1939	1942	rBV2	3771101	4616767	87.91%	10.495%
22	14.451	2131	2136	2147	rBV	303186	435061	8.28%	0.989%
23	14.557	2149	2154	2158	rBV	1174786	1276897	24.31%	2.903%
24	16.186	2426	2431	2439	rBV	754880	845579	16.10%	1.922%
25	16.703	2515	2519	2523	rBV2	44472	68199	1.30%	0.155%
26	17.156	2592	2596	2604	rVB4	44356	72156	1.37%	0.164%

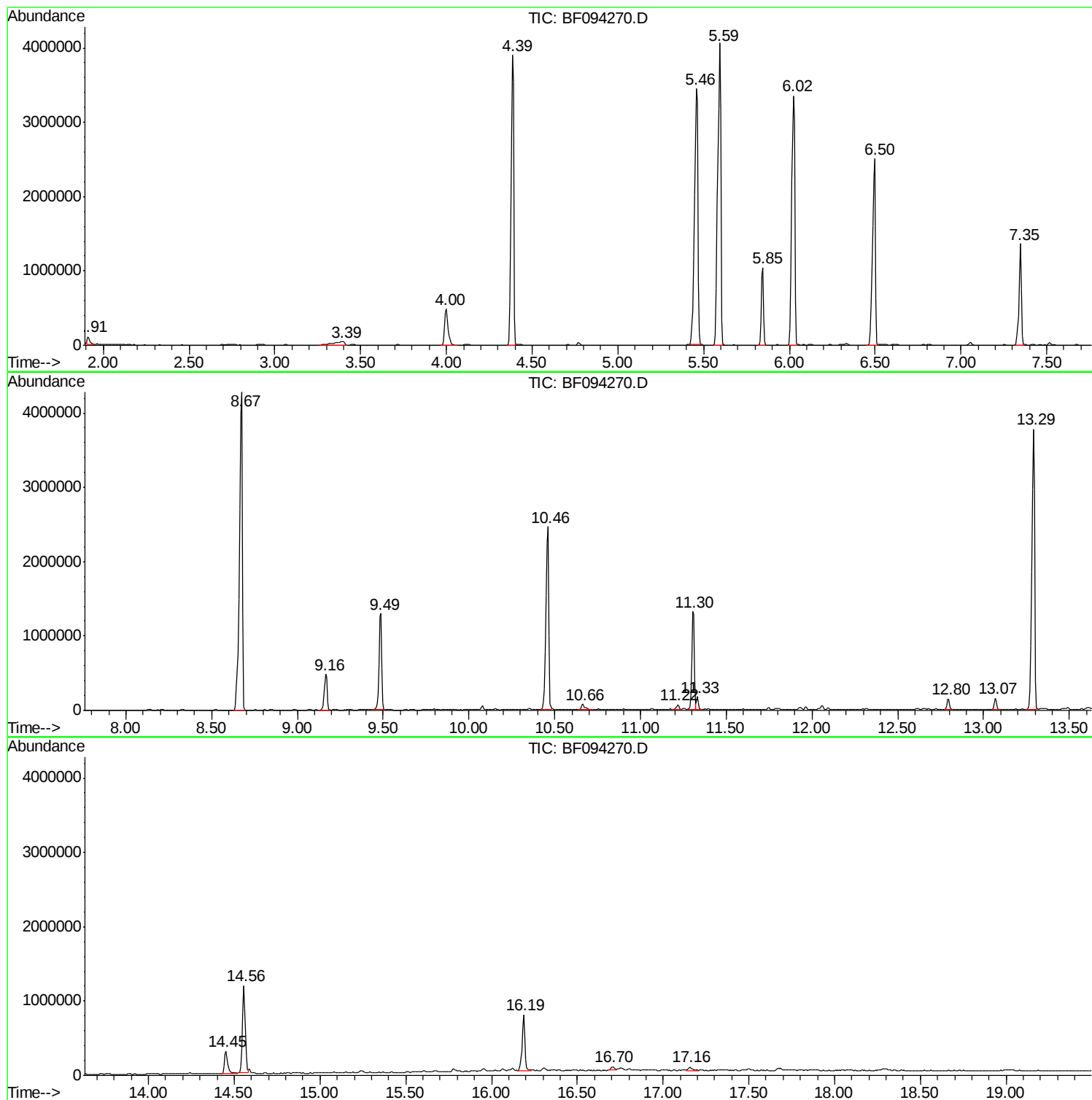
Sum of corrected areas: 43989676

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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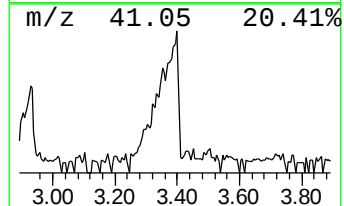
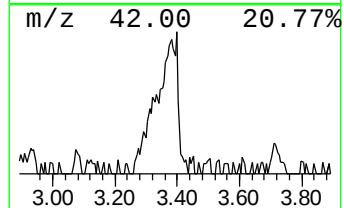
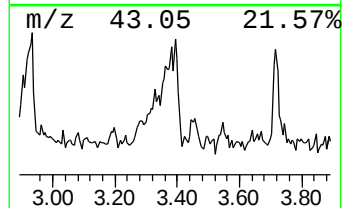
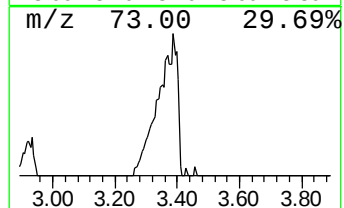
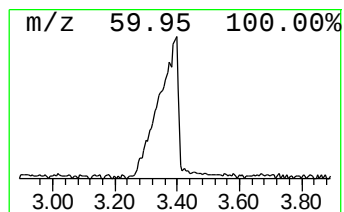
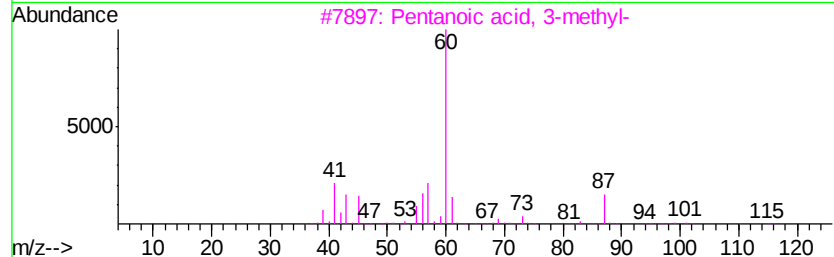
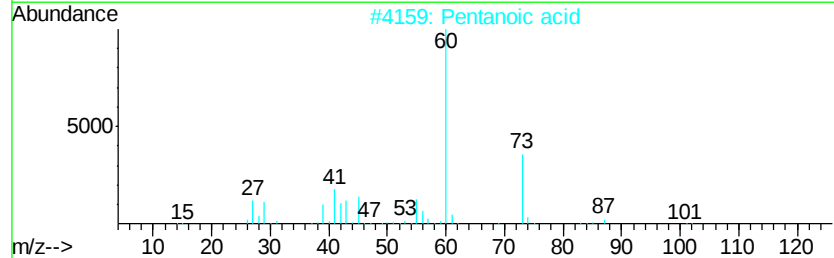
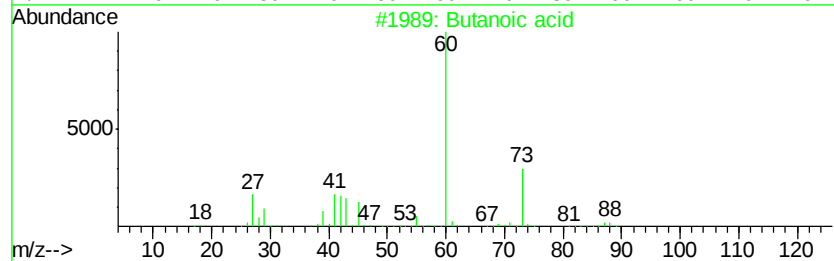
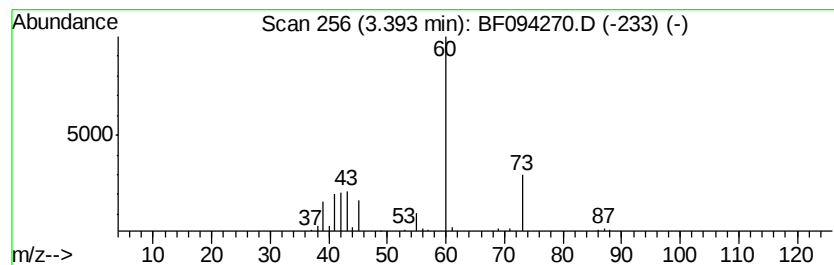
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.39	4.24 ng	207704	1,4-Dichlorobenzene-d4	5.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid	88	C4H8O2	000107-92-6	86
2		Pentanoic acid	102	C5H10O2	000109-52-4	39
3		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	33
4		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5		Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	9



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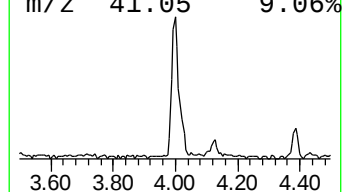
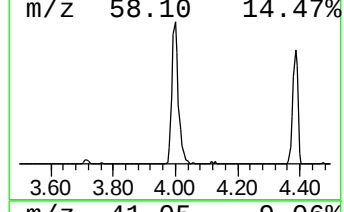
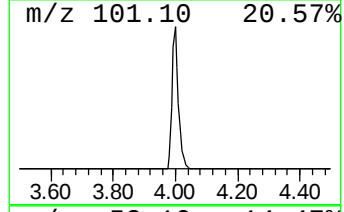
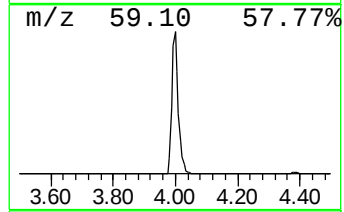
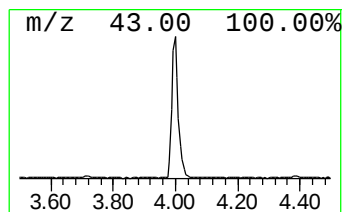
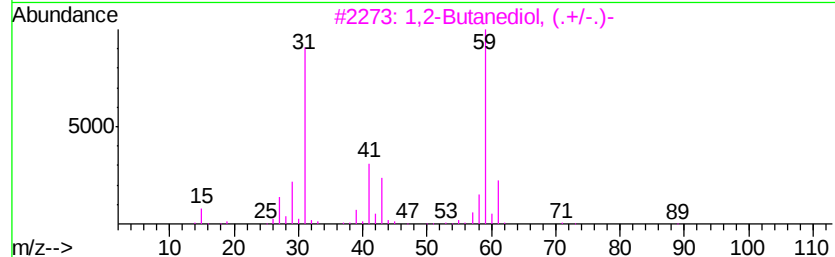
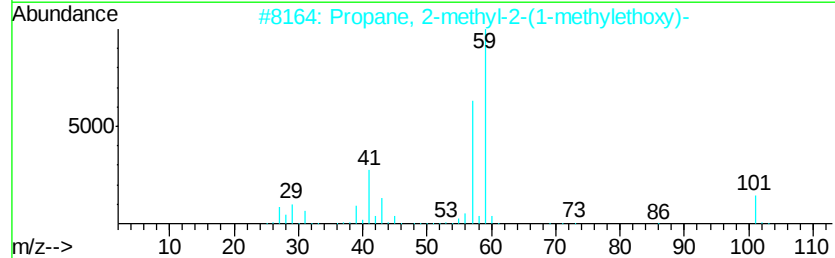
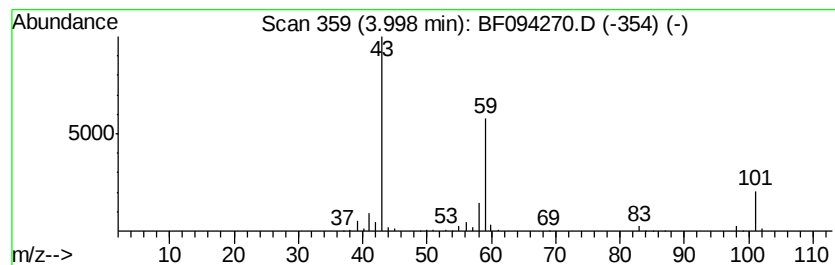
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	14.81 ng	724995	1,4-Dichlorobenzene-d4	5.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	25
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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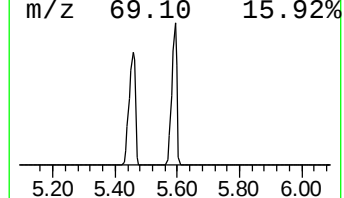
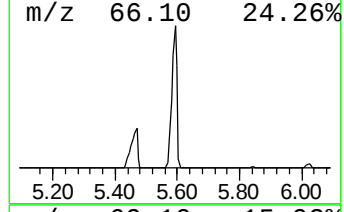
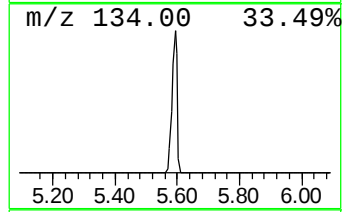
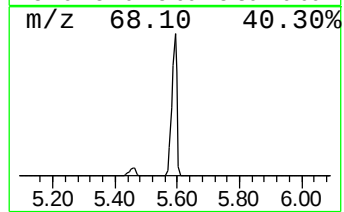
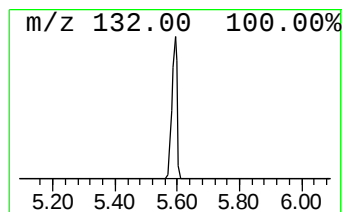
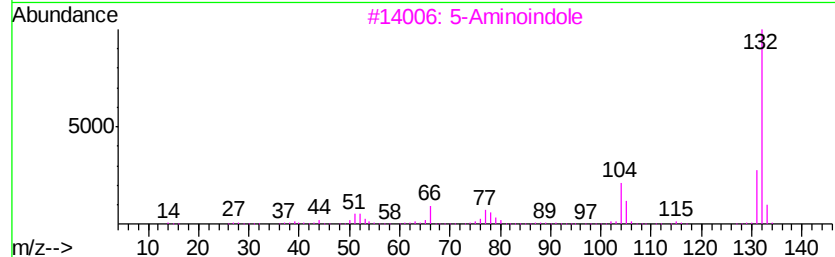
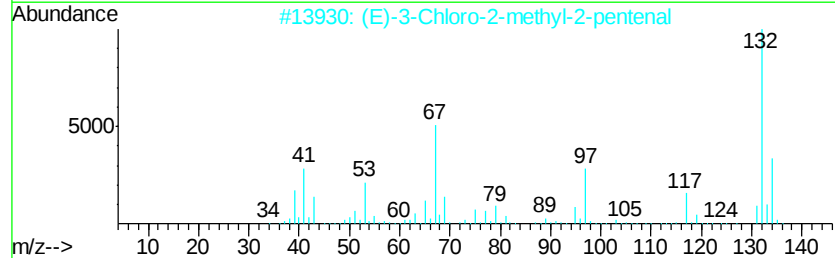
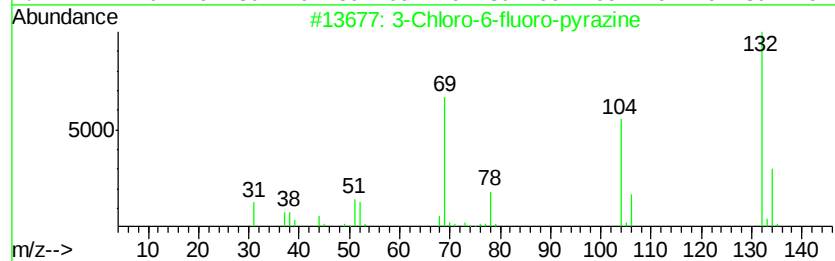
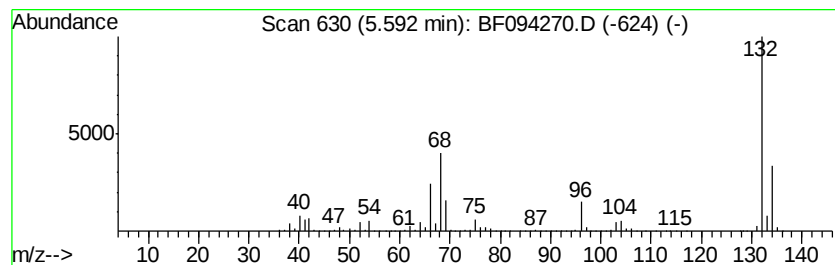
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Peak Number 3 unknown5.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	97.73 ng	4785460	1,4-Dichlorobenzene-d4	5.85

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		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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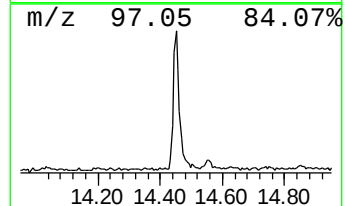
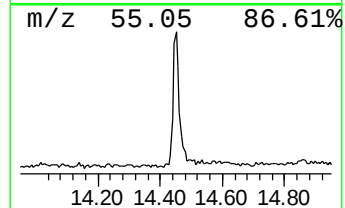
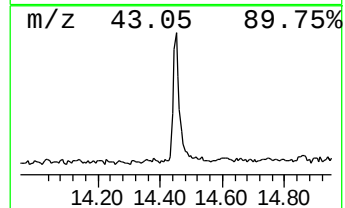
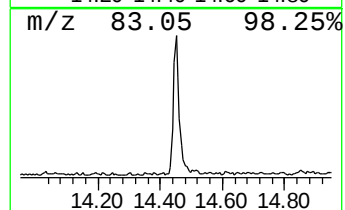
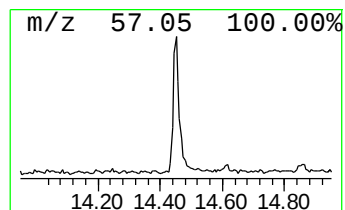
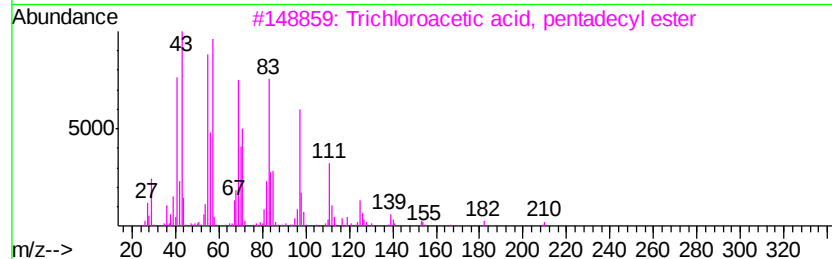
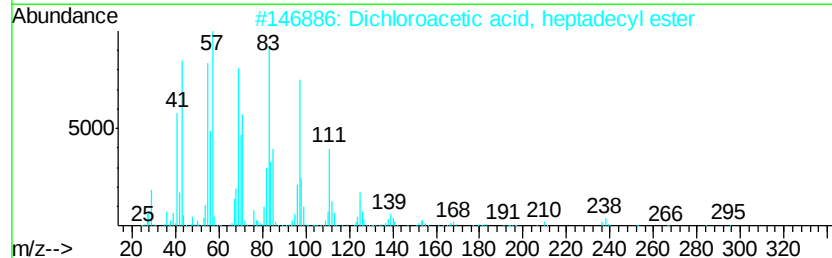
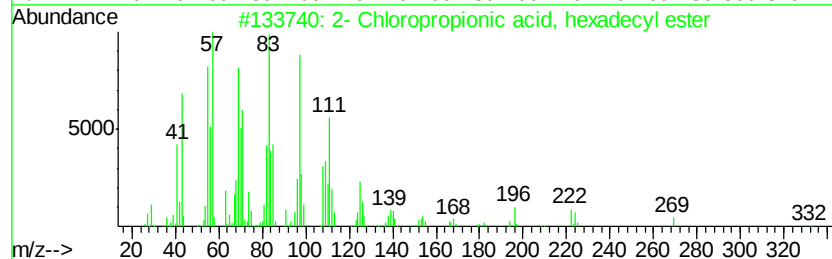
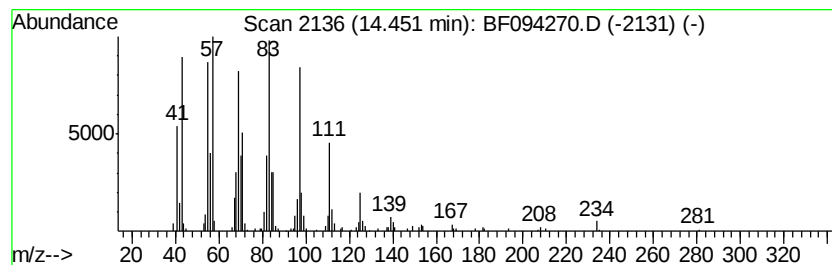
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Peak Number 6 2- Chloropropionic acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.45	6.81 ng	435061	Chrysene-d12		14.56		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91	
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91		
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91		
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91		
5	Cyclopentadecane	210	C15H30	000295-48-7	90		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid	3.39	4.2	ng	207704	1	5.85	979326	20.0
2-Pentanone, 4-hy...	4.00	14.8	ng	724995	1	5.85	979326	20.0
unknown5.59	5.59	97.7	ng	4785460	1	5.85	979326	20.0
2- Chloropropioni...	14.45	6.8	ng	435061	5	14.56	1276900	20.0