

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
 Data File : BG043376.D
 Acq On : 29 Oct 2019 16:23
 Operator : JU
 Sample : K5544-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 N-1

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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	3.190	13	17	27	rVB	124394	195349	7.55%	1.428%
2	5.129	341	347	355	rBV	90816	146009	5.64%	1.067%
3	5.610	422	429	444	rBV	435709	787322	30.43%	5.754%
4	7.209	691	701	718	rBV	467512	925563	35.77%	6.765%
5	7.567	753	762	775	rBV	493492	898393	34.72%	6.566%
6	8.025	833	840	850	rVB	128154	235161	9.09%	1.719%
7	8.348	887	895	905	rBV	382396	699080	27.02%	5.109%
8	9.189	1028	1038	1050	rBV	243721	527344	20.38%	3.854%
9	10.828	1309	1317	1338	rBV	144617	320772	12.40%	2.344%
10	13.272	1726	1733	1749	rBV	858654	1473974	56.96%	10.773%
11	14.100	1868	1874	1888	rBV	85617	163759	6.33%	1.197%
12	14.653	1960	1968	1983	rBV	294221	530837	20.51%	3.880%
13	16.139	2214	2221	2238	rBV	772200	1332528	51.50%	9.739%
14	17.397	2428	2435	2450	rBV	376706	679321	26.25%	4.965%
15	17.514	2450	2455	2466	rVB5	21987	41601	1.61%	0.304%
16	18.284	2582	2586	2599	rBV5	30965	69782	2.70%	0.510%
17	20.005	2873	2879	2893	rBV	1783151	2587652	100.00%	18.912%
18	21.310	3095	3101	3114	rBV8	36788	119511	4.62%	0.873%
19	21.662	3153	3161	3178	rBV	419341	815017	31.50%	5.957%
20	22.450	3290	3295	3300	rBV3	22262	34265	1.32%	0.250%
21	23.137	3406	3412	3418	rVB3	28849	53800	2.08%	0.393%
22	23.325	3439	3444	3452	rBV	25682	50670	1.96%	0.370%
23	23.930	3541	3547	3553	rBV4	30003	60044	2.32%	0.439%
24	24.858	3694	3705	3718	rBV	303138	897734	34.69%	6.561%
25	25.987	3889	3897	3899	rBV8	15651	36848	1.42%	0.269%

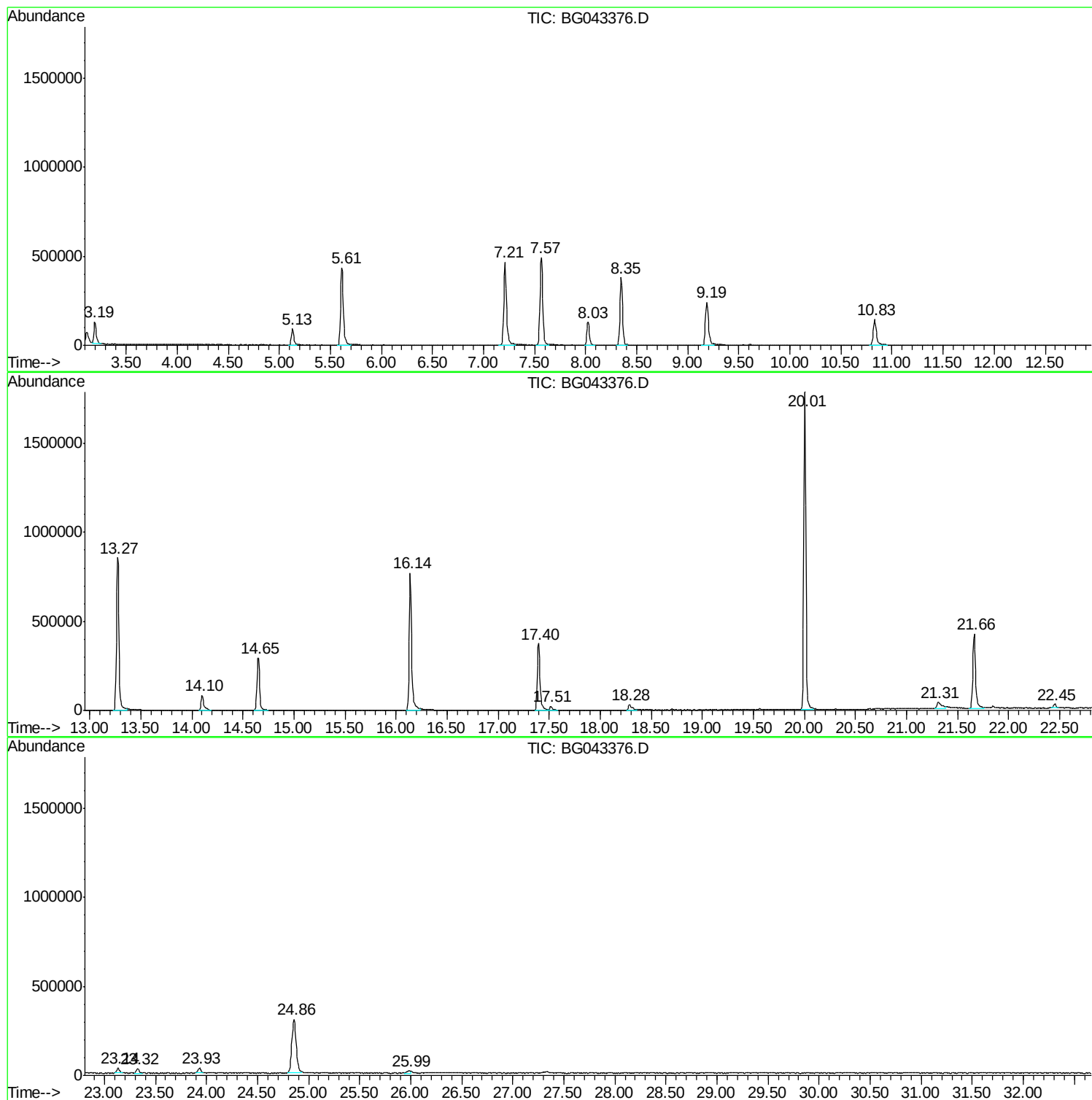
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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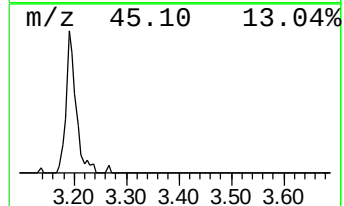
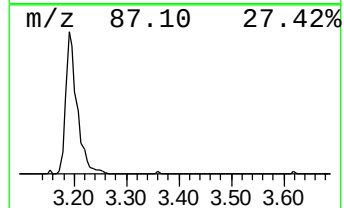
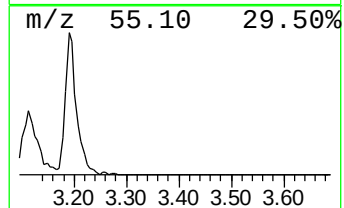
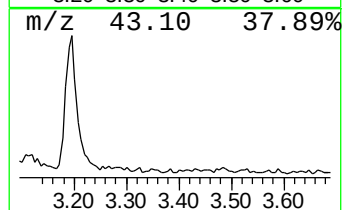
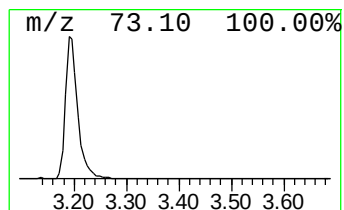
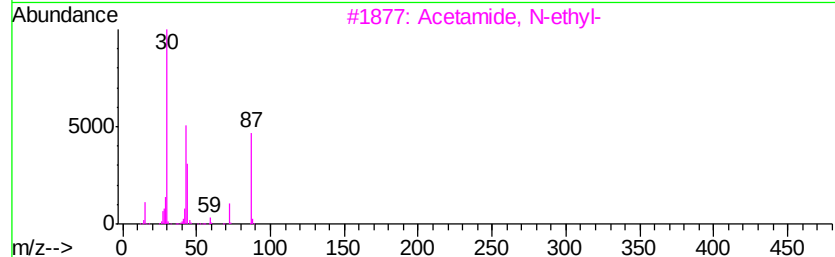
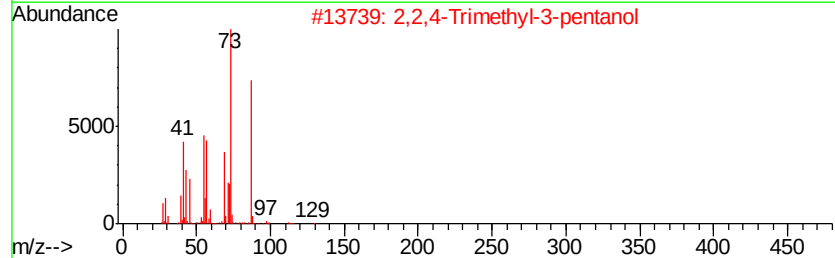
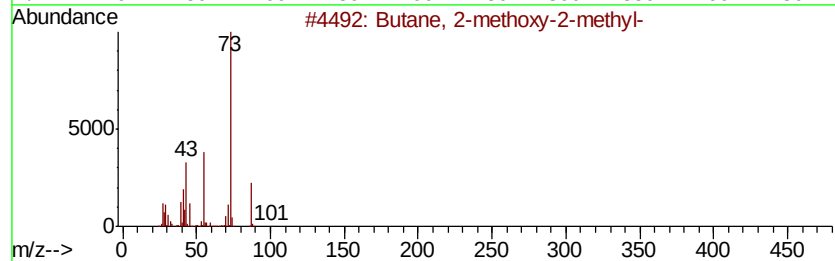
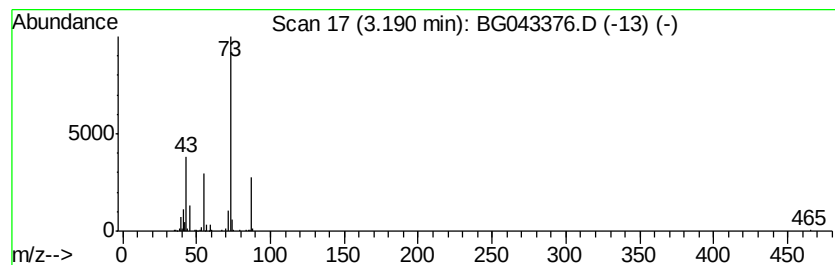
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.19	16.61 ng	195349	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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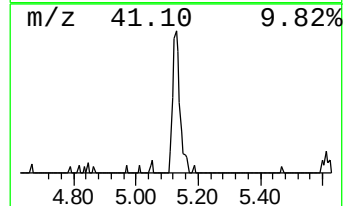
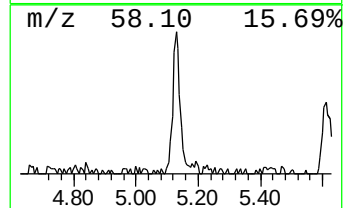
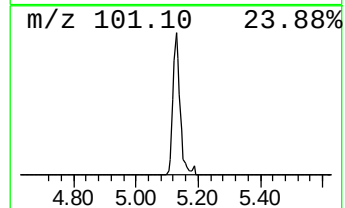
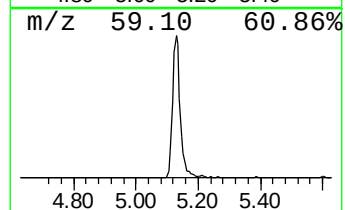
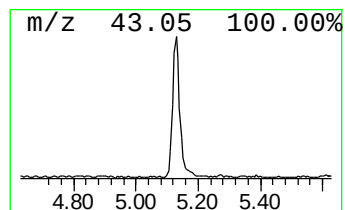
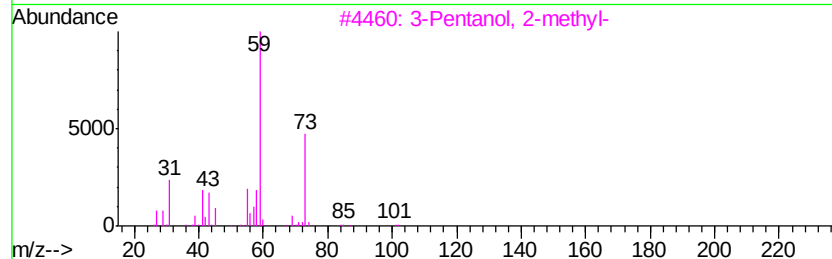
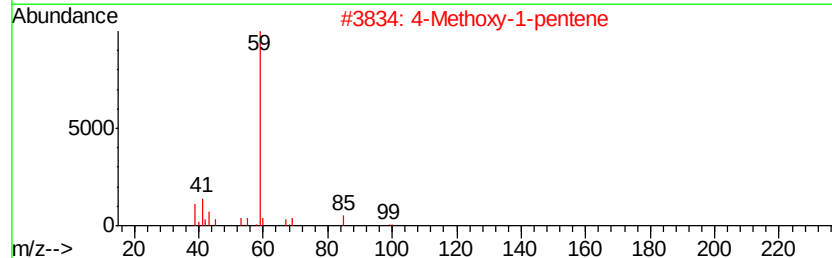
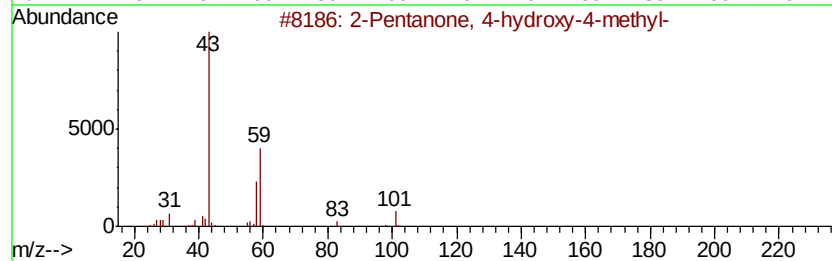
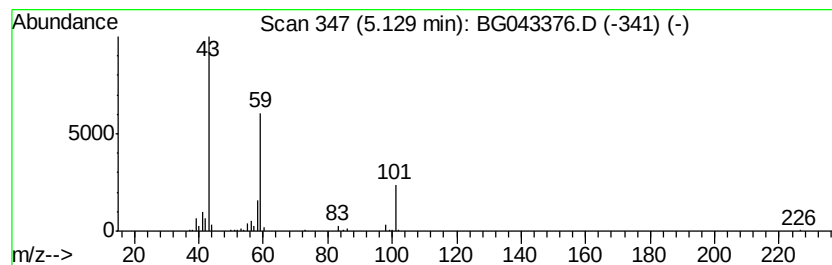
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	12.42 ng	146009	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		4-Methoxy-1-pentene	100	C6H12O	098386-09-5	25
3		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	23
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	9



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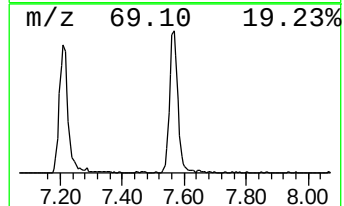
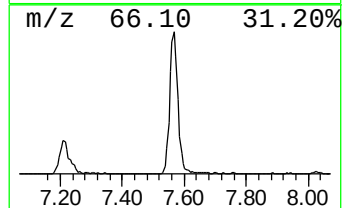
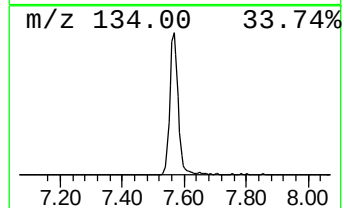
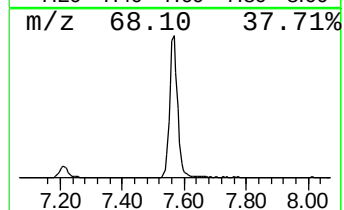
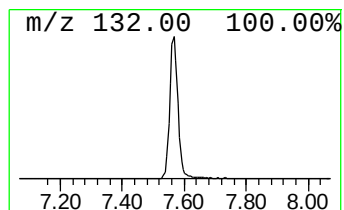
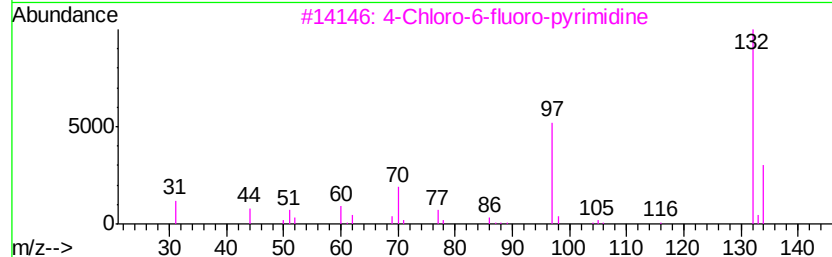
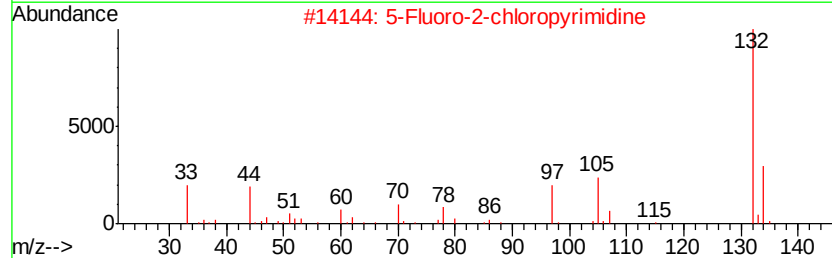
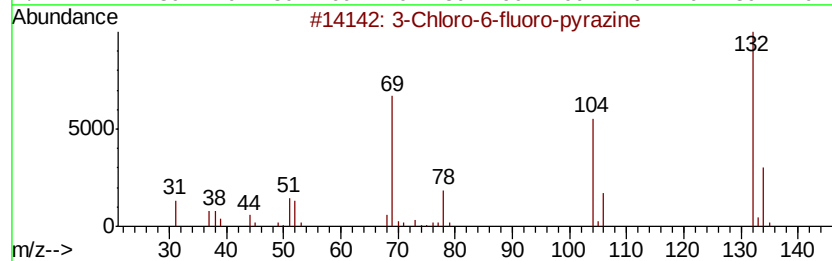
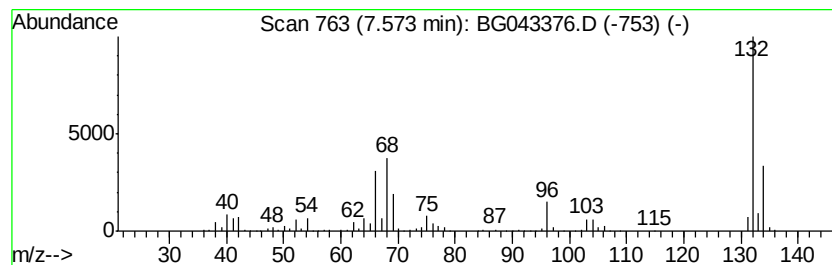
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Peak Number 3 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	76.41 ng	898393	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25



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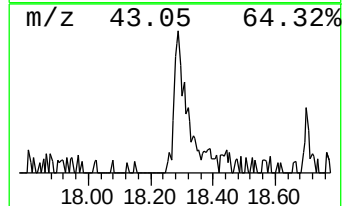
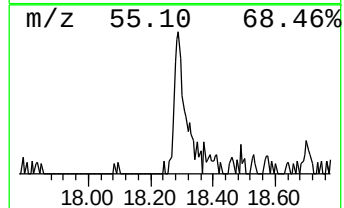
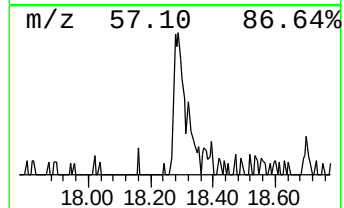
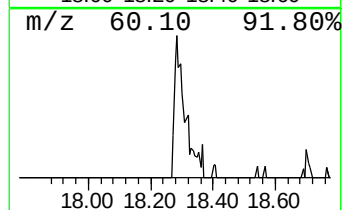
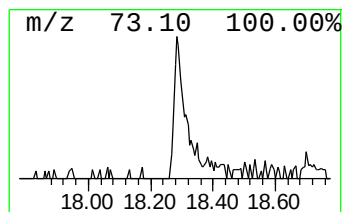
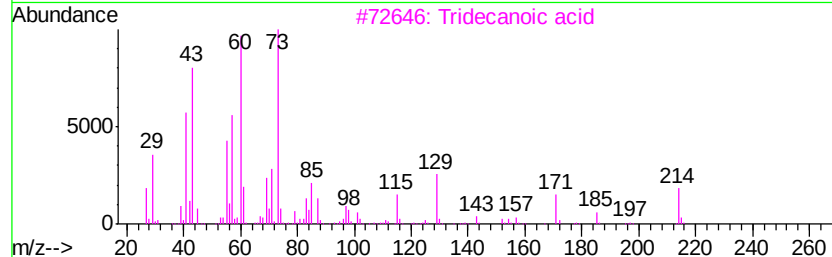
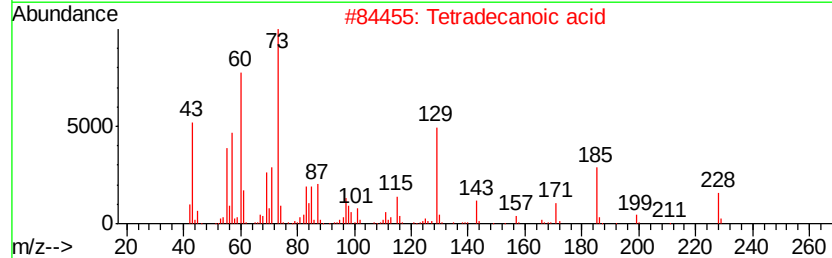
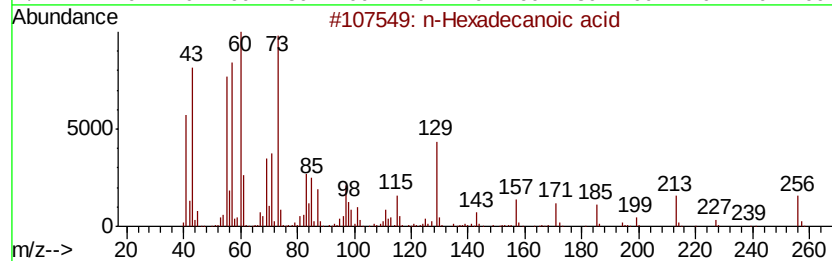
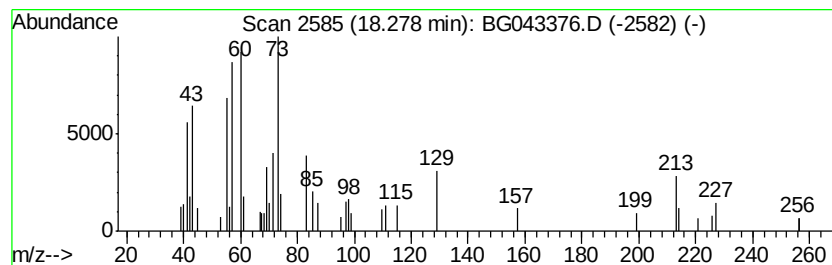
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.28	2.05 ng	69782	Phenanthrene-d10	17.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	42



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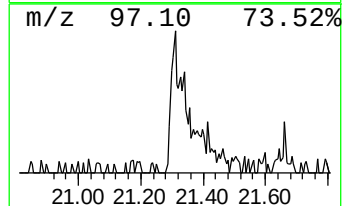
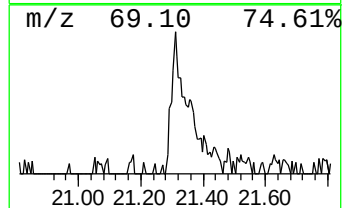
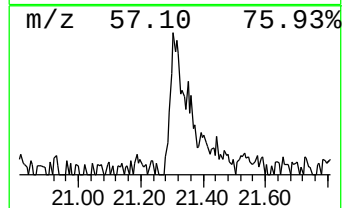
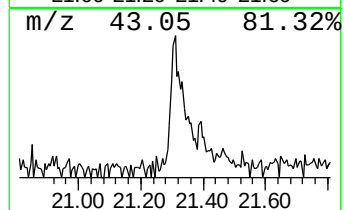
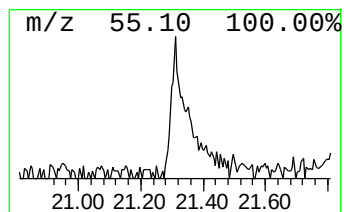
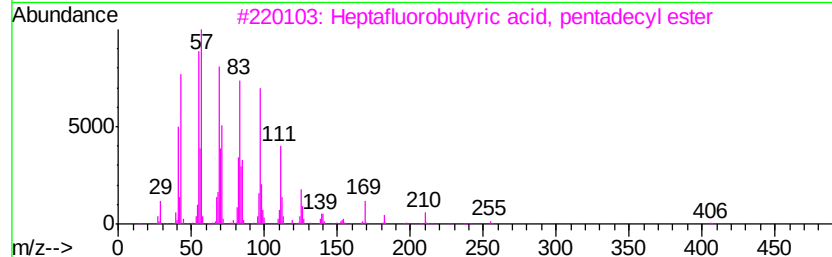
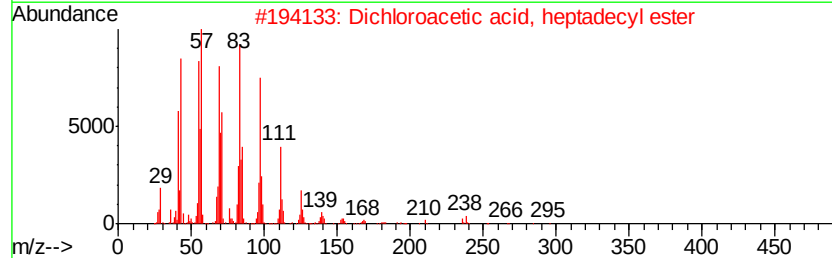
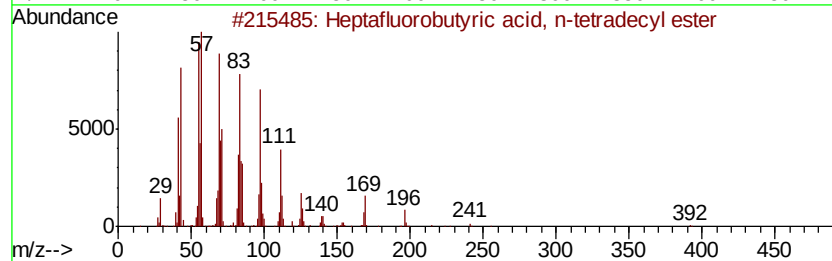
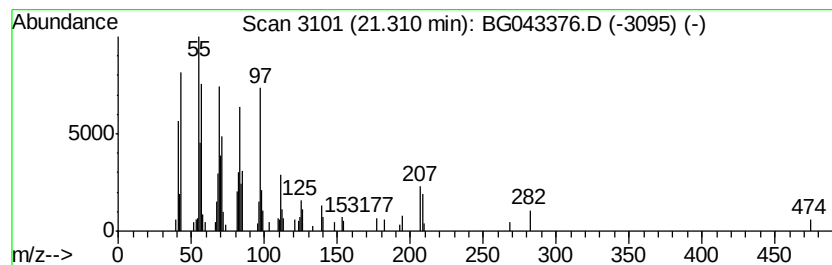
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Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.93 ng	119511	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3		Heptafluorobutyric acid, penta...	424	C19H31F7O2	959261-23-5	93
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.19	16.6	ng	195349	1	8.03	235161	20.0
2-Pentanone, 4-hy...	5.13	12.4	ng	146009	1	8.03	235161	20.0
unknown7.57	7.57	76.4	ng	898393	1	8.03	235161	20.0
n-Hexadecanoic acid	18.28	2.0	ng	69782	4	17.40	679321	20.0
Heptafluorobutyri...	21.31	2.9	ng	119511	5	21.66	815017	20.0