

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
 Data File : BG029304.D
 Acq On : 17 Oct 2017 16:54
 Operator : SJ/JU
 Sample : I5794-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ENV-106-5(15-20)

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_G\METHODS\8270-BG101617.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	5.247	327	333	345	rBV	186761	289104	7.32%	1.185%
2	5.722	404	414	428	rBV	1004212	1625160	41.12%	6.663%
3	7.321	676	686	704	rBV	1058830	1953565	49.43%	8.009%
4	7.702	741	751	767	rBV	1023605	1794712	45.41%	7.358%
5	8.167	823	830	838	rBV	223846	387138	9.80%	1.587%
6	8.496	877	886	897	rVB	729814	1264080	31.99%	5.182%
7	9.336	1020	1029	1040	rBV	617270	1104949	27.96%	4.530%
8	10.987	1303	1310	1318	rBV	348521	626920	15.86%	2.570%
9	13.413	1714	1723	1731	rBV	1781050	2766260	70.00%	11.341%
10	14.230	1855	1862	1873	rBV	476609	688546	17.42%	2.823%
11	14.788	1950	1957	1970	rVB2	601371	960568	24.31%	3.938%
12	16.128	2180	2185	2193	rVB	69028	102178	2.59%	0.419%
13	16.269	2202	2209	2224	rBV	1585040	2402897	60.80%	9.851%
14	17.526	2416	2423	2433	rVB	786933	1173937	29.70%	4.813%
15	18.390	2565	2570	2580	rBV	139492	215157	5.44%	0.882%
16	19.242	2711	2715	2724	rBV3	42510	69692	1.76%	0.286%
17	19.653	2781	2785	2789	rBV2	48556	57952	1.47%	0.238%
18	20.117	2857	2864	2874	rBV	2904716	3952053	100.00%	16.202%
19	21.416	3081	3085	3094	rVB	82090	136151	3.45%	0.558%
20	21.792	3143	3149	3158	rVB	782277	1351850	34.21%	5.542%
21	23.519	3437	3443	3452	rVB	54849	107016	2.71%	0.439%
22	24.160	3547	3552	3558	rVB4	24646	49046	1.24%	0.201%
23	25.106	3702	3713	3728	rBV2	412914	1312926	33.22%	5.383%

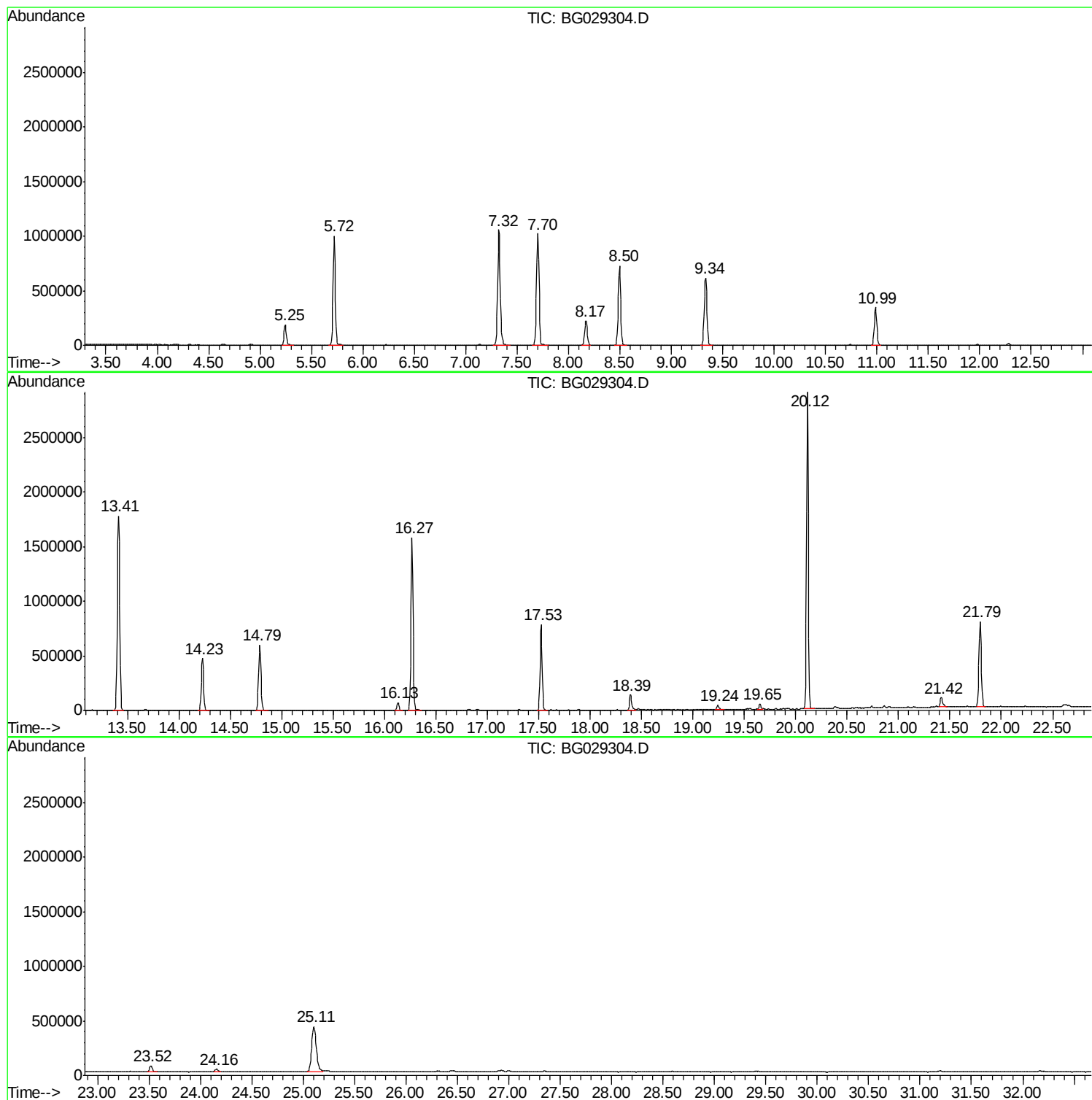
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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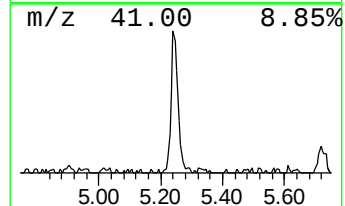
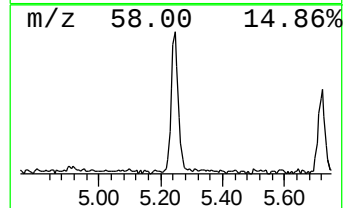
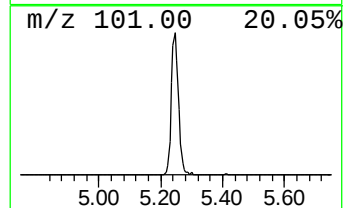
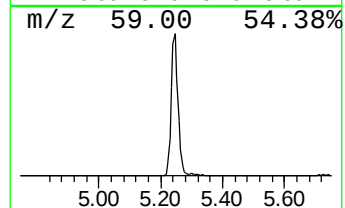
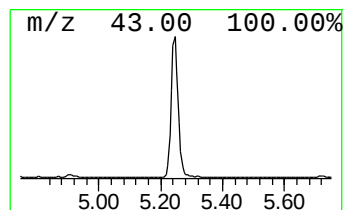
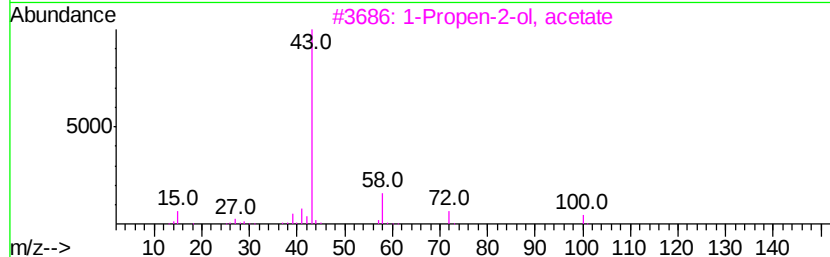
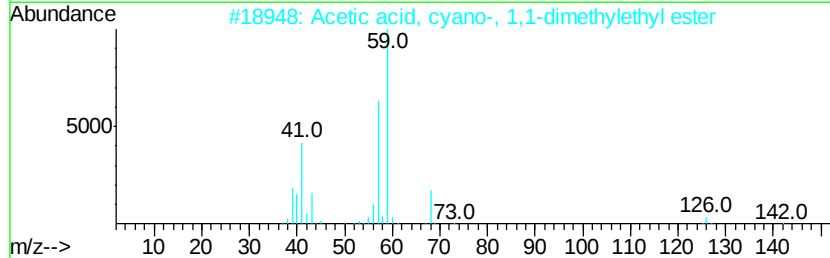
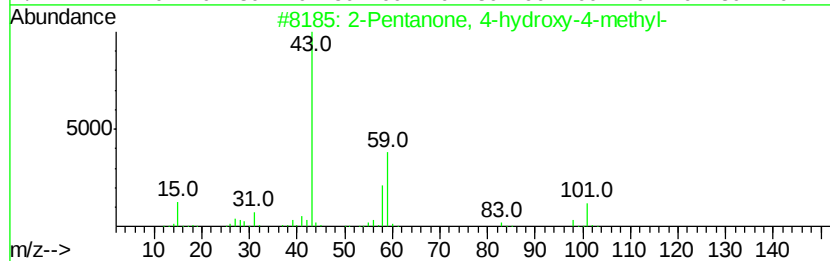
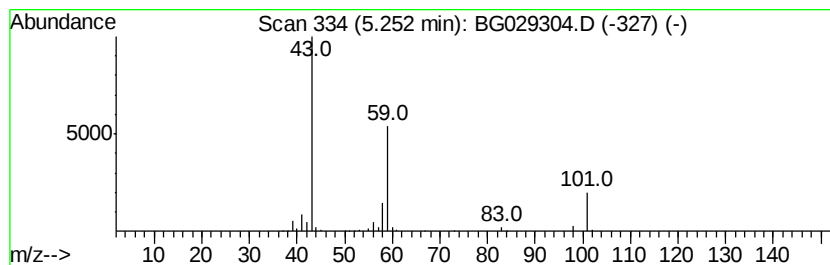
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	14.94 ng	289104	1,4-Dichlorobenzene-d4	8.17

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	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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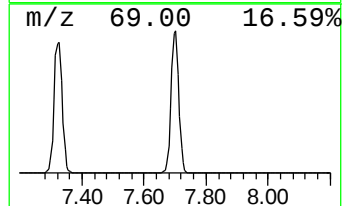
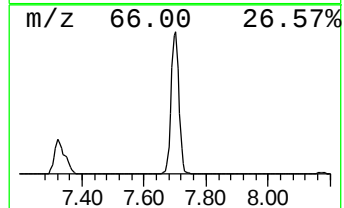
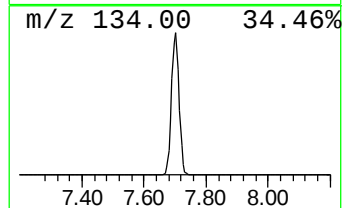
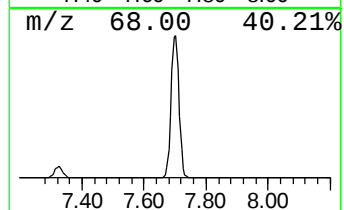
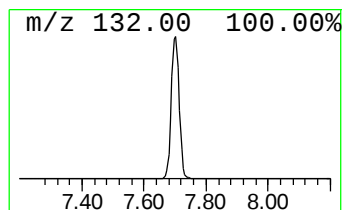
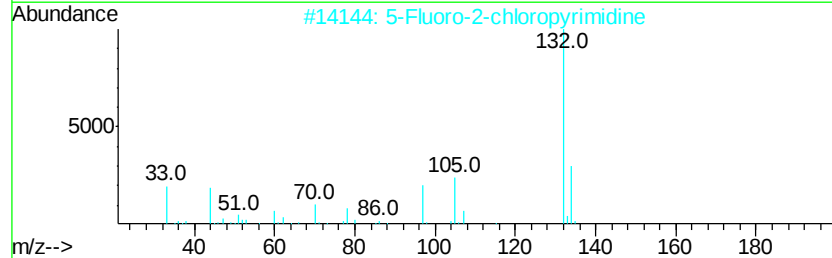
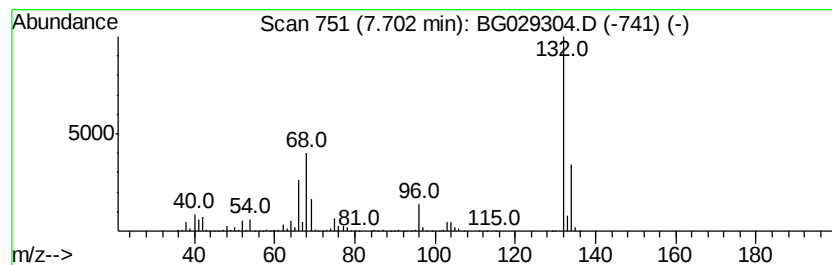
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	92.72 ng	1794710	1,4-Dichlorobenzene-d4	8.17

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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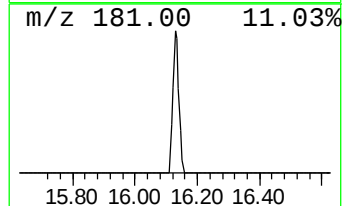
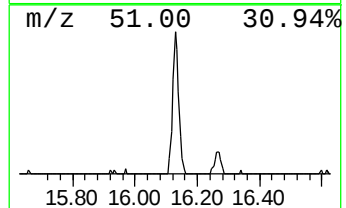
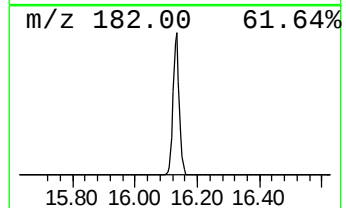
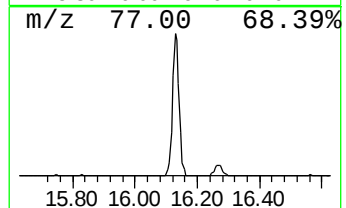
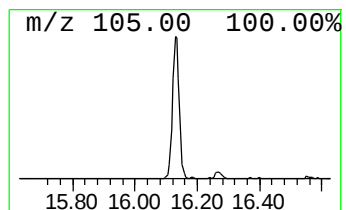
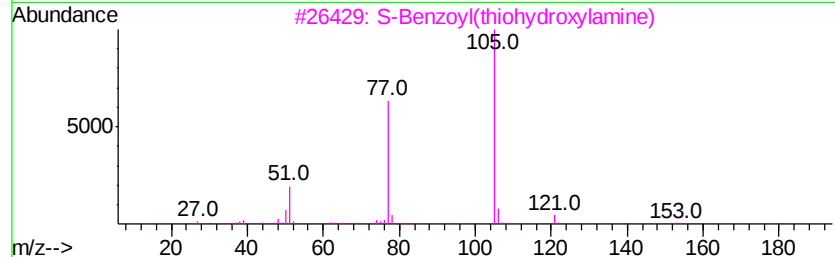
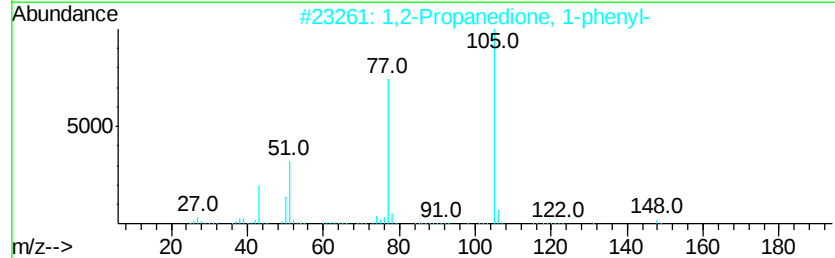
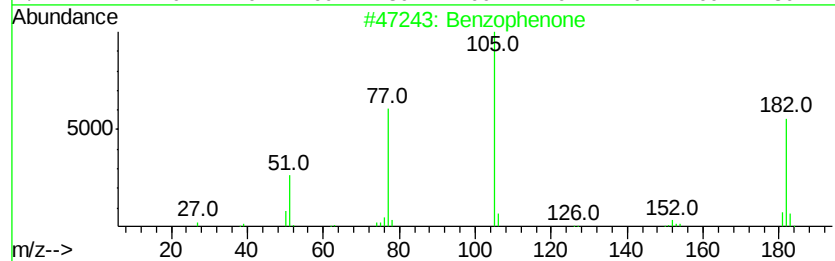
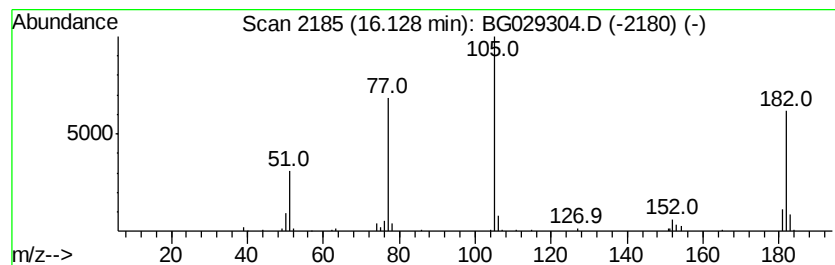
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.13 ng	102178	Acenaphthene-d10	14.79
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		1,2-Propanedione, 1-phenyl-	148 C9H8O2	000579-07-7 43
3		S-Benzoyl(thiohydroxylamine)	153 C7H7NOS	025740-80-1 43
4		Vinyl benzoate	148 C9H8O2	000769-78-8 43
5		Benzoic acid, phenyl ester	198 C13H10O2	000093-99-2 43



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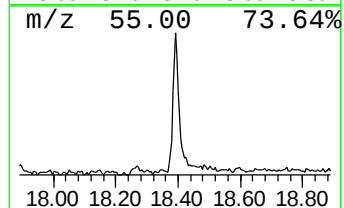
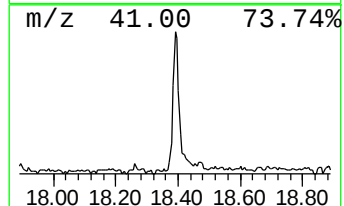
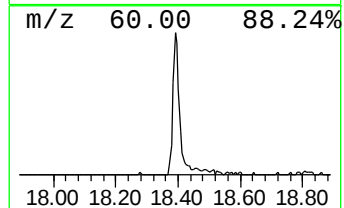
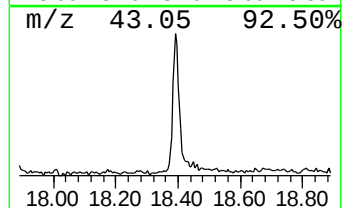
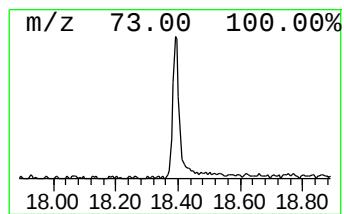
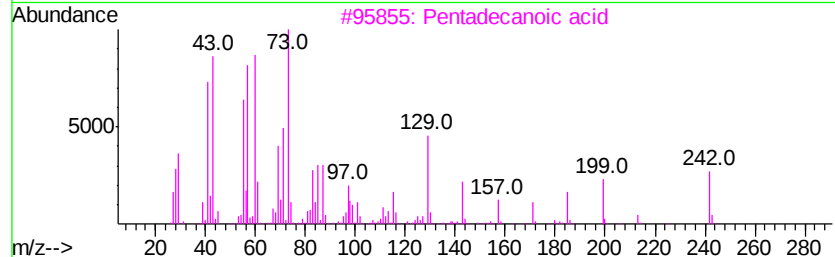
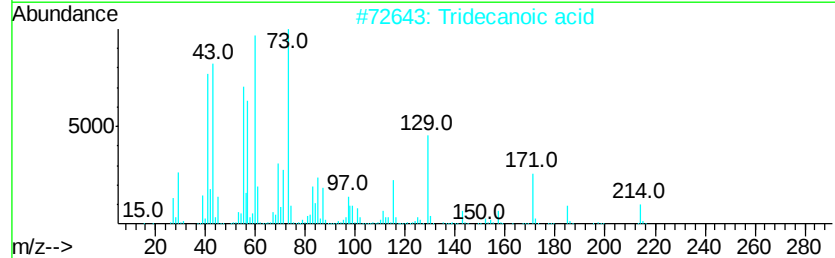
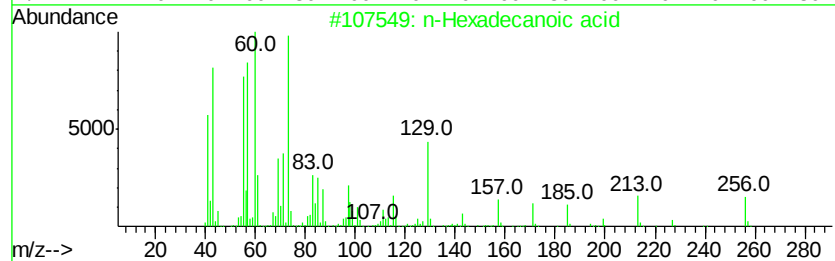
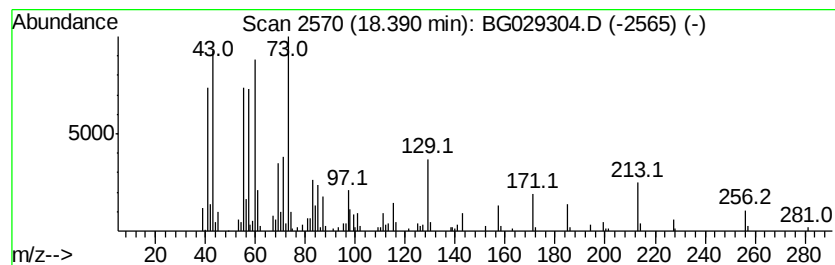
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.39	3.67 ng	215157	Phenanthrene-d10		17.53
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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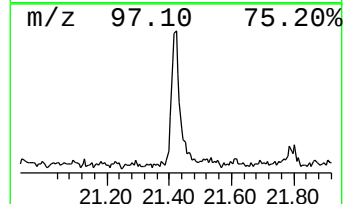
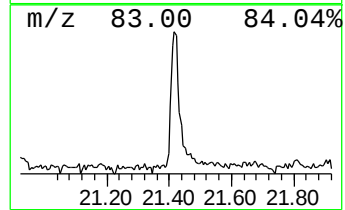
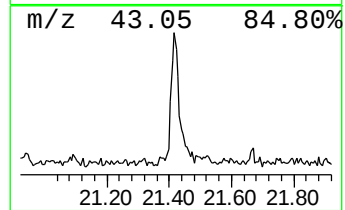
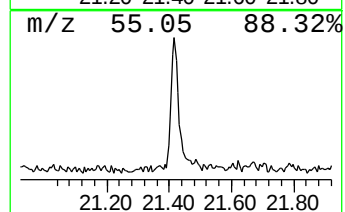
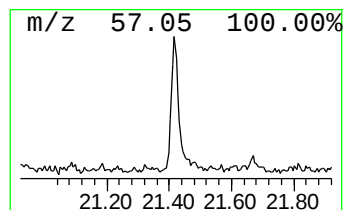
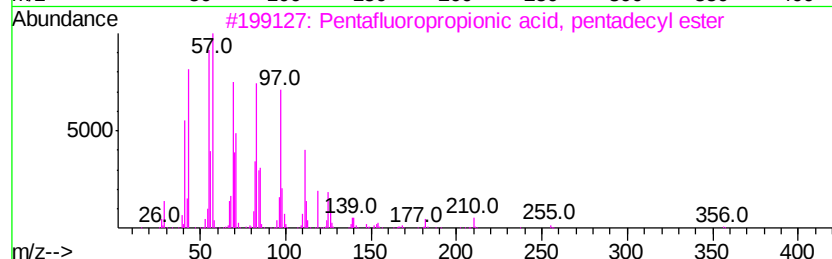
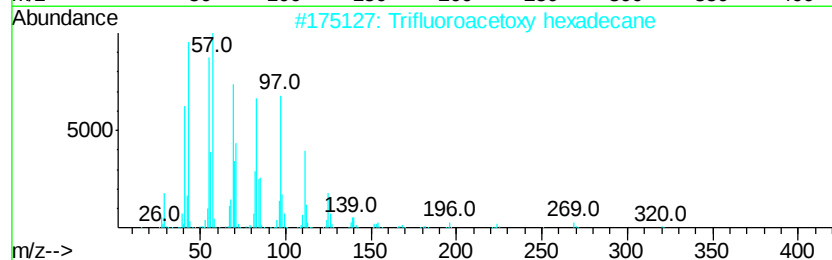
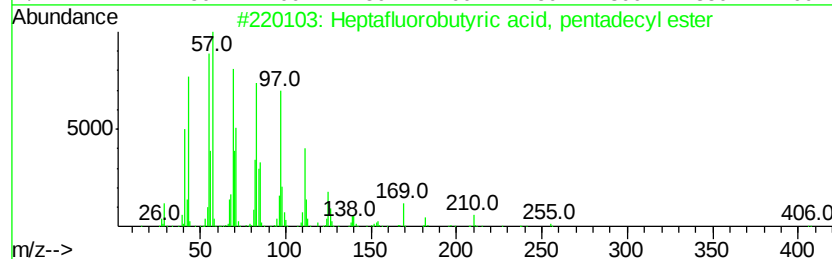
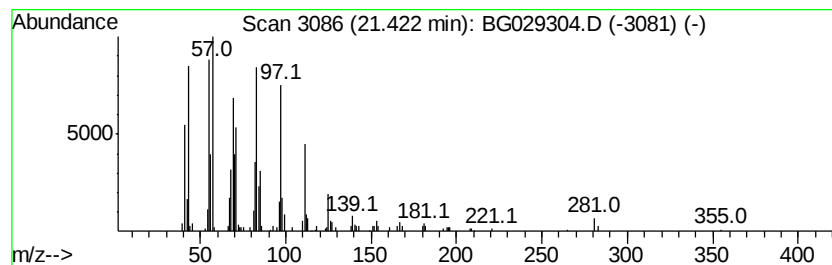
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Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	2.01 ng	136151	Chrysene-d12	21.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.25	14.9	ng	289104	1	8.17	387138	20.0
unknown7.70	7.70	92.7	ng	1794710	1	8.17	387138	20.0
Benzophenone	16.13	2.1	ng	102178	3	14.79	960568	20.0
n-Hexadecanoic acid	18.39	3.7	ng	215157	4	17.53	1173940	20.0
Heptafluorobutyri...	21.42	2.0	ng	136151	5	21.79	1351850	20.0