

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
 Data File : BF102396.D
 Acq On : 24 Jan 2018 18:18
 Operator : SJ/JU
 Sample : J1249-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AB-3(0-2)

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-BF012218.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	4.916	478	481	491	rVB	83935	120694	3.58%	0.443%
2	5.328	546	551	554	rBV	3018518	3064482	90.87%	11.238%
3	6.363	721	727	743	rBV	2690333	3372371	100.00%	12.367%
4	6.487	743	748	751	rBV	3383461	3166110	93.88%	11.610%
5	6.716	783	787	795	rBV	879440	757430	22.46%	2.778%
6	6.869	809	813	817	rBV	2640771	2367602	70.21%	8.682%
7	7.287	878	884	894	rBV	1922831	2083805	61.79%	7.641%
8	7.998	1001	1005	1008	rBV	1139567	1003386	29.75%	3.679%
9	8.557	1096	1100	1103	rBV	62077	56876	1.69%	0.209%
10	9.075	1183	1188	1191	rBV	3609772	3081524	91.38%	11.300%
11	9.469	1251	1255	1262	rBV	346199	301395	8.94%	1.105%
12	9.680	1288	1291	1295	rVB	78356	61734	1.83%	0.226%
13	9.751	1299	1303	1312	rVB	1251543	1125401	33.37%	4.127%
14	10.180	1372	1376	1379	rVB2	91006	78187	2.32%	0.287%
15	10.463	1419	1424	1430	rBV	151367	137076	4.06%	0.503%
16	10.539	1433	1437	1447	rVB	1759652	1654905	49.07%	6.069%
17	10.651	1453	1456	1463	rVB	68120	71734	2.13%	0.263%
18	11.233	1551	1555	1563	rBV	1165448	1009463	29.93%	3.702%
19	12.821	1820	1825	1828	rBV	2272430	2105915	62.45%	7.723%
20	13.710	1973	1976	1981	rBV	239053	272616	8.08%	1.000%
21	13.868	2000	2003	2008	rVB	699095	690226	20.47%	2.531%
22	15.298	2241	2246	2252	rBV	563467	686771	20.36%	2.518%

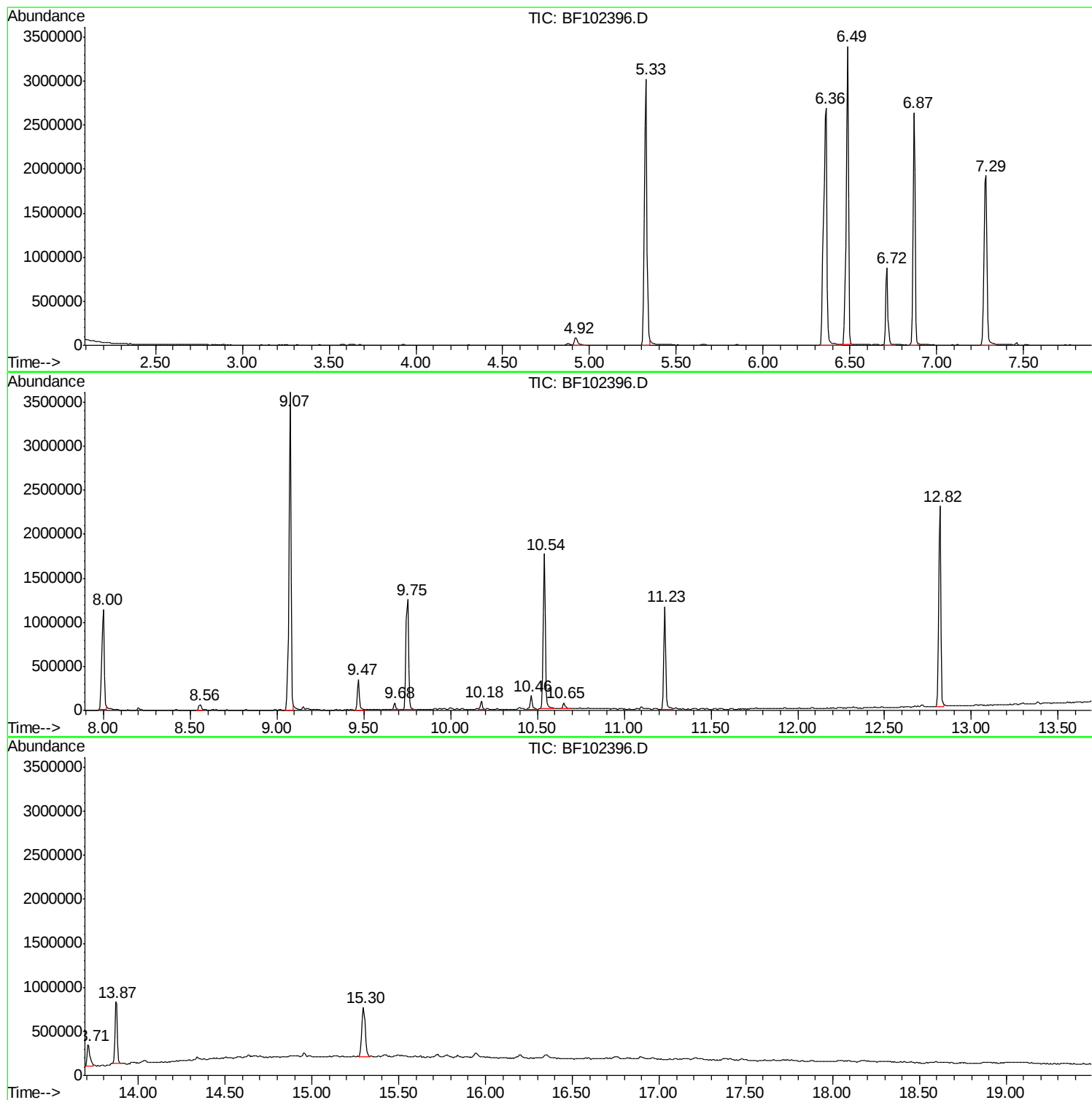
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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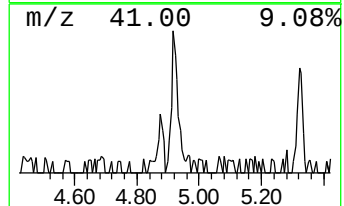
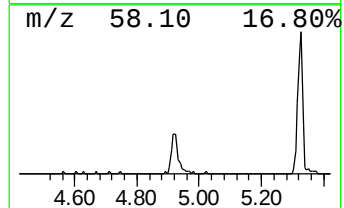
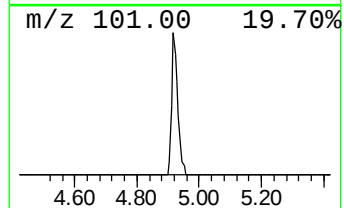
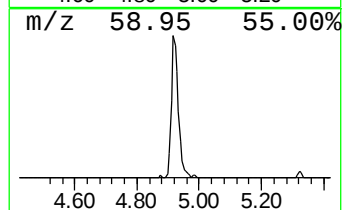
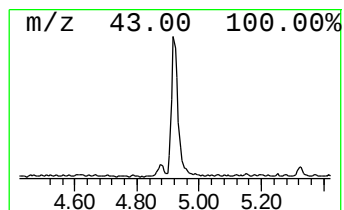
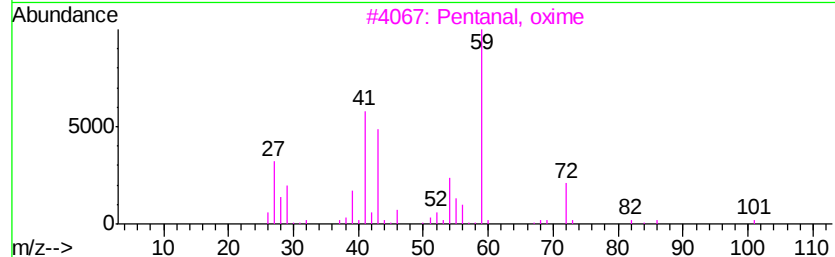
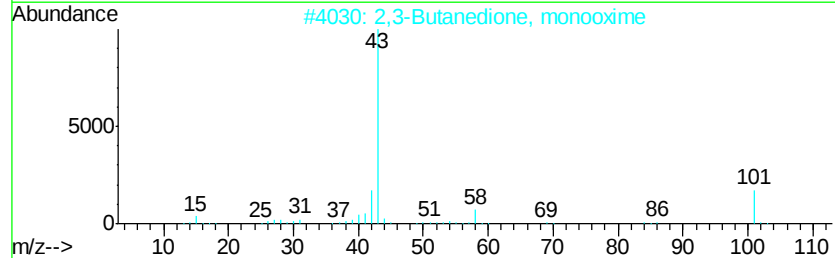
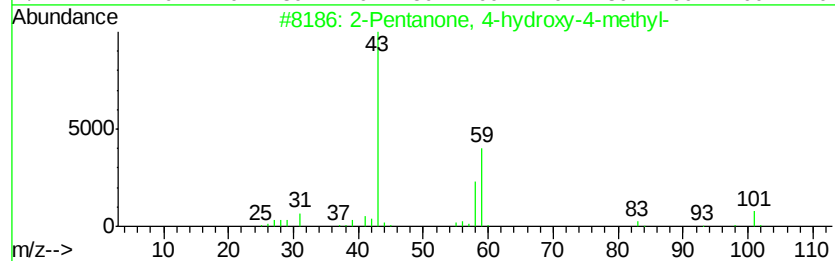
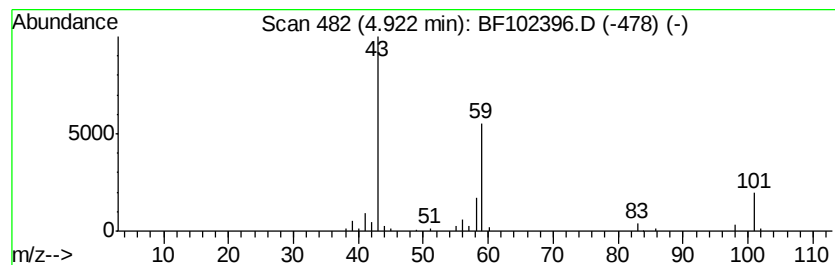
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.19 ng	120694	1,4-Dichlorobenzene-d4	6.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
3	Pentanal, oxime	101	C5H11NO	000628-79-5	9	
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	9	
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9	



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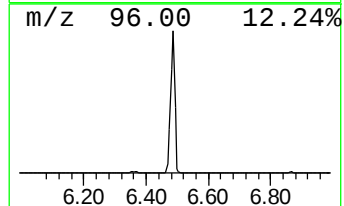
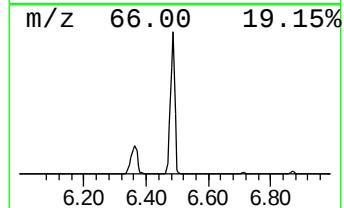
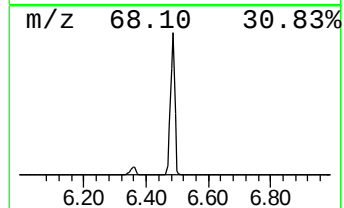
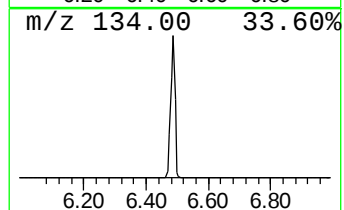
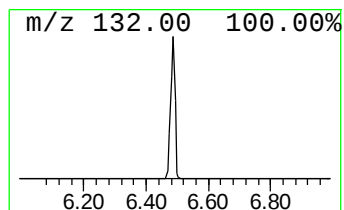
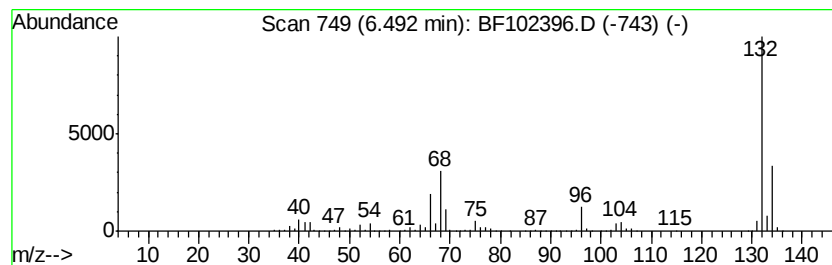
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	83.60 ng	3166110	1,4-Dichlorobenzene-d4	6.72

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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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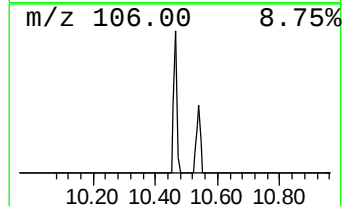
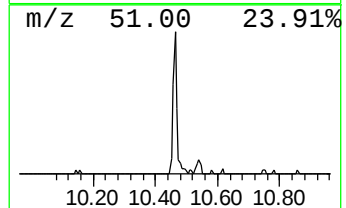
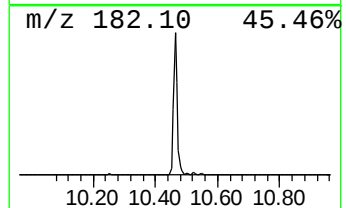
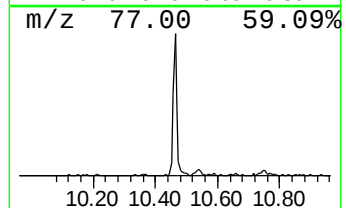
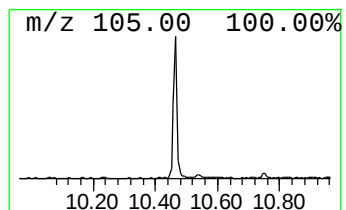
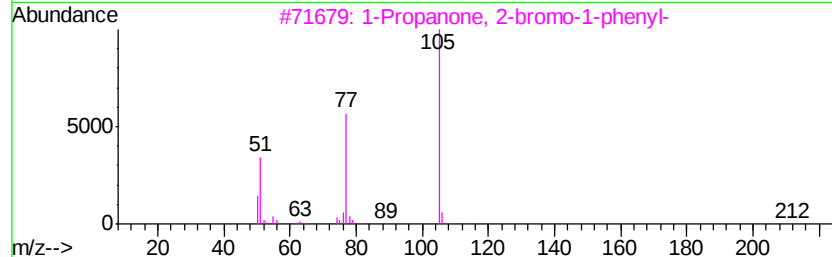
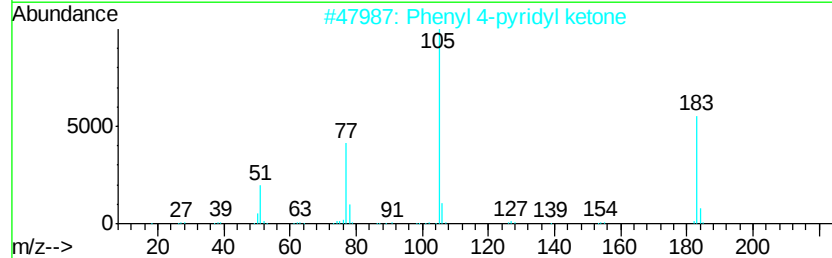
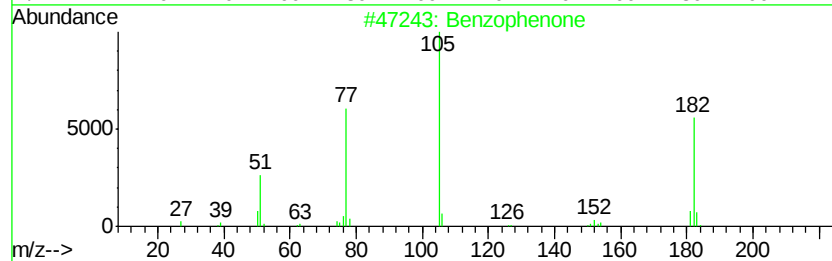
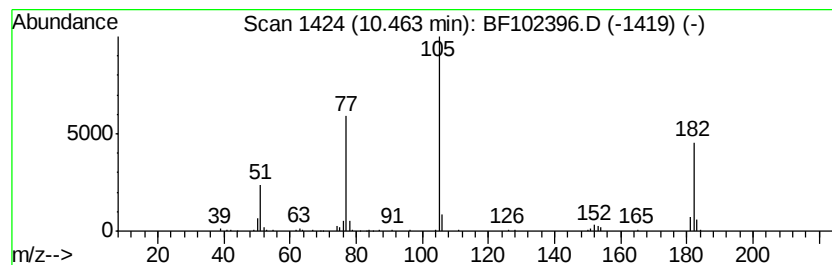
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Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.46	2.44 ng	137076	Acenaphthene-d10		9.75
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47



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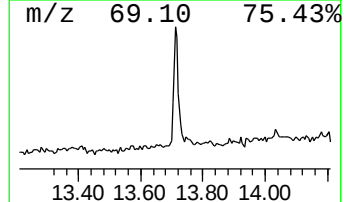
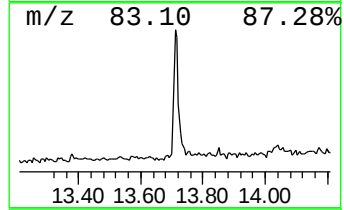
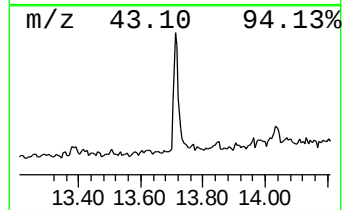
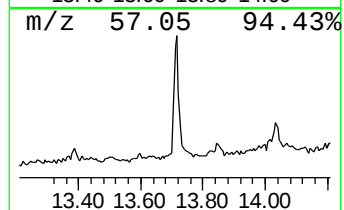
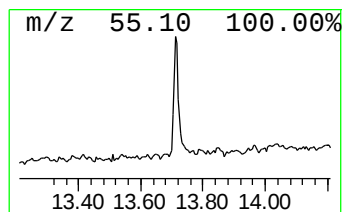
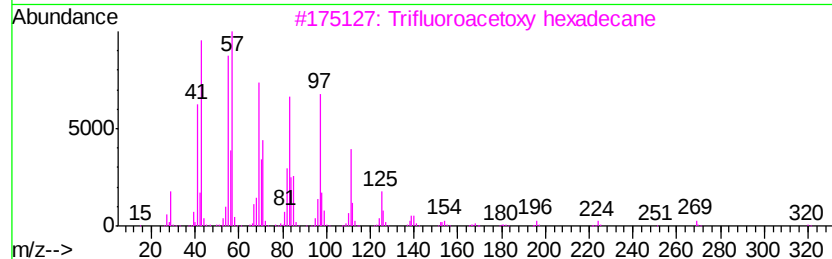
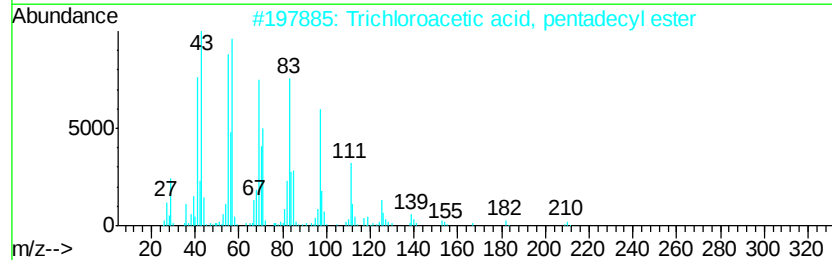
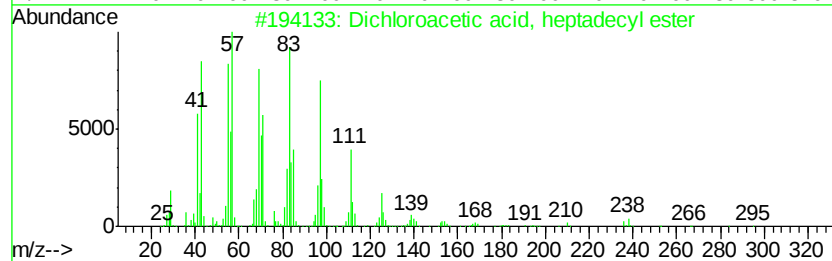
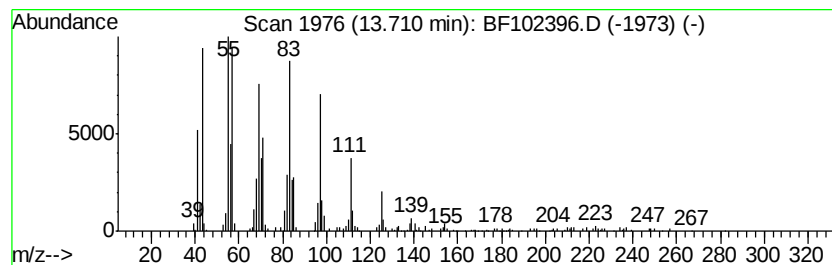
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	7.90 ng	272616	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	3.2	ng	120694	1	6.72	757430	20.0
unknown6.49	6.49	83.6	ng	3166110	1	6.72	757430	20.0
Benzophenone	10.46	2.4	ng	137076	3	9.75	1125400	20.0
Dichloroacetic ac...	13.71	7.9	ng	272616	5	13.87	690226	20.0