

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
 Data File : BG057070.D
 Acq On : 12 Apr 2023 19:22
 Operator : CG/JU
 Sample : 02292-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 IDW-SO-G2-041123

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057070.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.432	316	322	329	rVB2	21334	34718	4.19%	0.897%
2	5.914	395	404	413	rBV	189247	307974	37.20%	7.956%
3	7.535	673	680	688	rBV	195748	338958	40.94%	8.756%
4	8.405	822	828	836	rVB2	53249	86020	10.39%	2.222%
5	9.580	1019	1028	1038	rBV	108586	199080	24.05%	5.143%
6	11.248	1305	1312	1319	rVB	64615	114722	13.86%	2.964%
7	13.645	1713	1720	1728	rVB	317959	476684	57.58%	12.314%
8	15.019	1948	1954	1960	rVB	113610	171094	20.67%	4.420%
9	16.353	2175	2181	2188	rBV	14655	19126	2.31%	0.494%
10	16.494	2199	2205	2219	rBV	261367	405831	49.02%	10.484%
11	17.757	2414	2420	2426	rVB	156443	224536	27.12%	5.801%
12	18.591	2558	2562	2573	rBV2	25186	33700	4.07%	0.871%
13	19.842	2772	2775	2782	rBV7	8232	13263	1.60%	0.343%
14	20.324	2851	2857	2862	rVB	667682	827851	100.00%	21.386%
15	21.634	3075	3080	3093	rVB4	30180	60742	7.34%	1.569%
16	22.075	3149	3155	3161	rVB2	142863	243609	29.43%	6.293%
17	22.879	3286	3292	3295	rBV6	5705	13193	1.59%	0.341%
18	23.625	3414	3419	3425	rBV7	12952	30233	3.65%	0.781%
19	24.142	3504	3507	3511	rVB4	6960	9347	1.13%	0.241%
20	25.611	3743	3757	3767	rVB	83791	260285	31.44%	6.724%

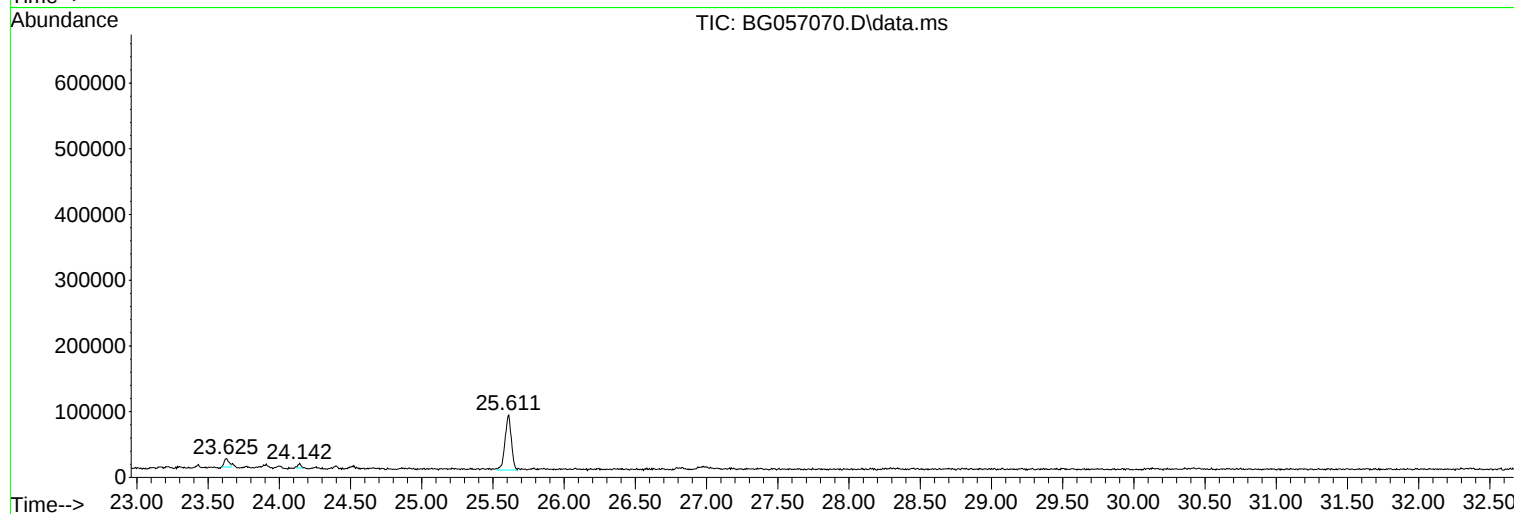
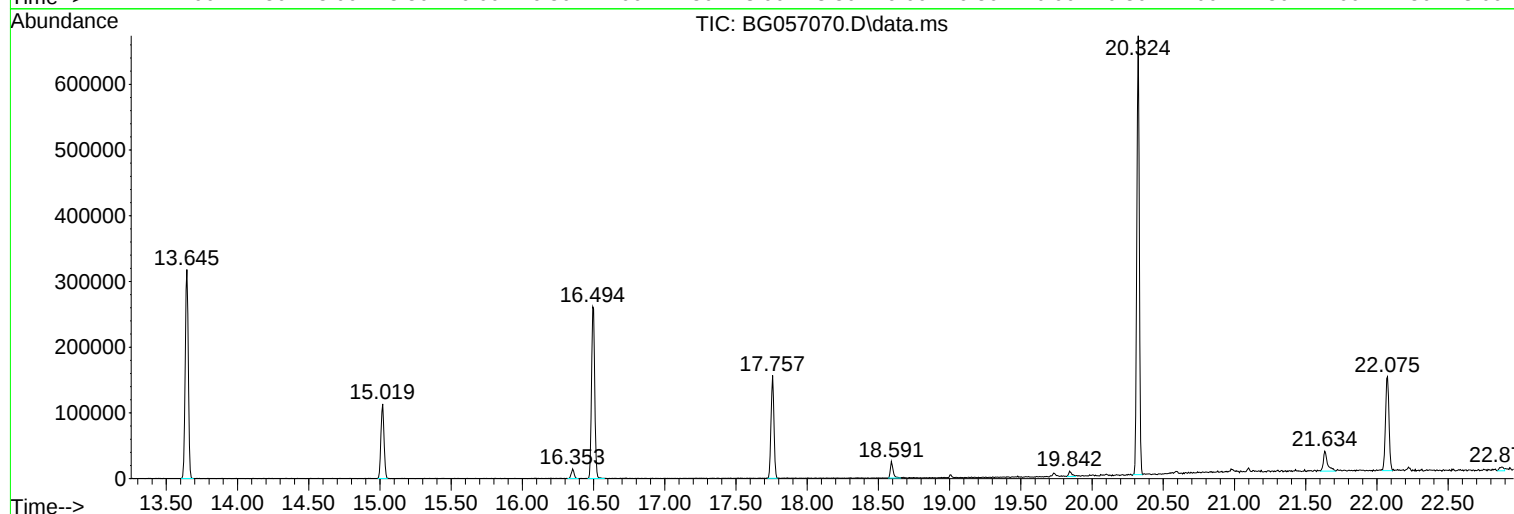
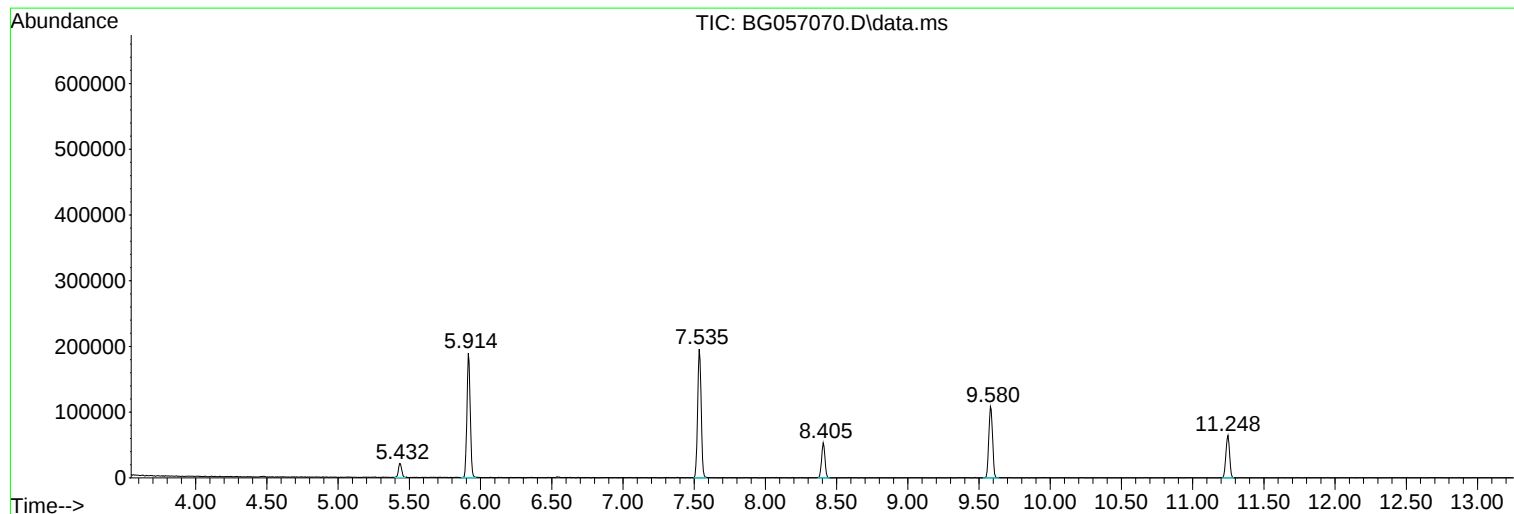
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BG057070.D
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Instrument :
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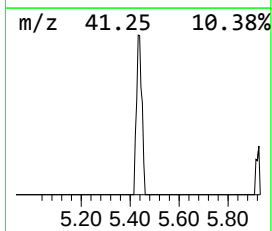
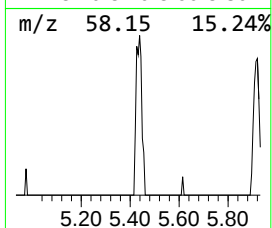
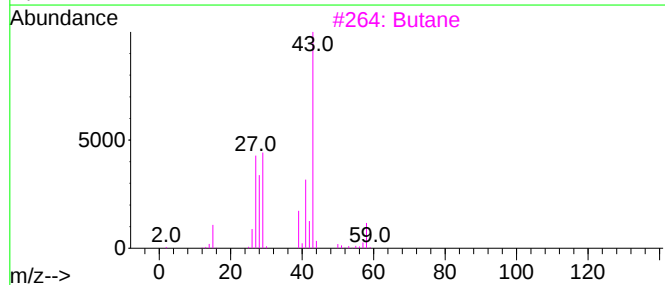
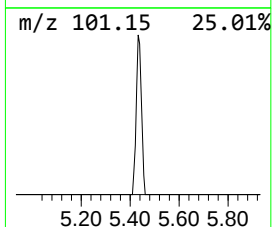
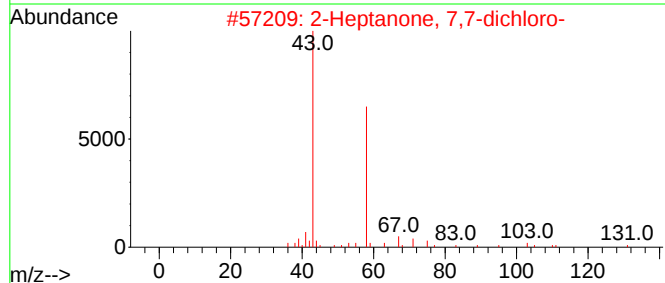
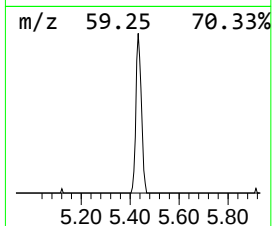
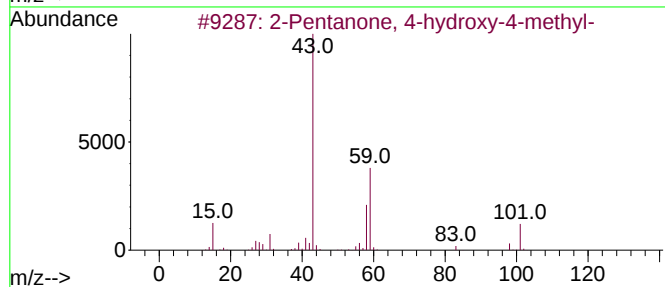
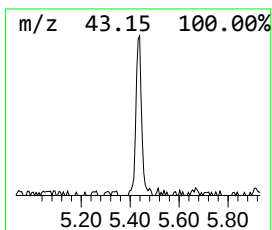
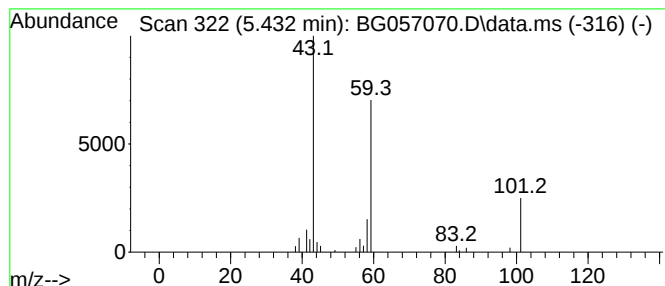
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.432	8.07 ng	34718	1,4-Dichlorobenzene-d4	8.405

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	12		
3	Butane	58	C4H10	000106-97-8	9		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Guanidine	59	CH5N3	000113-00-8	9		



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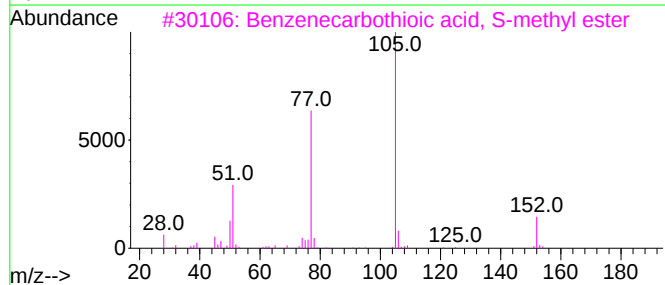
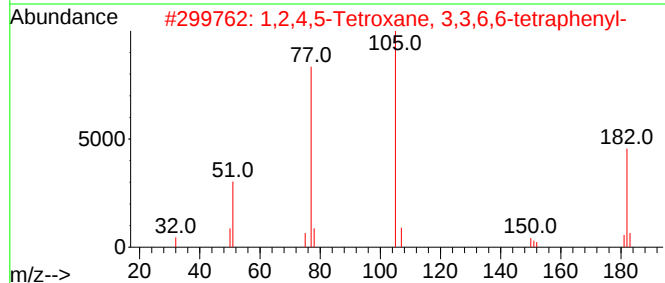
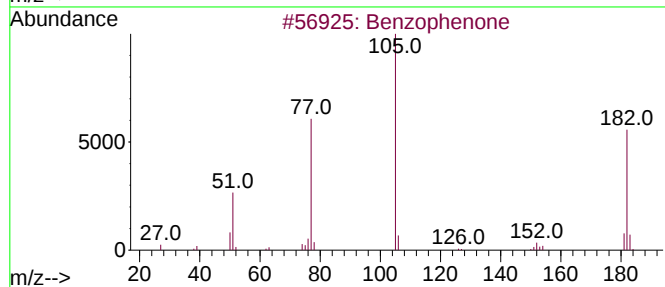
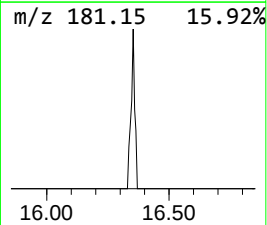
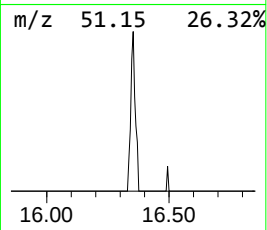
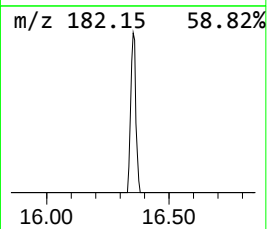
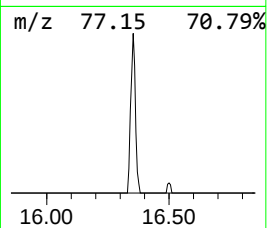
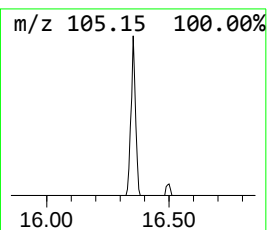
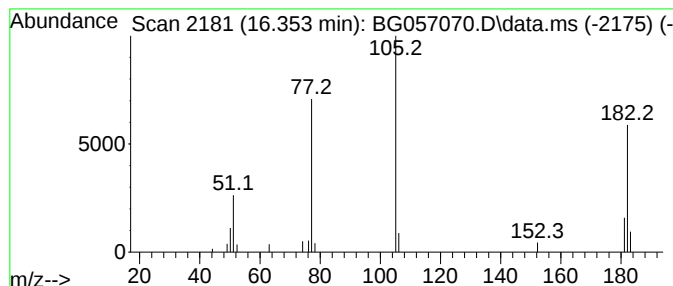
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.353	2.24 ng	19126	Acenaphthene-d10	15.020

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5			Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	43



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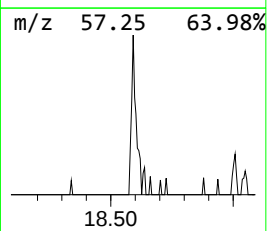
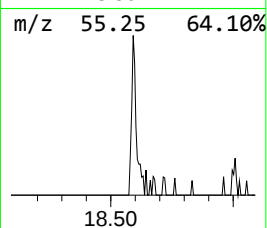
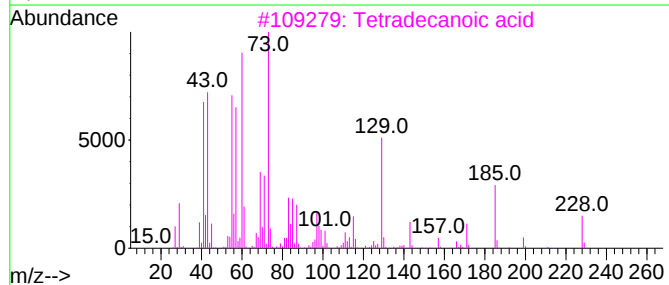
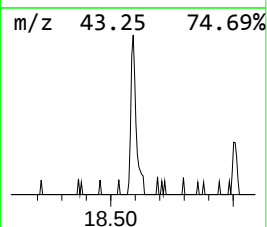
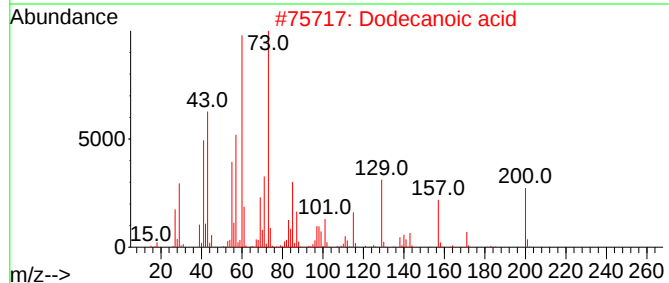
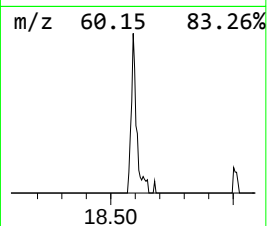
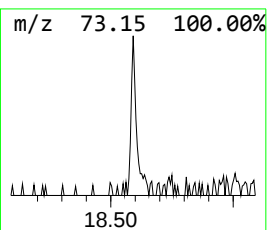
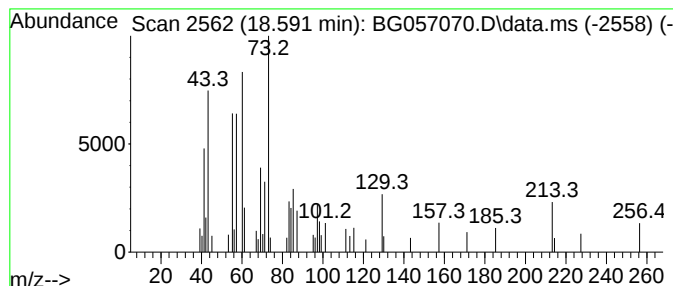
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.591	3.00 ng	33700	Phenanthrene-d10	17.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Dodecanoic acid	200	C12H24O2	000143-07-7	59
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	53
5			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	53



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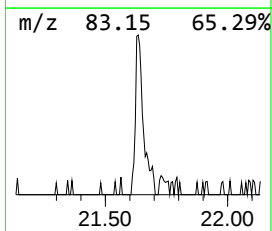
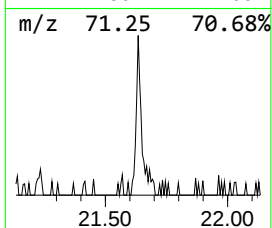
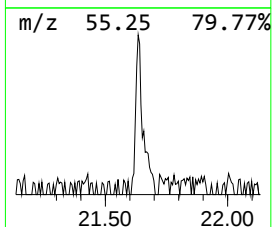
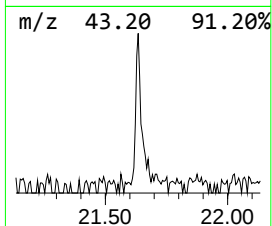
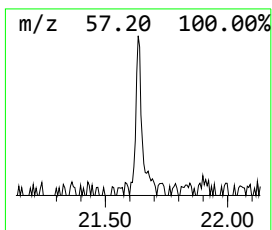
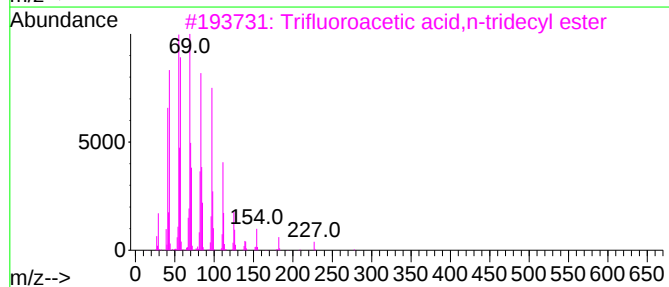
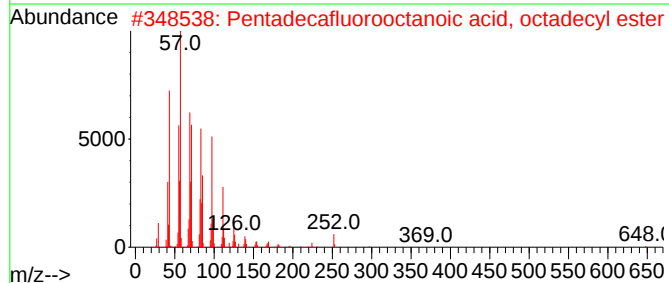
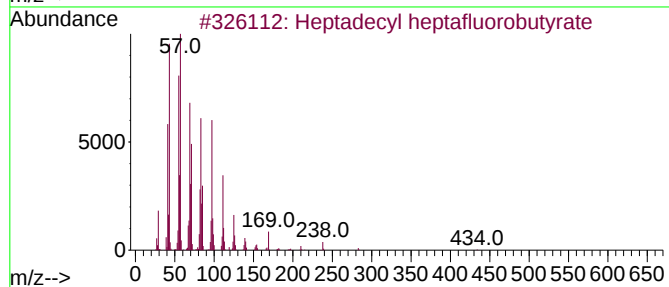
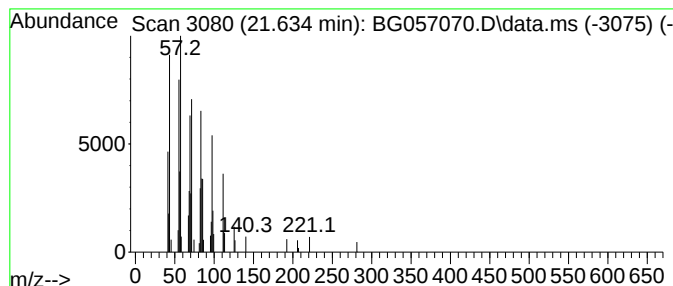
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.634	4.99 ng	60742	Chrysene-d12	22.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81
3			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	81
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	81
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	74



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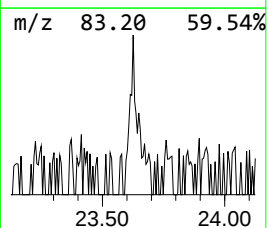
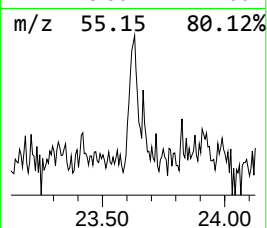
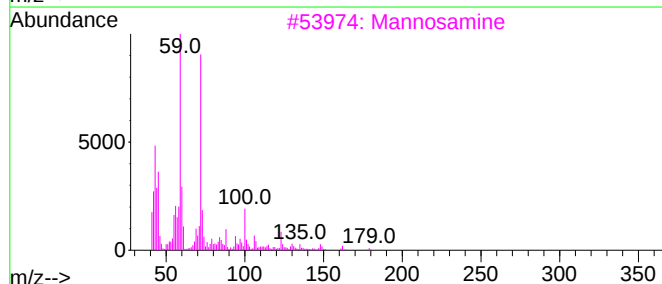
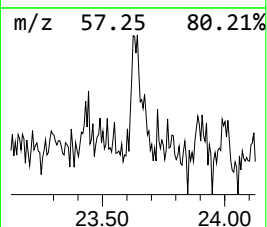
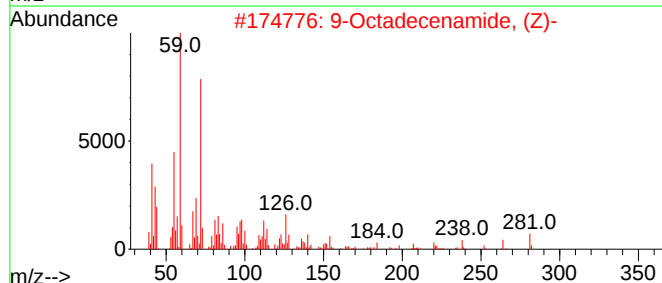
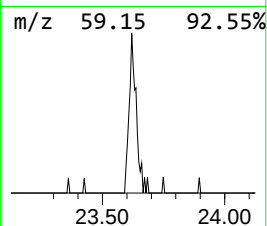
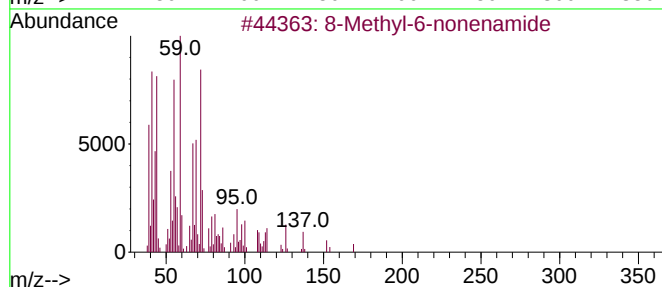
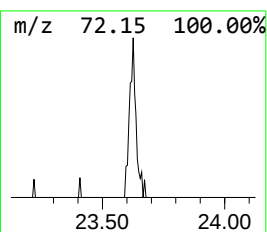
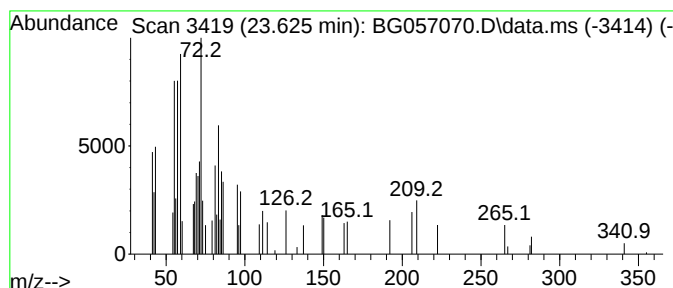
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown23.625 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.625	2.48 ng	30233	Chrysene-d12	22.069	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Methyl-6-nonenamide	169	C10H19NO	1000293-20-9	43
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	40
3	Mannosamine	179	C6H13NO5	006915-39-5	37
4	3-Dodecanone	184	C12H24O	001534-27-6	27
5	1-Octen-3-ol	128	C8H16O	003391-86-4	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.432	8.1	ng	34718	1	8.405	86020	20.0
Benzophenone	16.353	2.2	ng	19126	3	15.020	171094	20.0
n-Hexadecanoic ...	18.591	3.0	ng	33700	4	17.757	224536	20.0
Heptadecyl hept...	21.634	5.0	ng	60742	5	22.069	243609	20.0
unknown23.625	23.625	2.5	ng	30233	5	22.069	243609	20.0