

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
 Data File : BG057076.D
 Acq On : 12 Apr 2023 23:44
 Operator : CG/JU
 Sample : 02283-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230334-COMP-12

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: BG057076.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.435	317	323	329	rBV	41061	62102	4.36%	1.037%
2	5.916	398	405	418	rVB	366666	595919	41.85%	9.948%
3	7.538	673	681	691	rBV	373192	637904	44.80%	10.649%
4	8.401	823	828	835	rBB	52570	88724	6.23%	1.481%
5	9.582	1021	1029	1038	rVB	217114	380114	26.69%	6.346%
6	11.244	1303	1312	1320	rBV	69796	126683	8.90%	2.115%
7	13.641	1713	1720	1727	rBV	577019	888741	62.41%	14.837%
8	15.016	1948	1954	1961	rBV	115800	178335	12.52%	2.977%
9	16.355	2176	2182	2188	rBV2	25734	36650	2.57%	0.612%
10	16.496	2200	2206	2214	rBV	500729	753792	52.94%	12.584%
11	17.753	2414	2420	2427	rBV2	149096	230599	16.19%	3.850%
12	18.593	2558	2563	2568	rBV	35318	47604	3.34%	0.795%
13	20.326	2851	2858	2863	rBV	1109744	1423967	100.00%	23.772%
14	21.636	3076	3081	3089	rBV2	30772	51506	3.62%	0.860%
15	22.071	3149	3155	3162	rVB	143839	244068	17.14%	4.074%
16	25.607	3746	3757	3767	rVB2	80600	243499	17.10%	4.065%

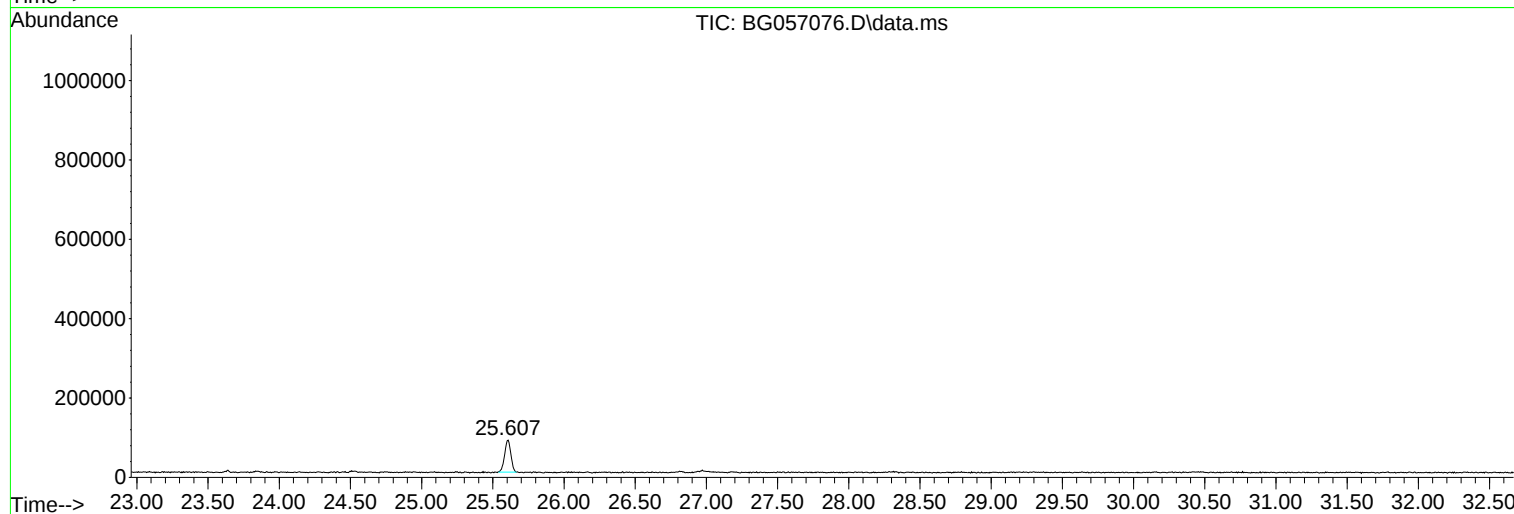
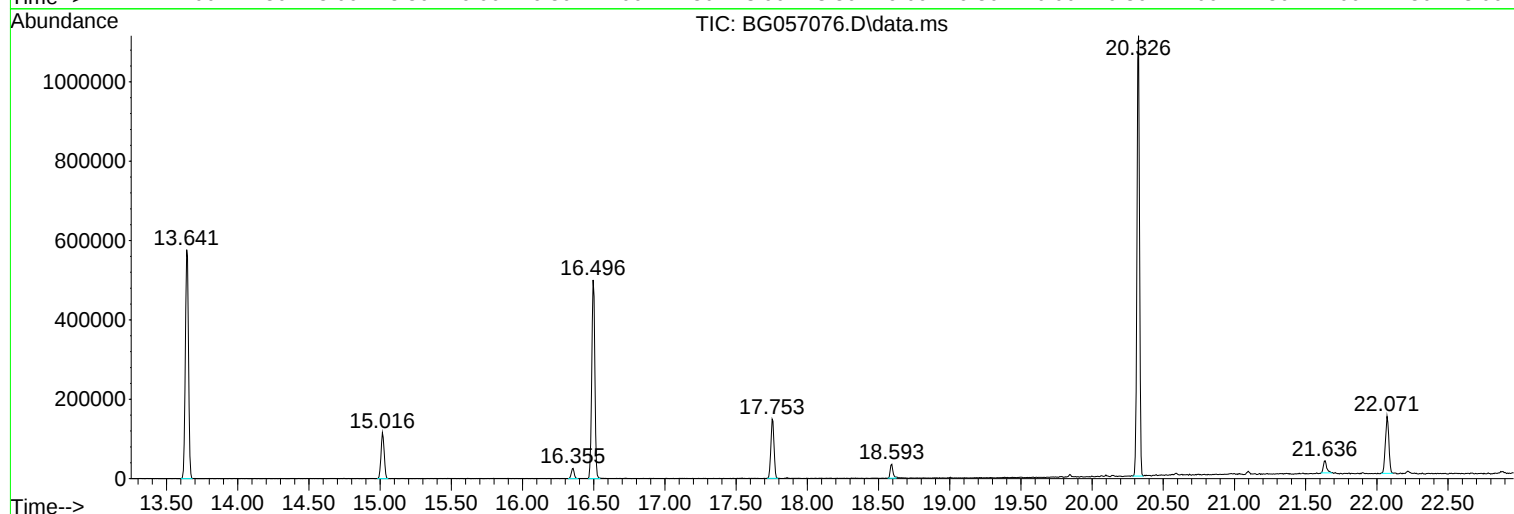
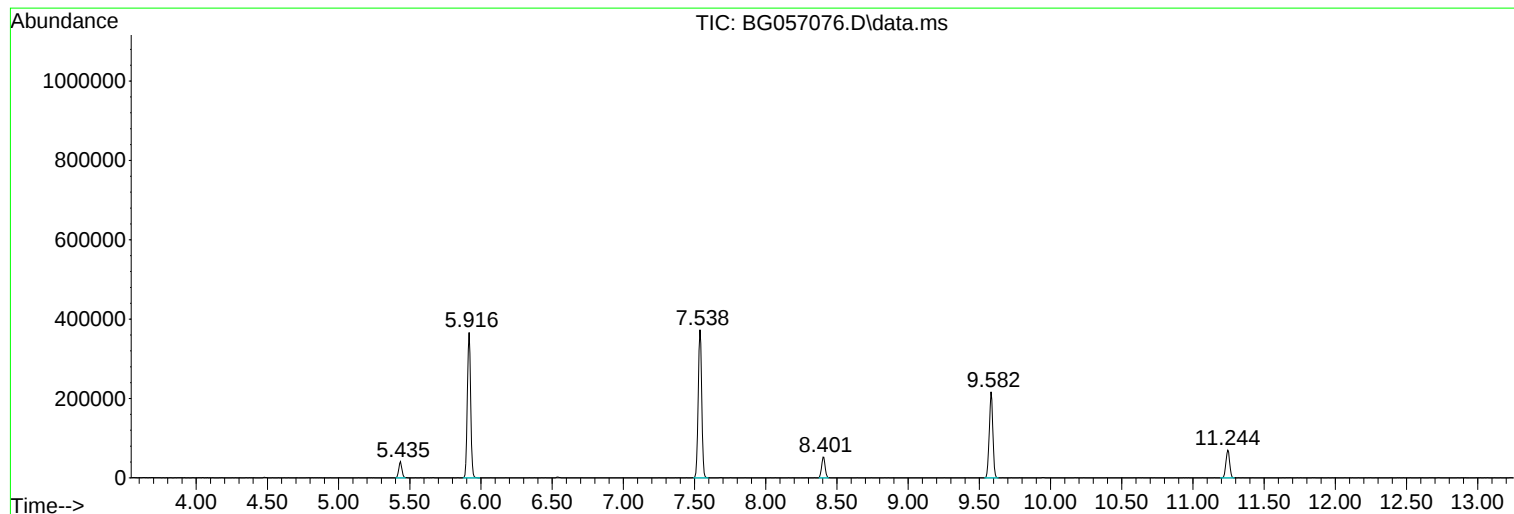
Sum of corrected areas: 5990207

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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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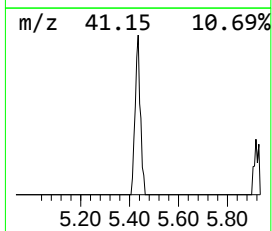
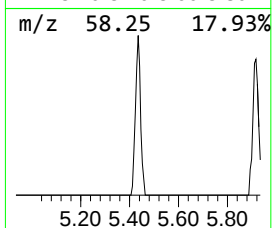
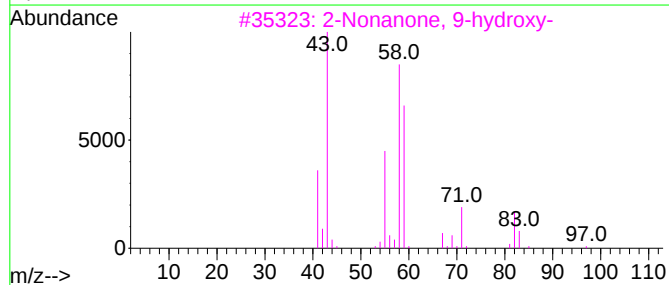
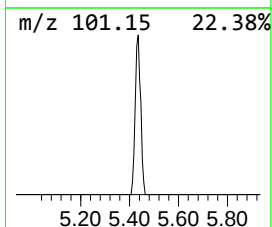
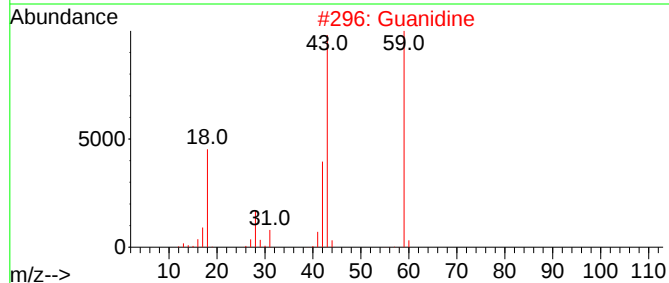
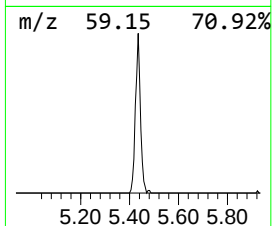
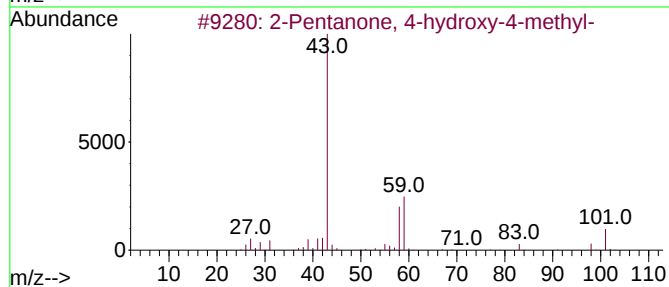
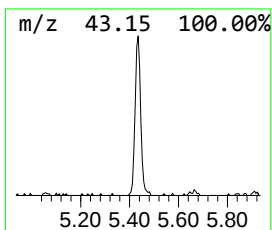
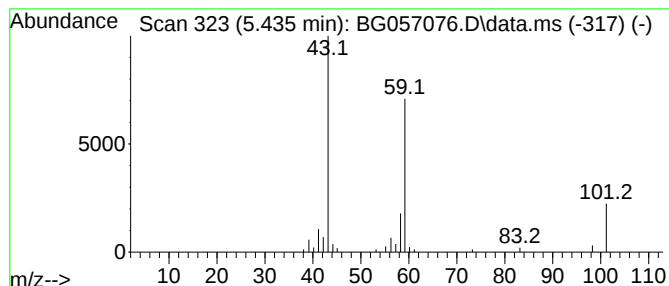
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.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.
5.435	14.00 ng	62102	1,4-Dichlorobenzene-d4	8.401

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Guanidine	59	CH5N3	000113-00-8	43		
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23		



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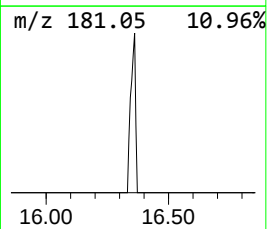
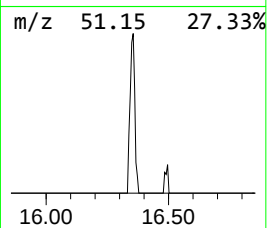
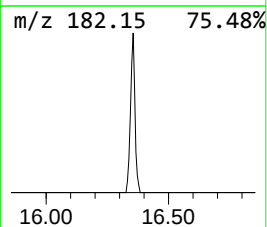
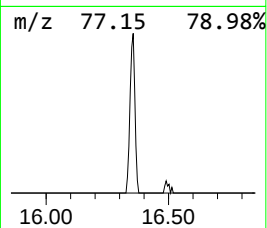
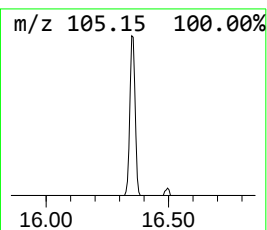
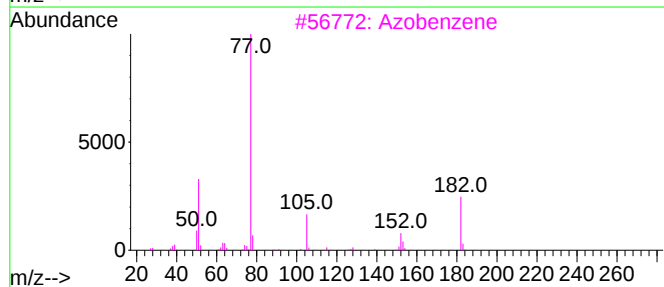
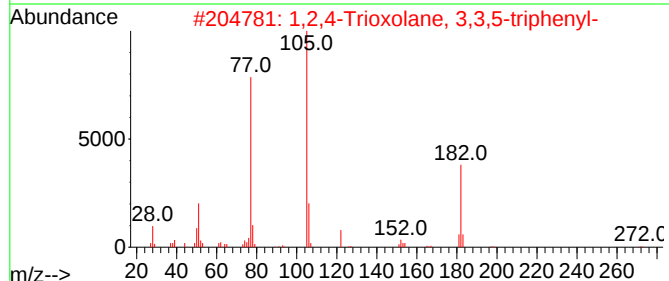
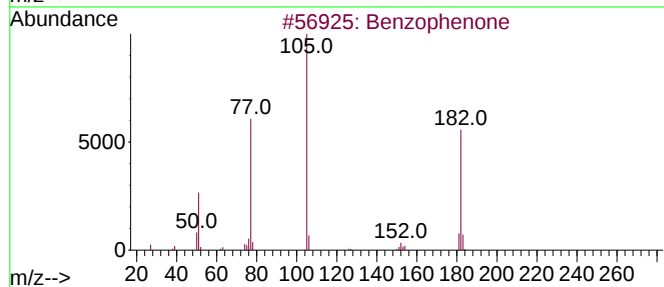
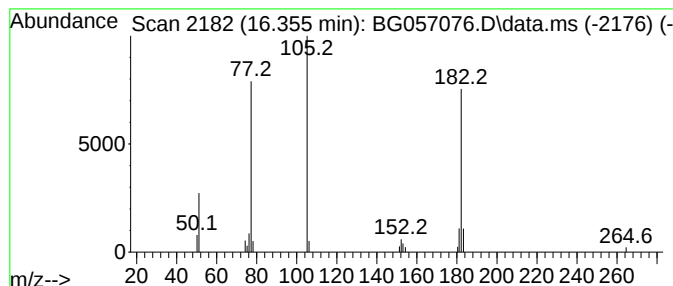
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.355	4.11 ng	36650	Acenaphthene-d10	15.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3			Azobenzene	182	C12H10N2	000103-33-3	43
4			4-Nitrophenyl benzoate	243	C13H9NO4	000959-22-8	38
5			1,3,5-Triazine-2,4,6-triamine, N...	182	C7H14N6	005606-16-6	38



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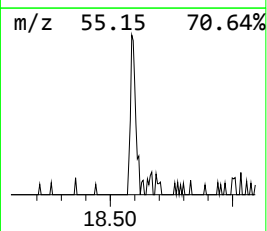
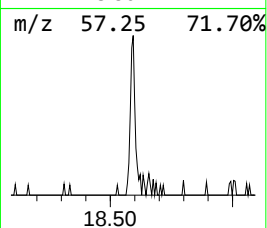
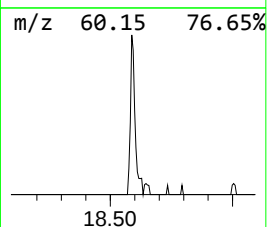
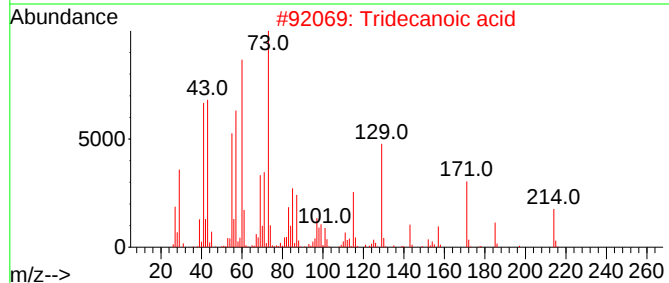
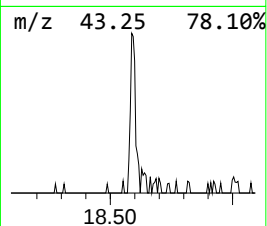
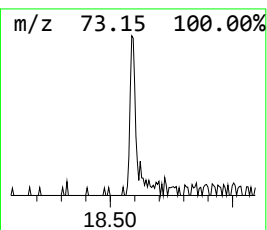
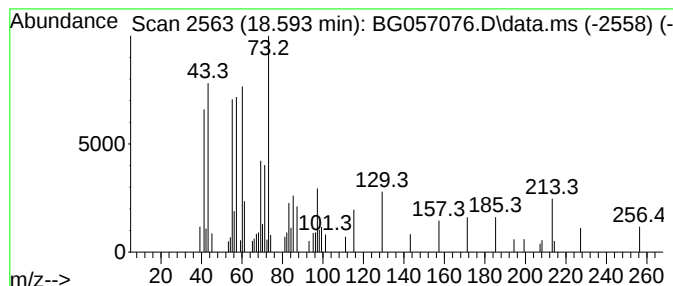
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.593	4.13 ng	47604	Phenanthrene-d10	17.753

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Octadecyl propyl ether	312	C21H44O	1000406-28-0	35
5			1,6-Dioxacycloheptadecan-7-one	256	C15H28O3	006707-60-4	18



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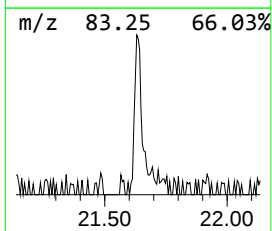
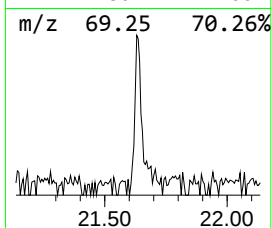
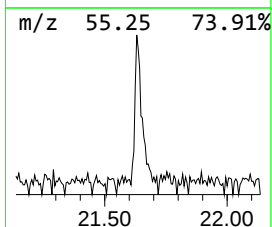
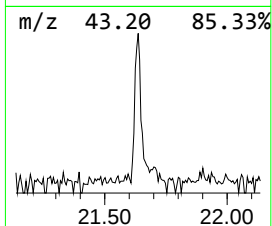
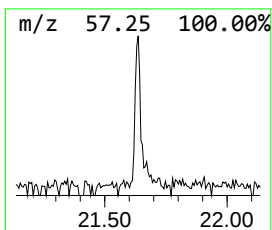
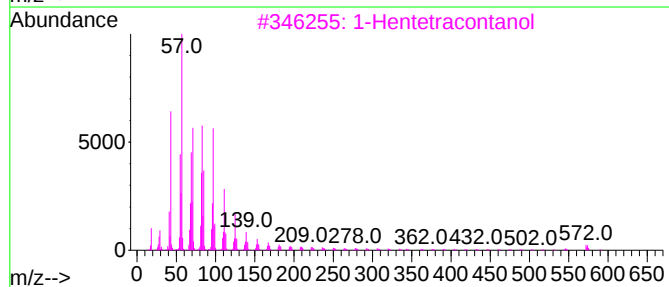
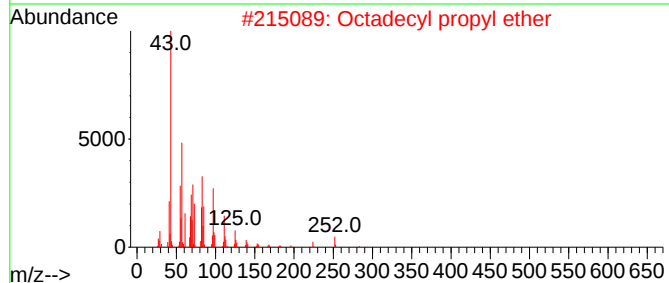
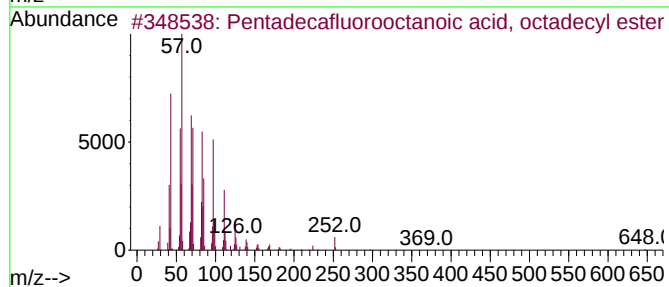
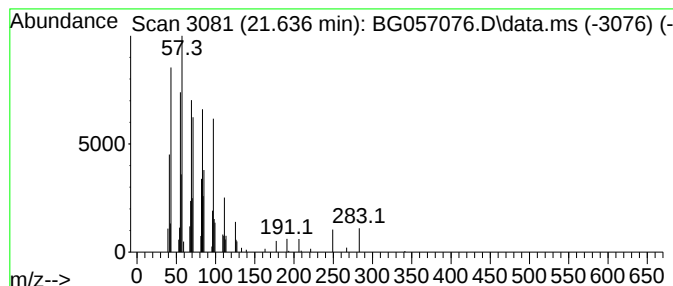
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.636	4.22 ng	51506	Chrysene-d12	22.071

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
2			Octadecyl propyl ether	312	C21H44O	1000406-28-0	83
3			1-Hentetracontanol	593	C41H84O	040710-42-7	83
4			17-Pentatriacontene	491	C35H70	006971-40-0	83
5			Hexadecyl propyl ether	284	C19H40O	1000406-27-9	74



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.435	14.0	ng	62102	1	8.401	88724	20.0
Benzophenone	16.355	4.1	ng	36650	3	15.016	178335	20.0
n-Hexadecanoic ...	18.593	4.1	ng	47604	4	17.753	230599	20.0
Pentadecafluoro...	21.636	4.2	ng	51506	5	22.071	244068	20.0