

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
 Data File : BG057830.D
 Acq On : 23 Jun 2023 5:59
 Operator : CG/JU
 Sample : 03327-07
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMPOSIT-TW-02

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057830.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.027	325	330	337	rBV	24644	37016	2.23%	0.353%
2	5.497	400	410	421	rBV	489333	782294	47.10%	7.452%
3	7.084	672	680	688	rBV	493521	833575	50.19%	7.940%
4	7.924	816	823	830	rVB	170100	280466	16.89%	2.672%
5	9.081	1012	1020	1030	rBV	302295	519652	31.29%	4.950%
6	10.727	1292	1300	1308	rBV	242792	424837	25.58%	4.047%
7	13.183	1711	1718	1728	rBV	764957	1177158	70.87%	11.213%
8	14.557	1945	1952	1959	rBV	364197	555874	33.47%	5.295%
9	15.909	2177	2182	2189	rVB	98349	138951	8.37%	1.324%
10	16.044	2198	2205	2215	rBV	565670	873504	52.59%	8.320%
11	17.301	2412	2419	2423	rBV	457748	678572	40.85%	6.464%
12	17.342	2423	2426	2431	rVB	49206	63797	3.84%	0.608%
13	18.188	2564	2570	2574	rBV2	91643	139535	8.40%	1.329%
14	18.371	2595	2601	2605	rBV3	12572	24853	1.50%	0.237%
15	19.352	2763	2768	2773	rBV	138211	187152	11.27%	1.783%
16	19.463	2782	2787	2793	rBV5	27055	43868	2.64%	0.418%
17	19.716	2820	2830	2837	rBV	121312	209924	12.64%	2.000%
18	19.916	2858	2864	2871	rBV	1285513	1660930	100.00%	15.821%
19	21.208	3080	3084	3093	rVV3	73118	135158	8.14%	1.287%
20	21.285	3093	3097	3102	rVB	54766	73248	4.41%	0.698%
21	21.549	3135	3142	3147	rBV3	442733	787982	47.44%	7.506%
22	21.743	3173	3175	3181	rVB3	26900	35887	2.16%	0.342%
23	23.706	3504	3509	3515	rBV	29768	73569	4.43%	0.701%
24	24.704	3670	3679	3697	rBV	243137	760594	45.79%	7.245%

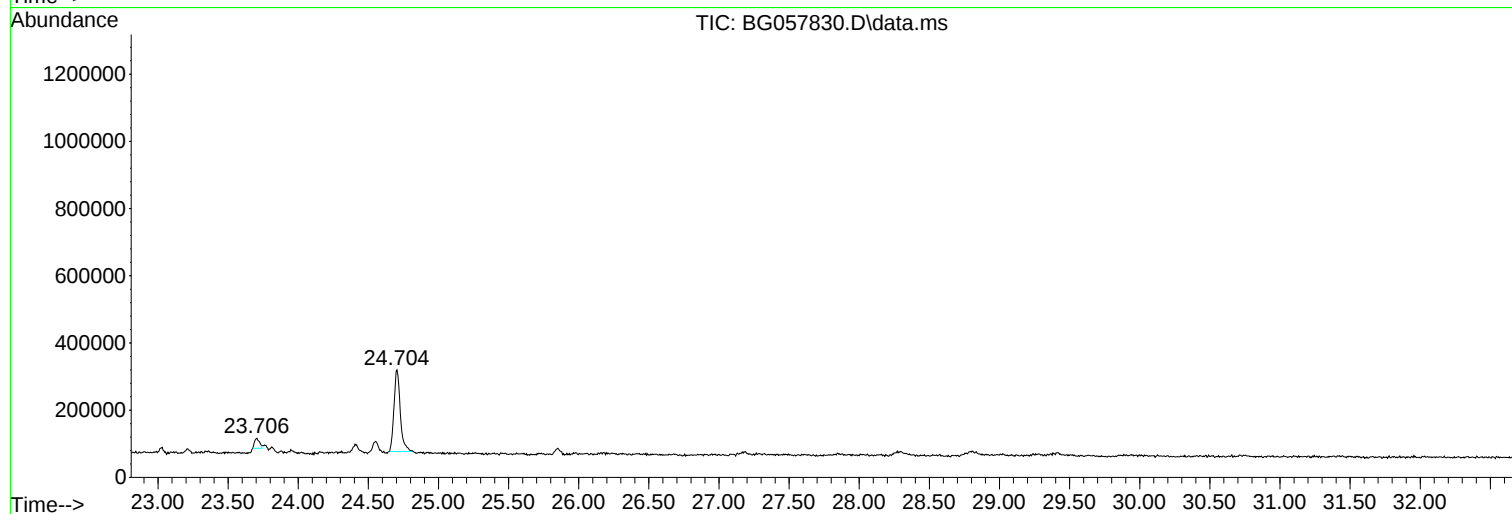
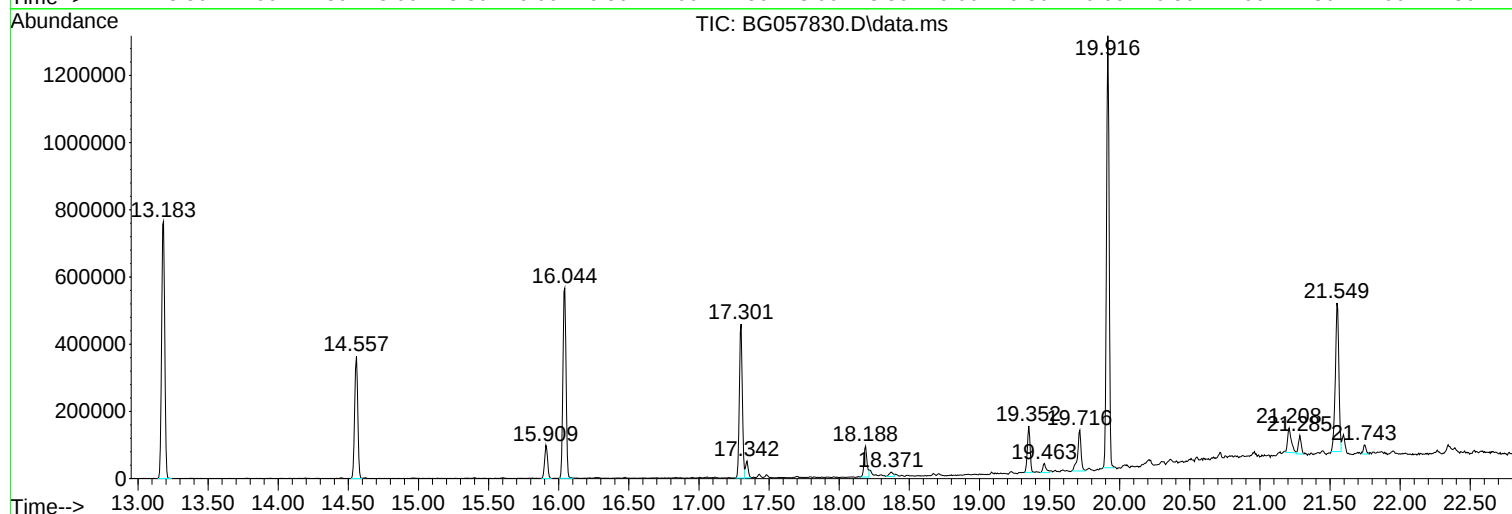
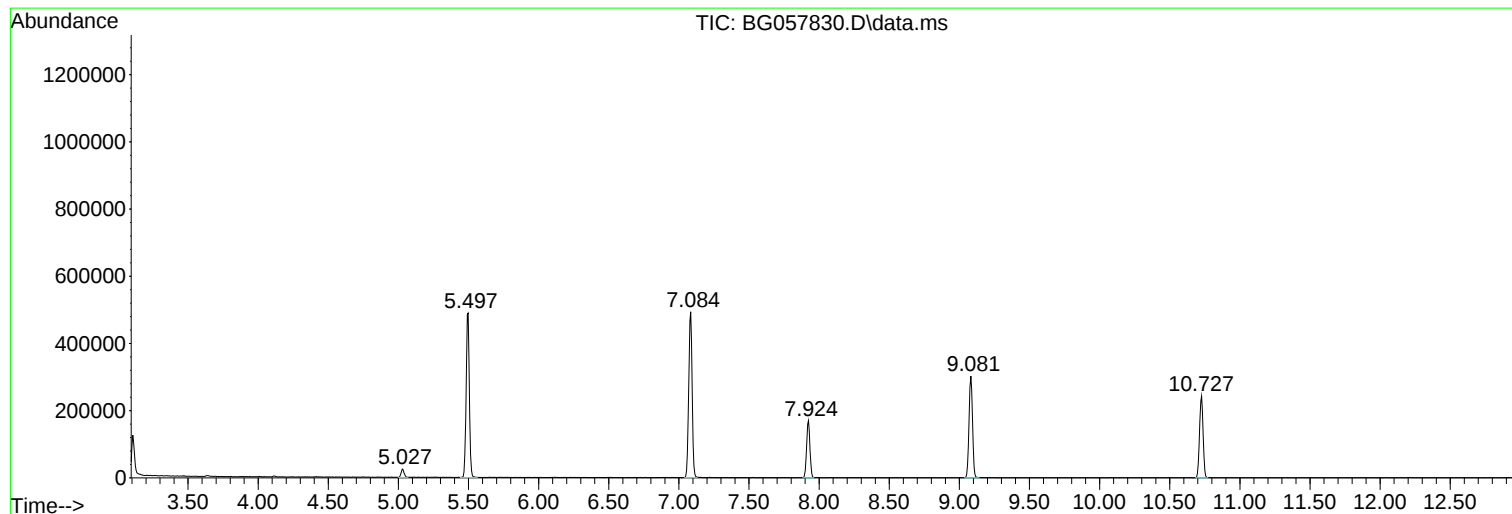
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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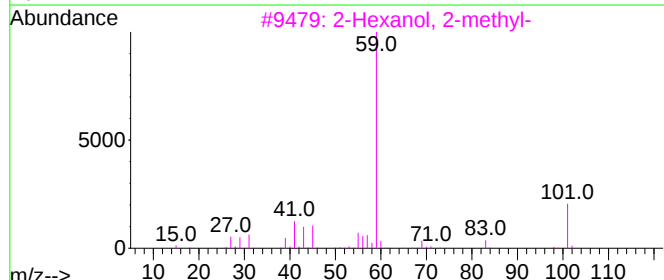
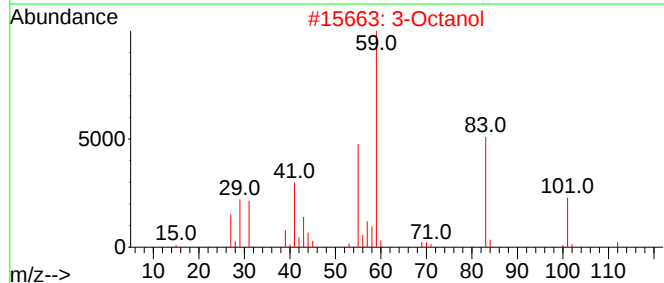
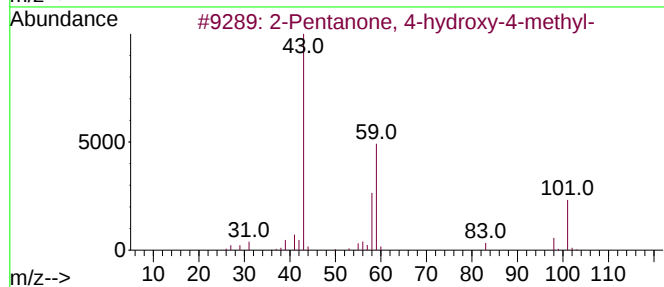
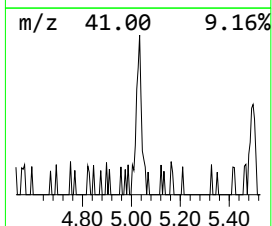
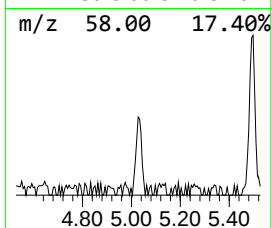
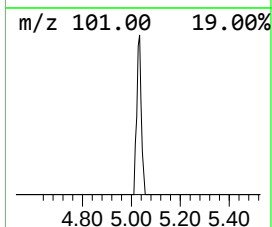
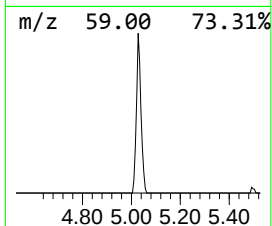
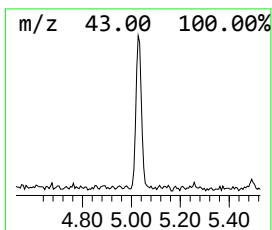
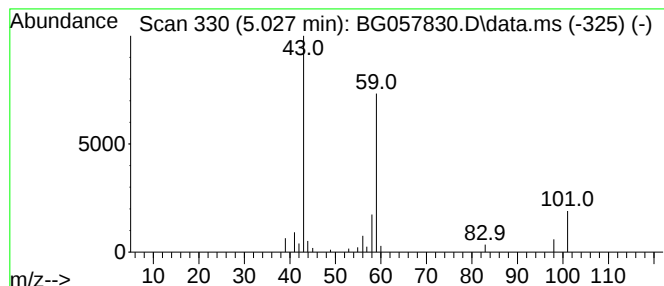
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.027	2.64 ng	37016	1,4-Dichlorobenzene-d4			7.924

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	3-Octanol	130	C8H18O	000589-98-0	38	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36	
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	33	
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	33	



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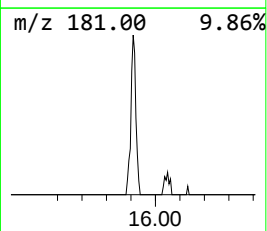
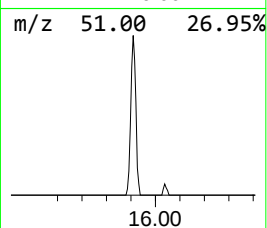
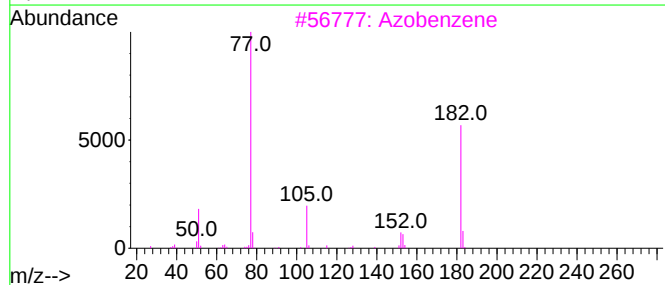
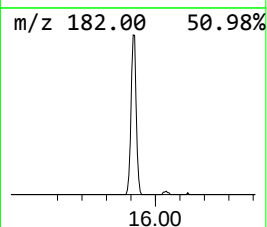
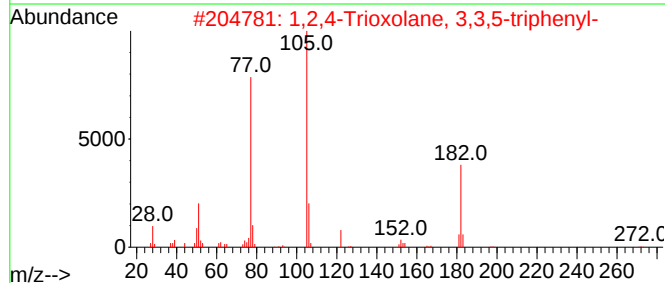
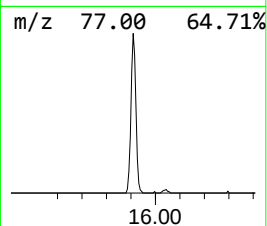
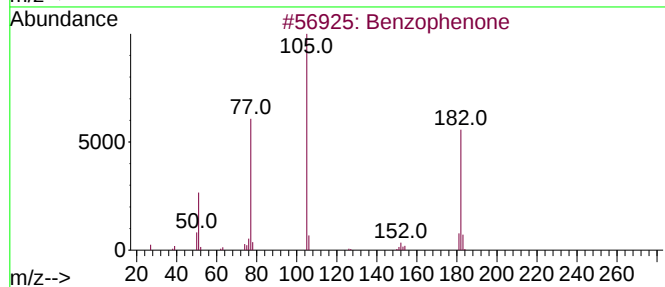
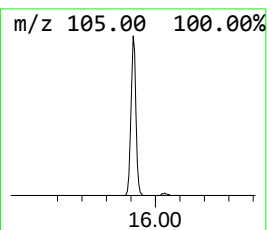
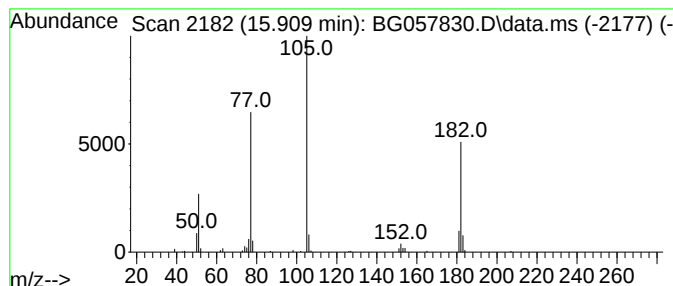
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.909	5.00 ng	138951	Acenaphthene-d10	14.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	80
3			Azobenzene	182	C12H10N2	000103-33-3	59
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



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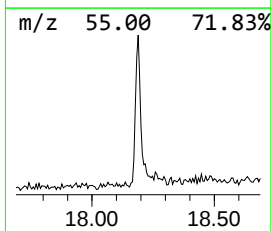
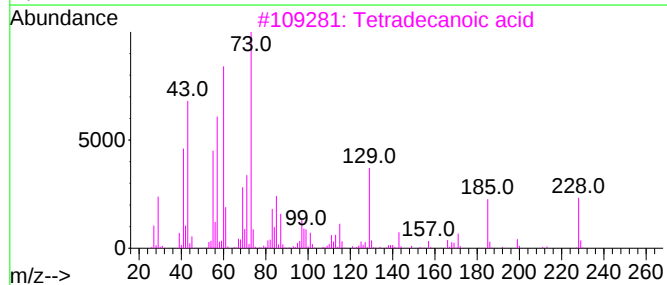
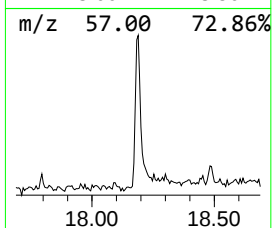
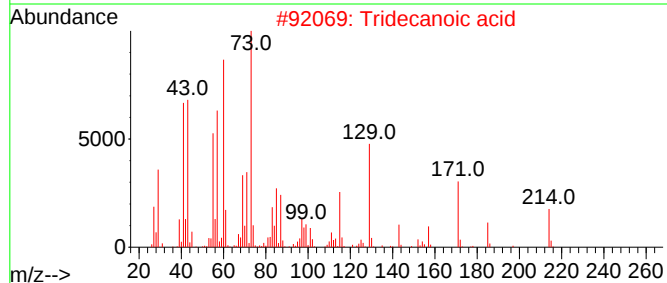
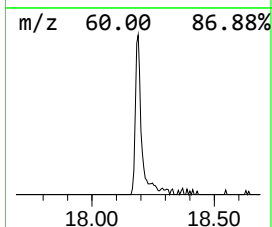
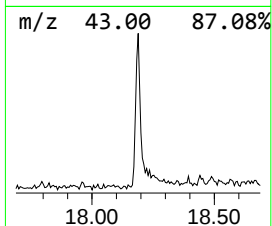
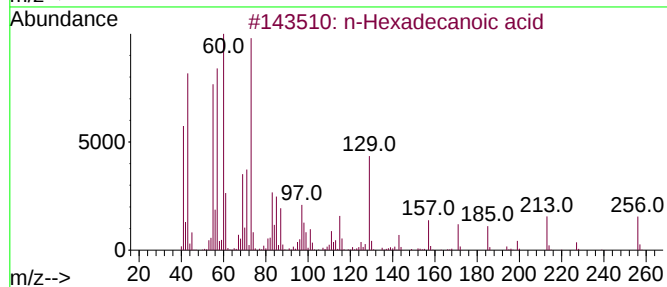
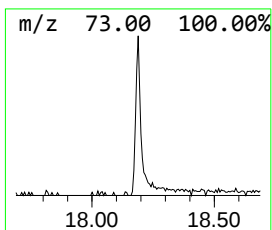
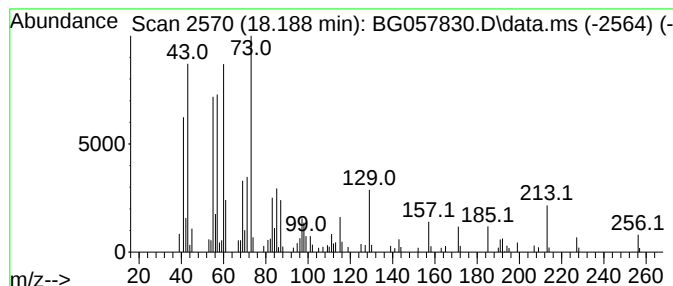
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.189	4.11 ng	139535	Phenanthrene-d10	17.301	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Nonanoic acid	158	C9H18O2	000112-05-0	60



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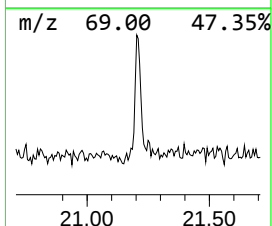
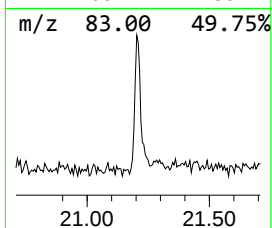
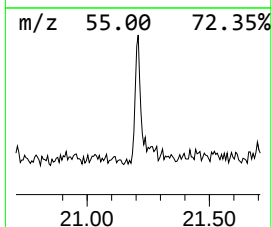
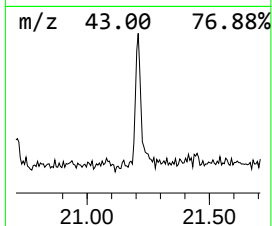
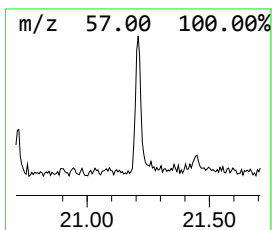
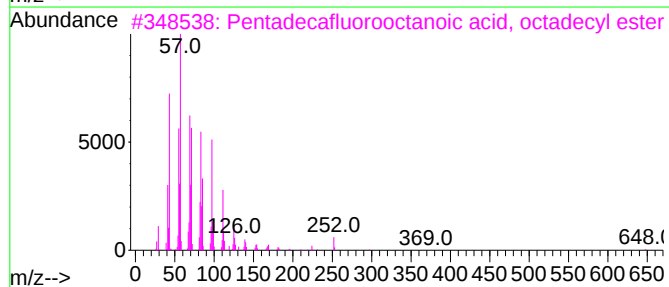
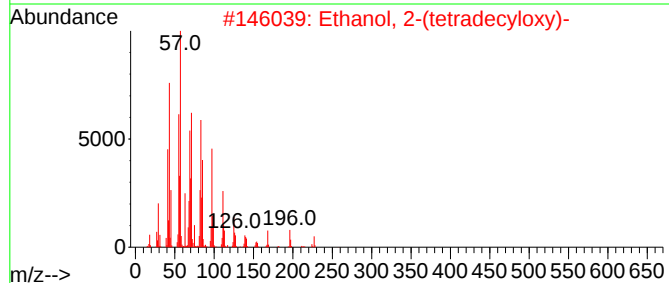
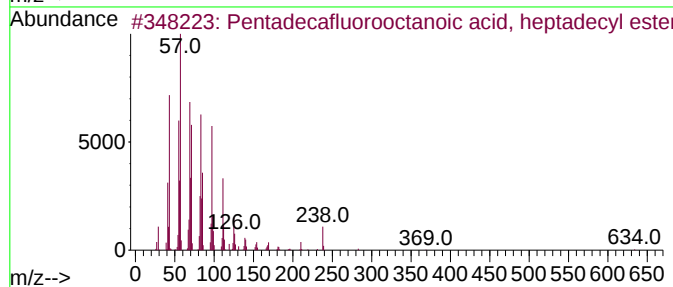
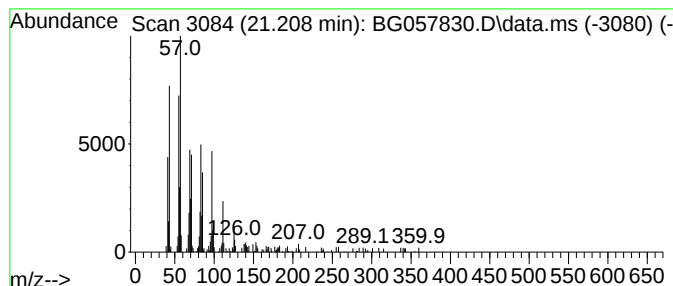
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.208	3.43 ng	135158	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, he...	652	C25H35F15O2	1000406-04-7	91
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	91
5			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.027	2.6	ng	37016	1	7.924	280466	20.0
Benzophenone	15.909	5.0	ng	138951	3	14.557	555874	20.0
n-Hexadecanoic ...	18.189	4.1	ng	139535	4	17.301	678572	20.0
Pentadecafluoro...	21.208	3.4	ng	135158	5	21.549	787982	20.0