

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052322\
 Data File : BG053670.D
 Acq On : 23 May 2022 18:49
 Operator : CG/JU
 Sample : N2968-08
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-44

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-BG050522.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053670.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.627	375	381	398	rBV	260269	450731	18.04%	4.232%
2	7.231	647	654	669	rBV	178314	335107	13.42%	3.147%
3	8.059	787	795	803	rBV	113075	196127	7.85%	1.842%
4	8.834	921	927	934	rBV	39306	73725	2.95%	0.692%
5	9.222	985	993	1003	rBV	432059	779857	31.22%	7.323%
6	10.867	1265	1273	1279	rBV	157126	287963	11.53%	2.704%
7	10.920	1279	1282	1290	rVB3	16322	29318	1.17%	0.275%
8	11.478	1371	1377	1381	rBV	13122	29357	1.18%	0.276%
9	13.311	1681	1689	1698	rVB	1201407	1864513	74.64%	17.508%
10	14.515	1883	1894	1910	rBV3	72570	208628	8.35%	1.959%
11	14.685	1917	1923	1930	rVB	262657	418026	16.74%	3.925%
12	16.177	2170	2177	2188	rBV	952706	1544173	61.82%	14.500%
13	17.434	2385	2391	2397	rBV	350568	527215	21.11%	4.951%
14	18.316	2537	2541	2552	rBV3	70323	133977	5.36%	1.258%
15	19.584	2753	2757	2761	rBV3	40652	60905	2.44%	0.572%
16	20.037	2828	2834	2840	rBV	1926061	2497912	100.00%	23.456%
17	21.335	3051	3055	3065	rVB2	78006	130644	5.23%	1.227%
18	21.711	3113	3119	3125	rVB2	324048	534810	21.41%	5.022%
19	24.971	3666	3674	3685	rVB2	187264	546510	21.88%	5.132%

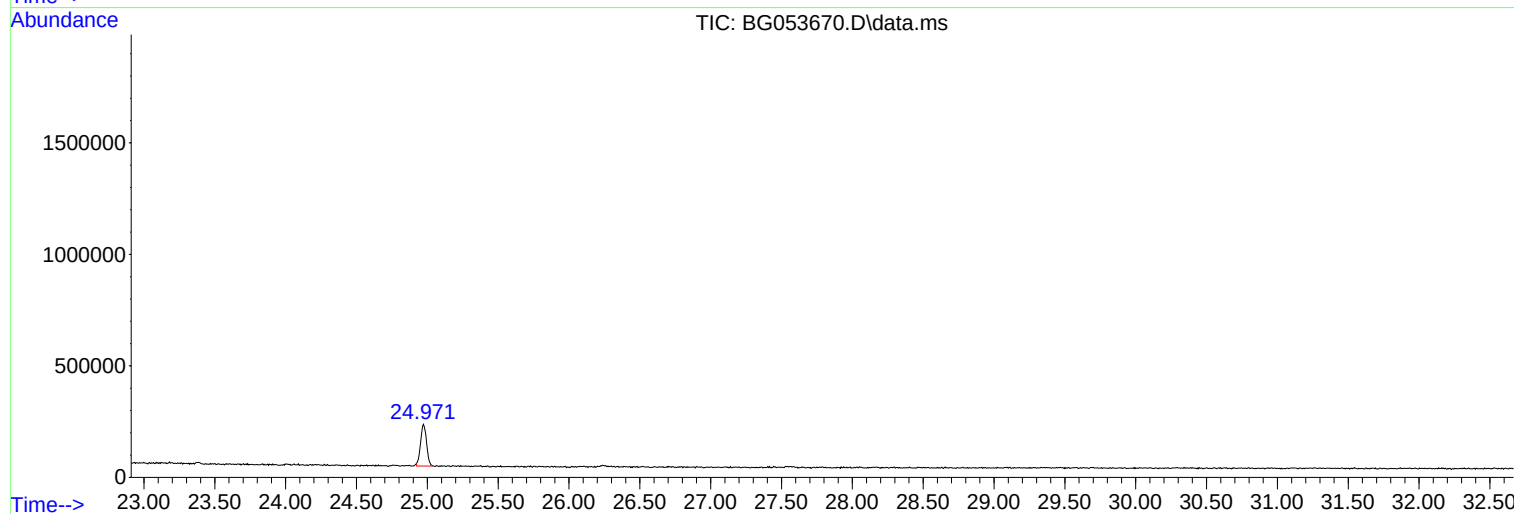
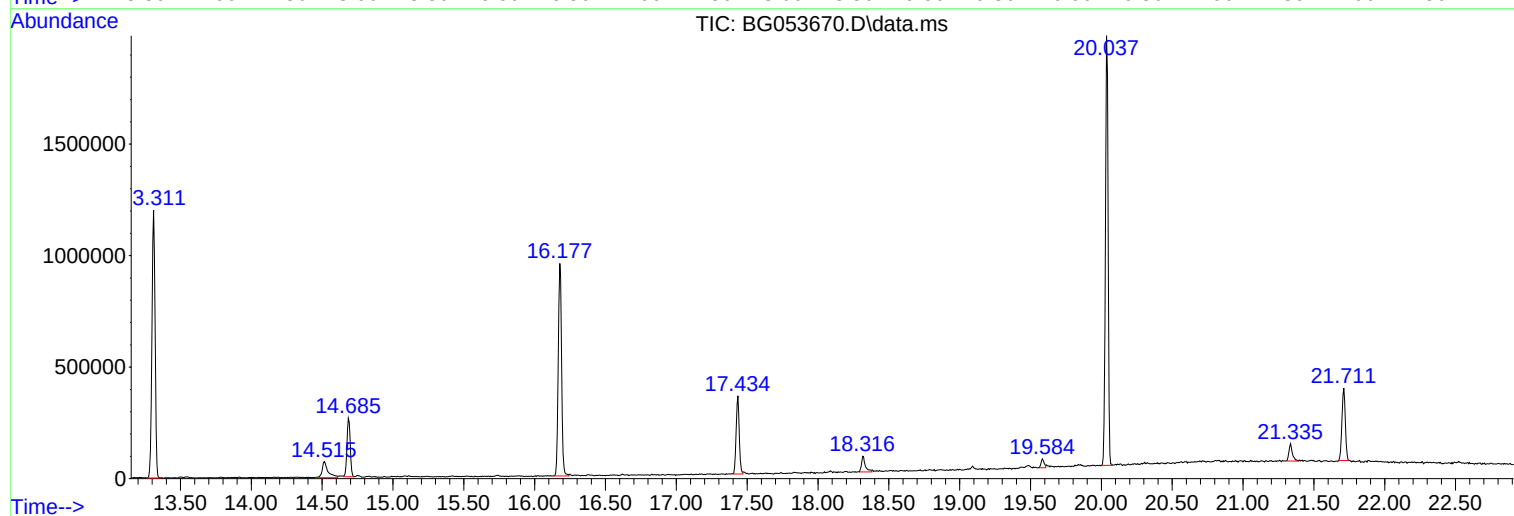
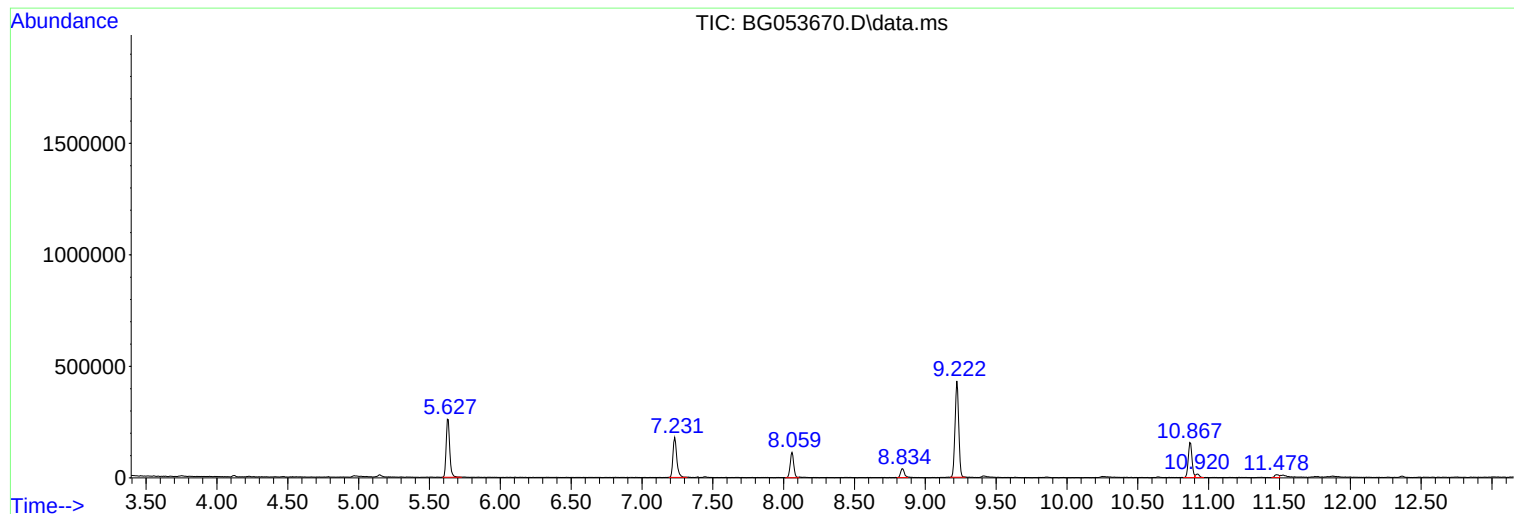
Sum of corrected areas: 10649498

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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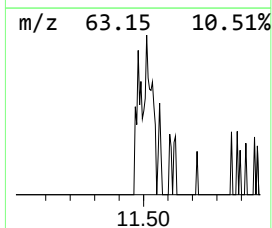
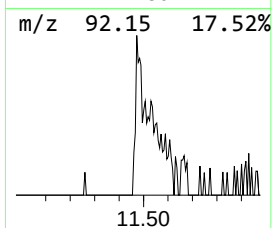
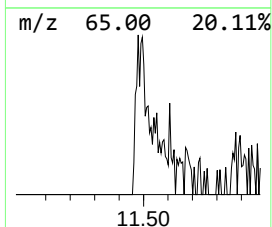
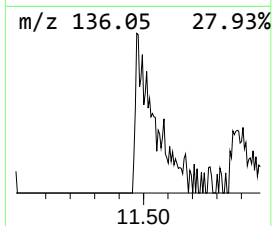
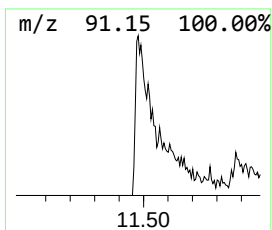
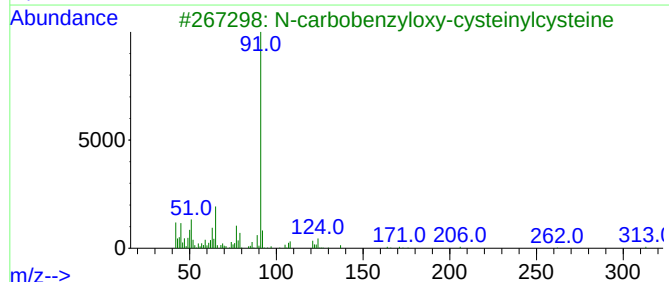
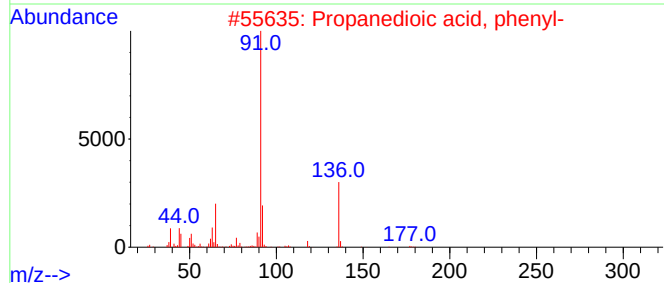
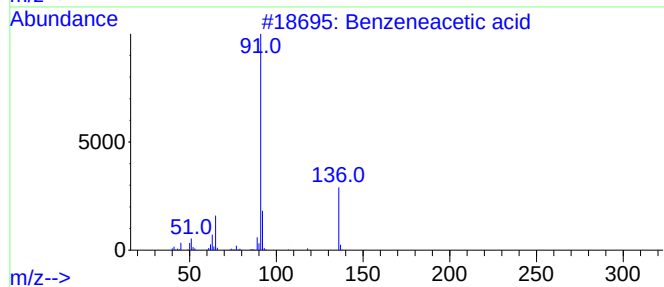
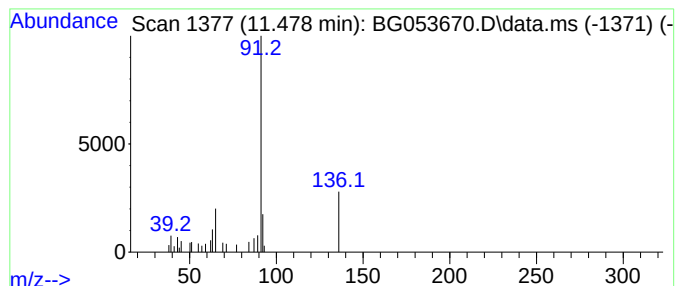
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzeneacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.478	2.04 ng	29357	Naphthalene-d8	10.867

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	72
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	72
3			N-carbobenzyloxy-cysteinylcysteine	358	C14H18N2O5S2	189388-08-7	53
4			5-Benzyloxy-2-nitrotoluene	243	C14H13NO3	022424-58-4	50
5			(1,3,3,3-Tetrafluoro-2-trifluoro...	304	C11H7F7S	075667-95-7	50



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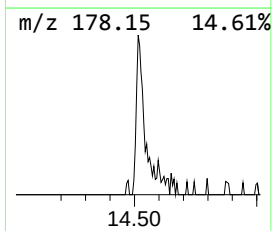
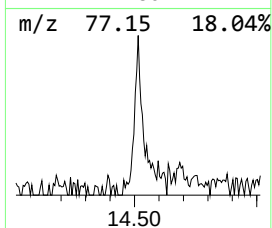
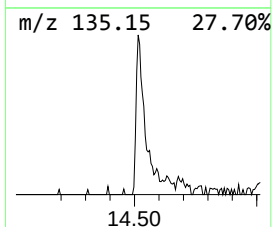
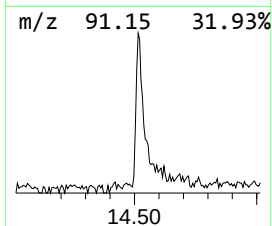
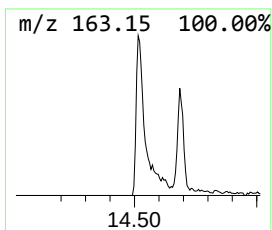
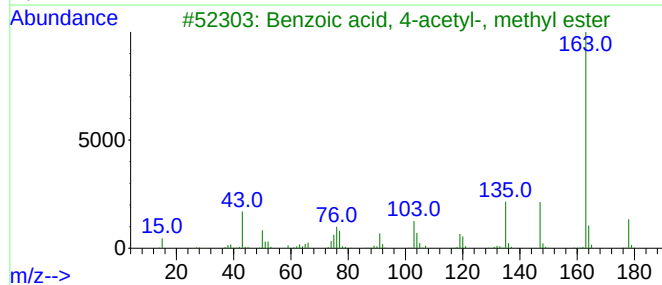
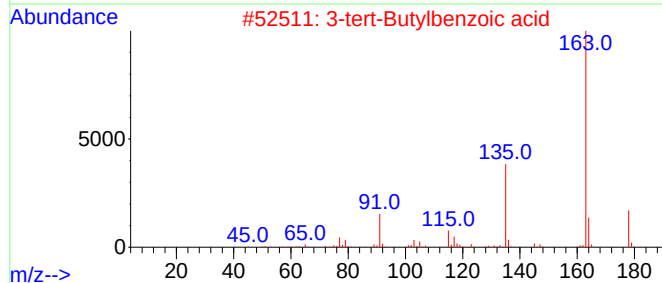
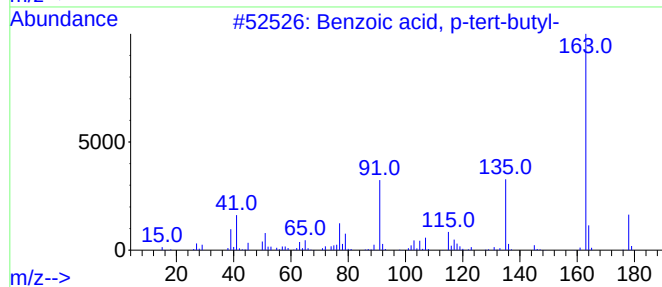
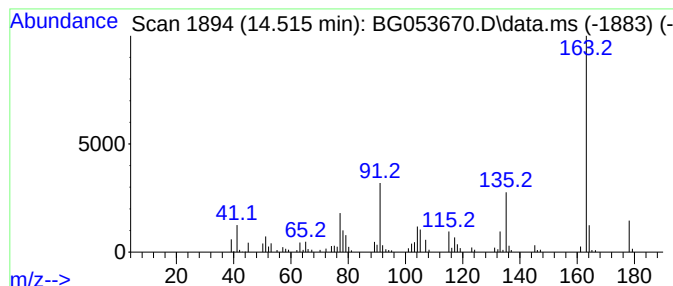
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzoic acid, p-tert-butyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	9.98 ng	208628	Acenaphthene-d10	14.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	94
2			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	81
3			Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
4			Benzoic acid, 4-(chlorocarbonyl)...	198	C9H7ClO3	007377-26-6	59
5			4-tert-Butyl-2,6-dimethylphenol	178	C12H18O	000879-97-0	59



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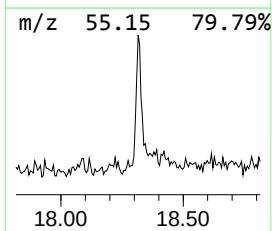
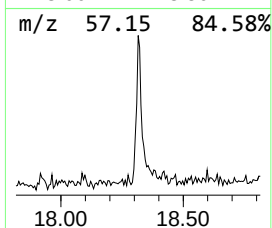
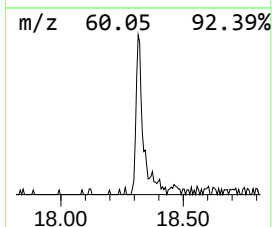
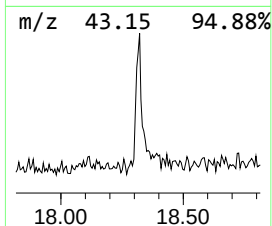
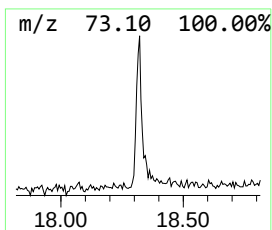
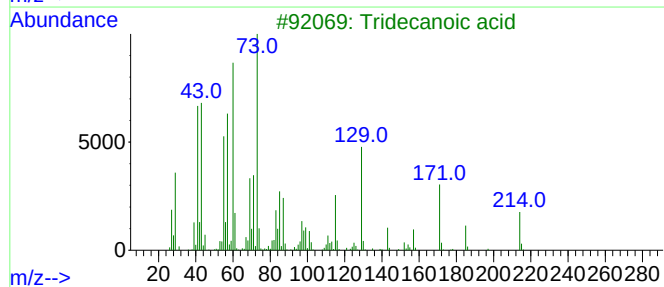
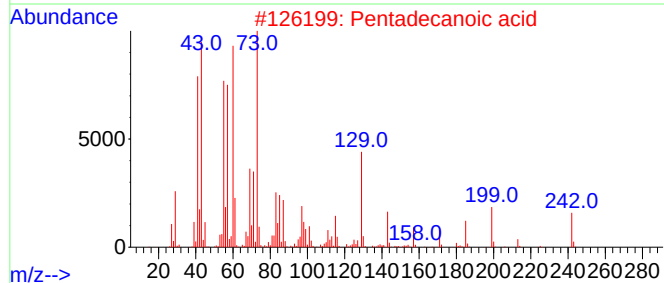
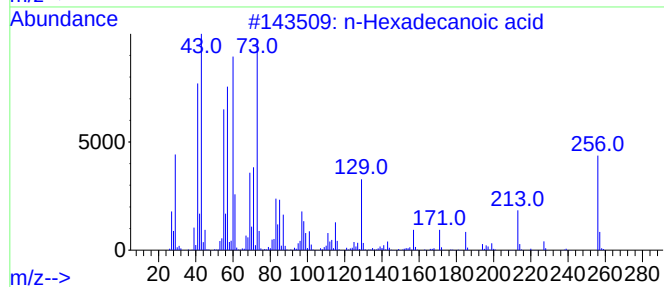
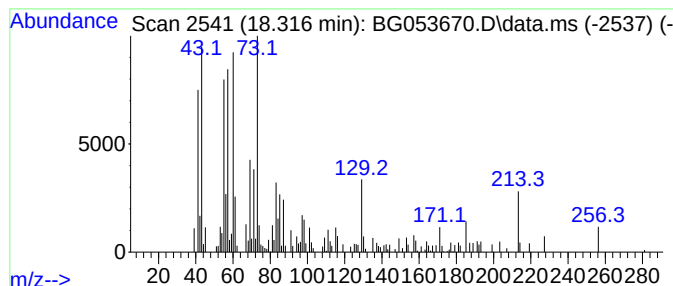
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.316	5.08 ng	133977	Phenanthrene-d10	17.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Undecanoic acid	186	C11H22O2	000112-37-8	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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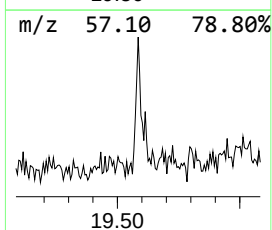
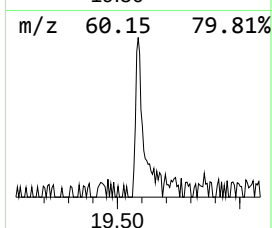
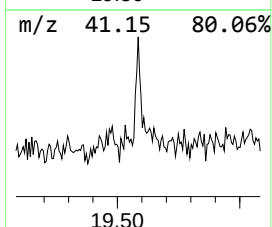
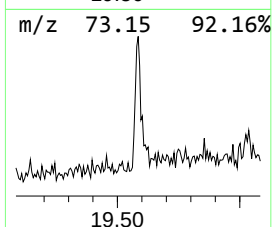
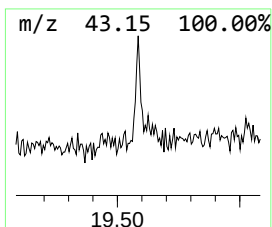
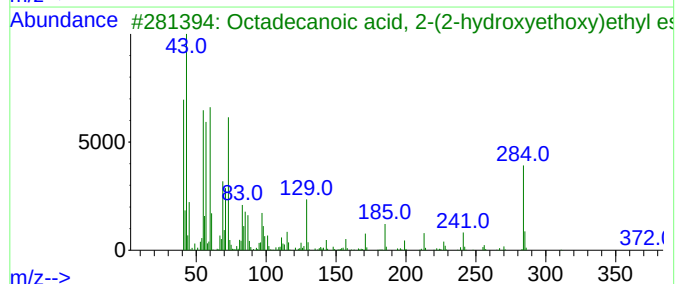
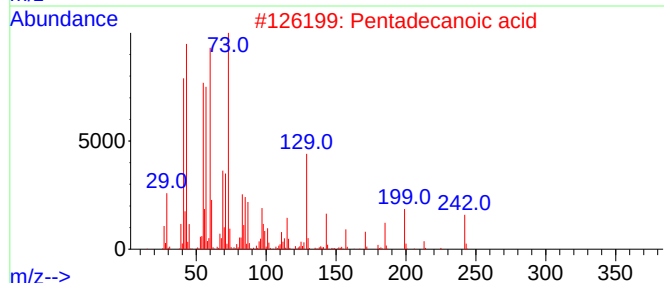
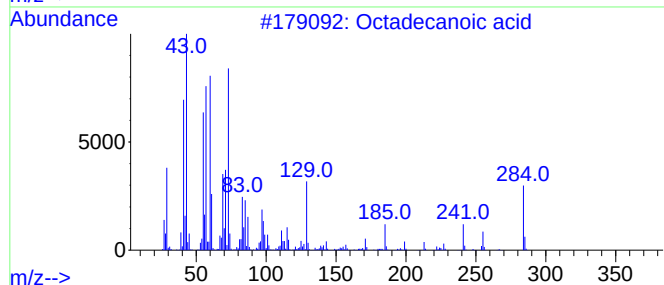
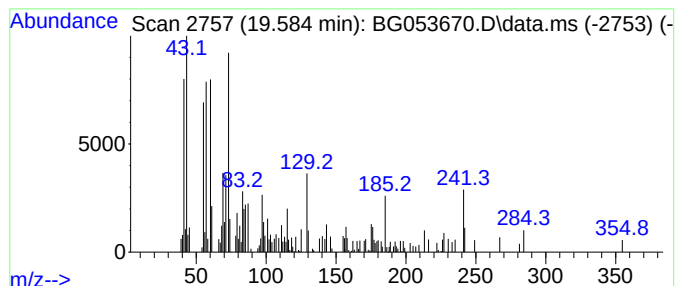
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.584	2.28 ng	60905	Chrysene-d12	21.711

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



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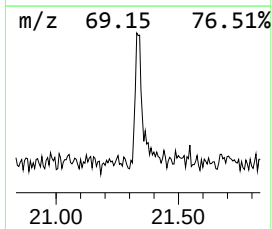
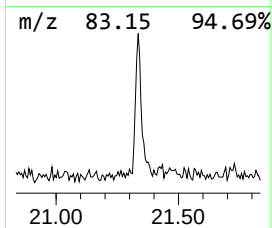
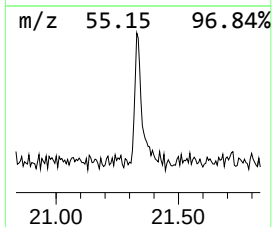
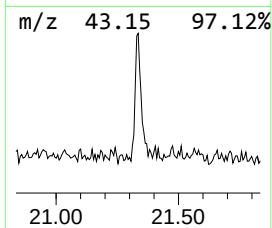
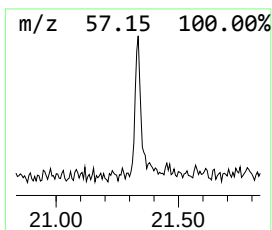
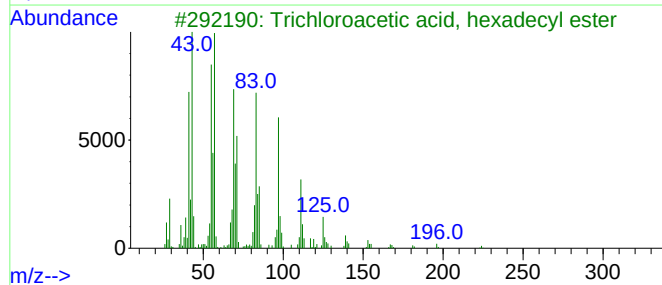
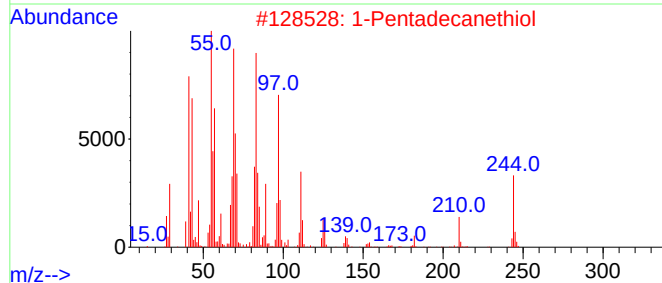
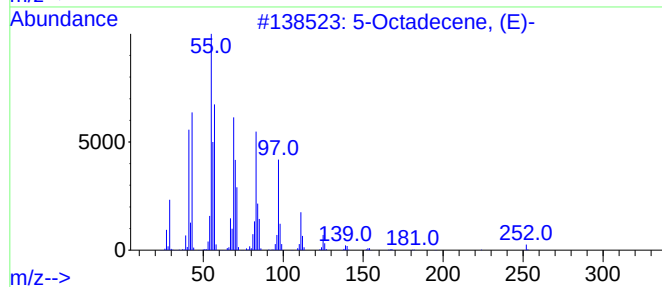
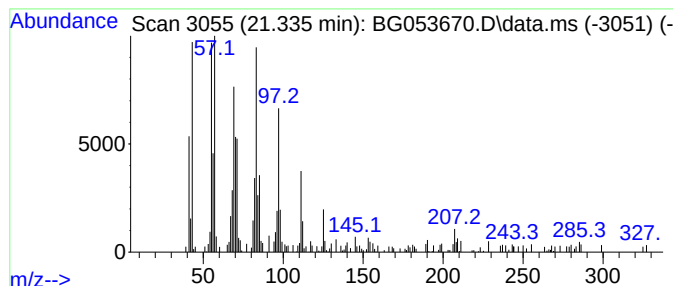
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.335	4.89 ng	130644	Chrysene-d12	21.711

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	94
2			1-Pentadecanethiol	244	C15H32S	025276-70-4	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	94



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzeneacetic acid	11.478	2.0	ng	29357	2	10.867	287963	20.0
Benzoic acid, p...	14.515	10.0	ng	208628	3	14.685	418026	20.0
n-Hexadecanoic ...	18.316	5.1	ng	133977	4	17.434	527215	20.0
Octadecanoic acid	19.584	2.3	ng	60905	5	21.711	534810	20.0
5-Octadecene, (E)-	21.335	4.9	ng	130644	5	21.711	534810	20.0