

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060922\
 Data File : BG053870.D
 Acq On : 9 Jun 2022 21:13
 Operator : CG/JU
 Sample : N3270-15
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-11E

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-BG060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053870.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.784	63	67	73	rBV	16576	26553	1.12%	0.282%
2	5.183	300	305	313	rBV2	14511	24298	1.02%	0.258%
3	5.653	378	385	400	rVB	426835	727990	30.71%	7.745%
4	7.245	647	656	667	rBV	437886	781388	32.96%	8.313%
5	8.091	793	800	807	rBV	77997	131613	5.55%	1.400%
6	9.248	989	997	1011	rVB	272161	496736	20.95%	5.284%
7	10.899	1269	1278	1287	rBV	105365	192882	8.14%	2.052%
8	13.338	1686	1693	1703	rBV	798027	1286315	54.26%	13.684%
9	14.713	1920	1927	1933	rBV	189565	311833	13.15%	3.317%
10	16.193	2172	2179	2191	rBV	721407	1183232	49.91%	12.588%
11	17.456	2387	2394	2401	rBV	281024	441460	18.62%	4.696%
12	18.120	2502	2507	2514	rVB2	39532	49938	2.11%	0.531%
13	19.284	2700	2705	2710	rVB	85465	98731	4.16%	1.050%
14	20.065	2831	2838	2844	rBV	1673333	2370833	100.00%	25.222%
15	21.369	3054	3060	3071	rBV	113730	183825	7.75%	1.956%
16	21.728	3114	3121	3132	rVB	309466	528744	22.30%	5.625%
17	24.995	3667	3677	3695	rVB2	175662	537438	22.67%	5.717%
18	26.340	3901	3906	3916	rVB2	8720	26121	1.10%	0.278%

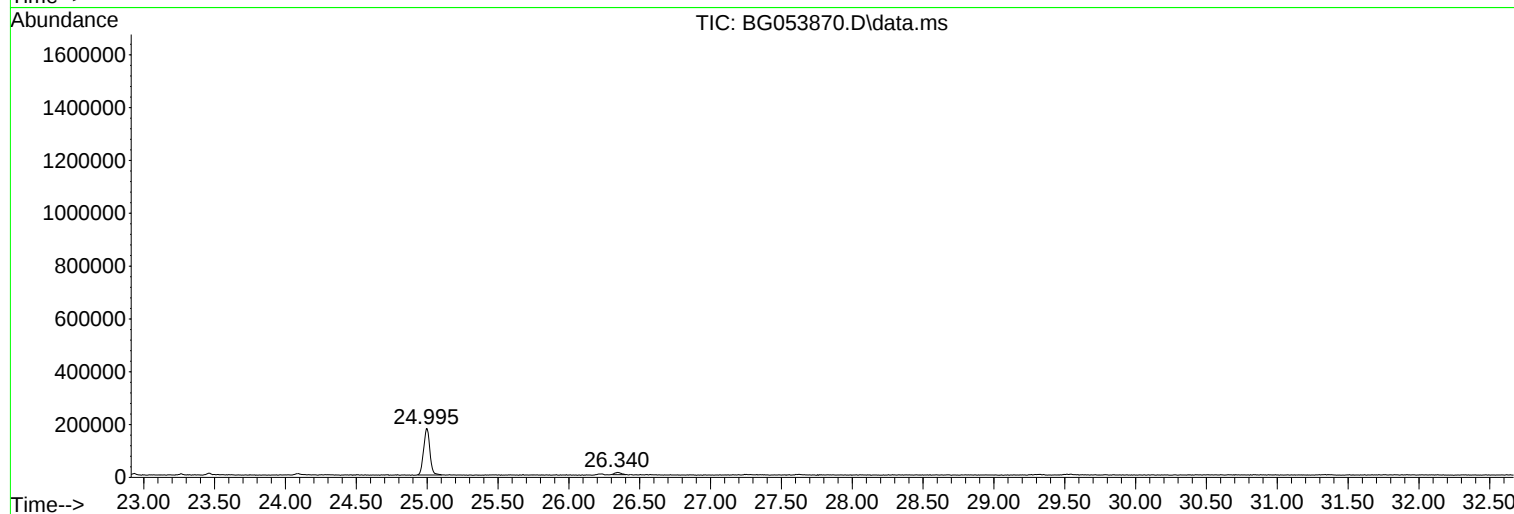
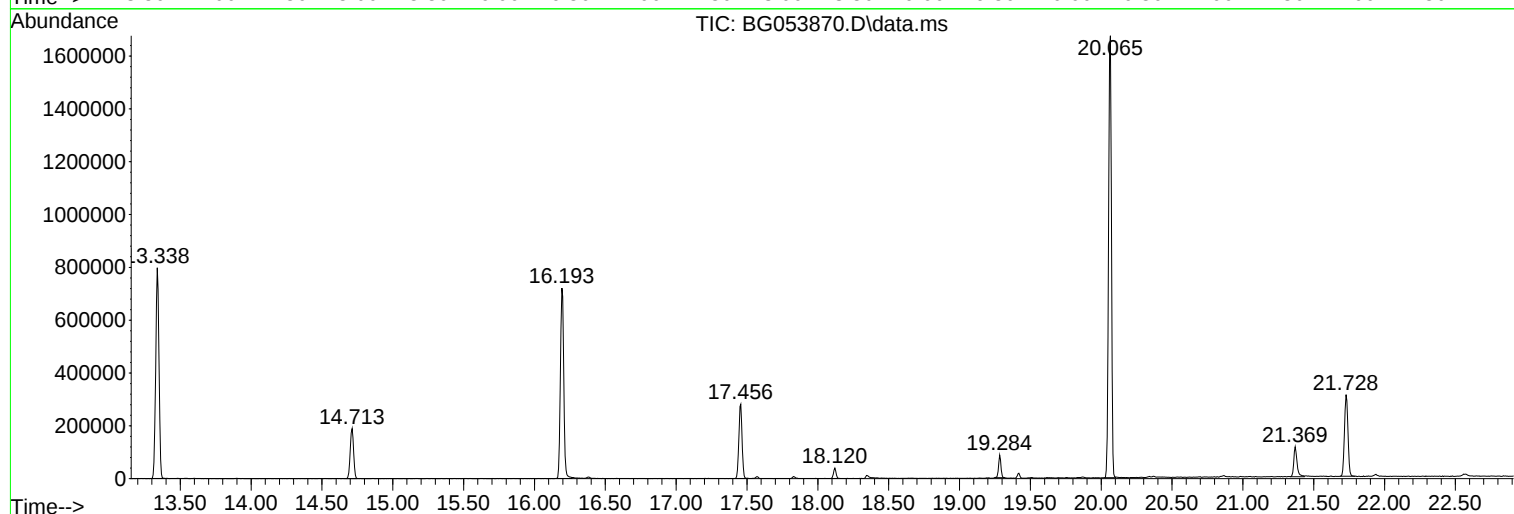
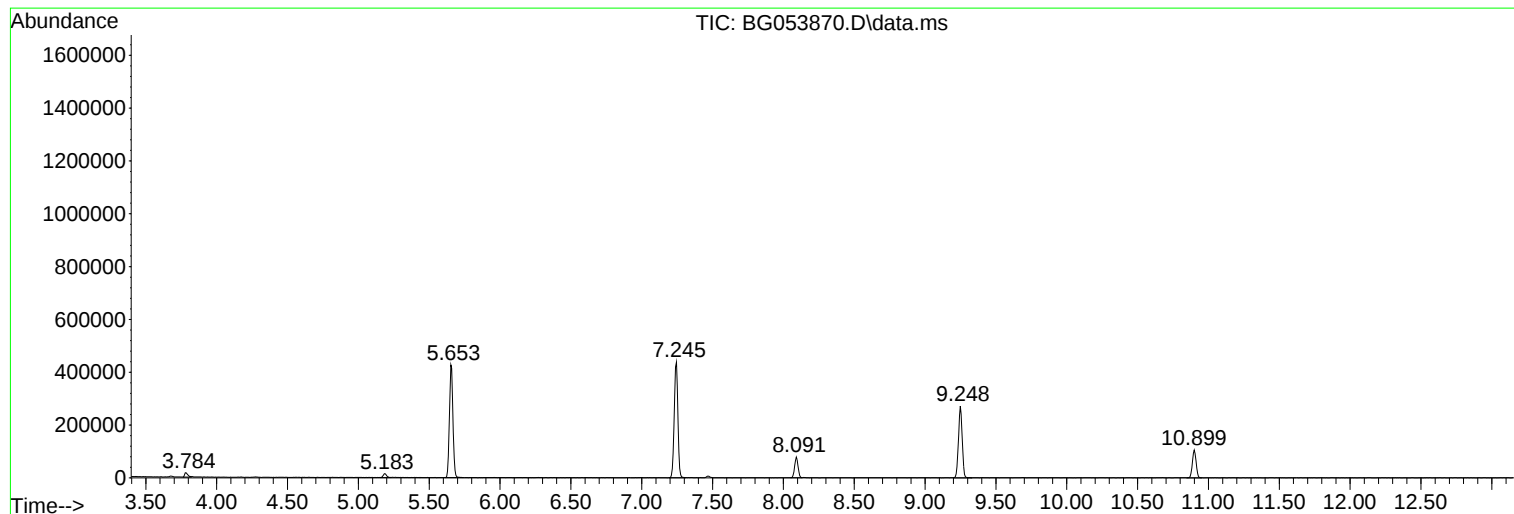
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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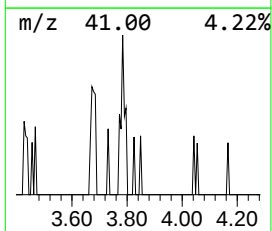
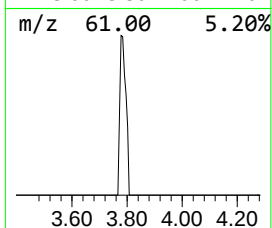
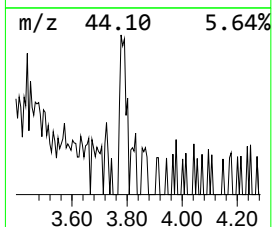
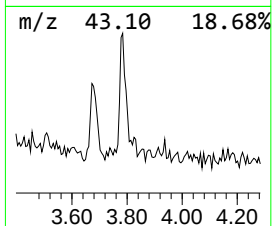
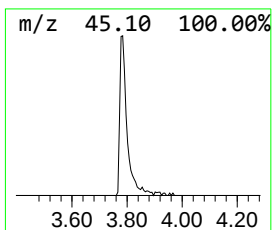
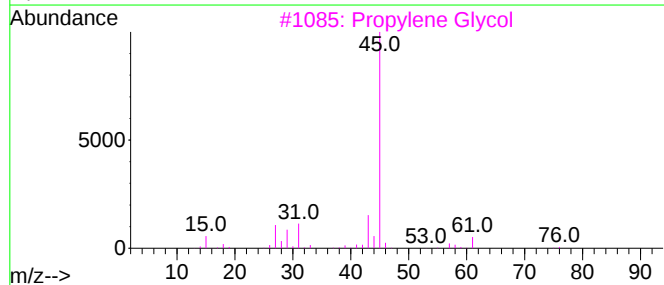
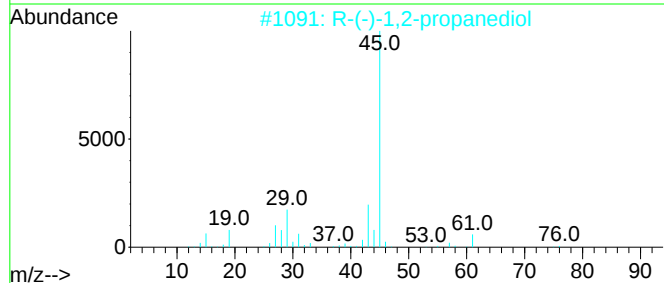
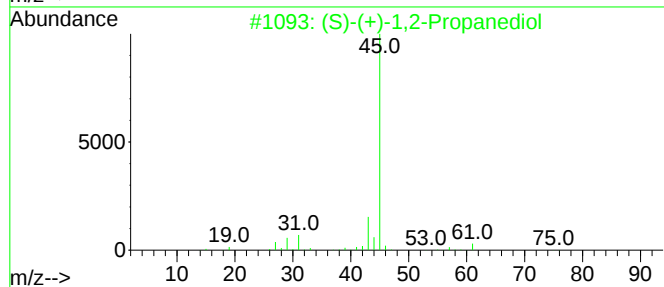
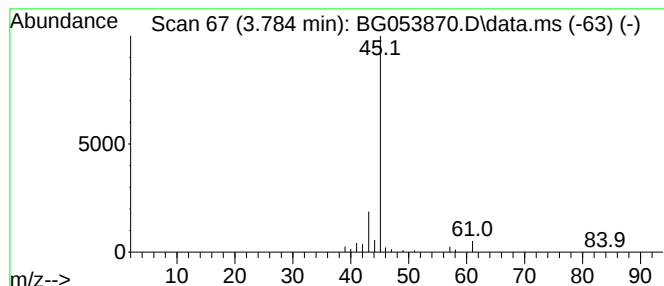
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.784 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.784	4.04 ng	26553	1,4-Dichlorobenzene-d4	8.091

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	43
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	40
3	Propylene Glycol			76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
5	Formamide			45	CH3NO	000075-12-7	5



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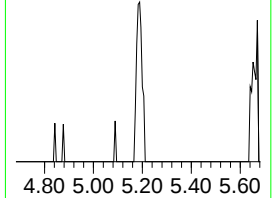
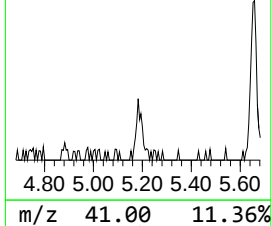
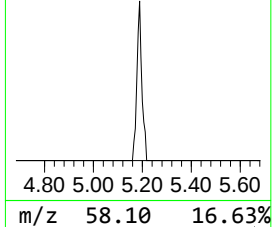
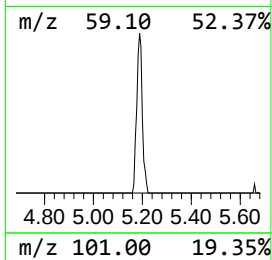
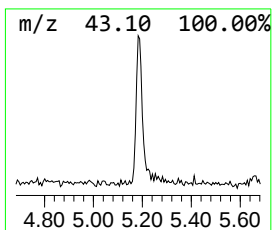
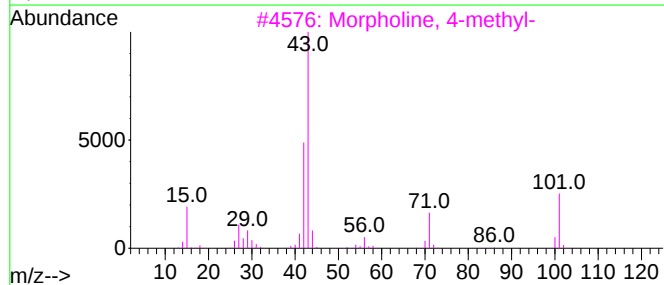
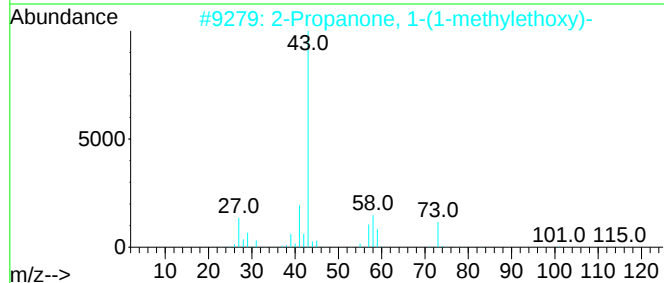
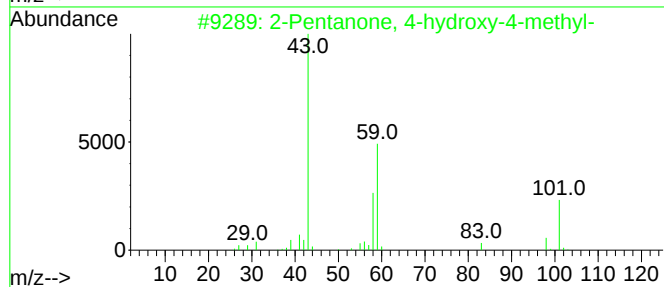
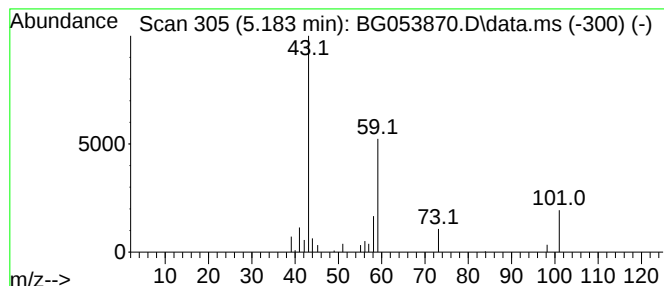
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.183	3.69 ng	24298	1,4-Dichlorobenzene-d4	8.091

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	10
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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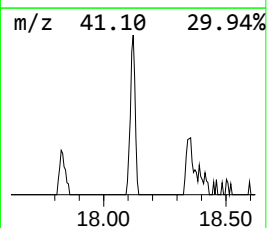
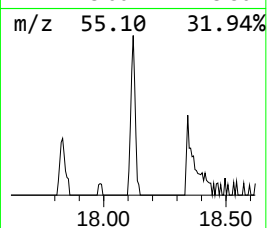
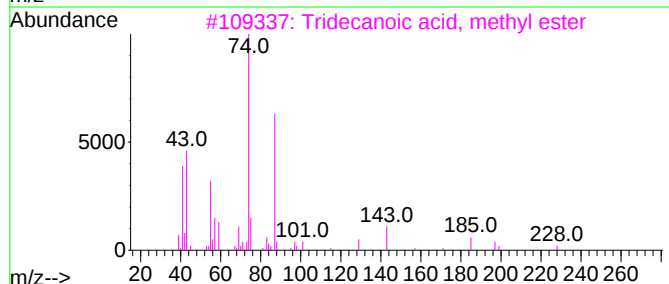
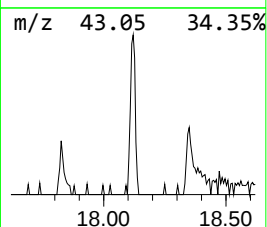
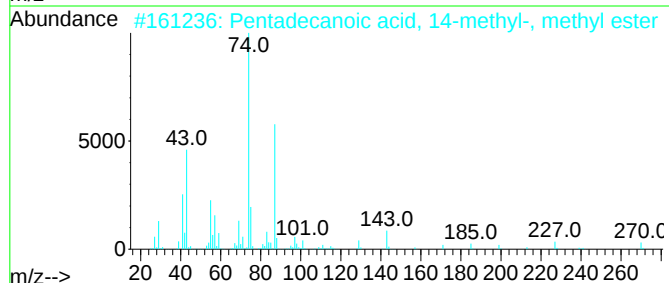
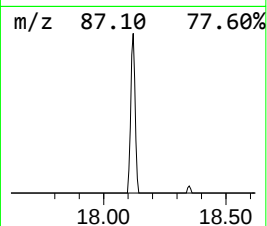
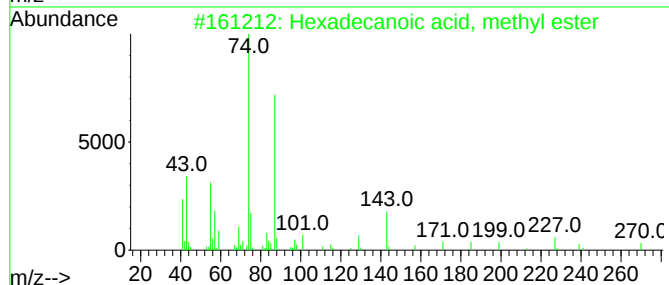
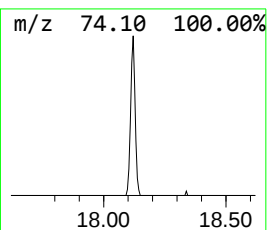
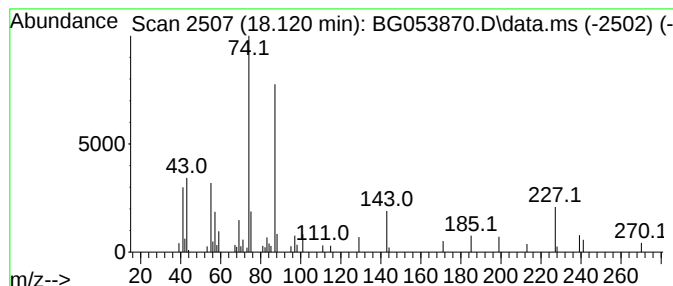
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.120	2.26 ng	49938	Phenanthrene-d10	17.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	72
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	72



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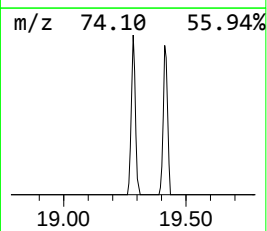
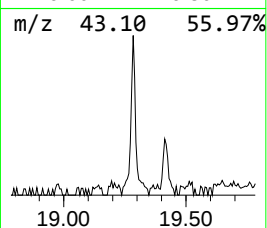
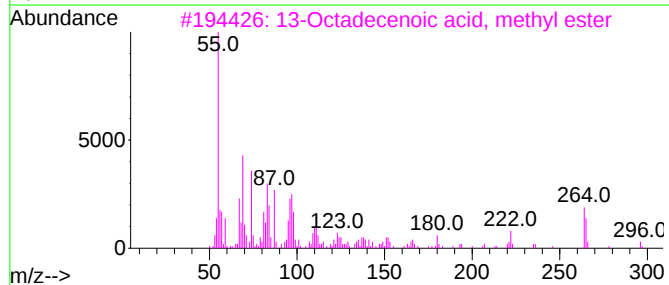
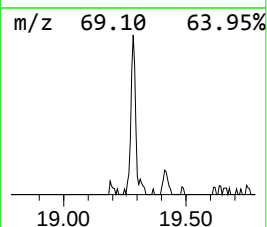
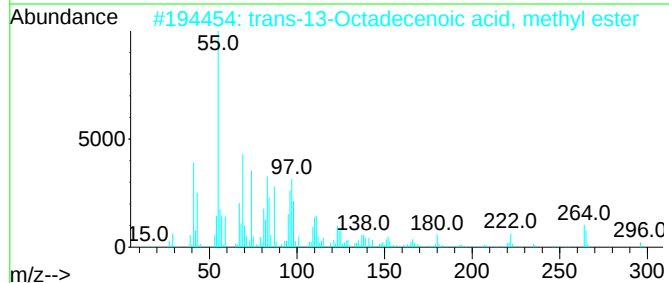
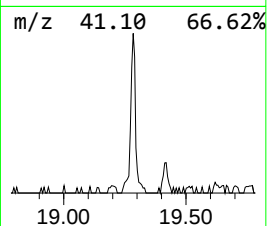
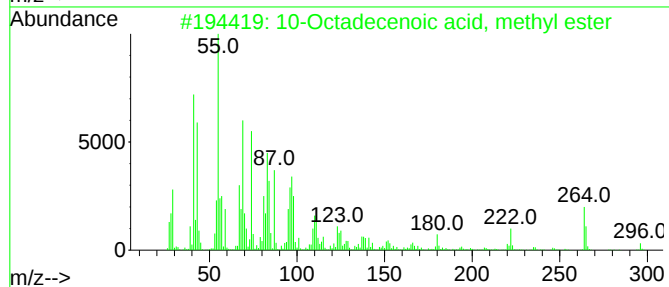
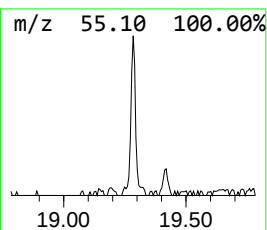
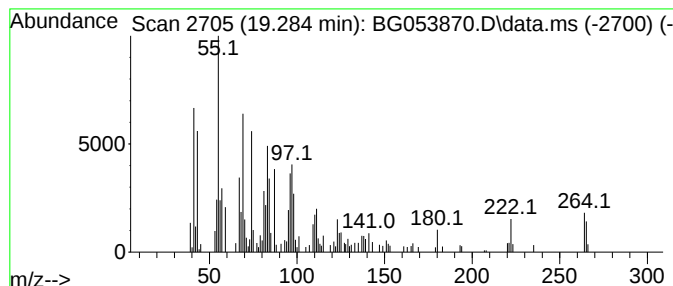
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Peak Number 4 10-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.284	4.47 ng	98731	Phenanthrene-d10	17.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2			trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	94
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
4			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91



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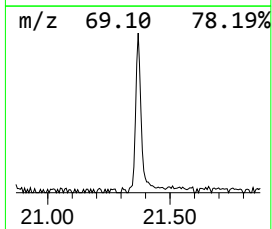
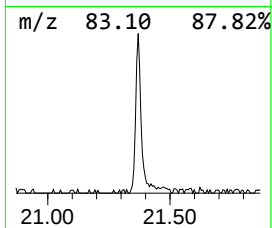
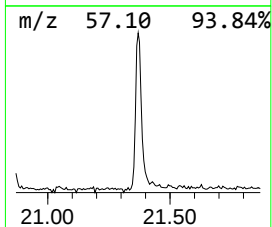
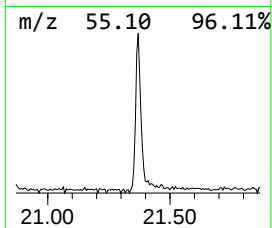
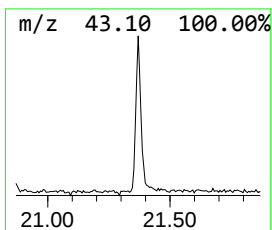
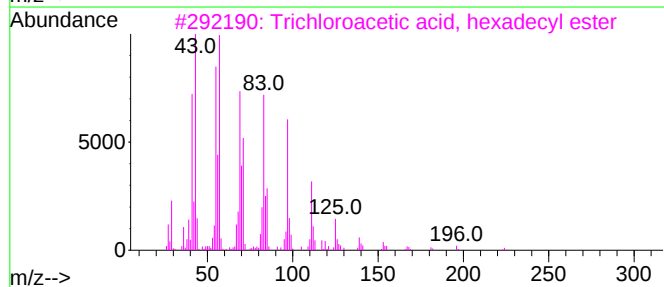
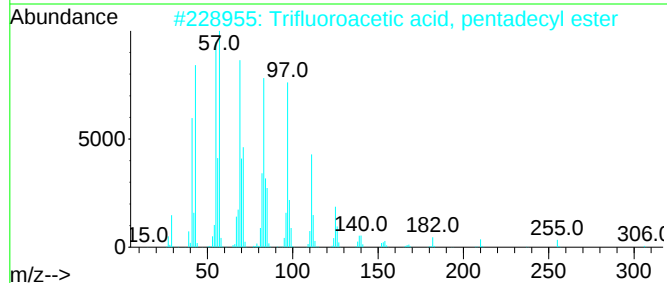
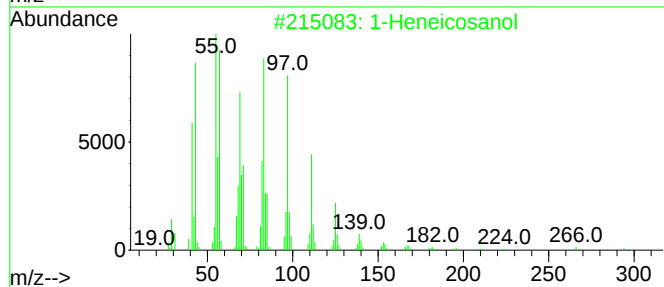
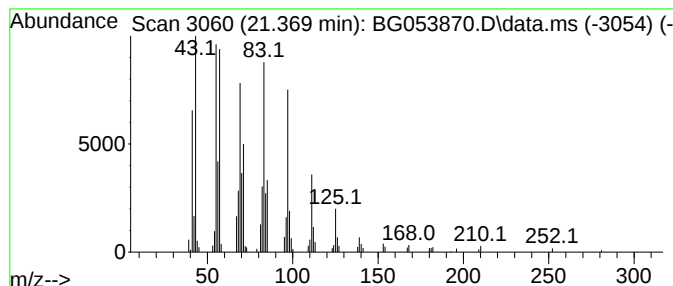
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.369	6.95 ng	183825	Chrysene-d12	21.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			1-Hexacosene	364	C26H52	018835-33-1	94
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.784	3.784	4.0	ng	26553	1	8.091	131613	20.0
2-Pentanone, 4-...	5.183	3.7	ng	24298	1	8.091	131613	20.0
Hexadecanoic ac...	18.120	2.3	ng	49938	4	17.456	441460	20.0
10-Octadecenoic...	19.284	4.5	ng	98731	4	17.456	441460	20.0
1-Heneicosanol	21.369	7.0	ng	183825	5	21.728	528744	20.0