

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062421\
 Data File : BG049085.D
 Acq On : 24 Jun 2021 18:54
 Operator : CG/JU
 Sample : M2795-10
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B4GW

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-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.155	13	20	29	rBV2	143903	332960	11.39%	2.909%
2	3.237	29	34	42	rVB	70709	129408	4.43%	1.131%
3	5.658	439	446	454	rBV	298023	484959	16.60%	4.237%
4	7.256	711	718	729	rBV	181229	323274	11.06%	2.825%
5	8.102	855	862	869	rBV	112452	199622	6.83%	1.744%
6	9.271	1053	1061	1069	rVB	405749	730737	25.01%	6.385%
7	10.687	1296	1302	1310	rBV	34554	60347	2.07%	0.527%
8	10.928	1335	1343	1350	rVB	144789	265911	9.10%	2.323%
9	13.366	1751	1758	1770	rBV	959822	1538420	52.65%	13.442%
10	14.747	1985	1993	2002	rBV	235009	368469	12.61%	3.220%
11	16.233	2239	2246	2259	rBV	959603	1523085	52.12%	13.308%
12	17.491	2454	2460	2469	rBV	317700	498492	17.06%	4.356%
13	18.378	2605	2611	2620	rBV	276908	411244	14.07%	3.593%
14	19.641	2822	2826	2839	rBV	218353	311430	10.66%	2.721%
15	20.099	2896	2904	2912	rBV	2236968	2922048	100.00%	25.532%
16	21.416	3123	3128	3137	rVB3	59535	109138	3.73%	0.954%
17	21.780	3183	3190	3198	rVB2	357167	601279	20.58%	5.254%
18	25.094	3746	3754	3768	rVB2	211093	633706	21.69%	5.537%

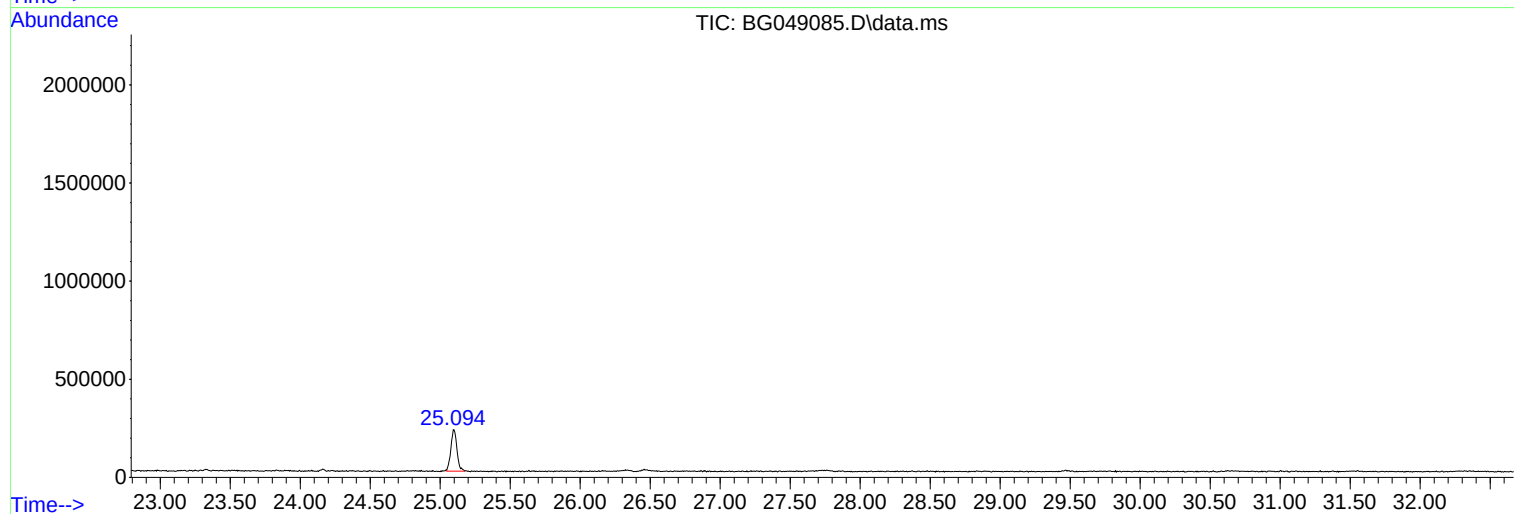
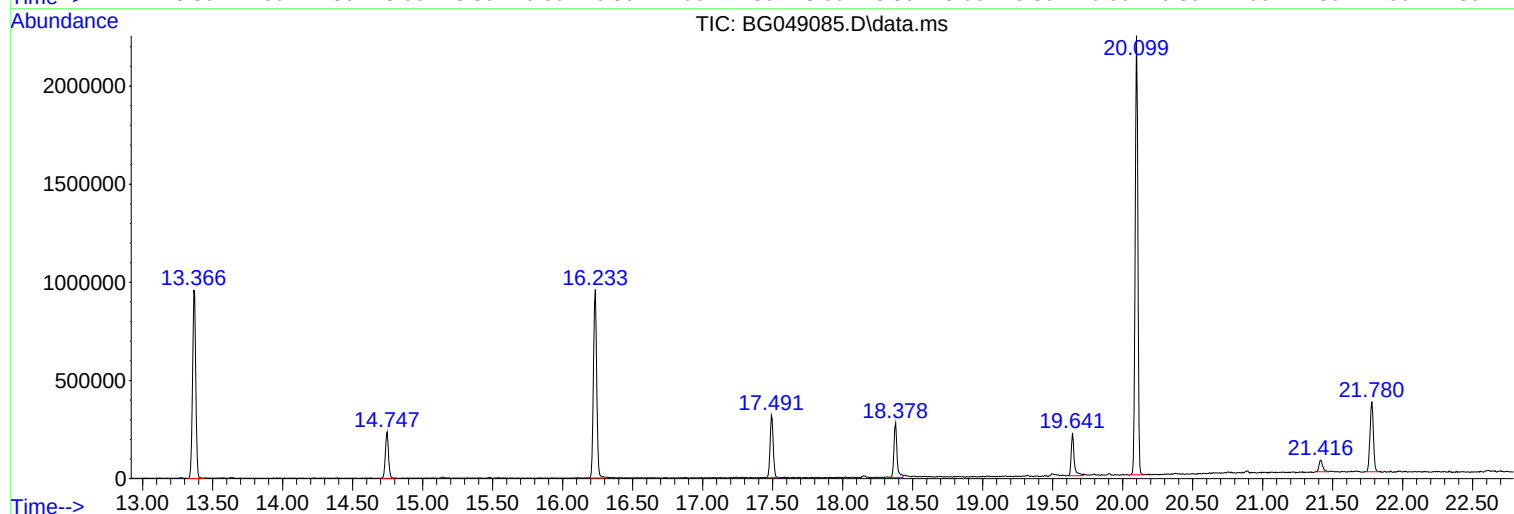
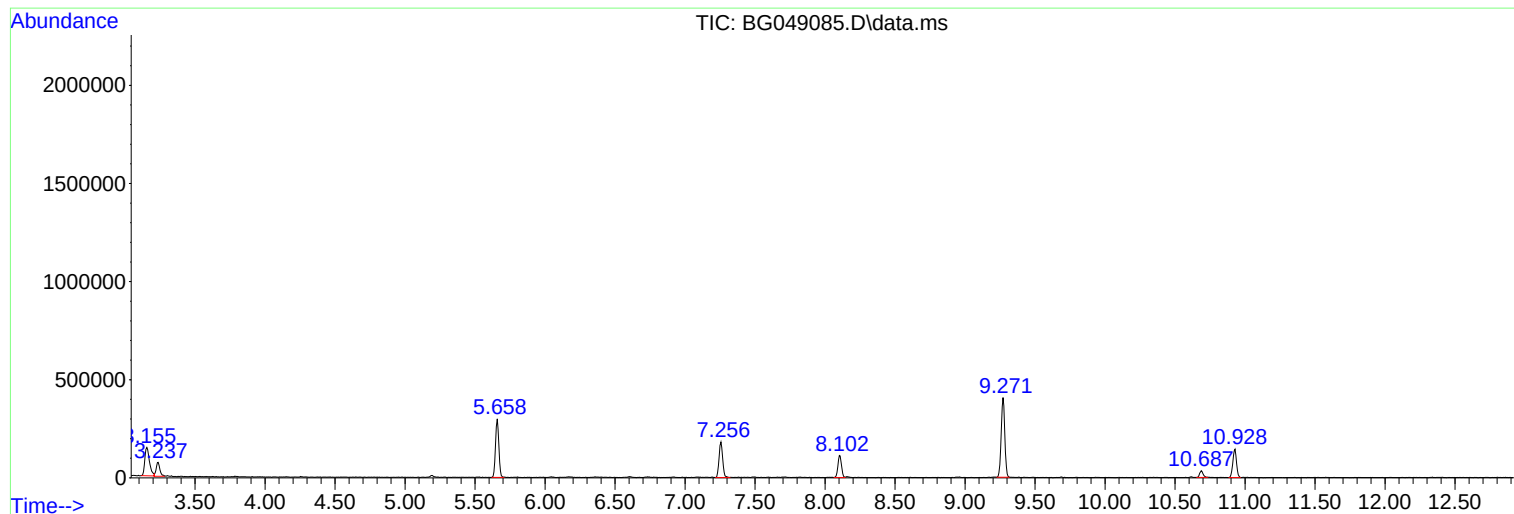
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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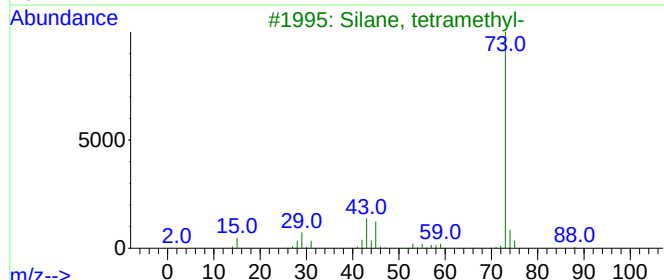
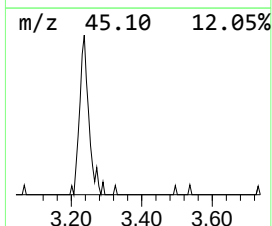
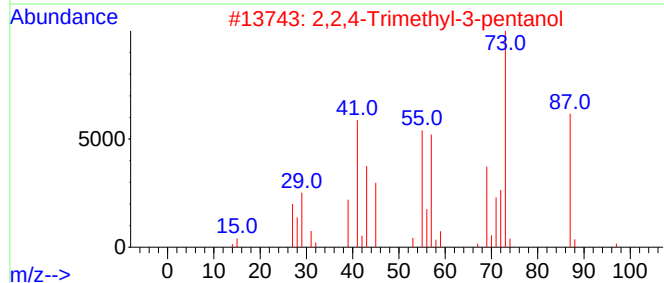
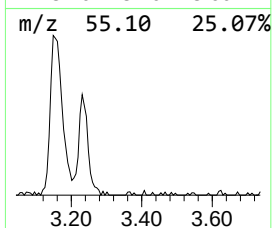
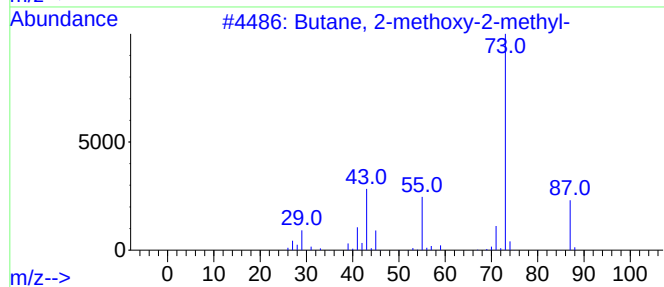
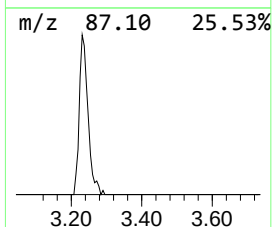
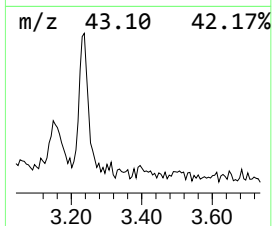
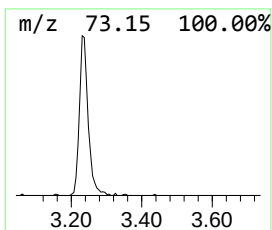
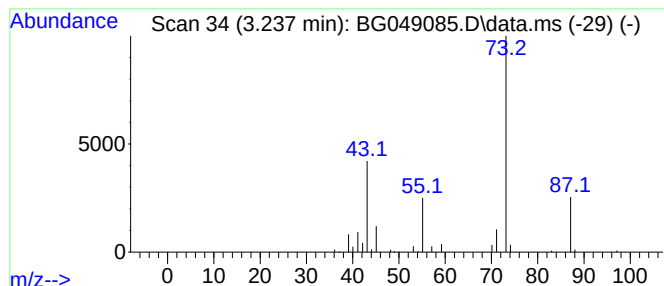
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.237	12.97 ng	129408	1,4-Dichlorobenzene-d4	8.108

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	78
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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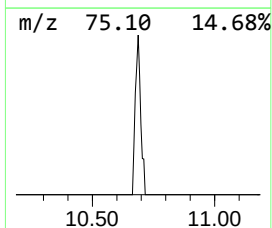
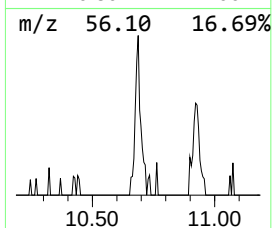
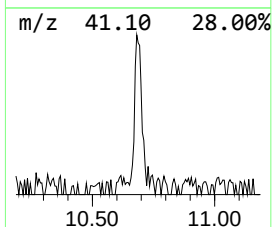
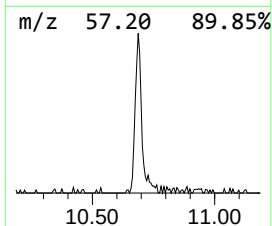
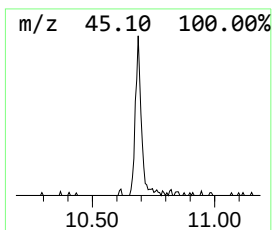
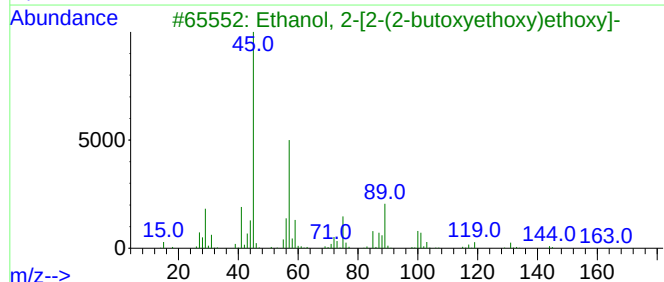
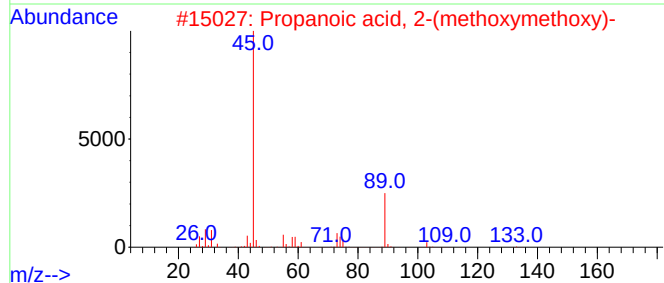
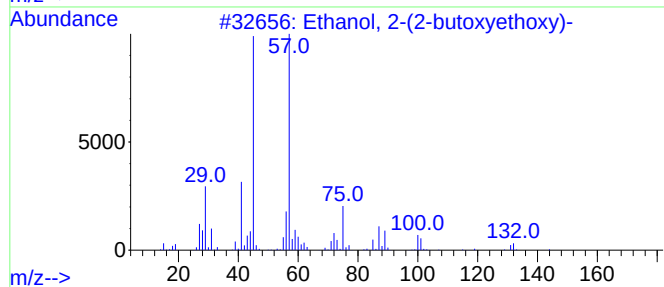
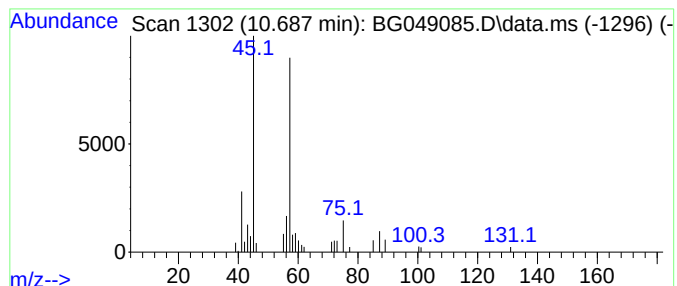
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.687	4.54 ng	60347	Naphthalene-d8	10.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4			(+)-5-Methyl-2-hexanol	116	C7H16O	111768-09-3	47
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45



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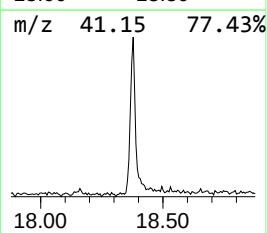
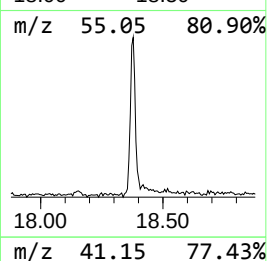
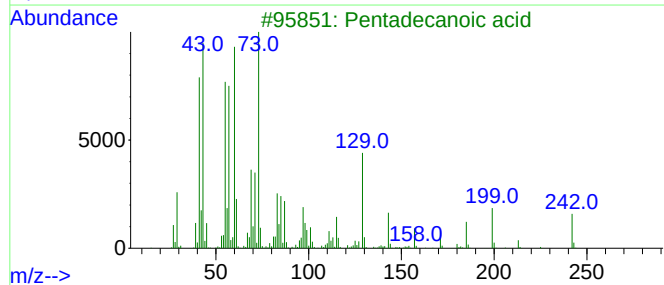
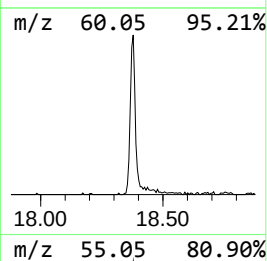
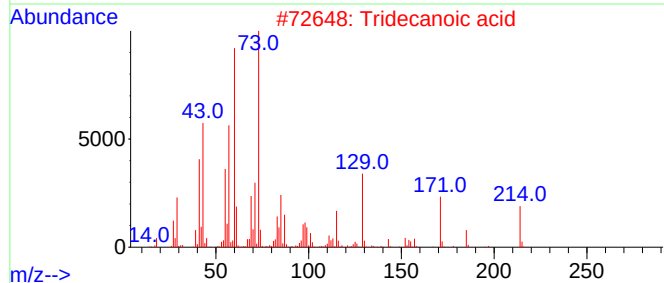
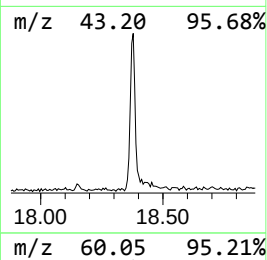
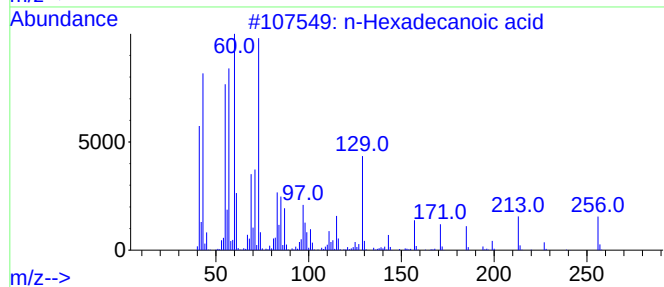
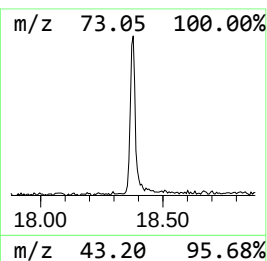
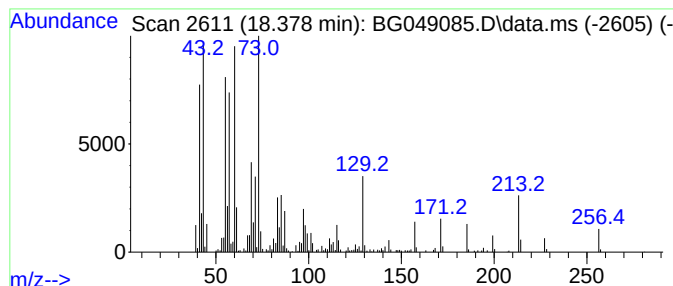
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.378	16.50 ng	411244	Phenanthrene-d10	17.491	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	62



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Instrument :
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ClientSampleId :
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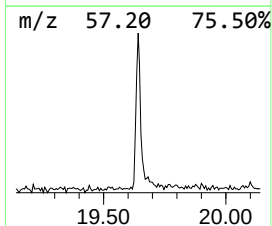
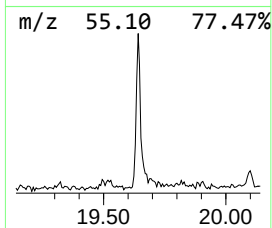
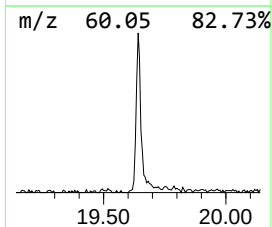
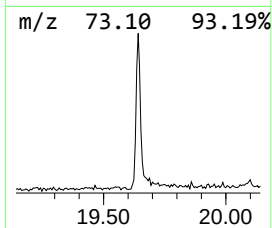
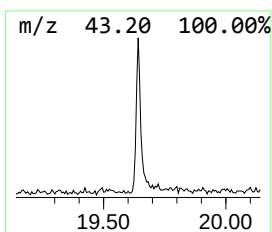
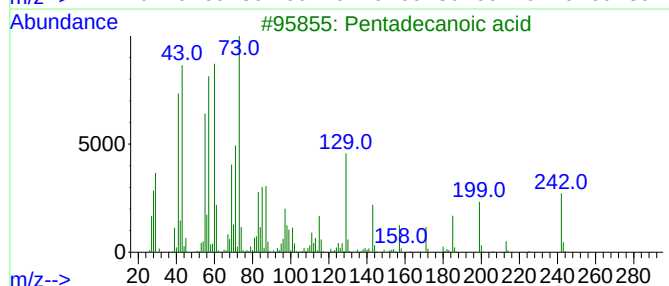
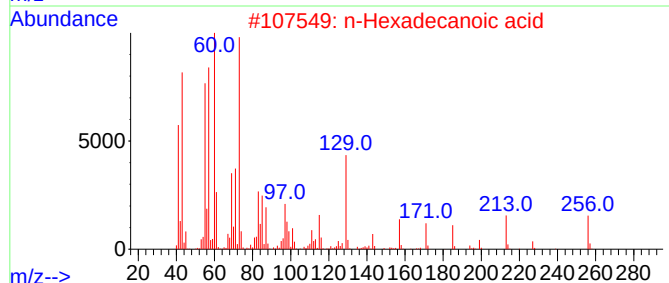
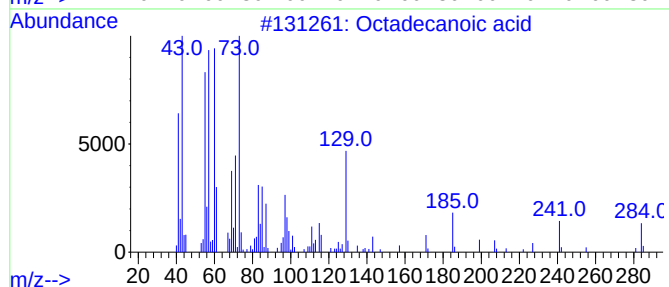
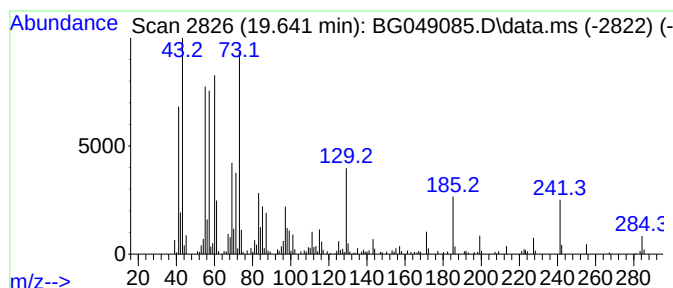
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.641	10.36 ng	311430	Chrysene-d12	21.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



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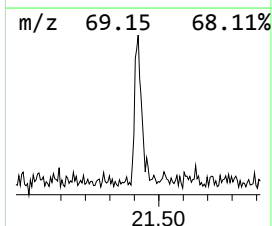
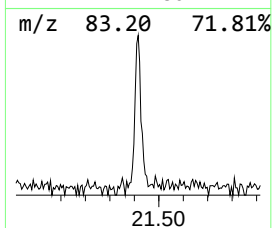
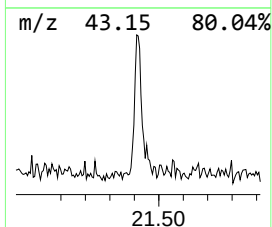
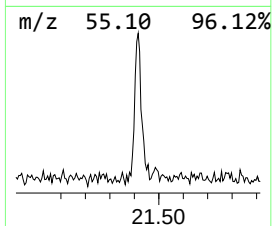
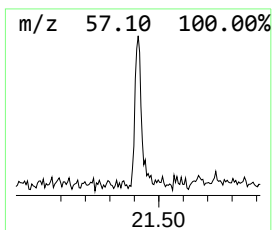
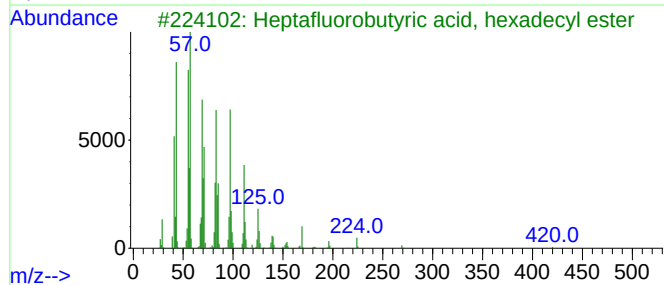
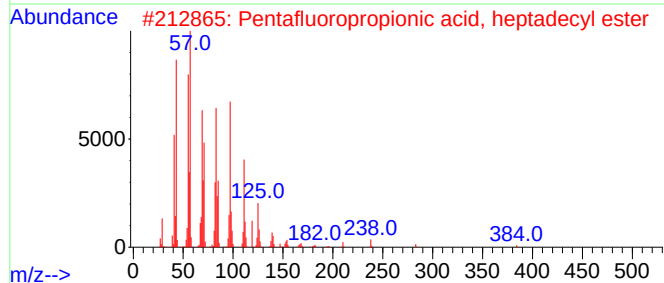
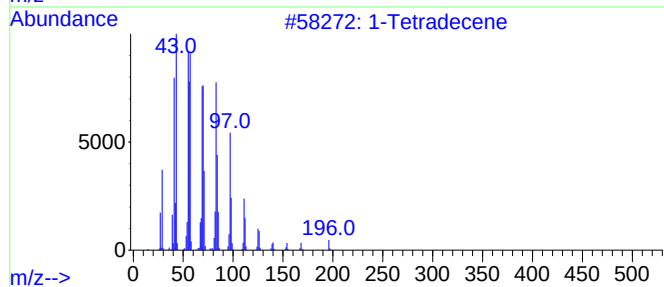
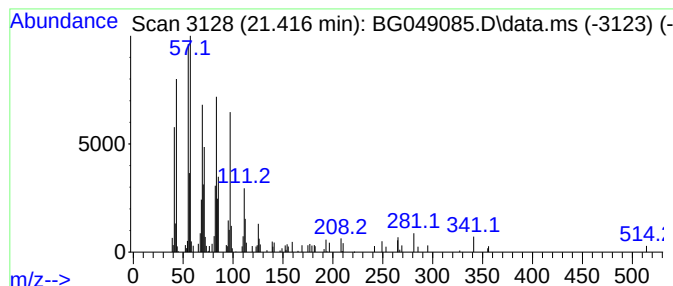
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Tetradecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	3.63 ng	109138	Chrysene-d12	21.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetradecene	196	C14H28	001120-36-1	89
2			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.237	13.0	ng	129408	1	8.108	199622	20.0
Ethanol, 2-(2-b...	10.687	4.5	ng	60347	2	10.928	265911	20.0
n-Hexadecanoic ...	18.378	16.5	ng	411244	4	17.491	498492	20.0
Octadecanoic acid	19.641	10.4	ng	311430	5	21.780	601279	20.0
1-Tetradecene	21.416	3.6	ng	109138	5	21.780	601279	20.0