

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
 Data File : BG053696.D
 Acq On : 25 May 2022 16:33
 Operator : CG/JU
 Sample : N2923-13
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P024-SS007-0006-01

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: BG053696.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.017	3	5	13	rVB3	37466	62094	3.58%	0.681%
2	3.099	14	19	34	rVB	228819	360606	20.77%	3.956%
3	5.555	430	437	447	rBV	375225	615422	35.45%	6.752%
4	7.158	703	710	727	rVB	393753	699207	40.28%	7.671%
5	7.987	843	851	858	rBV	100081	168457	9.70%	1.848%
6	9.150	1040	1049	1060	rBV	245653	438873	25.28%	4.815%
7	10.794	1323	1329	1336	rBV	127932	232780	13.41%	2.554%
8	13.244	1739	1746	1754	rVB	659699	999348	57.57%	10.964%
9	14.625	1974	1981	1988	rVB	215058	334958	19.30%	3.675%
10	16.117	2228	2235	2246	rBV	567430	893229	51.46%	9.800%
11	17.368	2442	2448	2454	rBV	293214	440836	25.40%	4.837%
12	18.255	2596	2599	2613	rVB3	79898	202243	11.65%	2.219%
13	19.524	2807	2815	2837	rVB2	207134	729323	42.02%	8.002%
14	19.976	2887	2892	2898	rBV	1332212	1735841	100.00%	19.044%
15	21.075	3074	3079	3082	rBV6	10498	22765	1.31%	0.250%
16	21.269	3108	3112	3123	rVB4	52772	90454	5.21%	0.992%
17	21.633	3168	3174	3182	rVB2	325162	531531	30.62%	5.832%
18	24.840	3710	3720	3731	rVB2	191261	556793	32.08%	6.109%

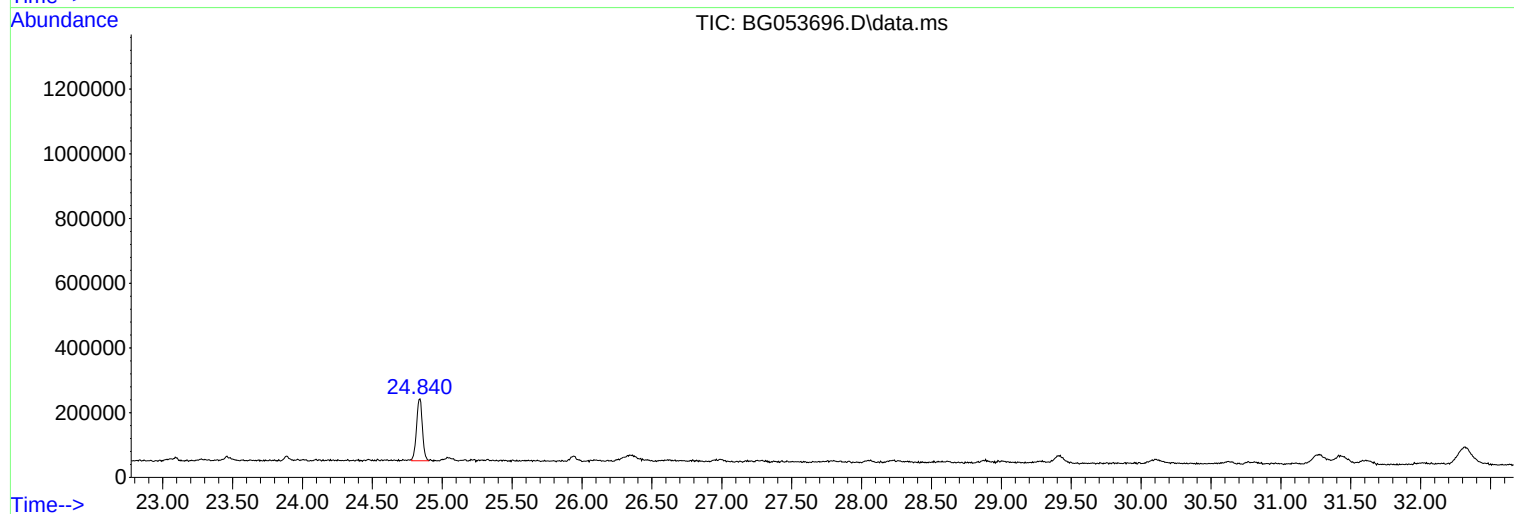
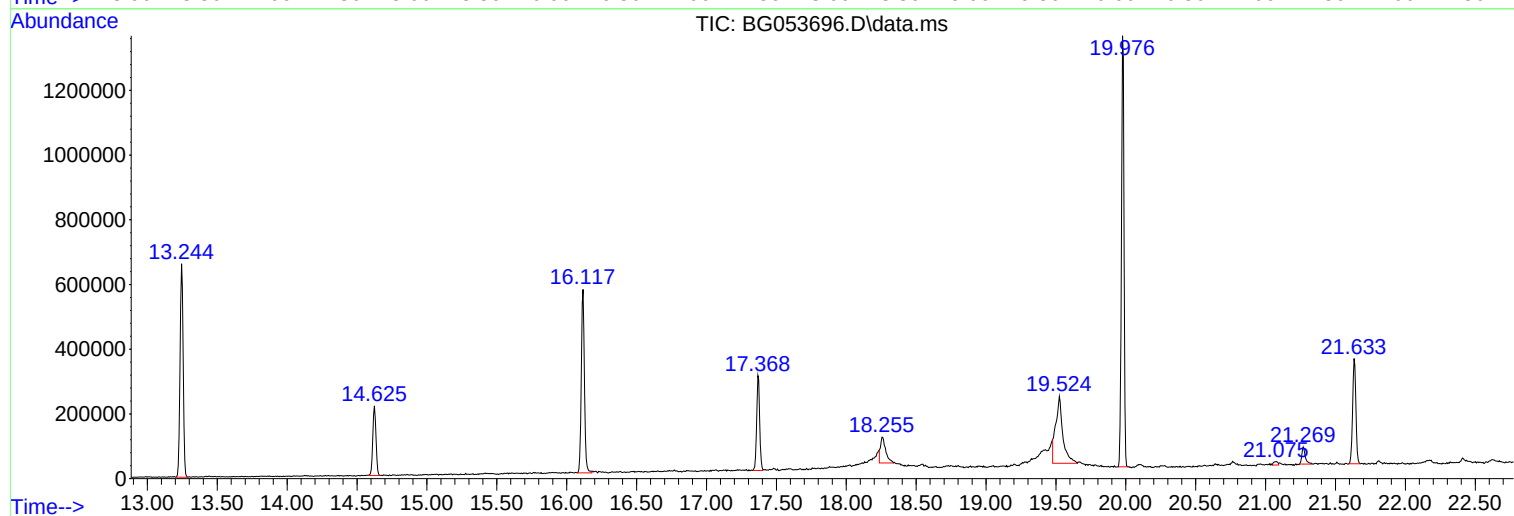
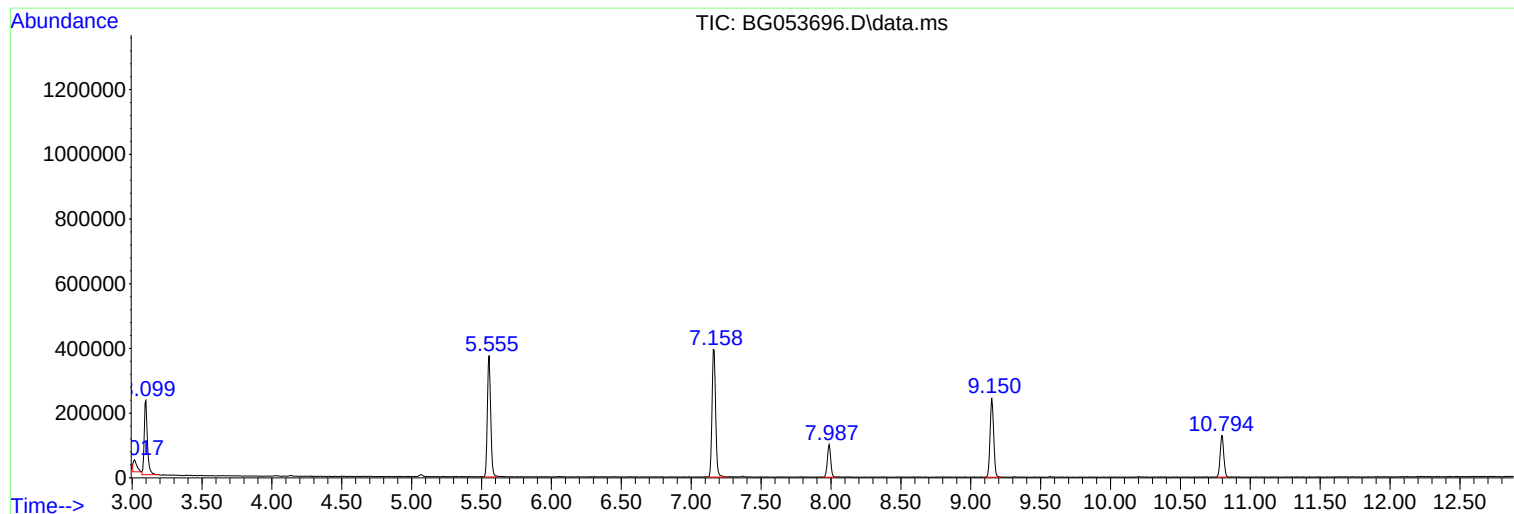
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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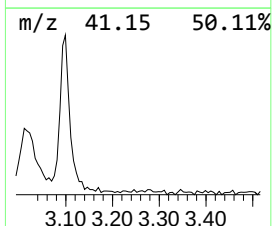
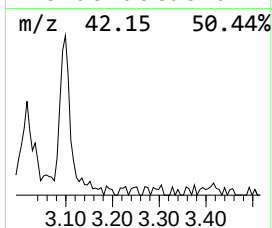
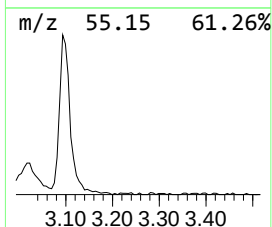
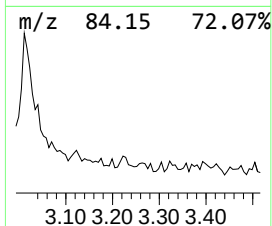
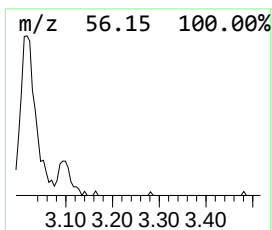
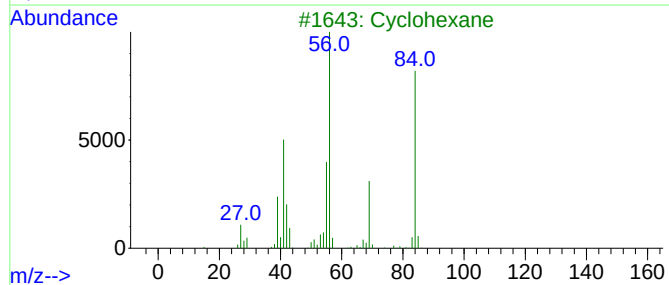
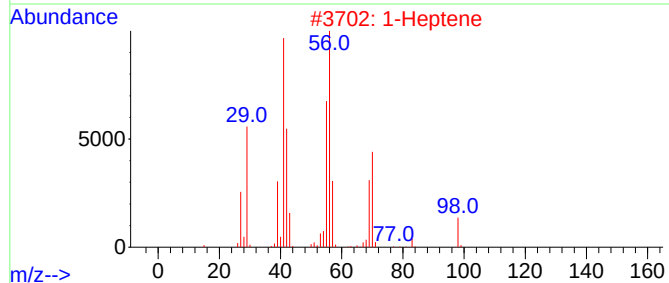
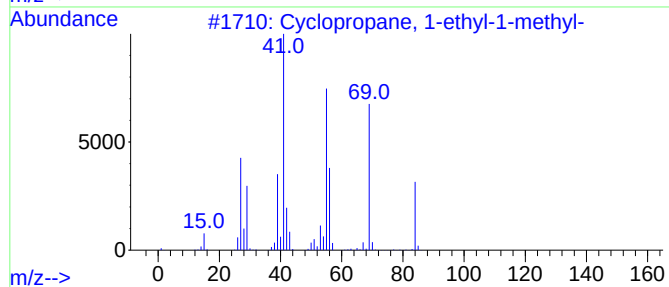
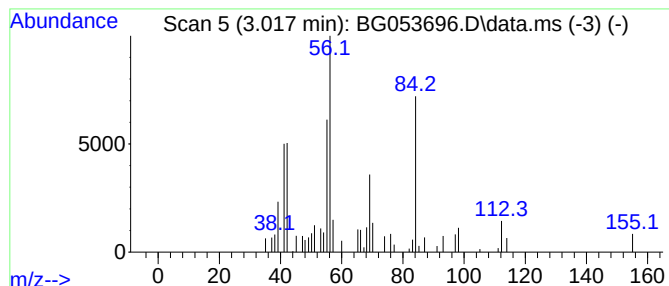
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopropane, 1-ethyl-1-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.017	7.37 ng	62094	1,4-Dichlorobenzene-d4	7.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	59
2			1-Heptene	98	C7H14	000592-76-7	49
3			Cyclohexane	84	C6H12	000110-82-7	47
4			Pent-4-enylamine	85	C5H11N	022537-07-1	47
5			Heptane, 4-methylene-	112	C8H16	015918-08-8	43



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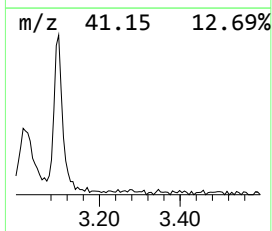
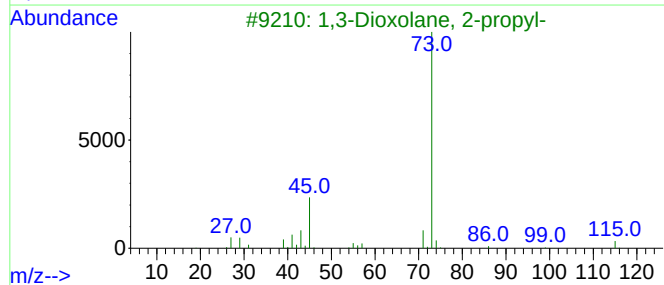
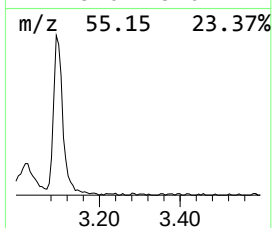
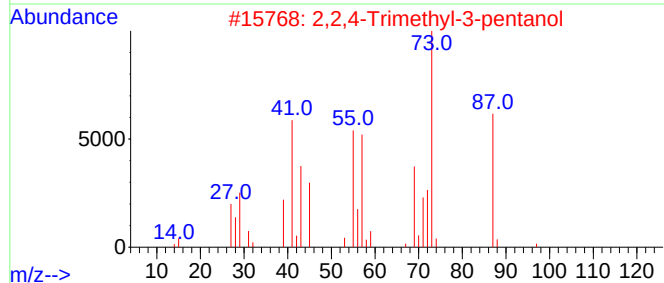
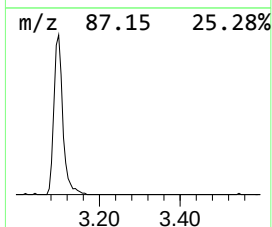
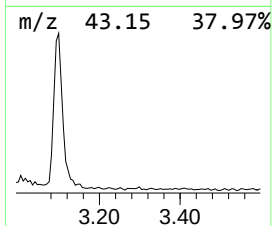
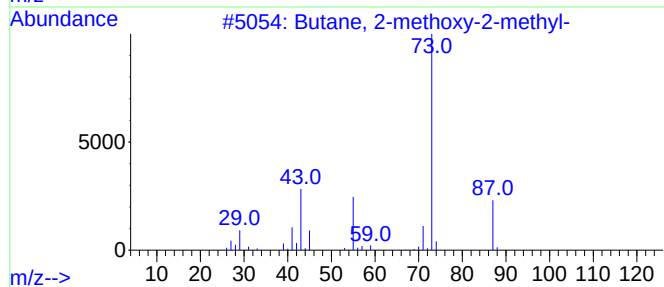
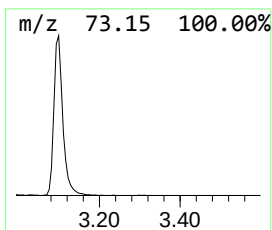
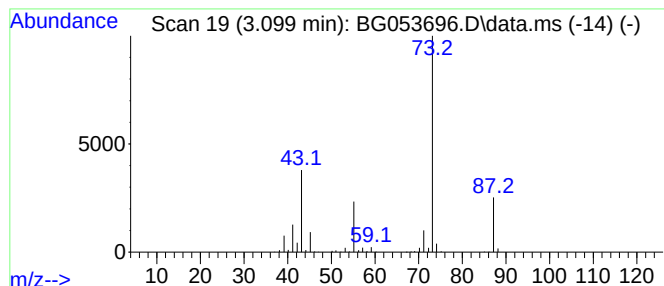
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.099	42.81 ng	360606	1,4-Dichlorobenzene-d4	7.987

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	64
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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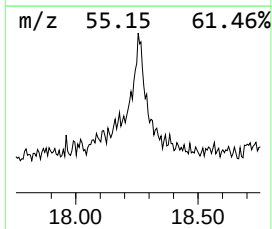
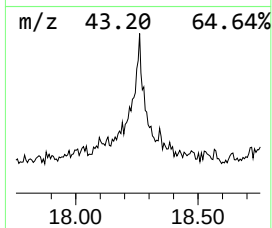
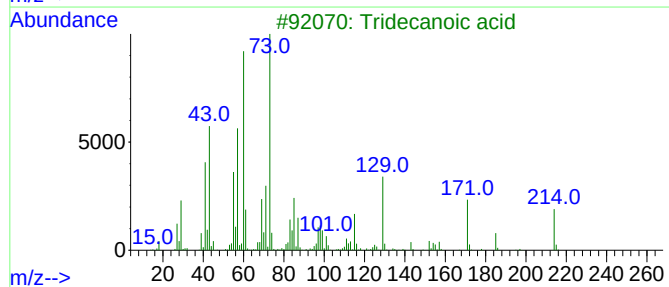
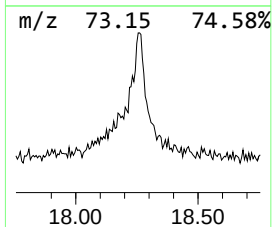
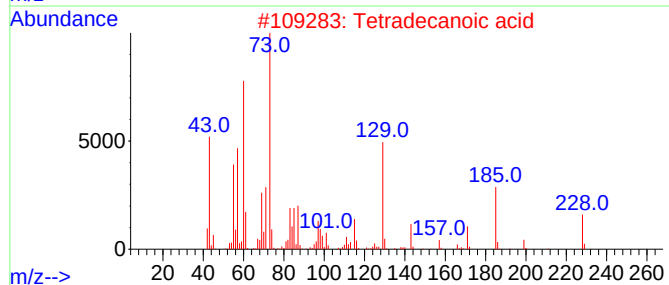
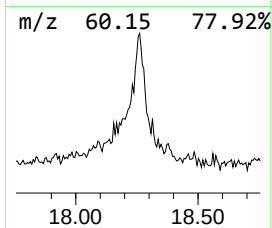
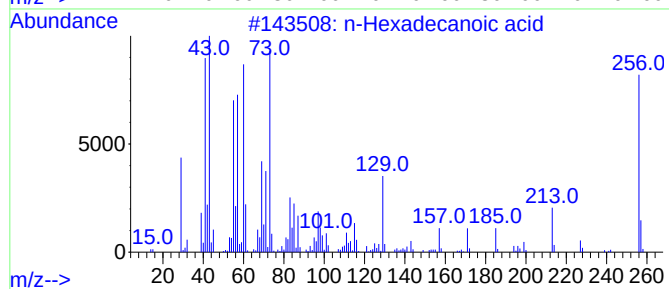
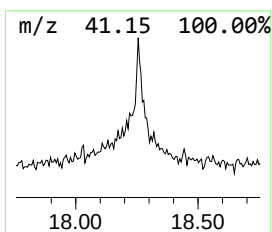
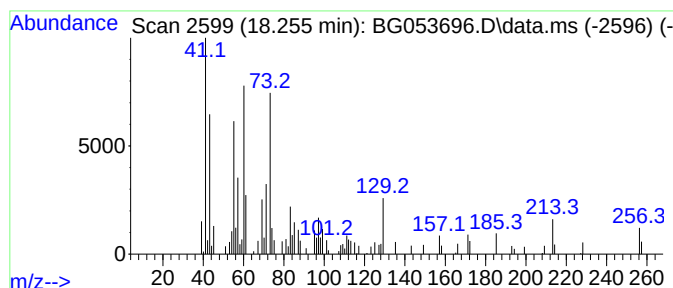
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.255	9.18 ng	202243	Phenanthrene-d10	17.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	47



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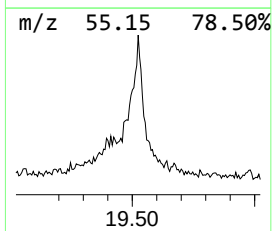
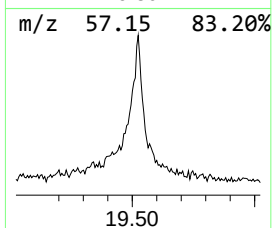
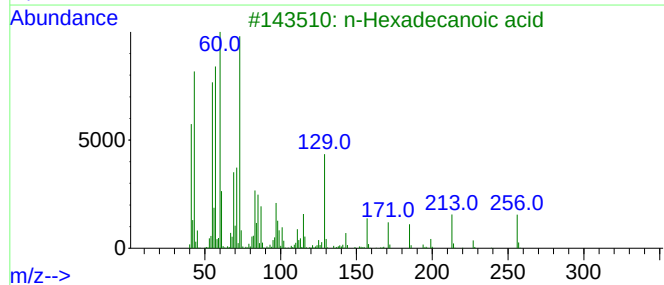
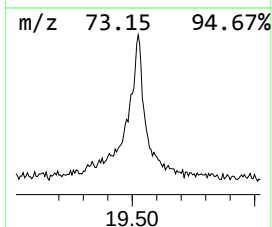
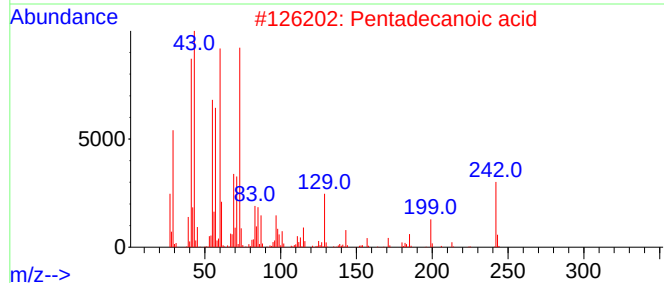
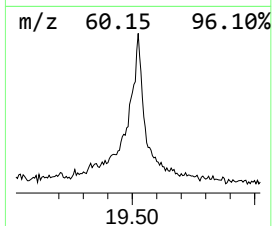
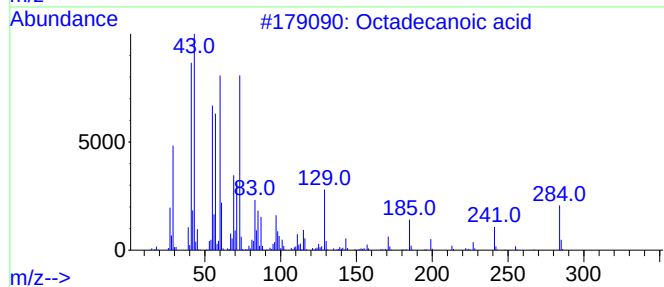
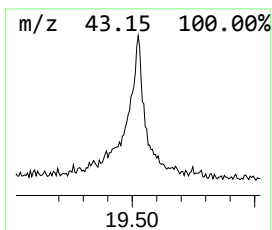
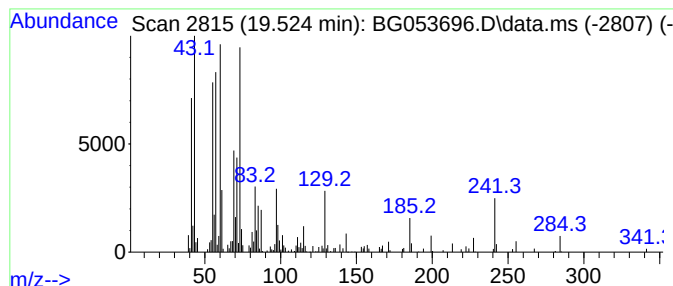
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.524	27.44 ng	729323	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	90
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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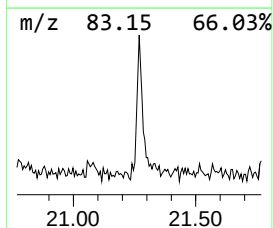
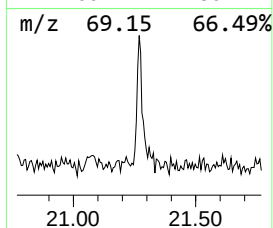
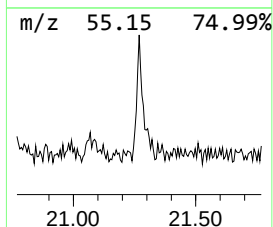
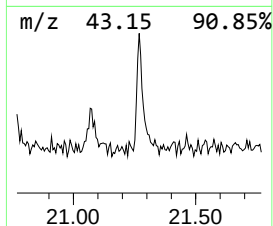
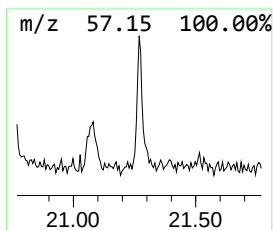
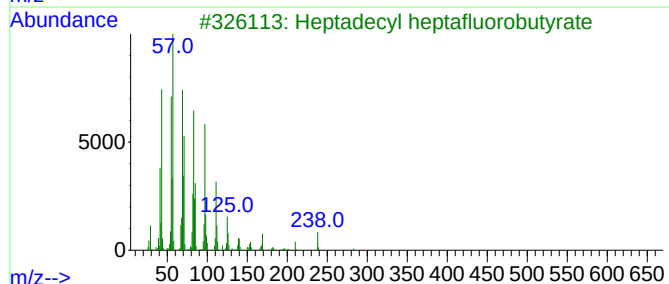
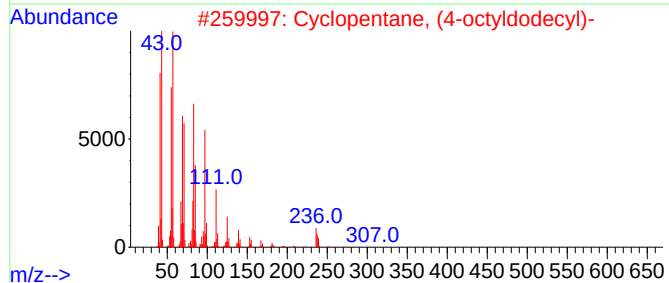
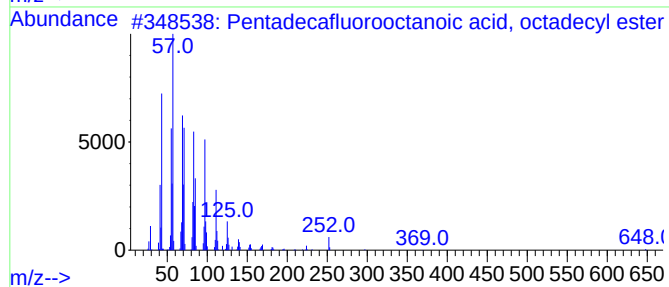
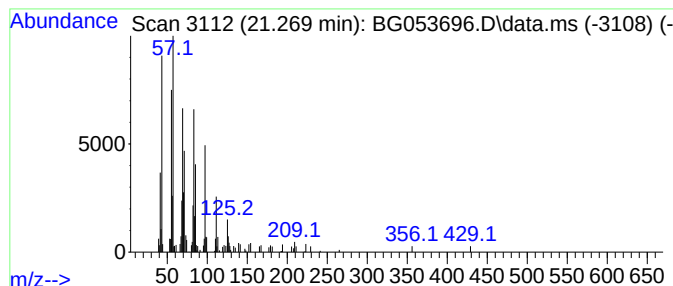
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.269	3.40 ng	90454	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
2			Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	86
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	80
5			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	74



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopropane, 1...	3.017	7.4	ng	62094	1	7.987	168457	20.0
Butane, 2-metho...	3.099	42.8	ng	360606	1	7.987	168457	20.0
n-Hexadecanoic ...	18.255	9.2	ng	202243	4	17.368	440836	20.0
Octadecanoic acid	19.524	27.4	ng	729323	5	21.633	531531	20.0
Pentadecafluoro...	21.269	3.4	ng	90454	5	21.633	531531	20.0