

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
 Data File : BG055116.D
 Acq On : 10 Oct 2022 17:22
 Operator : CG/JU
 Sample : N5052-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 551B-2

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-BG100322.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.367	8	13	31	rVB	855997	1304005	38.42%	9.588%
2	5.376	349	355	361	rVB	76736	114857	3.38%	0.845%
3	5.846	429	435	444	rBV	360411	566117	16.68%	4.163%
4	7.456	701	709	717	rBV	235158	404515	11.92%	2.974%
5	8.331	851	858	873	rVB	106691	183299	5.40%	1.348%
6	9.501	1049	1057	1065	rBV	400912	710036	20.92%	5.221%
7	10.905	1289	1296	1305	rBV	42547	81005	2.39%	0.596%
8	11.158	1332	1339	1347	rVB	141499	256896	7.57%	1.889%
9	13.566	1740	1749	1756	rBV	1117875	1718688	50.64%	12.638%
10	14.371	1880	1886	1893	rVB	339126	496551	14.63%	3.651%
11	14.935	1975	1982	1990	rVB	253000	393170	11.58%	2.891%
12	15.723	2104	2116	2121	rBV2	25821	36857	1.09%	0.271%
13	16.410	2226	2233	2248	rVB	1122510	1714423	50.52%	12.606%
14	17.668	2441	2447	2454	rBV	385682	569822	16.79%	4.190%
15	18.519	2588	2592	2600	rBV2	51167	84619	2.49%	0.622%
16	18.602	2601	2606	2612	rVB	100955	126141	3.72%	0.928%
17	18.943	2660	2664	2669	rBV	48911	54430	1.60%	0.400%
18	20.247	2880	2886	2891	rBV	2630705	3393872	100.00%	24.955%
19	21.563	3105	3110	3122	rBV2	40549	77493	2.28%	0.570%
20	21.963	3171	3178	3186	rVB2	366576	639651	18.85%	4.703%
21	25.406	3753	3764	3778	rVB2	220347	673423	19.84%	4.952%

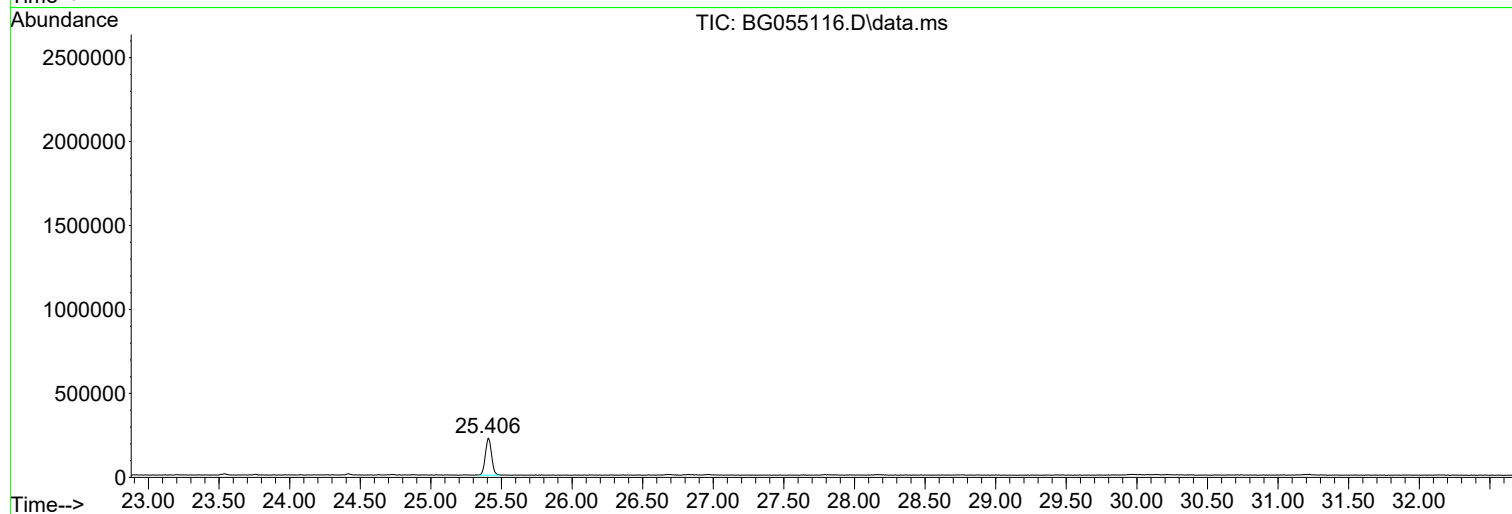
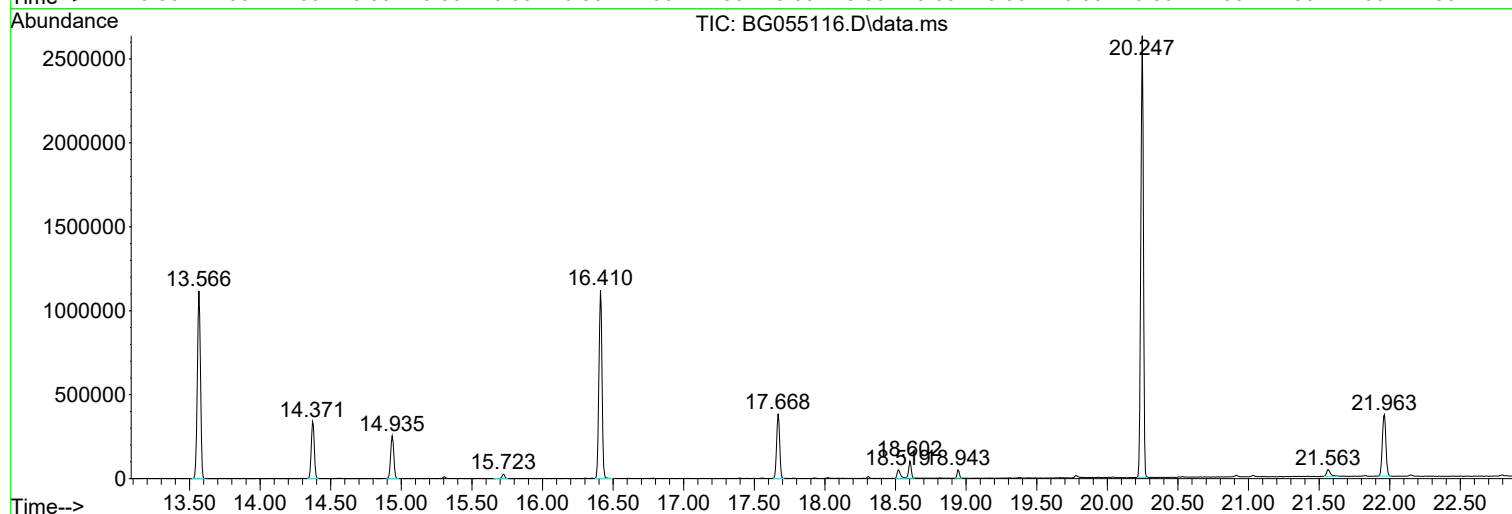
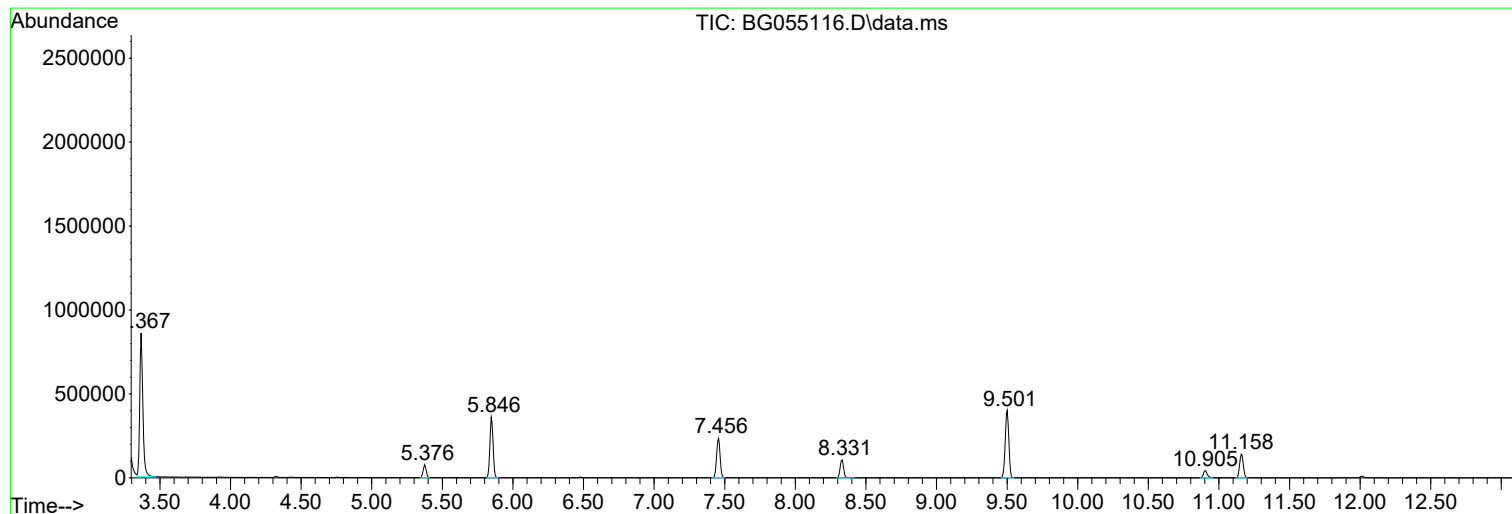
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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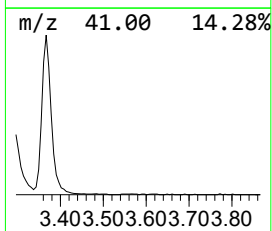
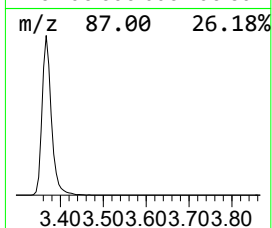
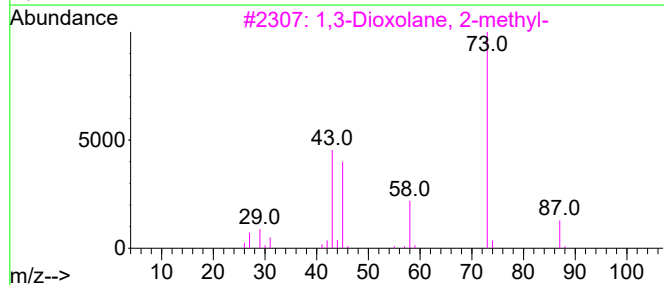
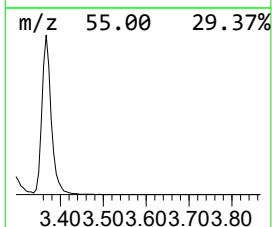
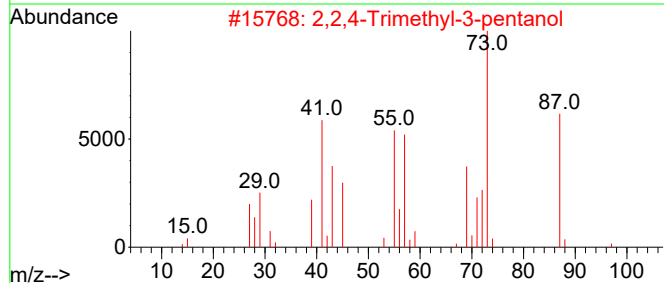
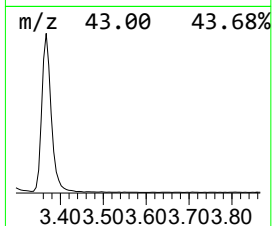
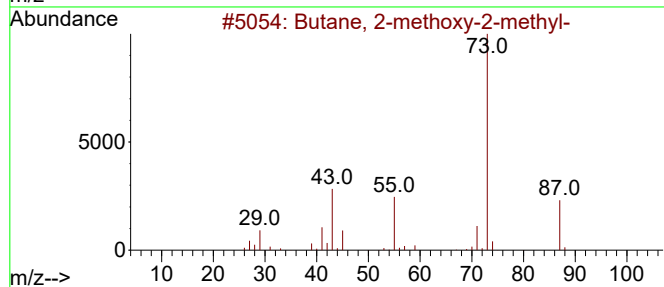
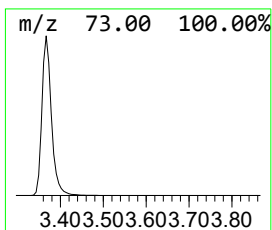
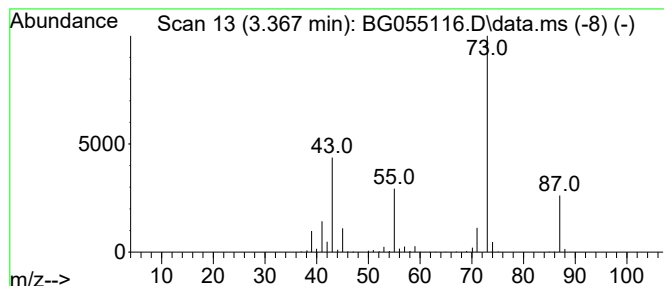
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.367	142.28 ng	1304010	1,4-Dichlorobenzene-d4	8.331

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	50
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16



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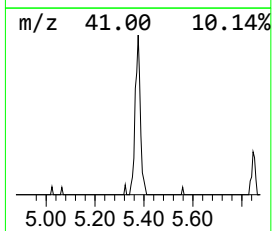
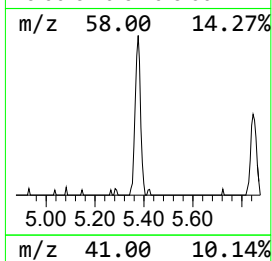
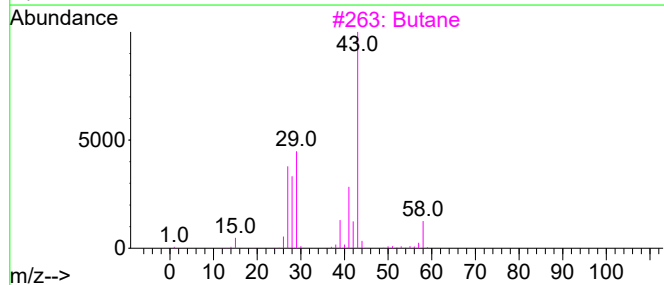
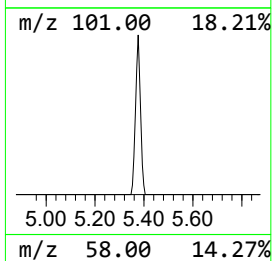
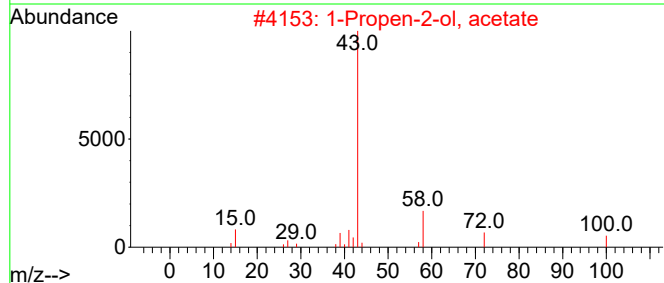
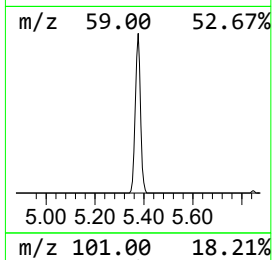
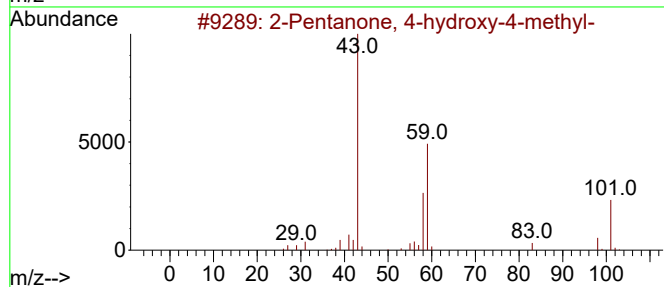
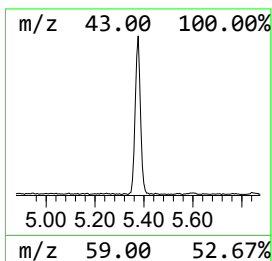
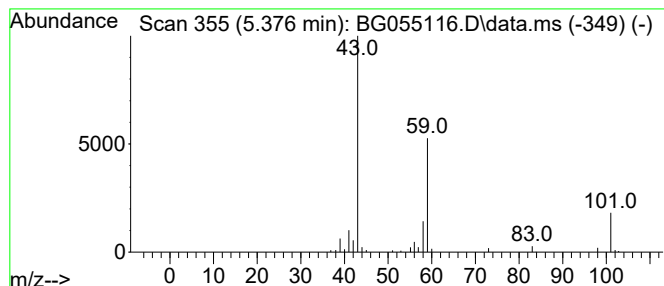
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.376	12.53 ng	114857	1,4-Dichlorobenzene-d4	8.331

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3			Butane	58	C4H10	000106-97-8	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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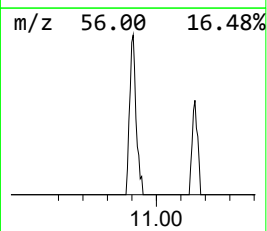
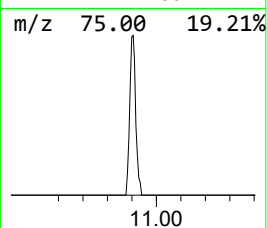
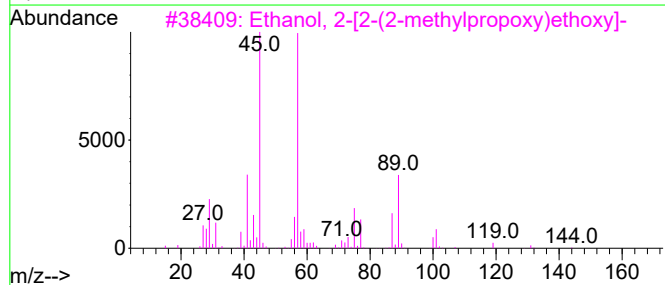
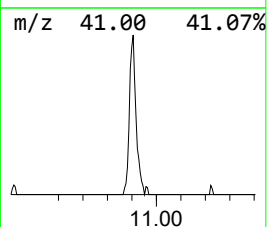
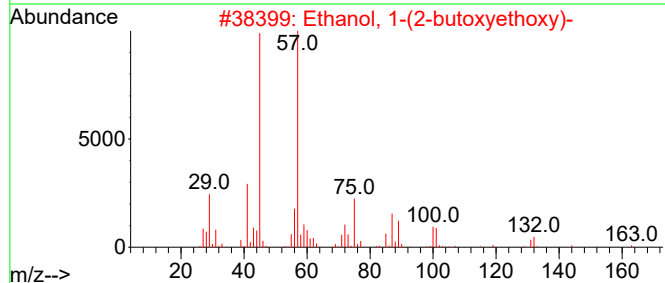
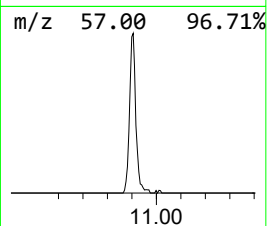
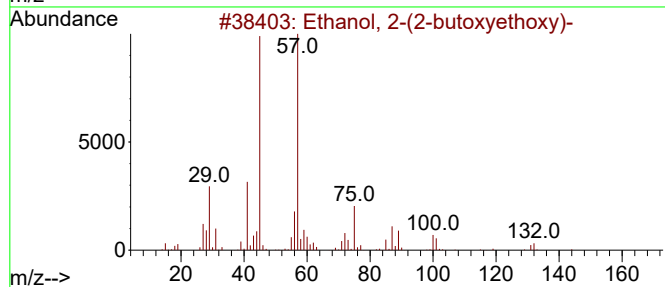
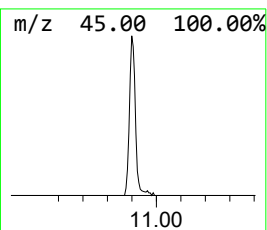
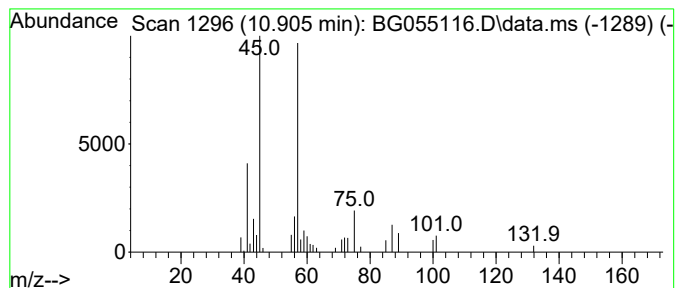
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.905	6.31 ng	81005	Naphthalene-d8	11.158

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45



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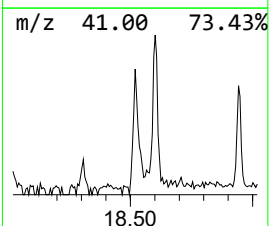
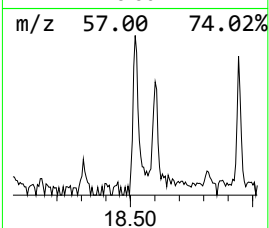
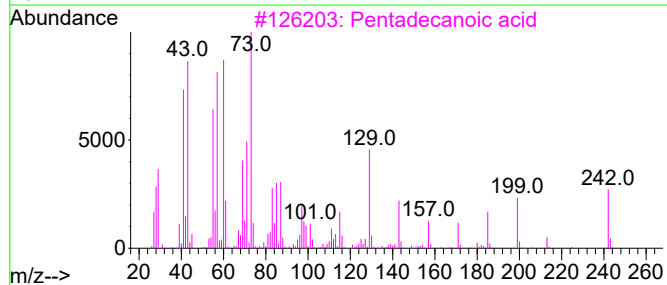
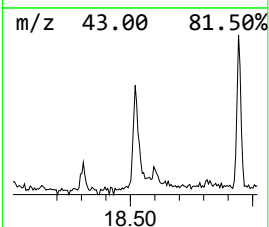
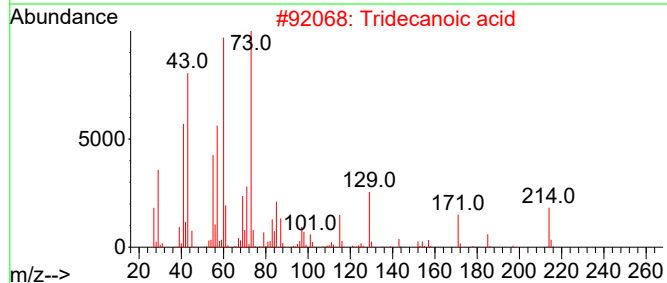
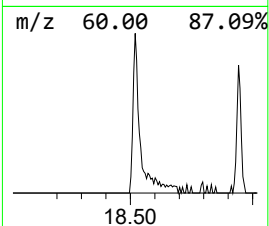
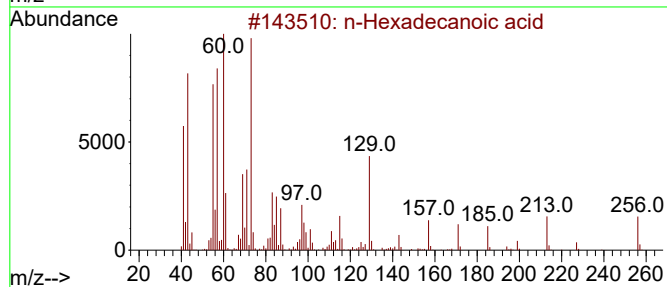
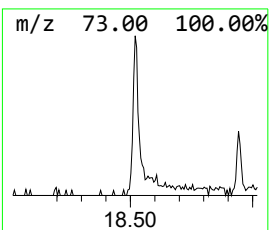
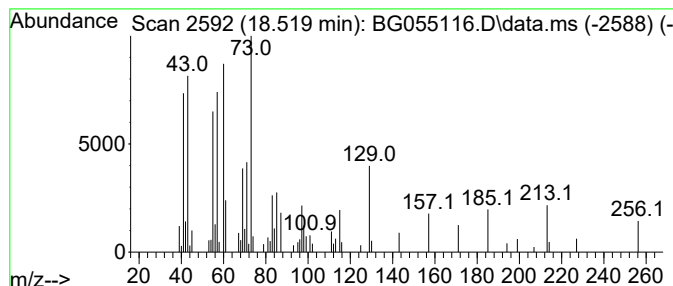
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.520	2.97 ng	84619	Phenanthrene-d10	17.668

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	15



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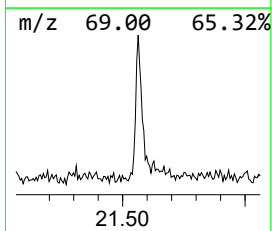
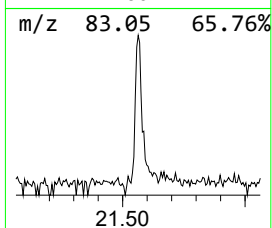
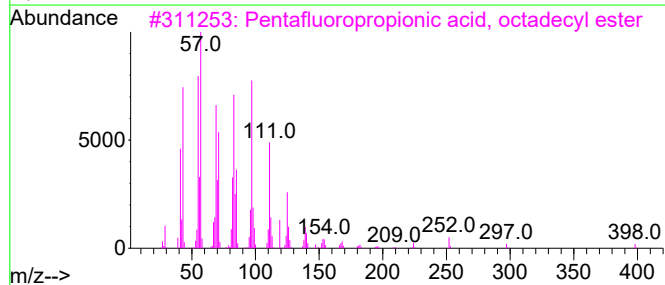
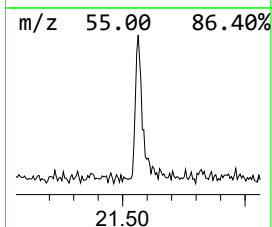
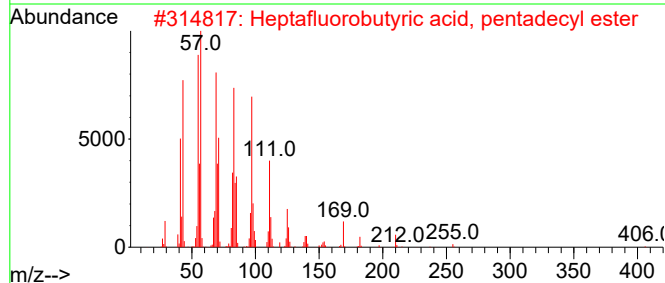
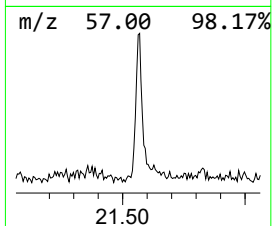
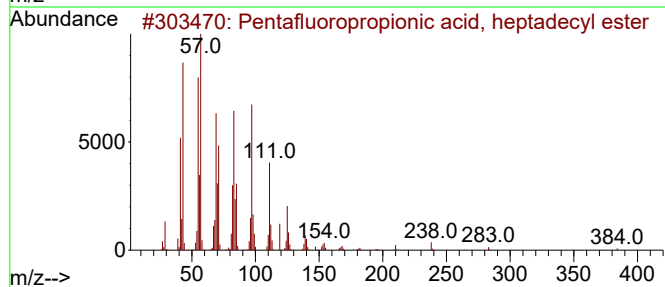
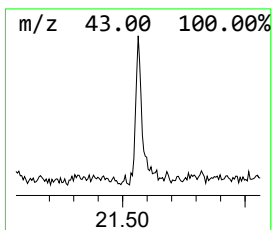
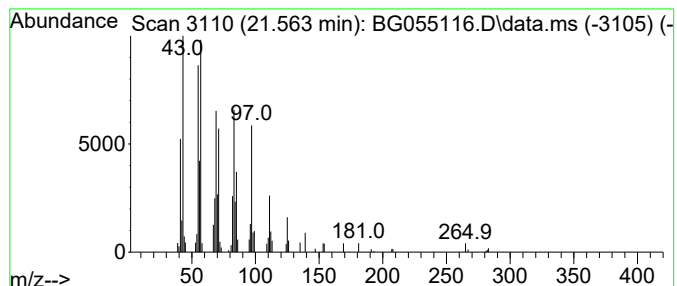
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.563	2.42 ng	77493	Chrysene-d12	21.962	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.367	142.3	ng	1304010	1	8.331	183299	20.0
2-Pentanone, 4-...	5.376	12.5	ng	114857	1	8.331	183299	20.0
Ethanol, 2-(2-b...	10.905	6.3	ng	81005	2	11.158	256896	20.0
n-Hexadecanoic ...	18.520	3.0	ng	84619	4	17.668	569822	20.0
Pentafluoroprop...	21.563	2.4	ng	77493	5	21.962	639651	20.0