

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
 Data File : BP006550.D
 Acq On : 06 Aug 2021 21:38
 Operator : CG/JU
 Sample : M3278-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MW-5

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_P\Methods\8270E-BP080321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	304	309	319	rVB	586131	800488	6.97%	1.606%
2	5.358	380	386	393	rVB	2132551	3064411	26.69%	6.147%
3	5.969	485	490	498	rVB	329020	480876	4.19%	0.965%
4	6.928	647	653	667	rVB	1215672	1916163	16.69%	3.844%
5	7.752	787	793	801	rVB	828586	1270679	11.07%	2.549%
6	8.910	982	990	1002	rBV	2744173	4401671	38.34%	8.830%
7	10.328	1225	1231	1242	rBV	410489	659576	5.75%	1.323%
8	10.534	1259	1266	1277	rBV	980565	1690132	14.72%	3.391%
9	13.004	1679	1686	1701	rBV	5571679	8333380	72.59%	16.717%
10	14.381	1910	1920	1933	rBV	1309062	1882965	16.40%	3.777%
11	15.875	2167	2174	2197	rBV	4031250	5907355	51.46%	11.851%
12	17.134	2381	2388	2398	rBV	1420849	2024852	17.64%	4.062%
13	17.822	2500	2505	2510	rBV	101438	127492	1.11%	0.256%
14	18.039	2537	2542	2548	rBV	180815	268030	2.33%	0.538%
15	19.275	2748	2752	2761	rBV2	103389	161862	1.41%	0.325%
16	19.710	2820	2826	2831	rBV	9681332	11479427	100.00%	23.029%
17	20.957	3034	3038	3045	rBV2	207184	292413	2.55%	0.587%
18	21.227	3080	3084	3092	rBV	1860821	2322346	20.23%	4.659%
19	22.327	3268	3271	3280	rVB2	130061	176856	1.54%	0.355%
20	23.557	3473	3480	3490	rVB2	1306522	2587796	22.54%	5.191%

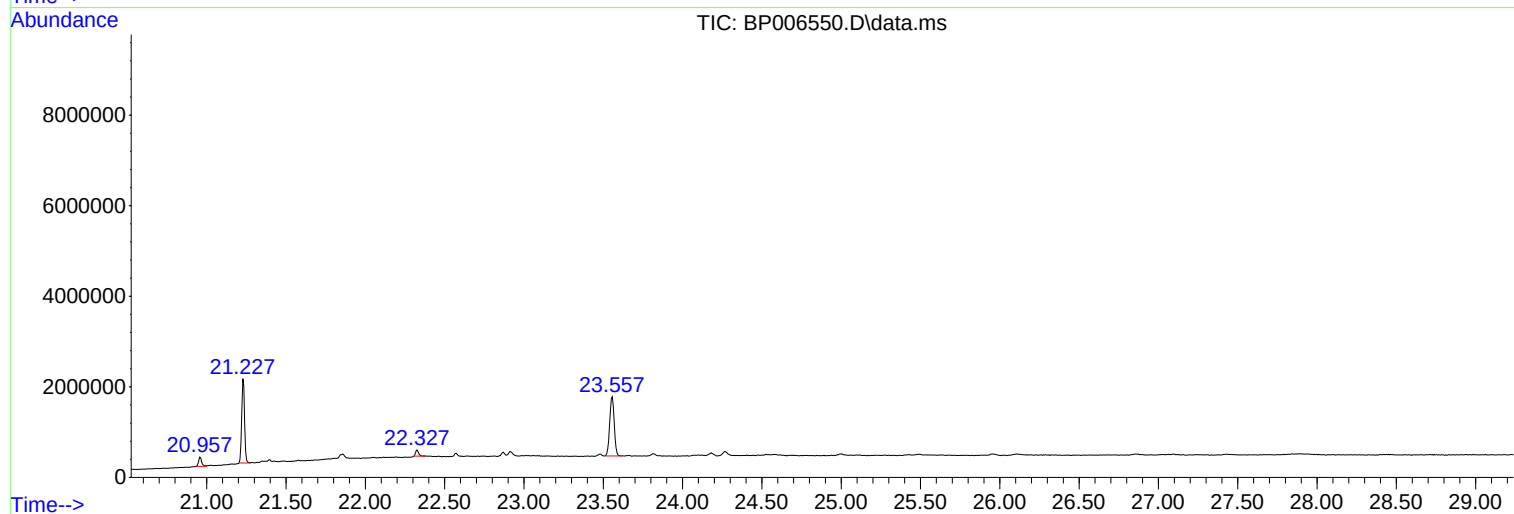
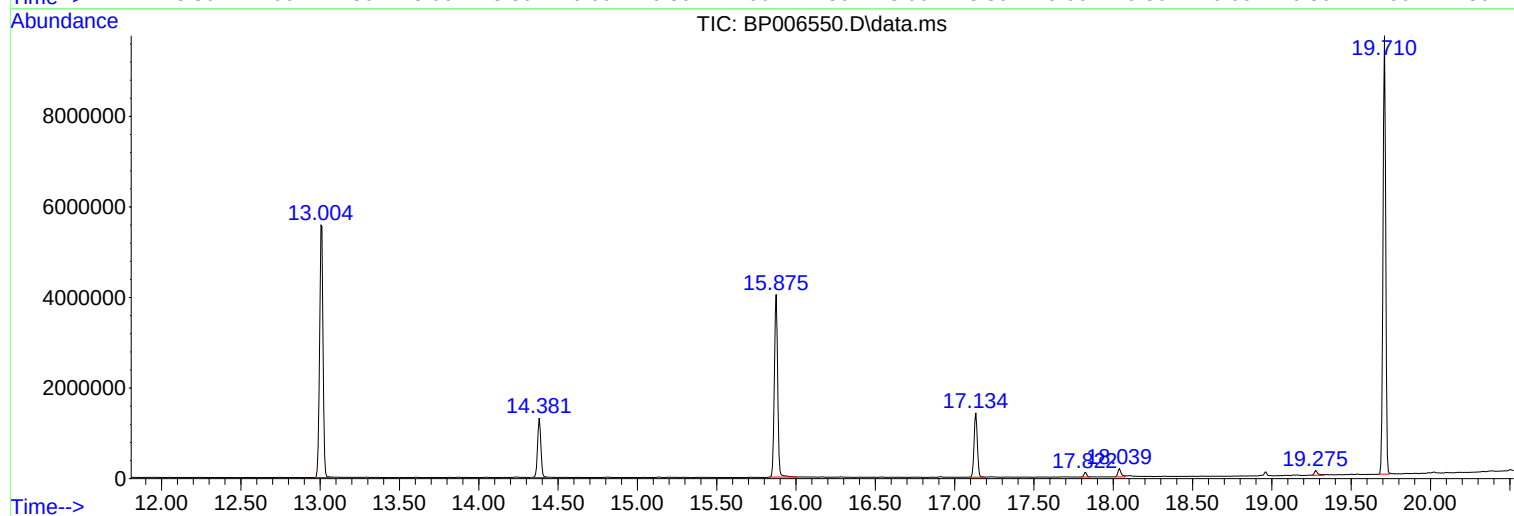
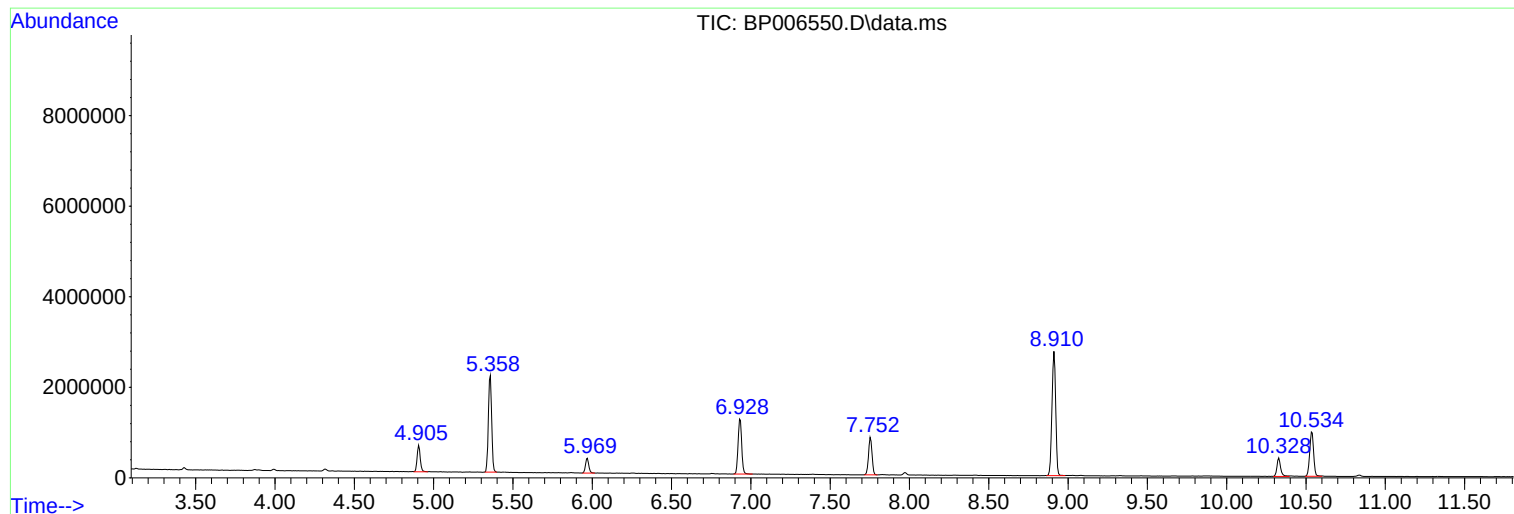
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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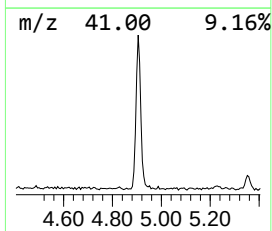
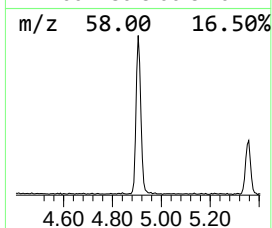
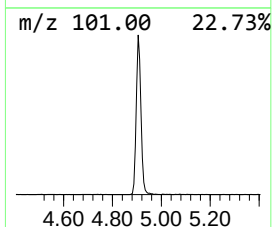
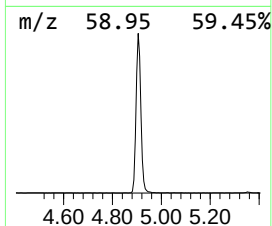
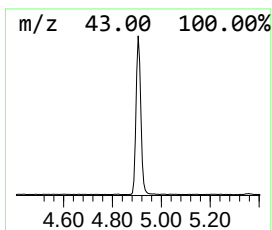
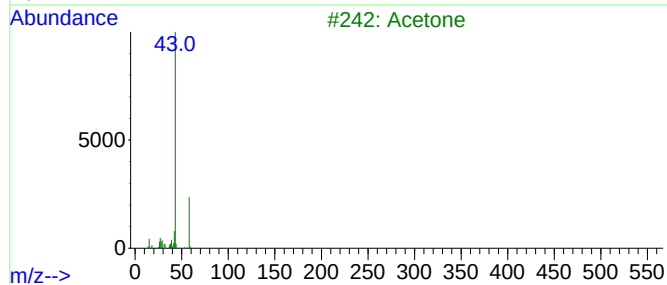
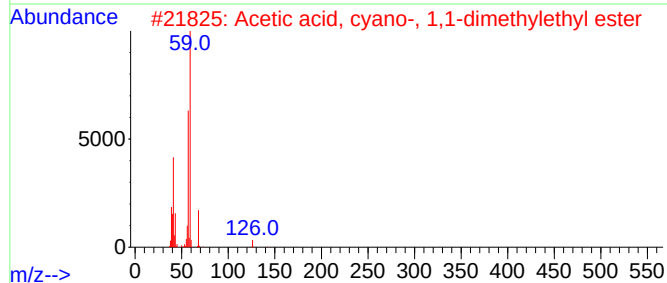
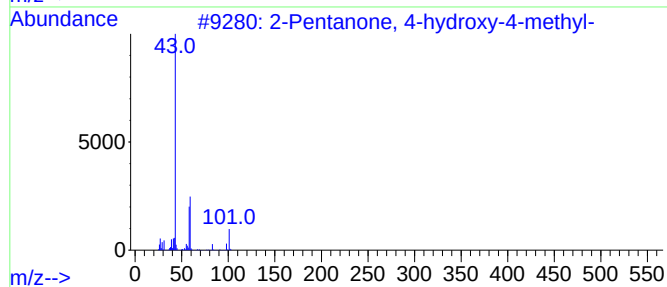
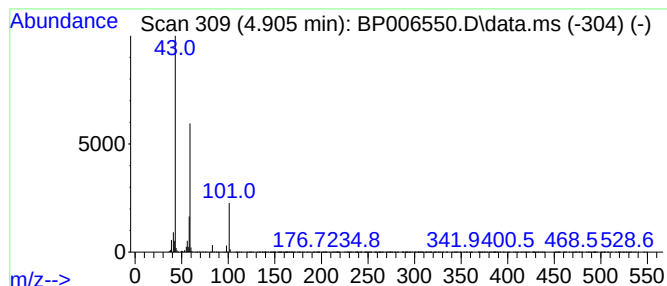
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	12.60 ng	800488	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
3	Acetone	58	C3H6O	000067-64-1	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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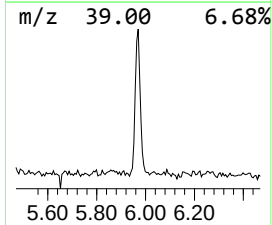
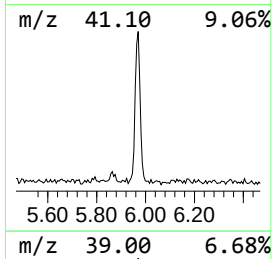
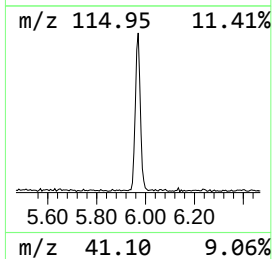
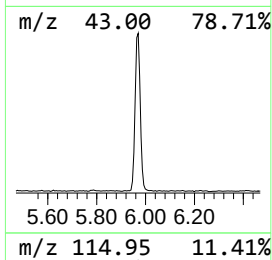
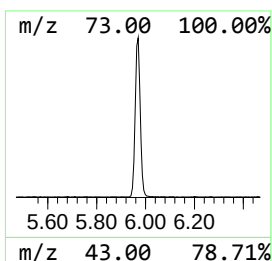
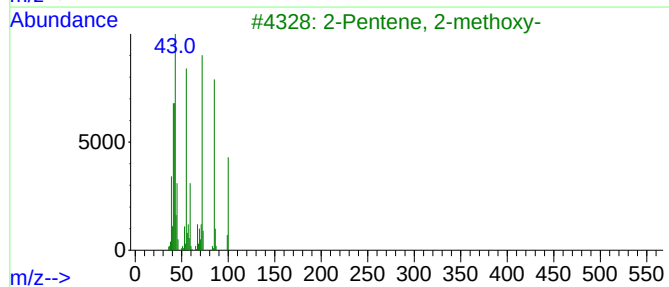
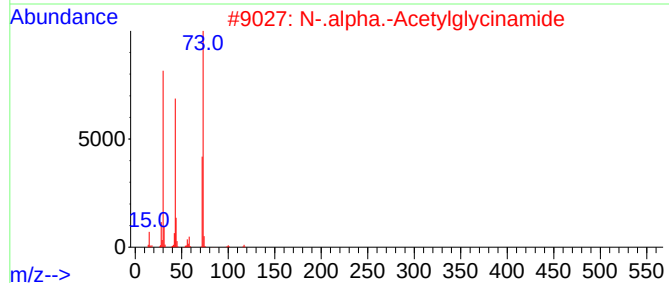
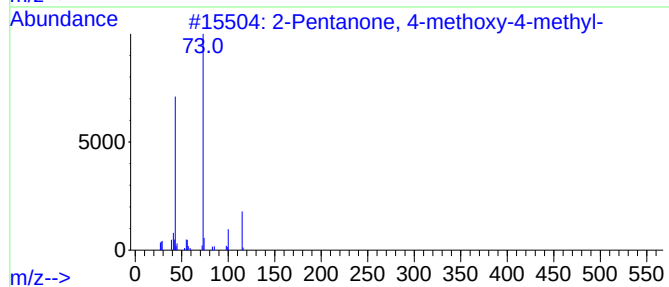
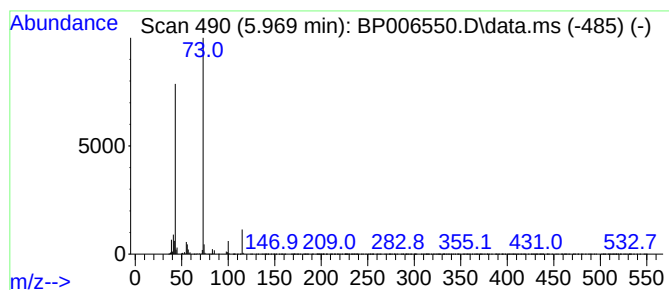
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	7.57 ng	480876	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	40
3			2-Pentene, 2-methoxy-	100	C6H12O	061142-47-0	14
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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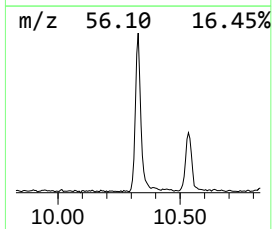
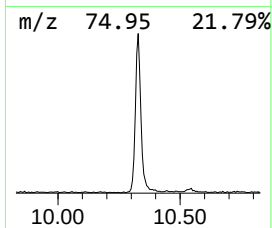
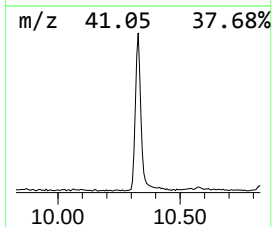
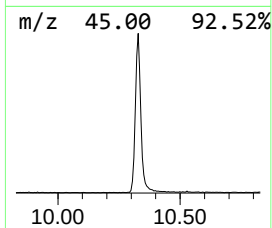
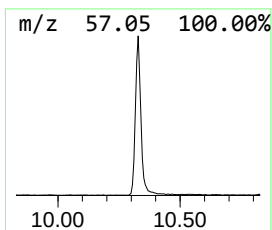
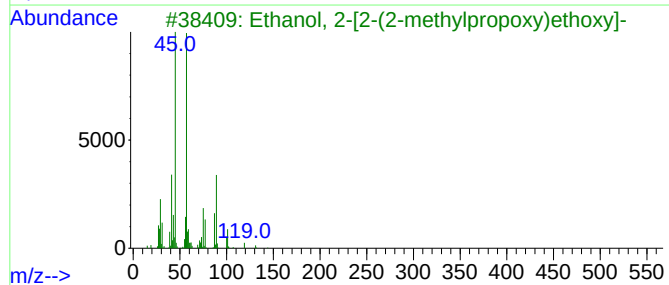
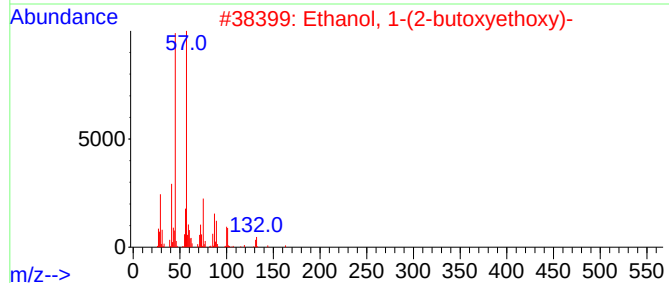
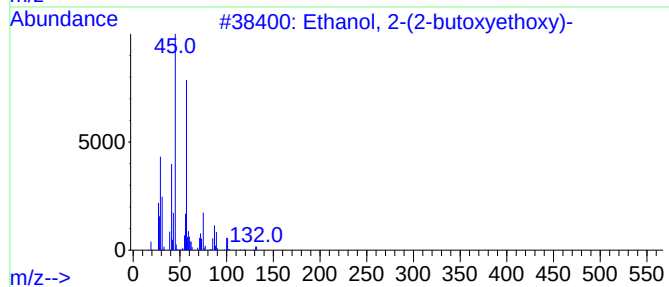
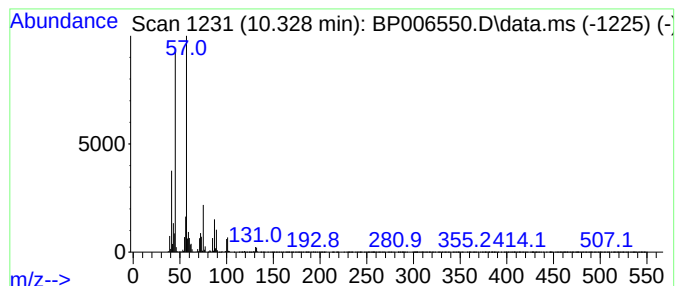
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	7.81 ng	659576	Naphthalene-d8	10.534

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	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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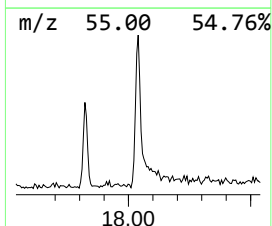
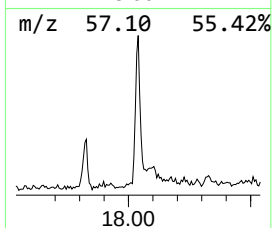
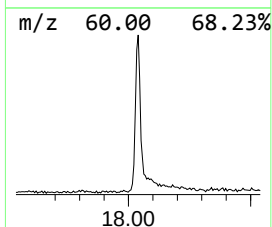
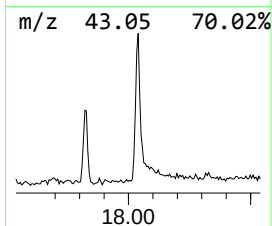
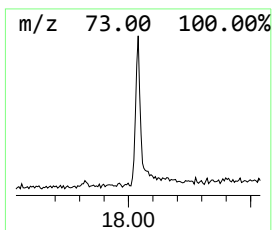
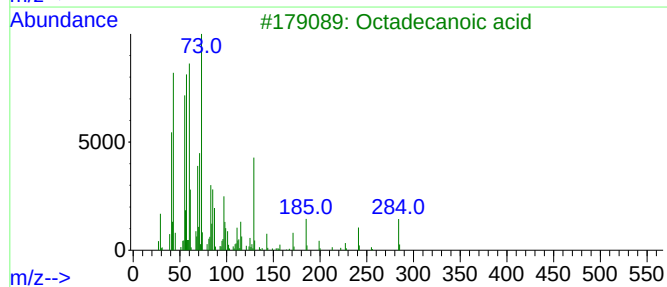
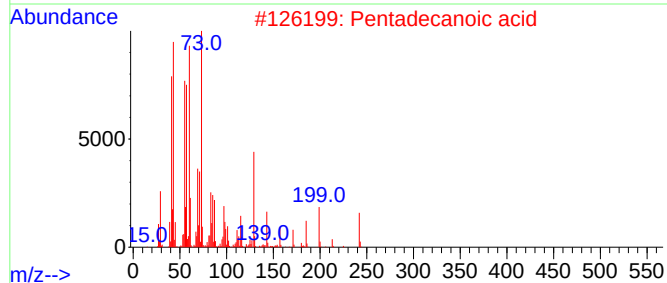
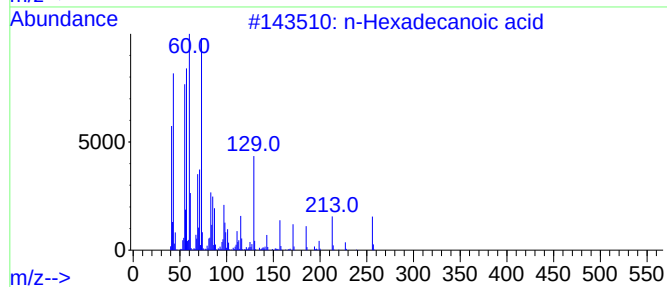
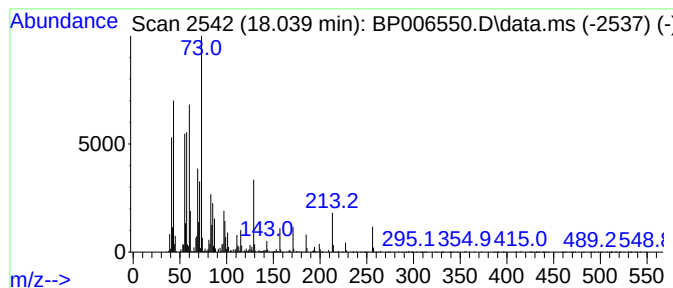
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	2.65 ng	268030	Phenanthrene-d10	17.134

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3			Octadecanoic acid	284	C18H36O2	000057-11-4	70
4			l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	62
5			Hexacosanoic acid	396	C26H52O2	000506-46-7	46



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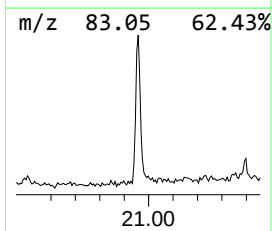
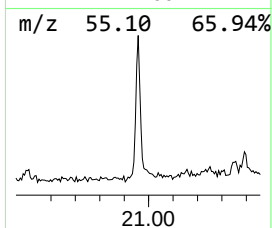
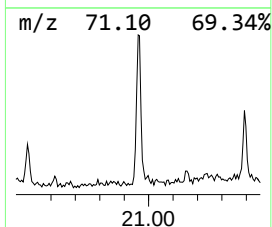
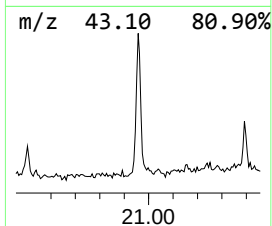
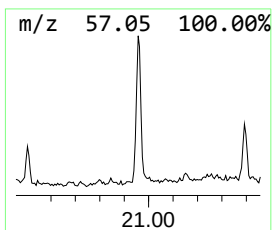
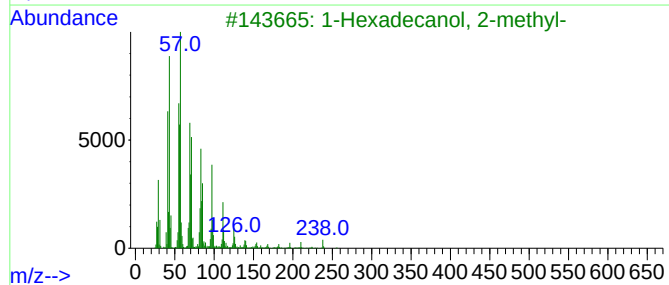
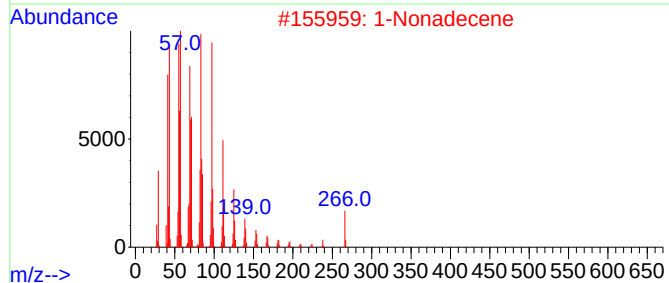
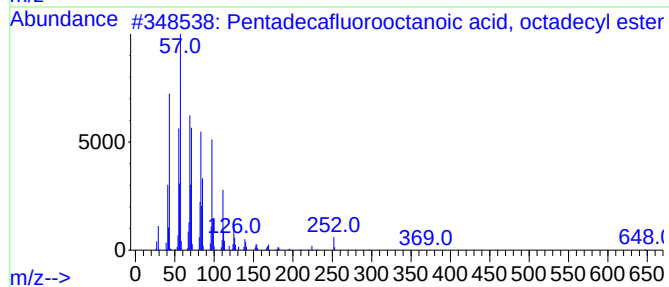
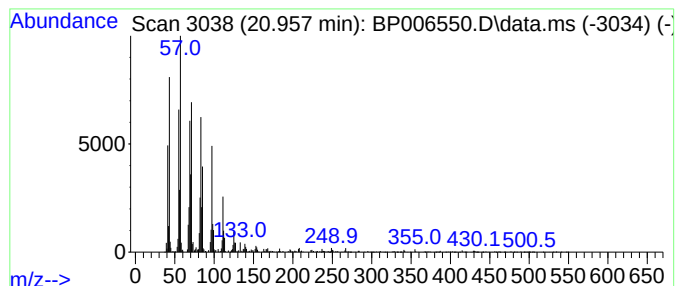
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	2.52 ng	292413	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Nonadecene	266	C19H38	018435-45-5	93
3			1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	93
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.905	12.6	ng	800488	1	7.752	1270680	20.0
2-Pentanone, 4-...	5.969	7.6	ng	480876	1	7.752	1270680	20.0
Ethanol, 2-(2-b...	10.328	7.8	ng	659576	2	10.534	1690130	20.0
n-Hexadecanoic ...	18.039	2.6	ng	268030	4	17.134	2024850	20.0
Pentadecafluoro...	20.957	2.5	ng	292413	5	21.227	2322350	20.0