

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
 Data File : BP006558.D
 Acq On : 07 Aug 2021 02:45
 Operator : CG/JU
 Sample : M3291-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 WC-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_P\Methods\8270E-BP080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006559.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.317	205	209	216	rVB	90712	129346	1.19%	0.204%
2	4.905	304	309	323	rVB	2334869	3337204	30.69%	5.258%
3	5.358	380	386	397	rVB	4372654	6152942	56.58%	9.694%
4	5.969	485	490	502	rVB	449259	661646	6.08%	1.042%
5	6.934	647	654	667	rBV	4158408	6422157	59.05%	10.118%
6	7.752	787	793	801	rVB	901641	1365157	12.55%	2.151%
7	8.910	982	990	1000	rBV	2526088	4151647	38.18%	6.541%
8	10.328	1224	1231	1241	rBV	1008194	1519366	13.97%	2.394%
9	10.534	1259	1266	1276	rVB	1161414	1937331	17.81%	3.052%
10	13.004	1679	1686	1702	rBV	5359152	7920701	72.83%	12.479%
11	14.381	1911	1920	1928	rBV	1615277	2364996	21.75%	3.726%
12	15.869	2167	2173	2183	rBV	4159237	5996386	55.14%	9.448%
13	17.128	2381	2387	2400	rBV	1820569	2680387	24.65%	4.223%
14	17.822	2500	2505	2513	rBV	187440	216093	1.99%	0.340%
15	18.039	2537	2542	2551	rBV	330227	492374	4.53%	0.776%
16	18.957	2695	2698	2702	rVB	151760	158474	1.46%	0.250%
17	19.275	2748	2752	2762	rBV	144899	216693	1.99%	0.341%
18	19.710	2820	2826	2831	rBV	8670053	10875189	100.00%	17.134%
19	20.951	3033	3037	3045	rBV	563894	770332	7.08%	1.214%
20	21.227	3079	3084	3089	rBV	2402001	2849579	26.20%	4.490%
21	21.392	3109	3112	3118	rVB	133376	142959	1.31%	0.225%
22	21.845	3186	3189	3196	rVB3	112596	161760	1.49%	0.255%
23	23.551	3473	3479	3491	rVB2	1495925	2947144	27.10%	4.643%

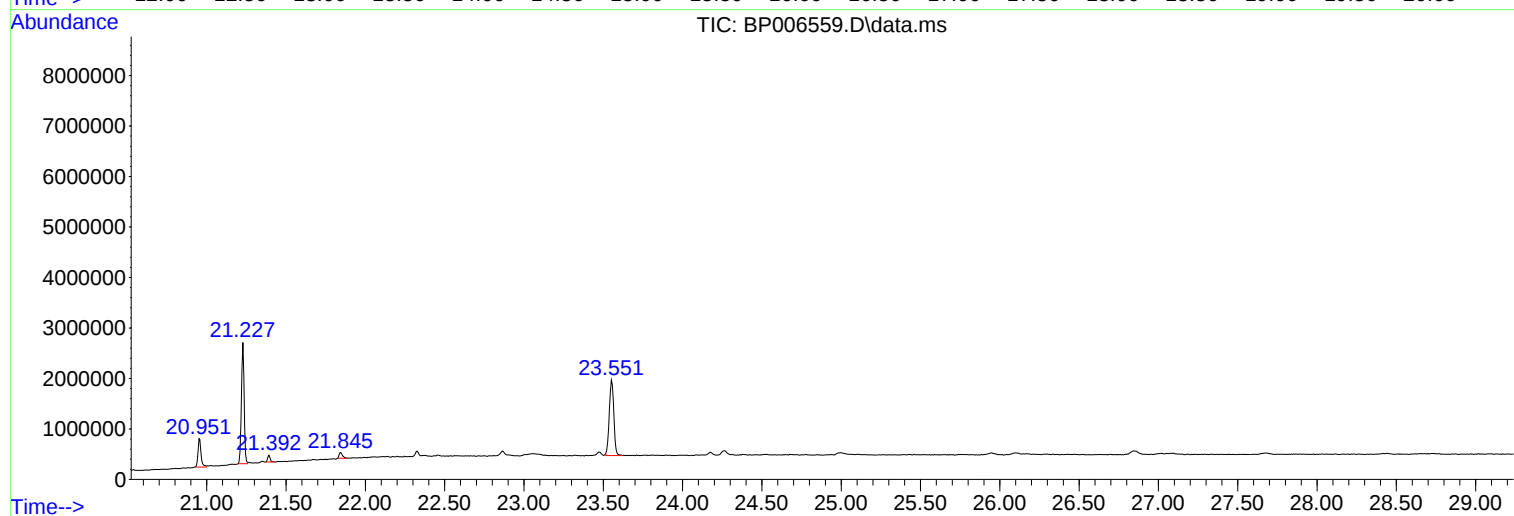
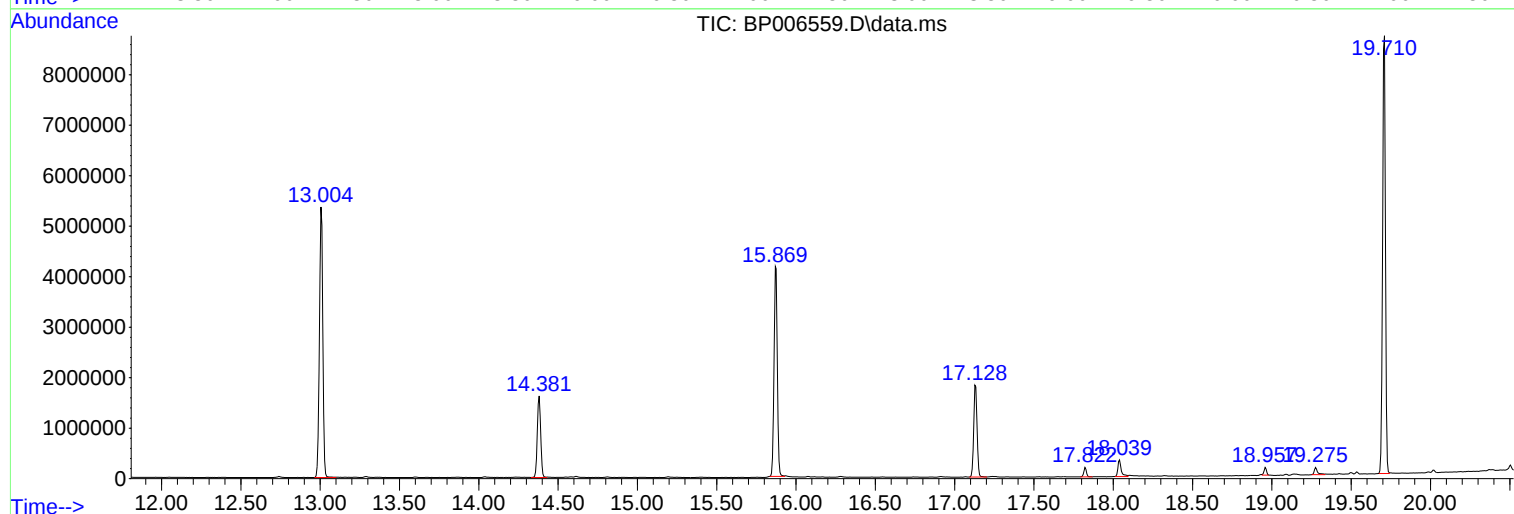
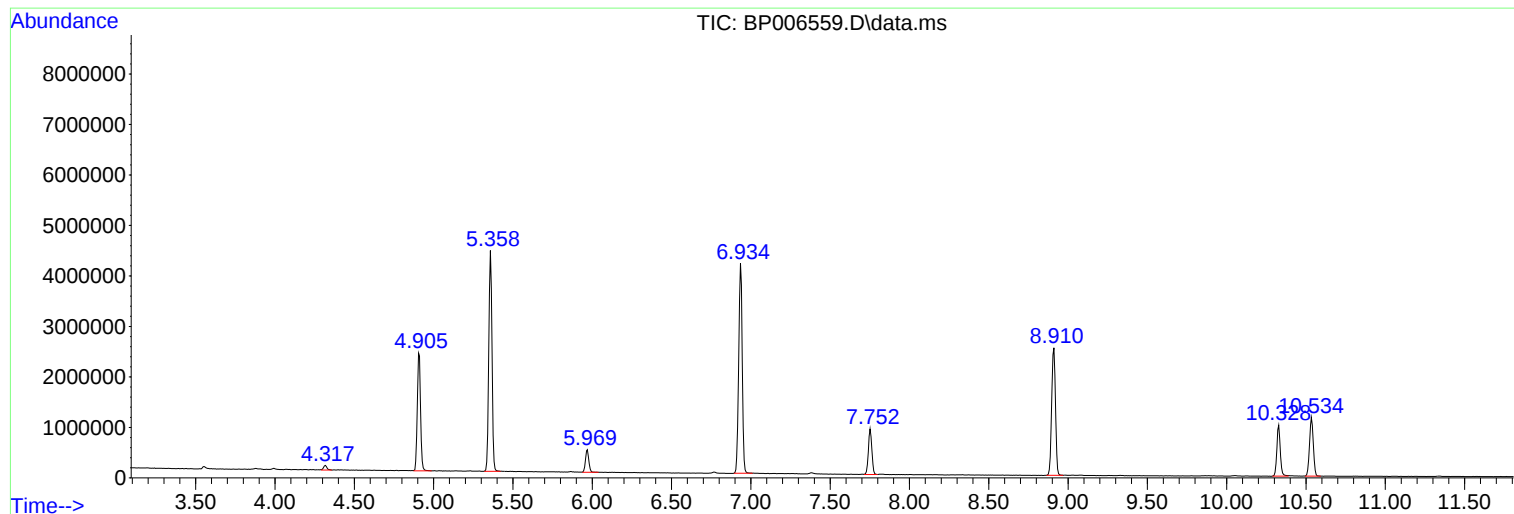
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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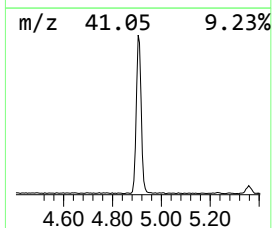
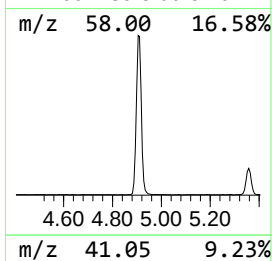
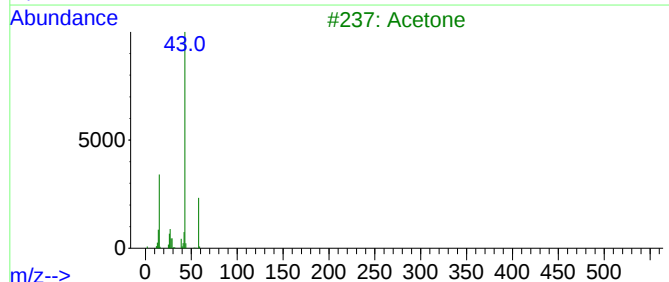
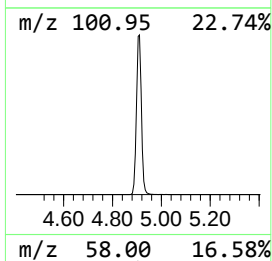
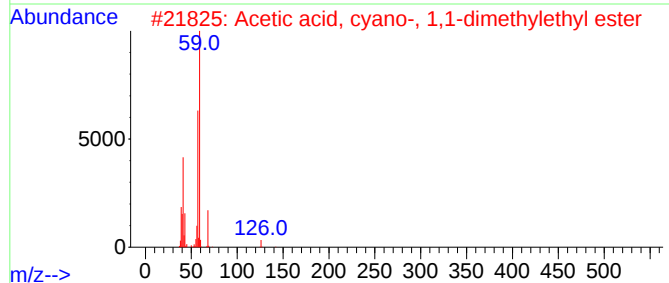
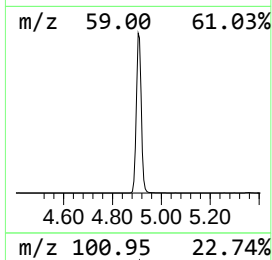
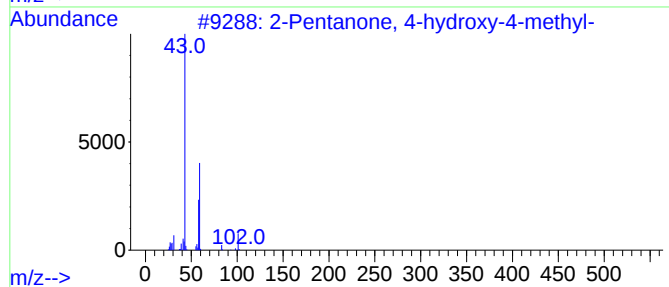
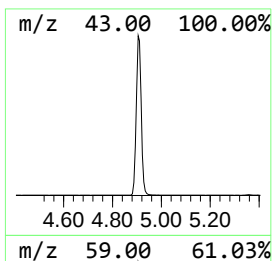
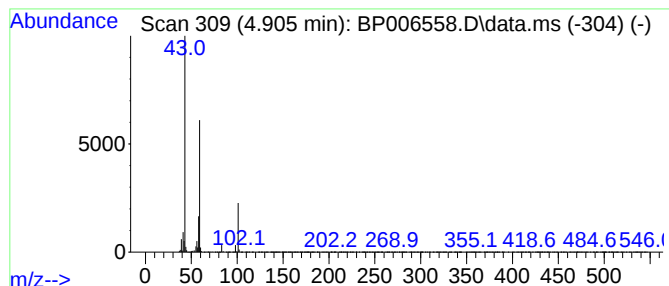
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	48.89 ng	3337200	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	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	Acetone	58	C3H6O	000067-64-1	10		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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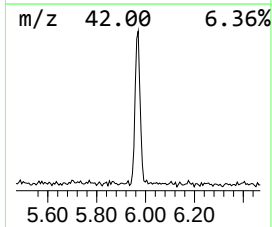
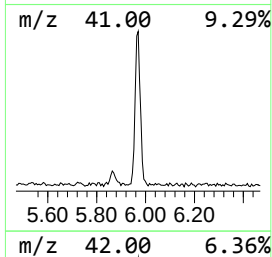
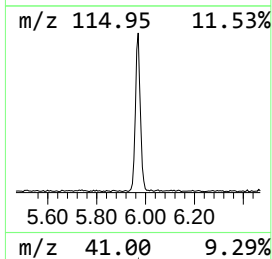
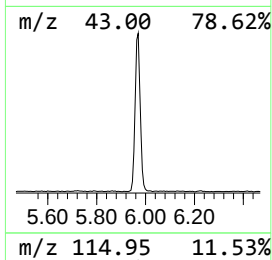
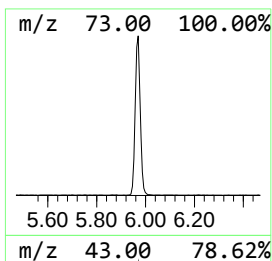
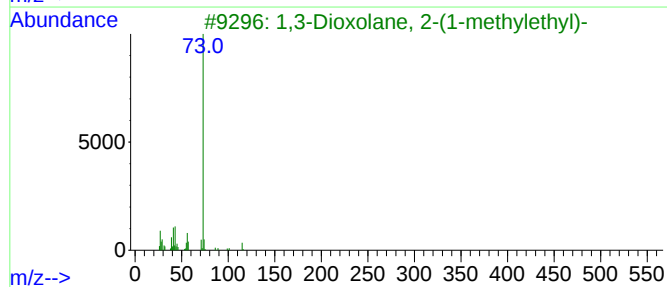
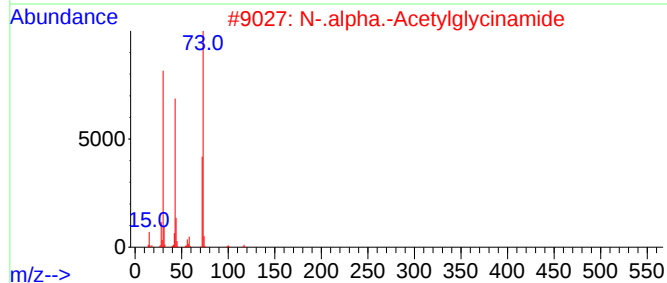
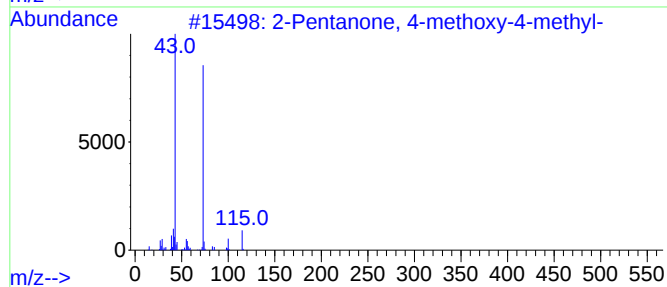
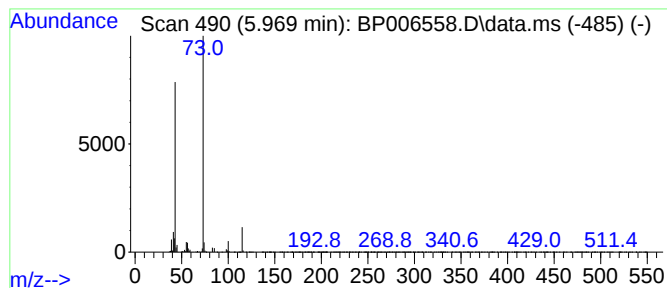
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	9.69 ng	661646	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			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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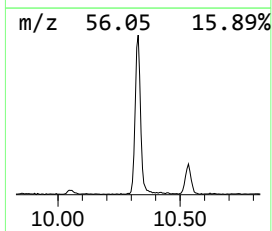
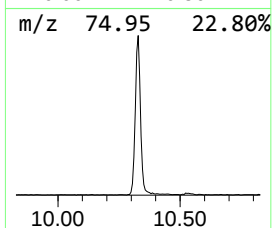
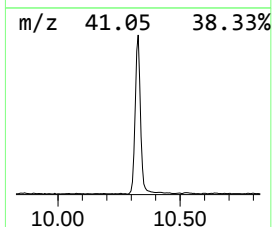
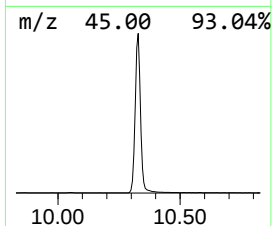
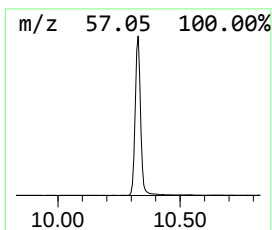
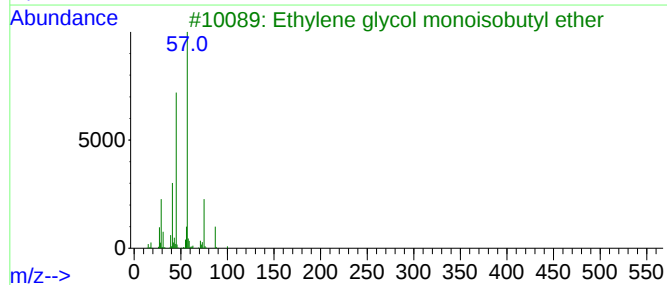
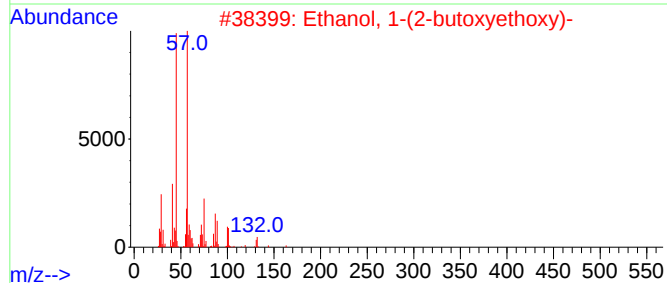
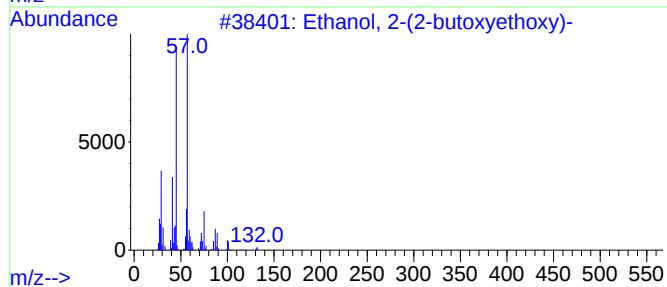
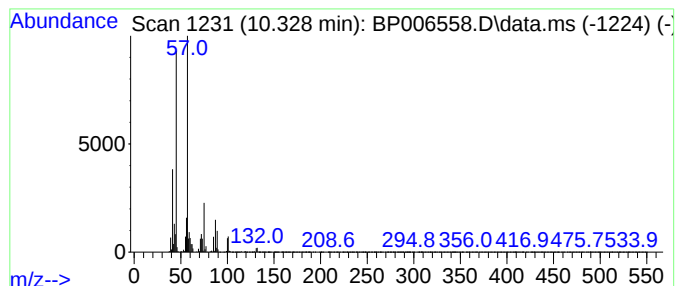
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	15.69 ng	1519370	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	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	47



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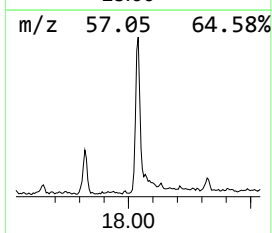
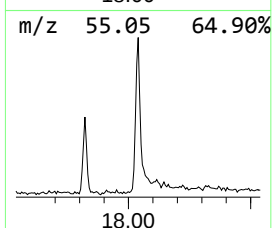
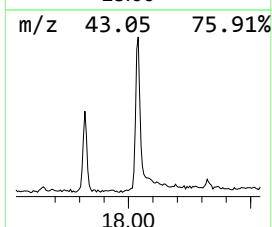
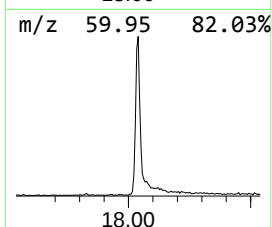
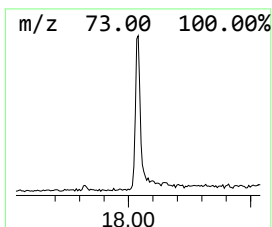
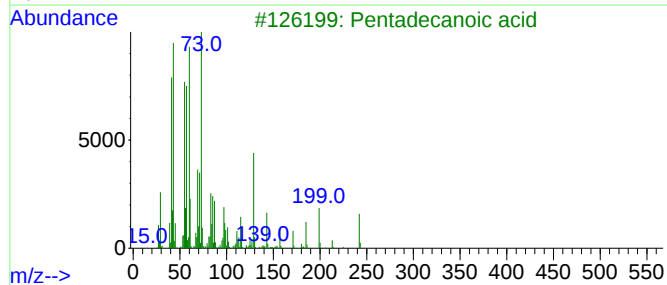
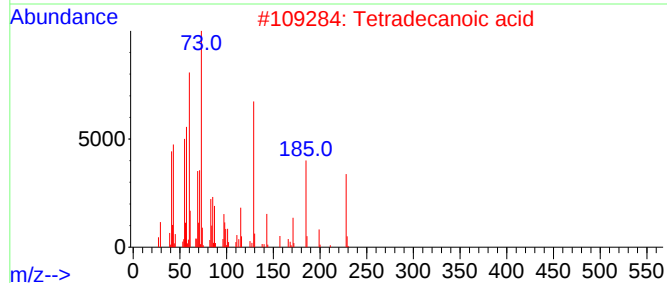
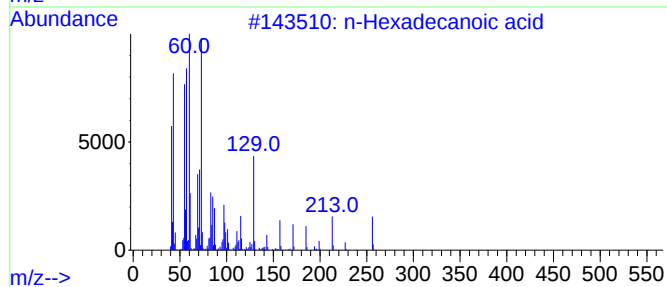
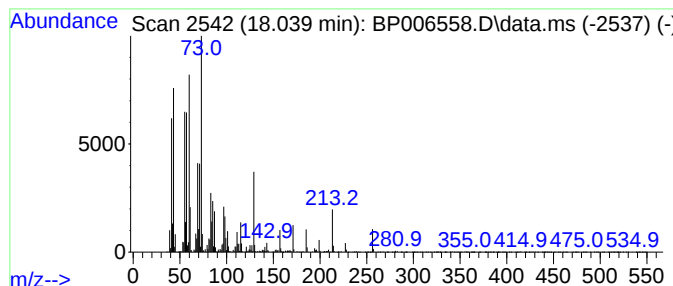
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	3.67 ng	492374	Phenanthrene-d10	17.128

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Octadecanoic acid	284	C18H36O2	000057-11-4	87
5		Tridecanoic acid	214	C13H26O2	000638-53-9	68



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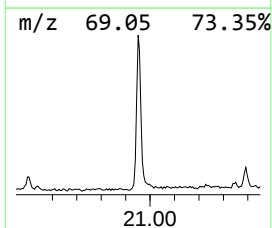
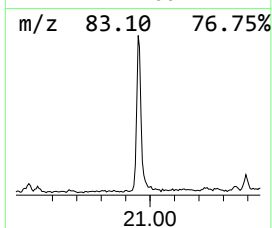
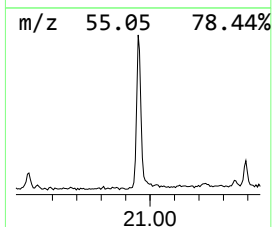
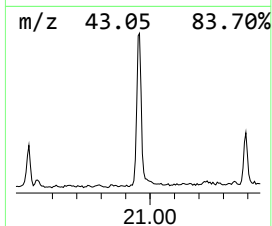
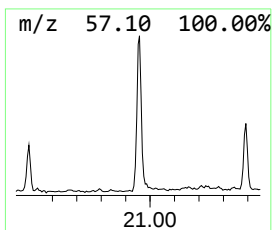
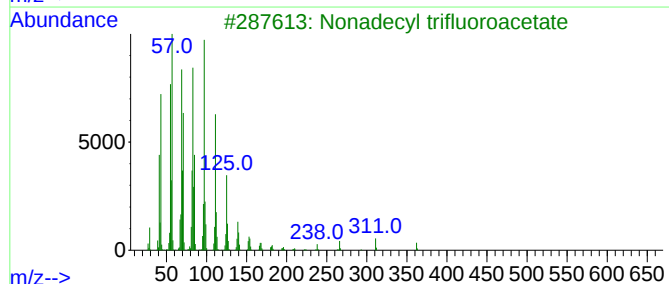
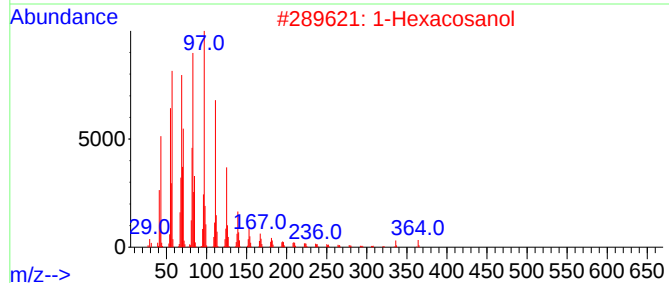
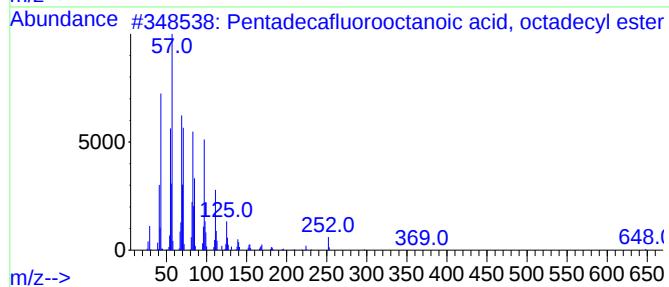
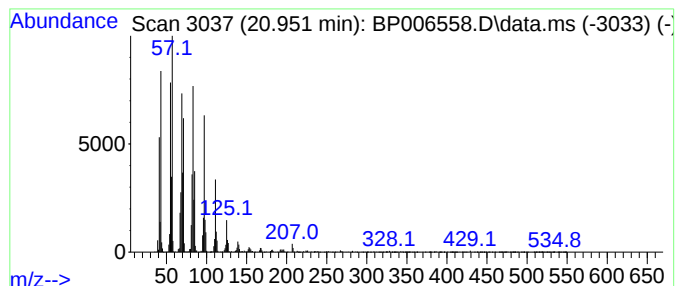
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.951	5.41 ng	770332	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-Hexacosanol	382	C26H54O	000506-52-5	91
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.905	48.9	ng	3337200	1	7.752	1365160	20.0
2-Pentanone, 4-...	5.969	9.7	ng	661646	1	7.752	1365160	20.0
Ethanol, 2-(2-b...	10.328	15.7	ng	1519370	2	10.534	1937330	20.0
n-Hexadecanoic ...	18.039	3.7	ng	492374	4	17.128	2680390	20.0
Pentadecafluoro...	20.951	5.4	ng	770332	5	21.227	2849580	20.0