

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
 Data File : BP006521.D
 Acq On : 05 Aug 2021 23:46
 Operator : CG/JU
 Sample : M3279-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20210572-COM-45

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: BP006521.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	rBV	1923018	2779691	27.56%	4.190%
2	5.358	380	386	395	rBV	5248947	7290742	72.29%	10.989%
3	5.969	485	490	497	rVB	413701	599859	5.95%	0.904%
4	6.934	647	654	667	rVB	4823438	7729057	76.63%	11.649%
5	7.757	786	794	801	rBV	909027	1440505	14.28%	2.171%
6	8.910	982	990	1005	rBV	2949225	4904626	48.63%	7.392%
7	10.328	1225	1231	1251	rBV	493378	813651	8.07%	1.226%
8	10.540	1259	1267	1274	rBV	1231410	2036532	20.19%	3.069%
9	13.010	1678	1687	1701	rBV	5763955	8352832	82.82%	12.589%
10	14.381	1911	1920	1929	rBV	1650974	2533263	25.12%	3.818%
11	15.875	2168	2174	2190	rBV	5270156	7310152	72.48%	11.018%
12	17.133	2382	2388	2402	rBV	2009340	2881645	28.57%	4.343%
13	18.039	2537	2542	2551	rBV	239147	350129	3.47%	0.528%
14	19.151	2726	2731	2737	rBV	58873	107940	1.07%	0.163%
15	19.274	2749	2752	2759	rBV2	102674	154040	1.53%	0.232%
16	19.710	2820	2826	2831	rBV	8606810	10085779	100.00%	15.201%
17	20.957	3034	3038	3048	rBV	385676	555553	5.51%	0.837%
18	21.157	3069	3072	3076	rBV	141137	139168	1.38%	0.210%
19	21.227	3079	3084	3095	rBV	2359285	3163210	31.36%	4.768%
20	23.557	3473	3480	3491	rVB2	1574802	3119742	30.93%	4.702%

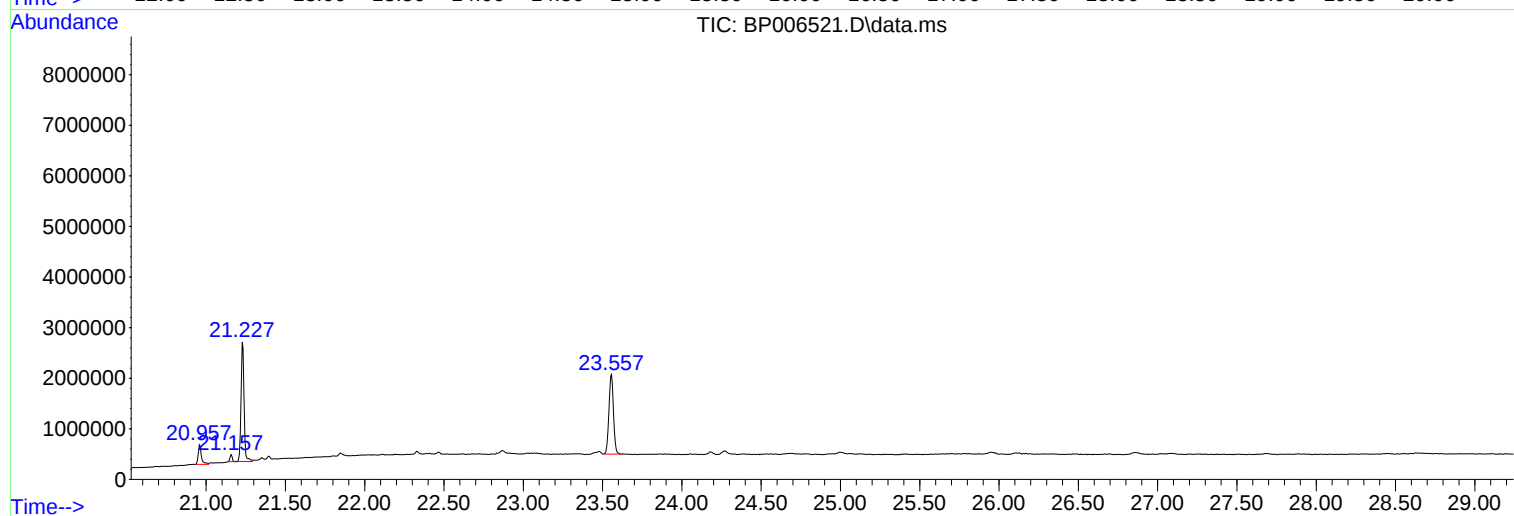
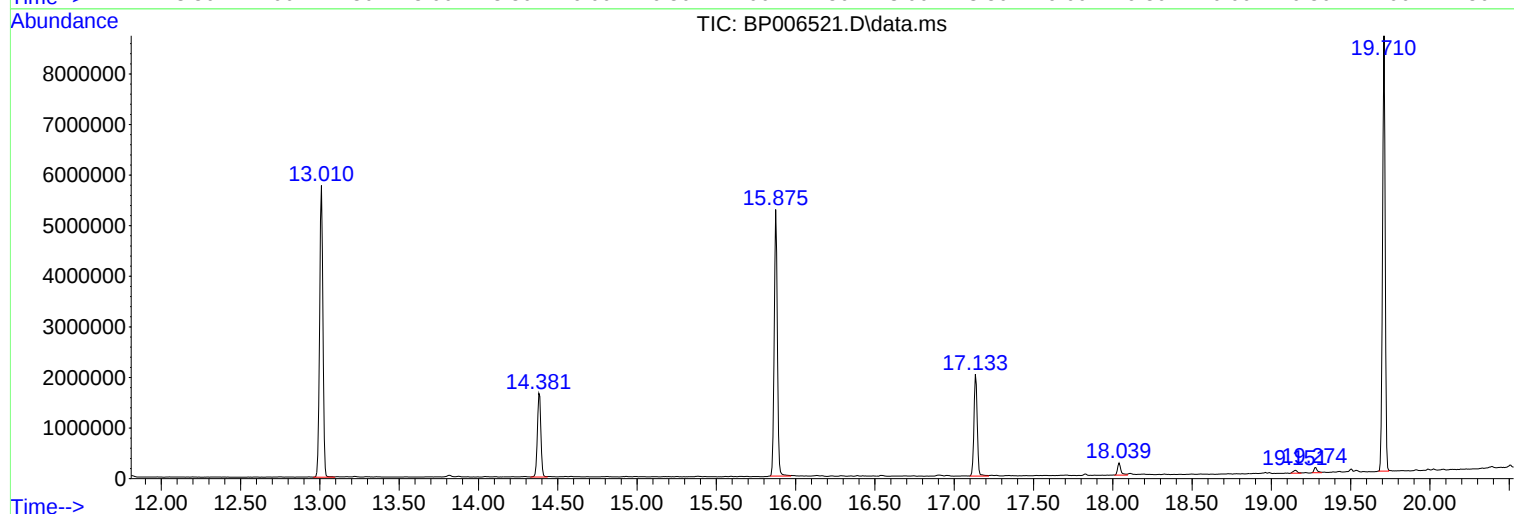
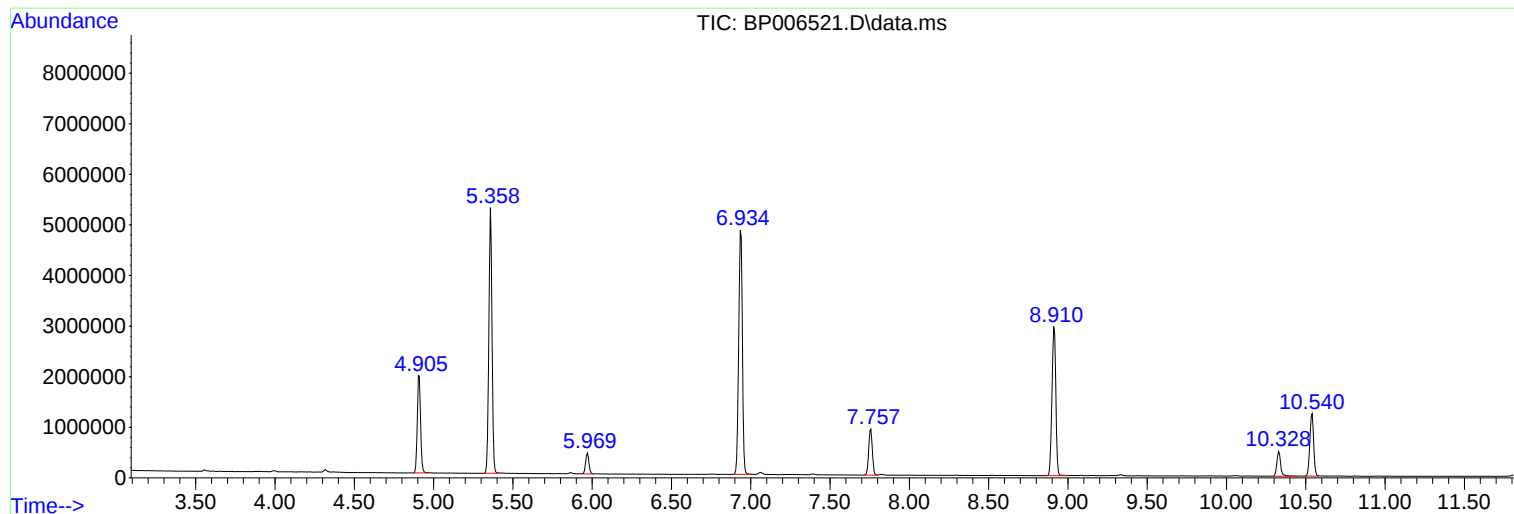
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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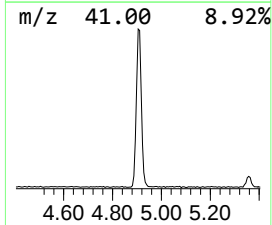
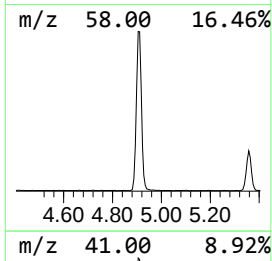
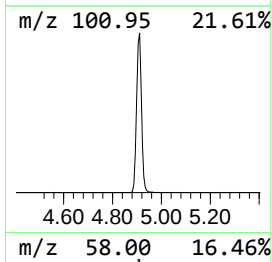
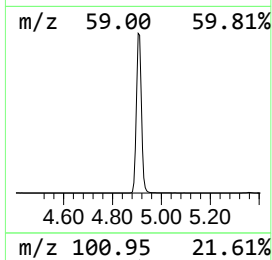
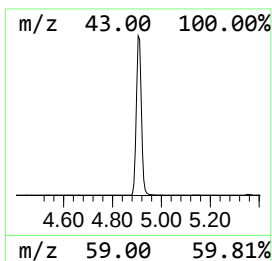
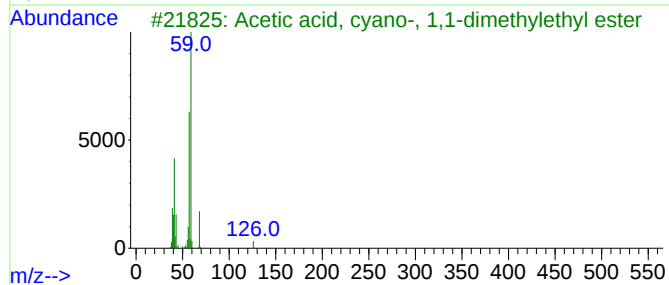
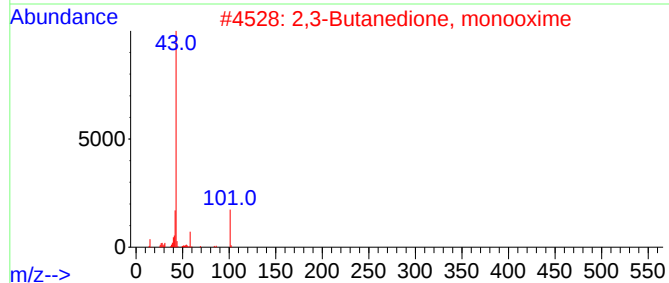
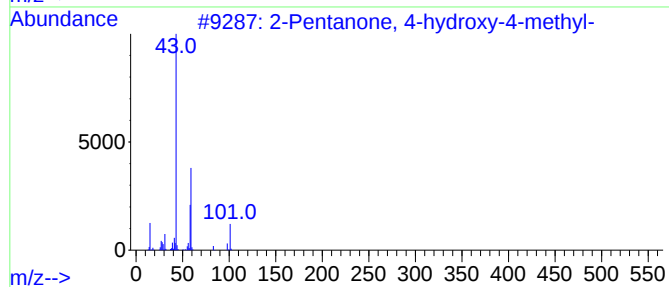
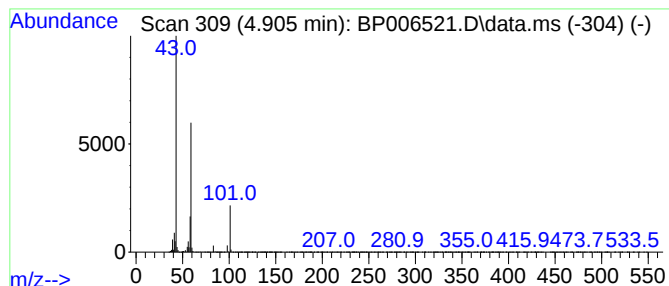
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	38.59 ng	2779690	1,4-Dichlorobenzene-d4	7.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Acetone	58	C3H6O	000067-64-1	10		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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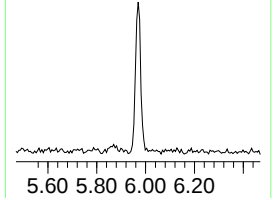
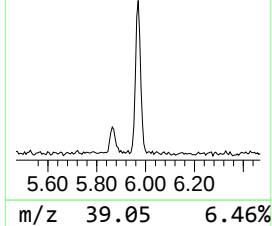
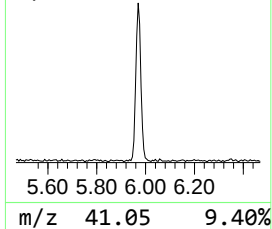
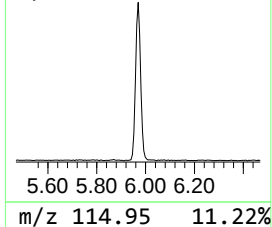
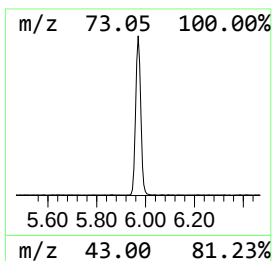
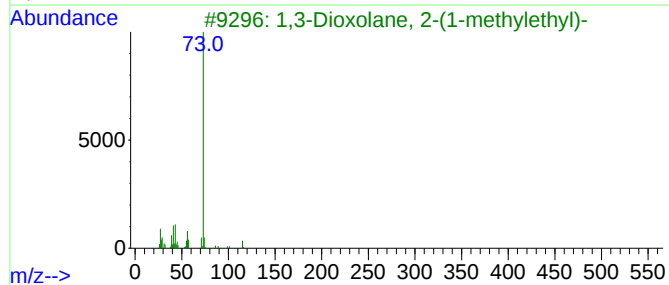
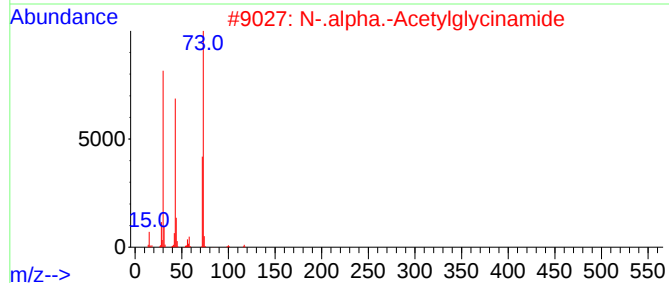
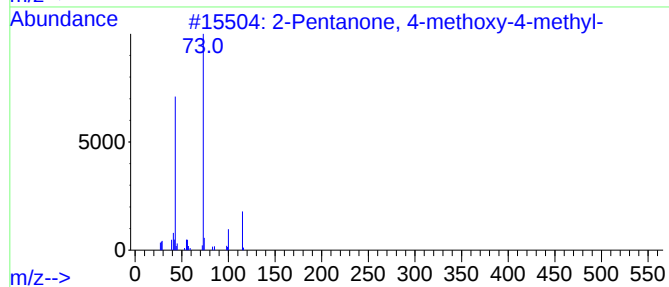
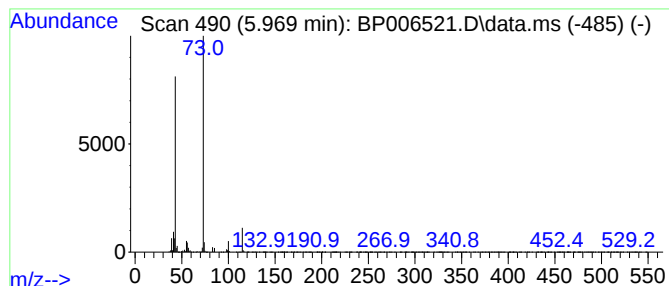
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	8.33 ng	599859	1,4-Dichlorobenzene-d4	7.757

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	33
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5			Ethanone, 1-(3-ethyloxiranyl)-	114	C6H10O2	017257-81-7	10



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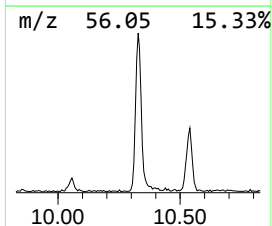
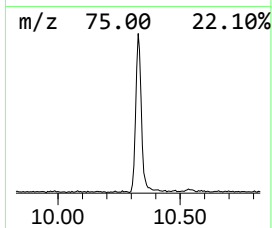
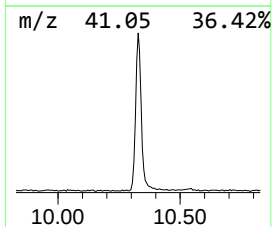
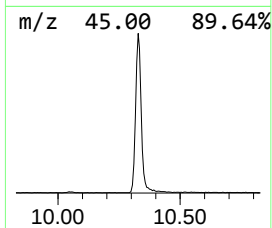
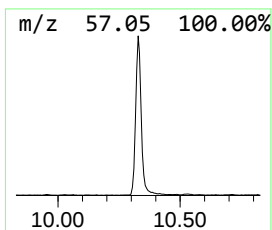
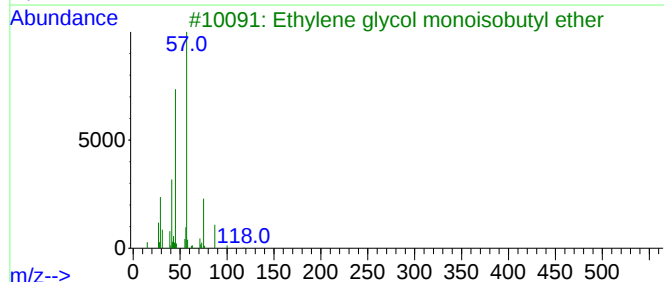
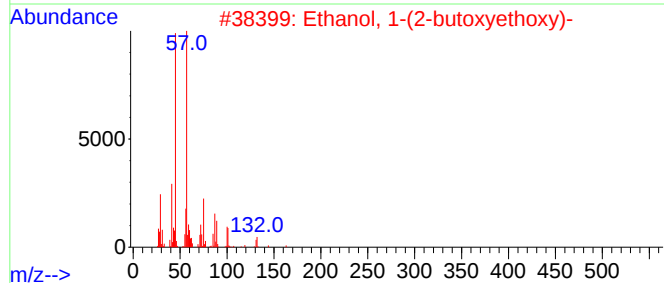
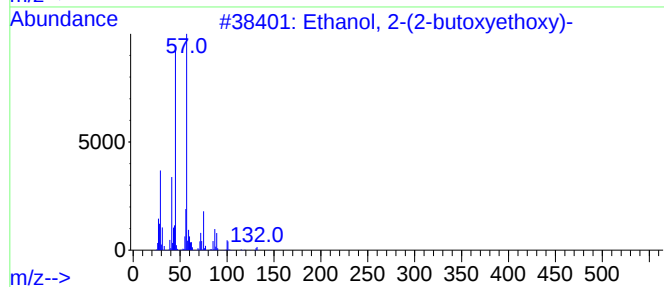
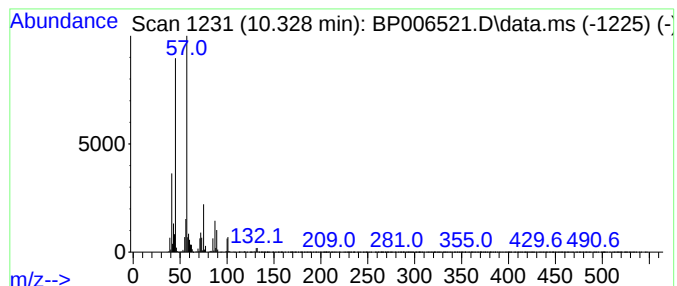
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	7.99 ng	813651	Naphthalene-d8	10.540

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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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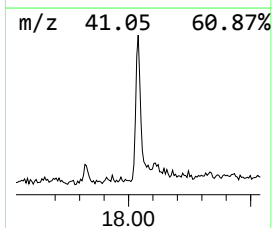
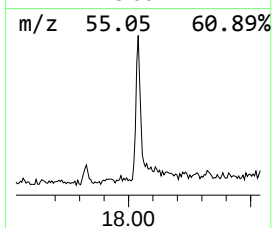
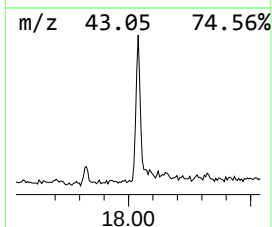
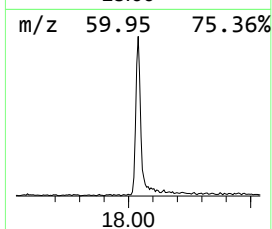
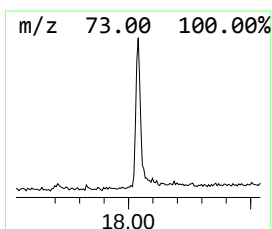
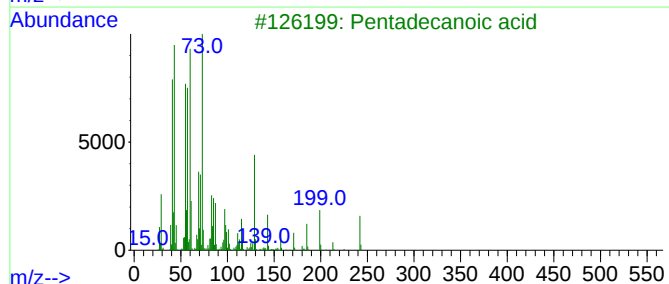
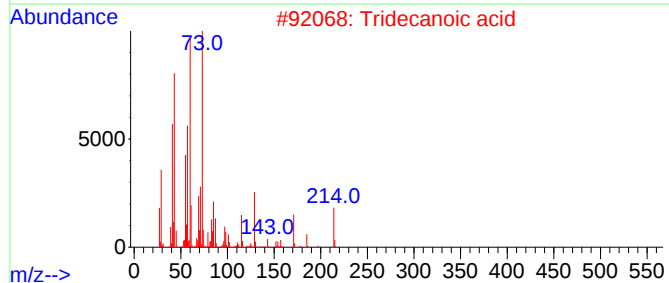
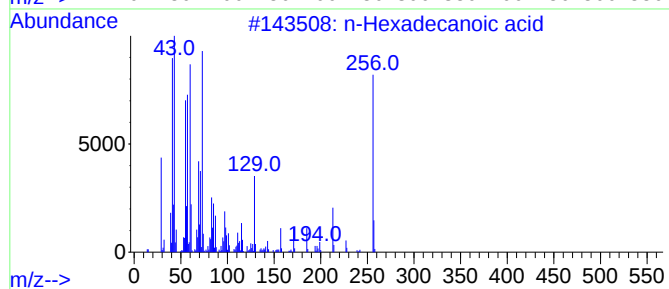
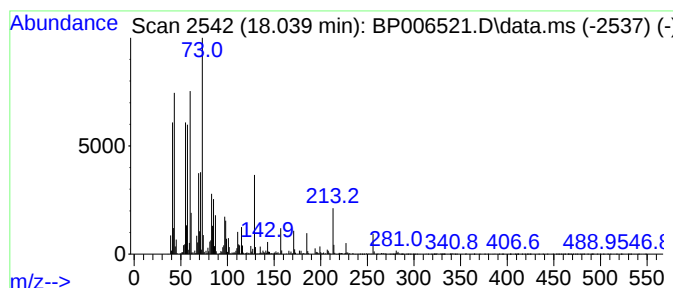
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	2.43 ng	350129	Phenanthrene-d10	17.133

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Octadecanoic acid	284	C18H36O2	000057-11-4	64
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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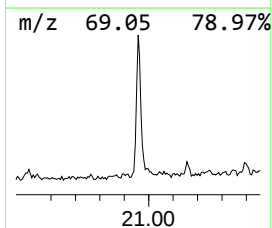
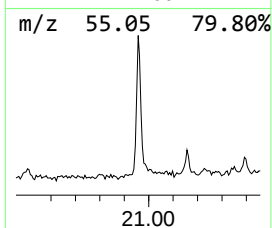
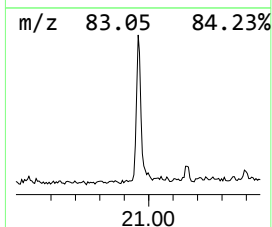
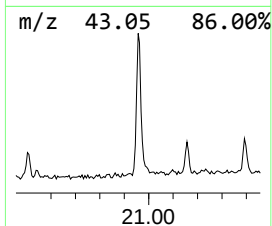
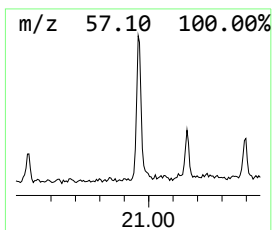
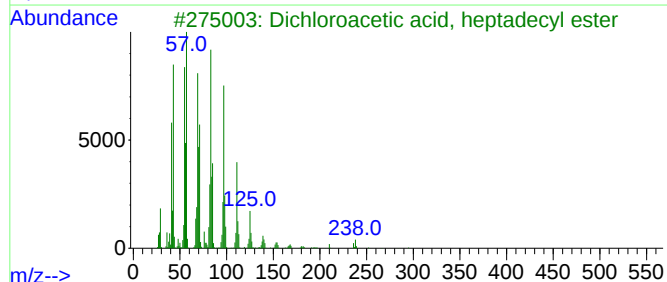
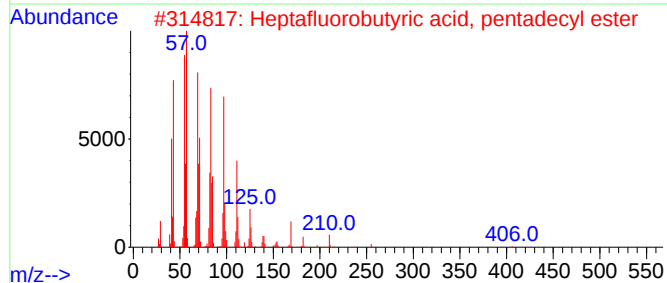
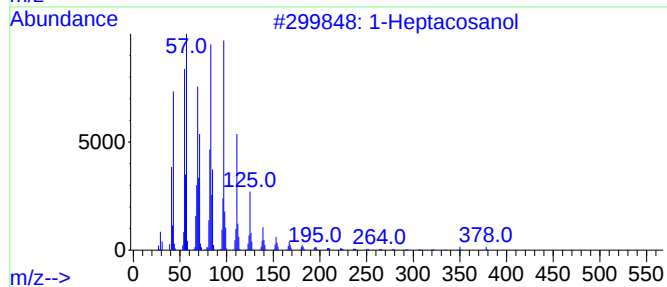
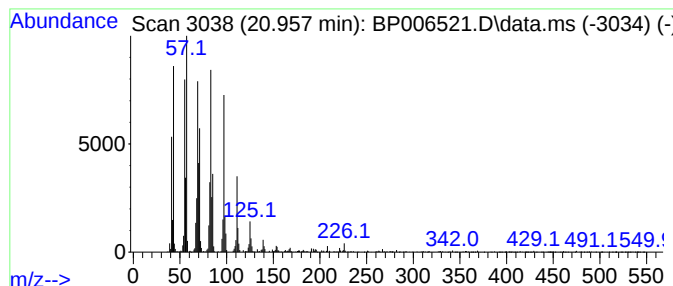
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Peak Number 5 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.51 ng	555553	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.905	38.6	ng	2779690	1	7.757	1440510	20.0
2-Pentanone, 4-...	5.969	8.3	ng	599859	1	7.757	1440510	20.0
Ethanol, 2-(2-b...	10.328	8.0	ng	813651	2	10.540	2036530	20.0
n-Hexadecanoic ...	18.039	2.4	ng	350129	4	17.133	2881650	20.0
1-Heptacosanol	20.957	3.5	ng	555553	5	21.227	3163210	20.0