

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080621\
 Data File : BP006557.D
 Acq On : 07 Aug 2021 02:11
 Operator : CG/JU
 Sample : M3279-07
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20210577-COM-50

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: BP006558.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	320	rVB	2061116	2869245	23.79%	4.289%
2	5.358	380	386	394	rBV	5343636	7470984	61.94%	11.168%
3	5.969	485	490	498	rVB	409751	609080	5.05%	0.911%
4	6.934	647	654	666	rBV	4853216	7640516	63.34%	11.422%
5	7.752	787	793	801	rVB	887353	1342345	11.13%	2.007%
6	8.910	982	990	1000	rBV	3035398	4921175	40.80%	7.357%
7	10.328	1224	1231	1247	rBV	597510	940941	7.80%	1.407%
8	10.534	1258	1266	1273	rBV	1168613	1841818	15.27%	2.753%
9	13.004	1677	1686	1699	rBV	5950194	8908672	73.86%	13.317%
10	14.381	1909	1920	1929	rBV	1540791	2191154	18.17%	3.276%
11	15.875	2167	2174	2190	rBV	4884534	6991224	57.96%	10.451%
12	17.133	2381	2388	2401	rBV	1688713	2501700	20.74%	3.740%
13	18.033	2537	2541	2551	rBV	185756	299297	2.48%	0.447%
14	19.704	2820	2825	2831	rBV	9925777	12062133	100.00%	18.031%
15	20.951	3033	3037	3045	rBV	403856	565461	4.69%	0.845%
16	21.227	3079	3084	3092	rBV	2266709	2784152	23.08%	4.162%
17	23.551	3473	3479	3488	rVB2	1509274	2954983	24.50%	4.417%

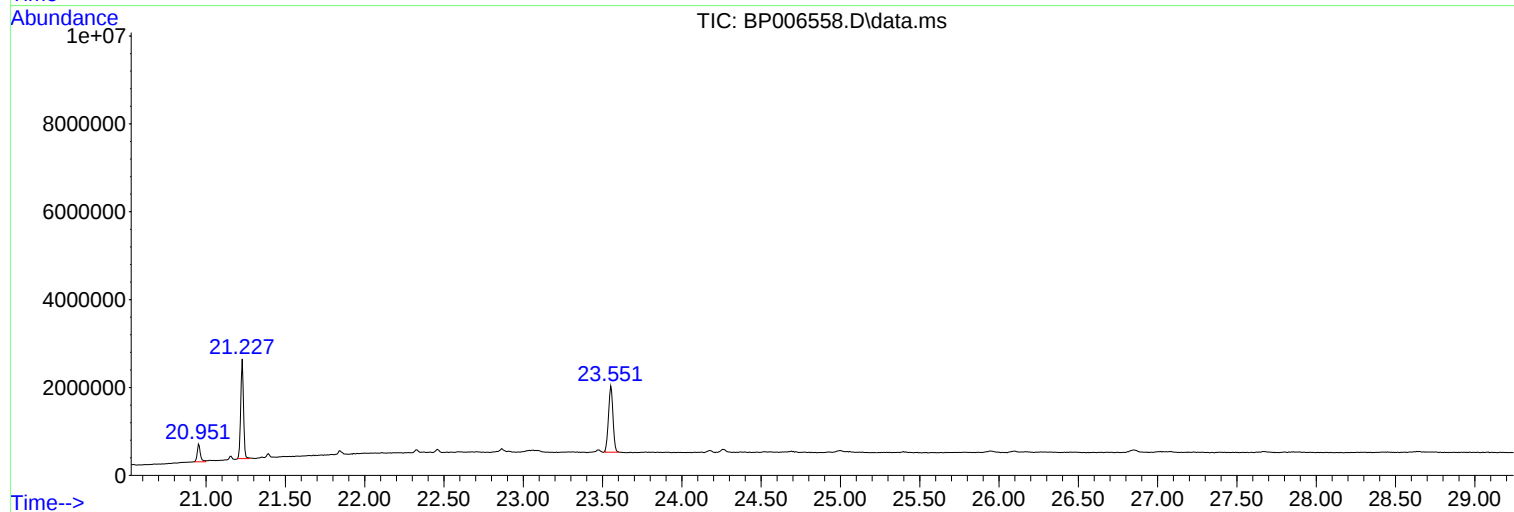
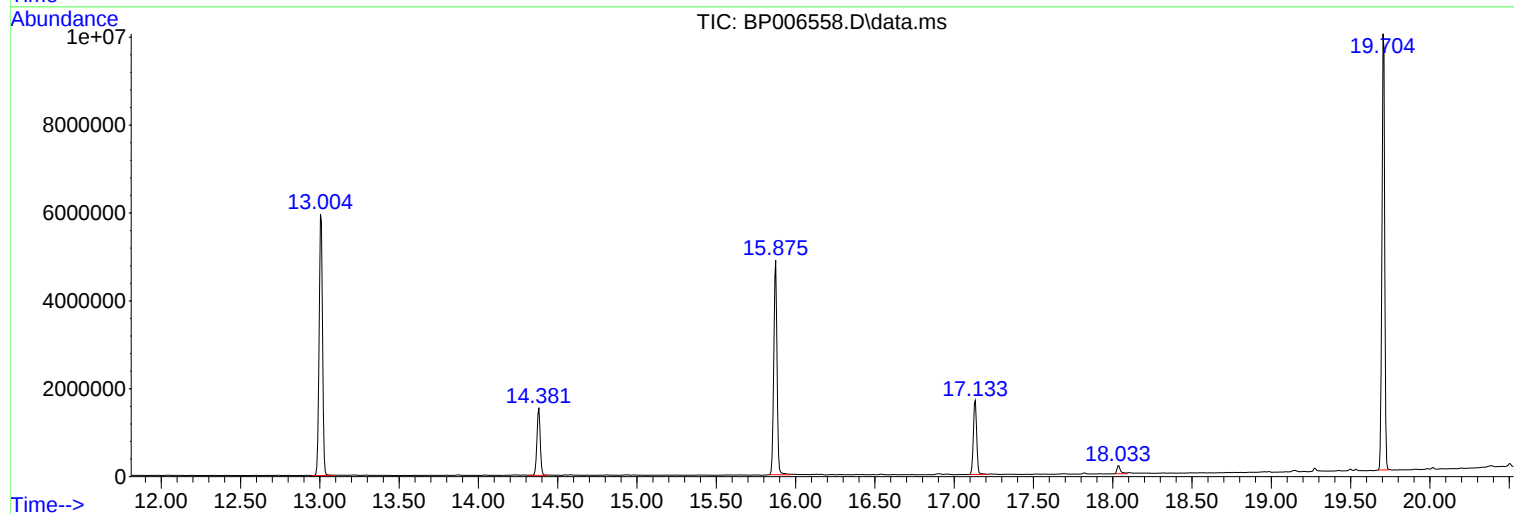
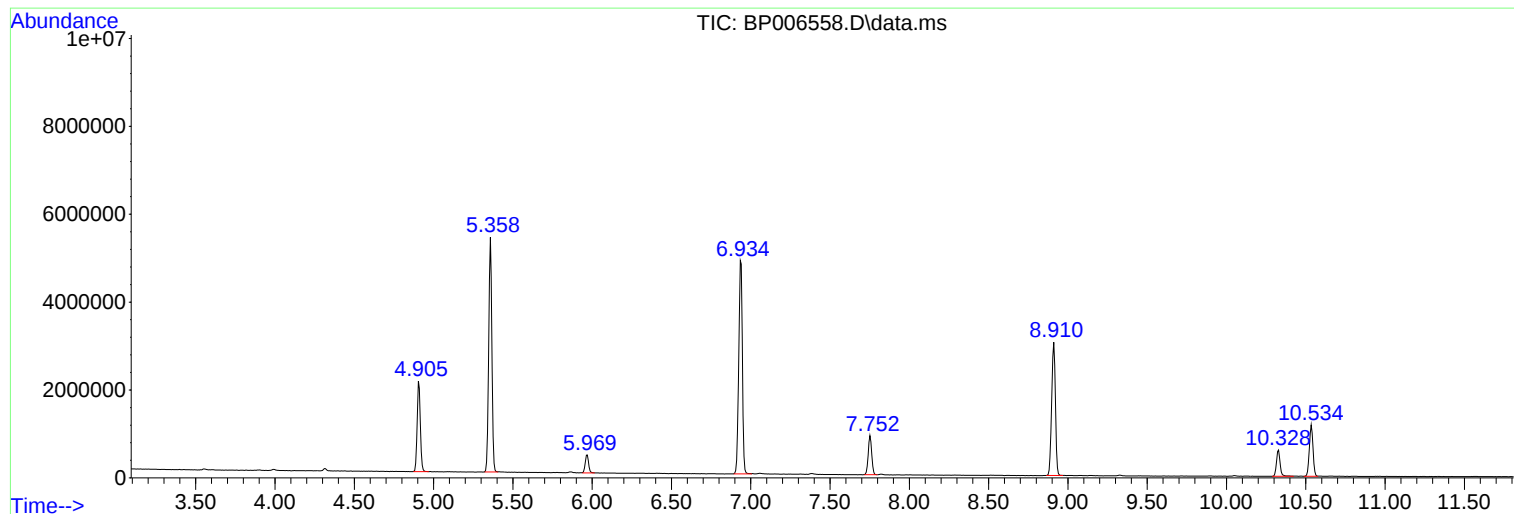
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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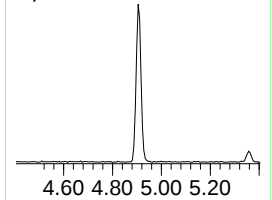
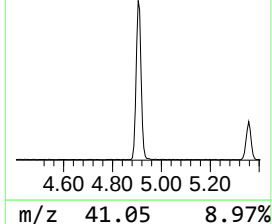
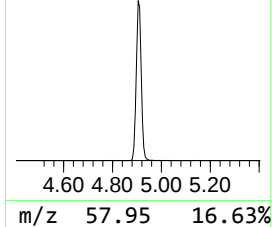
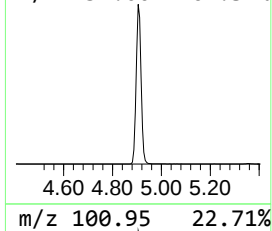
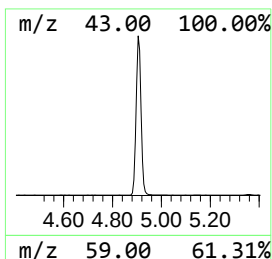
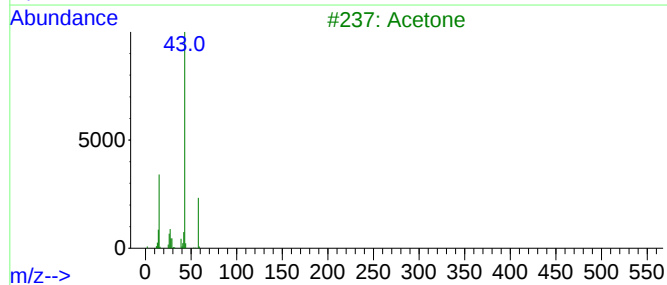
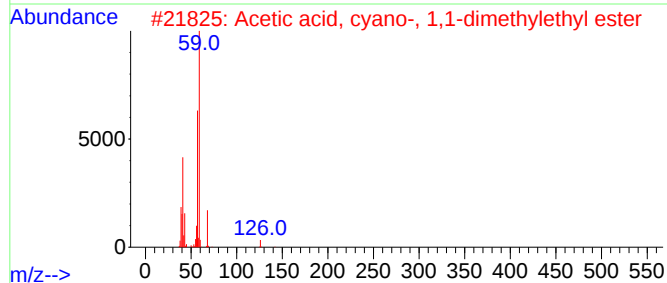
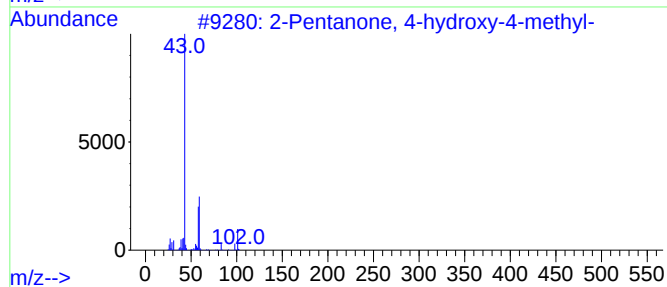
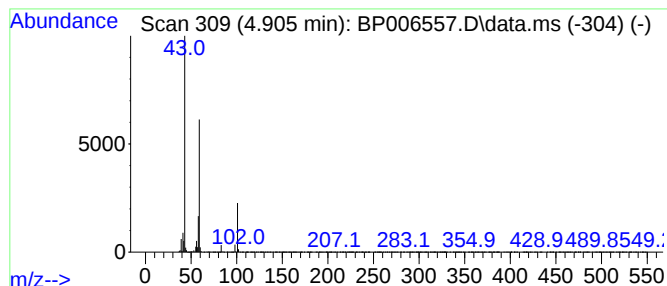
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	42.75 ng	2869250	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	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	Acetone	58	C3H6O	000067-64-1	10		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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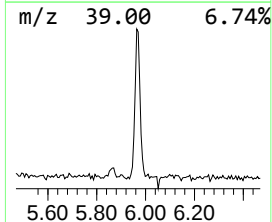
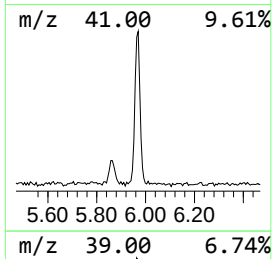
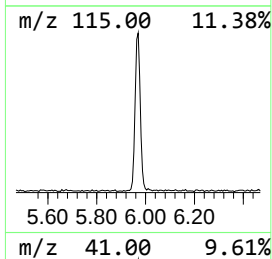
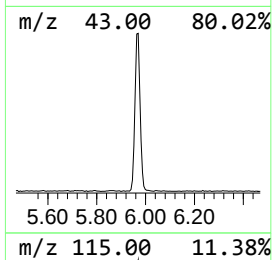
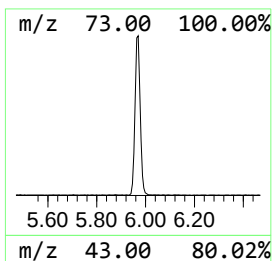
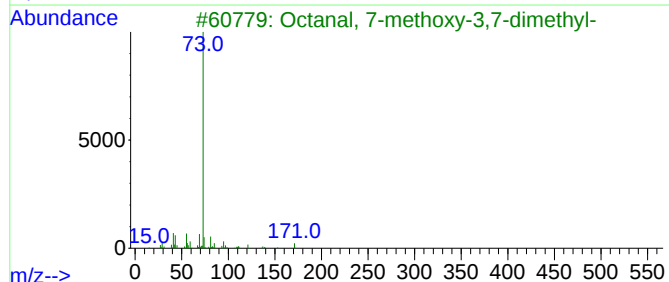
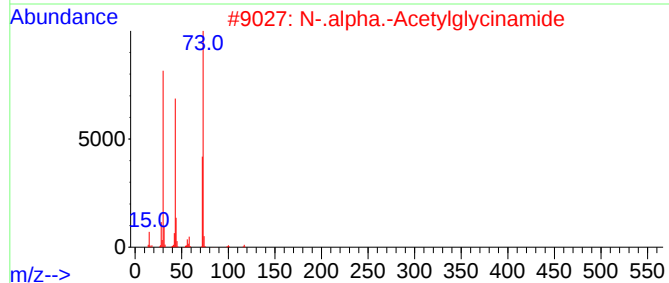
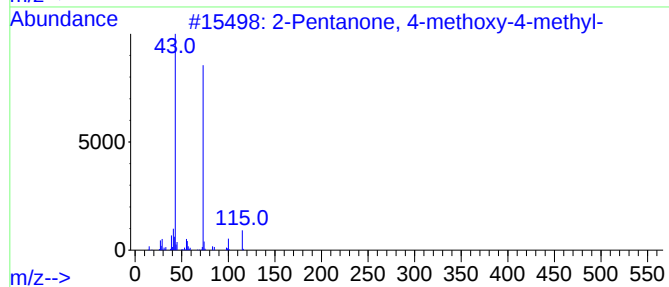
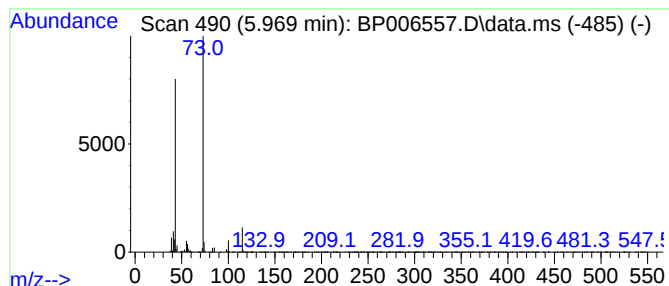
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	9.07 ng	609080	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	33
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	16
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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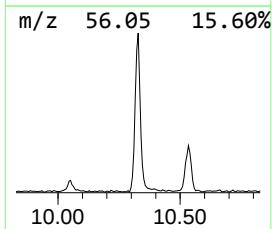
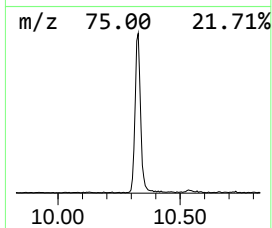
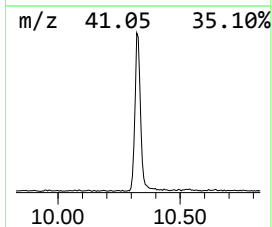
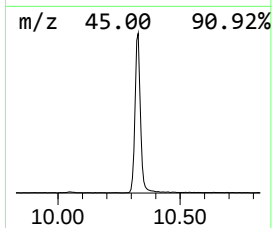
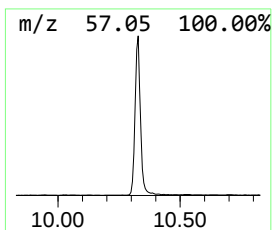
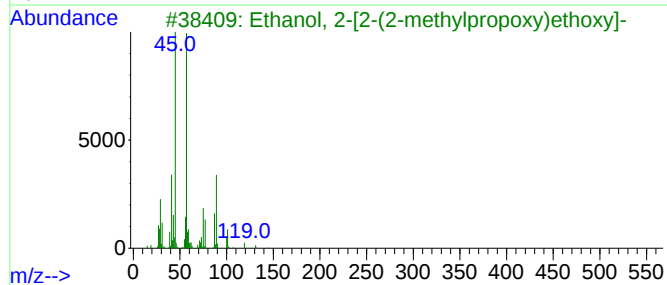
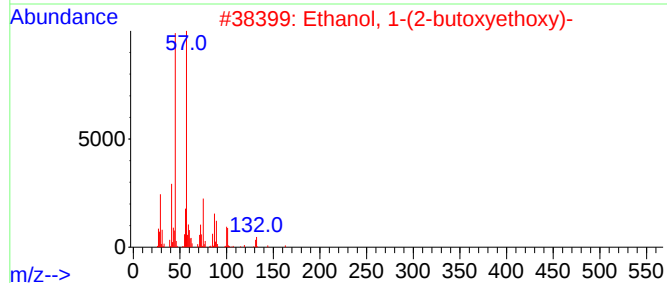
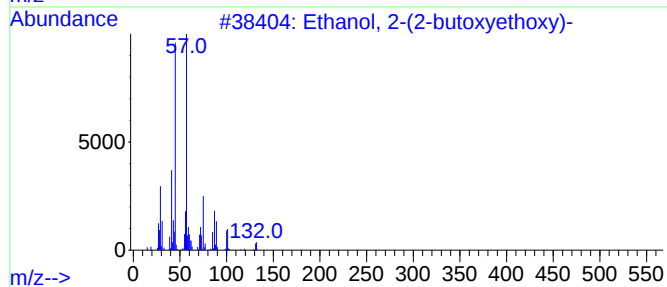
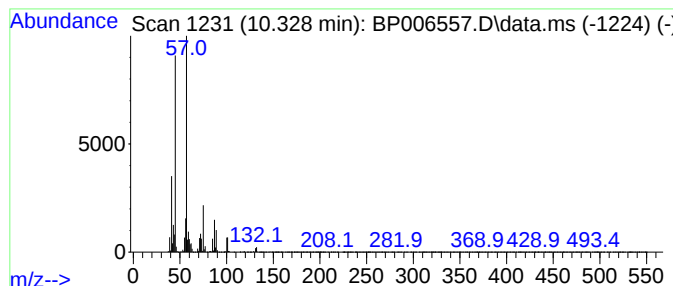
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	10.22 ng	940941	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			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50



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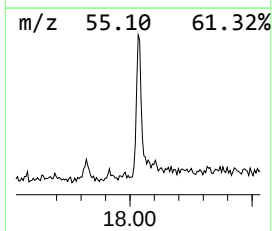
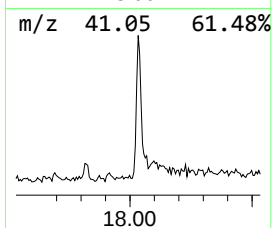
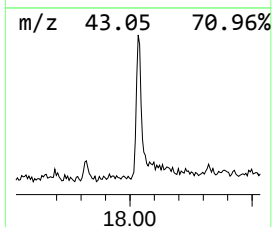
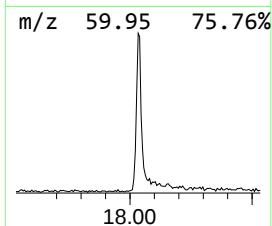
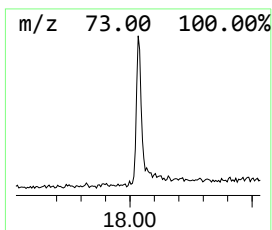
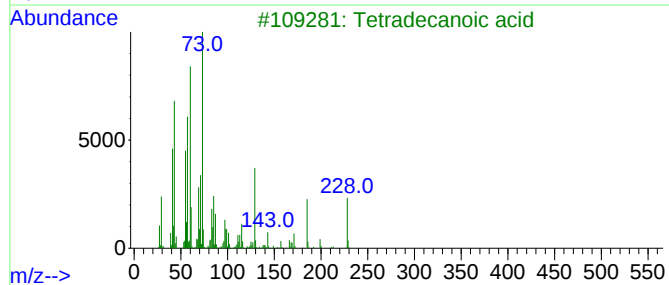
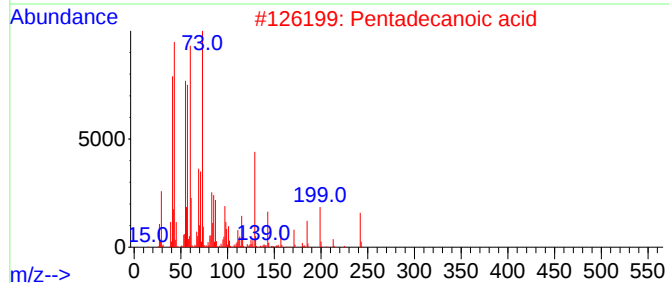
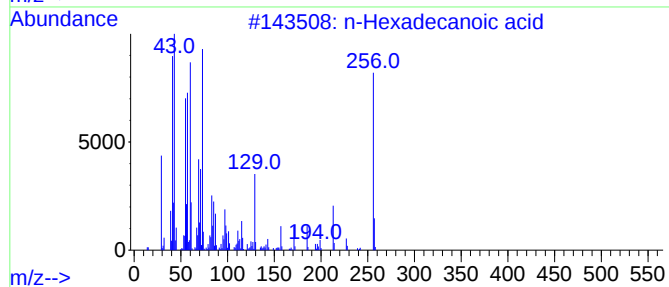
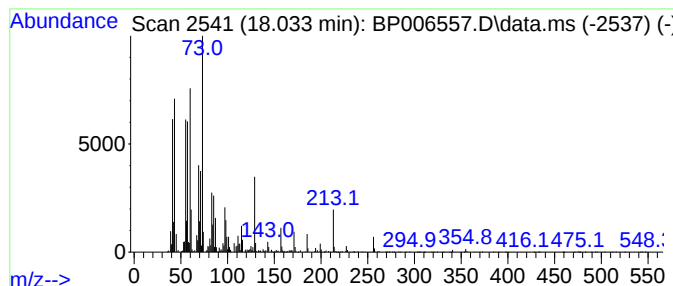
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.033	2.39 ng	299297	Phenanthrene-d10	17.133

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	68
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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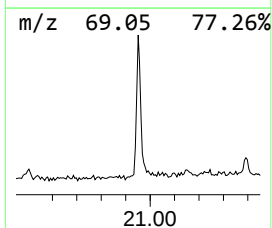
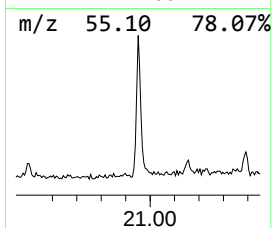
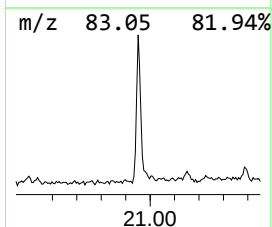
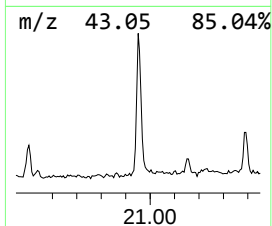
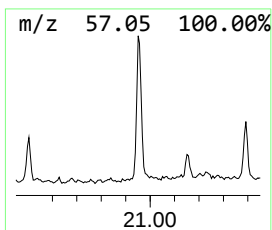
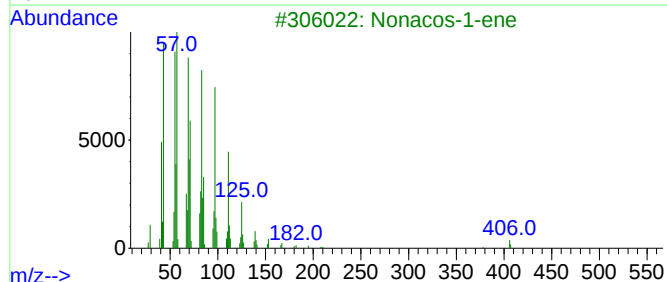
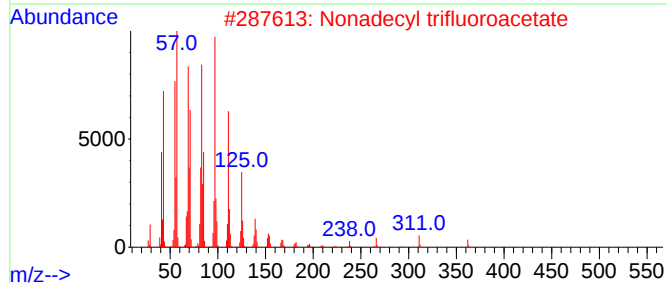
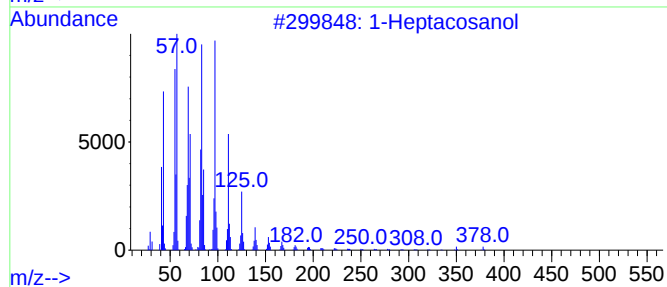
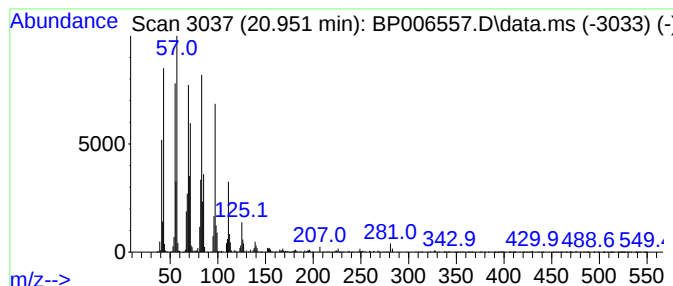
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.951	4.06 ng	565461	Chrysene-d12	21.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	94
2			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3			Nonacos-1-ene	406	C29H58	018835-35-3	91
4			1-Hexacosanol	382	C26H54O	000506-52-5	91
5			1-Hexacosene	364	C26H52	018835-33-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.905	42.8	ng	2869250	1	7.752	1342350	20.0
2-Pentanone, 4-...	5.969	9.1	ng	609080	1	7.752	1342350	20.0
Ethanol, 2-(2-b...	10.328	10.2	ng	940941	2	10.534	1841820	20.0
n-Hexadecanoic ...	18.033	2.4	ng	299297	4	17.133	2501700	20.0
1-Heptacosanol	20.951	4.1	ng	565461	5	21.227	2784150	20.0