

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121423\
 Data File : BG060025.D
 Acq On : 14 Dec 2023 23:46
 Operator : MA/JU
 Sample : 05632-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RW1

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060025.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.138	4	8	33	rVB	813691	1765984	18.76%	4.834%
2	5.065	330	336	342	rBV	117975	193965	2.06%	0.531%
3	5.524	405	414	426	rBV	698217	1238921	13.16%	3.391%
4	7.110	676	684	690	rBV	518086	883599	9.39%	2.418%
5	7.956	821	828	836	rBV	329607	573187	6.09%	1.569%
6	9.113	1018	1025	1033	rBV	1101522	1962758	20.85%	5.372%
7	10.759	1297	1305	1311	rBV	466963	836540	8.89%	2.290%
8	11.287	1390	1395	1400	rBV	135571	211035	2.24%	0.578%
9	11.352	1400	1406	1411	rVB	181412	287066	3.05%	0.786%
10	13.214	1715	1723	1731	rBV	3399072	5280078	56.08%	14.452%
11	14.589	1948	1957	1966	rBV	854464	1365282	14.50%	3.737%
12	16.082	2204	2211	2220	rBV	3757543	5633583	59.84%	15.420%
13	17.339	2419	2425	2431	rBV	1335159	1938191	20.59%	5.305%
14	18.232	2572	2577	2585	rBV2	253239	348730	3.70%	0.955%
15	19.507	2790	2794	2800	rBV3	99237	118732	1.26%	0.325%
16	19.965	2865	2872	2877	rBV	7013725	9414529	100.00%	25.769%
17	21.611	3144	3152	3165	rVB	1268524	2039229	21.66%	5.582%
18	24.331	3608	3615	3623	rVB7	49028	140790	1.50%	0.385%
19	24.801	3685	3695	3710	rVB	757839	2152942	22.87%	5.893%
20	25.618	3829	3834	3843	rVB	52089	149873	1.59%	0.410%

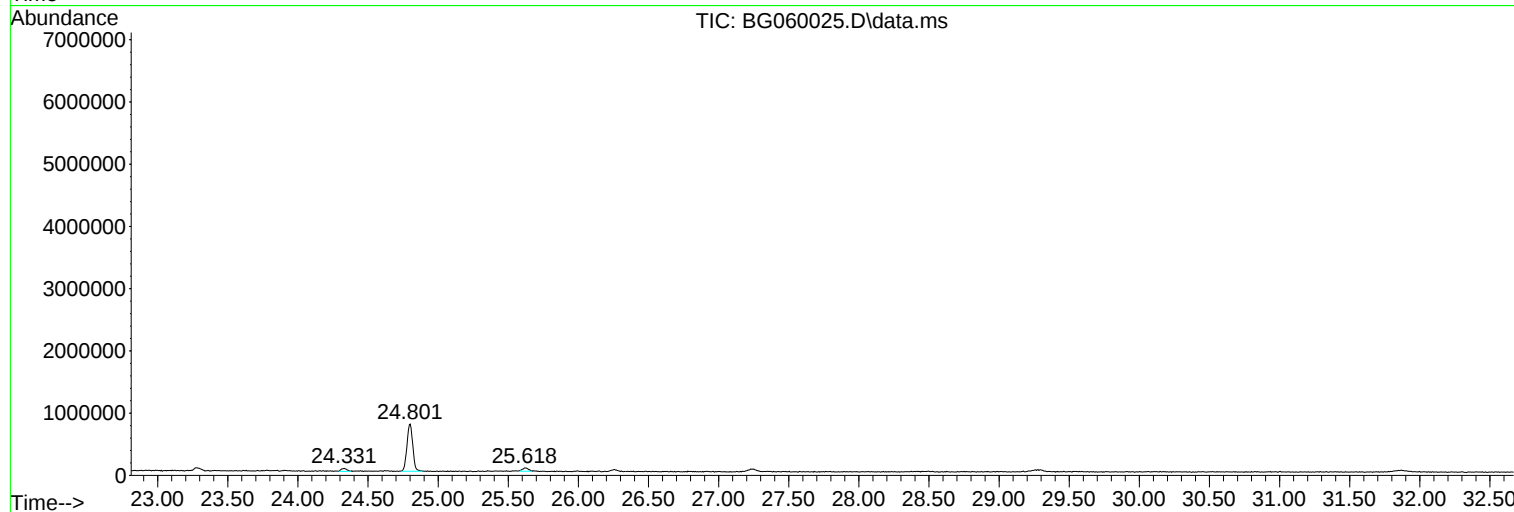
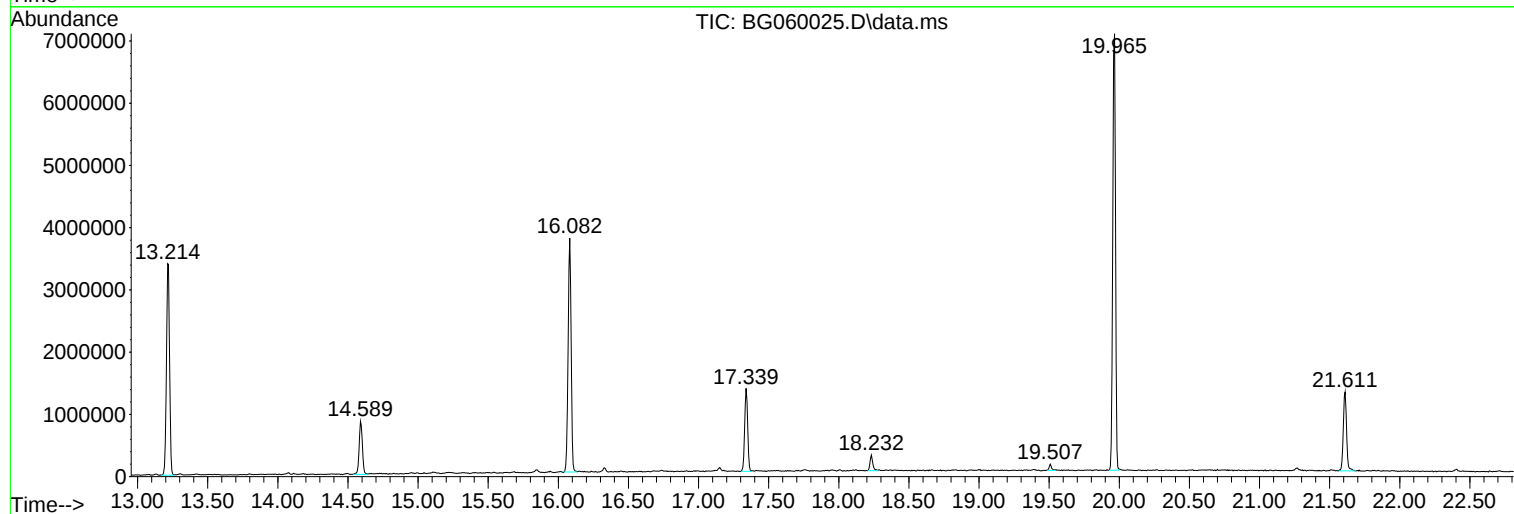
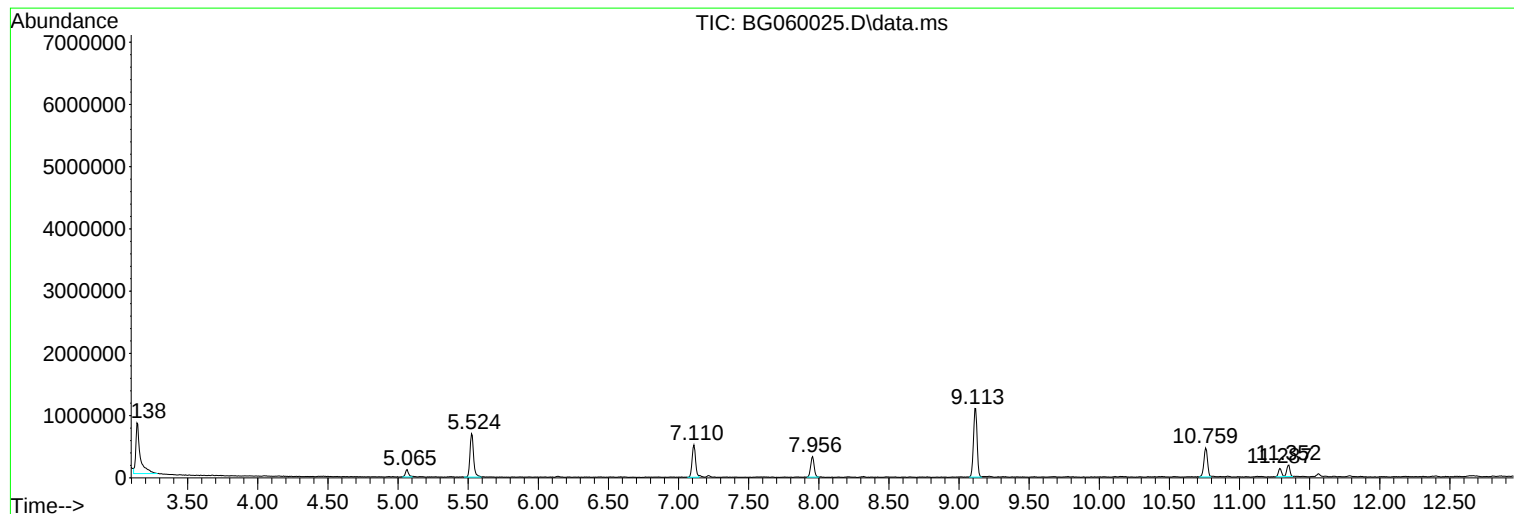
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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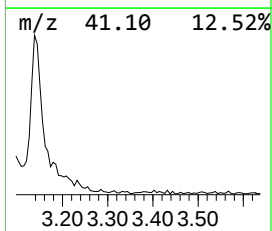
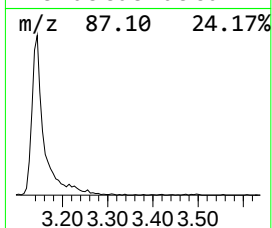
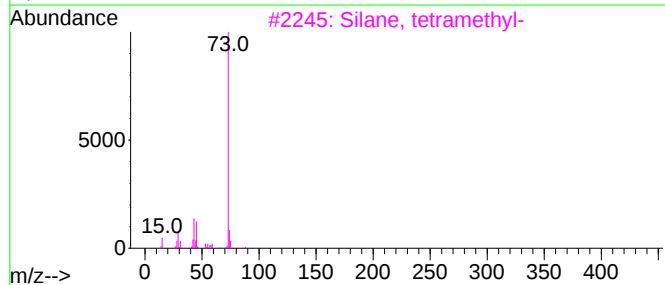
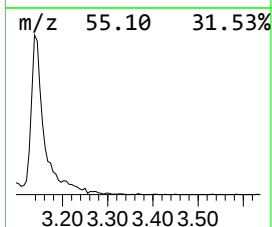
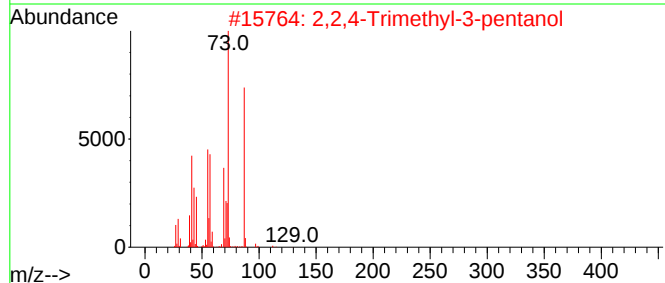
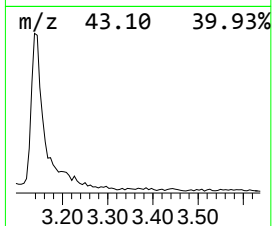
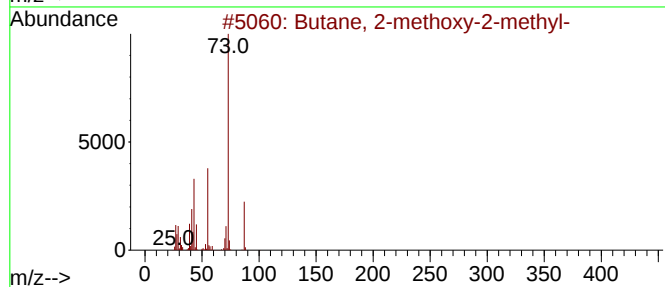
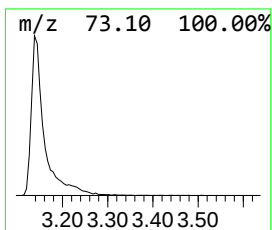
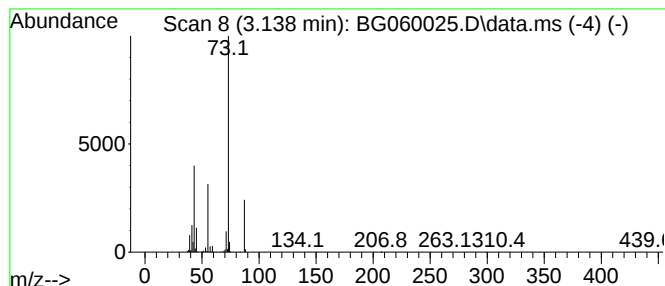
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.138	61.62 ng	1765980	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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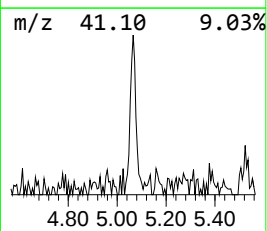
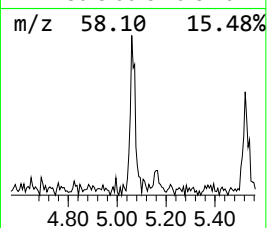
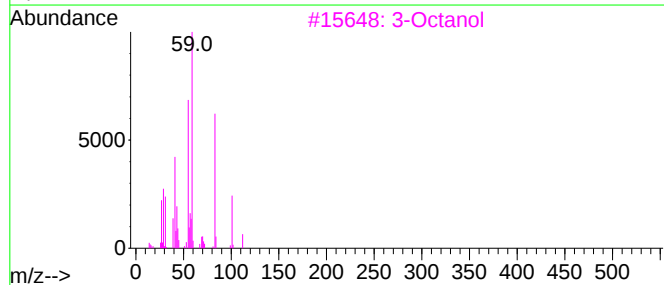
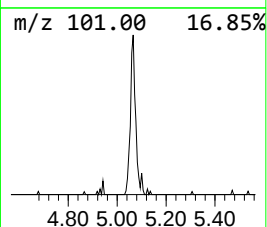
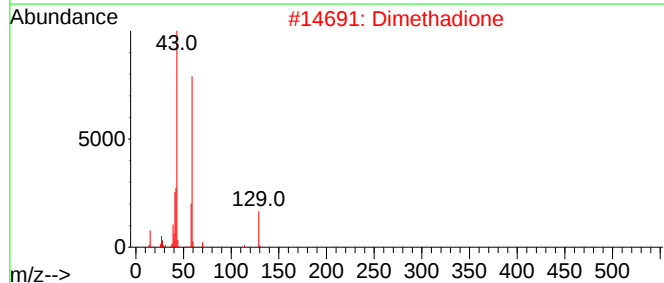
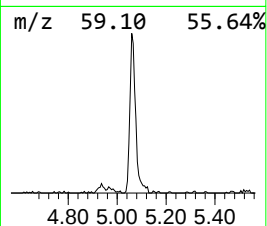
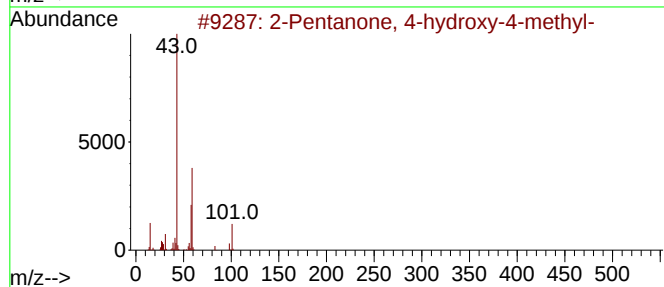
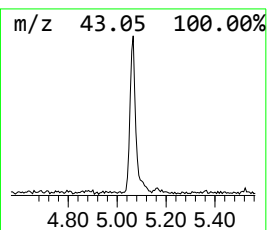
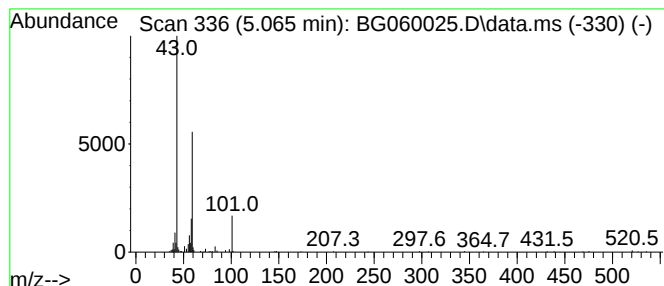
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.065	6.77 ng	193965	1,4-Dichlorobenzene-d4	7.956

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Dimethadione	129	C5H7NO3	000695-53-4	40
3		3-Octanol	130	C8H18O	000589-98-0	38
4		Acetic acid, chloro-, 1,1-dimeth...	150	C6H11ClO2	000107-59-5	37
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	37



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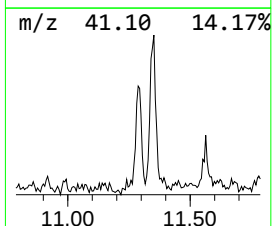
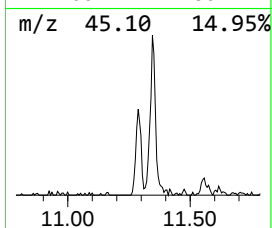
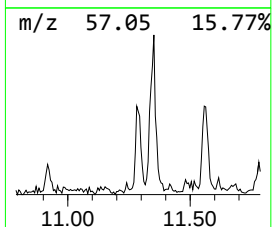
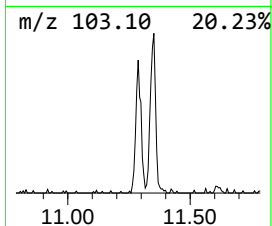
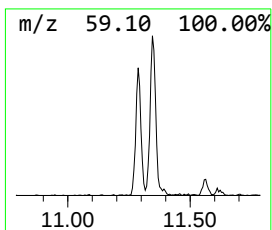
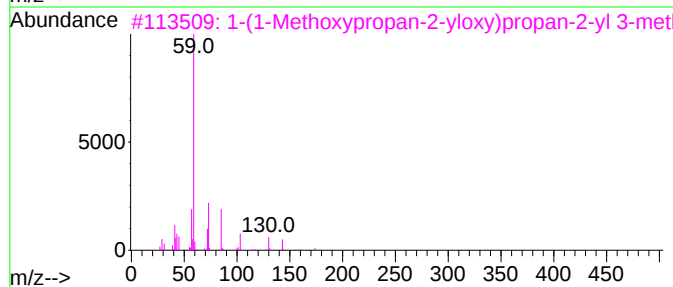
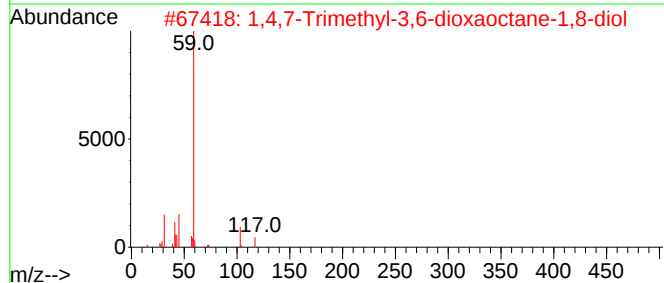
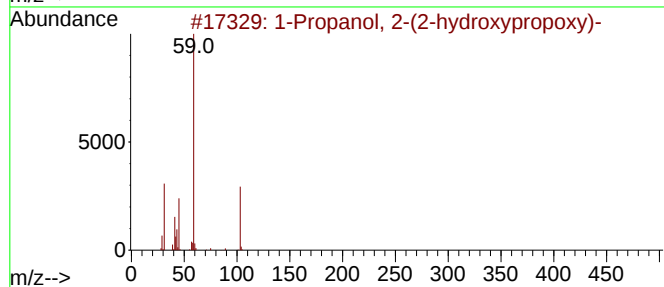
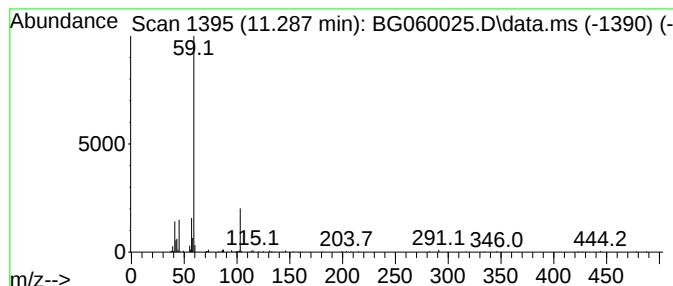
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Peak Number 3 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.287	5.05 ng	211035	Naphthalene-d8	10.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
2			1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	72
3			1-(1-Methoxypropan-2-yloxy)propan...	232	C12H24O4	1000367-13-2	59
4			d1-Erythro-0-methylthreonine	133	C5H11NO3	1000214-70-7	59
5			2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	59



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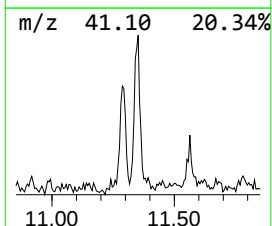
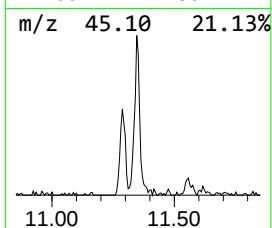
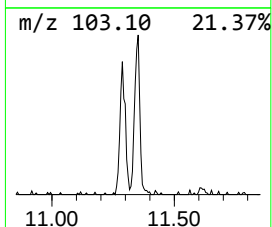
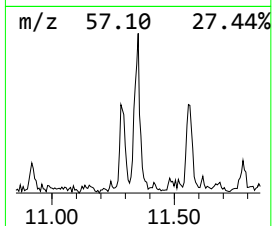
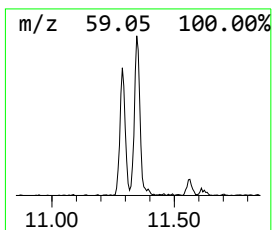
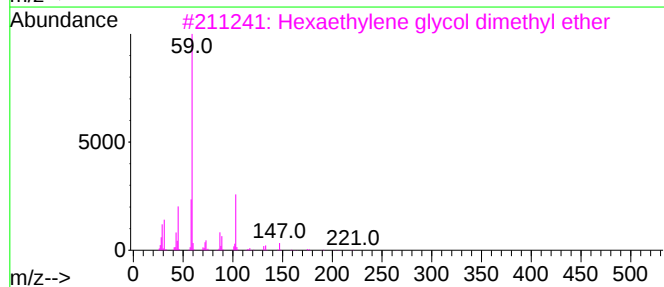
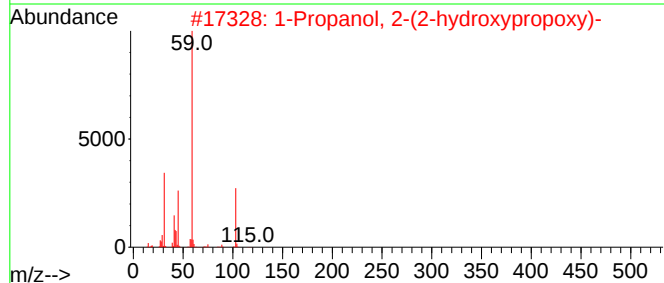
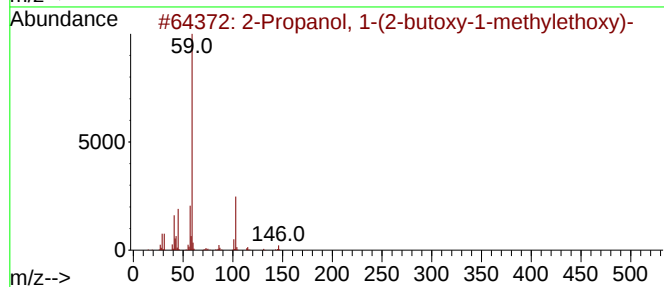
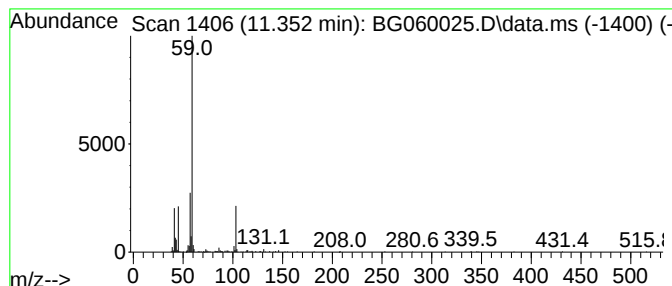
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.352	6.86 ng	287066	Naphthalene-d8	10.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	78
2			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3			Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	64
4			Methyl 2,5,8,11,14,17,20,23-octa...	412	C18H36O10	1000366-81-2	64
5			Methyl 2,5,8,11,14,17,20-heptaox...	368	C16H32O9	1010366-81-3	64



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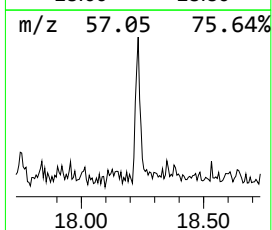
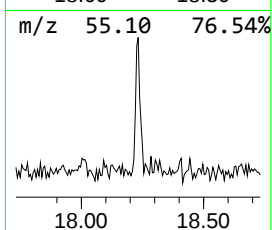
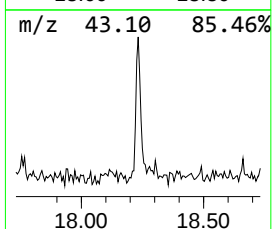
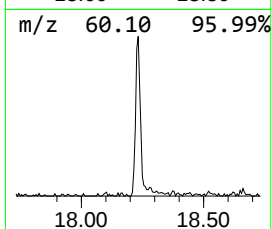
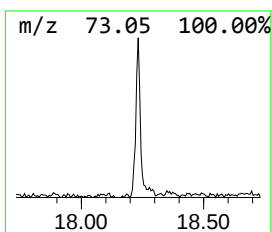
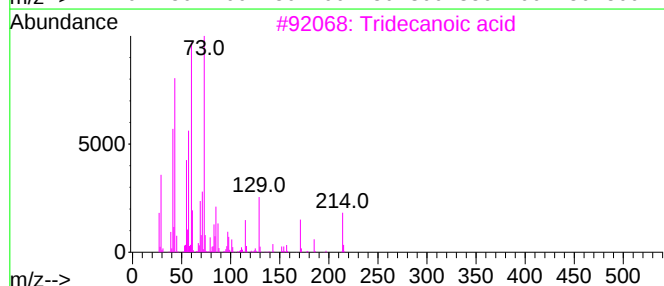
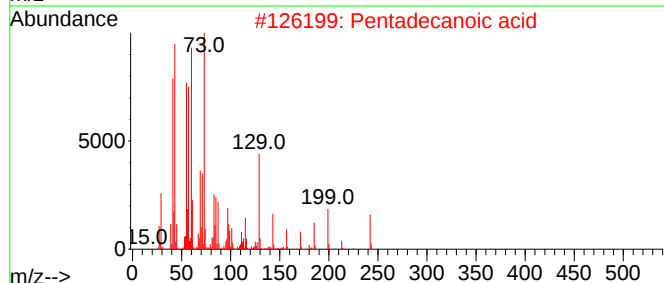
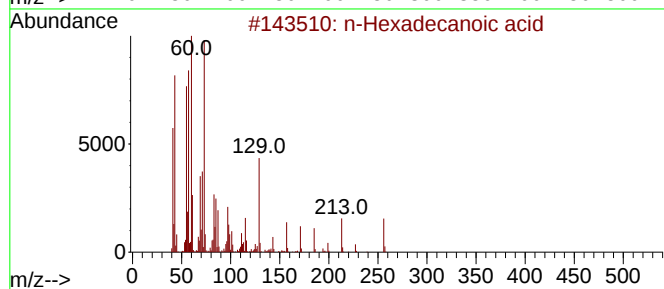
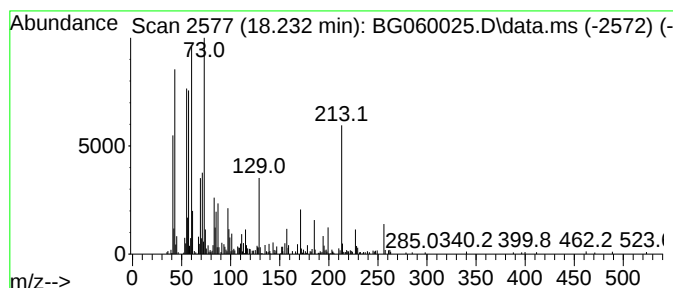
Instrument :
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.232	3.60 ng	348730	Phenanthrene-d10	17.339	
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	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.138	61.6	ng	1765980	1	7.956	573187	20.0
2-Pentanone, 4-...	5.065	6.8	ng	193965	1	7.956	573187	20.0
1-Propanol, 2-(...	11.287	5.0	ng	211035	2	10.759	836540	20.0
2-Propanol, 1-(...	11.352	6.9	ng	287066	2	10.759	836540	20.0
n-Hexadecanoic ...	18.232	3.6	ng	348730	4	17.339	1938190	20.0