

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033021\
 Data File : BM029275.D
 Acq On : 30 Mar 2021 18:12
 Operator : CG/JU
 Sample : M1812-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-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_M\Methods\8270-BM032621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.999	15	19	24	rBV	529445	581843	11.88%	2.178%
2	3.040	24	26	37	rVB	99308	122861	2.51%	0.460%
3	4.893	336	341	352	rBV	100211	149746	3.06%	0.561%
4	5.340	411	417	426	rBV	1754134	2582182	52.74%	9.668%
5	6.916	677	685	697	rBV	1746940	2784325	56.87%	10.425%
6	7.745	819	826	835	rVB	420928	670084	13.69%	2.509%
7	8.892	1013	1021	1034	rBV	1081309	1787216	36.50%	6.692%
8	10.528	1291	1299	1307	rBV	527639	884826	18.07%	3.313%
9	12.998	1711	1719	1731	rBV	2473550	3726460	76.11%	13.952%
10	13.827	1851	1860	1869	rBV	52660	85429	1.74%	0.320%
11	14.374	1946	1953	1963	rBV	737133	1127785	23.03%	4.223%
12	15.857	2199	2205	2214	rBV	1759805	2445124	49.94%	9.155%
13	17.109	2412	2418	2428	rBV	872536	1243205	25.39%	4.655%
14	18.009	2566	2571	2578	rBV	110650	166049	3.39%	0.622%
15	19.292	2783	2789	2794	rBV7	28877	53730	1.10%	0.201%
16	19.733	2858	2864	2872	rBV	4089692	4896198	100.00%	18.332%
17	21.003	3076	3080	3088	rBV	424583	609302	12.44%	2.281%
18	21.062	3088	3090	3097	rVB	47636	60868	1.24%	0.228%
19	21.280	3122	3127	3132	rBV	1096878	1317118	26.90%	4.931%
20	23.515	3501	3507	3515	rVB	764724	1414284	28.89%	5.295%

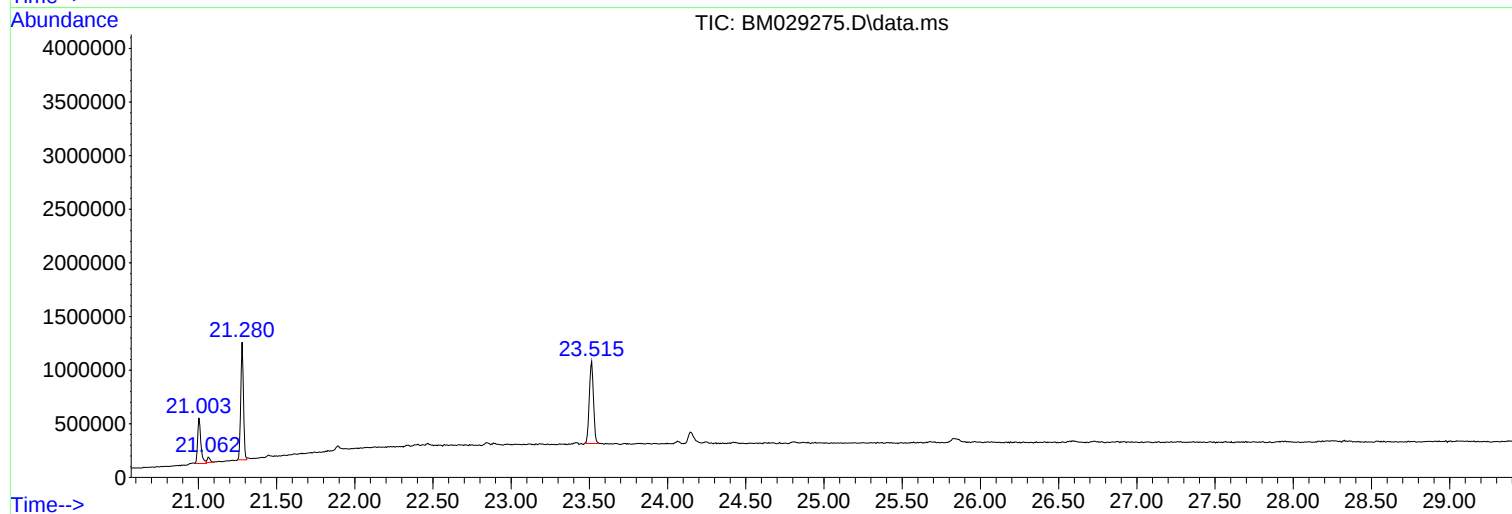
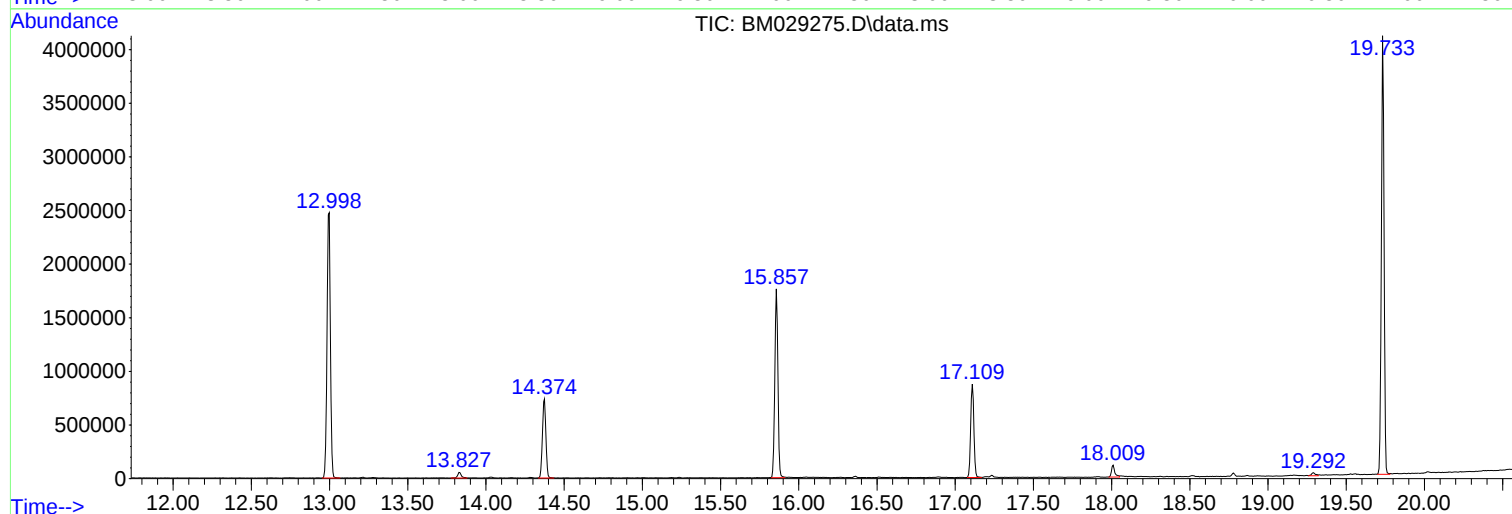
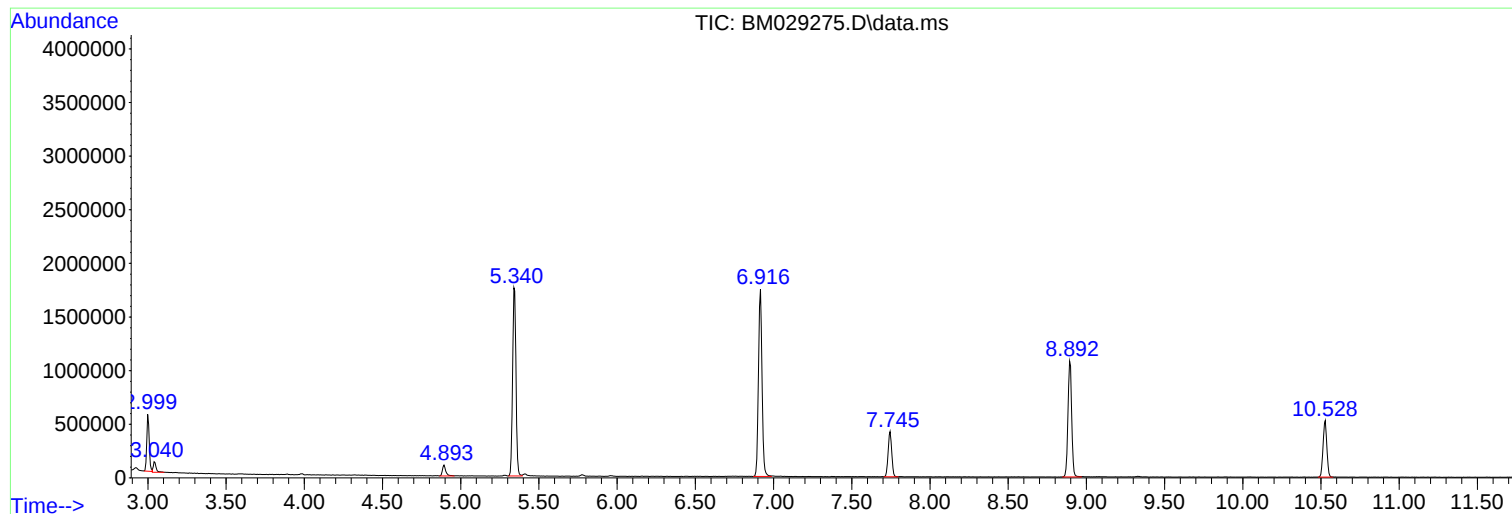
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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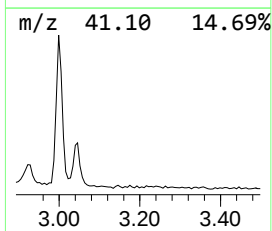
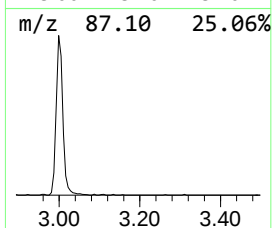
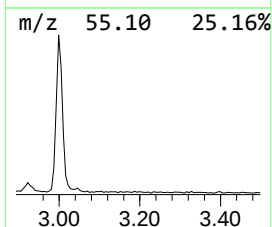
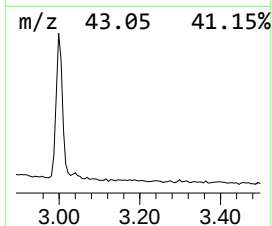
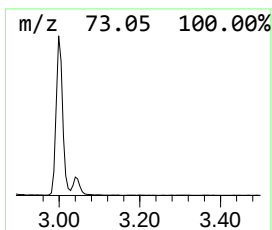
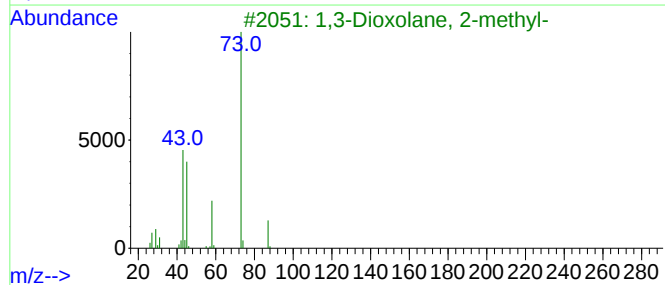
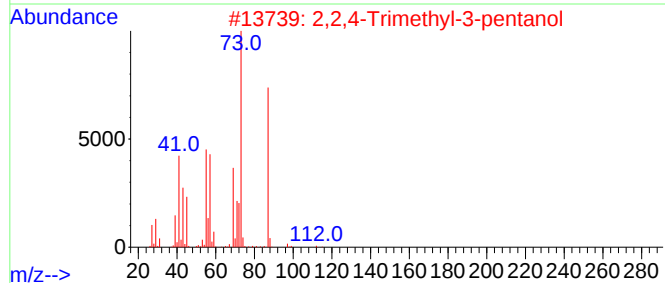
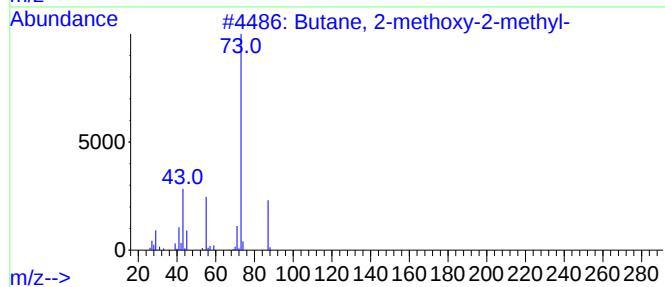
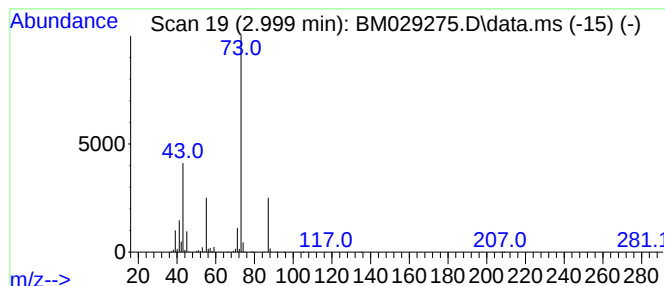
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.999	17.37 ng	581843	1,4-Dichlorobenzene-d4	7.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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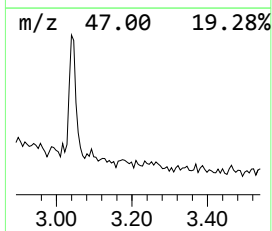
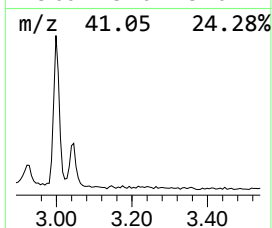
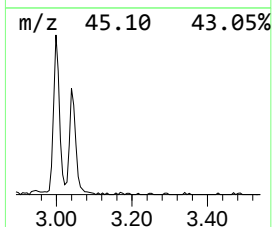
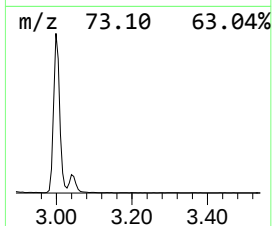
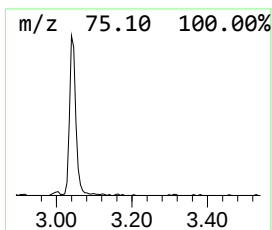
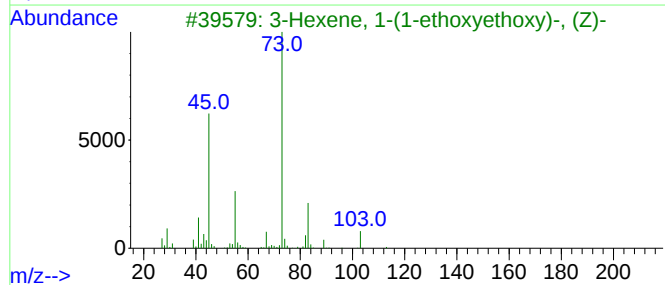
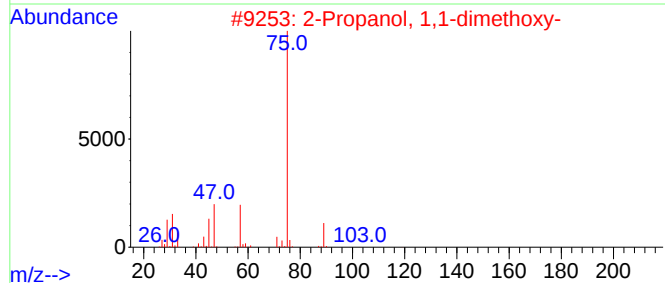
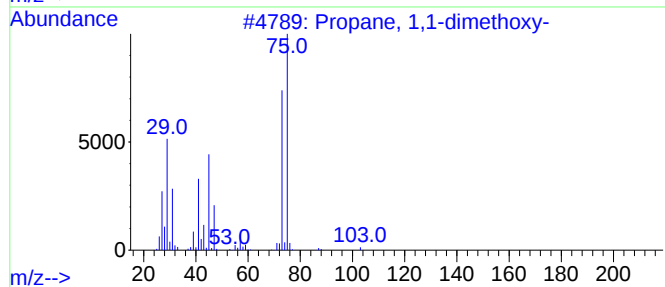
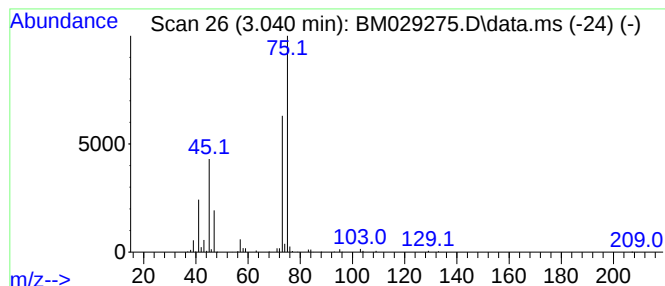
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.040	3.67 ng	122861	1,4-Dichlorobenzene-d4	7.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	33
3			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10
4			1-Butanol, 3-(1-ethoxyethoxy)-2-...	176	C9H20O3	059410-44-5	9
5			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9



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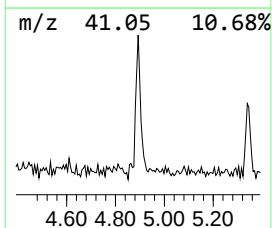
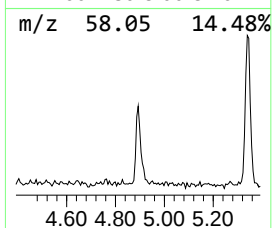
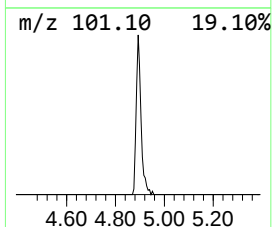
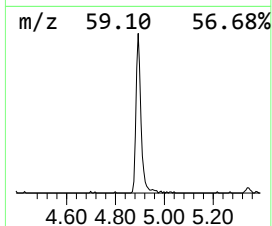
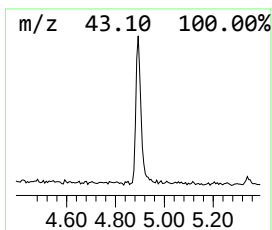
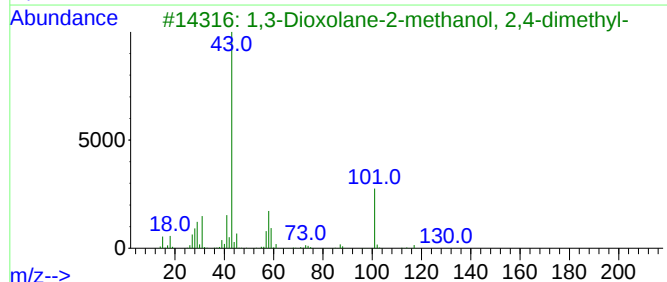
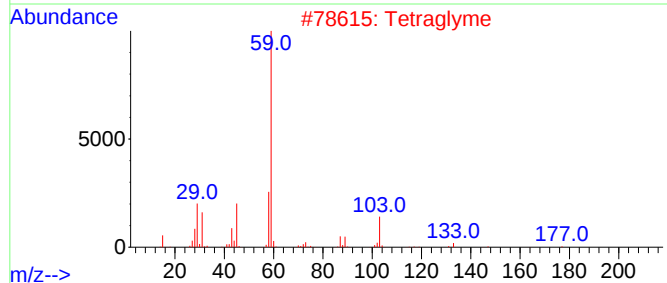
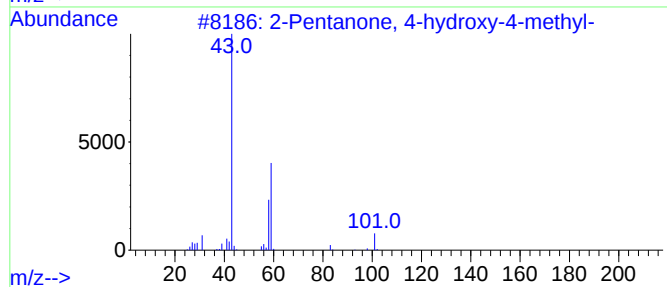
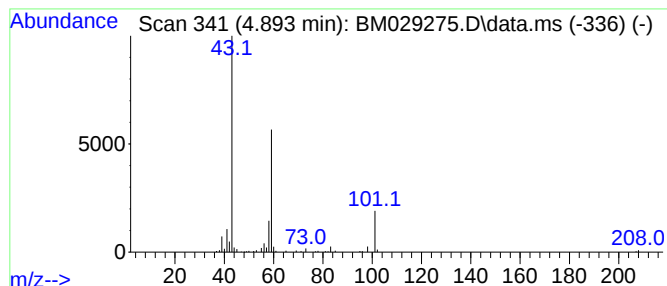
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	4.47 ng	149746	1,4-Dichlorobenzene-d4	7.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	Tetraglyme	222	C10H22O5	000143-24-8	25		
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		



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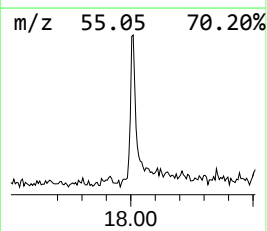
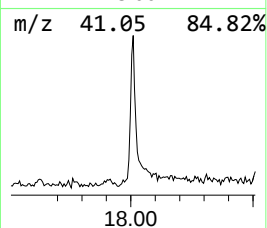
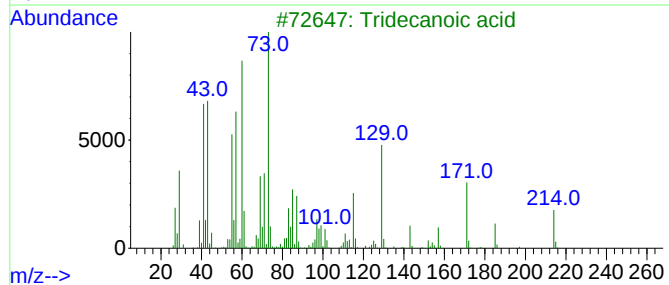
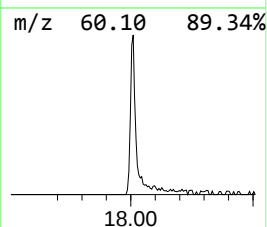
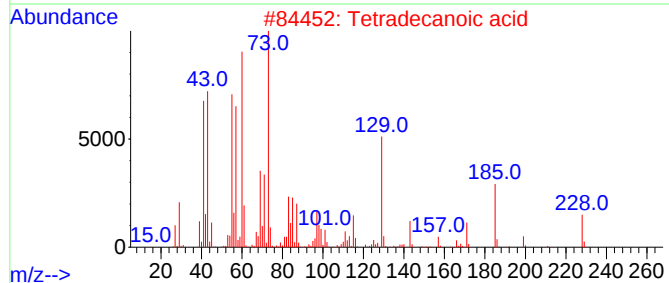
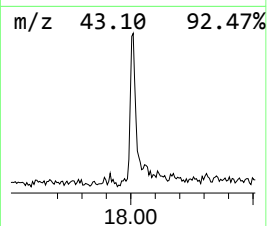
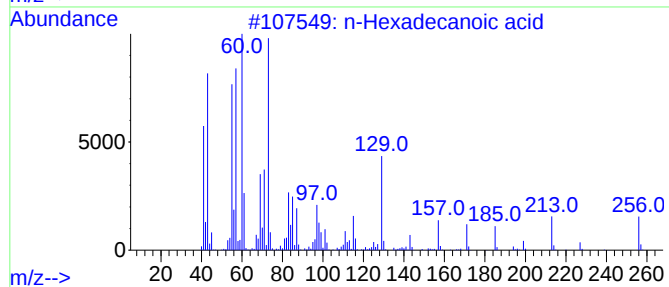
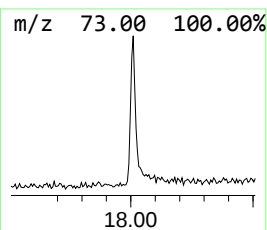
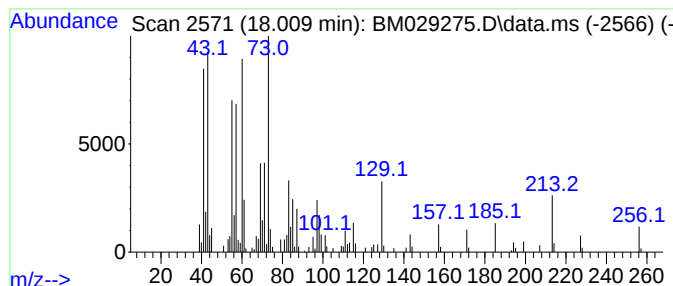
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.009	2.67 ng	166049	Phenanthrene-d10	17.110

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	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	94
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	25



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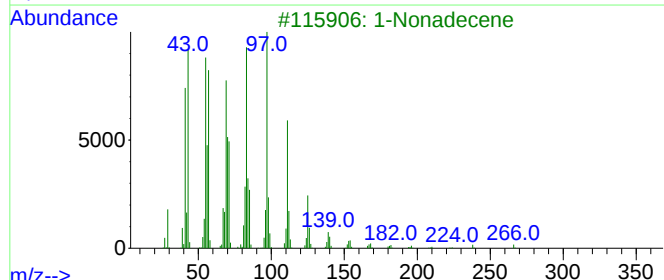
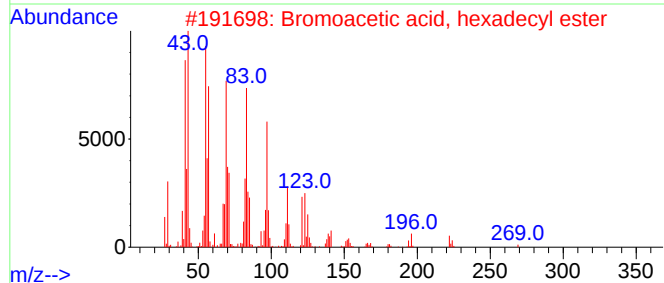
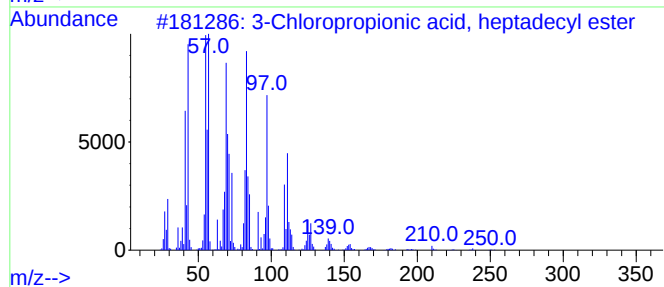
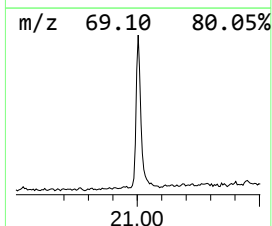
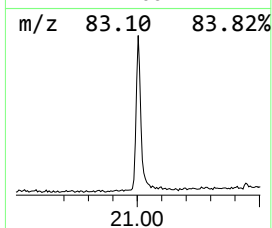
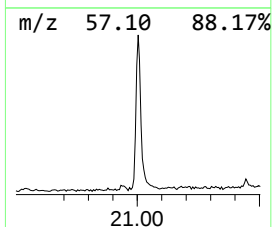
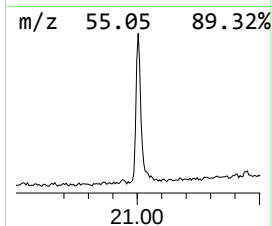
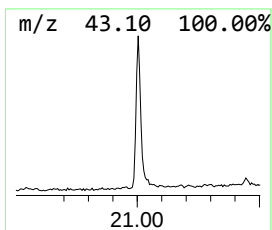
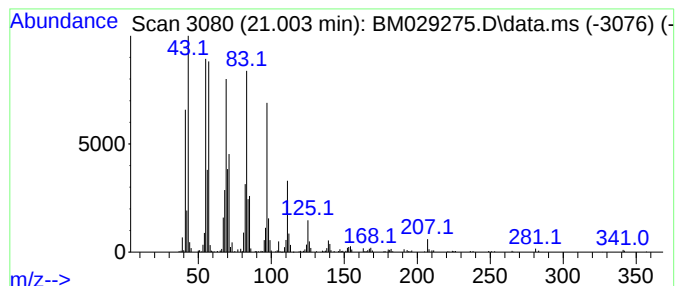
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Chloropropionic acid, hep... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.003	9.25 ng	609302	Chrysene-d12	21.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.999	17.4	ng	581843	1	7.745	670084	20.0
Propane, 1,1-di...	3.040	3.7	ng	122861	1	7.745	670084	20.0
2-Pentanone, 4-...	4.893	4.5	ng	149746	1	7.745	670084	20.0
n-Hexadecanoic ...	18.009	2.7	ng	166049	4	17.110	1243210	20.0
3-Chloropropion...	21.003	9.3	ng	609302	5	21.280	1317120	20.0