

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102621\
 Data File : VU045403.D
 Acq On : 26 Oct 2021 16:11
 Operator : SY/MD
 Sample : I.BLK
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VU1027

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:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M

Title : SW846 8260

Signal : TIC: VU045403.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.295	1213	1230	1243	rBV	194295	409241	21.72%	3.560%
2	5.379	1243	1256	1279	rVB	308339	642170	34.08%	5.586%
3	5.706	1341	1358	1379	rBV	224209	460393	24.43%	4.004%
4	6.163	1449	1500	1514	rBV3	93114	707856	37.56%	6.157%
5	6.253	1517	1528	1594	rVB	588352	1496209	79.40%	13.014%
6	7.903	2027	2041	2069	rBV	791683	1347918	71.53%	11.724%
7	9.420	2500	2513	2538	rBV	719110	1181215	62.68%	10.274%
8	10.636	2879	2891	2914	rBV	564997	899206	47.72%	7.821%
9	11.816	3244	3258	3276	rBV	779025	1204844	63.94%	10.480%
10	13.211	3684	3692	3699	rBV2	23088	34440	1.83%	0.300%
11	13.635	3811	3824	3853	rBV	1193434	1884410	100.00%	16.390%
12	14.253	4010	4016	4037	rVB2	28302	52826	2.80%	0.459%
13	14.658	4131	4142	4162	rBV	374296	645728	34.27%	5.616%
14	14.989	4236	4245	4257	rBV4	57127	104786	5.56%	0.911%
15	15.610	4429	4438	4453	rBV3	35384	64834	3.44%	0.564%
16	15.950	4534	4544	4558	rBV3	8558	19355	1.03%	0.168%
17	16.021	4559	4566	4583	rVB8	10130	20239	1.07%	0.176%
18	16.346	4656	4667	4684	rBV	122166	231307	12.27%	2.012%
19	17.153	4910	4918	4928	rVB8	11615	19572	1.04%	0.170%
20	17.220	4930	4939	4950	rVV	47842	70511	3.74%	0.613%

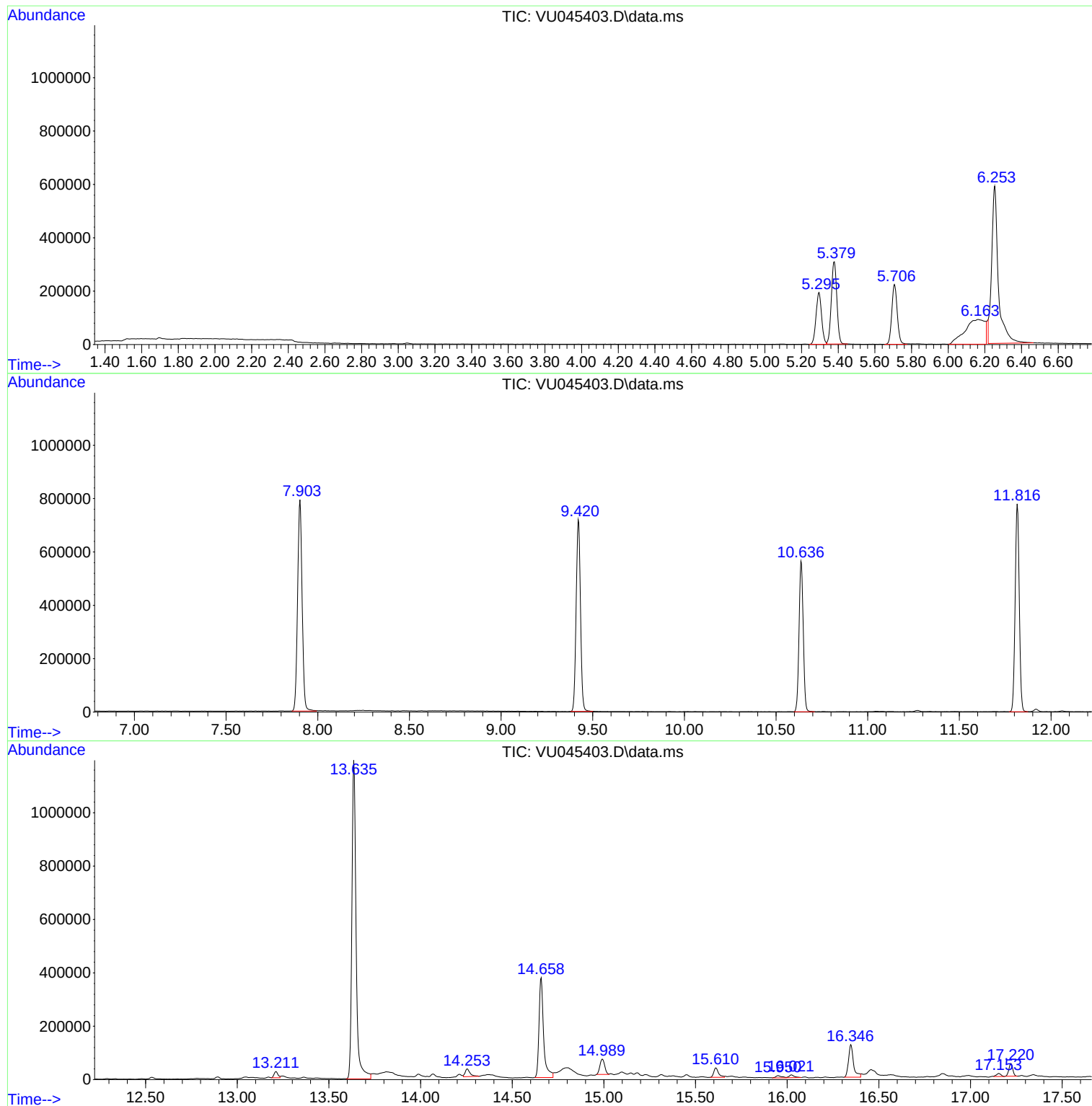
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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



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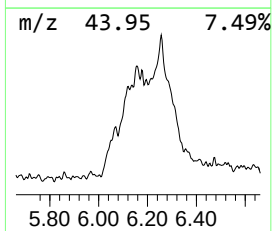
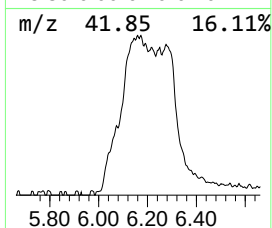
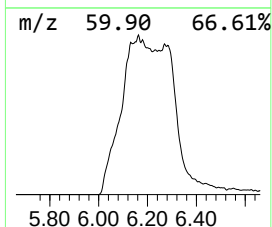
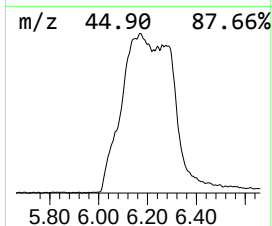
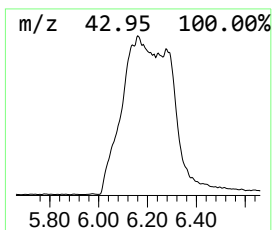
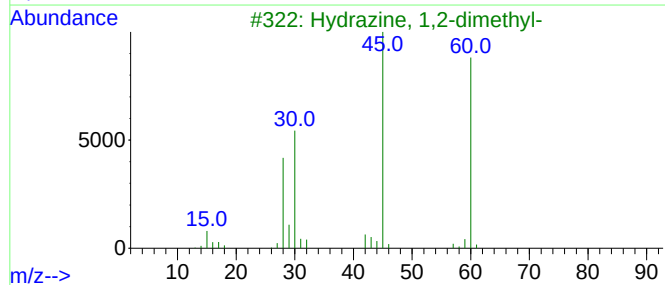
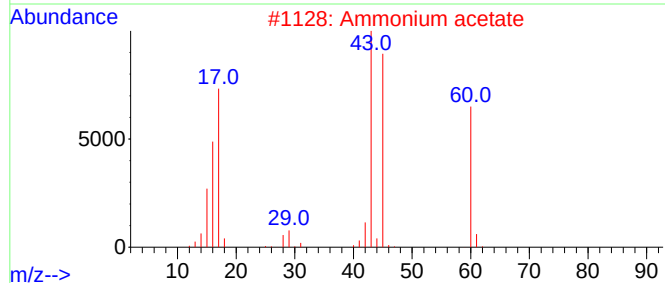
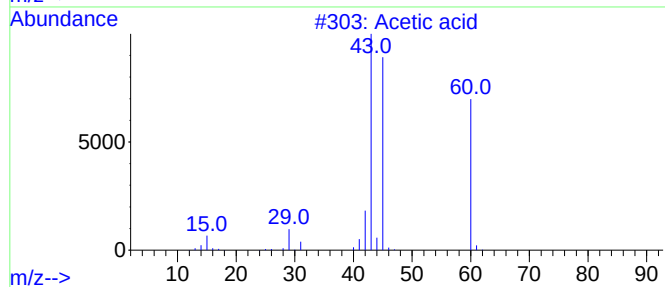
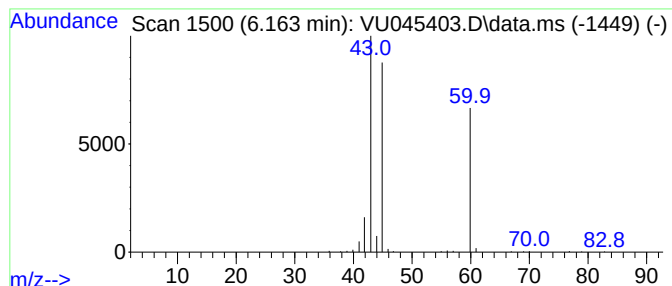
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.163	23.66 ug/l	707856	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid	60	C2H4O2	000064-19-7	91
2		Ammonium acetate	77	C2H7NO2	000631-61-8	83
3		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
4		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5		n-Butyl nitrite	103	C4H9NO2	000544-16-1	9



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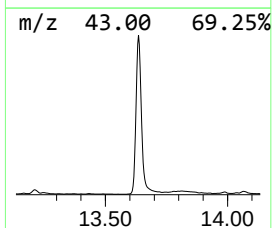
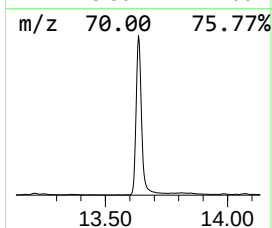
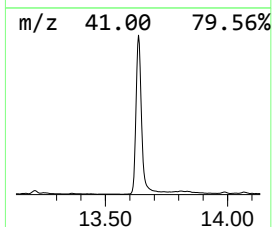
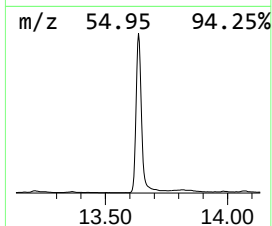
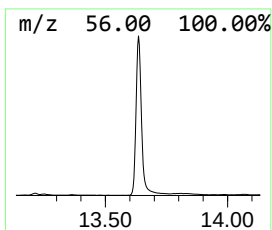
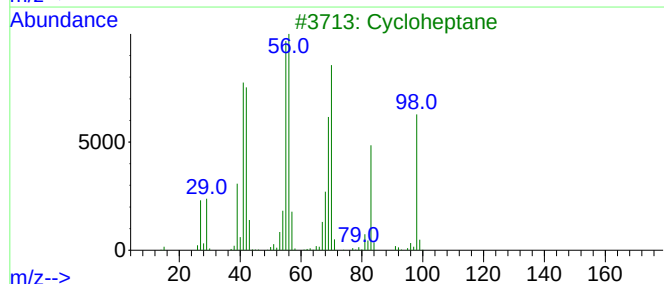
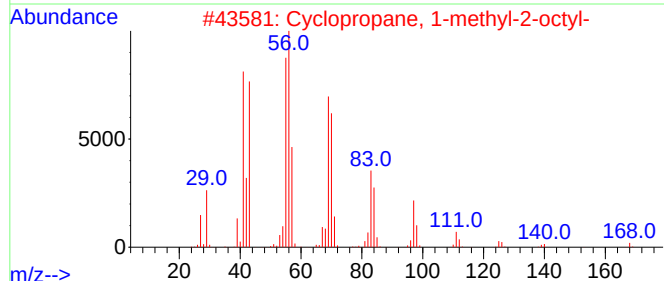
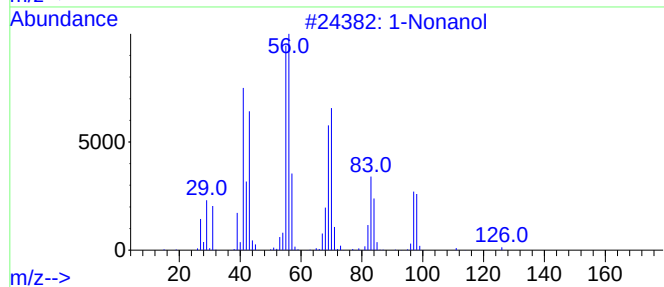
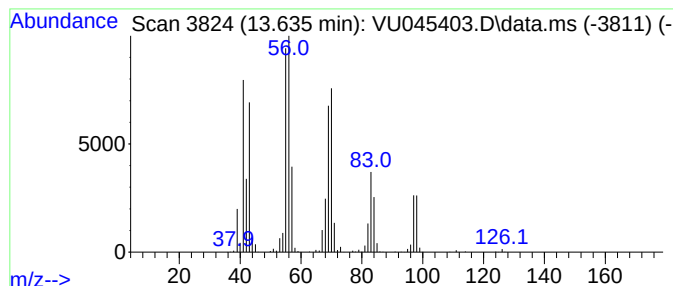
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.635	78.20 ug/l	1884410	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	91
2			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
3			Cycloheptane	98	C7H14	000291-64-5	74
4			Isopropylcyclobutane	98	C7H14	000872-56-0	68
5			1-Decanol	158	C10H22O	000112-30-1	64



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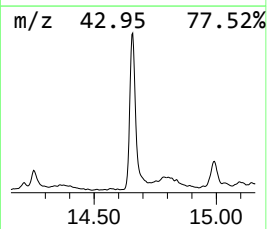
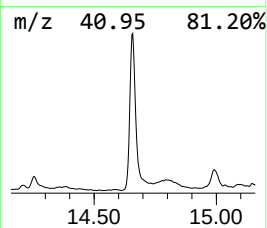
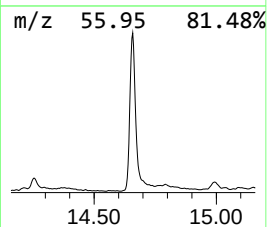
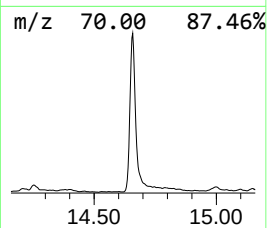
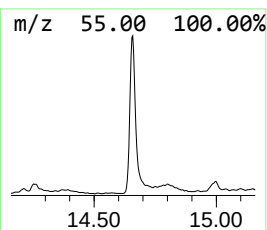
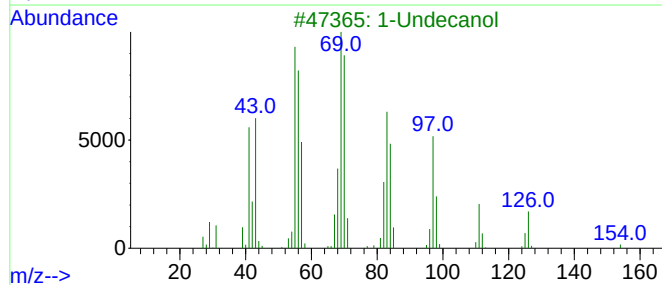
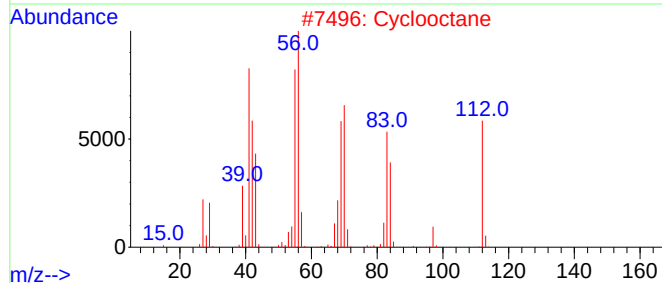
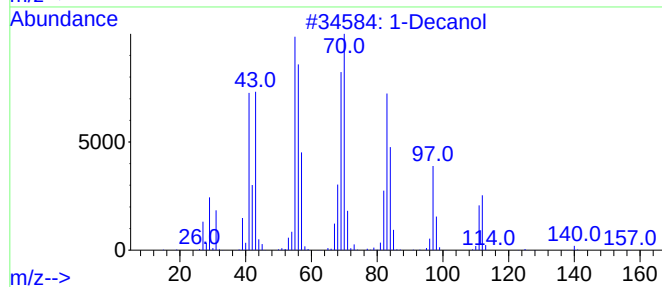
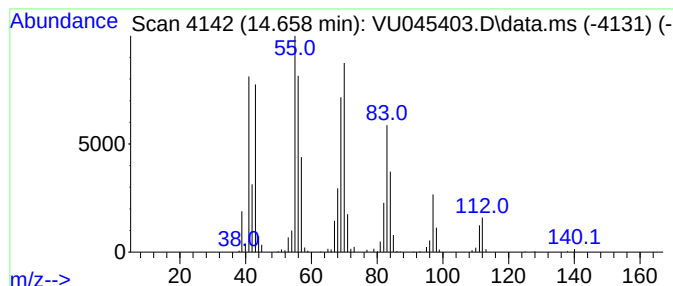
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Peak Number 3 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.658	26.80 ug/l	645728	1,4-Dichlorobenzene-d4	11.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol	158	C10H22O	000112-30-1	91
2	Cyclooctane	112	C8H16	000292-64-8	87
3	1-Undecanol	172	C11H24O	000112-42-5	86
4	1-Dodecanol	186	C12H26O	000112-53-8	83
5	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	72



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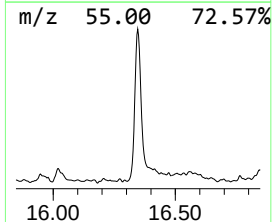
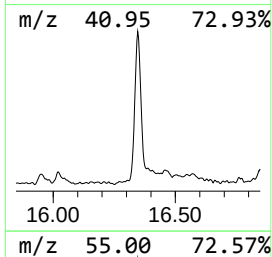
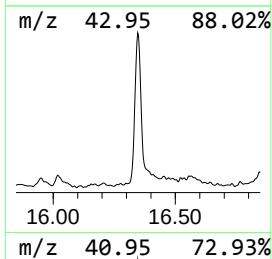
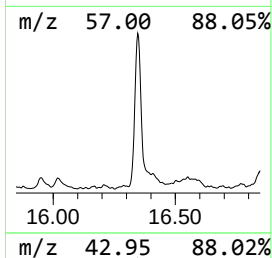
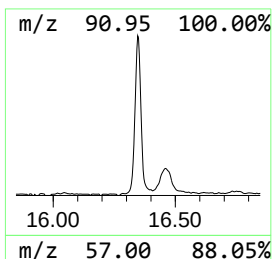
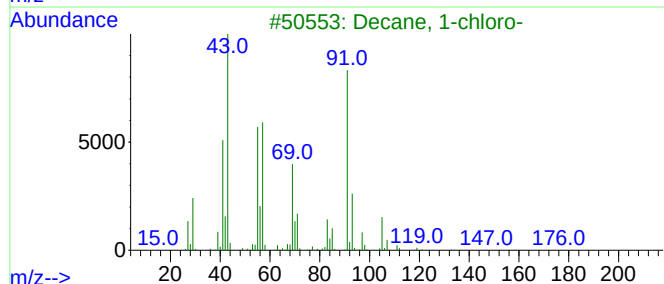
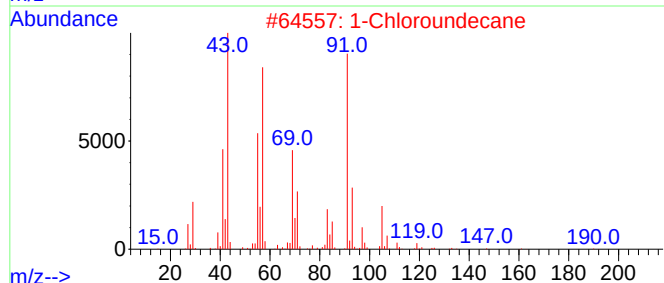
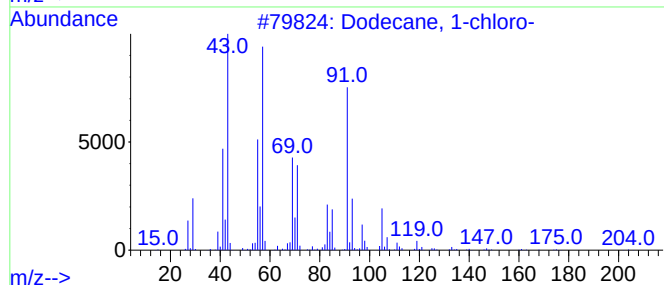
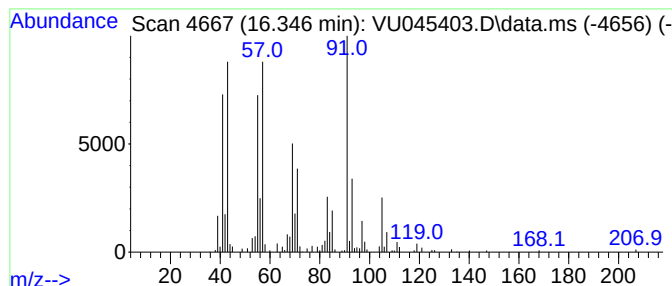
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.346	9.60 ug/l	231307	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	91
2			1-Chloroundecane	190	C11H23Cl	002473-03-2	91
3			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	80
4			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	59
5			Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid	6.163	23.7	ug/l	707856	2	6.253	1496210	50.0
1-Nonanol	13.635	78.2	ug/l	1884410	4	11.816	1204840	50.0
1-Decanol	14.658	26.8	ug/l	645728	4	11.816	1204840	50.0
Dodecane, 1-chl...	16.346	9.6	ug/l	231307	4	11.816	1204840	50.0