

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN030321\
 Data File : VN066126.D
 Acq On : 3 Mar 2021 16:08
 Operator : JC/MD
 Sample : M1507-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP-30771-73-77

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_N\methods\82N030221W.M
 Title : SW846 8260

Signal : TIC: VN066126.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.811	14	22	38	rVB2	46195	65509	17.56%	2.176%
2	1.988	70	77	83	rBV3	4254	6360	1.70%	0.211%
3	2.174	122	135	146	rVB3	4599	11639	3.12%	0.387%
4	2.306	166	176	188	rVB	30223	47870	12.83%	1.590%
5	3.248	460	469	486	rVB4	3613	9463	2.54%	0.314%
6	3.666	588	599	618	rBV2	2627	6453	1.73%	0.214%
7	3.788	622	637	654	rBV	9177	24581	6.59%	0.816%
8	4.032	695	713	728	rBV	7913	23182	6.21%	0.770%
9	6.499	1461	1480	1504	rBV2	43834	132418	35.50%	4.398%
10	6.782	1548	1568	1588	rBV4	7336	23723	6.36%	0.788%
11	7.550	1790	1807	1818	rBV4	46285	116129	31.13%	3.857%
12	7.624	1818	1830	1847	rVB	78729	183324	49.14%	6.089%
13	7.994	1927	1945	1964	rBV3	81916	216435	58.02%	7.188%
14	8.547	2102	2117	2138	rBV	130126	271711	72.84%	9.024%
15	8.753	2170	2181	2202	rBV	23732	54209	14.53%	1.800%
16	9.126	2290	2297	2311	rVB5	3412	6601	1.77%	0.219%
17	10.055	2571	2586	2597	rBV	205615	373038	100.00%	12.390%
18	10.119	2597	2606	2626	rVB	75526	139204	37.32%	4.623%
19	10.839	2821	2830	2842	rVB5	3529	6422	1.72%	0.213%
20	11.376	2984	2997	3018	rBV	195741	352509	94.50%	11.708%
21	11.479	3022	3029	3043	rVB2	12163	19841	5.32%	0.659%
22	11.585	3050	3062	3079	rBV	44519	85303	22.87%	2.833%
23	11.920	3154	3166	3176	rBV	20871	36633	9.82%	1.217%
24	12.373	3295	3307	3326	rBV	149633	267247	71.64%	8.876%
25	12.624	3379	3385	3392	rBV3	3806	6215	1.67%	0.206%
26	12.701	3402	3409	3418	rVB7	3170	4973	1.33%	0.165%
27	12.887	3454	3467	3478	rBV8	5569	10900	2.92%	0.362%
28	13.010	3497	3505	3512	rBV2	6156	8960	2.40%	0.298%
29	13.074	3518	3525	3538	rBV4	7254	12538	3.36%	0.416%
30	13.312	3587	3599	3616	rBV	167221	301672	80.87%	10.019%
31	13.424	3622	3634	3655	rBV	56616	126559	33.93%	4.203%
32	14.611	3997	4003	4014	rVB6	12299	18819	5.04%	0.625%
33	15.077	4141	4148	4161	rBV5	18596	40421	10.84%	1.343%

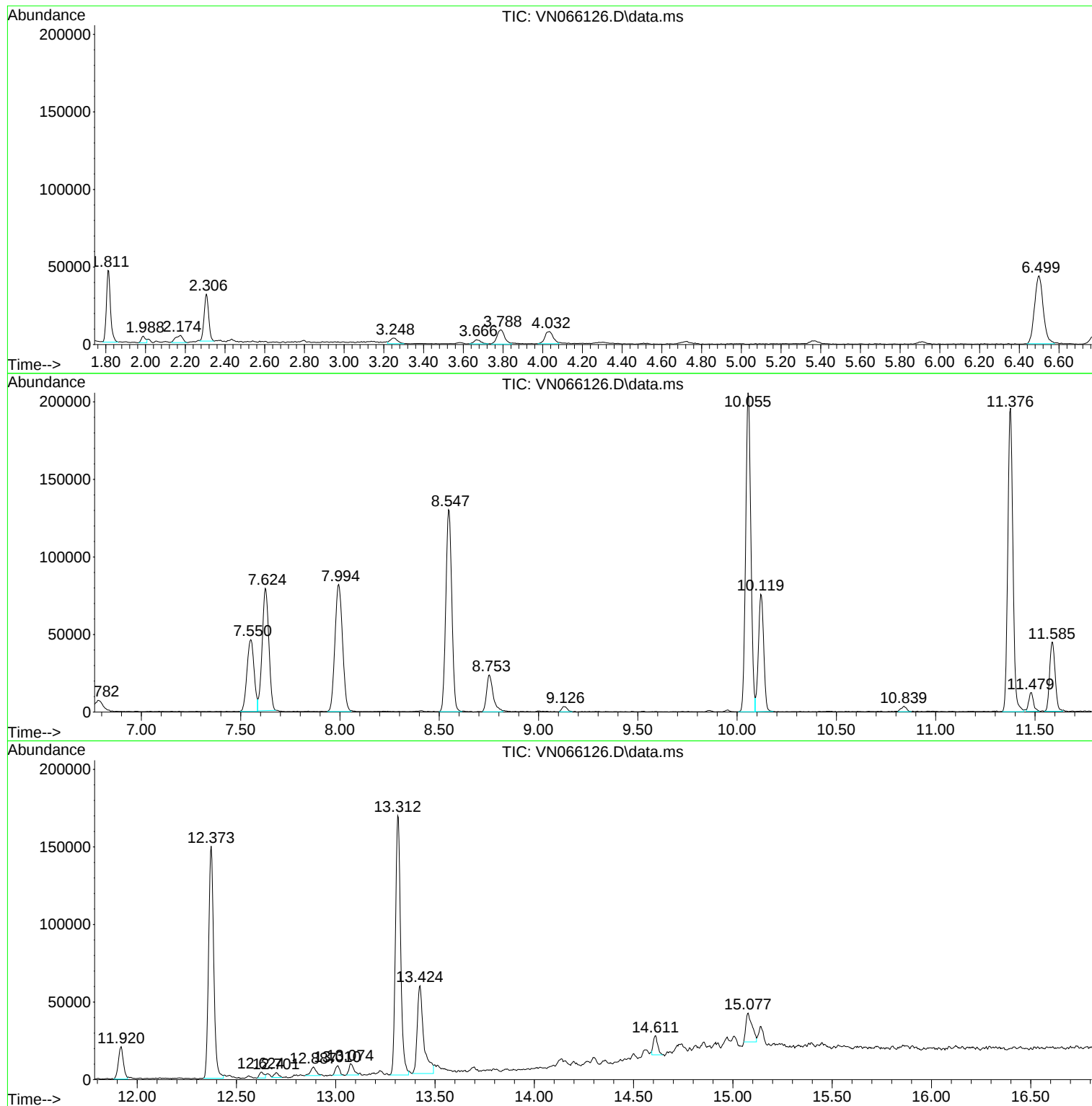
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COMP-30771-73-77

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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



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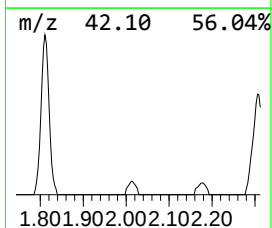
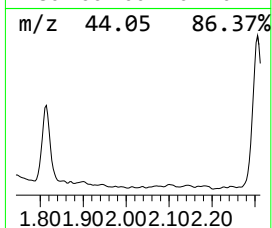
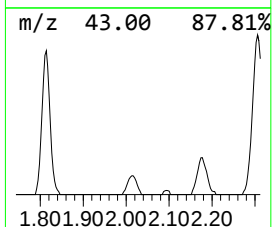
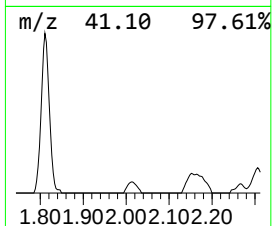
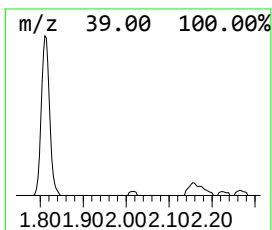
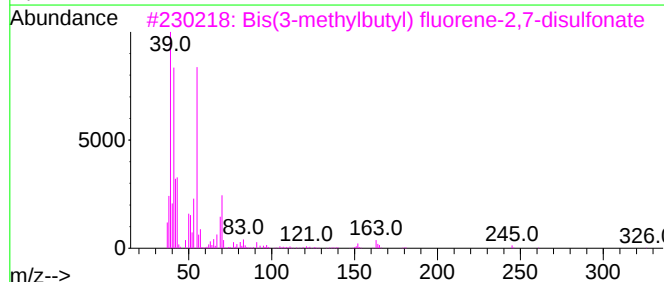
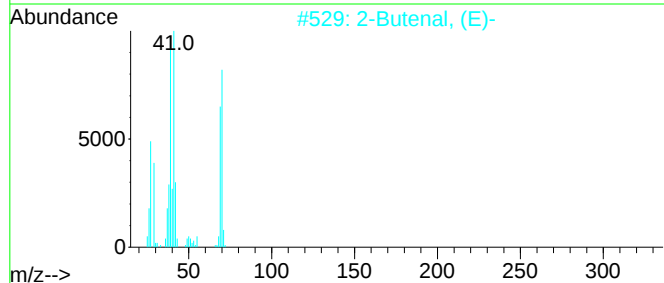
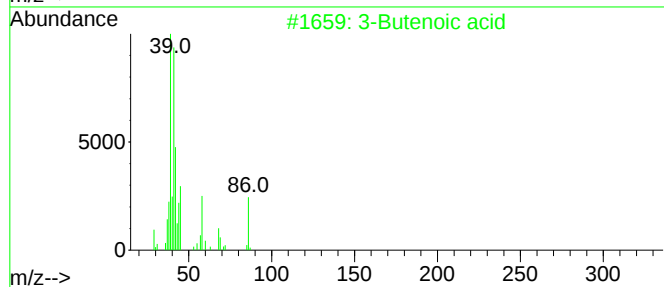
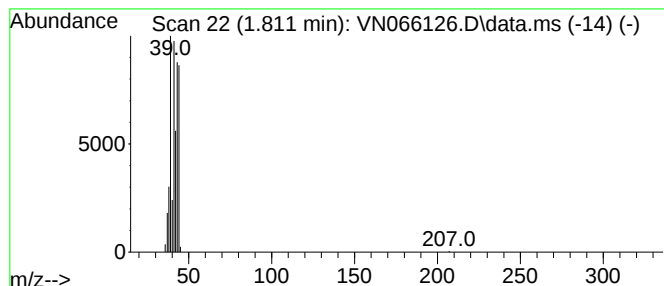
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Quant Title : SW846 8260

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

Peak Number 1 3-Butenoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.811	17.87 ug/l	65509	Pentafluorobenzene	7.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Butenoic acid	86	C4H6O2	000625-38-7	72
2			2-Butenal, (E)-	70	C4H6O	000123-73-9	64
3			Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	64
4			Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	53
5			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	53



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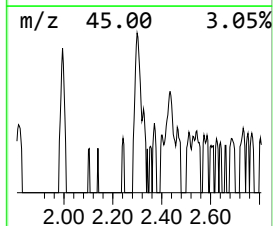
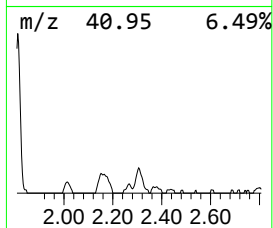
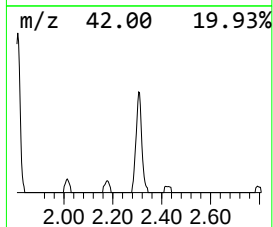
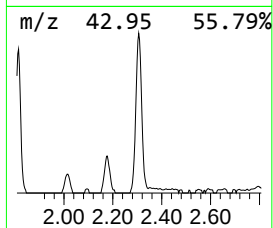
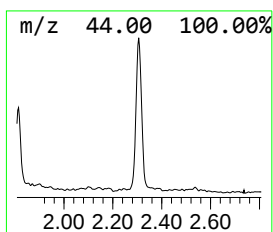
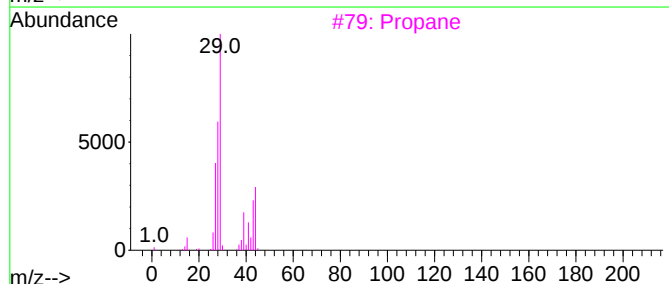
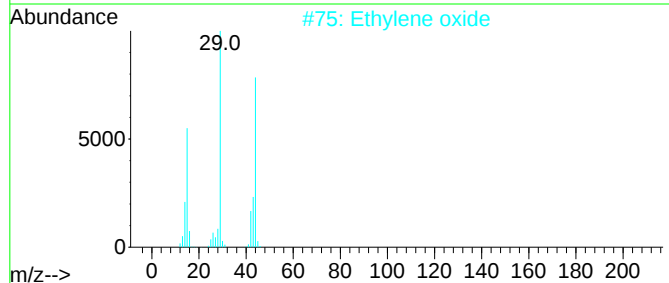
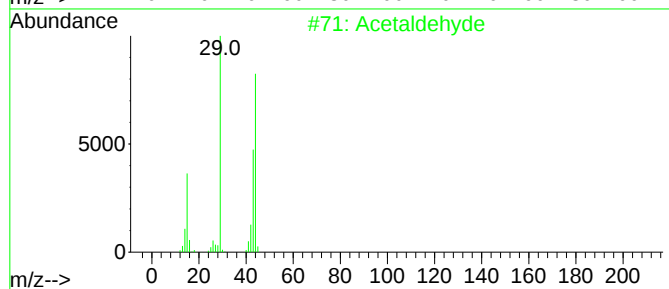
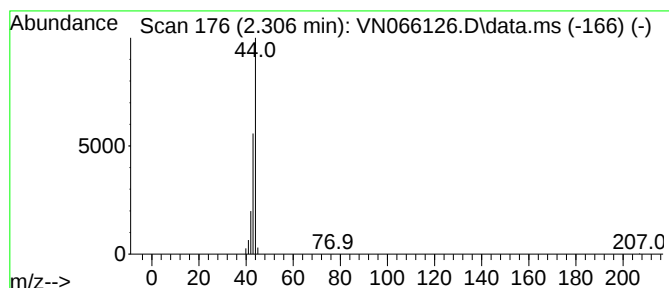
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Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	13.06 ug/l	47870	Pentafluorobenzene	7.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			L-Alanine, methyl ester	103	C4H9NO2	010065-72-2	4
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	4



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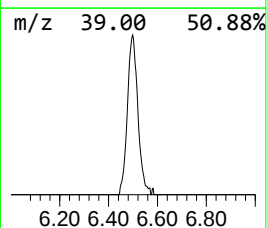
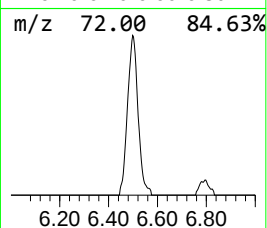
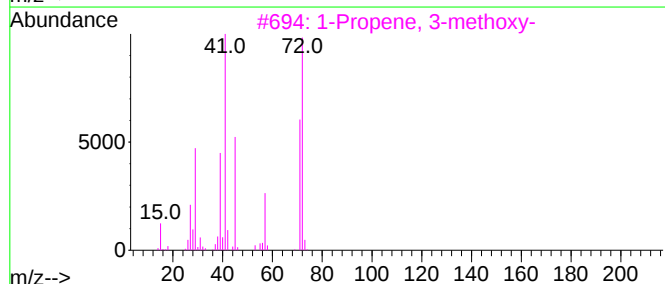
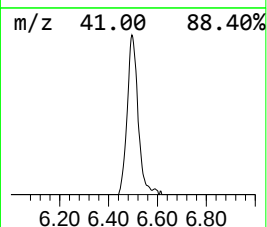
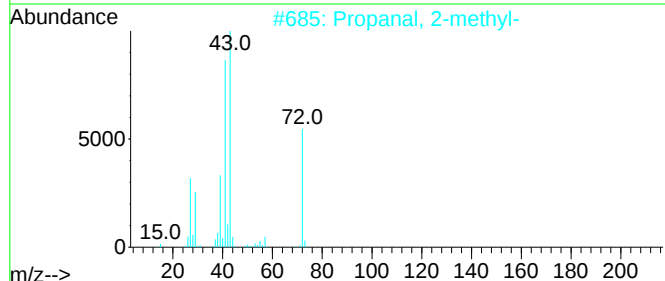
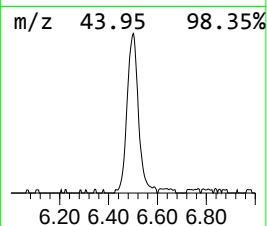
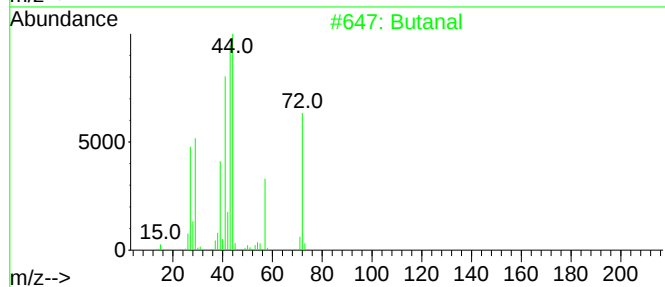
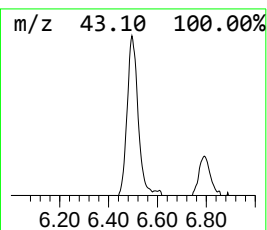
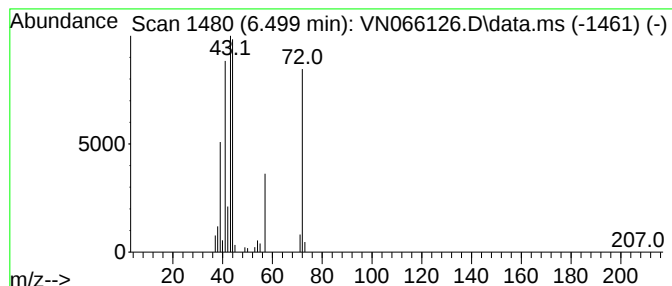
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030221W.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.499	36.12 ug/l	132418	Pentafluorobenzene	7.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4			Isobutylene epoxide	72	C4H8O	000558-30-5	27
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	25



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

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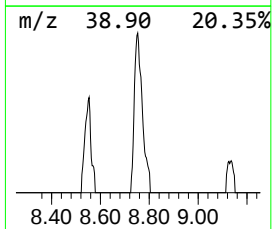
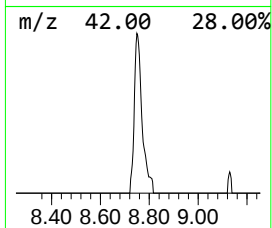
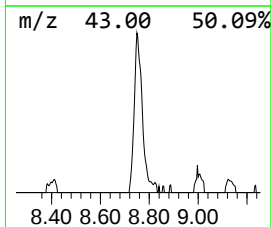
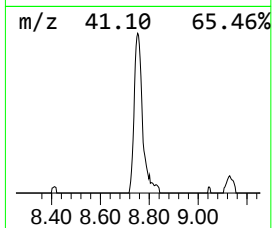
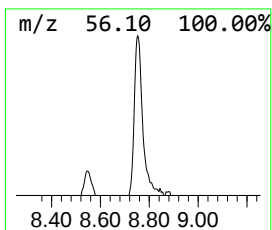
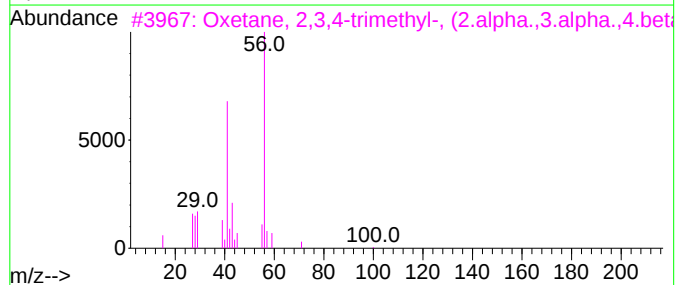
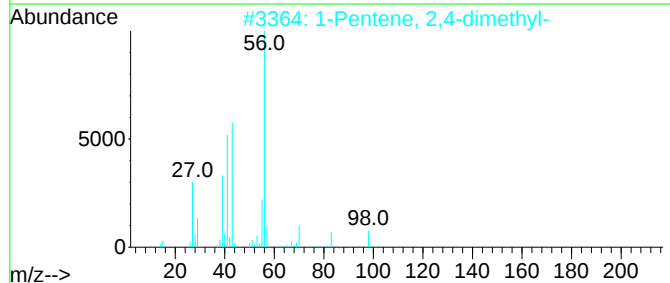
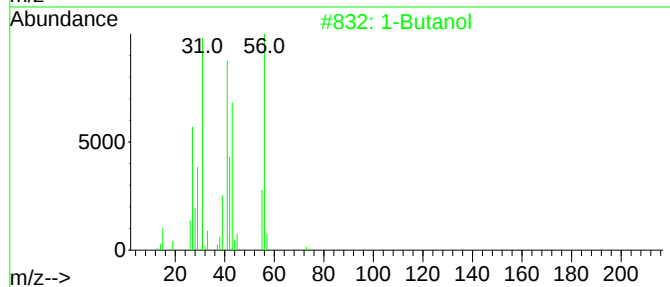
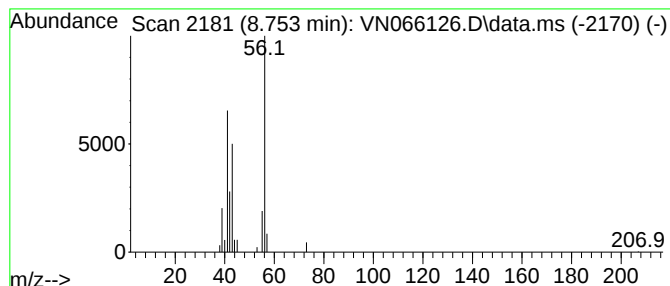
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	9.98 ug/l	54209	1,4-Difluorobenzene	8.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	83
2			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	38
3			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	38
4			1-Hexanol	102	C6H14O	000111-27-3	9
5			2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	9



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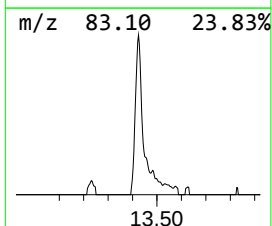
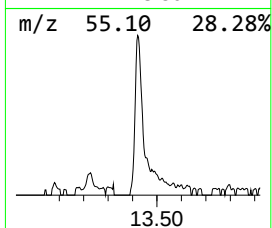
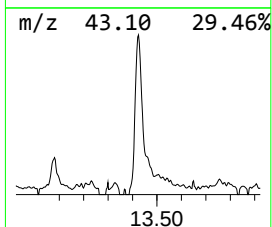
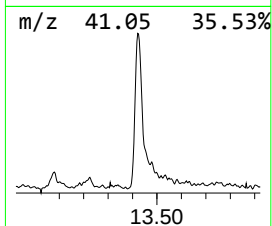
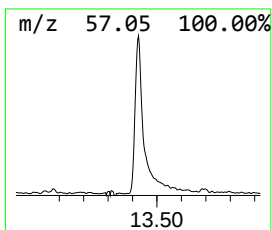
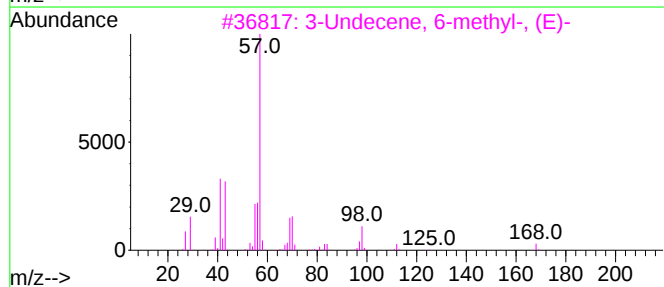
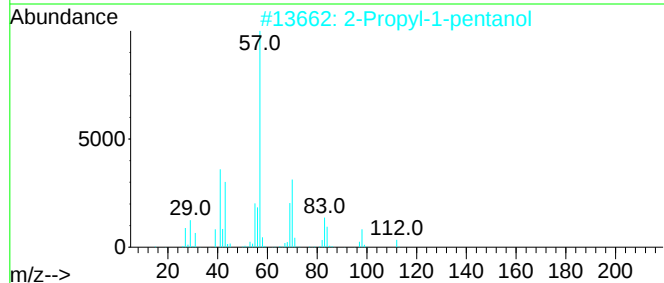
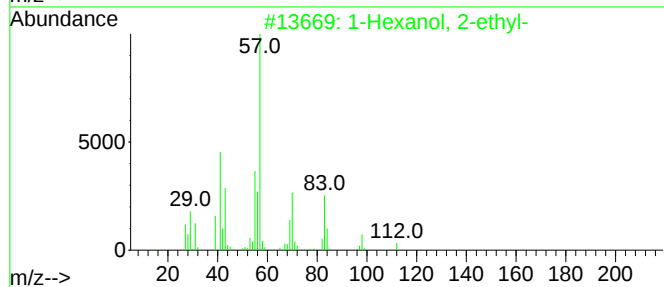
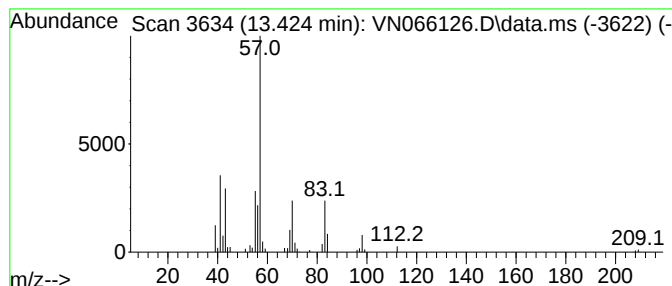
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.424	20.98 ug/l	126559	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	47
4			2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	47
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Butenoic acid	1.811	17.9	ug/l	65509	1	7.624	183324	50.0
Acetaldehyde	2.306	13.1	ug/l	47870	1	7.624	183324	50.0
Butanal	6.499	36.1	ug/l	132418	1	7.624	183324	50.0
1-Butanol	8.753	10.0	ug/l	54209	2	8.547	271711	50.0
1-Hexanol, 2-et...	13.424	21.0	ug/l	126559	4	13.312	301672	50.0