

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060925\
 Data File : VN086896.D
 Acq On : 09 Jun 2025 11:55
 Operator : JC\MD
 Sample : Q2216-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3851

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\82N060625W.M
 Title : SW846 8260

Signal : TIC: VN086896.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.112	21	27	40	rVB	104065	170768	8.85%	1.398%
2	2.354	61	68	73	rBV	15937	26331	1.37%	0.216%
3	2.524	90	97	111	rBV2	83850	183292	9.50%	1.500%
4	4.448	415	424	433	rBV	16283	50526	2.62%	0.414%
5	4.548	433	441	453	rVB2	16456	50705	2.63%	0.415%
6	5.530	596	608	633	rVB	92022	343322	17.80%	2.810%
7	8.177	1046	1058	1062	rBV	232457	571634	29.64%	4.679%
8	8.230	1062	1067	1081	rVB	454503	1043128	54.08%	8.538%
9	8.588	1118	1128	1137	rBV	252446	588054	30.49%	4.813%
10	8.977	1187	1194	1202	rVB5	11439	25521	1.32%	0.209%
11	9.106	1207	1216	1233	rVB	678225	1398688	72.52%	11.448%
12	9.465	1269	1277	1283	rVV4	9148	26654	1.38%	0.218%
13	9.535	1284	1289	1296	rVB	10446	20841	1.08%	0.171%
14	9.912	1345	1353	1364	rVB	240502	489020	25.35%	4.003%
15	10.453	1439	1445	1451	rBV2	15642	34257	1.78%	0.280%
16	10.565	1457	1464	1471	rBV	1037087	1928799	100.00%	15.787%
17	10.630	1471	1475	1487	rVV2	53127	119922	6.22%	0.982%
18	11.071	1543	1550	1558	rBV2	22016	56714	2.94%	0.464%
19	11.865	1677	1685	1695	rBV	875248	1583167	82.08%	12.958%
20	11.965	1696	1702	1709	rBV2	26586	56742	2.94%	0.464%
21	12.071	1713	1720	1725	rBV	41134	82998	4.30%	0.679%
22	12.394	1770	1775	1779	rBV	16049	31055	1.61%	0.254%
23	12.847	1845	1852	1862	rVB	675171	1173057	60.82%	9.601%
24	13.176	1901	1908	1915	rBV3	35698	89013	4.61%	0.729%
25	13.476	1953	1959	1968	rVB8	26803	73408	3.81%	0.601%
26	13.788	2005	2012	2022	rVB	907820	1564171	81.10%	12.803%
27	14.118	2063	2068	2078	rVB5	47114	104470	5.42%	0.855%
28	14.212	2080	2084	2088	rBV5	23455	43393	2.25%	0.355%
29	14.365	2108	2110	2118	rVB7	26927	58125	3.01%	0.476%
30	14.629	2150	2155	2157	rBV4	37946	66863	3.47%	0.547%
31	14.859	2189	2194	2207	rVB2	60757	162873	8.44%	1.333%

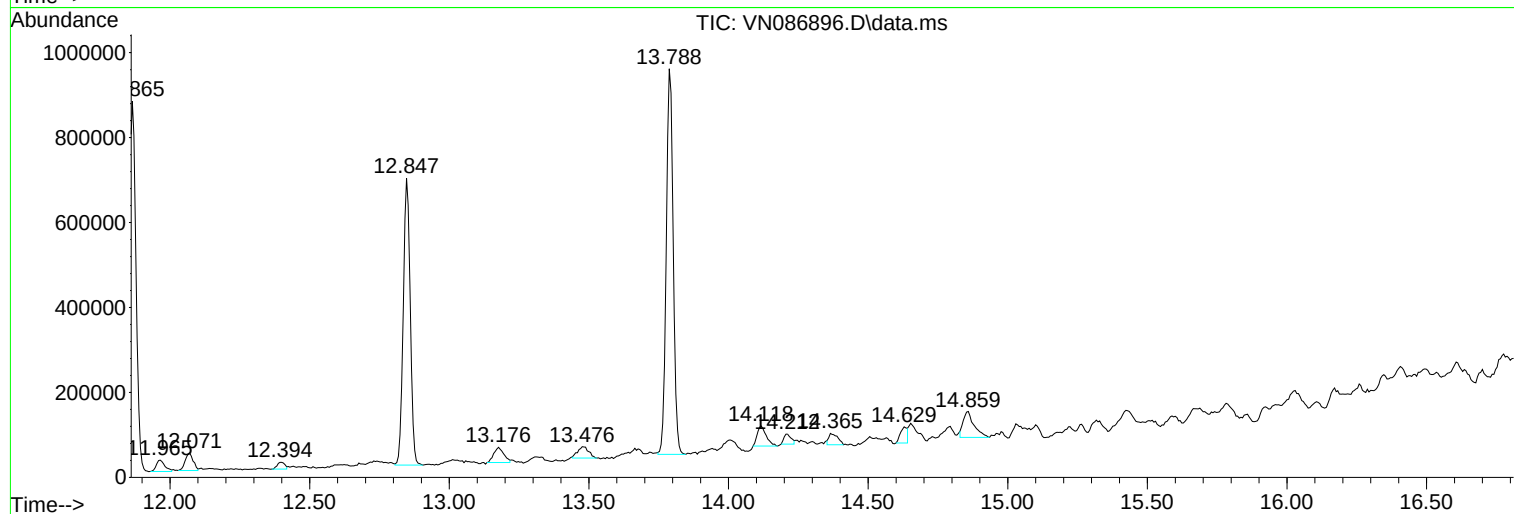
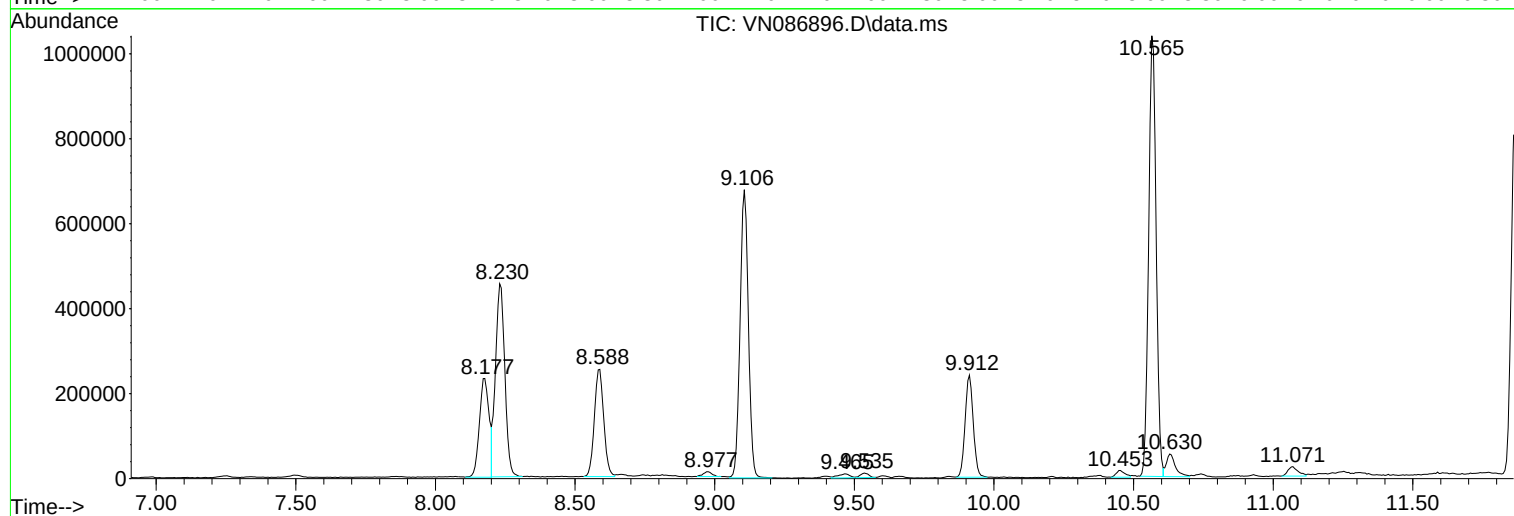
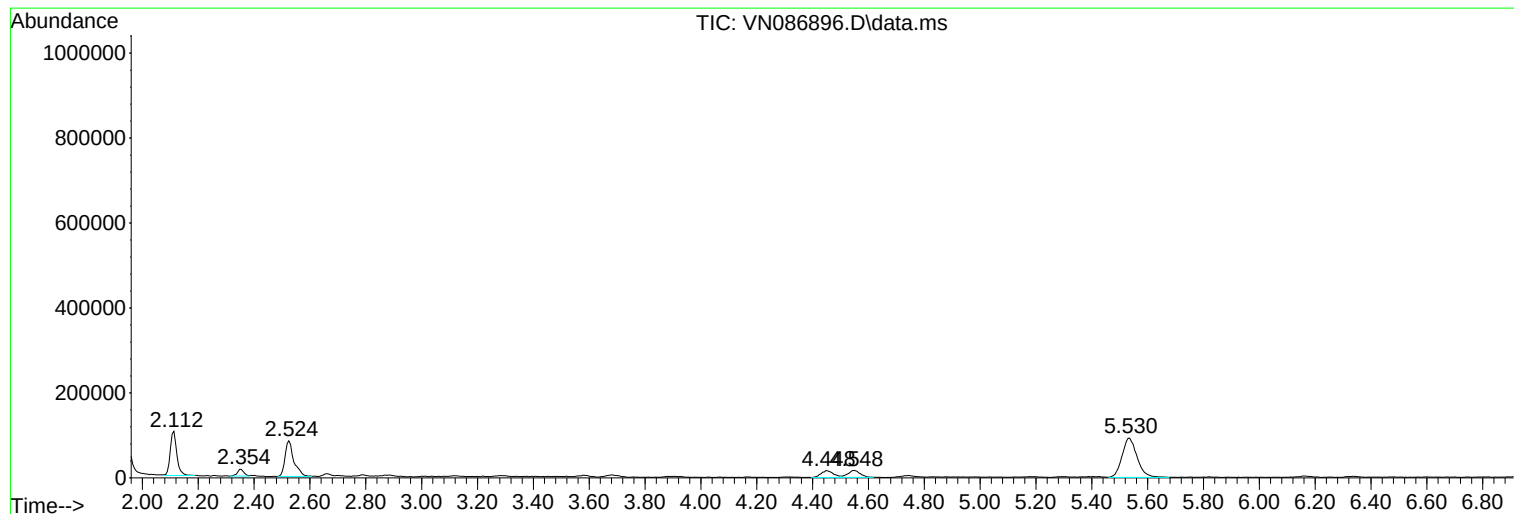
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



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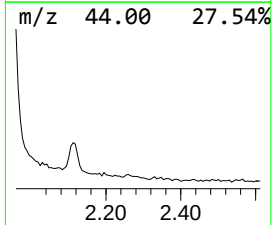
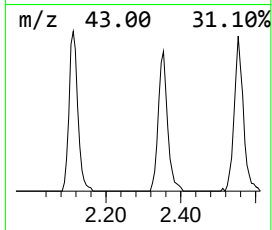
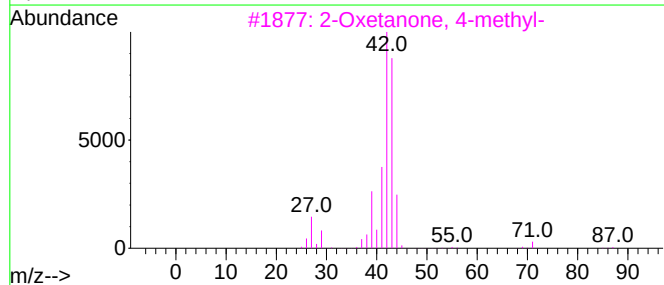
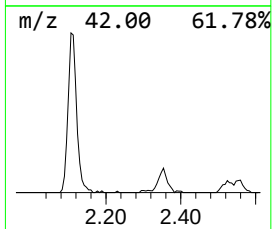
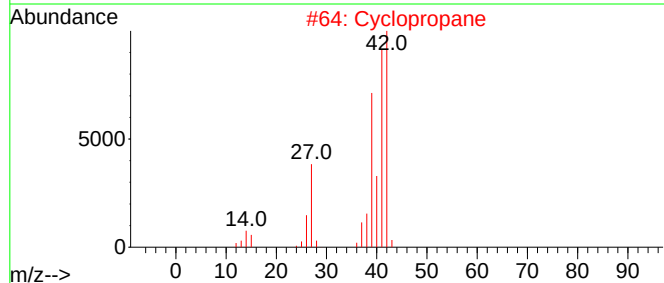
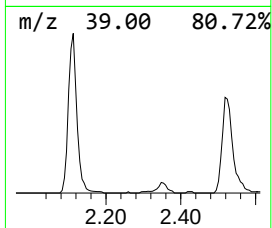
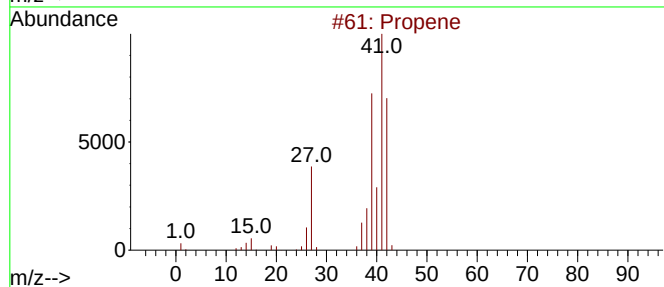
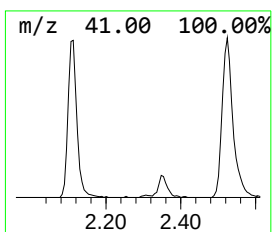
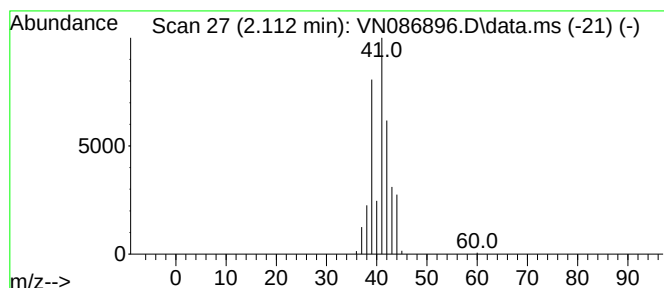
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Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.112	8.19 ug/l	170768	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	9
3			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4
4			4-Amino-1-butanol	89	C4H11NO	013325-10-5	2
5			Methylenecyclopropane	54	C4H6	006142-73-0	2



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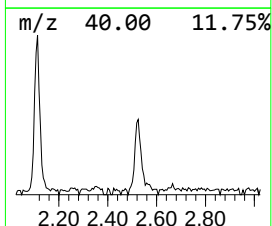
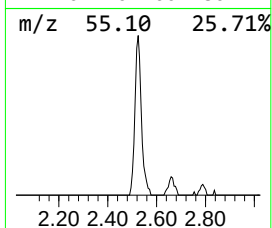
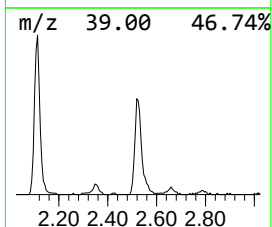
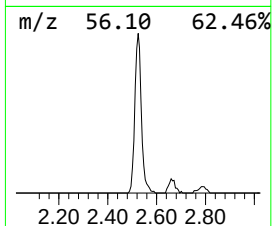
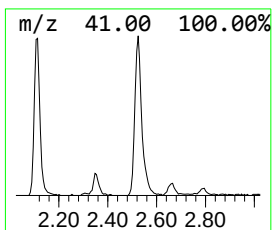
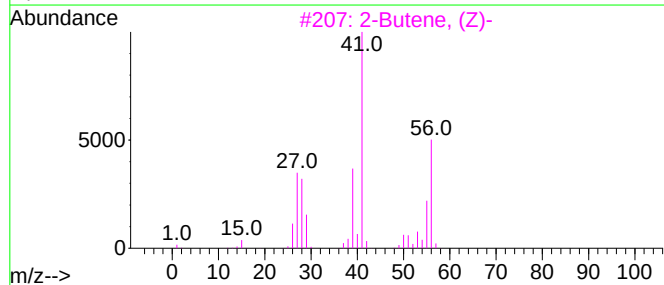
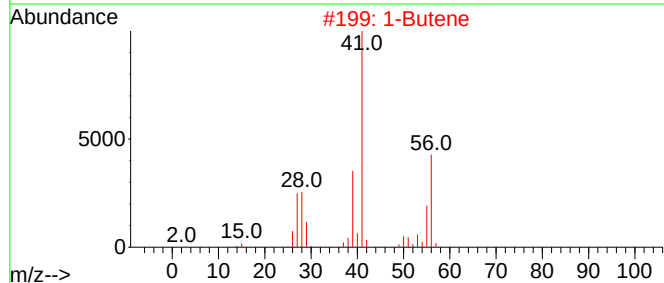
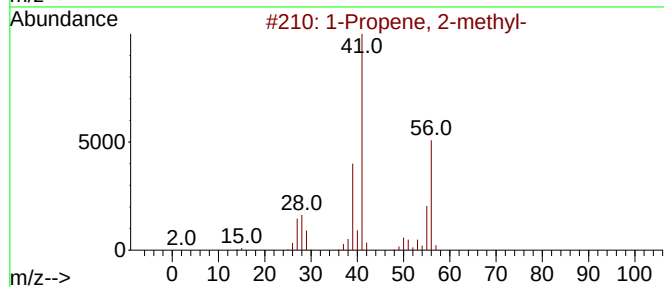
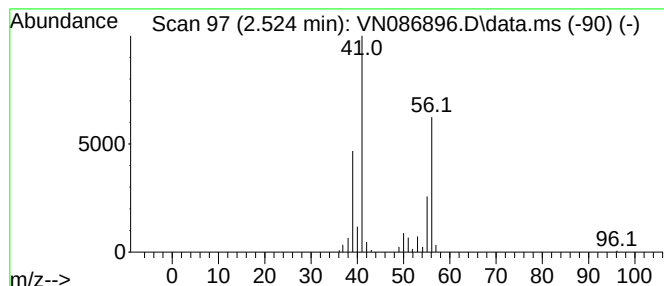
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.524	8.79 ug/l	183292	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2		1-Butene	56	C4H8	000106-98-9	87
3		2-Butene, (Z)-	56	C4H8	000590-18-1	80
4		2-Butene, (E)-	56	C4H8	000624-64-6	80
5		2-Butene	56	C4H8	000107-01-7	72



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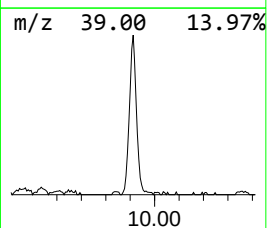
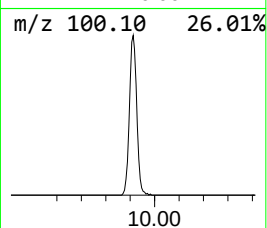
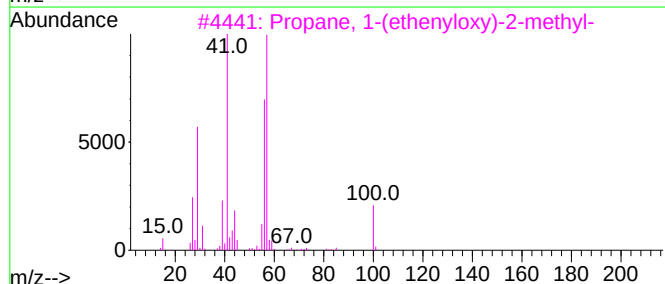
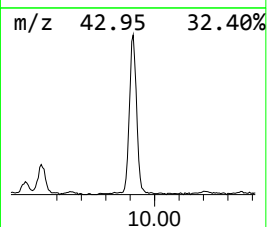
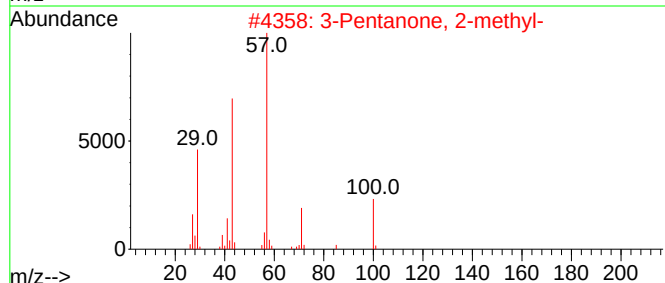
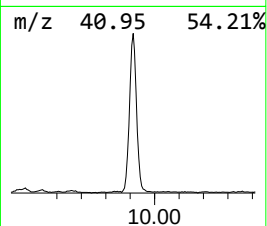
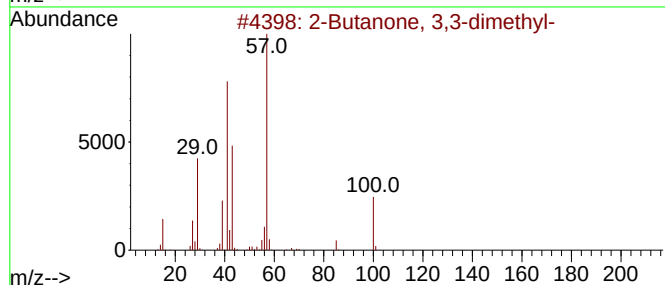
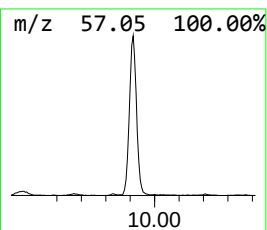
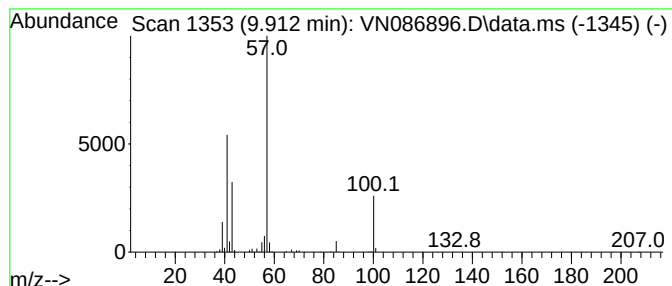
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.912	17.48 ug/l	489020	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	78
2			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
3			Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	50
4			3,3-Dimethyl-2-oxobutanoic acid	130	C6H10O3	000815-17-8	40
5			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	38



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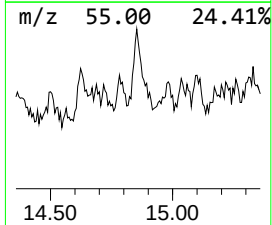
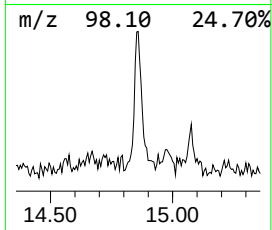
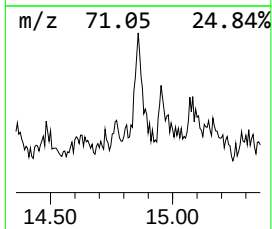
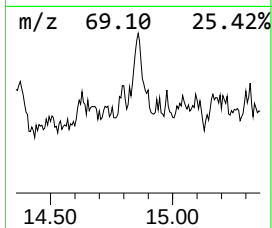
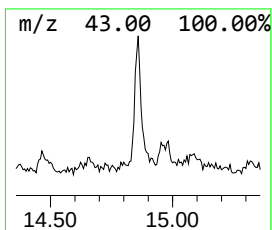
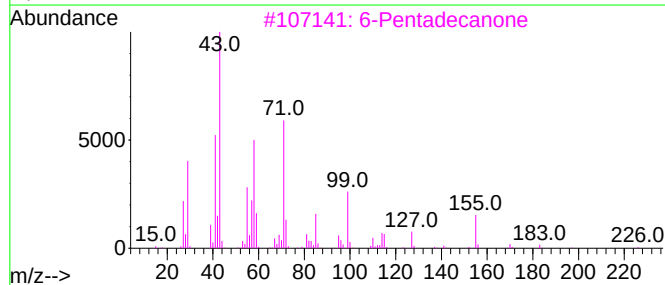
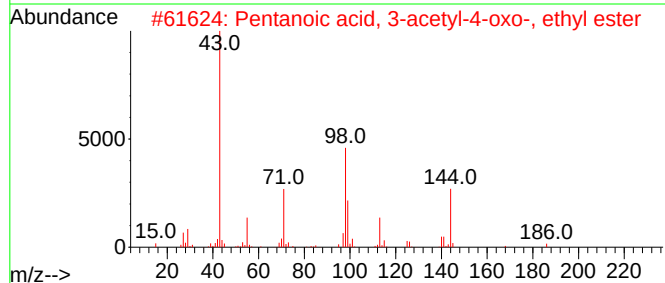
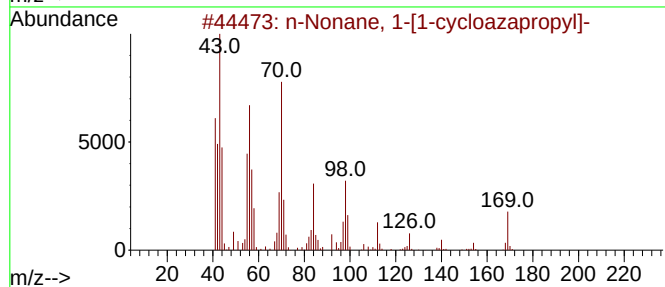
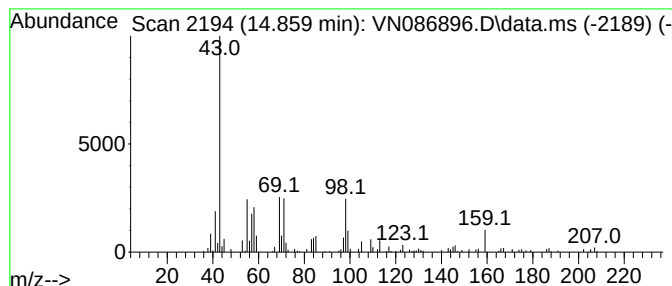
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Peak Number 4 n-Nonane, 1-[1-cycloazaprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.859	5.21 ug/l	162873	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonane, 1-[1-cycloazapropyl]-	169	C11H23N	014924-95-9	53
2			Pentanoic acid, 3-acetyl-4-oxo-,...	186	C9H14O4	018835-02-4	43
3			6-Pentadecanone	226	C15H30O	001001-45-2	38
4			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	25
5			5-Decanone	156	C10H20O	000820-29-1	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propene	2.112	8.2	ug/l	170768	1	8.230	1043130	50.0
1-Propene, 2-me...	2.524	8.8	ug/l	183292	1	8.230	1043130	50.0
2-Butanone, 3,3...	9.912	17.5	ug/l	489020	2	9.106	1398690	50.0
n-Nonane, 1-[1-...	14.859	5.2	ug/l	162873	4	13.788	1564170	50.0