

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060925\
 Data File : VN086892.D
 Acq On : 09 Jun 2025 10:29
 Operator : JC\MD
 Sample : Q2216-01
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3898

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: VN086892.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.759	975	987	1003	rBV	438445	1151485	9.14%	3.716%
2	8.171	1045	1057	1060	rBV	243625	551437	4.38%	1.780%
3	8.224	1060	1066	1077	rVV2	821856	1970521	15.64%	6.359%
4	8.330	1077	1084	1094	rVB2	105176	259123	2.06%	0.836%
5	8.447	1094	1104	1119	rBV	474474	1123238	8.91%	3.625%
6	8.582	1119	1127	1138	rVB	267096	608452	4.83%	1.964%
7	8.706	1138	1148	1157	rBV5	54137	151894	1.21%	0.490%
8	8.965	1184	1192	1205	rVB	207512	429488	3.41%	1.386%
9	9.100	1205	1215	1227	rBV	685631	1436940	11.40%	4.637%
10	10.565	1455	1464	1469	rBV	1057326	1991428	15.80%	6.427%
11	10.629	1469	1475	1489	rVB	6984280	12601770	100.00%	40.669%
12	11.865	1676	1685	1695	rBV	874754	1581419	12.55%	5.104%
13	11.965	1695	1702	1710	rVV	375764	652108	5.17%	2.105%
14	12.065	1710	1719	1731	rBV	1383621	2704049	21.46%	8.727%
15	12.394	1763	1775	1785	rBV	318802	587756	4.66%	1.897%
16	12.847	1846	1852	1864	rVB	648249	1110055	8.81%	3.582%
17	13.159	1898	1905	1912	rVB3	82742	177000	1.40%	0.571%
18	13.788	2006	2012	2021	rVB	846290	1435391	11.39%	4.632%
19	14.100	2060	2065	2072	rBV2	95599	146235	1.16%	0.472%
20	14.953	2201	2210	2218	rVV4	99708	181497	1.44%	0.586%
21	15.053	2219	2227	2240	rVB8	33416	134913	1.07%	0.435%

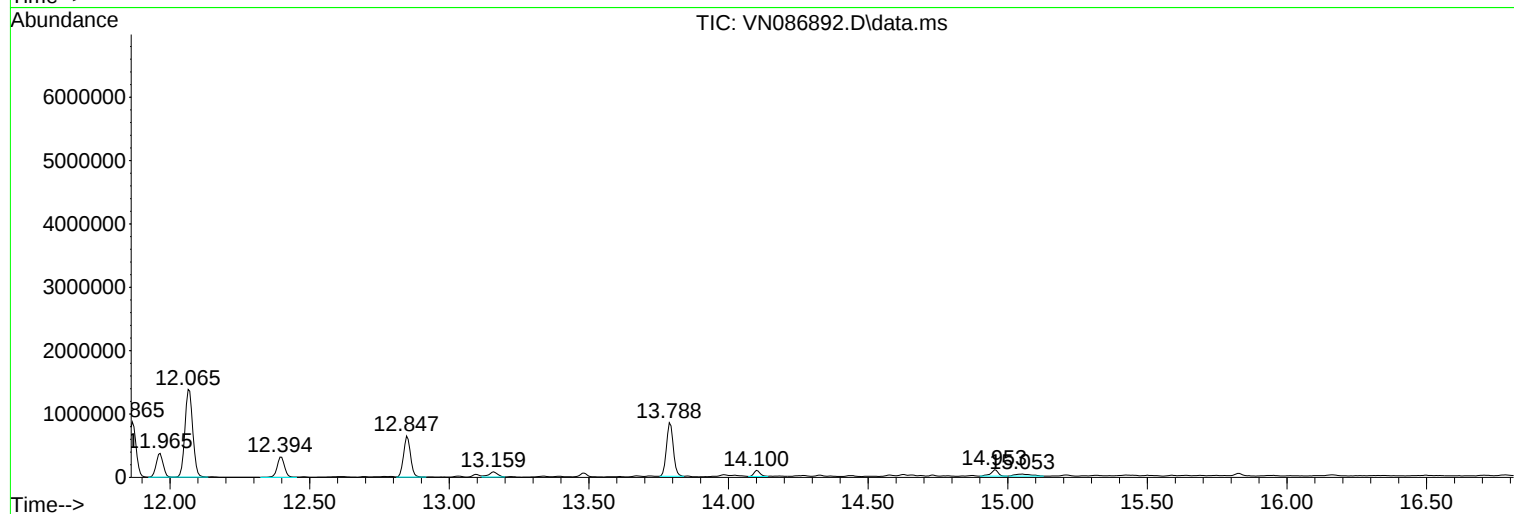
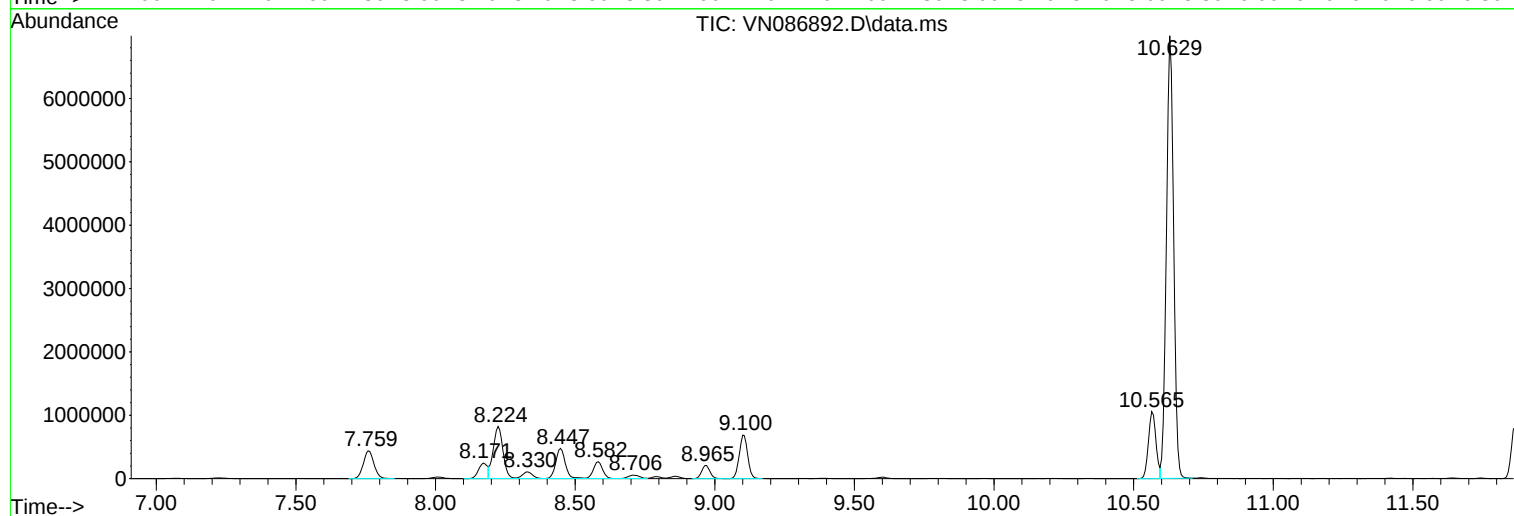
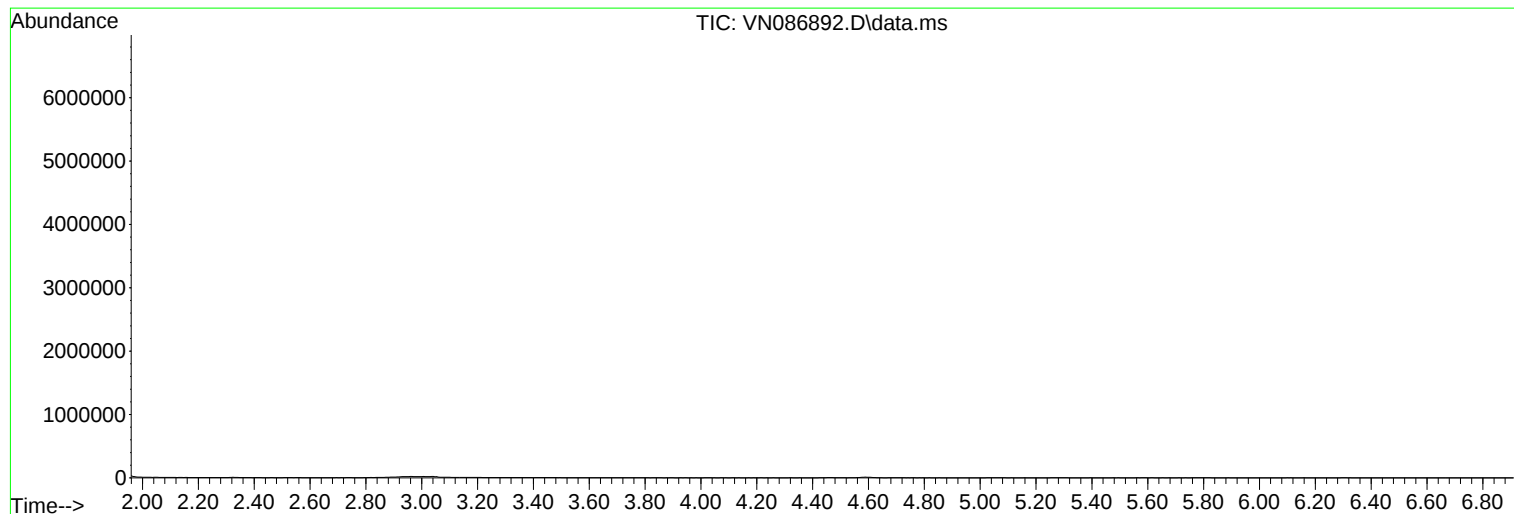
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3898

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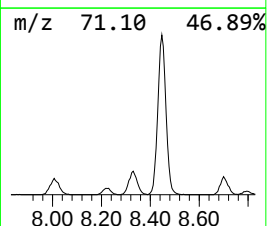
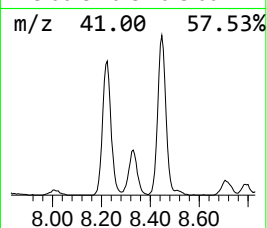
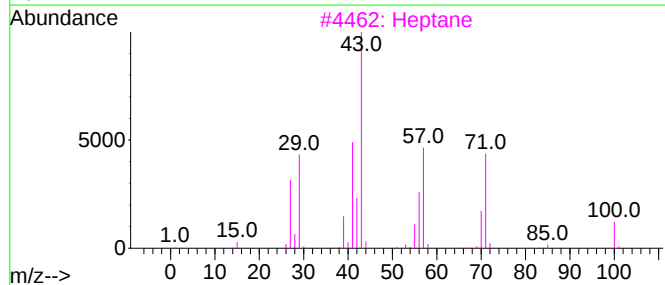
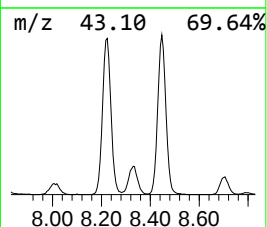
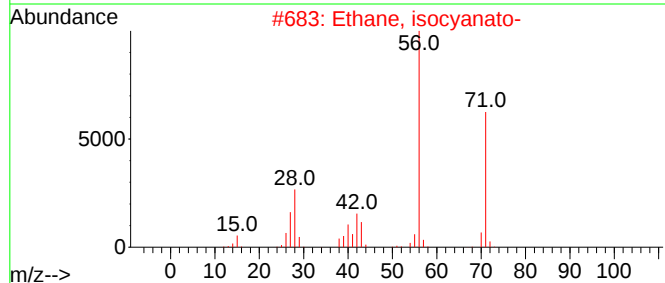
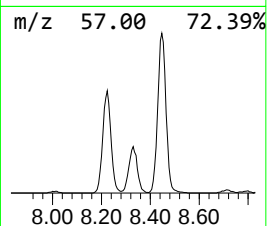
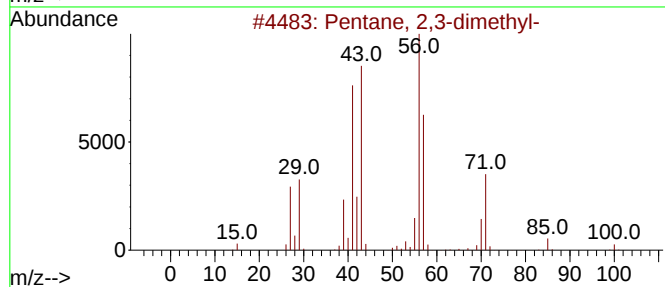
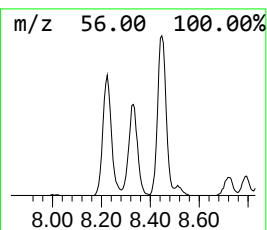
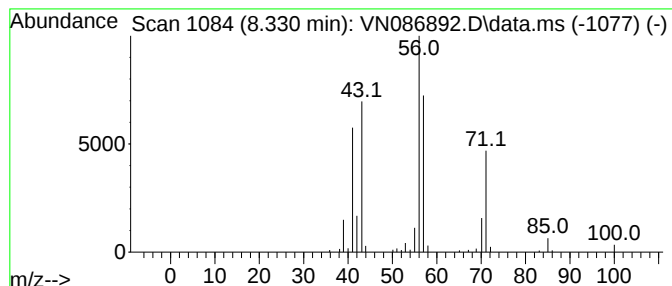
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.330	6.57 ug/l	259123	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Ethane, isocyanato-	71	C3H5NO	000109-90-0	59
3			Heptane	100	C7H16	000142-82-5	47
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43



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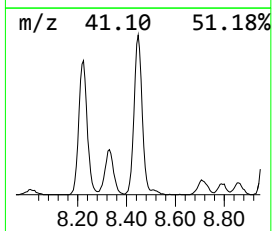
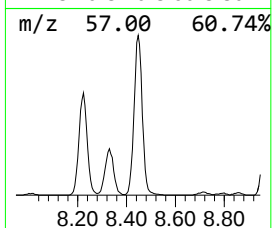
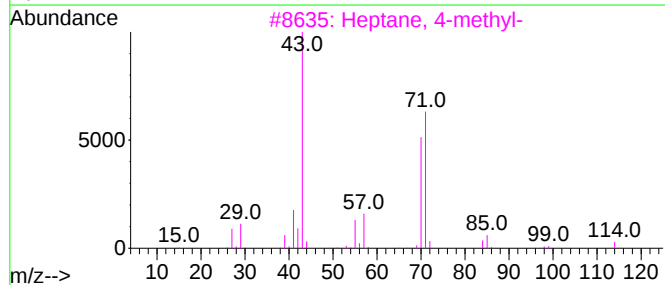
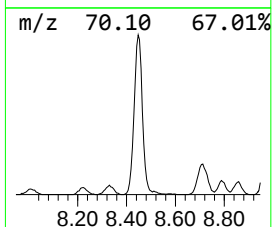
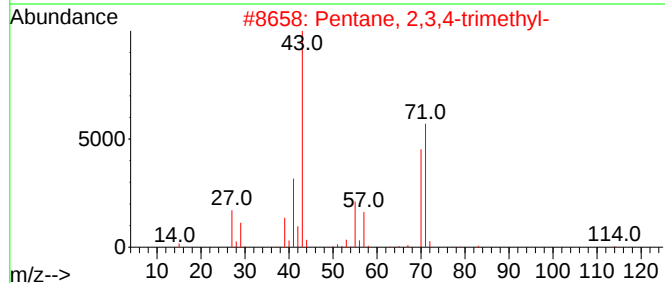
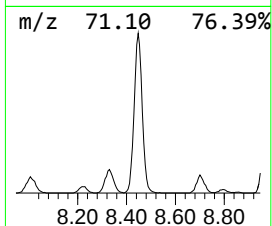
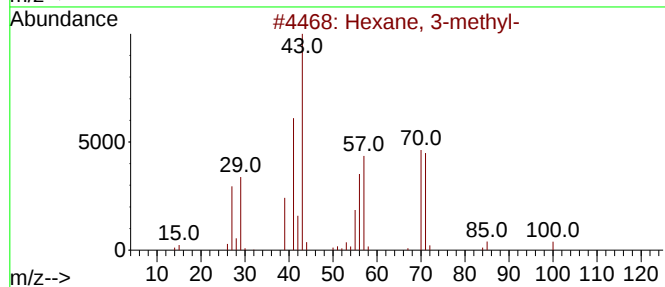
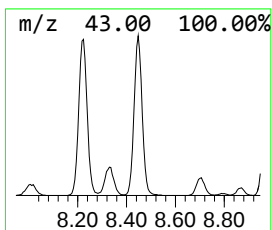
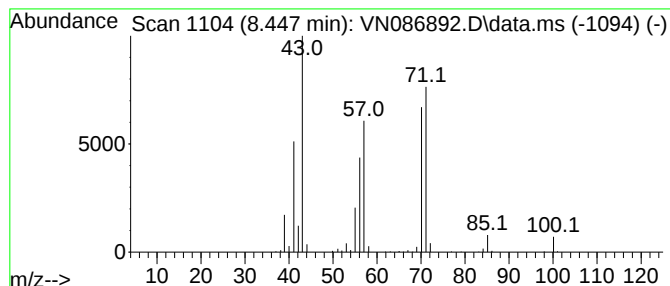
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.447	28.50 ug/l	1123240	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	95	
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59	
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59	
4	Diisoamyl ether	158	C10H22O	000544-01-4	59	
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	59	



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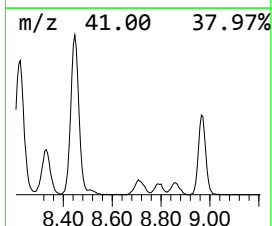
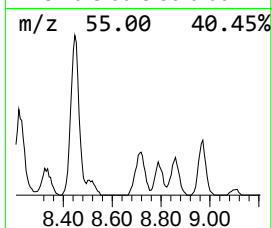
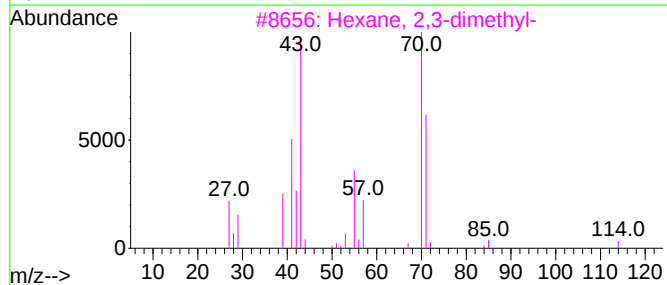
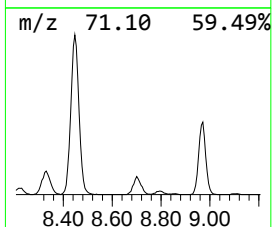
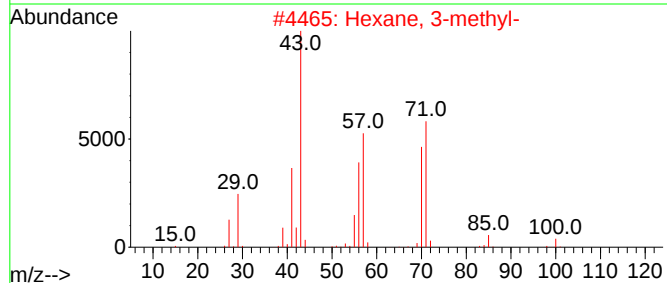
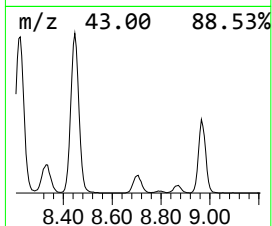
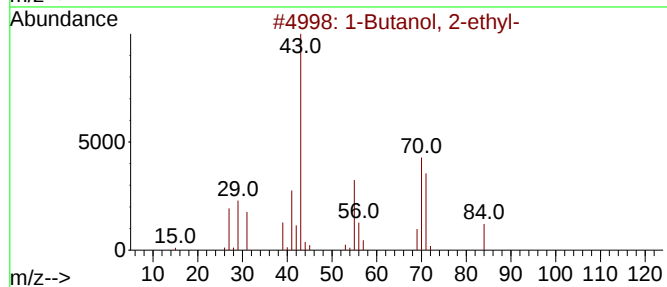
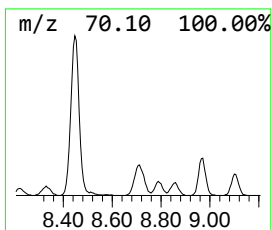
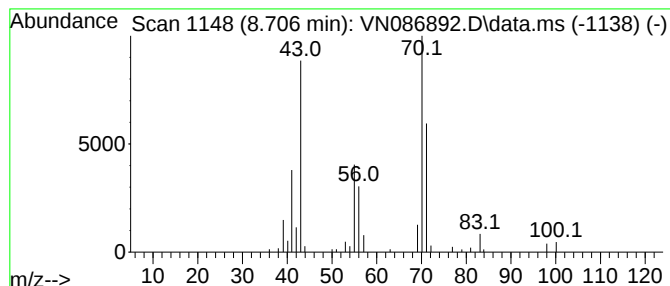
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Quant Title : SW846 8260

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

Peak Number 3 1-Butanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.706	5.29 ug/l	151894	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-ethyl-			102	C6H14O	000097-95-0	53
2	Hexane, 3-methyl-			100	C7H16	000589-34-4	47
3	Hexane, 2,3-dimethyl-			114	C8H18	000584-94-1	45
4	1-Pentanol, 2-methyl-			102	C6H14O	000105-30-6	42
5	Butane, 1-bromo-3-methyl-			150	C5H11Br	000107-82-4	38



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Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

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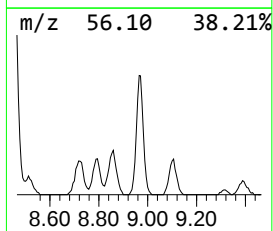
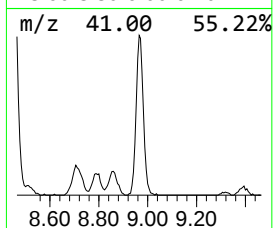
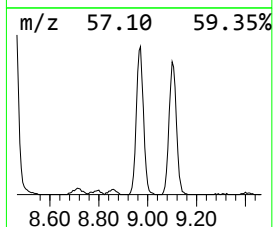
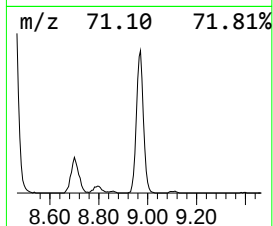
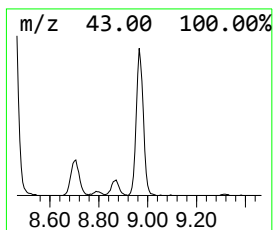
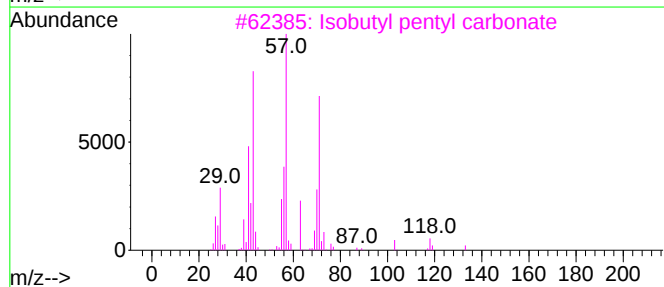
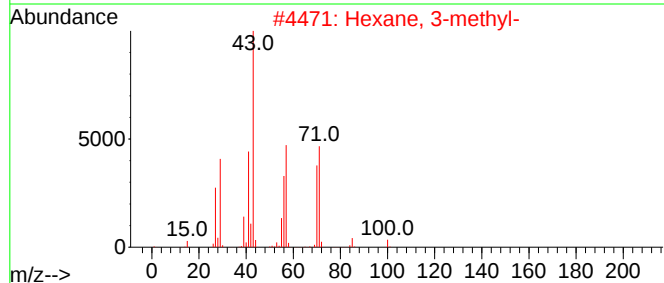
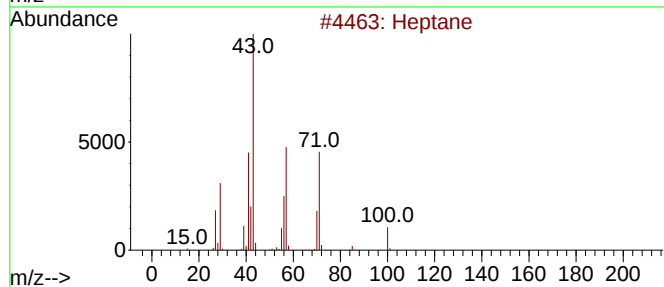
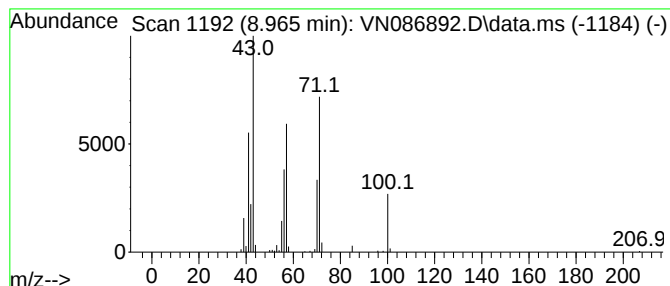
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 4 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	14.94 ug/l	429488	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
3			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	50
4			1,1-Dimethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-99-2	47
5			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	46



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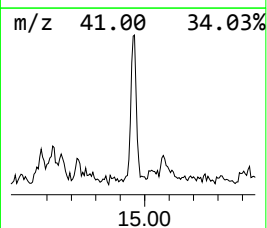
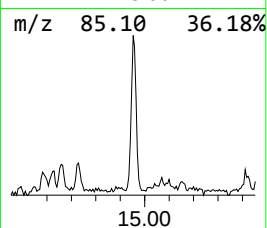
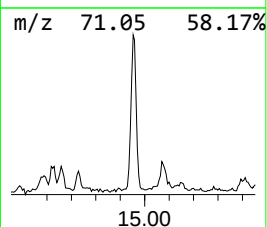
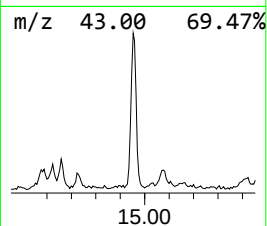
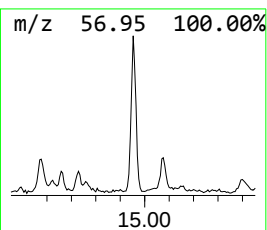
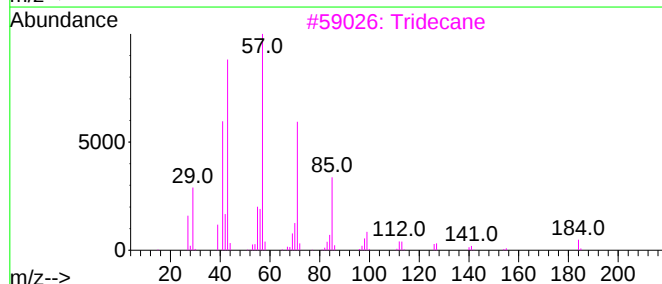
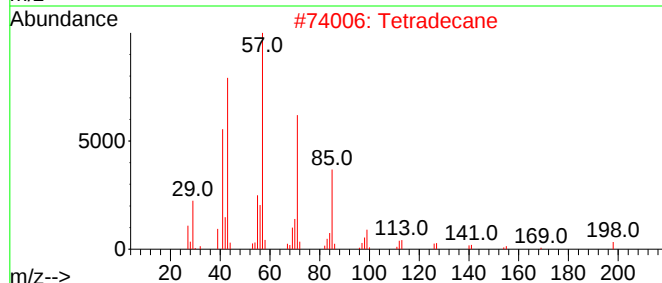
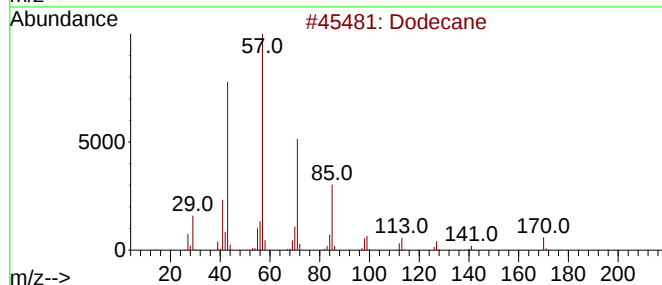
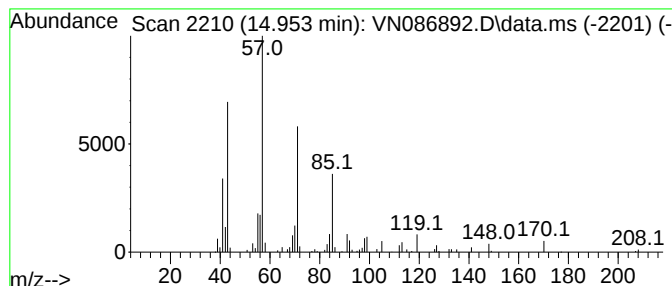
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Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.953	6.32 ug/l	181497	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Tetradecane	198	C14H30	000629-59-4	83
3			Tridecane	184	C13H28	000629-50-5	80
4			Pentadecane	212	C15H32	000629-62-9	80
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.330	6.6	ug/l	259123	1	8.230	1970520	50.0
Hexane, 3-methyl-	8.447	28.5	ug/l	1123240	1	8.230	1970520	50.0
1-Butanol, 2-et...	8.706	5.3	ug/l	151894	2	9.106	1436940	50.0
Heptane	8.965	14.9	ug/l	429488	2	9.106	1436940	50.0
Dodecane	14.953	6.3	ug/l	181497	4	13.788	1435390	50.0