

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100925\
 Data File : VX048084.D
 Acq On : 09 Oct 2025 14:20
 Operator : JC/MD
 Sample : Q3311-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2S

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_X\Method\82X091625W.M
 Title : SW846 8260

Signal : TIC: VX048084.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.380	42	48	54	rBV	13623	18236	1.40%	0.207%
2	1.758	104	110	127	rBV	202008	333011	25.59%	3.788%
3	1.965	139	144	154	rBV	14917	24706	1.90%	0.281%
4	2.349	201	207	217	rBV	6700	16471	1.27%	0.187%
5	2.788	270	279	287	rBV	25188	67329	5.17%	0.766%
6	2.873	287	293	312	rVB4	29963	97445	7.49%	1.109%
7	3.105	322	331	350	rBV2	64353	163011	12.52%	1.854%
8	3.733	426	434	443	rBV5	5704	13940	1.07%	0.159%
9	3.837	443	451	459	rBV4	7559	19909	1.53%	0.226%
10	4.306	519	528	539	rVB3	17335	50062	3.85%	0.569%
11	4.483	550	557	568	rVB2	27544	76155	5.85%	0.866%
12	5.373	693	703	712	rBV3	97427	314559	24.17%	3.578%
13	5.464	712	718	723	rVV3	32317	95363	7.33%	1.085%
14	5.544	723	731	746	rVB	131416	400852	30.80%	4.560%
15	5.836	770	779	787	rBV7	4426	13135	1.01%	0.149%
16	5.946	787	797	809	rBV	109951	319906	24.58%	3.639%
17	6.153	823	831	832	rBV4	10394	19948	1.53%	0.227%
18	6.239	843	845	856	rVB4	8913	22580	1.73%	0.257%
19	6.751	919	929	941	rBV	265619	771838	59.30%	8.780%
20	7.117	982	989	992	rBV2	29844	64717	4.97%	0.736%
21	7.866	1100	1112	1119	rBV3	60236	206208	15.84%	2.346%
22	7.940	1119	1124	1130	rVB2	21009	39451	3.03%	0.449%
23	8.129	1151	1155	1160	rVV2	9489	17720	1.36%	0.202%
24	8.488	1205	1214	1224	rVB	74496	129942	9.98%	1.478%
25	8.635	1232	1238	1254	rVB	537634	910093	69.93%	10.353%
26	8.805	1262	1266	1270	rBV3	11594	21523	1.65%	0.245%
27	9.074	1304	1310	1317	rVB4	11235	26391	2.03%	0.300%
28	9.147	1317	1322	1332	rVB3	21175	43613	3.35%	0.496%
29	9.256	1332	1340	1360	rBV3	840796	1301514	100.00%	14.806%
30	9.415	1360	1366	1369	rBV	38288	64491	4.96%	0.734%
31	9.445	1369	1371	1375	rVV	31453	45627	3.51%	0.519%
32	9.482	1375	1377	1386	rVB3	15599	22069	1.70%	0.251%
33	9.744	1415	1420	1427	rVB2	17213	26205	2.01%	0.298%
34	9.842	1427	1436	1444	rBV4	8899	19418	1.49%	0.221%
35	9.958	1451	1455	1460	rVB	22135	32266	2.48%	0.367%
36	10.037	1460	1468	1482	rBV	682390	976035	74.99%	11.103%

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Peak separation: 5

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37	10.945	1612	1617	1626	rBV	217162	292075	22.44%	3.323%
38	11.061	1631	1636	1654	rVB	507854	718068	55.17%	8.168%
39	11.695	1734	1740	1745	rBV	11045	14720	1.13%	0.167%
40	11.872	1764	1769	1775	rVB	21626	26492	2.04%	0.301%
41	12.006	1785	1791	1799	rBV	712049	953609	73.27%	10.848%

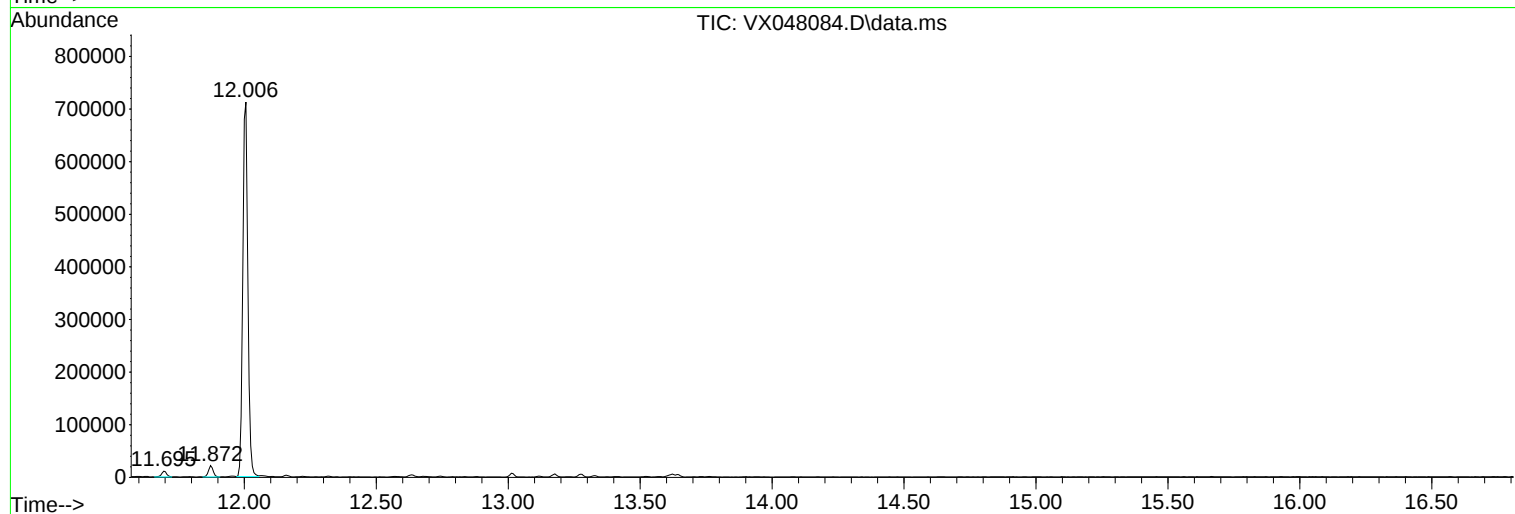
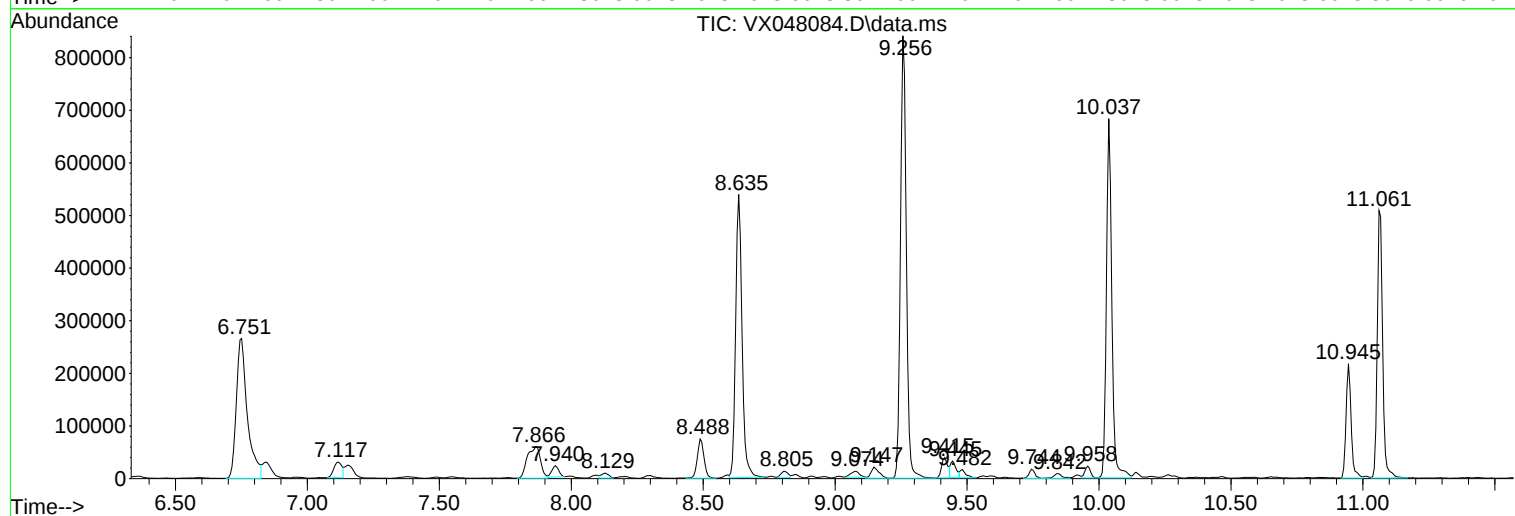
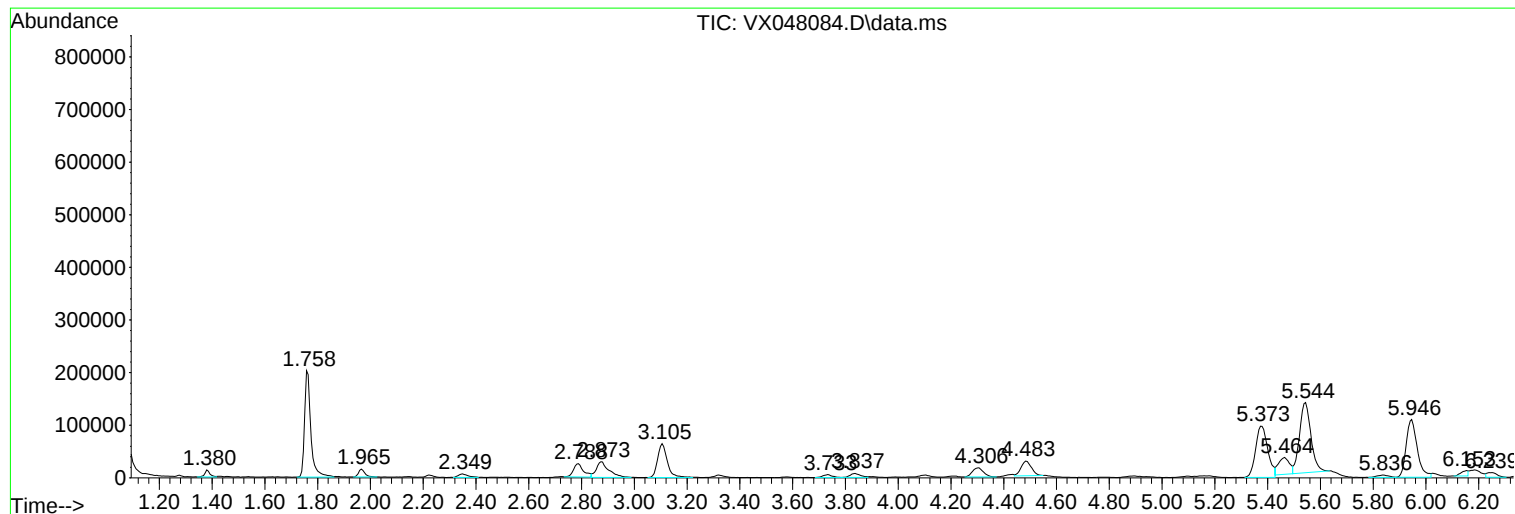
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091625W.M
Quant Title : SW846 8260

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



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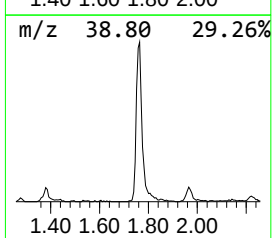
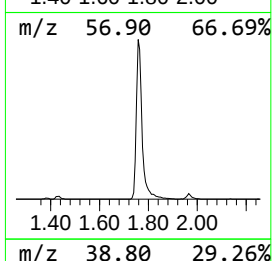
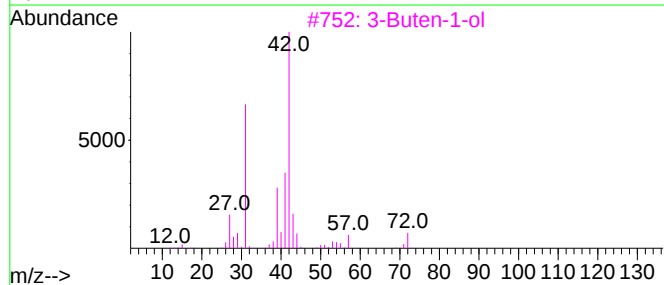
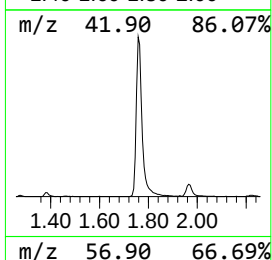
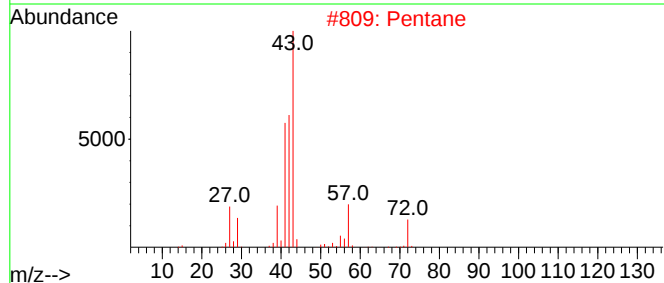
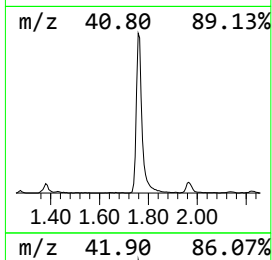
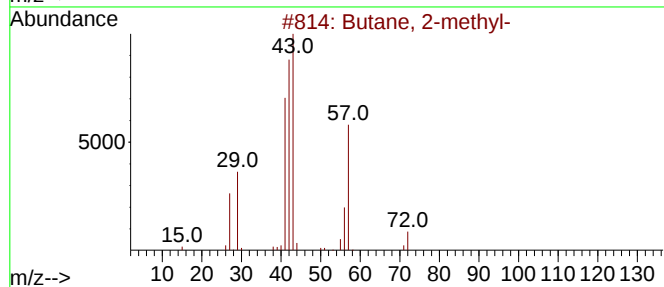
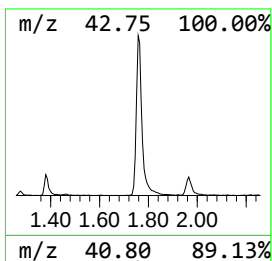
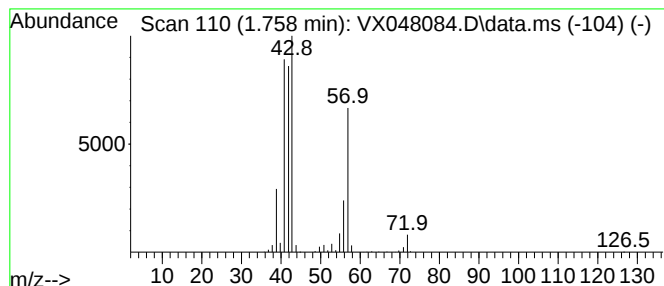
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091625W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.758	41.54 ug/l	333011	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			Pentane	72	C5H12	000109-66-0	42
3			3-Buten-1-ol	72	C4H8O	000627-27-0	38
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	27
5			1-Butene	56	C4H8	000106-98-9	10



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2S

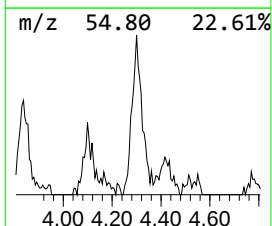
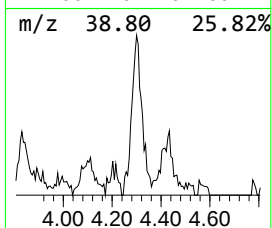
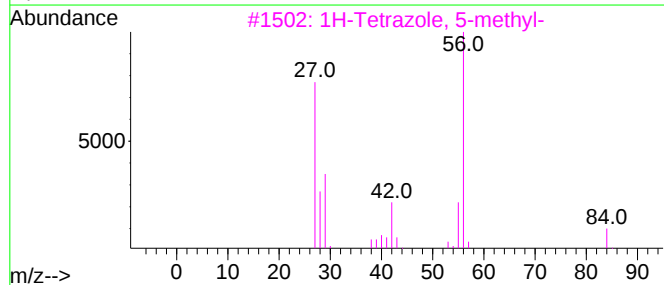
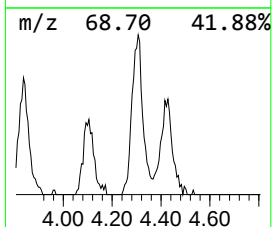
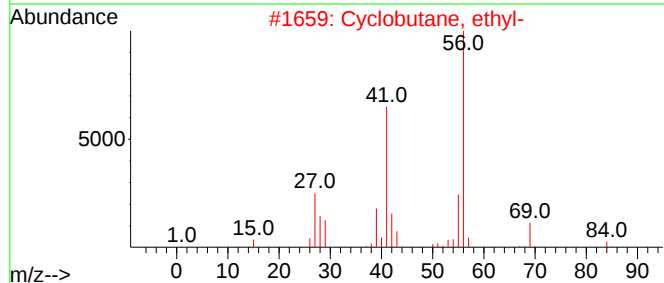
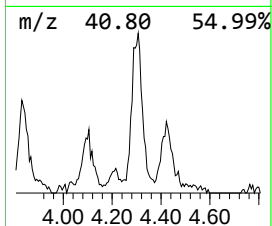
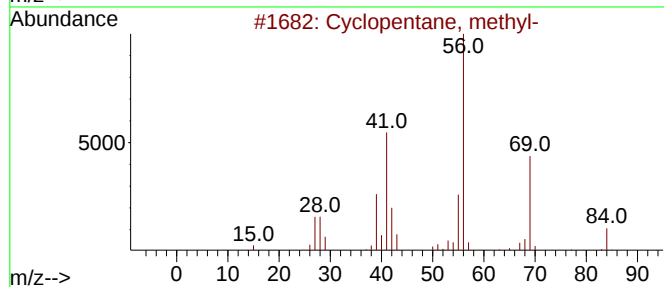
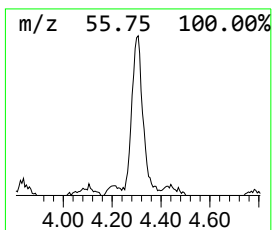
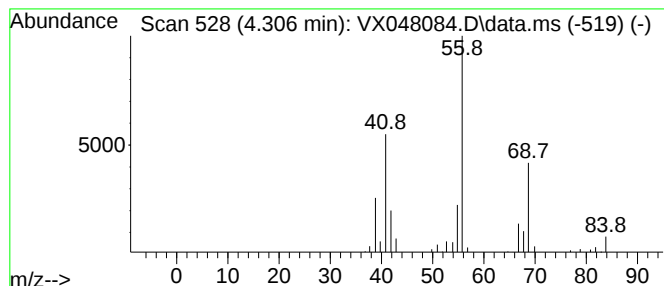
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091625W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	6.24 ug/l	50062	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	58
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53
5			Cyclobutane	56	C4H8	000287-23-0	47



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Instrument :
MSVOA_X
ClientSampleId :
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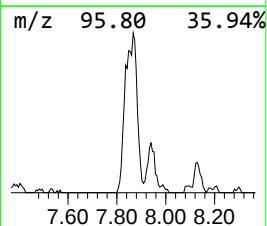
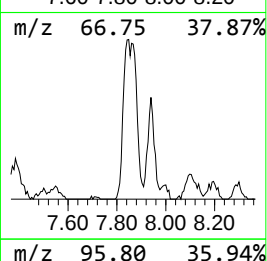
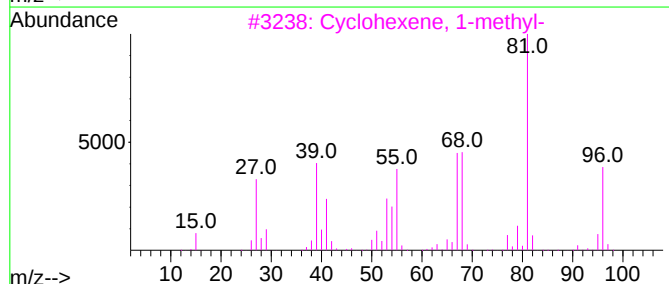
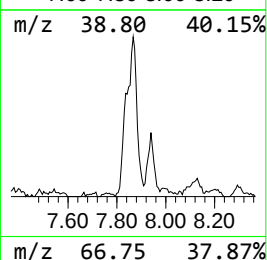
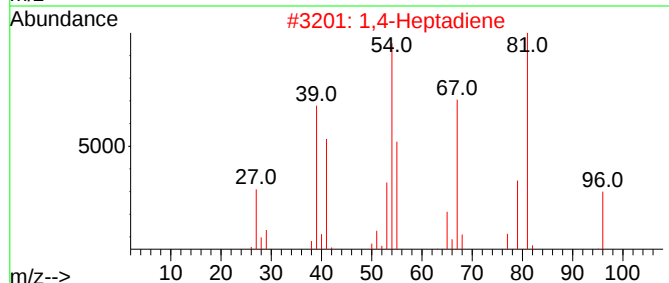
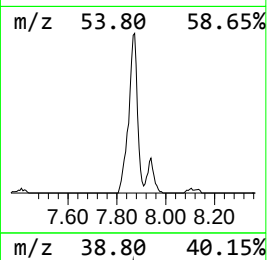
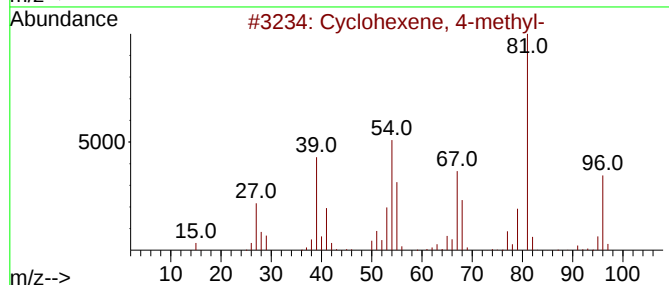
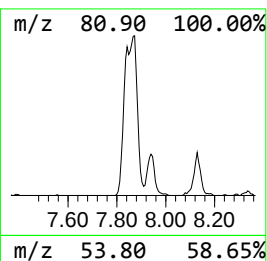
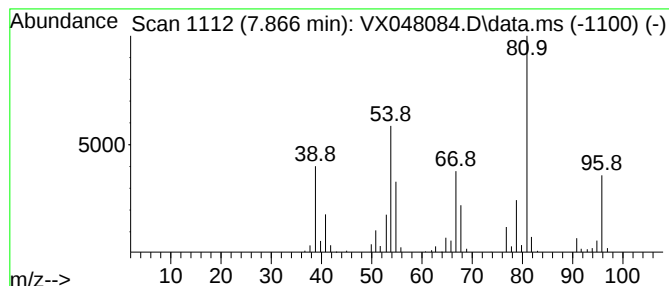
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091625W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclohexene, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	13.36 ug/l	206208	1,4-Difluorobenzene	6.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	96
2			1,4-Heptadiene	96	C7H12	005675-22-9	76
3			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	70
4			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	64
5			2,4-Heptadiene, (E,E)-	96	C7H12	002384-94-3	62



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Instrument :
MSVOA_X
ClientSampleId :
MW-2S

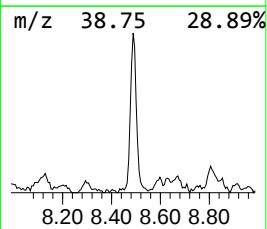
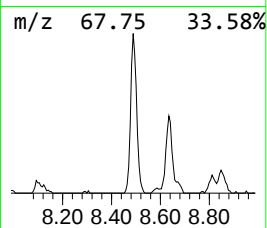
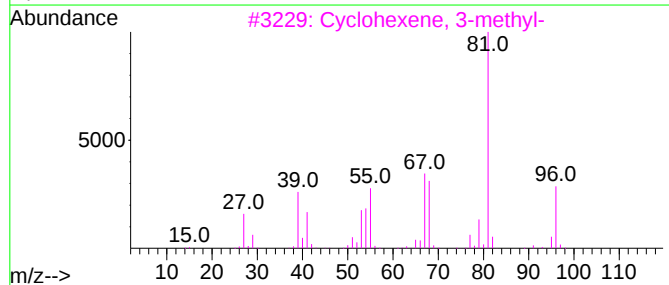
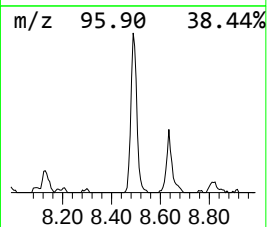
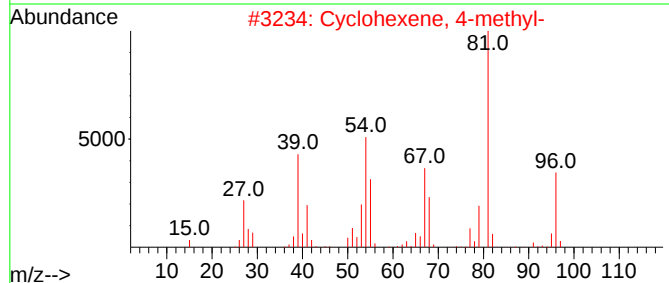
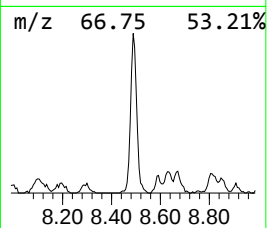
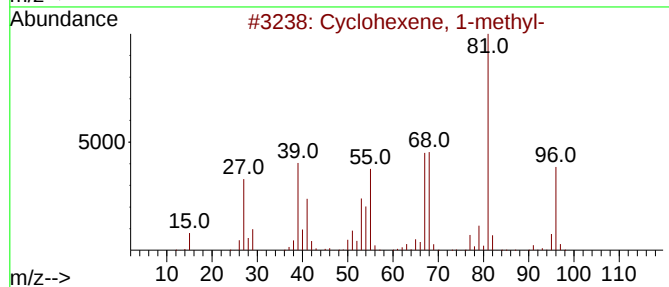
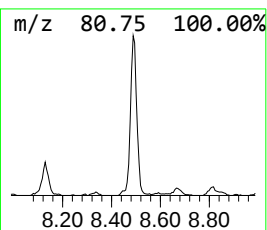
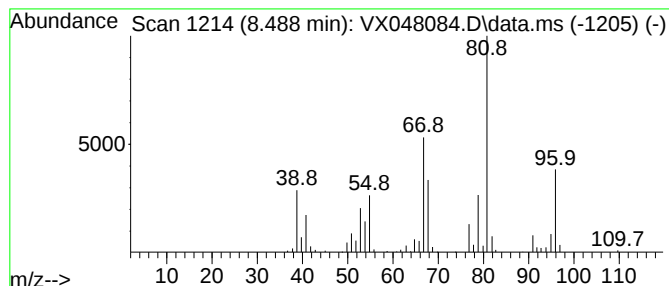
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.488	6.66 ug/l	129942	Chlorobenzene-d5	10.037

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	94
2			Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	90
3			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	87
4			2,4-Hexadiene, 2-methyl-	96	C7H12	028823-41-8	81
5			2,4-Hexadiene, 3-methyl-	96	C7H12	028823-42-9	81



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.758	41.5	ug/l	333011	1	5.544	400852	50.0
Cyclopentane, m...	4.306	6.2	ug/l	50062	1	5.544	400852	50.0
Cyclohexene, 4-...	7.866	13.4	ug/l	206208	2	6.751	771838	50.0
Cyclohexene, 1-...	8.488	6.7	ug/l	129942	3	10.037	976035	50.0