

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051625\
 Data File : VX046250.D
 Acq On : 16 May 2025 18:02
 Operator : JC/MD
 Sample : Q2072-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-4

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.739	101	107	117	rVB	30739	42269	9.88%	1.428%
2	2.123	165	170	178	rVV2	3694	7297	1.71%	0.247%
3	2.331	198	204	209	rBV	18055	35739	8.35%	1.208%
4	2.379	209	212	220	rVB	3807	6661	1.56%	0.225%
5	2.776	270	277	282	rBV2	11860	25830	6.04%	0.873%
6	2.873	287	293	304	rVB3	11119	26533	6.20%	0.897%
7	3.093	321	329	339	rBB2	8395	19219	4.49%	0.649%
8	3.837	442	451	459	rBV4	4852	13154	3.07%	0.444%
9	4.294	518	526	536	rVB3	6345	17204	4.02%	0.581%
10	4.434	538	549	561	rVB8	5022	18174	4.25%	0.614%
11	5.166	664	669	682	rVB7	3381	11079	2.59%	0.374%
12	5.385	693	705	715	rBV3	53839	161170	37.66%	5.446%
13	5.550	723	732	743	rBV	67403	193062	45.11%	6.524%
14	5.952	790	798	811	rBV	57676	157151	36.72%	5.310%
15	6.092	815	821	828	rVV9	2494	8276	1.93%	0.280%
16	6.239	832	845	855	rVV3	19675	63229	14.77%	2.137%
17	6.360	857	865	874	rVB4	4056	11099	2.59%	0.375%
18	6.757	922	930	942	rBV	126348	311194	72.71%	10.515%
19	6.976	959	966	976	rBV2	5867	13609	3.18%	0.460%
20	7.165	989	997	1006	rVB2	13794	31544	7.37%	1.066%
21	7.379	1023	1032	1039	rVB5	1599	4453	1.04%	0.150%
22	7.494	1044	1051	1056	rBV5	2030	4478	1.05%	0.151%
23	7.878	1101	1114	1121	rBV8	5093	17691	4.13%	0.598%
24	7.982	1123	1131	1142	rVB2	13511	32651	7.63%	1.103%
25	8.104	1142	1151	1162	rBV4	12770	29327	6.85%	0.991%
26	8.305	1178	1184	1192	rBV5	4517	8823	2.06%	0.298%
27	8.500	1210	1216	1221	rBV5	3999	7448	1.74%	0.252%
28	8.647	1231	1240	1253	rBV	271883	427972	100.00%	14.461%
29	8.982	1289	1295	1300	rVB6	2141	4576	1.07%	0.155%
30	9.159	1319	1324	1333	rVB2	9595	16517	3.86%	0.558%
31	9.427	1364	1368	1371	rBV2	4041	5985	1.40%	0.202%
32	9.762	1418	1423	1428	rBV5	3000	4919	1.15%	0.166%
33	10.049	1465	1470	1484	rBV	268745	385529	90.08%	13.027%
34	10.963	1614	1620	1625	rBV	8513	12345	2.88%	0.417%
35	11.079	1634	1639	1653	rBV	226462	288308	67.37%	9.742%
36	11.610	1722	1726	1732	rBV	10755	14233	3.33%	0.481%

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Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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37	11.866	1763	1768	1769	rBV	12002	13948	3.26%	0.471%
38	11.890	1769	1772	1778	rVB	18267	21572	5.04%	0.729%
39	12.018	1788	1793	1804	rBV	268801	345013	80.62%	11.658%
40	12.176	1815	1819	1825	rVB2	3886	5155	1.20%	0.174%
41	12.469	1862	1867	1872	rVB	18421	23918	5.59%	0.808%
42	12.695	1900	1904	1912	rBV	23388	32831	7.67%	1.109%
43	13.030	1954	1959	1963	rBV	3885	5076	1.19%	0.172%
44	13.134	1971	1976	1979	rBV	4574	6102	1.43%	0.206%
45	13.188	1983	1985	1991	rVB2	3896	5194	1.21%	0.176%
46	13.292	1997	2002	2007	rBV3	7348	9357	2.19%	0.316%
47	13.347	2007	2011	2014	rVV3	3932	4758	1.11%	0.161%
48	13.426	2020	2024	2029	rVB2	3646	5033	1.18%	0.170%
49	13.542	2039	2043	2047	rVB2	9010	11645	2.72%	0.393%
50	13.658	2052	2062	2068	rVB	17260	31075	7.26%	1.050%

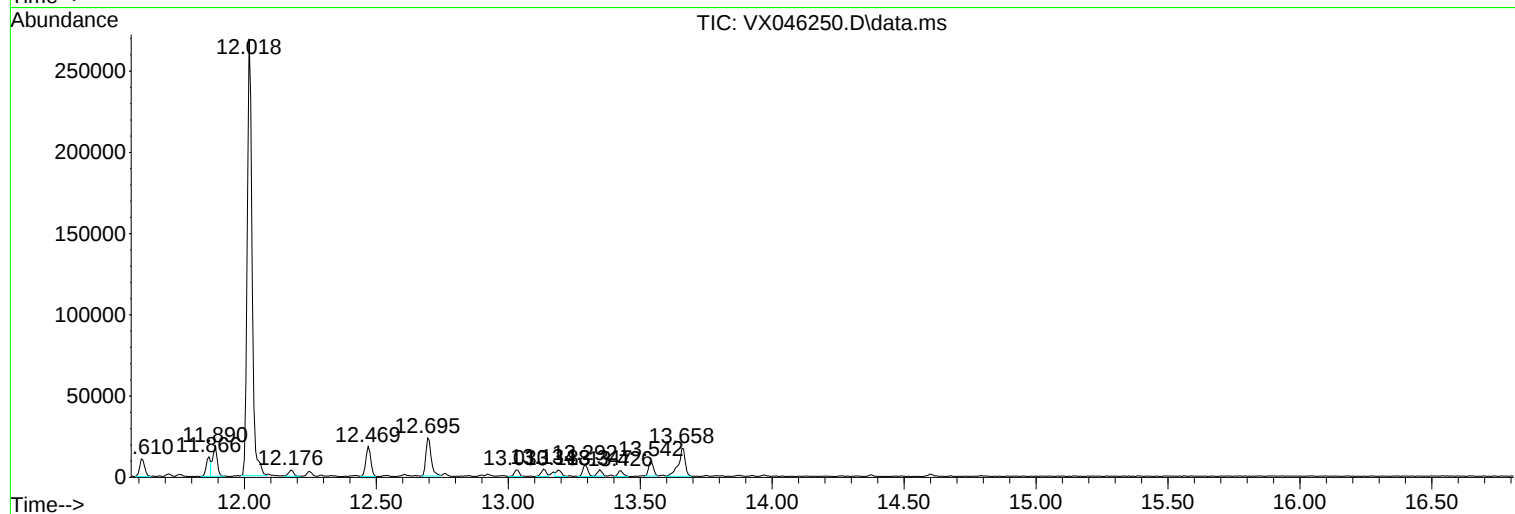
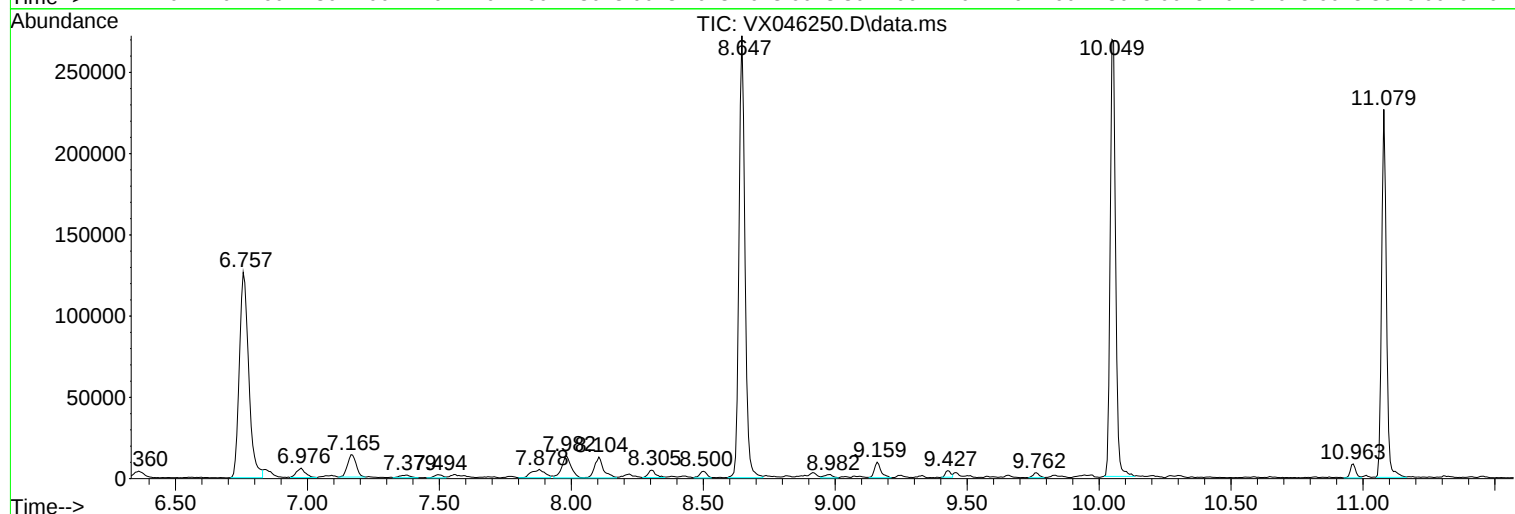
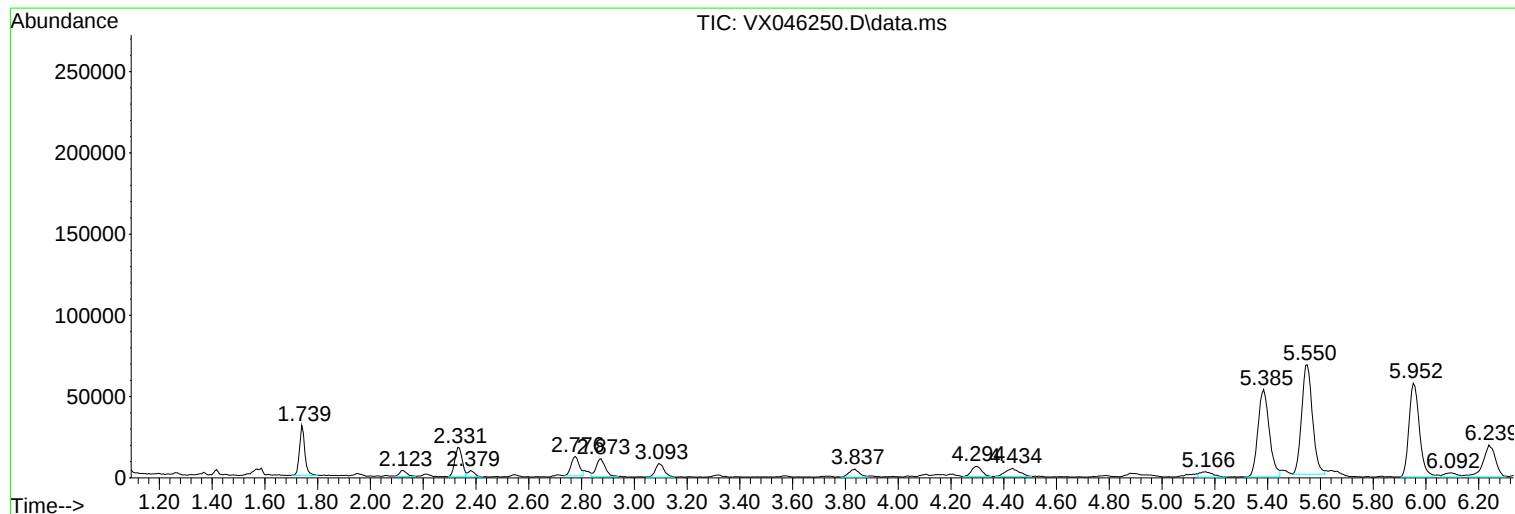
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



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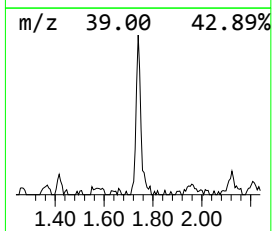
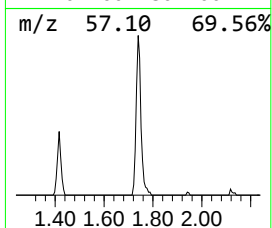
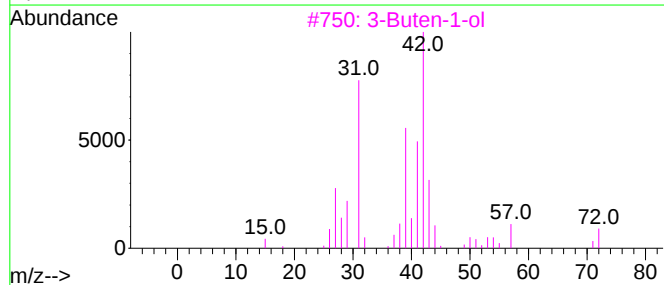
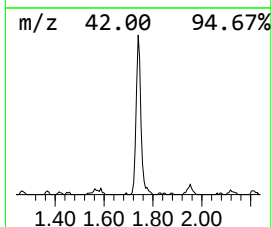
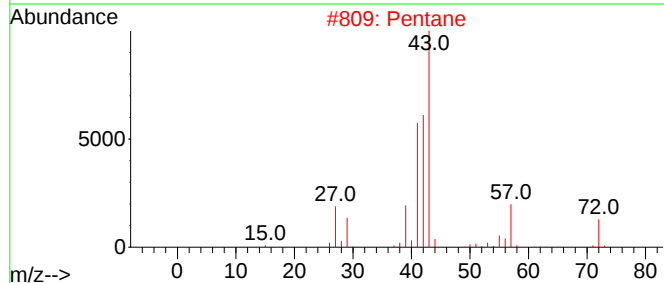
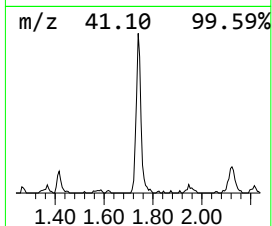
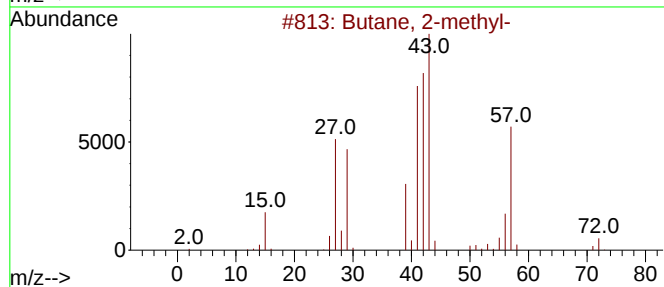
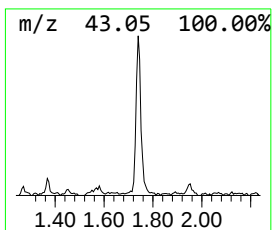
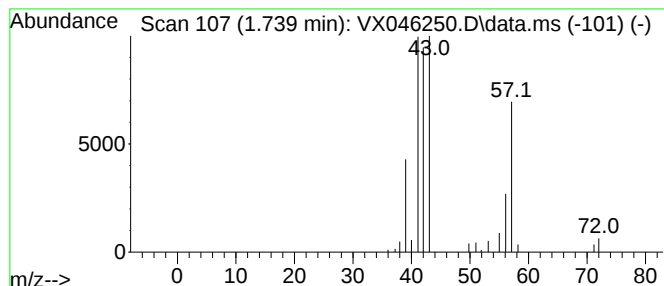
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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.
1.739	10.95 ug/l	42269	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	33
4			1-Butene	56	C4H8	000106-98-9	10
5			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10



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Instrument :
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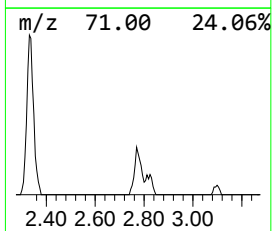
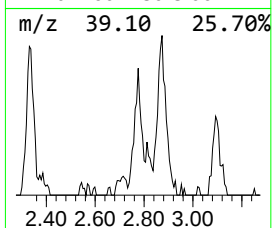
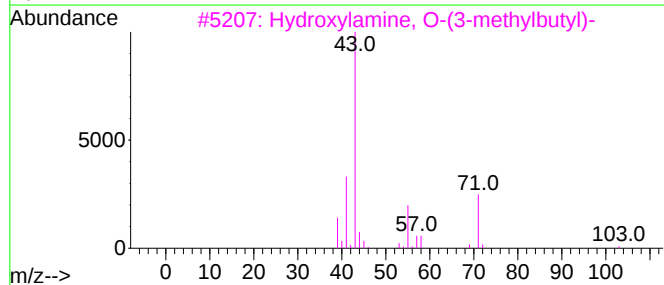
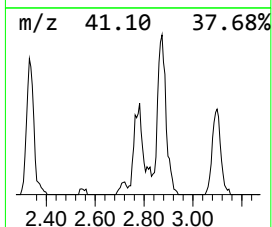
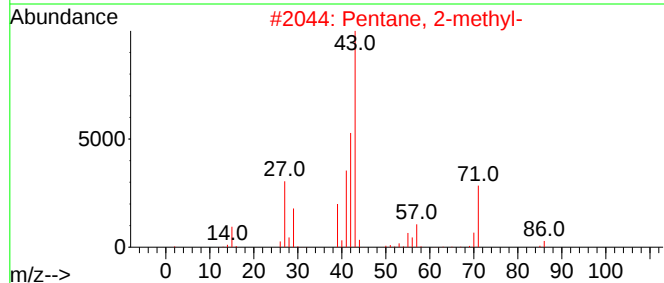
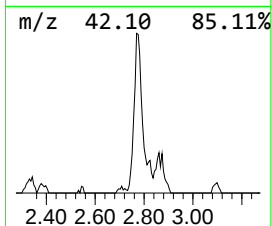
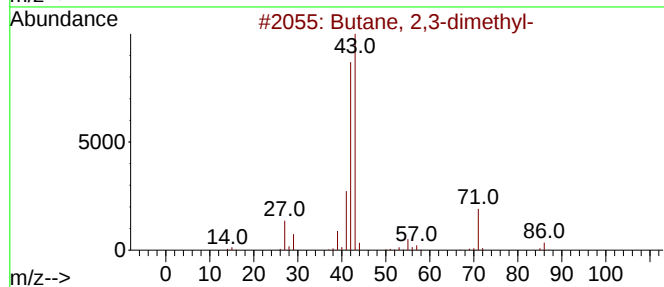
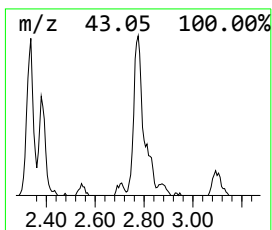
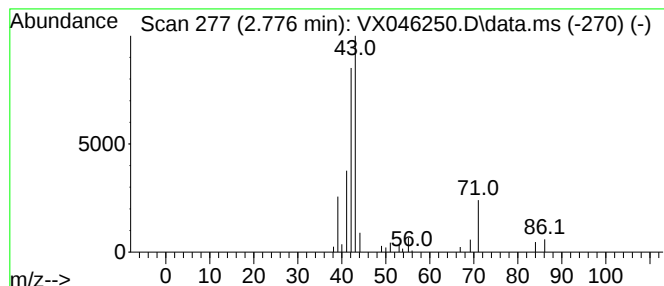
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.776	6.69 ug/l	25830	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	23
3			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	9
4			2-Oxetanone, 4-methylene-	84	C4H4O2	000674-82-8	5
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	5



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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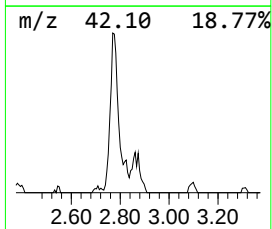
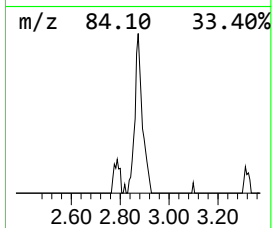
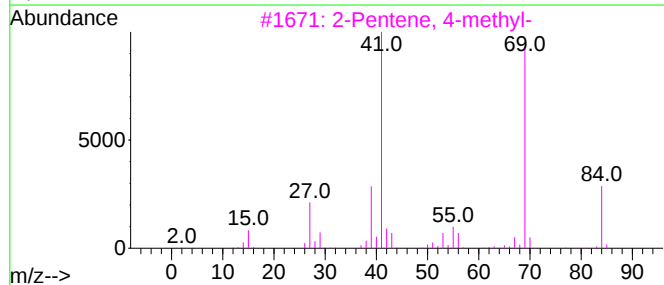
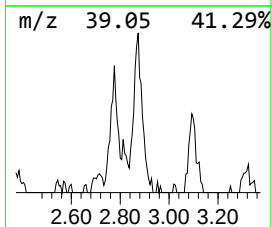
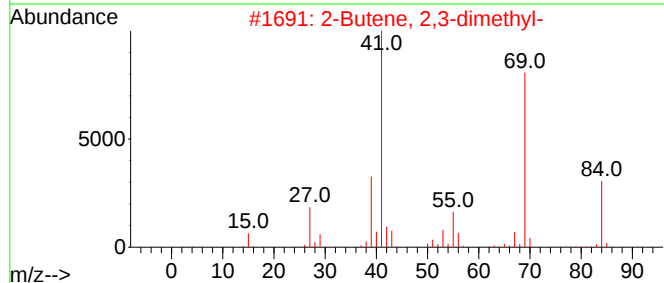
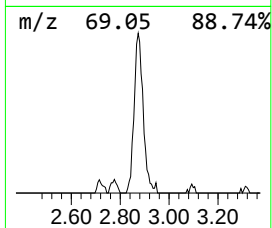
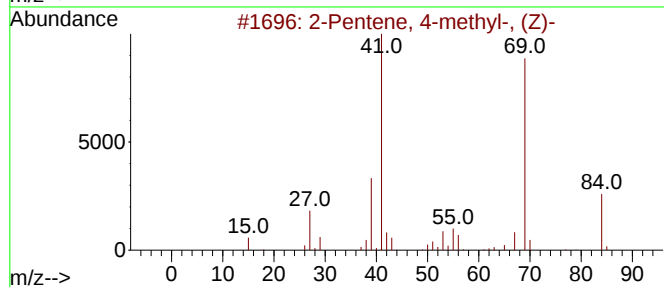
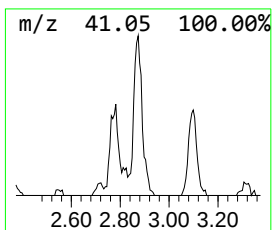
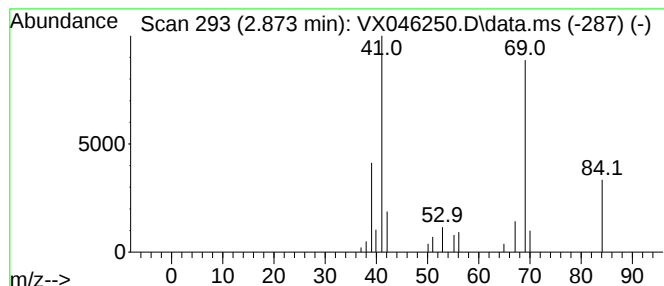
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Pentene, 4-methyl-, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.873	6.87 ug/l	26533	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4-methyl-, (Z)-			84	C6H12	000691-38-3	74
2	2-Butene, 2,3-dimethyl-			84	C6H12	000563-79-1	72
3	2-Pentene, 4-methyl-			84	C6H12	004461-48-7	64
4	2-Pentene, 4-methyl-, (E)-			84	C6H12	000674-76-0	64
5	1-Butene, 2,3-dimethyl-			84	C6H12	000563-78-0	64



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Instrument :
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ClientSampleId :
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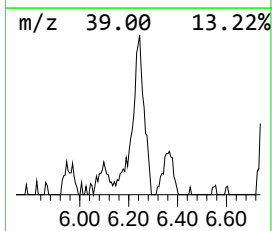
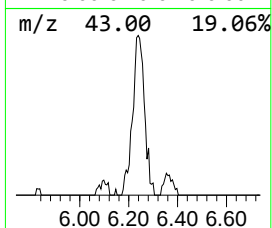
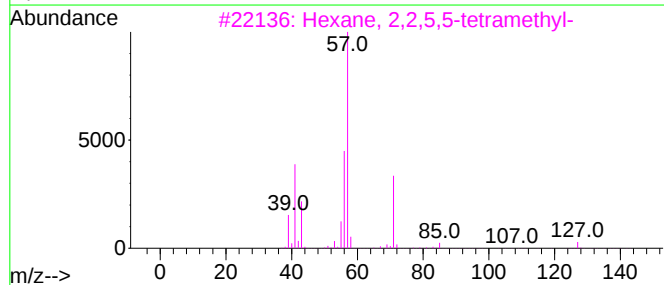
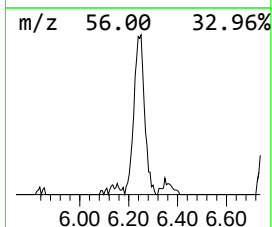
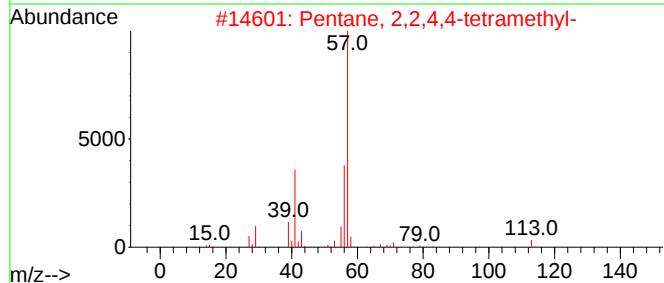
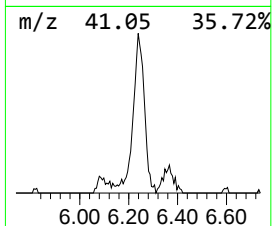
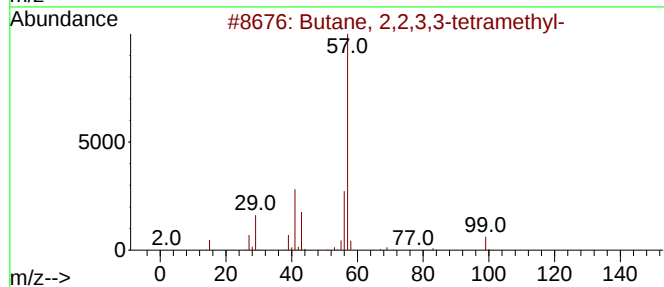
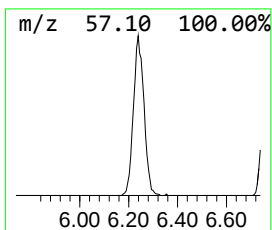
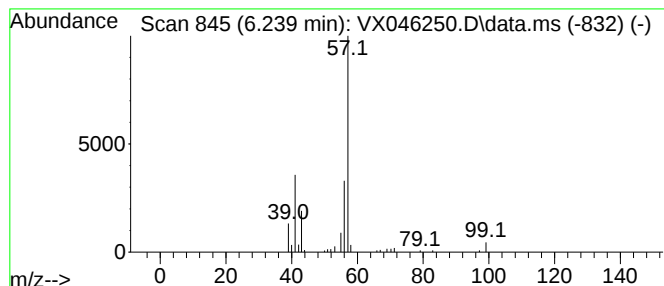
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	10.16 ug/l	63229	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	47
4			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	45
5			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	45



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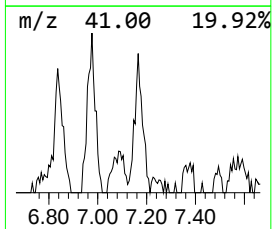
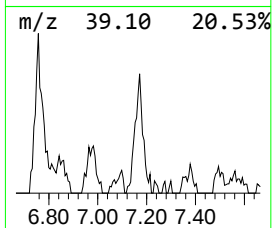
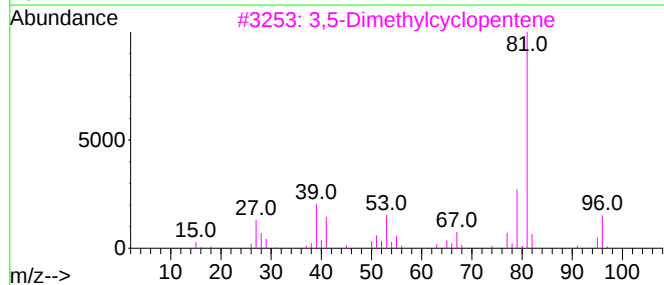
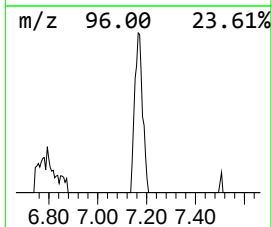
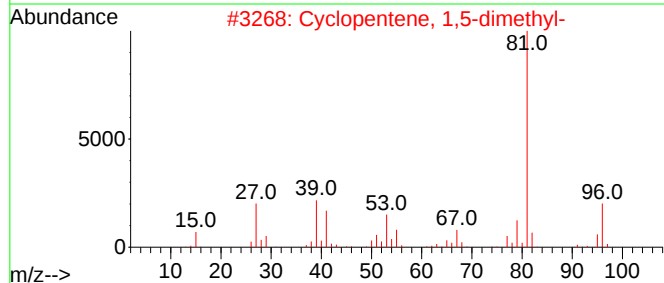
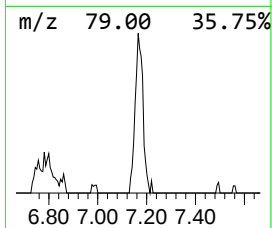
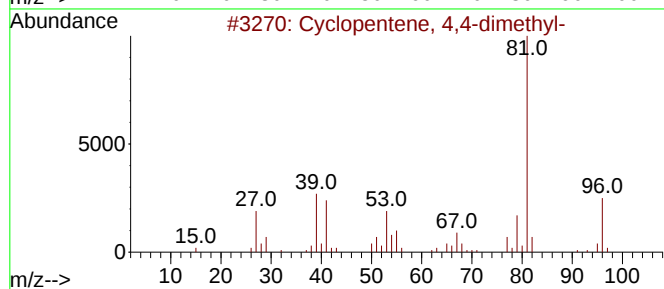
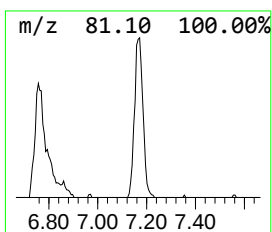
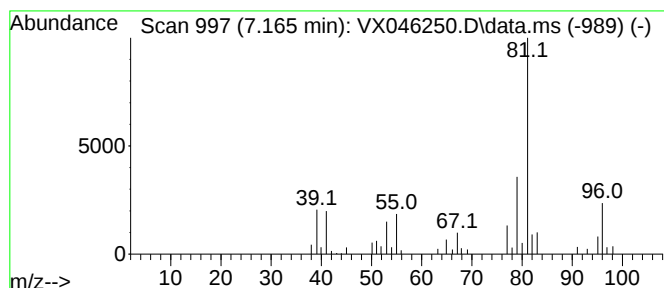
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentene, 4,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.165	5.07 ug/l	31544	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	80
2			Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	72
3			3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	72
4			Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	64
5			Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051625\
Data File : VX046250.D
Acq On : 16 May 2025 18:02
Operator : JC/MD
Sample : Q2072-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

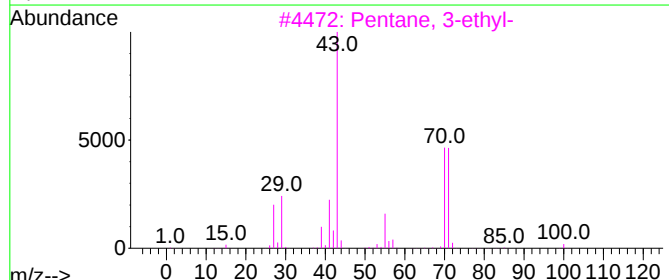
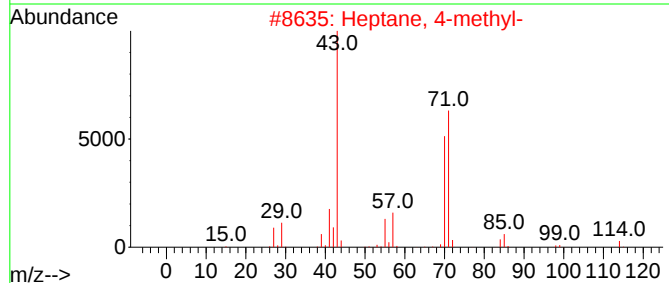
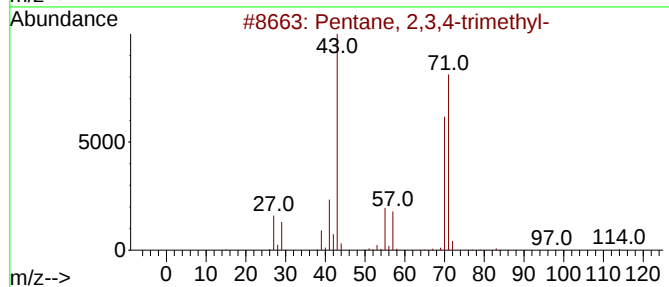
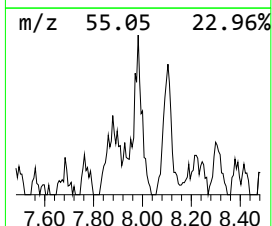
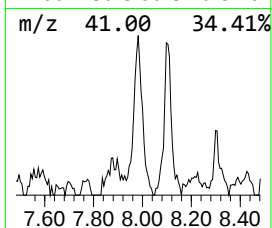
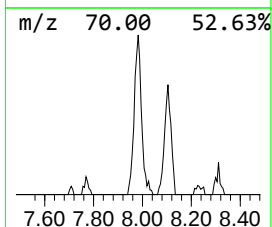
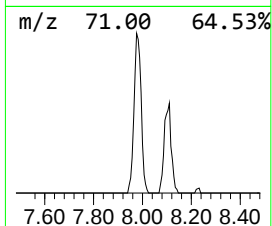
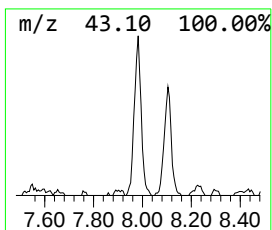
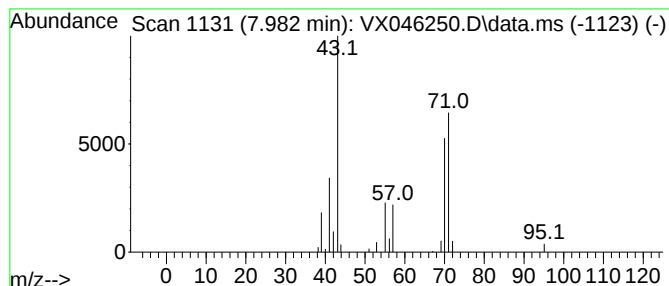
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	5.25 ug/l	32651	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	78
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78
5			Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051625\
Data File : VX046250.D
Acq On : 16 May 2025 18:02
Operator : JC/MD
Sample : Q2072-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
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-	1.739	10.9	ug/l	42269	1	5.550	193062	50.0
Butane, 2,3-dim...	2.776	6.7	ug/l	25830	1	5.550	193062	50.0
2-Pentene, 4-me...	2.873	6.9	ug/l	26533	1	5.550	193062	50.0
Butane, 2,2,3,3...	6.239	10.2	ug/l	63229	2	6.757	311194	50.0
Cyclopentene, 4...	7.165	5.1	ug/l	31544	2	6.757	311194	50.0
Pentane, 2,3,4-...	7.982	5.3	ug/l	32651	2	6.757	311194	50.0