

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX103125\
 Data File : VX048425.D
 Acq On : 31 Oct 2025 12:43
 Operator : JC/MD
 Sample : Q3494-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW3

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\82X102925W.M
 Title : SW846 8260

Signal : TIC: VX048425.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	45	48	58	rVB	13072	21175	2.17%	0.276%
2	1.557	73	77	85	rVB2	11333	16251	1.66%	0.212%
3	1.764	105	111	116	rBV	16104	25881	2.65%	0.338%
4	1.965	139	144	153	rVB4	6657	15525	1.59%	0.203%
5	2.221	181	186	195	rVB3	8841	16491	1.69%	0.215%
6	2.373	203	211	216	rBV	6724	14089	1.44%	0.184%
7	2.526	229	236	246	rBV2	7610	22879	2.34%	0.299%
8	2.782	270	278	285	rBV2	14179	33251	3.41%	0.434%
9	2.873	288	293	300	rVB2	5726	11160	1.14%	0.146%
10	4.202	500	511	522	rBV3	24900	81134	8.31%	1.059%
11	5.373	690	703	716	rBV2	87366	284050	29.09%	3.706%
12	5.538	721	730	738	rBV	122656	377432	38.66%	4.924%
13	5.946	786	797	804	rBV	102046	291491	29.85%	3.803%
14	6.025	804	810	827	rVB2	89230	259953	26.62%	3.392%
15	6.239	833	845	875	rVB	224963	727635	74.52%	9.494%
16	6.745	919	928	950	rBV	247342	641377	65.69%	8.368%
17	7.360	1020	1029	1038	rVB5	4601	12811	1.31%	0.167%
18	7.488	1038	1050	1055	rBV2	21517	50316	5.15%	0.656%
19	7.549	1055	1060	1062	rVV4	15820	31885	3.27%	0.416%
20	7.586	1062	1066	1075	rVB	21580	48320	4.95%	0.630%
21	7.970	1120	1129	1141	rBV	167531	346191	35.46%	4.517%
22	8.092	1141	1149	1158	rBV	264113	545704	55.89%	7.120%
23	8.171	1158	1162	1176	rVB4	6766	16078	1.65%	0.210%
24	8.372	1189	1195	1199	rBV3	5472	11100	1.14%	0.145%
25	8.635	1221	1238	1246	rBV	541187	976375	100.00%	12.739%
26	9.147	1317	1322	1325	rBV	11008	17820	1.83%	0.232%
27	9.183	1325	1328	1333	rVB3	7747	10905	1.12%	0.142%
28	9.439	1362	1370	1374	rBV	17948	30299	3.10%	0.395%
29	9.482	1374	1377	1385	rVB7	6181	14250	1.46%	0.186%
30	9.653	1398	1405	1412	rVB9	3880	11109	1.14%	0.145%
31	9.744	1412	1420	1424	rBV5	6443	13509	1.38%	0.176%
32	10.037	1462	1468	1482	rBV	604217	873067	89.42%	11.391%
33	10.287	1505	1509	1515	rVB	11940	18955	1.94%	0.247%
34	10.366	1515	1522	1530	rBV7	5480	13028	1.33%	0.170%
35	11.061	1631	1636	1641	rBV	526631	703071	72.01%	9.173%
36	11.725	1742	1745	1751	rVB2	13199	18002	1.84%	0.235%

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37	11.847	1757	1765	1768	rBV2	8301	17327	1.77%	0.226%
38	11.914	1772	1776	1780	rVV	19958	24680	2.53%	0.322%
39	12.006	1785	1791	1802	rBV	669368	911962	93.40%	11.898%
40	12.103	1803	1807	1810	rVV2	14005	20834	2.13%	0.272%
41	12.128	1810	1811	1818	rVB	13325	13078	1.34%	0.171%
42	12.201	1818	1823	1825	rBV	18516	25491	2.61%	0.333%
43	12.225	1825	1827	1832	rVB2	17228	20181	2.07%	0.263%
44	12.914	1936	1940	1944	rVB3	10056	14939	1.53%	0.195%
45	13.274	1995	1999	2005	rVB4	8698	13467	1.38%	0.176%

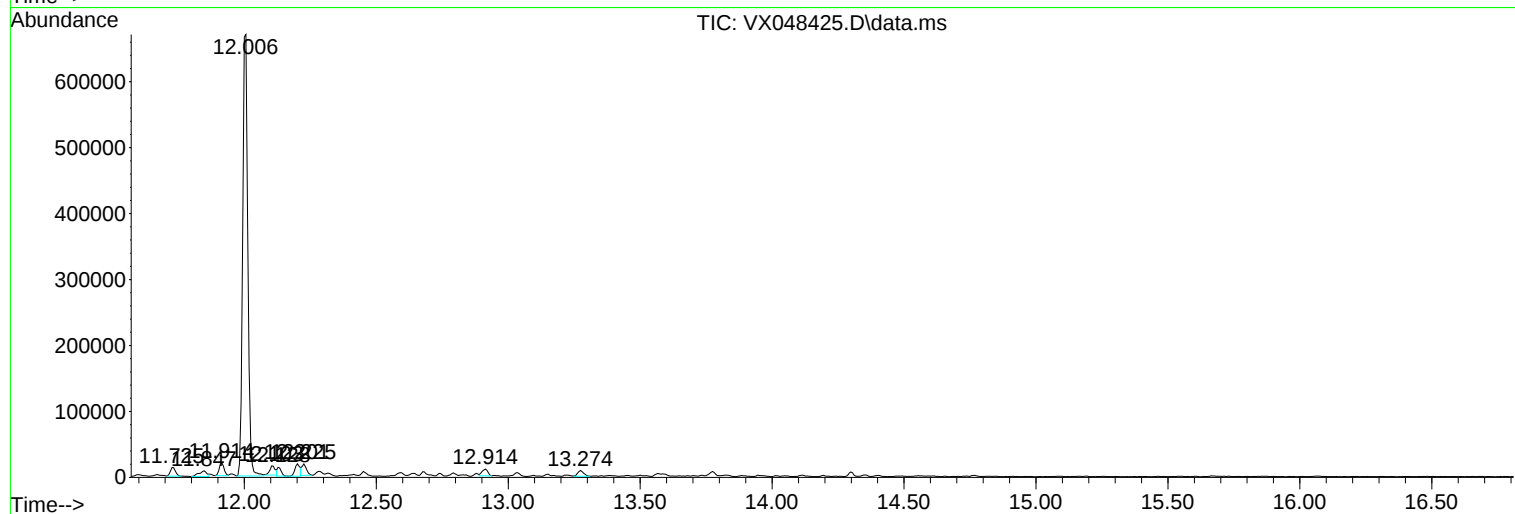
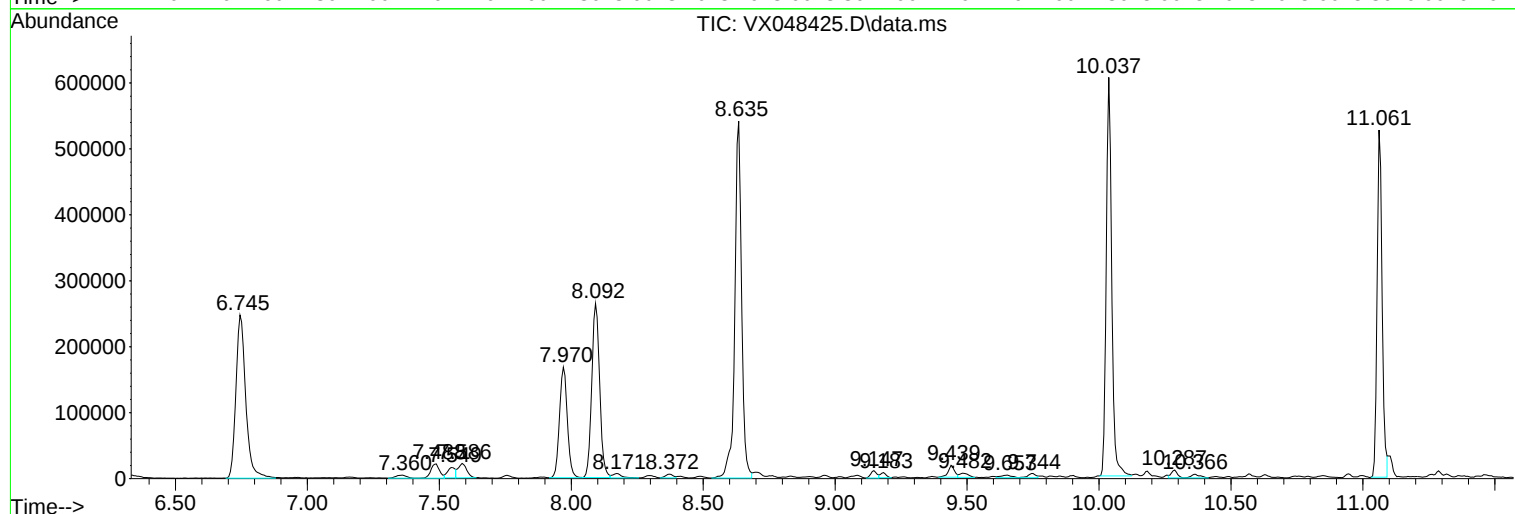
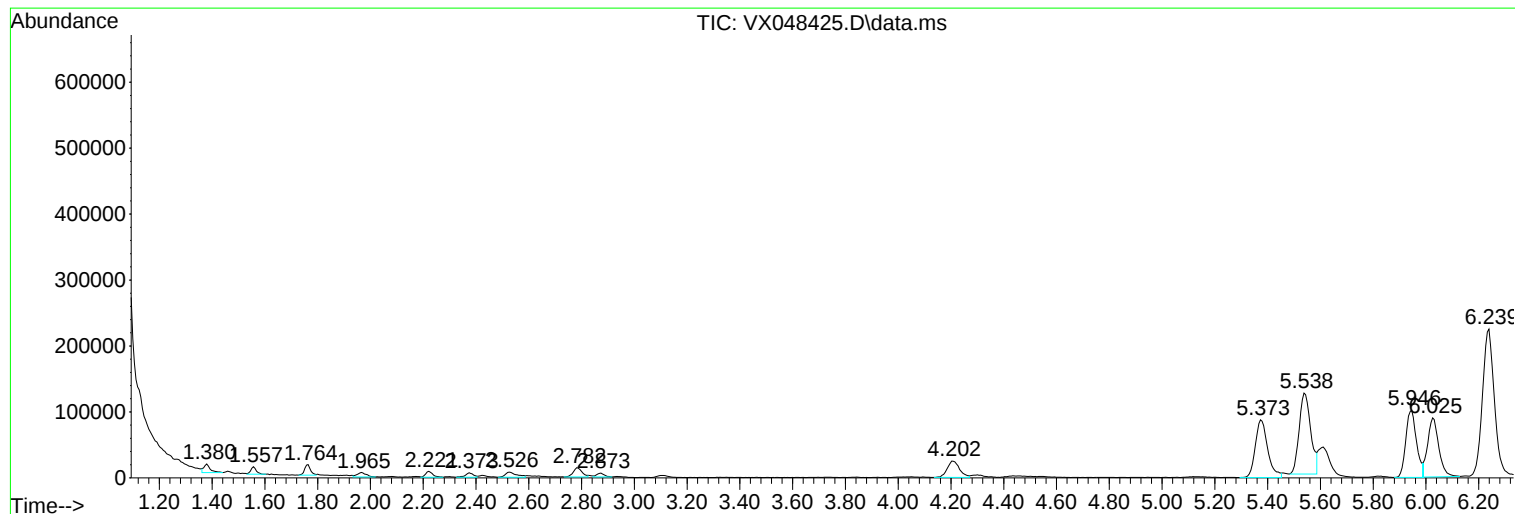
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

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



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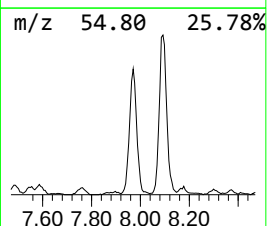
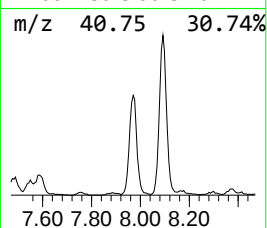
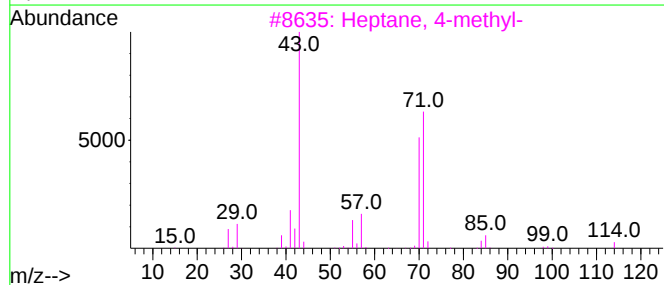
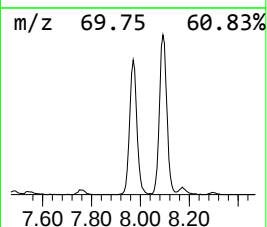
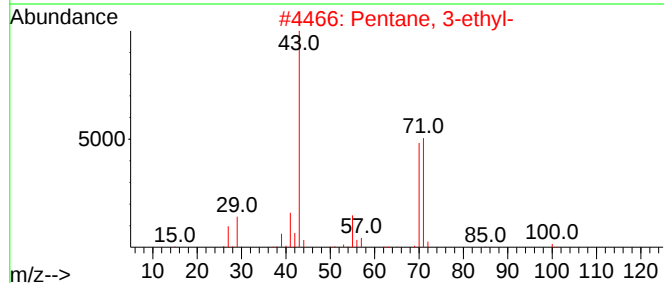
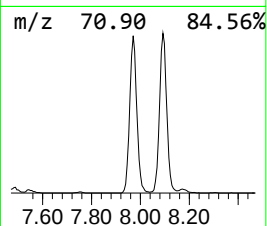
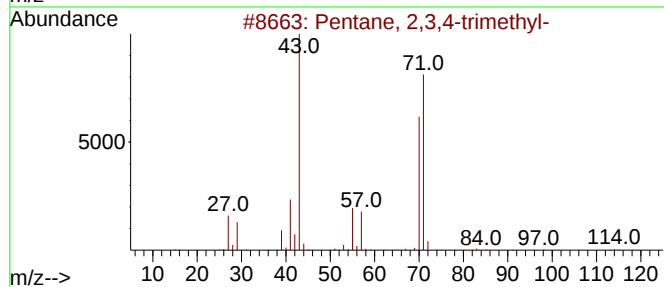
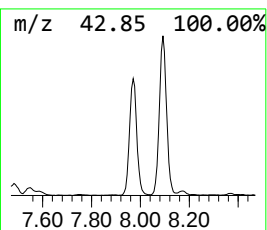
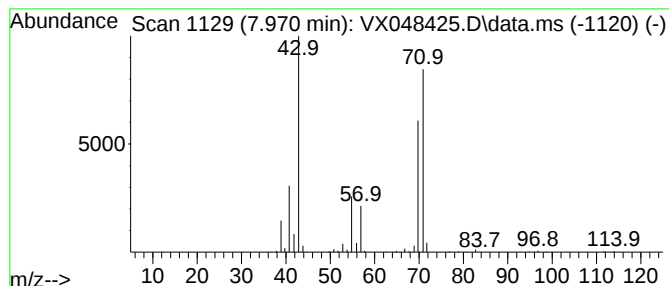
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.970	26.99 ug/l	346191	1,4-Difluorobenzene	6.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	78



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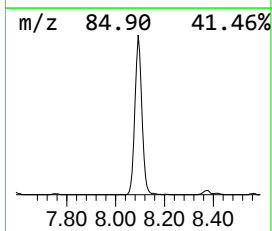
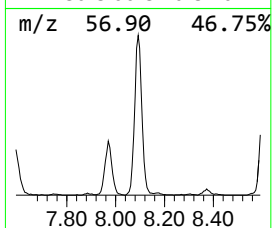
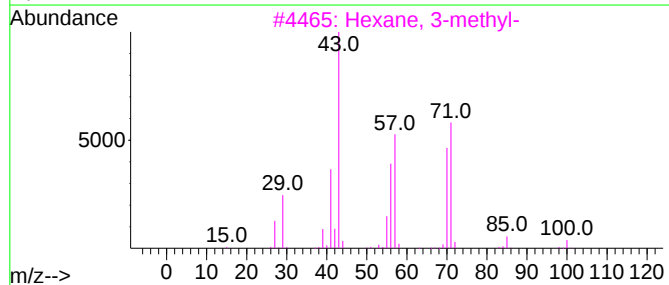
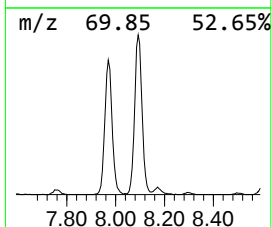
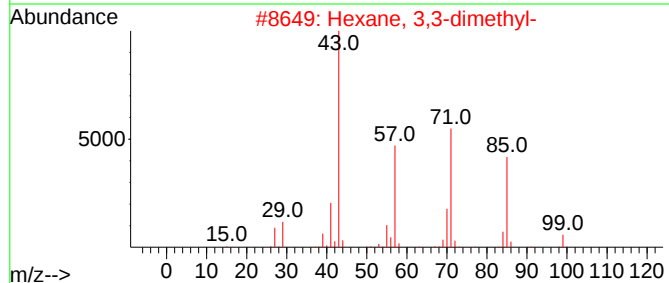
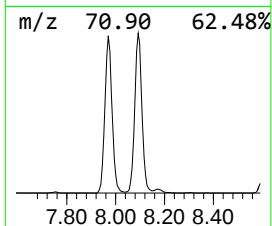
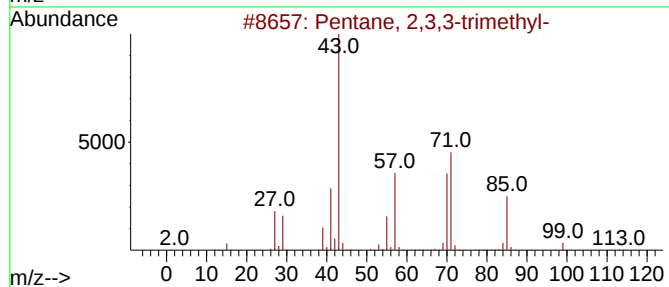
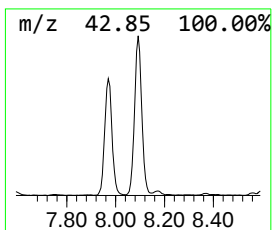
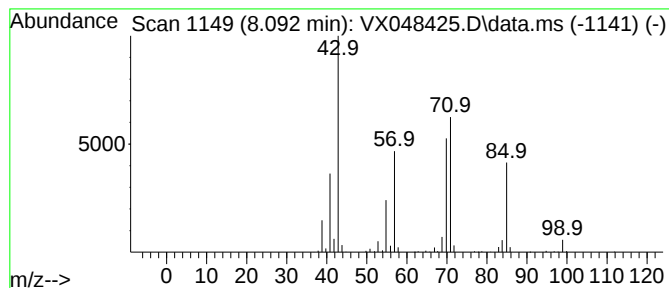
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	42.54 ug/l	545704	1,4-Difluorobenzene	6.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3,4-...	7.970	27.0	ug/l	346191	2	6.745	641377	50.0
Pentane, 2,3,3-...	8.092	42.5	ug/l	545704	2	6.745	641377	50.0