

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112125\
 Data File : VX048646.D
 Acq On : 21 Nov 2025 11:15
 Operator : JC/MD
 Sample : Q3685-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 4197

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\82X110725W.M
 Title : SW846 8260

Signal : TIC: VX048646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	57	61	85	rBV	332743	539433	22.29%	4.343%
2	2.050	151	158	174	rBV	1246905	2420144	100.00%	19.486%
3	2.294	194	198	204	rVB2	15520	29720	1.23%	0.239%
4	2.373	205	211	228	rVV	94926	188710	7.80%	1.519%
5	2.514	229	234	247	rVB	90652	175614	7.26%	1.414%
6	2.697	259	264	275	rVB	15329	32078	1.33%	0.258%
7	2.940	296	304	318	rVB2	20451	55265	2.28%	0.445%
8	3.824	439	449	465	rBV2	39954	116047	4.80%	0.934%
9	4.702	585	593	608	rBV	12743	40391	1.67%	0.325%
10	5.373	691	703	720	rBV2	124690	404139	16.70%	3.254%
11	5.538	720	730	754	rVB	196309	619032	25.58%	4.984%
12	5.940	786	796	815	rVV3	118043	357494	14.77%	2.878%
13	6.086	815	820	835	rVB2	9141	27289	1.13%	0.220%
14	6.745	918	928	947	rBV	365941	954905	39.46%	7.689%
15	7.196	996	1002	1012	rBV2	15540	41700	1.72%	0.336%
16	7.568	1056	1063	1078	rBV2	36418	92841	3.84%	0.748%
17	8.635	1231	1238	1247	rBV	703626	1170555	48.37%	9.425%
18	9.013	1293	1300	1313	rBV2	36430	73298	3.03%	0.590%
19	9.220	1329	1334	1346	rBV	33951	67631	2.79%	0.545%
20	9.500	1375	1380	1399	rBV	305793	508563	21.01%	4.095%
21	10.037	1462	1468	1487	rBV	880452	1269179	52.44%	10.219%
22	10.567	1548	1555	1566	rBV	90738	158319	6.54%	1.275%
23	10.841	1596	1600	1612	rVB2	25775	46165	1.91%	0.372%
24	11.061	1631	1636	1645	rBV	685498	961160	39.71%	7.739%
25	11.604	1719	1725	1728	rBV2	30326	41556	1.72%	0.335%
26	11.640	1728	1731	1735	rVV3	20392	29183	1.21%	0.235%
27	11.908	1772	1775	1780	rVB2	28930	36659	1.51%	0.295%
28	12.000	1785	1790	1800	rVV	996485	1346555	55.64%	10.842%
29	12.201	1818	1823	1831	rBV	323321	438439	18.12%	3.530%
30	12.573	1879	1884	1896	rBV2	65007	104102	4.30%	0.838%
31	12.841	1923	1928	1934	rBV2	19492	28113	1.16%	0.226%
32	14.237	2154	2157	2168	rVB2	36201	45447	1.88%	0.366%

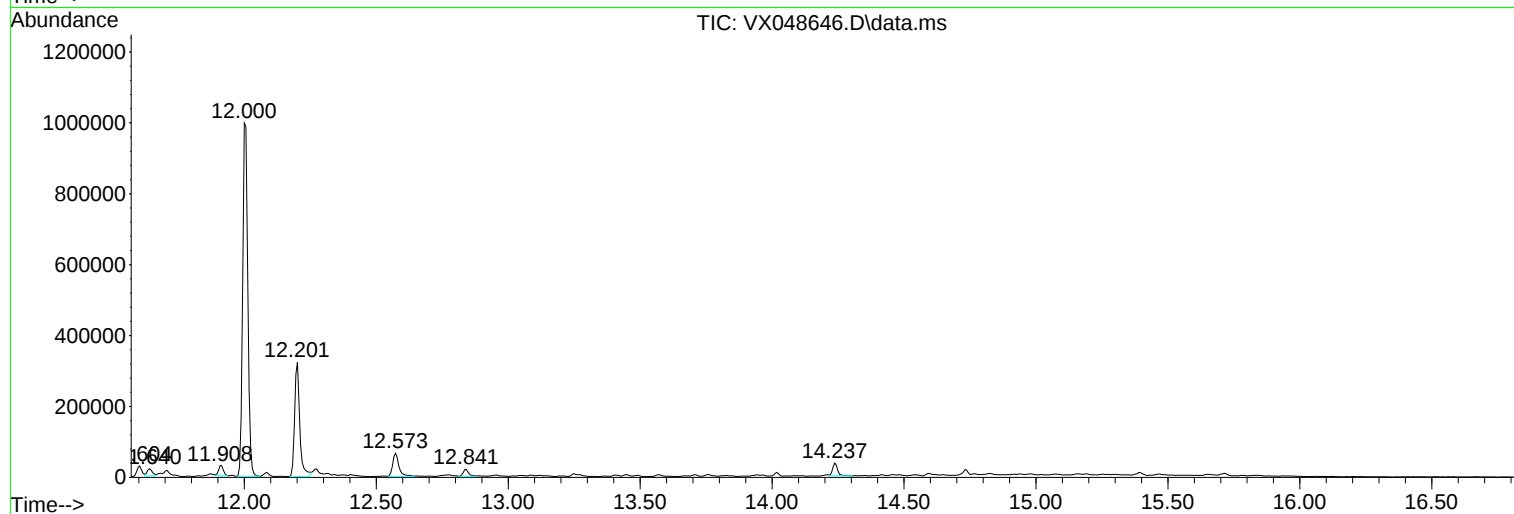
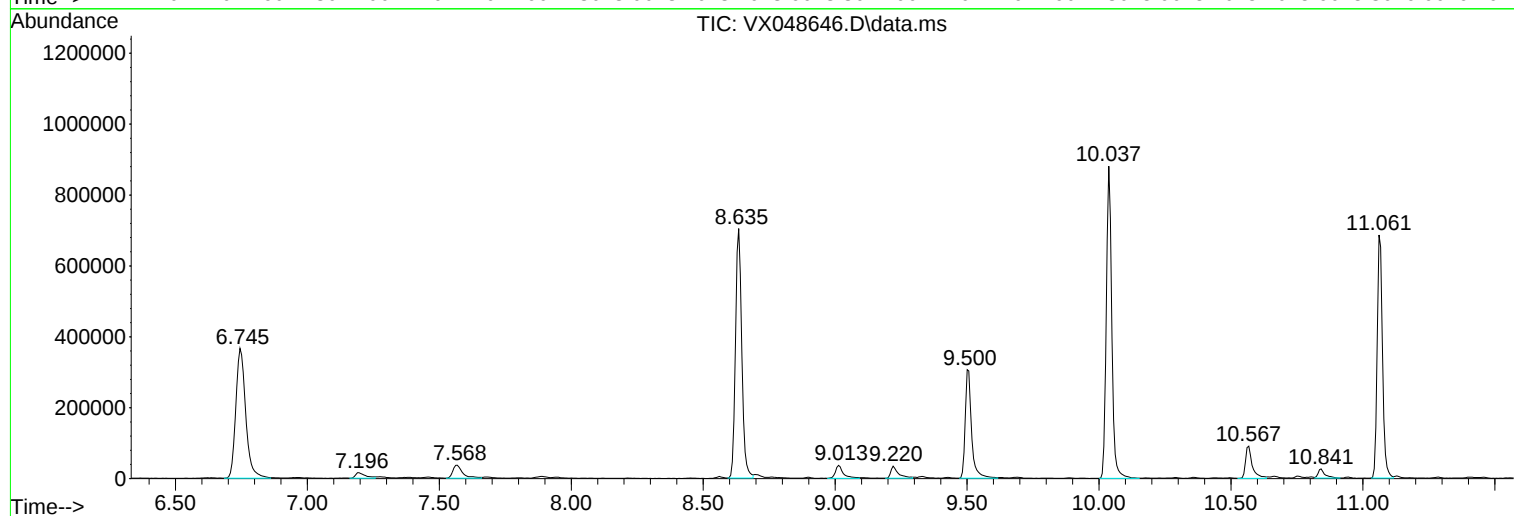
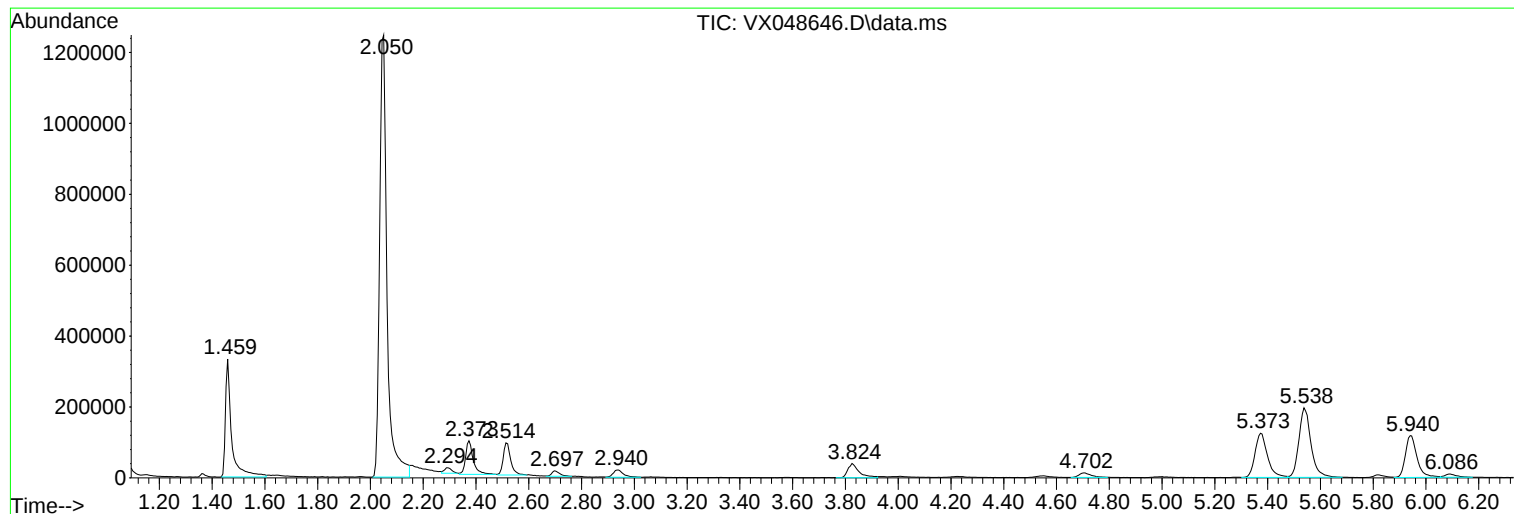
Sum of corrected areas: 12419726

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110725W.M
Quant Title : SW846 8260

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



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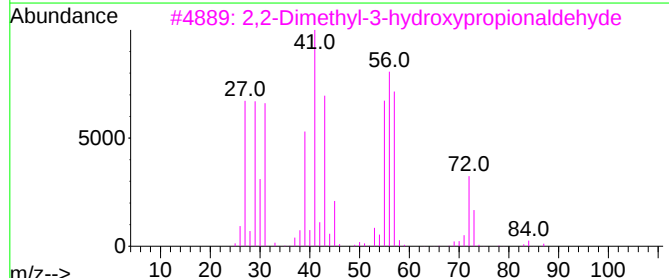
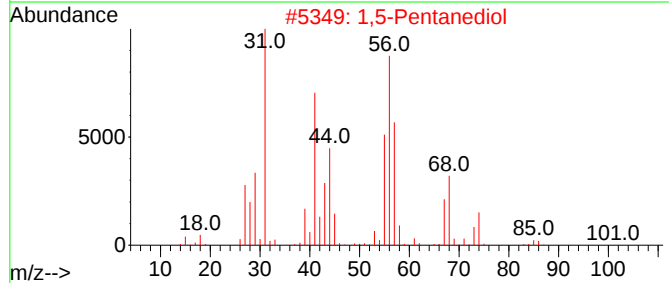
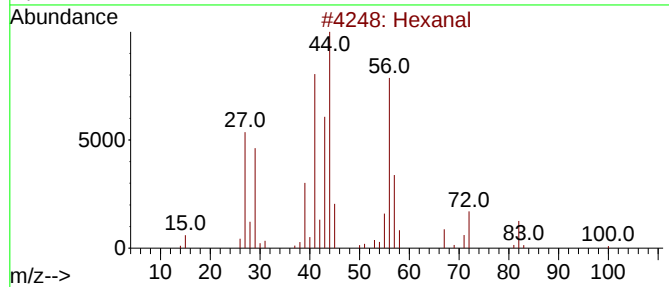
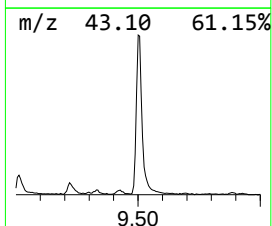
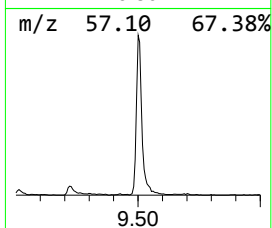
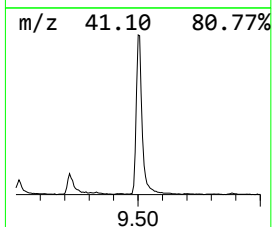
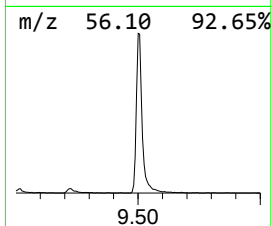
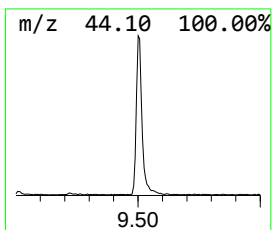
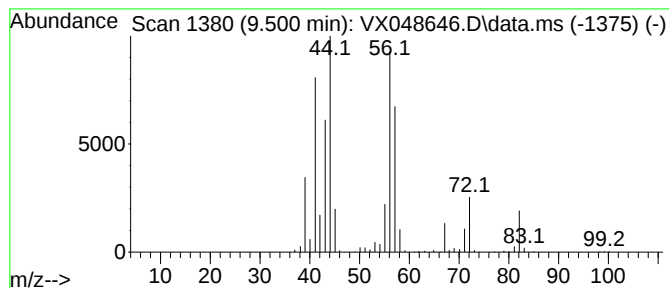
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110725W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.500	20.04 ug/l	508563	Chlorobenzene-d5	10.037

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	91
2			1,5-Pentanediol	104	C5H12O2	000111-29-5	28
3			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	25
4			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	22
5			Butanal, 3-methyl-	86	C5H10O	000590-86-3	16



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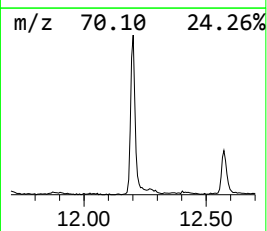
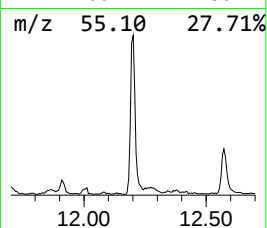
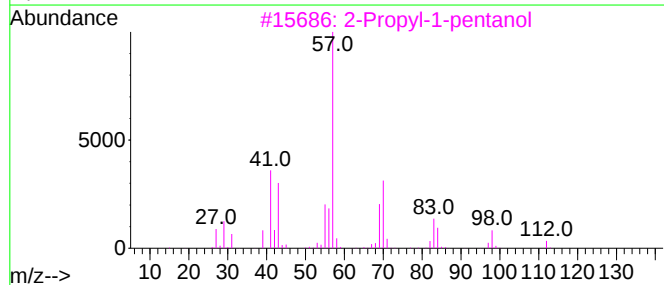
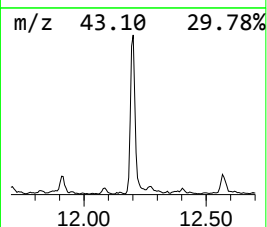
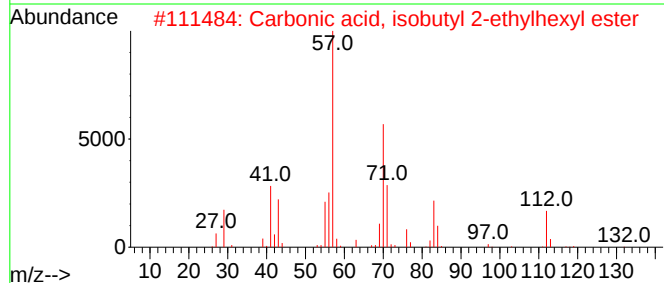
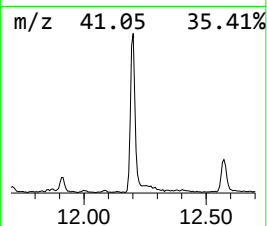
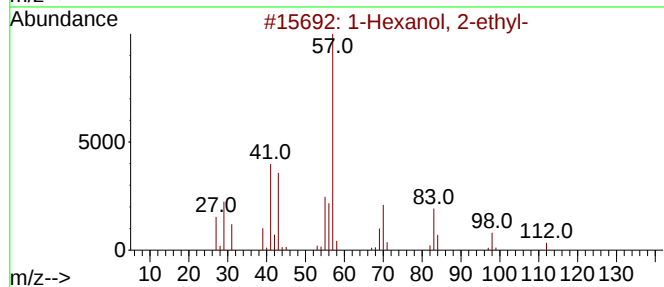
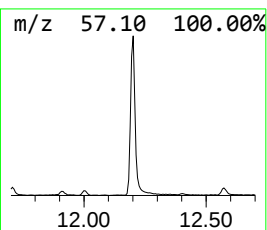
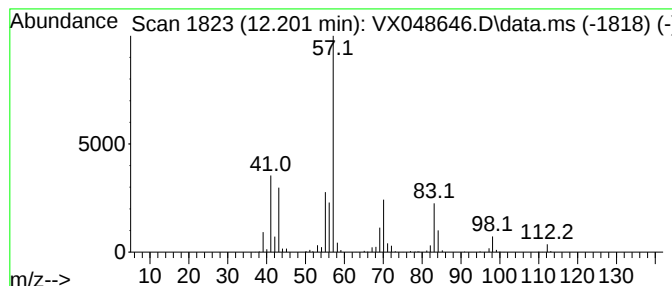
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Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.201	16.28 ug/l	438439	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	9.500	20.0	ug/l	508563	3	10.037	1269180	50.0
1-Hexanol, 2-et...	12.201	16.3	ug/l	438439	4	12.006	1346560	50.0