

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112125\
 Data File : VX048647.D
 Acq On : 21 Nov 2025 11:36
 Operator : JC/MD
 Sample : Q3685-02 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 4198

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: VX048647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	115	rBV	7582365	11086421	100.00%	44.634%
2	2.051	151	158	193	rBV	1899078	3743413	33.77%	15.071%
3	2.288	193	197	205	rVV	56226	118601	1.07%	0.477%
4	2.374	205	211	224	rVB	185099	351364	3.17%	1.415%
5	2.514	229	234	249	rVB	76038	164133	1.48%	0.661%
6	3.825	441	449	460	rBV2	61690	174486	1.57%	0.702%
7	5.373	693	703	718	rBV	131331	420284	3.79%	1.692%
8	5.538	720	730	756	rVB	191351	607155	5.48%	2.444%
9	5.946	787	797	812	rBV	134222	386888	3.49%	1.558%
10	6.745	917	928	948	rBV	360071	933124	8.42%	3.757%
11	7.568	1056	1063	1070	rBV3	49301	114203	1.03%	0.460%
12	8.635	1232	1238	1248	rBV	755764	1240039	11.19%	4.992%
13	9.013	1291	1300	1325	rBV	191587	379761	3.43%	1.529%
14	9.220	1330	1334	1346	rBV	58343	112590	1.02%	0.453%
15	9.507	1375	1381	1398	rVB	112781	187897	1.69%	0.756%
16	10.037	1462	1468	1486	rBV	919260	1311820	11.83%	5.281%
17	10.561	1549	1554	1570	rBV	208801	352137	3.18%	1.418%
18	11.067	1631	1637	1652	rBV	728974	1042530	9.40%	4.197%
19	12.006	1785	1791	1799	rBV	1013310	1352103	12.20%	5.444%
20	12.201	1817	1823	1831	rBV	580802	759487	6.85%	3.058%

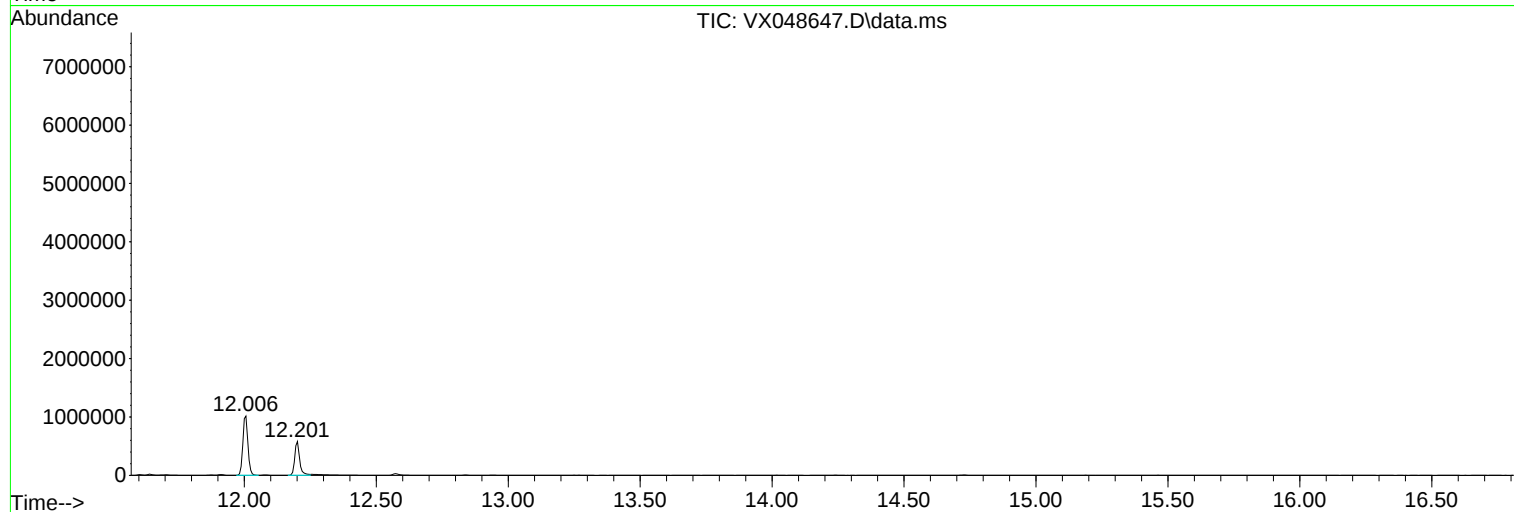
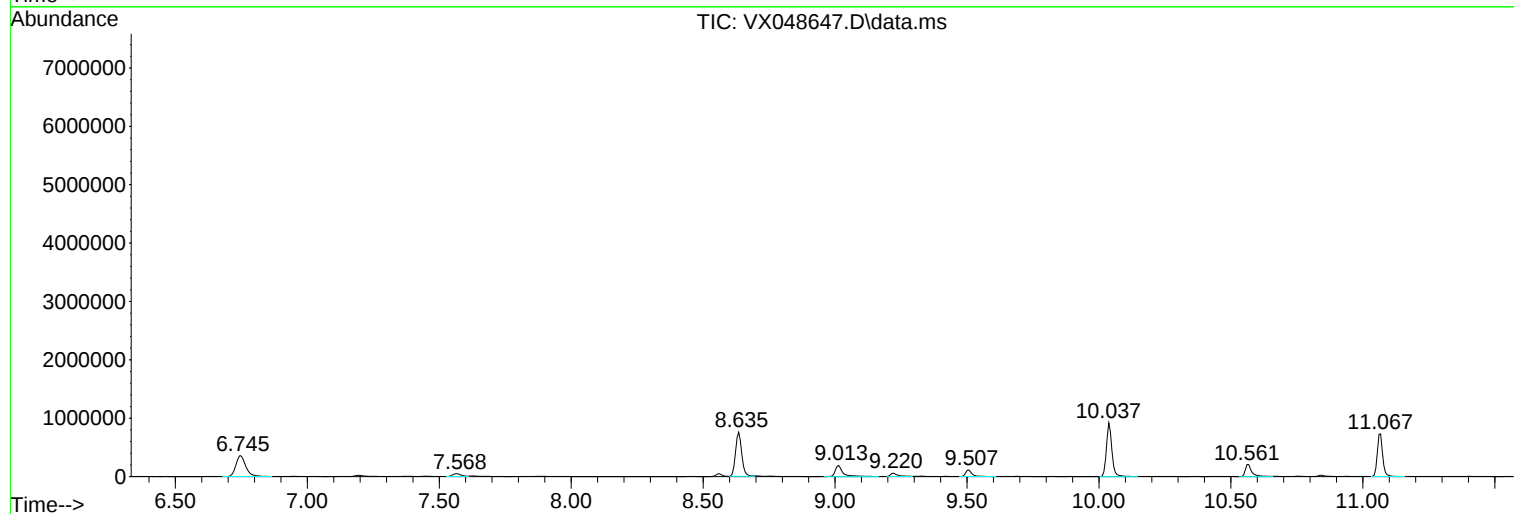
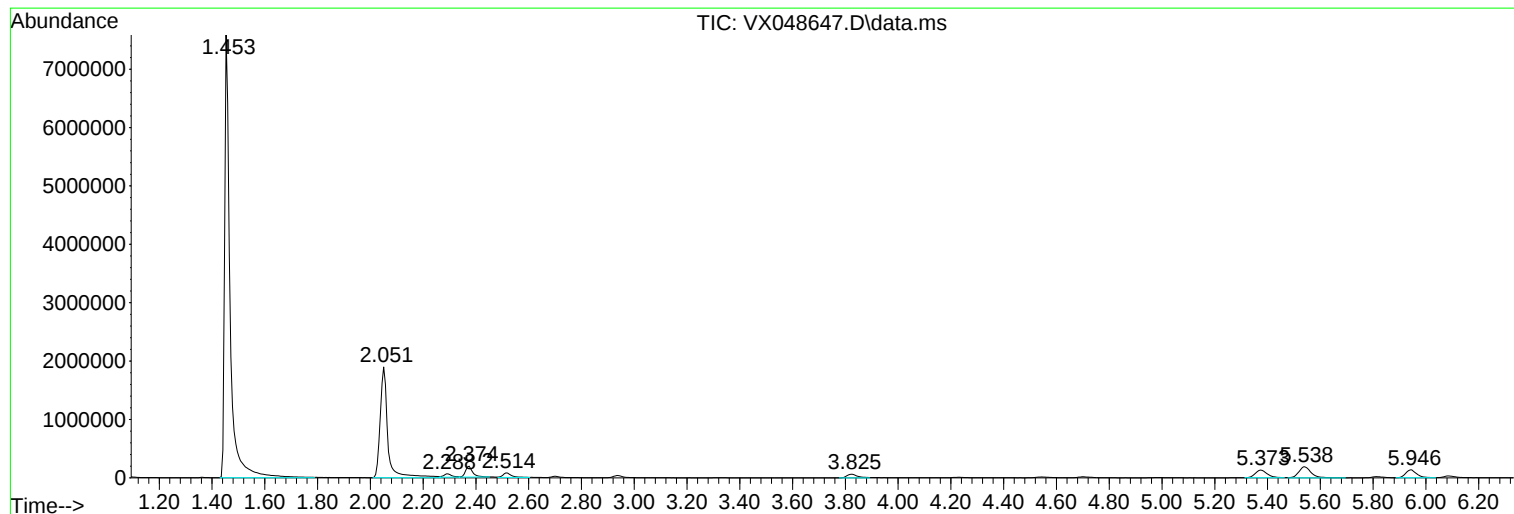
Sum of corrected areas: 24838436

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112125\
Data File : VX048647.D
Acq On : 21 Nov 2025 11:36
Operator : JC/MD
Sample : Q3685-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4198

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112125\
Data File : VX048647.D
Acq On : 21 Nov 2025 11:36
Operator : JC/MD
Sample : Q3685-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4198

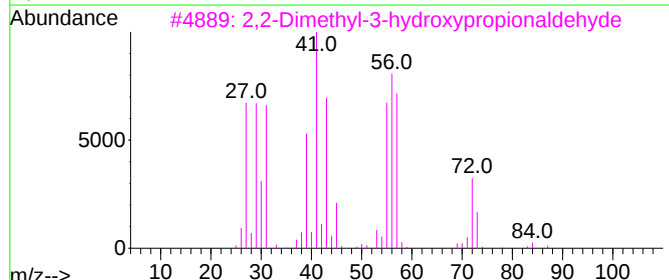
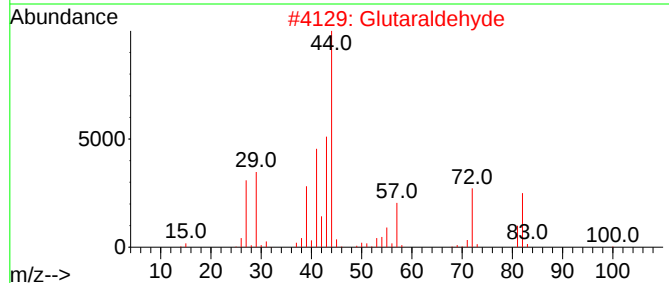
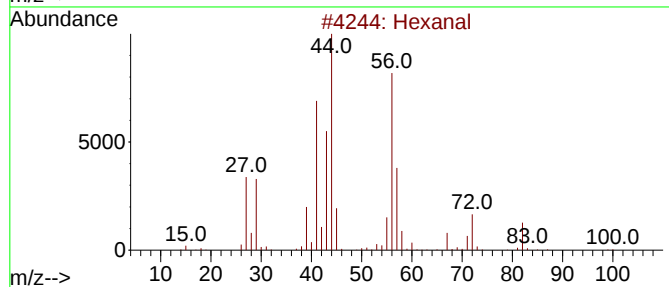
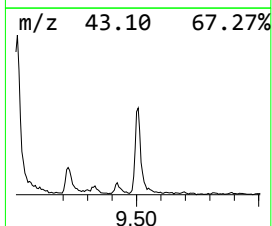
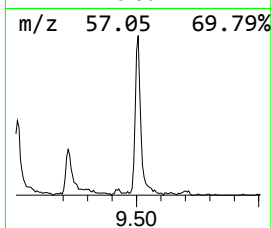
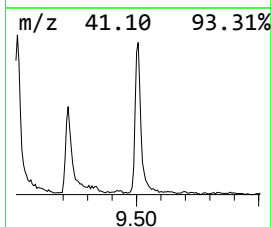
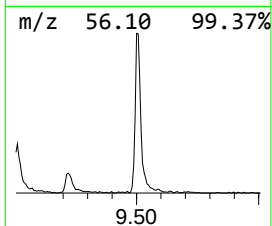
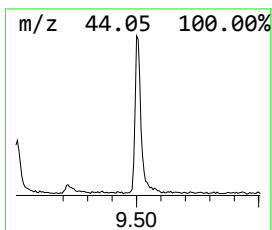
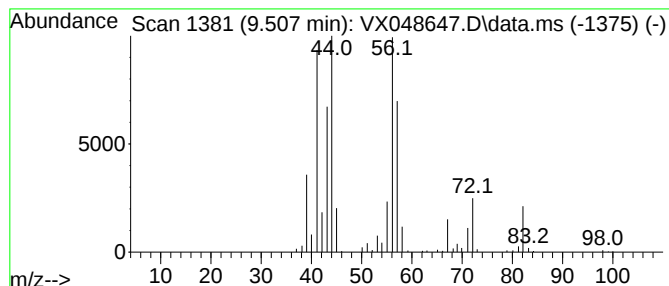
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X110725W.M
Quant Title : SW846 8260

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

Peak Number 8 Hexanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.507	7.16 ug/l	187897	Chlorobenzene-d5	10.037

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	94
2			Glutaraldehyde	100	C5H8O2	000111-30-8	43
3			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	25
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	16
5			Butanal	72	C4H8O	000123-72-8	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112125\
Data File : VX048647.D
Acq On : 21 Nov 2025 11:36
Operator : JC/MD
Sample : Q3685-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
4198

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	9.507	7.2	ug/l	187897	3	10.037	1311820	50.0