

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080425\
 Data File : VX047226.D
 Acq On : 04 Aug 2025 14:44
 Operator : JC/MD
 Sample : Q2759-04 200X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 LIQUID-DRUMS

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\82X072125W.M
 Title : SW846 8260

Signal : TIC: VX047226.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.063	154	160	177	rBV2	20521	61359	2.23%	0.327%
2	5.391	692	706	722	rBV4	244801	780931	28.36%	4.156%
3	5.556	722	733	763	rVB2	417678	1295747	47.05%	6.895%
4	5.958	788	799	823	rBV	260448	756289	27.46%	4.024%
5	6.757	921	930	953	rBV	711907	1844528	66.98%	9.815%
6	8.647	1233	1240	1259	rBV	1440234	2302723	83.61%	12.254%
7	10.049	1465	1470	1490	rVB	1631754	2291111	83.19%	12.192%
8	11.079	1633	1639	1653	rBV	1333810	1705039	61.91%	9.073%
9	11.476	1698	1704	1711	rVB2	29581	45580	1.66%	0.243%
10	11.750	1746	1749	1758	rVB	31450	45642	1.66%	0.243%
11	12.018	1788	1793	1800	rBV	1956817	2329894	84.60%	12.398%
12	12.091	1800	1805	1811	rVB3	16254	37073	1.35%	0.197%
13	12.317	1837	1842	1848	rVB5	20305	38067	1.38%	0.203%
14	12.420	1854	1859	1863	rBV	63038	71268	2.59%	0.379%
15	12.579	1881	1885	1899	rBV	2253337	2753969	100.00%	14.655%
16	12.969	1945	1949	1955	rVB4	25816	47625	1.73%	0.253%
17	13.158	1977	1980	1985	rVB2	17428	28359	1.03%	0.151%
18	13.262	1993	1997	2000	rBV	69598	93598	3.40%	0.498%
19	13.292	2000	2002	2007	rVB3	49196	57023	2.07%	0.303%
20	13.420	2019	2023	2032	rVB2	110004	167119	6.07%	0.889%
21	13.579	2046	2049	2055	rBV4	29346	47519	1.73%	0.253%
22	13.731	2070	2074	2078	rBV6	21768	35356	1.28%	0.188%
23	13.768	2078	2080	2087	rVB2	19957	37077	1.35%	0.197%
24	13.847	2087	2093	2097	rBV6	33744	65467	2.38%	0.348%
25	14.036	2120	2124	2127	rVB	69422	71942	2.61%	0.383%
26	14.188	2145	2149	2167	rBV2	461711	843641	30.63%	4.489%
27	14.475	2193	2196	2205	rVB6	37904	87446	3.18%	0.465%
28	14.609	2215	2218	2220	rBV2	76143	94390	3.43%	0.502%
29	14.633	2220	2222	2225	rVV	71840	84757	3.08%	0.451%
30	14.664	2225	2227	2232	rVB3	31620	41810	1.52%	0.222%
31	14.749	2238	2241	2244	rBV	65402	79653	2.89%	0.424%
32	14.780	2244	2246	2250	rVV3	36286	46492	1.69%	0.247%
33	14.847	2254	2257	2261	rVB6	24135	29581	1.07%	0.157%
34	15.182	2308	2312	2314	rBV3	32709	47325	1.72%	0.252%
35	15.207	2314	2316	2320	rVB4	42537	46417	1.69%	0.247%
36	15.371	2339	2343	2346	rBV5	29369	44535	1.62%	0.237%

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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

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Title : SW846 8260

37	15.414	2347	2350	2354	rVB5	37106	46731	1.70%	0.249%
38	15.481	2356	2361	2367	rBV6	59644	116821	4.24%	0.622%
39	15.609	2378	2382	2385	rBV3	37965	55841	2.03%	0.297%
40	16.084	2456	2460	2472	rBV3	59737	116456	4.23%	0.620%

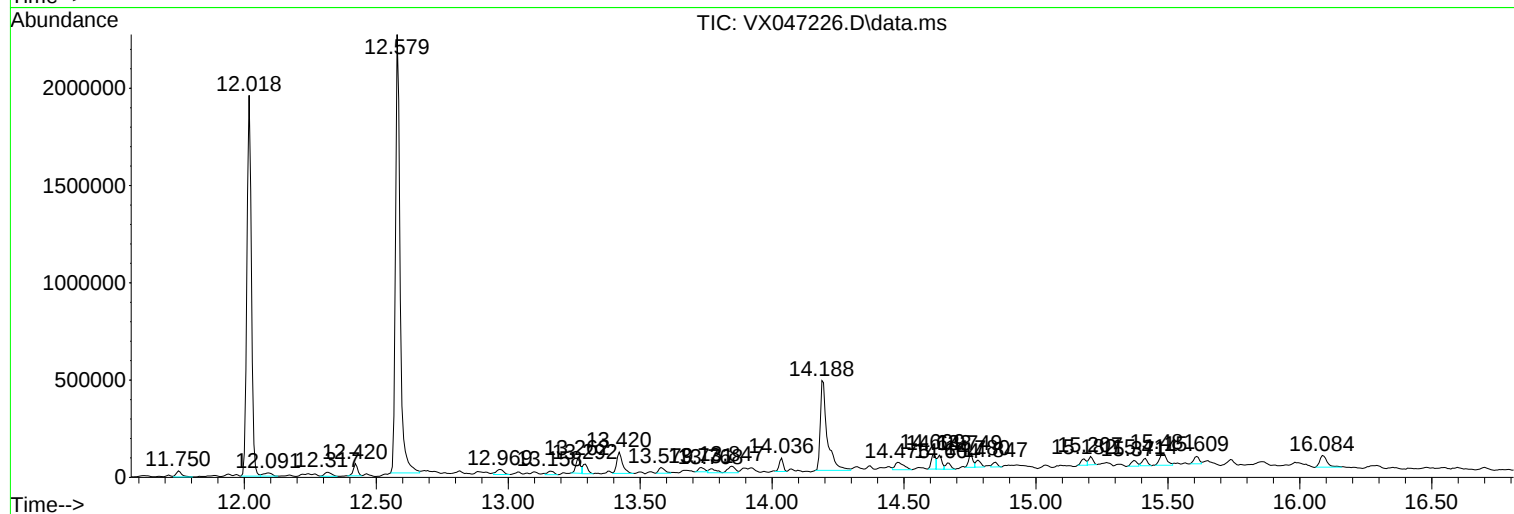
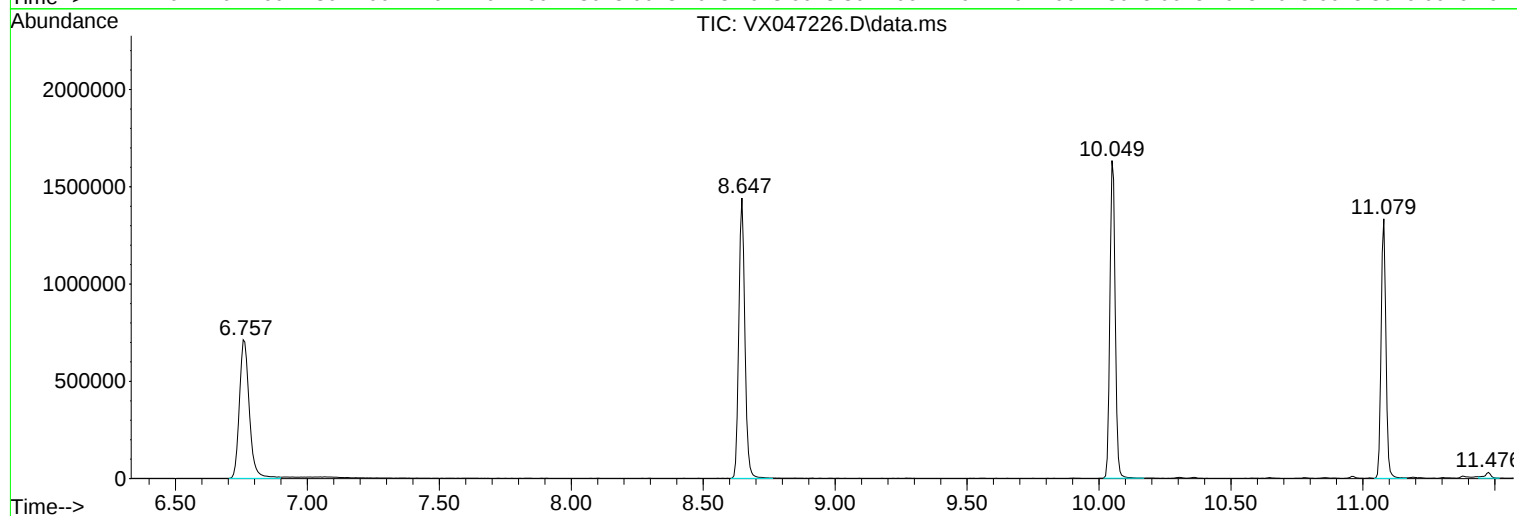
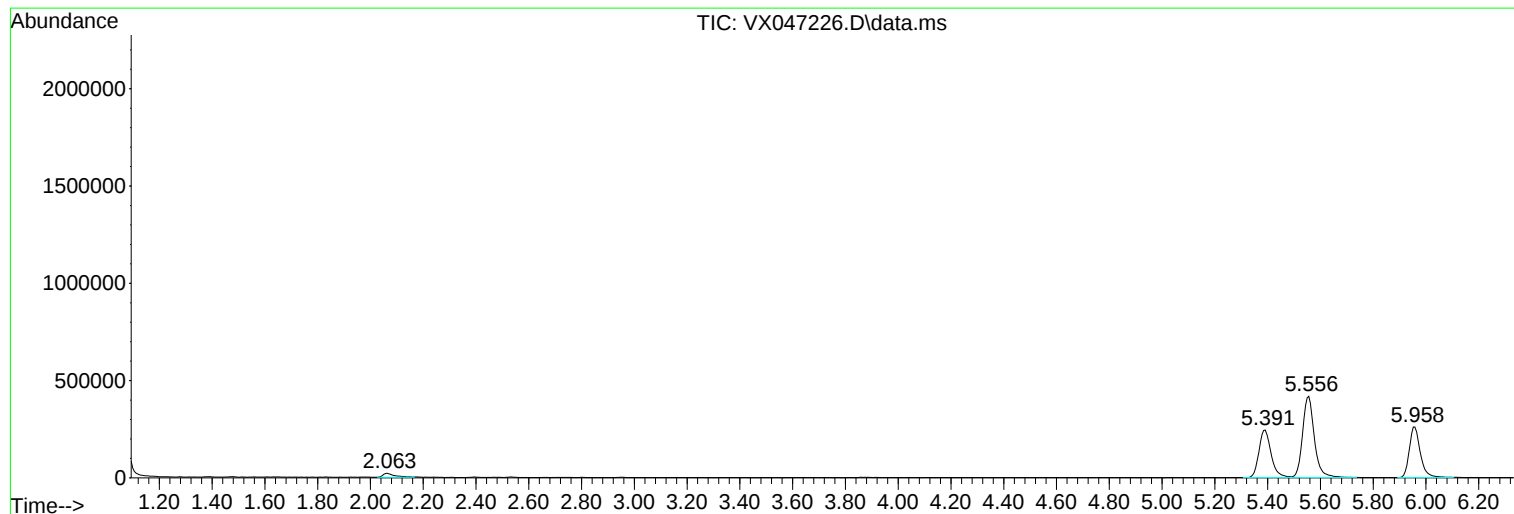
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
LIQUID-DRUMS

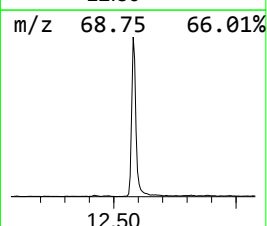
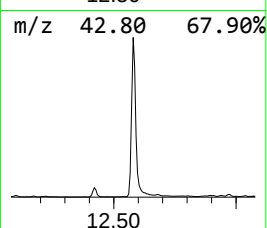
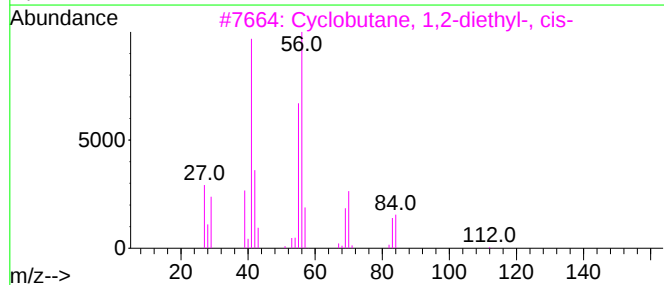
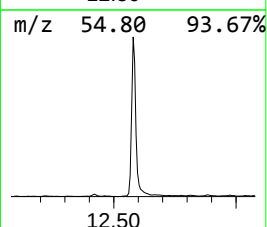
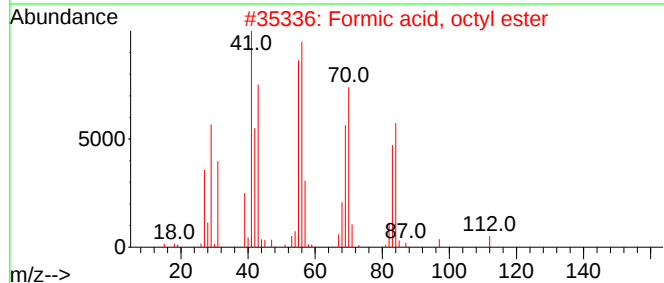
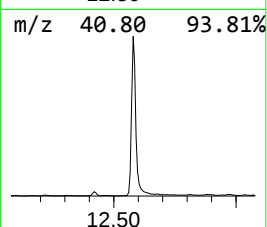
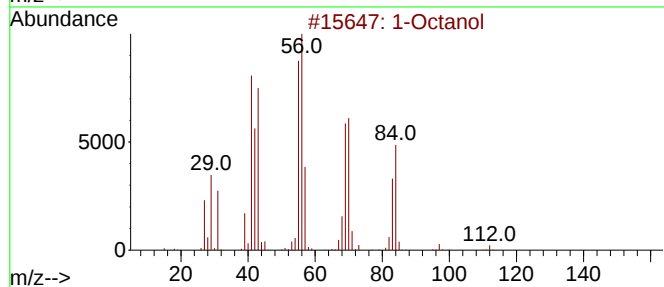
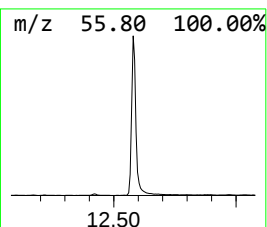
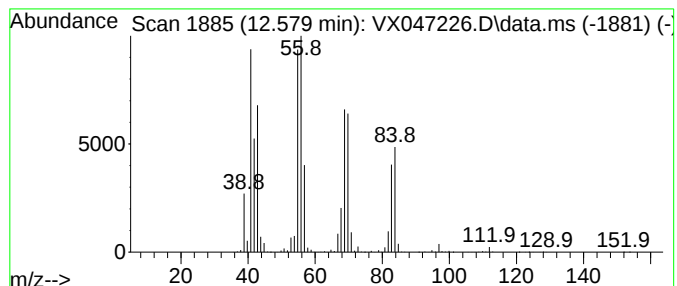
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072125W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.579	59.10 ug/l	2753970	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	91
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	64
4			1-Hexene	84	C6H12	000592-41-6	47
5			Formic acid, heptyl ester	144	C8H16O2	000112-23-2	47



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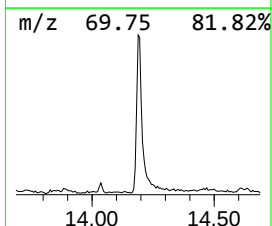
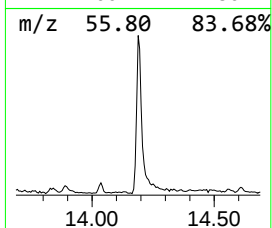
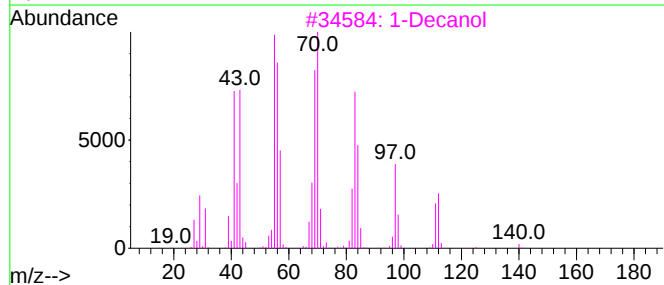
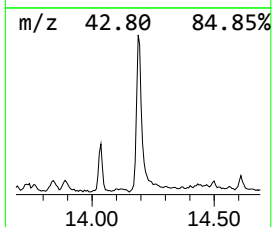
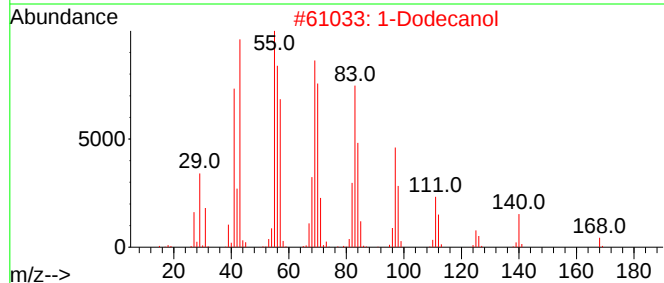
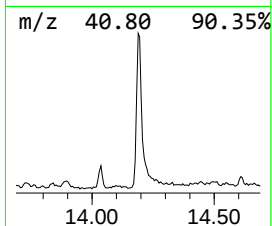
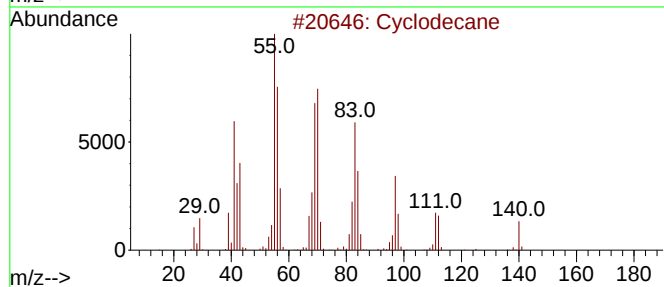
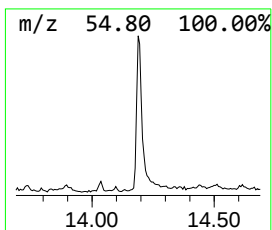
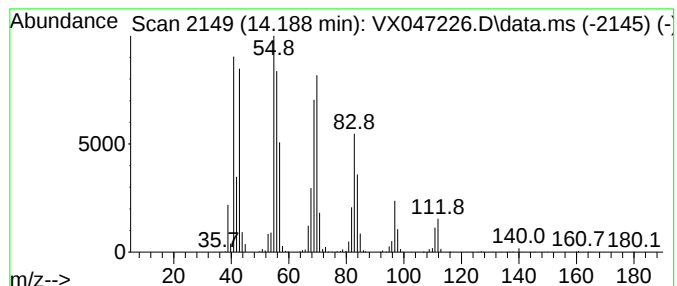
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.188	18.10 ug/l	843641	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclodecane	140	C10H20	000293-96-9	96
2			1-Dodecanol	186	C12H26O	000112-53-8	91
3			1-Decanol	158	C10H22O	000112-30-1	91
4			Cyclooctane	112	C8H16	000292-64-8	87
5			Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	81



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Octanol	12.579	59.1	ug/l	2753970	4	12.018	2329890	50.0
Cyclodecane	14.188	18.1	ug/l	843641	4	12.018	2329890	50.0