

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060225\
 Data File : VX046456.D
 Acq On : 02 Jun 2025 19:52
 Operator : JC/MD
 Sample : Q2169-03 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 303-PPR-2

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: VX046456.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.587	70	82	83	rBV2	5178	13020	2.79%	0.375%
2	1.611	83	86	89	rVB2	5942	7999	1.72%	0.230%
3	3.434	378	385	394	rVB5	2200	4795	1.03%	0.138%
4	5.379	694	704	721	rBV	53791	160677	34.45%	4.624%
5	5.544	721	731	747	rVB	78250	223139	47.84%	6.421%
6	5.952	787	798	815	rBV2	61677	169465	36.34%	4.877%
7	6.757	921	930	943	rBV	142287	336898	72.24%	9.695%
8	8.647	1234	1240	1248	rBV	295725	466380	100.00%	13.421%
9	8.714	1248	1251	1259	rVB2	12709	22263	4.77%	0.641%
10	10.049	1465	1470	1487	rBV	302877	429694	92.13%	12.366%
11	10.195	1489	1494	1501	rVB	10399	14559	3.12%	0.419%
12	10.299	1506	1511	1518	rBV	41269	56009	12.01%	1.612%
13	10.640	1560	1567	1574	rBV	25232	33741	7.23%	0.971%
14	11.079	1634	1639	1649	rBV	255270	329783	70.71%	9.490%
15	11.305	1672	1676	1683	rBV	3787	4824	1.03%	0.139%
16	11.378	1683	1688	1696	rVV	18557	33241	7.13%	0.957%
17	11.451	1696	1700	1710	rVB3	10169	16716	3.58%	0.481%
18	11.616	1722	1727	1735	rVB2	9047	16924	3.63%	0.487%
19	11.750	1745	1749	1759	rVB	40829	52612	11.28%	1.514%
20	12.018	1788	1793	1800	rBV	325355	402942	86.40%	11.596%
21	12.085	1800	1804	1815	rVB	20403	28872	6.19%	0.831%
22	12.244	1822	1830	1833	rBV3	15622	32240	6.91%	0.928%
23	12.317	1838	1842	1850	rVB3	9146	15202	3.26%	0.437%
24	12.420	1852	1859	1863	rBV6	4322	6391	1.37%	0.184%
25	12.463	1863	1866	1873	rVB2	3994	5122	1.10%	0.147%
26	12.530	1873	1877	1879	rBV	5039	6822	1.46%	0.196%
27	12.585	1881	1886	1900	rVV	110251	193227	41.43%	5.561%
28	12.701	1900	1905	1912	rVB3	7830	17054	3.66%	0.491%
29	12.920	1938	1941	1944	rVV2	4502	5550	1.19%	0.160%
30	12.963	1944	1948	1955	rVB	8885	12945	2.78%	0.373%
31	13.164	1977	1981	1985	rBV2	7252	8521	1.83%	0.245%
32	13.292	1992	2002	2007	rVB3	19206	35714	7.66%	1.028%
33	13.420	2019	2023	2027	rBV	17531	25458	5.46%	0.733%
34	13.585	2046	2050	2054	rBV4	4921	7118	1.53%	0.205%
35	13.774	2077	2081	2088	rVB	14971	22407	4.80%	0.645%
36	13.847	2089	2093	2098	rVB4	6682	10156	2.18%	0.292%

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37	13.926	2100	2106	2110	rBV3	6124	9865	2.12%	0.284%
38	14.036	2121	2124	2127	rBV2	6155	5477	1.17%	0.158%
39	14.073	2127	2130	2136	rVB3	4102	6305	1.35%	0.181%
40	14.188	2145	2149	2154	rBV	36863	63928	13.71%	1.840%
41	14.371	2176	2179	2183	rVB5	5534	6318	1.35%	0.182%
42	14.475	2192	2196	2207	rVB7	8846	15681	3.36%	0.451%
43	14.609	2214	2218	2220	rBV3	13480	17468	3.75%	0.503%
44	14.633	2220	2222	2226	rVB	15911	20153	4.32%	0.580%
45	14.755	2238	2242	2243	rBV	8106	8438	1.81%	0.243%
46	14.780	2243	2246	2251	rVV2	11143	14895	3.19%	0.429%
47	14.902	2262	2266	2269	rBV6	2718	4697	1.01%	0.135%
48	15.188	2308	2313	2314	rBV4	4305	7344	1.57%	0.211%
49	15.206	2314	2316	2323	rVB3	9864	12725	2.73%	0.366%
50	15.487	2357	2362	2368	rBV2	14640	25753	5.52%	0.741%
51	15.609	2379	2382	2386	rVB4	5660	8313	1.78%	0.239%
52	16.371	2502	2507	2518	rVB4	9074	19096	4.09%	0.550%

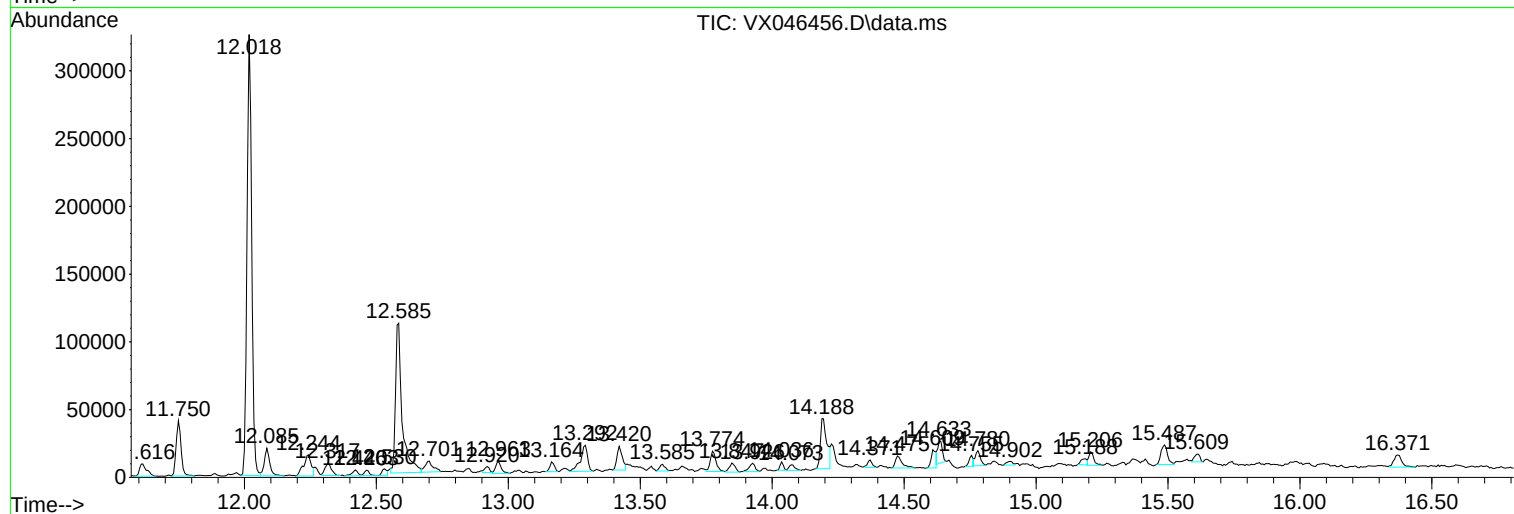
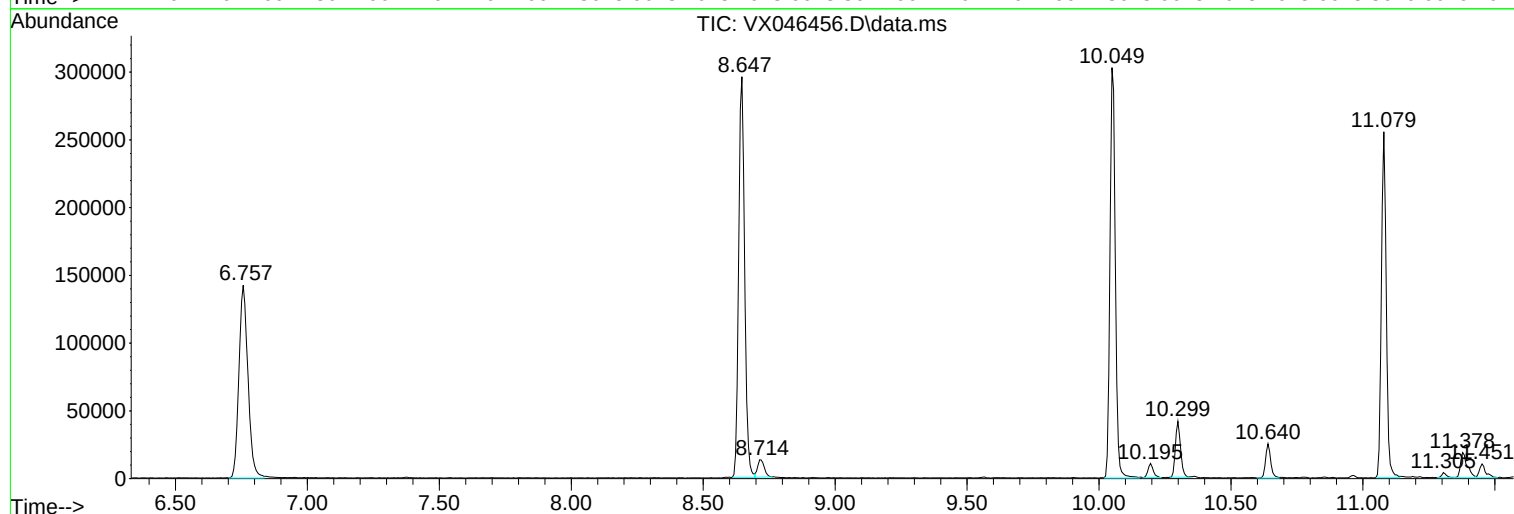
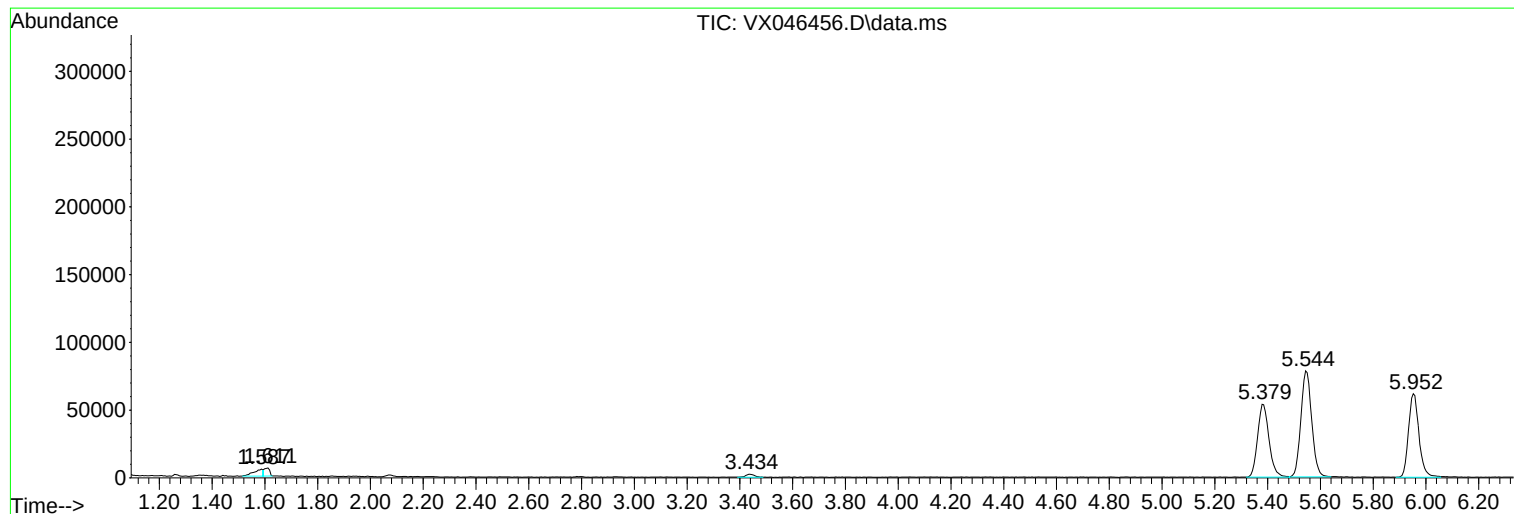
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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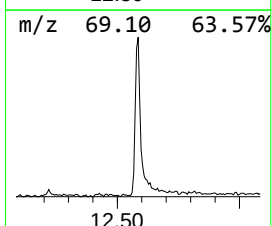
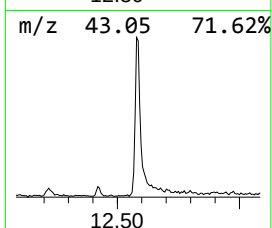
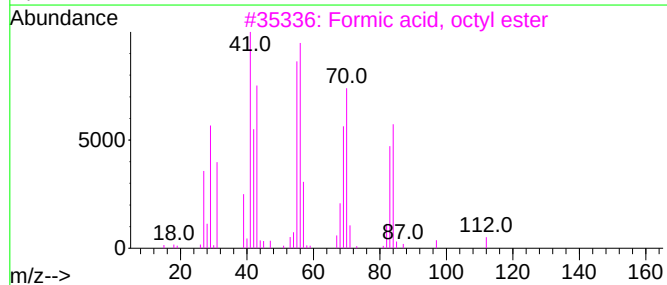
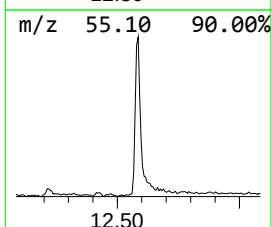
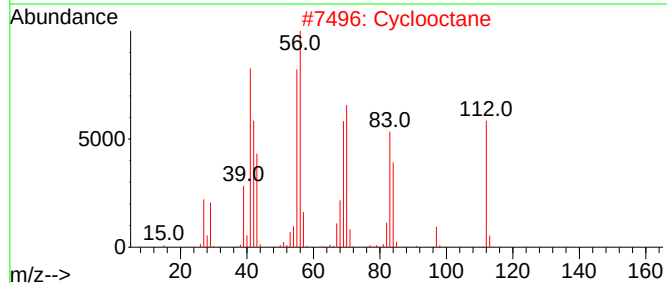
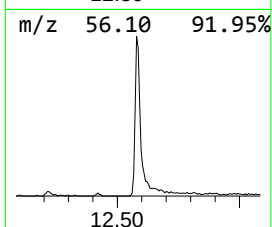
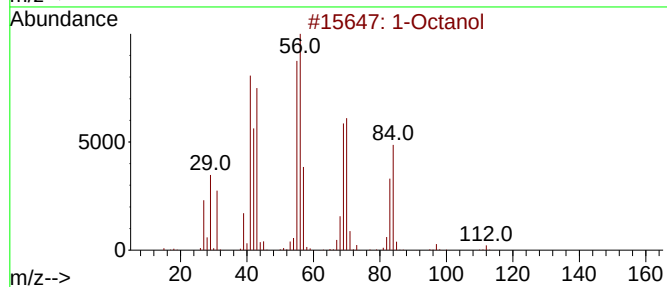
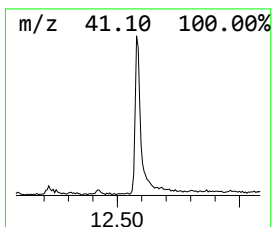
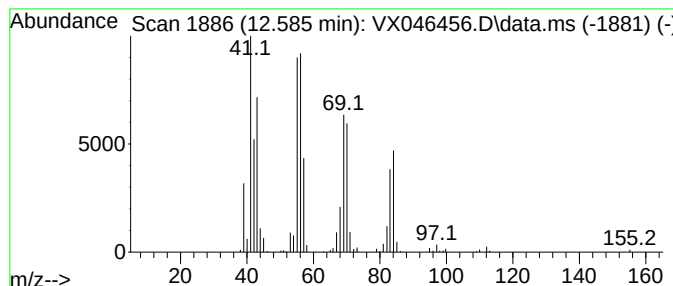
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	23.98 ug/l	193227	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	Cyclooctane			112	C8H16	000292-64-8	90
3	Formic acid, octyl ester			158	C9H18O2	000112-32-3	90
4	Octyl chloroformate			192	C9H17ClO2	007452-59-7	78
5	1-Hexene			84	C6H12	000592-41-6	47



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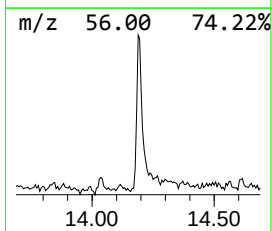
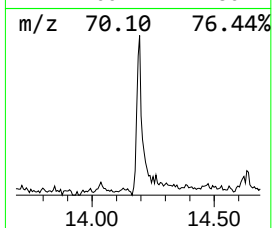
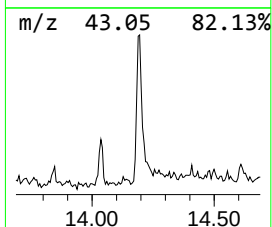
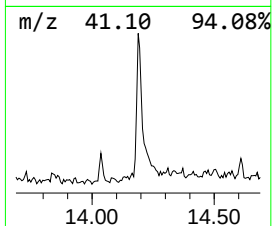
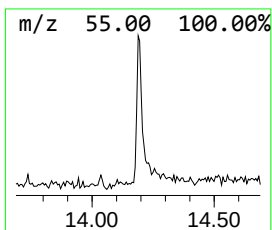
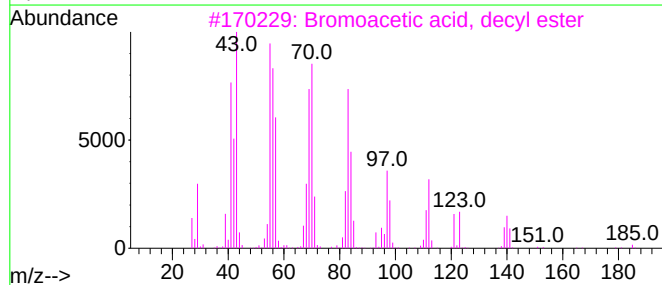
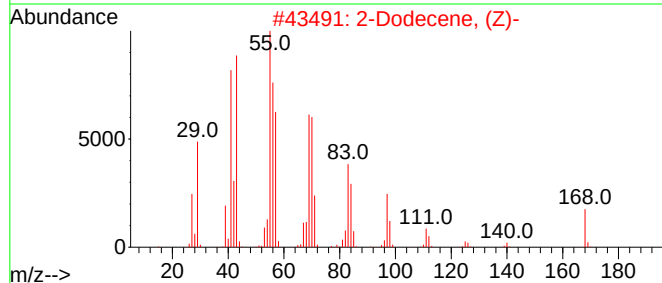
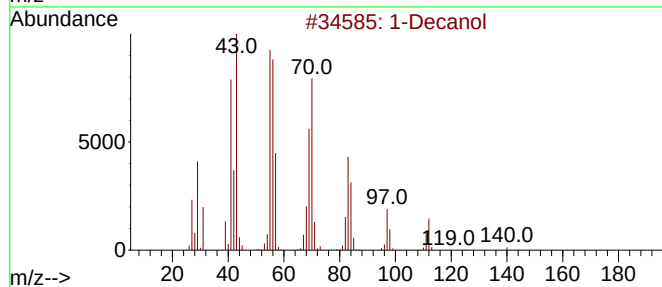
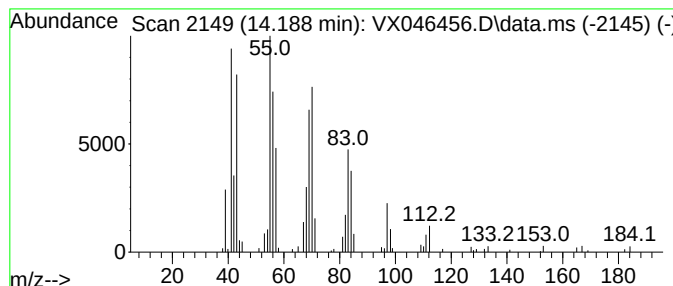
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.188	7.93 ug/l	63928	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol			158	C10H22O	000112-30-1	91
2	2-Dodecene, (Z)-			168	C12H24	007206-26-0	86
3	Bromoacetic acid, decyl ester			278	C12H23BrO2	005436-93-1	86
4	2-Dodecene, (E)-			168	C12H24	007206-13-5	86
5	Cyclopropane, 1-ethyl-2-heptyl-			168	C12H24	074663-86-8	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Octanol	12.585	24.0	ug/l	193227	4	12.018	402942	50.0
1-Decanol	14.188	7.9	ug/l	63928	4	12.018	402942	50.0