

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
 Data File : VX035578.D
 Acq On : 10 May 2023 11:39
 Operator : JC/MD
 Sample : VX0510MBL01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0510MBL01

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035578.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.788	273	279	289	rVB	7380	15018	1.04%	0.160%
2	5.379	692	704	720	rBV	168521	498482	34.40%	5.323%
3	5.544	720	731	749	rVB	294790	841091	58.05%	8.981%
4	5.946	787	797	816	rBV2	162197	438590	30.27%	4.683%
5	6.757	919	930	944	rBV	445240	1068655	73.76%	11.411%
6	8.647	1232	1240	1256	rBV	930116	1448897	100.00%	15.471%
7	9.275	1337	1343	1347	rBV2	10596	33090	2.28%	0.353%
8	10.049	1465	1470	1481	rVB	899098	1262376	87.13%	13.480%
9	11.079	1633	1639	1653	rBV	820576	1014933	70.05%	10.837%
10	12.018	1788	1793	1806	rBV	953303	1224923	84.54%	13.080%
11	13.536	2031	2042	2048	rBV4	17214	58533	4.04%	0.625%
12	13.688	2061	2067	2070	rBV2	15330	20653	1.43%	0.221%
13	13.969	2106	2113	2117	rBV6	10806	24254	1.67%	0.259%
14	14.012	2117	2120	2127	rVB9	7341	15200	1.05%	0.162%
15	14.457	2189	2193	2199	rVB7	11947	16257	1.12%	0.174%
16	15.182	2303	2312	2317	rBV8	32294	98665	6.81%	1.054%
17	15.249	2320	2323	2330	rVV2	23046	38866	2.68%	0.415%
18	15.322	2330	2335	2342	rVB4	17594	31107	2.15%	0.332%
19	15.542	2364	2371	2382	rBV	333053	522222	36.04%	5.576%
20	15.688	2391	2395	2406	rVB7	21311	52640	3.63%	0.562%
21	15.981	2439	2443	2447	rBV6	11456	22233	1.53%	0.237%
22	16.048	2452	2454	2459	rVV5	11654	18486	1.28%	0.197%
23	16.115	2461	2465	2470	rVB6	10626	17334	1.20%	0.185%
24	16.468	2517	2523	2536	rVB	293842	527187	36.39%	5.629%
25	16.645	2547	2552	2570	rVB10	16762	55404	3.82%	0.592%

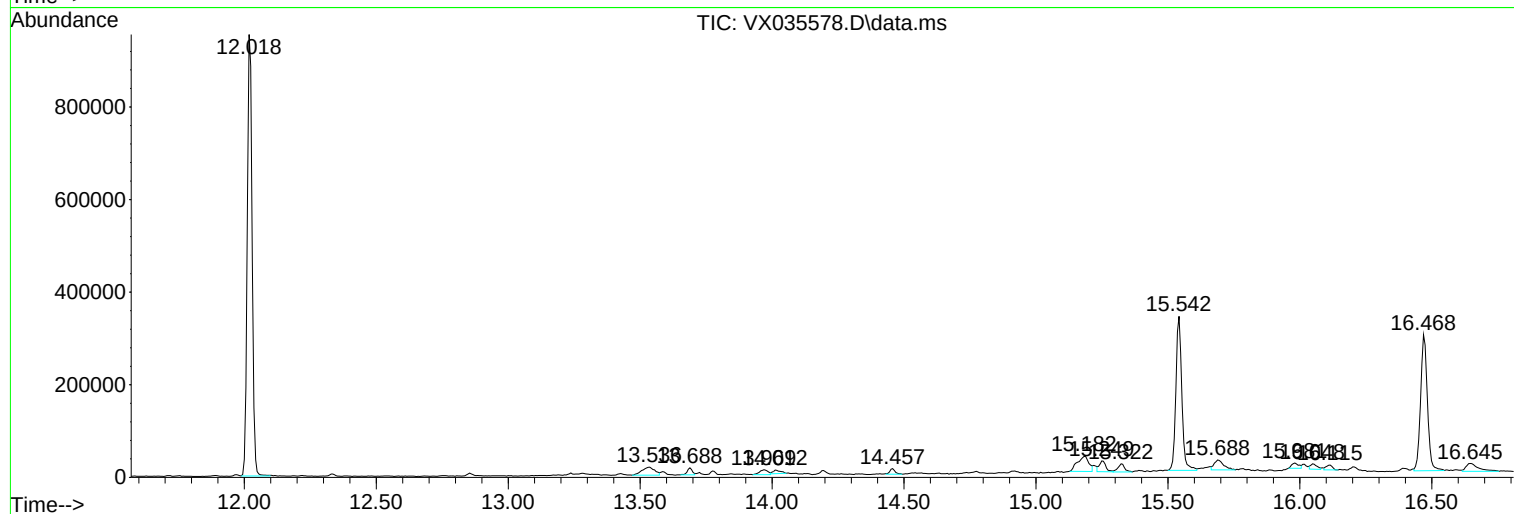
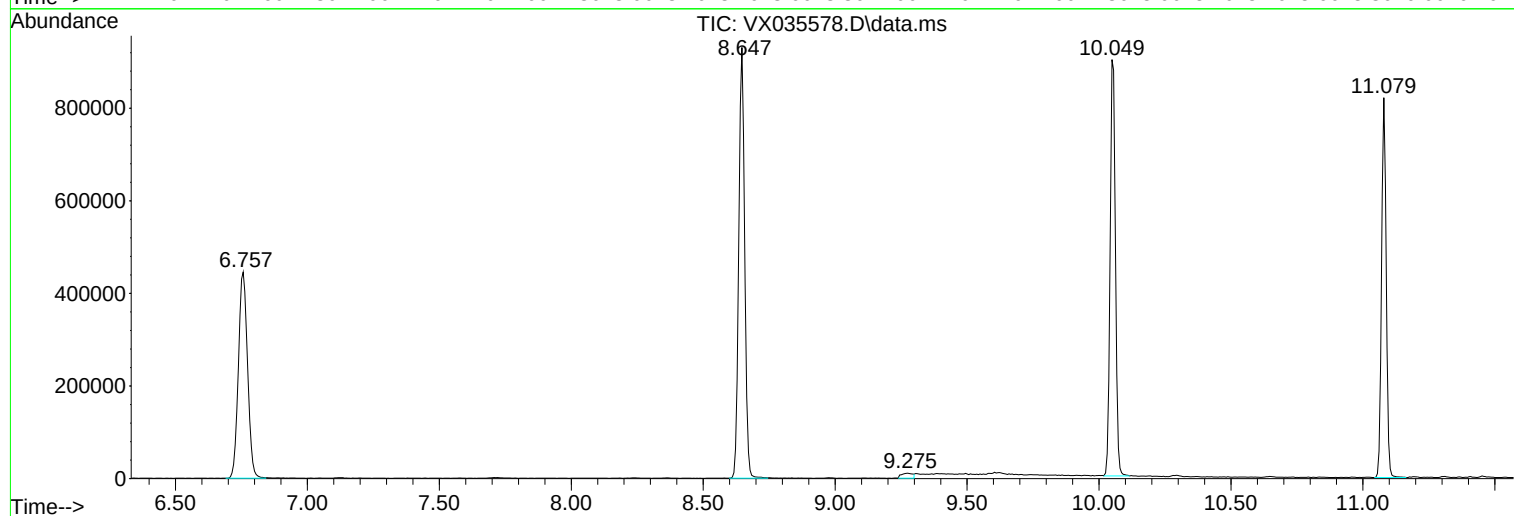
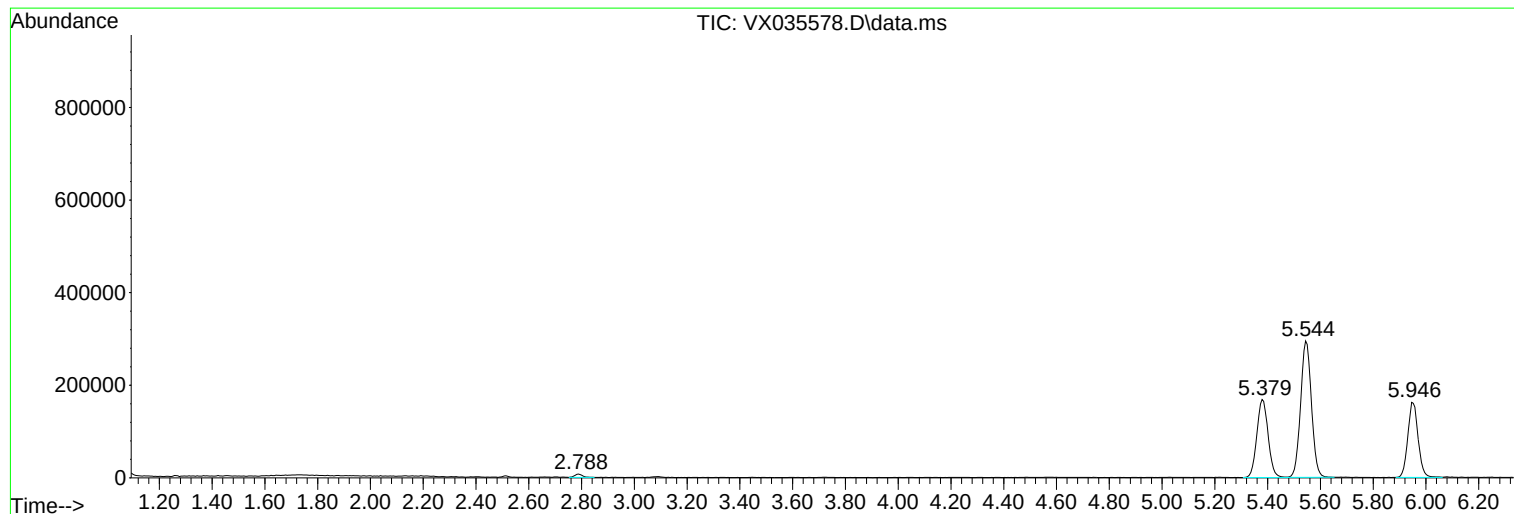
Sum of corrected areas: 9365096

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Instrument :
MSVOA_X
ClientSampleId :
VX0510MBL01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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Instrument :
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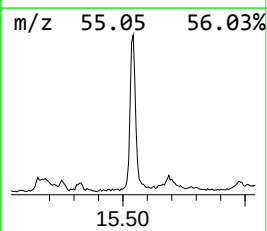
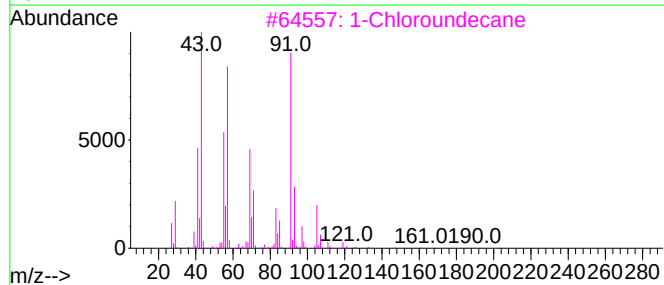
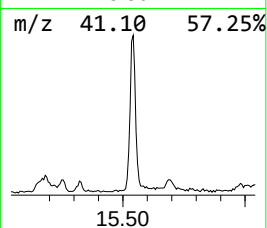
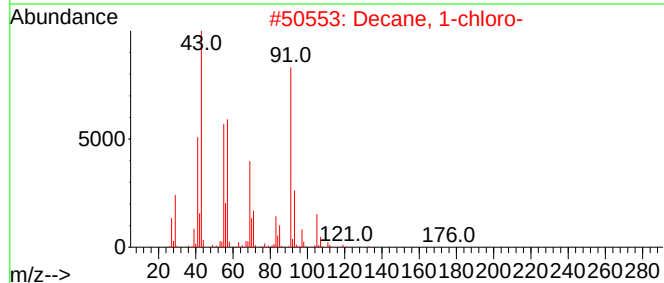
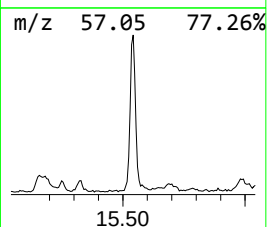
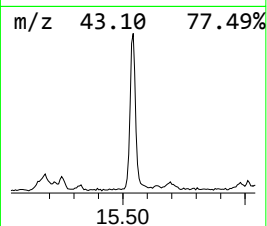
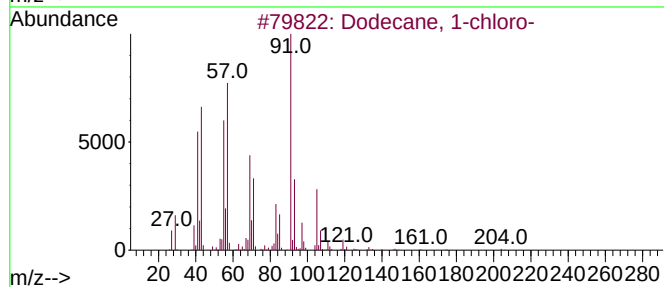
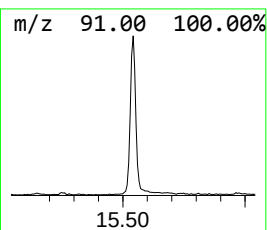
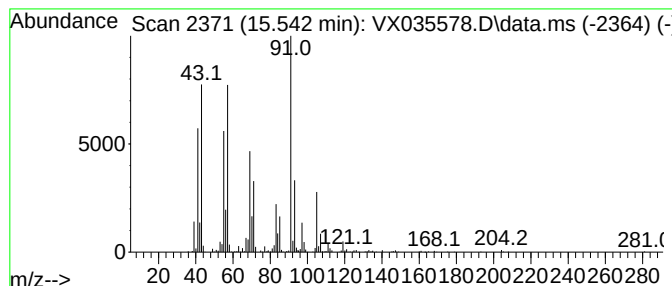
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 1 Dodecane, 1-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	21.32 ug/l	522222	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	98
2			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	86
3			1-Chloroundecane	190	C11H23Cl	002473-03-2	80
4			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	64
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	49



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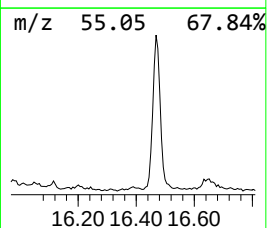
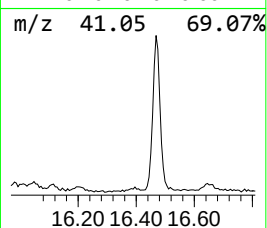
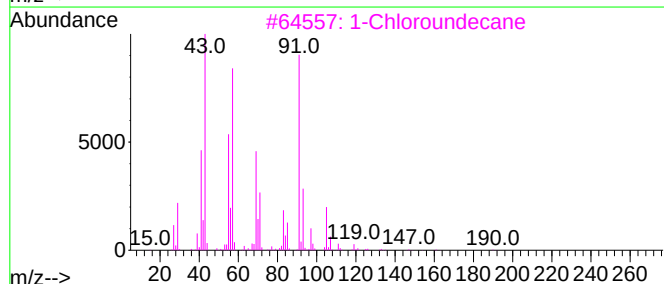
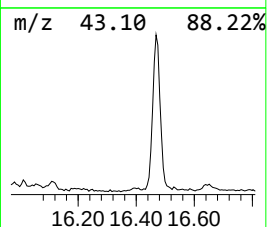
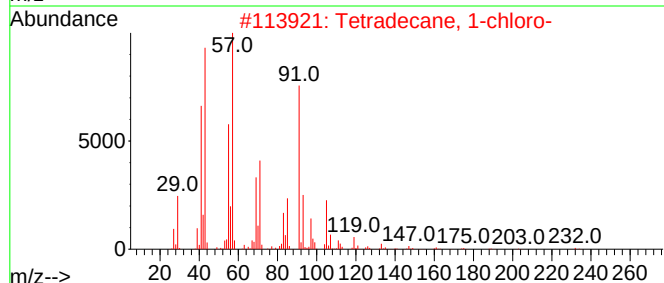
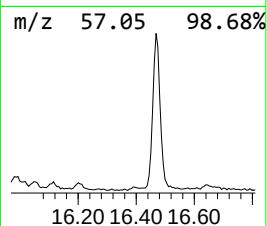
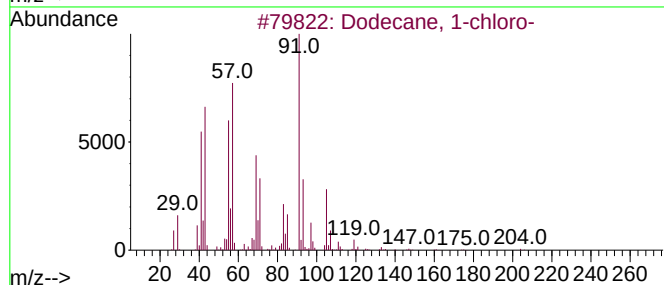
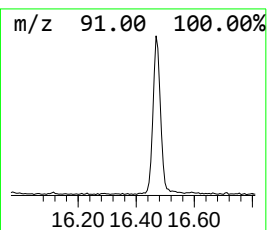
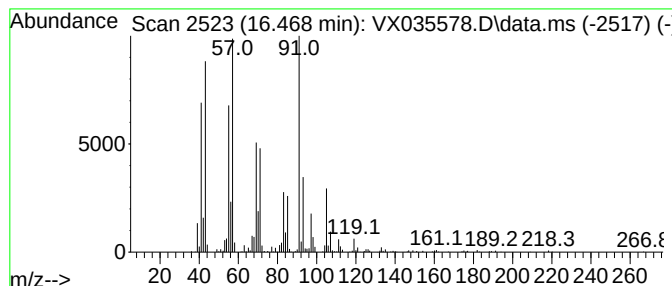
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Quant Title : SW846 8260

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

Peak Number 2 Tetradecane, 1-chloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.468	21.52 ug/l	527187	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	91
2			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	91
3			1-Chloroundecane	190	C11H23Cl	002473-03-2	58
4			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	52
5			Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dodecane, 1-chl...	15.542	21.3	ug/l	522222	4	12.018	1224920	50.0
Tetradecane, 1-...	16.468	21.5	ug/l	527187	4	12.018	1224920	50.0