

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
 Data File : VX035582.D
 Acq On : 10 May 2023 13:30
 Operator : JC/MD
 Sample : 02666-01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BU-02-050823

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: VX035582.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.379	694	704	720	rVB2	161350	472298	32.10%	5.303%
2	5.544	720	731	745	rVB2	293556	840529	57.12%	9.438%
3	5.952	786	798	814	rBV	163906	438907	29.83%	4.928%
4	6.757	920	930	944	rBV	449082	1075008	73.06%	12.071%
5	7.202	997	1003	1016	rVB4	5679	14791	1.01%	0.166%
6	8.647	1231	1240	1250	rBV	943560	1471434	100.00%	16.523%
7	10.055	1464	1471	1481	rBV	886079	1296813	88.13%	14.562%
8	10.299	1506	1511	1519	rVB3	9769	15577	1.06%	0.175%
9	11.085	1633	1640	1648	rBV	699920	1043612	70.92%	11.719%
10	12.024	1788	1794	1804	rBV	1018419	1284928	87.32%	14.428%
11	13.542	2033	2043	2049	rBV6	19403	65569	4.46%	0.736%
12	13.963	2109	2112	2117	rBV6	7669	14953	1.02%	0.168%
13	15.182	2303	2312	2316	rBV9	23345	63261	4.30%	0.710%
14	15.255	2321	2324	2329	rVV4	15680	24005	1.63%	0.270%
15	15.322	2331	2335	2341	rVB4	11885	19082	1.30%	0.214%
16	15.542	2365	2371	2386	rVB	249116	367359	24.97%	4.125%
17	15.688	2391	2395	2407	rVB	12704	37037	2.52%	0.416%
18	16.109	2461	2464	2470	rVB8	8026	14840	1.01%	0.167%
19	16.469	2516	2523	2536	rVB	190103	345488	23.48%	3.879%

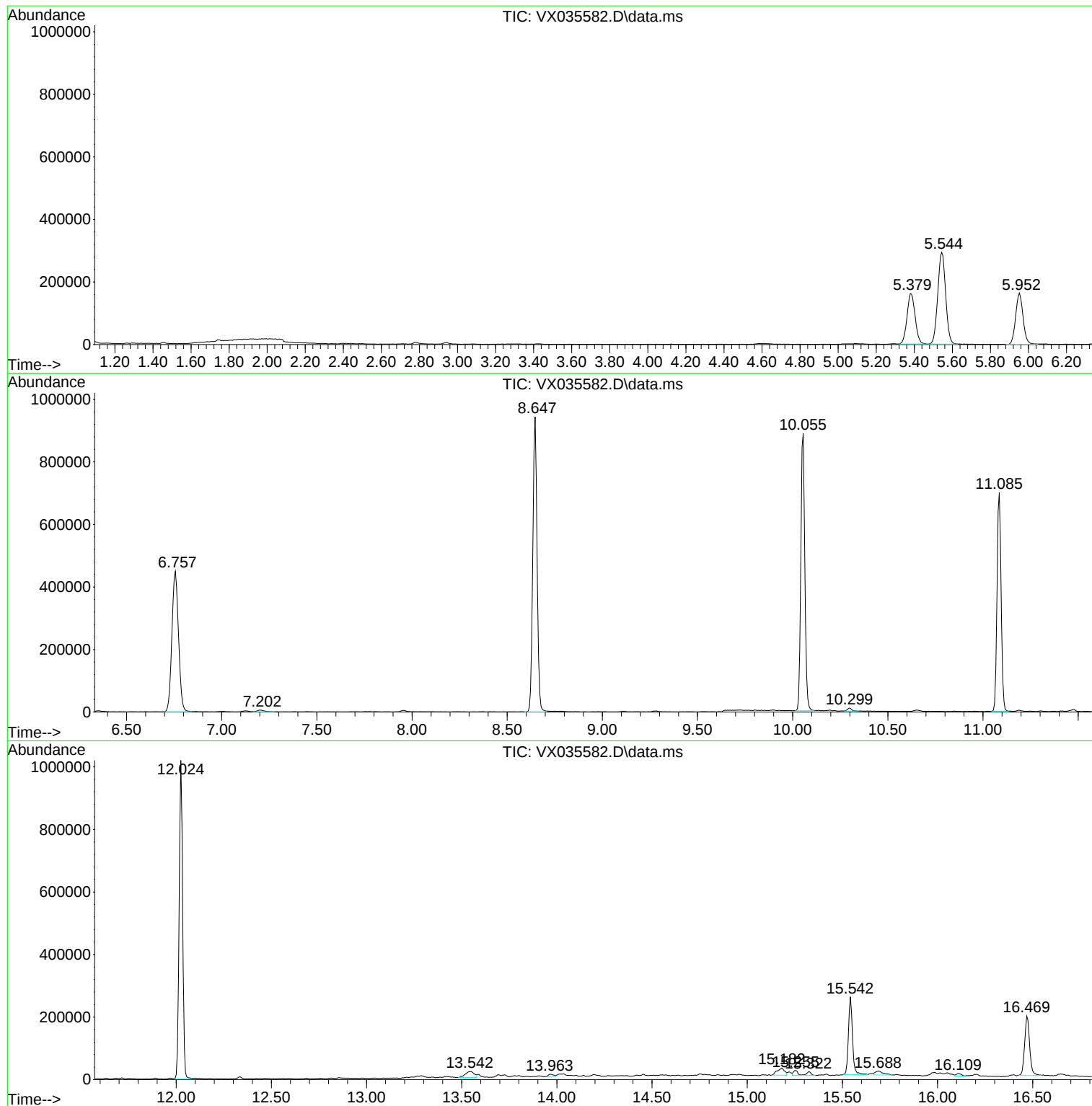
Sum of corrected areas: 8905491

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BU-02-050823

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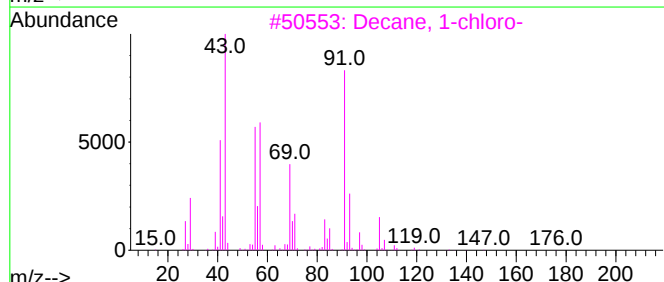
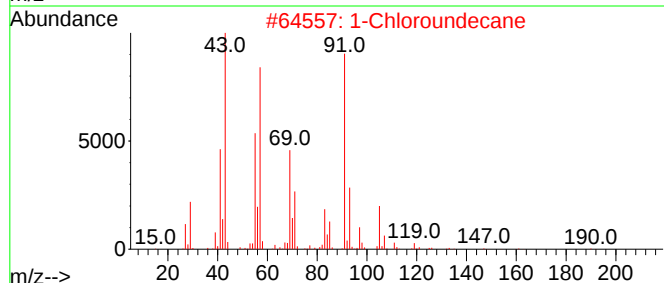
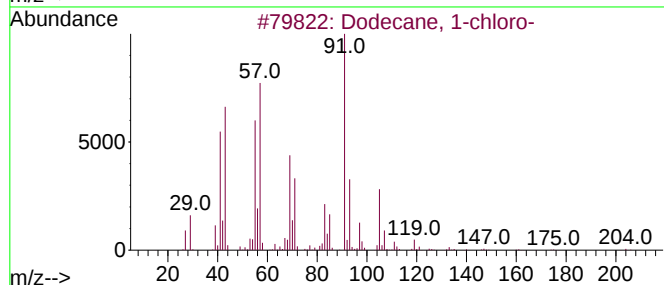
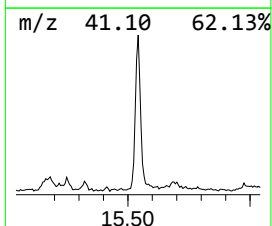
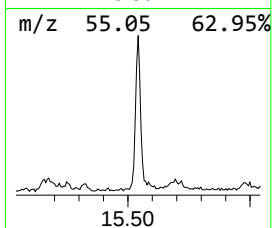
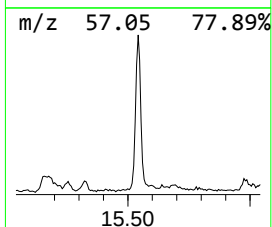
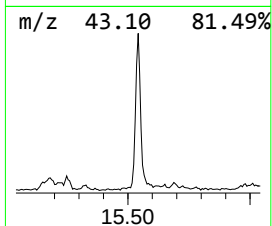
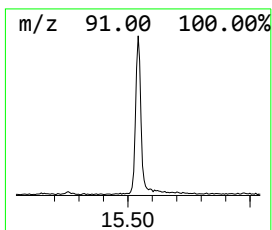
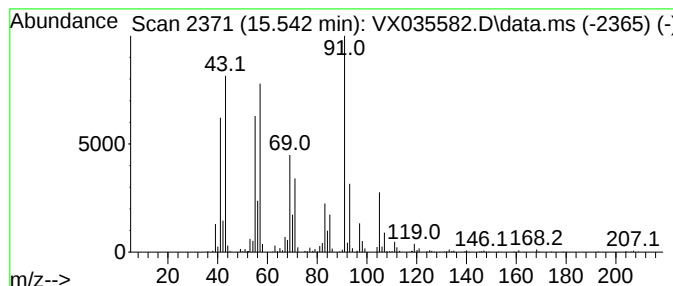
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	14.29 ug/l	367359	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	96
2			1-Chloroundecane	190	C11H23Cl	002473-03-2	86
3			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	86
4			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	53
5			Nonane, 1-chloro-	162	C9H19Cl	002473-01-0	52



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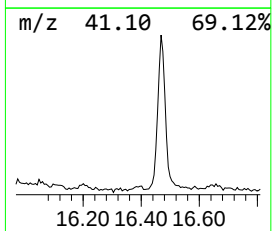
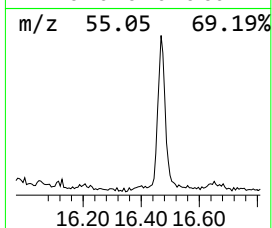
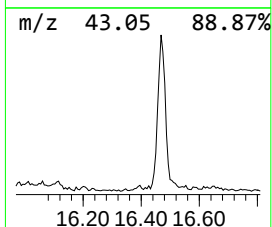
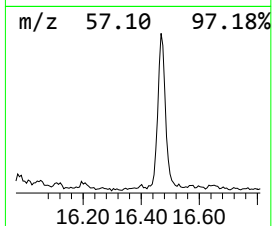
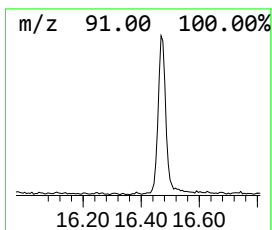
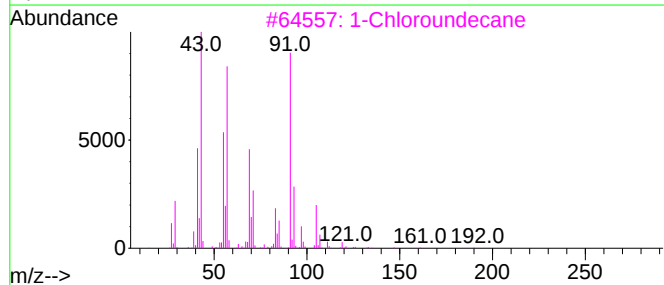
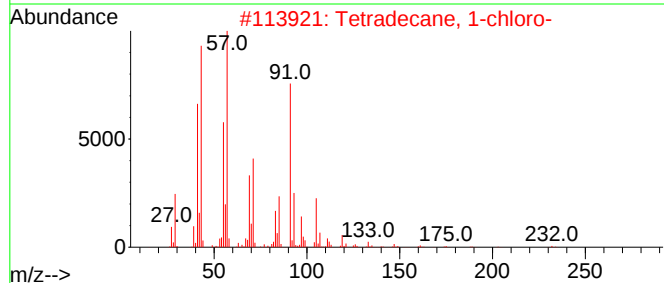
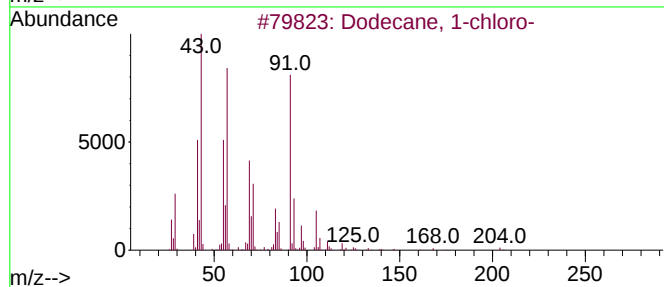
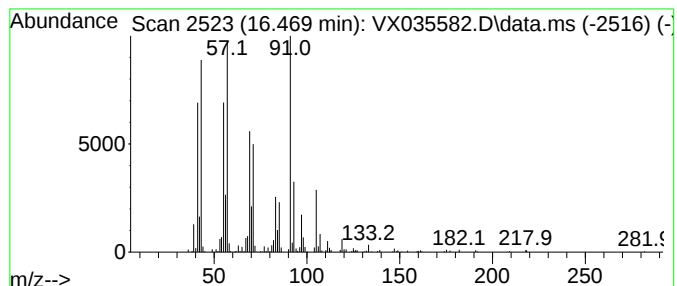
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Peak Number 2 Tetradecane, 1-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.468	13.44 ug/l	345488	1,4-Dichlorobenzene-d4	12.024

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	87
3			1-Chloroundecane	190	C11H23Cl	002473-03-2	80
4			Oxalic acid, allyl undecyl ester	284	C16H28O4	1000309-23-9	52
5			Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	52



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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
Dodecane, 1-chl...	15.542	14.3	ug/l	367359	4	12.024	1284930	50.0
Tetradecane, 1-...	16.468	13.4	ug/l	345488	4	12.024	1284930	50.0