

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041725\
Data File : VN086320.D
Acq On : 17 Apr 2025 14:29
Operator : JC\MD
Sample : Q1818-02
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3833

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_N\methods\82N041525W.M

Title : SW846 8260

Signal : TIC: VN086320.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.565	1454	1464	1468	rBV	701826	1290219	1.14%	0.694%
2	10.629	1468	1475	1488	rVB	2736815	5111255	4.50%	2.748%
3	11.959	1693	1701	1711	rBV	17320033	29623813	26.08%	15.929%
4	12.071	1711	1720	1739	rVB2	53923550	113602172	100.00%	61.085%
5	12.394	1766	1775	1785	rBV	19524341	32720386	28.80%	17.594%
6	14.759	2168	2177	2187	rVB	633412	1145702	1.01%	0.616%
7	14.953	2204	2210	2216	rBV	905147	1309456	1.15%	0.704%
8	15.823	2352	2358	2369	rVB	663484	1171263	1.03%	0.630%

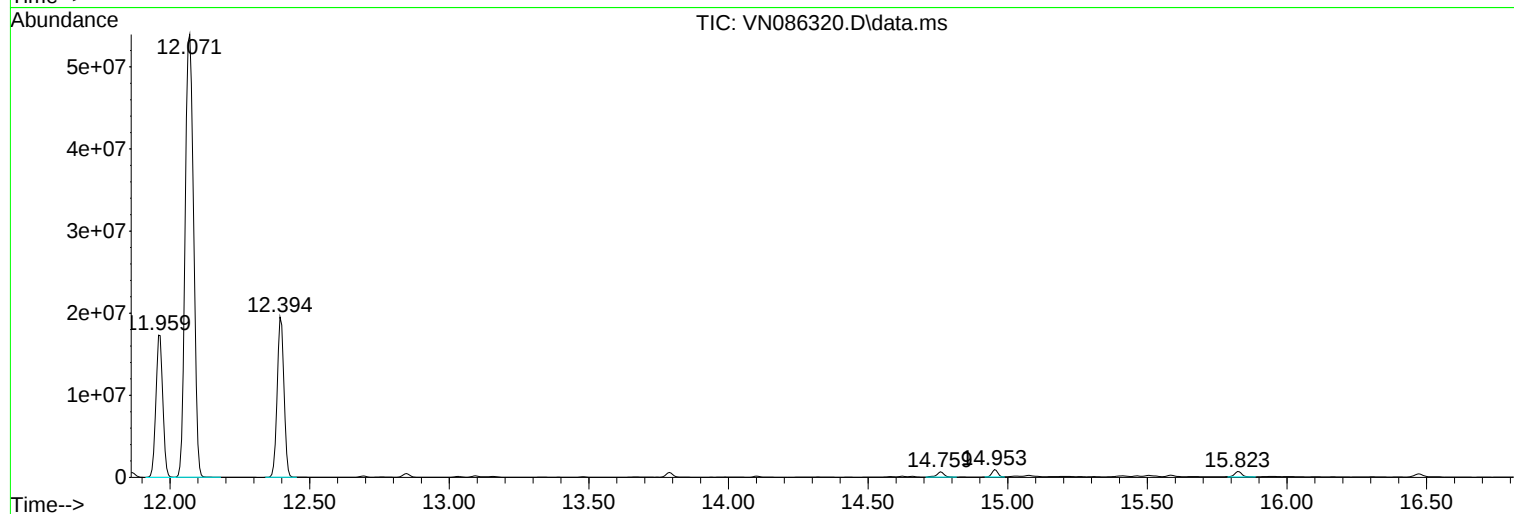
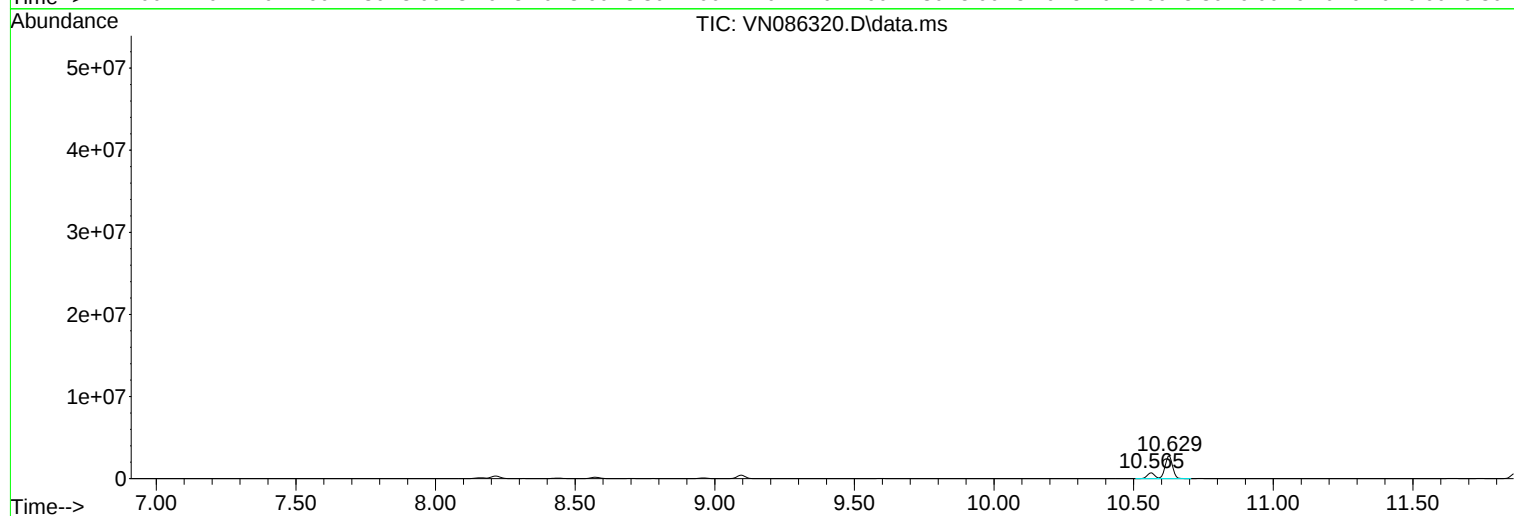
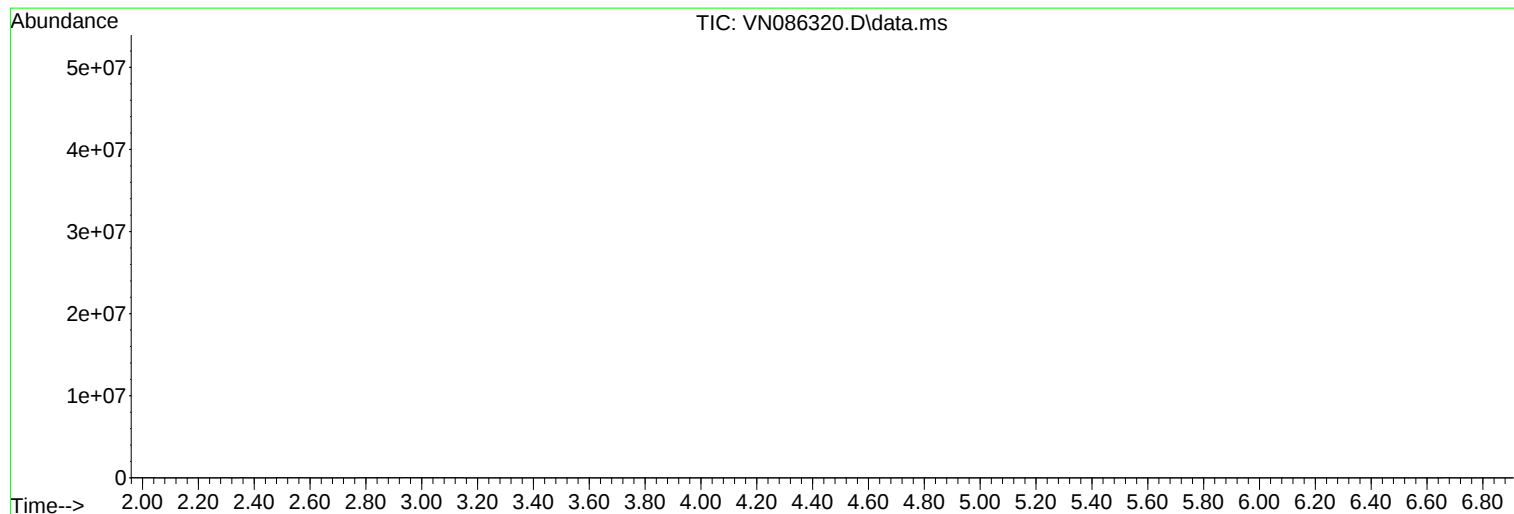
Sum of corrected areas: 185974266

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



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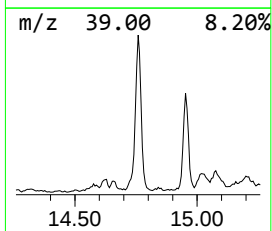
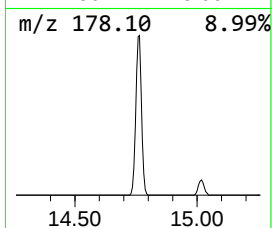
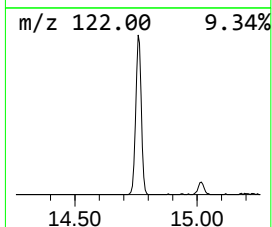
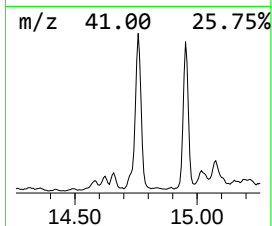
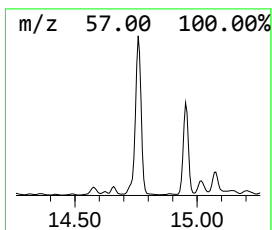
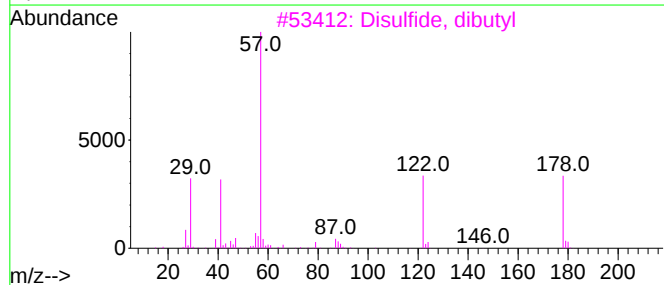
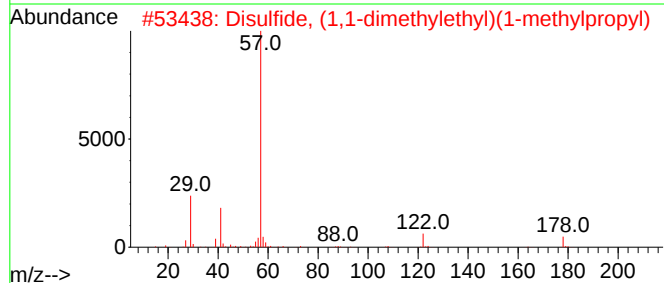
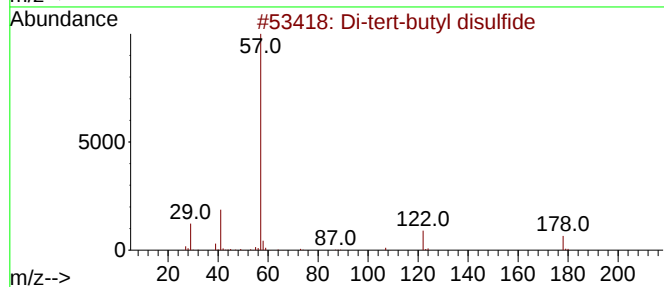
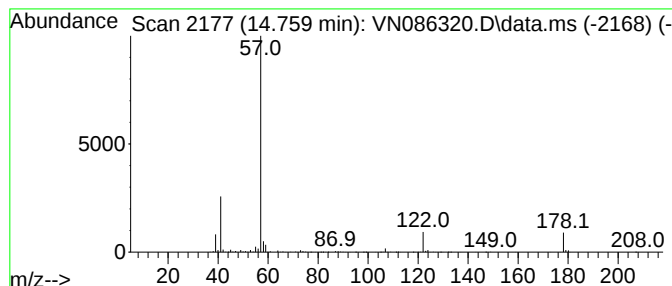
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 1 Di-tert-butyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.759	50.00 ug/l	1145700	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	91
2			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	72
3			Disulfide, dibutyl	178	C8H18S2	000629-45-8	64
4			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	56
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	35



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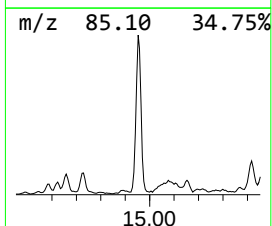
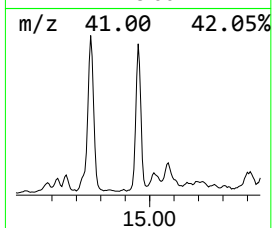
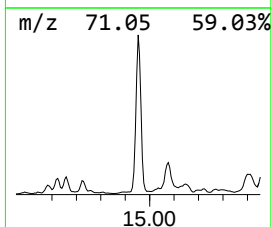
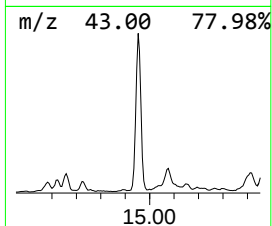
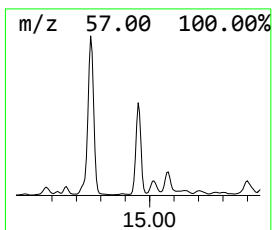
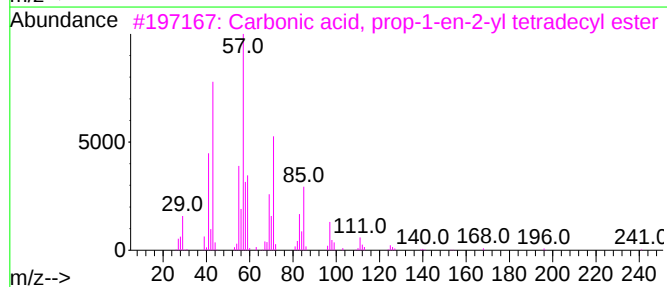
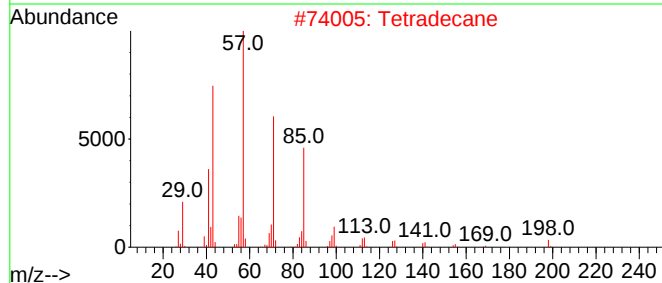
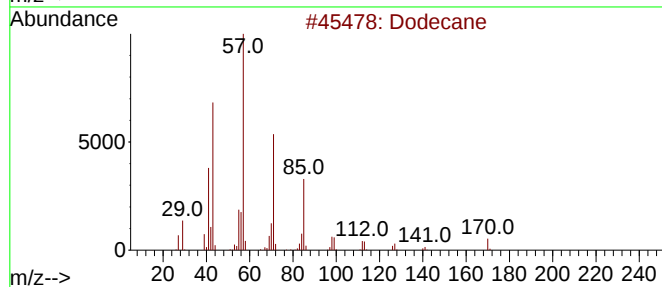
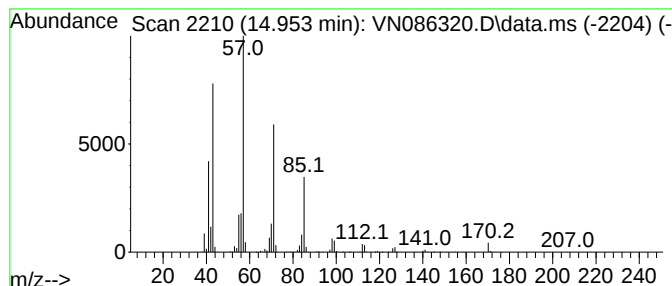
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Peak Number 2 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.953	57.15 ug/l	1309460	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Tetradecane	198	C14H30	000629-59-4	90
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
4			Pentadecane	212	C15H32	000629-62-9	86
5			Hexadecane	226	C16H34	000544-76-3	86



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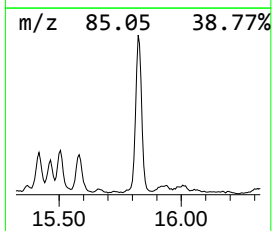
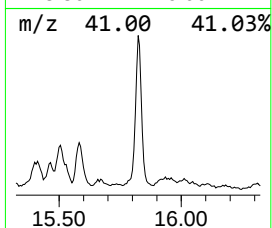
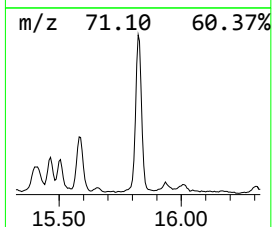
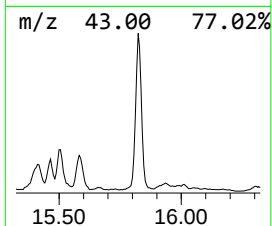
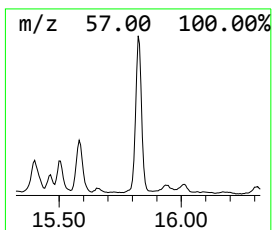
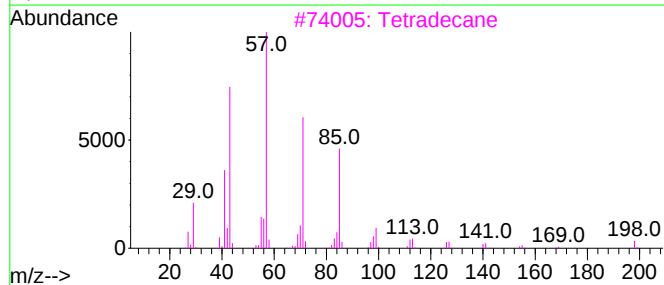
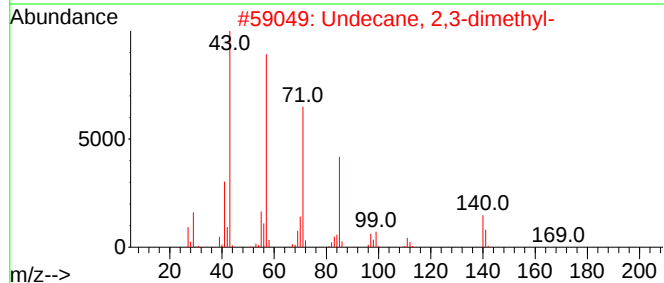
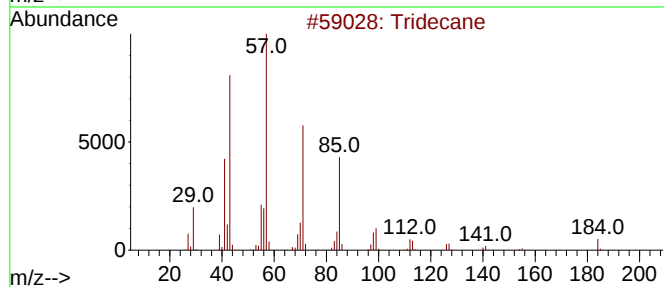
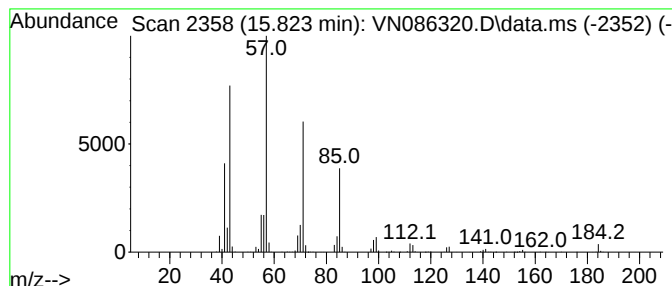
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Peak Number 3 Tridecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	51.12 ug/l	1171260	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Dodecane	170	C12H26	000112-40-3	90
5			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Di-tert-butyl d...	14.759	50.0	ug/l	1145700	4	13.788	1145700	50.0
Dodecane	14.953	57.1	ug/l	1309460	4	13.788	1145700	50.0
Tridecane	15.823	51.1	ug/l	1171260	4	13.788	1145700	50.0