

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051023\
 Data File : VX035586.D
 Acq On : 10 May 2023 15:14
 Operator : JC/MD
 Sample : 02658-05 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 507

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: VX035586.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.154	164	175	176	rBV3	6403	16061	1.08%	0.158%
2	2.294	194	198	208	rVB	12494	23034	1.54%	0.227%
3	5.385	692	705	721	rBV2	171444	504105	33.75%	4.960%
4	5.550	721	732	748	rVB	305598	863217	57.80%	8.494%
5	5.952	787	798	813	rBV2	167519	449819	30.12%	4.426%
6	6.757	921	930	945	rBV	461003	1102012	73.79%	10.843%
7	8.647	1231	1240	1259	rBV	959622	1493520	100.00%	14.695%
8	10.055	1465	1471	1482	rVB	914021	1296171	86.79%	12.754%
9	11.079	1633	1639	1649	rBV	842349	1048140	70.18%	10.313%
10	11.475	1697	1704	1708	rVB2	13470	17414	1.17%	0.171%
11	11.969	1780	1785	1788	rBV2	38707	47120	3.15%	0.464%
12	12.018	1788	1793	1801	rVV	1049319	1303932	87.31%	12.830%
13	12.103	1801	1807	1816	rVB	209576	277512	18.58%	2.731%
14	12.579	1878	1885	1894	rBV	34211	45261	3.03%	0.445%
15	12.817	1919	1924	1928	rBV	56173	70233	4.70%	0.691%
16	12.969	1945	1949	1957	rVB2	14357	21192	1.42%	0.209%
17	13.067	1962	1965	1967	rBV	14022	16836	1.13%	0.166%
18	13.097	1967	1970	1979	rVB	25508	38968	2.61%	0.383%
19	13.268	1994	1998	2004	rVB2	21316	27541	1.84%	0.271%
20	13.420	2019	2023	2031	rBV	55053	85691	5.74%	0.843%
21	13.512	2033	2038	2048	rBV3	50546	114091	7.64%	1.123%
22	13.707	2063	2070	2072	rBV	64018	91608	6.13%	0.901%
23	13.859	2089	2095	2097	rBV3	16360	24761	1.66%	0.244%
24	13.890	2097	2100	2107	rVB3	23799	37567	2.52%	0.370%
25	14.194	2146	2150	2163	rBV3	34812	73380	4.91%	0.722%
26	14.402	2180	2184	2188	rBV	43085	51023	3.42%	0.502%
27	14.451	2188	2192	2195	rBV4	12823	18351	1.23%	0.181%
28	14.615	2215	2219	2224	rVV6	14673	21933	1.47%	0.216%
29	14.670	2225	2228	2232	rVB3	13149	15752	1.05%	0.155%
30	15.042	2284	2289	2293	rBV6	10903	17513	1.17%	0.172%
31	15.182	2302	2312	2320	rVV9	34774	115036	7.70%	1.132%
32	15.249	2321	2323	2331	rVB4	24315	38548	2.58%	0.379%
33	15.322	2331	2335	2340	rVB4	14643	23963	1.60%	0.236%
34	15.377	2340	2344	2348	rBV5	12936	19627	1.31%	0.193%
35	15.542	2365	2371	2380	rBV	239404	354916	23.76%	3.492%
36	15.981	2436	2443	2446	rBV8	12858	26983	1.81%	0.265%

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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	16.468	2517	2523	2538	rVB	198376	354985	23.77%	3.493%
38	16.657	2549	2554	2560	rVB10	6787	15318	1.03%	0.151%

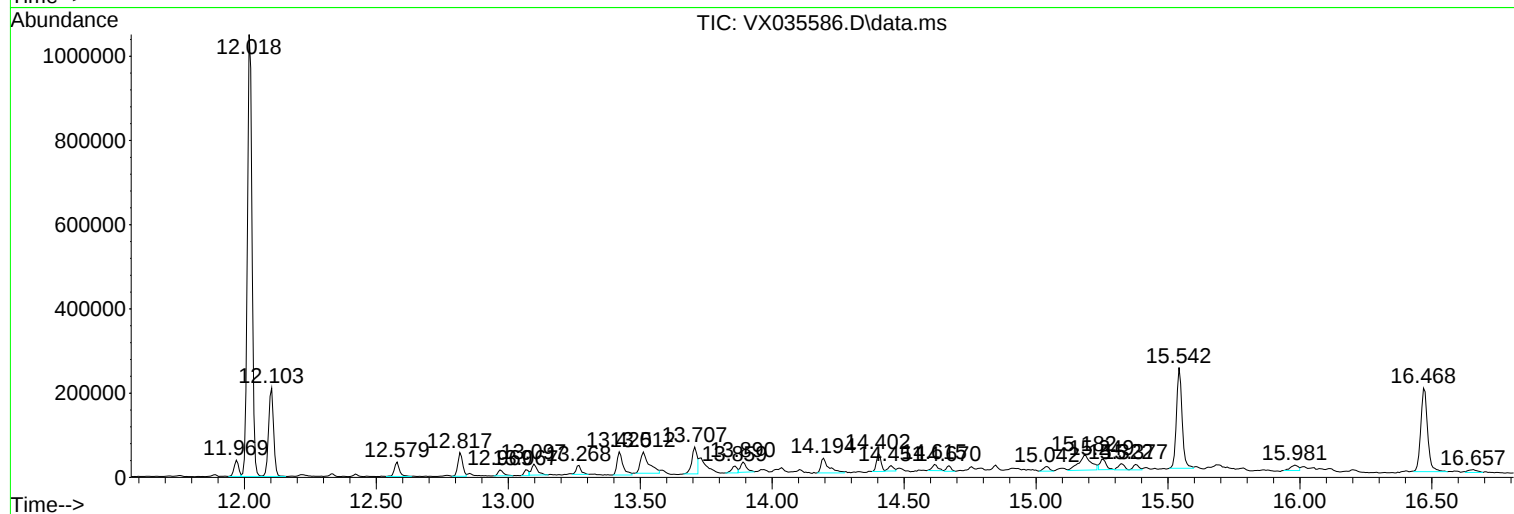
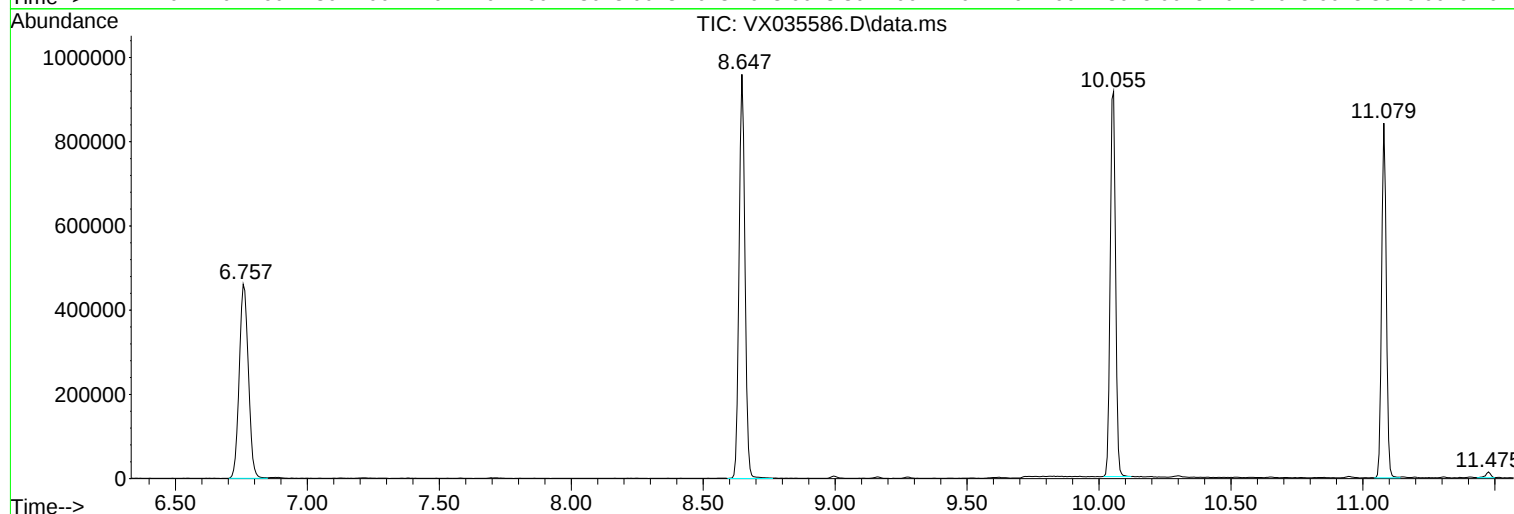
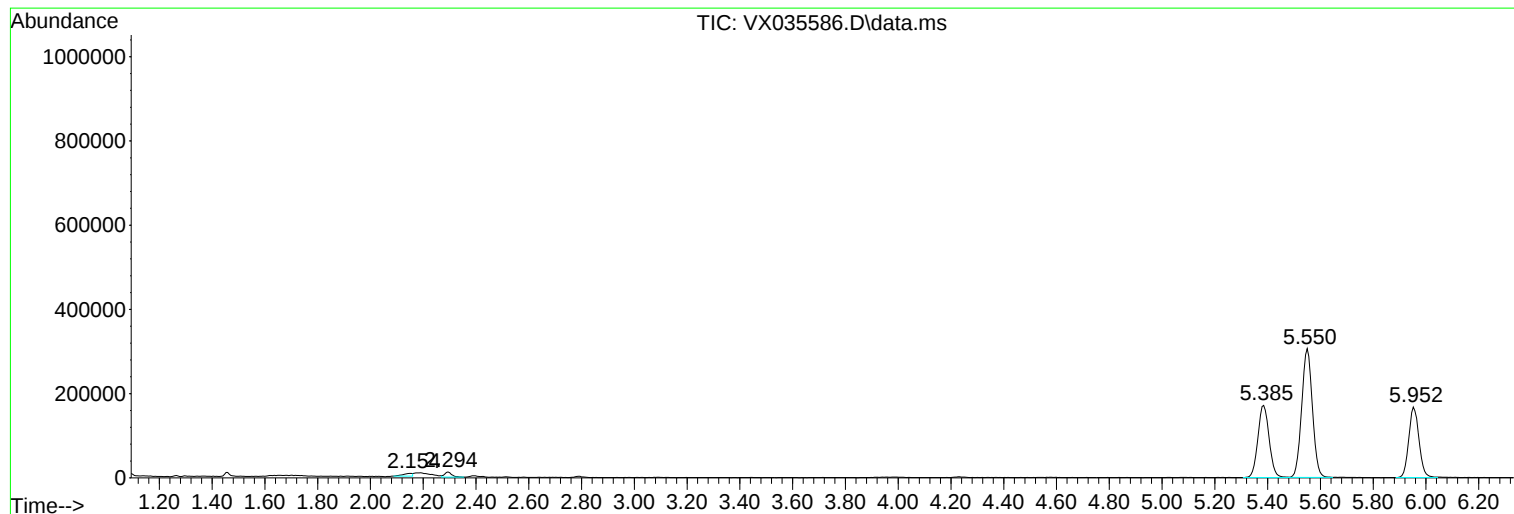
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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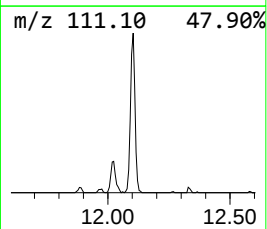
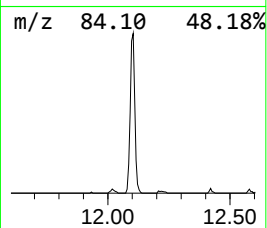
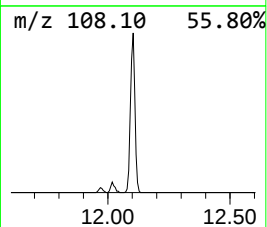
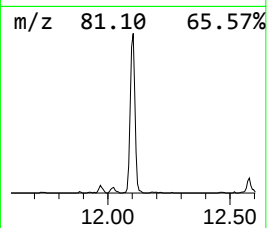
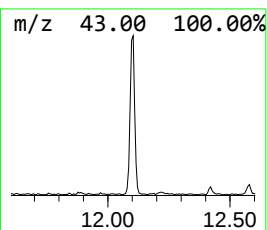
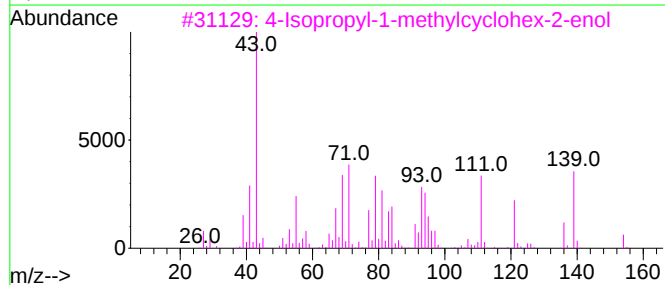
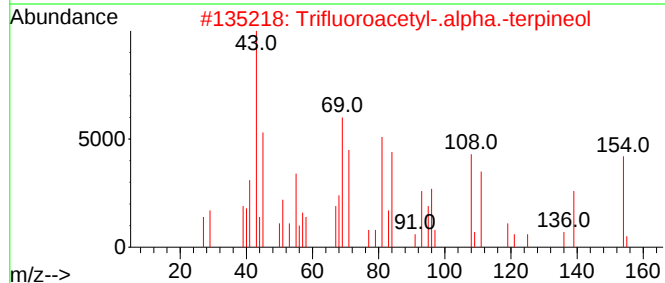
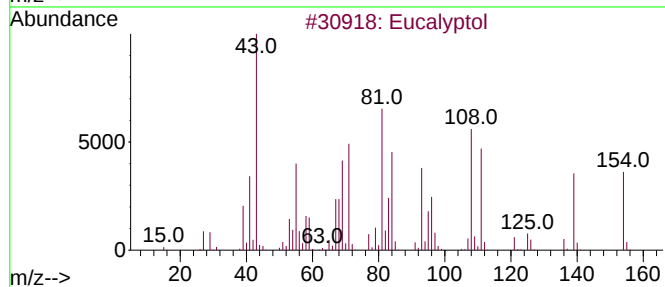
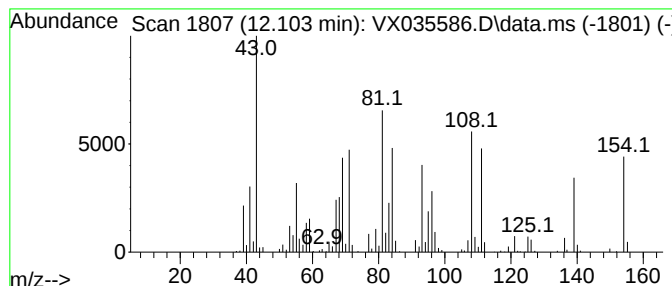
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	10.64 ug/l	277512	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	90
3			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	37
4			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5			2-Acetyl-cyclohexanone	154	C9H14O2	006126-53-0	22



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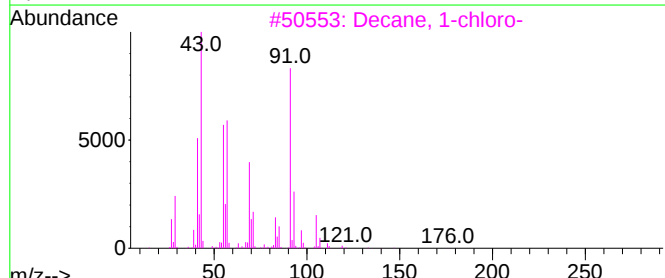
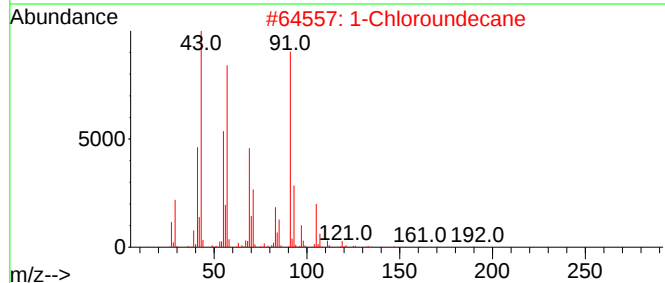
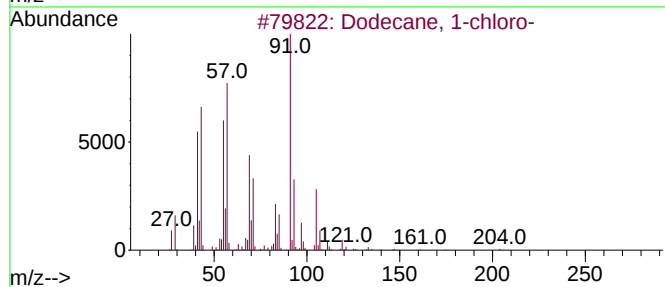
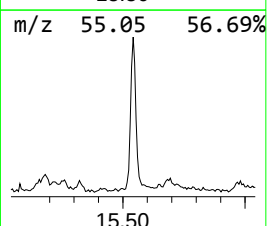
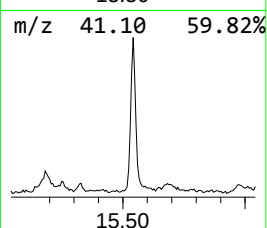
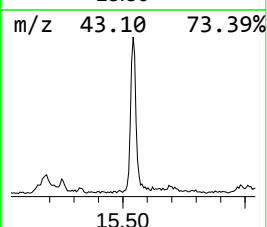
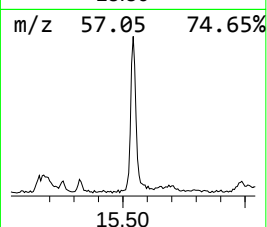
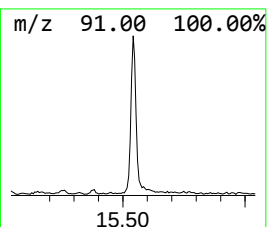
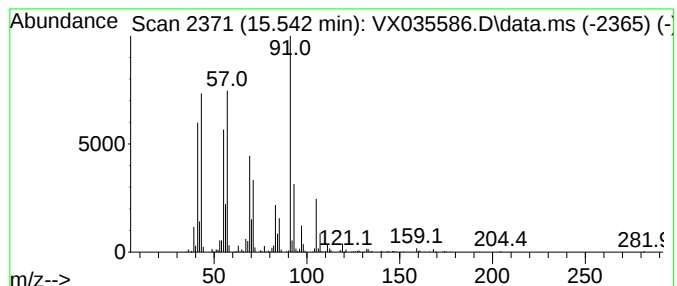
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.542	13.61 ug/l	354916	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			1-Chloroundecane	190	C11H23Cl	002473-03-2	91
3			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	87
4			n-Dodecylpyridinium chloride	283	C17H30ClN	000104-74-5	80
5			Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	58



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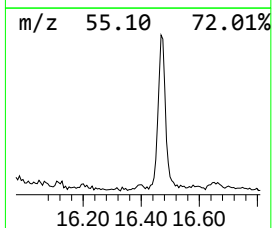
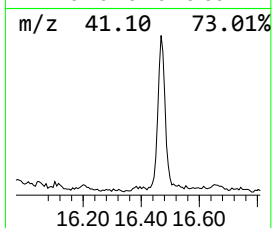
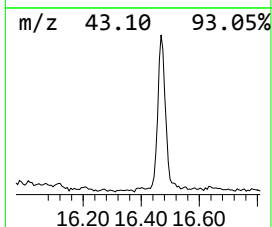
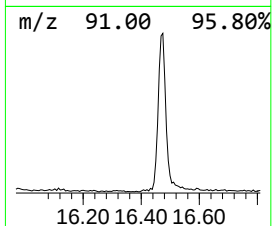
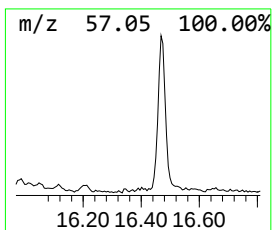
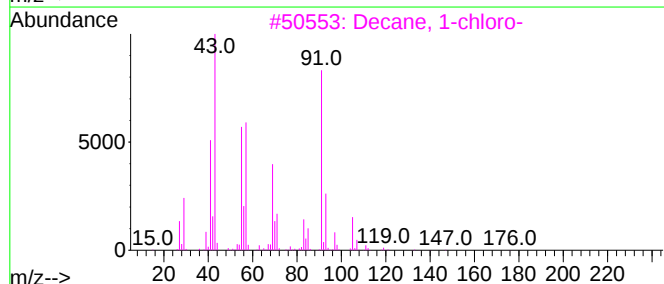
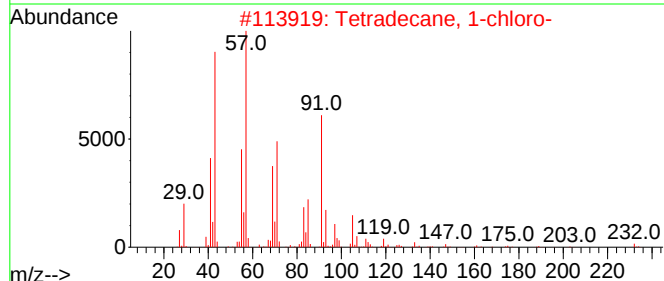
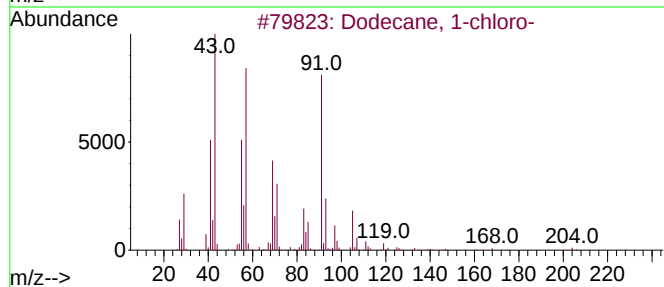
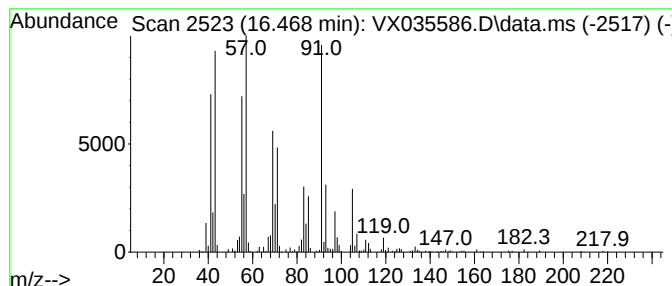
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 3 Tetradecane, 1-chloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.468	13.61 ug/l	354985	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	90
3			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	58
4			Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	52
5			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	49



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Eucalyptol	12.103	10.6	ug/l	277512	4	12.018	1303930	50.0
Dodecane, 1-chl...	15.542	13.6	ug/l	354916	4	12.018	1303930	50.0
Tetradecane, 1-...	16.468	13.6	ug/l	354985	4	12.018	1303930	50.0