

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091125\
 Data File : VN087804.D
 Acq On : 11 Sep 2025 17:30
 Operator : JC\MD
 Sample : Q3083-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW4S

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\82N082125W.M

Title : SW846 8260

Signal : TIC: VN087804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.147	27	33	39	rVB2	31468	53457	1.74%	0.293%
2	3.959	328	341	360	rBV	1145217	3065453	100.00%	16.783%
3	4.430	413	421	432	rVB4	22965	74586	2.43%	0.408%
4	6.659	787	800	815	rBV3	108173	342991	11.19%	1.878%
5	7.424	921	930	940	rBV2	29048	81439	2.66%	0.446%
6	7.829	987	999	1012	rBV	181150	487113	15.89%	2.667%
7	8.147	1043	1053	1058	rBV	306542	741519	24.19%	4.060%
8	8.206	1058	1063	1077	rVB	379171	890888	29.06%	4.878%
9	8.559	1114	1123	1131	rBV	337523	775307	25.29%	4.245%
10	8.641	1131	1137	1154	rVB2	103120	257100	8.39%	1.408%
11	9.082	1199	1212	1223	rBV	734164	1501971	49.00%	8.223%
12	9.576	1289	1296	1304	rVB3	24955	55238	1.80%	0.302%
13	10.547	1452	1461	1469	rBV	1173280	2149972	70.14%	11.771%
14	10.647	1473	1478	1486	rVB2	42579	86883	2.83%	0.476%
15	11.847	1671	1682	1695	rBV2	1062472	2496831	81.45%	13.670%
16	12.723	1826	1831	1836	rVB2	34214	51153	1.67%	0.280%
17	12.829	1836	1849	1858	rBV	817849	1501997	49.00%	8.223%
18	12.912	1858	1863	1869	rVB6	26517	54999	1.79%	0.301%
19	13.400	1940	1946	1953	rBV5	34719	72194	2.36%	0.395%
20	13.600	1970	1980	1981	rBV5	21093	45335	1.48%	0.248%
21	13.717	1994	2000	2003	rBV2	295145	476923	15.56%	2.611%
22	13.770	2003	2009	2021	rVB	1095616	2023264	66.00%	11.077%
23	13.970	2039	2043	2047	rVB4	21294	35525	1.16%	0.194%
24	14.088	2059	2063	2069	rVB7	26955	50027	1.63%	0.274%
25	14.306	2096	2100	2107	rVB3	36132	58209	1.90%	0.319%
26	14.417	2114	2119	2125	rVB3	22620	41482	1.35%	0.227%
27	14.500	2127	2133	2136	rVV3	27954	51227	1.67%	0.280%
28	14.547	2136	2141	2147	rVV2	120593	219846	7.17%	1.204%
29	14.629	2149	2155	2161	rVV	76950	142183	4.64%	0.778%
30	14.688	2161	2165	2173	rVB6	23731	48077	1.57%	0.263%
31	14.911	2196	2203	2208	rBV7	22051	46605	1.52%	0.255%
32	15.011	2214	2220	2226	rBV5	29074	70449	2.30%	0.386%
33	15.253	2255	2261	2262	rBV3	32444	46449	1.52%	0.254%
34	15.964	2376	2382	2393	rVB4	25228	52797	1.72%	0.289%
35	16.223	2416	2426	2433	rBV2	49215	115639	3.77%	0.633%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Title : SW846 8260

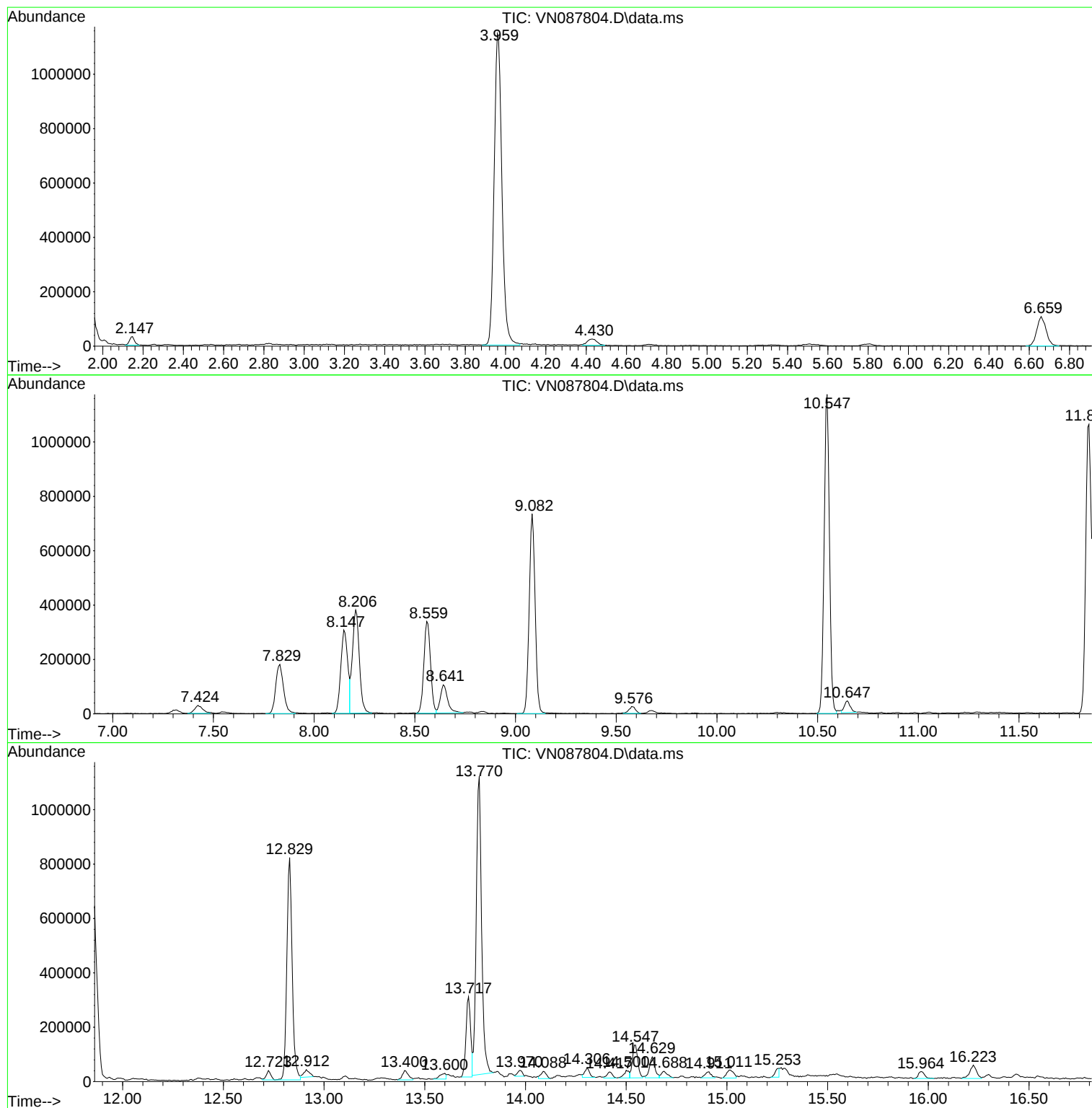
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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



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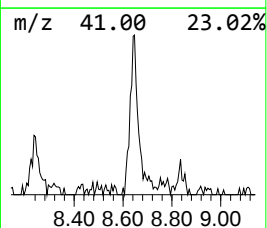
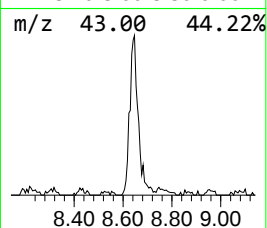
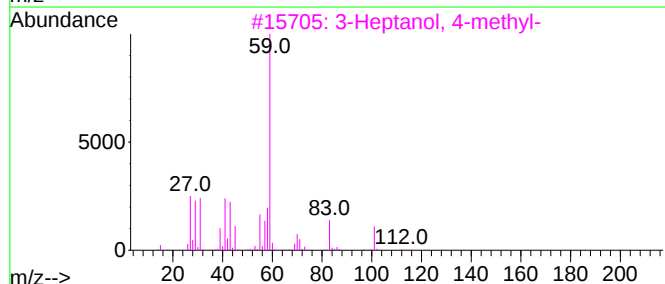
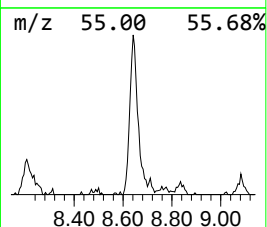
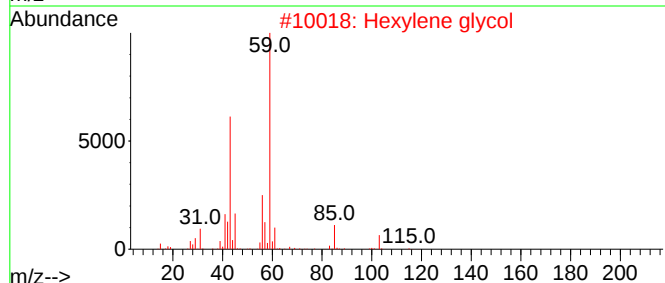
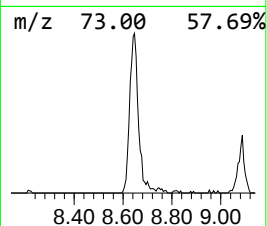
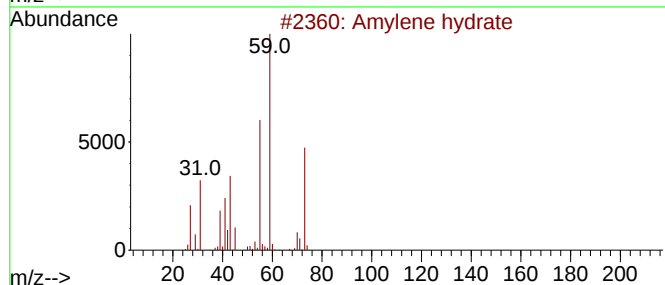
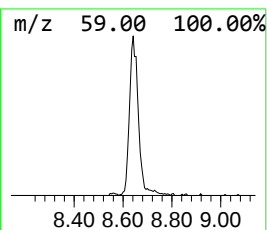
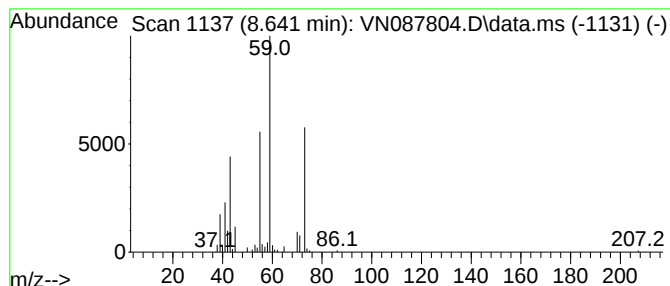
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.641	14.43 ug/l	257100	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			Hexylene glycol	118	C6H14O2	000107-41-5	42
3			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	40
4			1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	013588-28-8	39
5			2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	38



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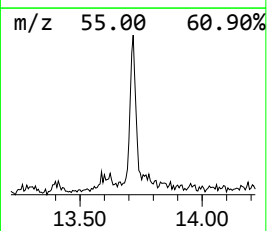
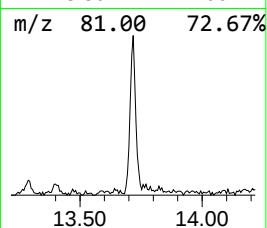
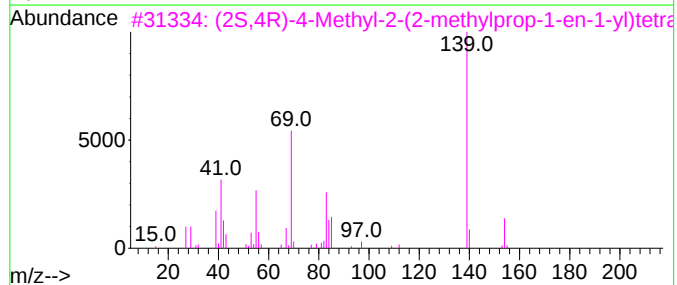
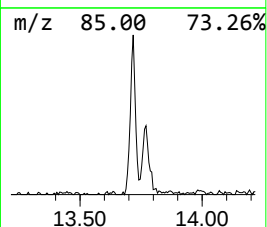
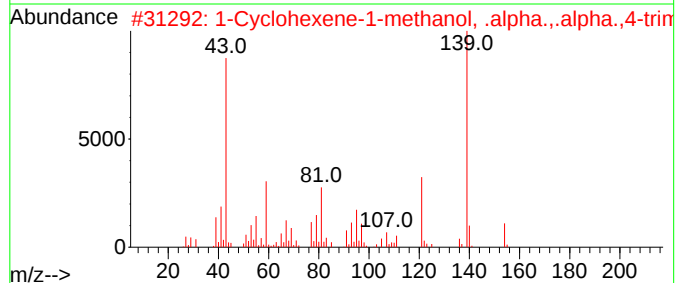
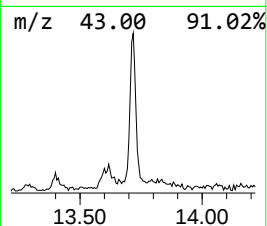
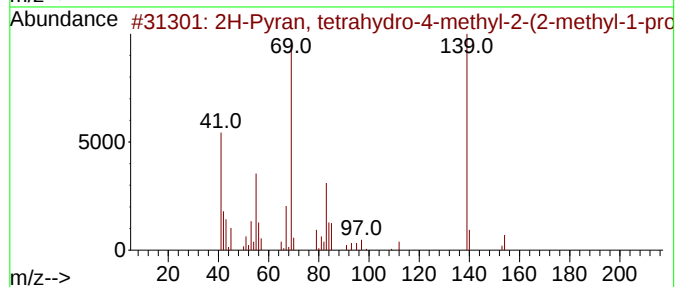
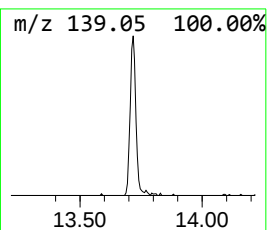
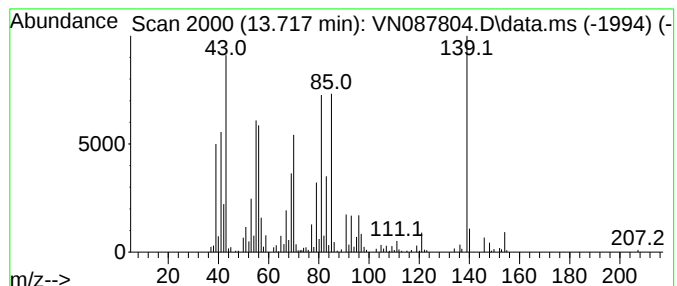
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.717 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.717	11.79 ug/l	476923	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyran, tetrahydro-4-methyl-2-...	154	C10H18O	016409-43-1	43
2			1-Cyclohexene-1-methanol, .alpha...	154	C10H18O	018479-65-7	25
3			(2S,4R)-4-Methyl-2-(2-methylprop...	154	C10H18O	003033-23-6	22
4			2-Octyn-1-ol, 7-[(tetrahydro-2H-...	226	C13H22O3	077758-37-3	22
5			Methyl 5-[(4-fluorophenoxy)methy...	250	C13H11FO4	402739-03-1	22



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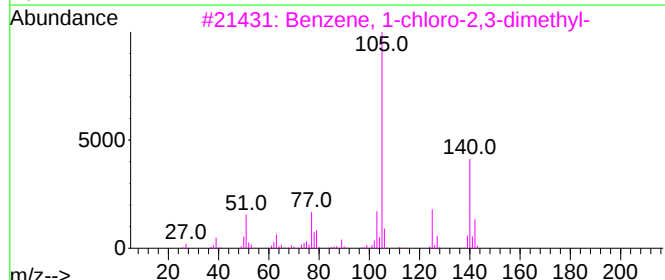
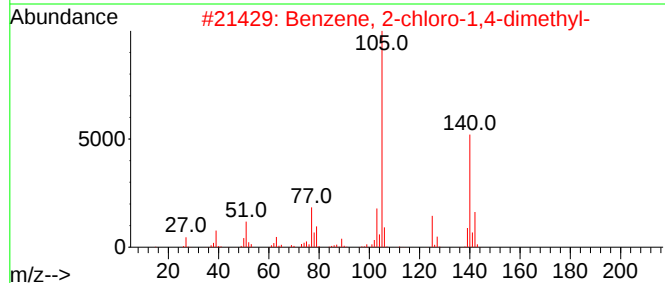
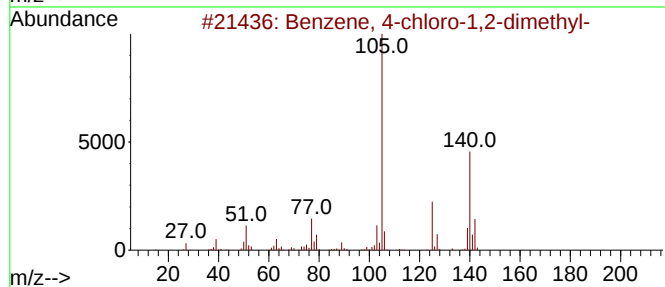
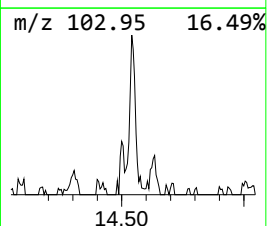
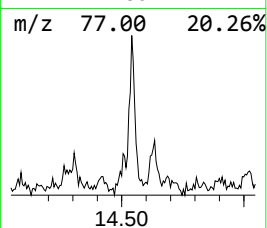
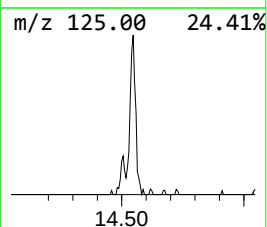
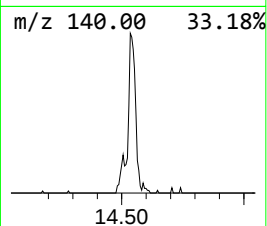
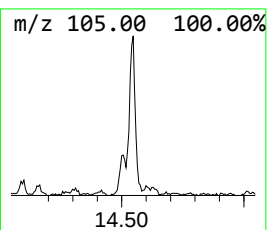
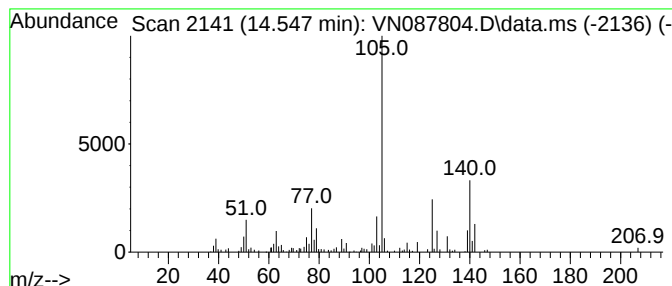
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 4-chloro-1,2-dimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.547	5.43 ug/l	219846	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-chloro-1,2-dimethyl-	140	C8H9Cl	000615-60-1	91
2			Benzene, 2-chloro-1,4-dimethyl-	140	C8H9Cl	000095-72-7	83
3			Benzene, 1-chloro-2,3-dimethyl-	140	C8H9Cl	000608-23-1	80
4			m-Xylene, 5-chloro-	140	C8H9Cl	000556-97-8	76
5			Benzene, 1-(chloromethyl)-3-methyl-	140	C8H9Cl	000620-19-9	74



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	8.641	14.4	ug/l	257100	1	8.206	890888	50.0
unknown13.717	13.717	11.8	ug/l	476923	4	13.770	2023260	50.0
Benzene, 4-chlo...	14.547	5.4	ug/l	219846	4	13.770	2023260	50.0