

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091525\
 Data File : VN087825.D
 Acq On : 15 Sep 2025 10:50
 Operator : JC\MD
 Sample : Q3083-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 8 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: VN087825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.142	27	32	40	rVB	29340	50352	1.77%	0.355%
2	3.959	331	341	362	rBV	1077214	2843353	100.00%	20.057%
3	4.430	411	421	431	rVB4	27980	96640	3.40%	0.682%
4	6.659	788	800	815	rBV3	96388	307629	10.82%	2.170%
5	7.306	901	910	921	rBV4	14090	41257	1.45%	0.291%
6	7.424	921	930	939	rBV2	28334	80419	2.83%	0.567%
7	7.830	987	999	1012	rBV	176024	469101	16.50%	3.309%
8	8.147	1043	1053	1058	rBV	209729	513870	18.07%	3.625%
9	8.206	1058	1063	1076	rVB	278639	642571	22.60%	4.533%
10	8.559	1115	1123	1131	rBV	229090	521154	18.33%	3.676%
11	8.641	1131	1137	1153	rVB	99250	254424	8.95%	1.795%
12	9.083	1203	1212	1224	rBV	490617	1018786	35.83%	7.186%
13	9.582	1289	1297	1304	rVB4	28905	62553	2.20%	0.441%
14	9.677	1304	1313	1321	rVB6	11332	31587	1.11%	0.223%
15	10.547	1450	1461	1469	rBV	771898	1439622	50.63%	10.155%
16	10.647	1472	1478	1487	rVB3	37419	84885	2.99%	0.599%
17	11.847	1674	1682	1693	rBV2	702453	1783431	62.72%	12.580%
18	12.723	1826	1831	1838	rVB4	29764	47160	1.66%	0.333%
19	12.829	1838	1849	1859	rBV	506617	990740	34.84%	6.989%
20	12.912	1859	1863	1870	rVB8	20245	44137	1.55%	0.311%
21	13.406	1940	1947	1952	rBV5	32245	64264	2.26%	0.453%
22	13.594	1969	1979	1987	rBV10	20341	70792	2.49%	0.499%
23	13.718	1993	2000	2004	rBV	261407	450531	15.85%	3.178%
24	13.770	2004	2009	2021	rVV	704420	1385313	48.72%	9.772%
25	14.088	2059	2063	2070	rVB7	25090	46812	1.65%	0.330%
26	14.306	2097	2100	2108	rVB2	29255	52085	1.83%	0.367%
27	14.417	2114	2119	2125	rVB4	20008	41712	1.47%	0.294%
28	14.506	2125	2134	2136	rBV7	26071	53840	1.89%	0.380%
29	14.541	2136	2140	2148	rVV3	100529	191752	6.74%	1.353%
30	14.629	2149	2155	2160	rVV	62966	117961	4.15%	0.832%
31	14.688	2161	2165	2173	rVB6	18573	40605	1.43%	0.286%
32	14.900	2195	2201	2213	rVB6	21783	56937	2.00%	0.402%
33	15.017	2213	2221	2226	rVB6	28407	76494	2.69%	0.540%
34	15.259	2253	2262	2264	rBV7	29447	59962	2.11%	0.423%
35	15.970	2376	2383	2396	rVB2	23828	60070	2.11%	0.424%
36	16.229	2418	2427	2435	rVB2	37498	83884	2.95%	0.592%

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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

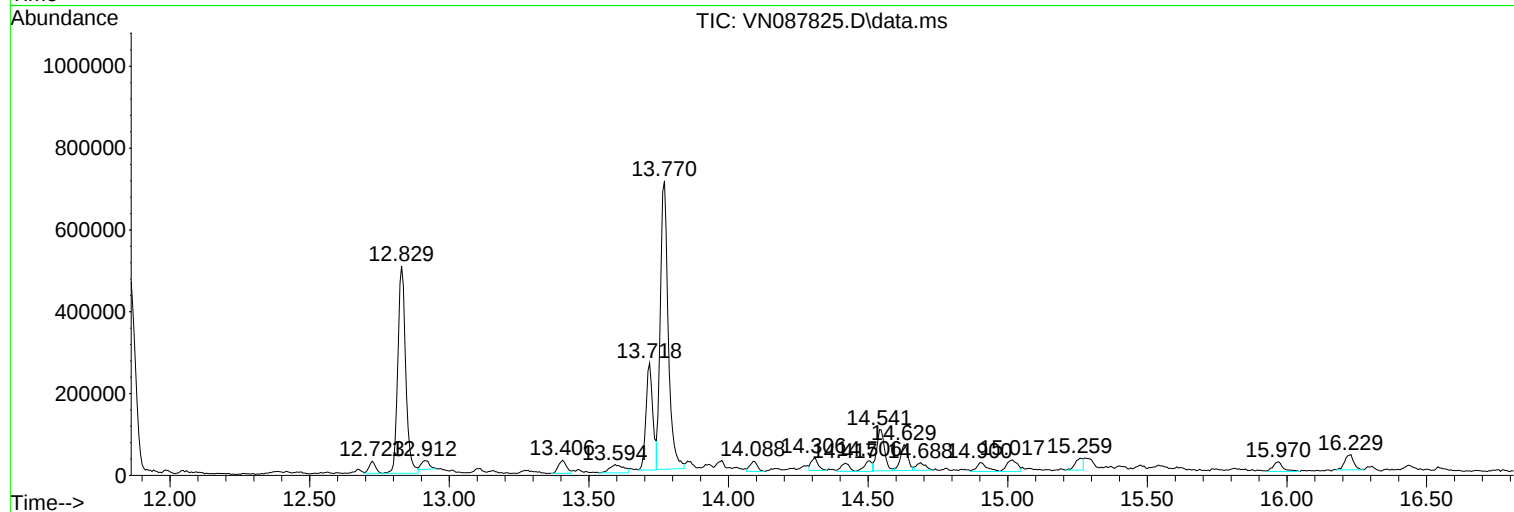
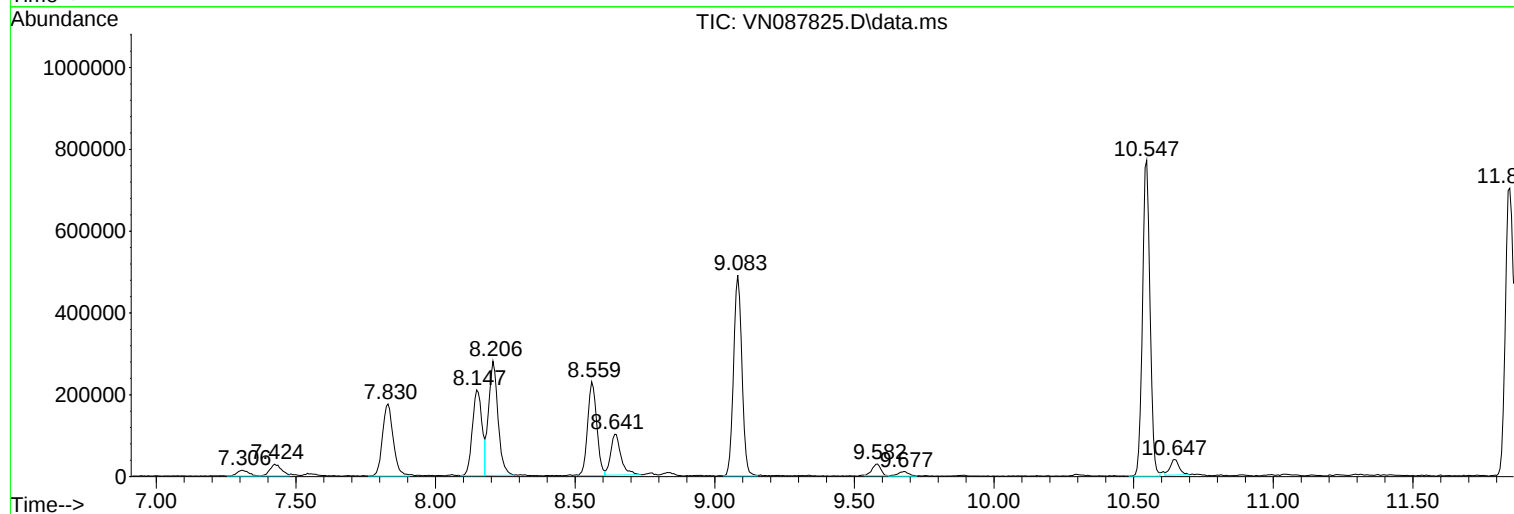
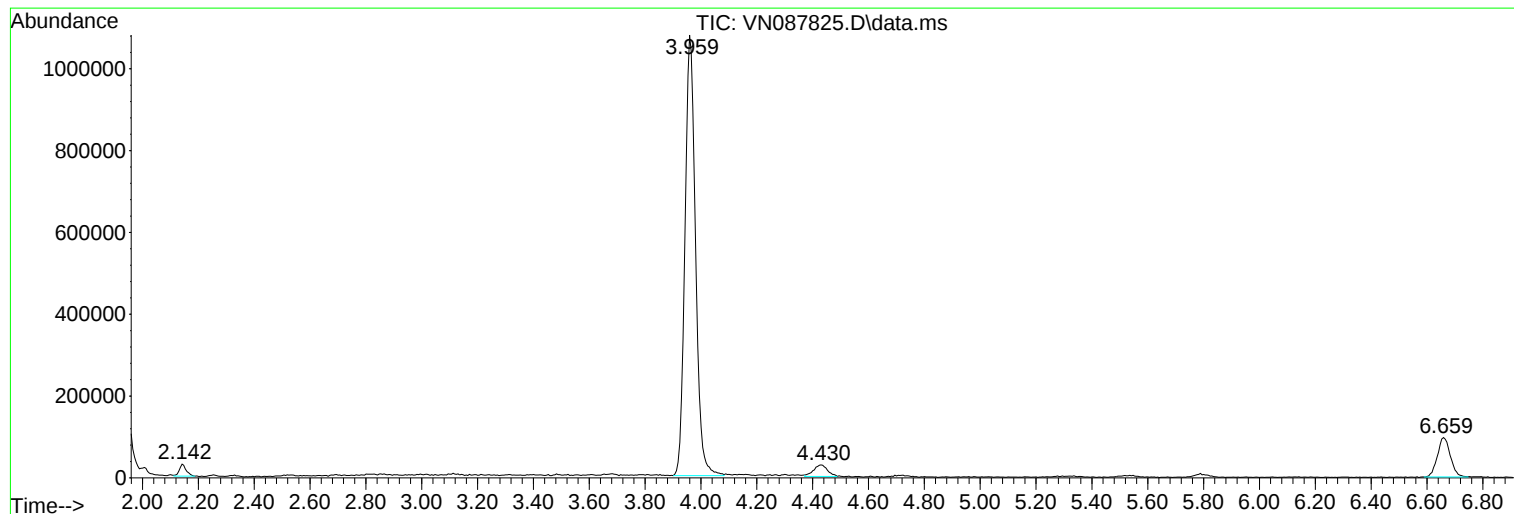
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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



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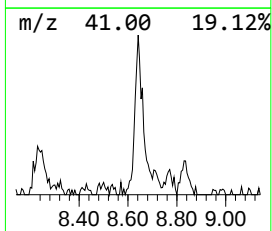
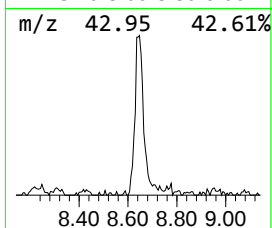
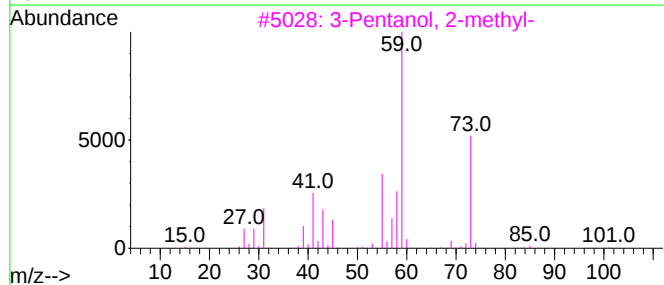
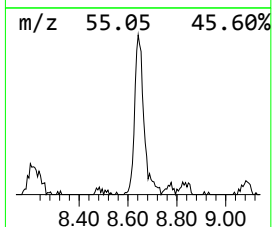
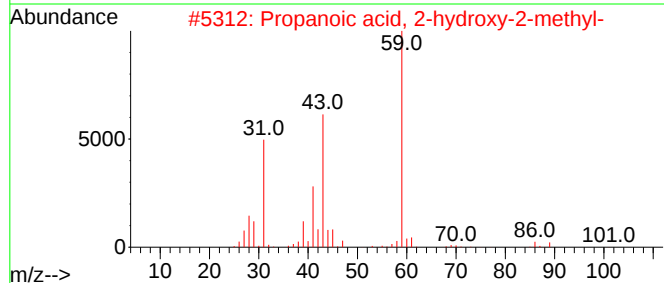
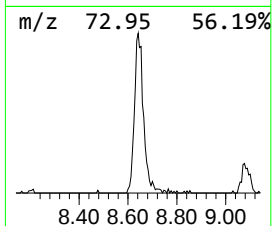
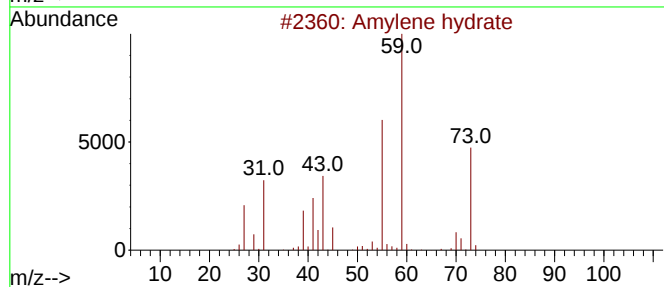
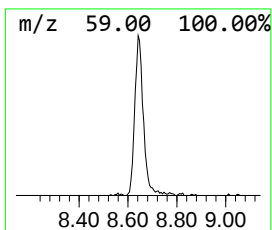
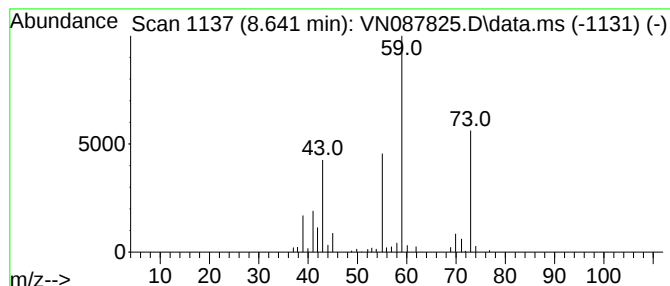
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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

Peak Number 2 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.641	19.80 ug/l	254424	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	74
2			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	42
3			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
4			Butanamide	87	C4H9NO	000541-35-5	38
5			HEX-5-EN-3-OL	100	C6H12O	000688-99-3	38



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Instrument :
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ClientSampleId :
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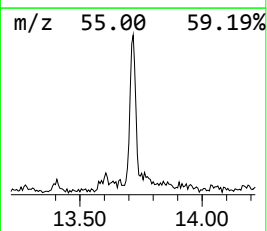
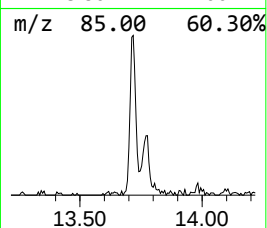
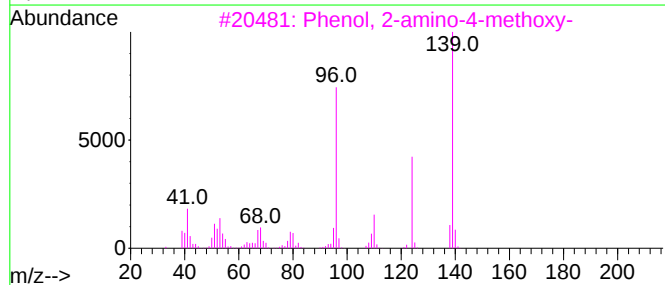
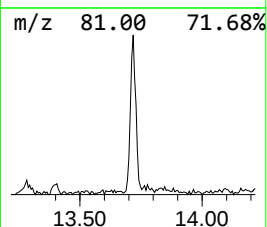
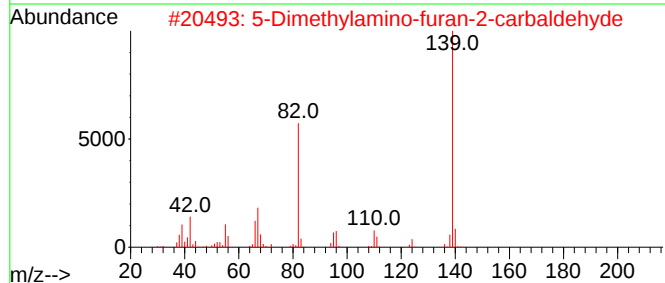
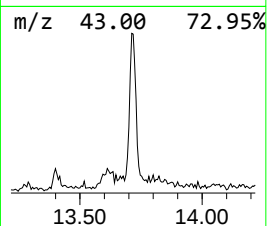
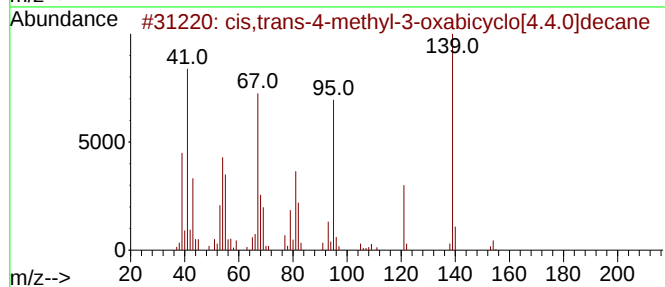
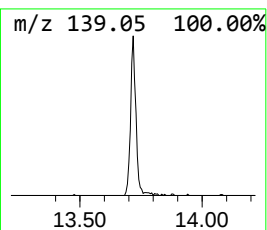
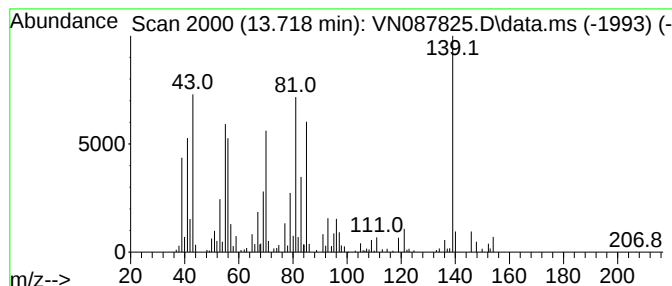
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Peak Number 3 unknown13.717 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.717	16.26 ug/l	450531	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,trans-4-methyl-3-oxabicyclo[...]	154	C10H18O	1000216-89-8	25
2			5-Dimethylamino-furan-2-carbalde...	139	C7H9NO2	1000317-69-8	25
3			Phenol, 2-amino-4-methoxy-	139	C7H9NO2	1000317-14-7	25
4			2-Amino-4-hydroxy-3,6-dimethylpy...	139	C6H9N3O	033796-41-7	22
5			1-Hexanol, 6-[(tetrahydro-2H-pyr...	202	C11H22O3	028659-22-5	18



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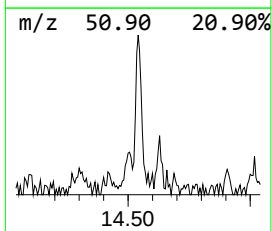
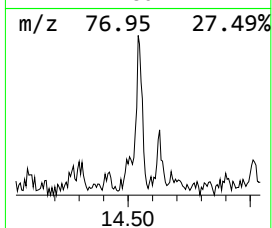
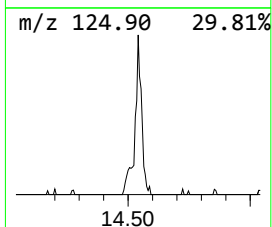
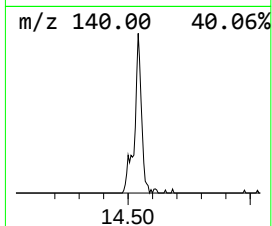
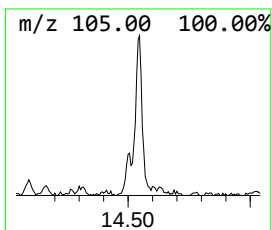
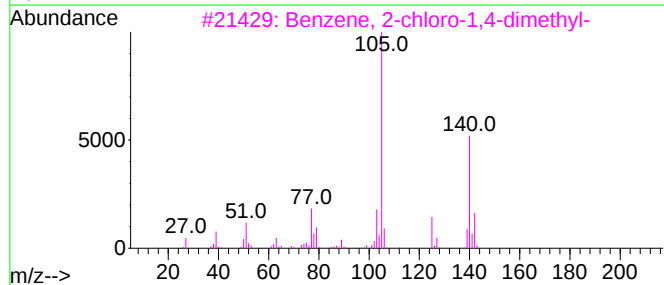
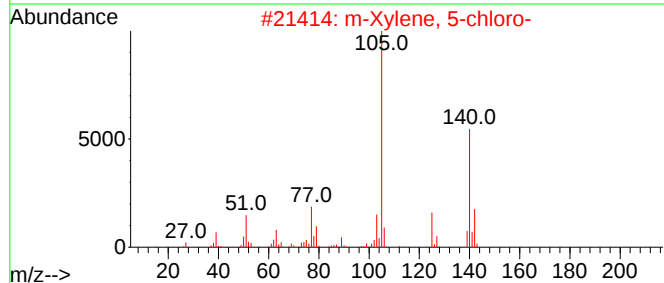
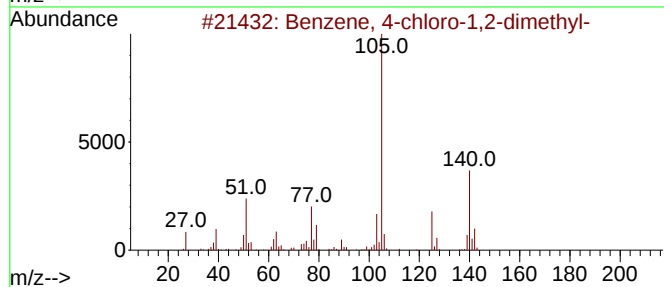
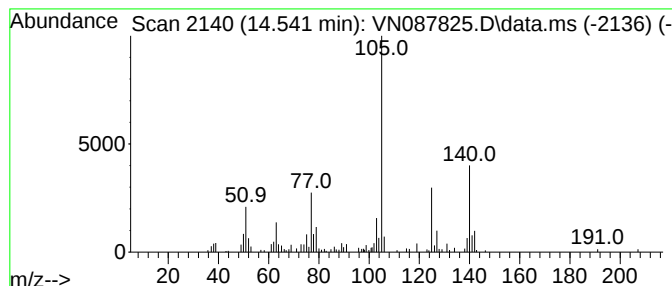
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.541	6.92 ug/l	191752	1,4-Dichlorobenzene-d4	13.771

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-chloro-1,2-dimethyl-	140	C8H9Cl	000615-60-1	94
2			m-Xylene, 5-chloro-	140	C8H9Cl	000556-97-8	93
3			Benzene, 2-chloro-1,4-dimethyl-	140	C8H9Cl	000095-72-7	91
4			Benzene, 1-(chloromethyl)-3-methyl-	140	C8H9Cl	000620-19-9	81
5			Benzene, 1-chloro-2,3-dimethyl-	140	C8H9Cl	000608-23-1	76



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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	19.8	ug/l	254424	1	8.206	642571	50.0
unknown13.717	13.717	16.3	ug/l	450531	4	13.771	1385310	50.0
Benzene, 4-chlo...	14.541	6.9	ug/l	191752	4	13.771	1385310	50.0