

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062822\
 Data File : VN073226.D
 Acq On : 29 Jun 2022 03:06
 Operator : JC\MD
 Sample : N3409-09 20X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-4

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\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073226.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	190	196	204	rBV3	11416	25221	1.24%	0.135%
2	5.222	555	567	570	rBV3	8307	20781	1.02%	0.112%
3	7.057	872	879	890	rVB3	9906	28492	1.40%	0.153%
4	7.239	900	910	925	rBV	23451	68662	3.38%	0.369%
5	7.951	1020	1031	1036	rBV	231043	557563	27.44%	2.994%
6	8.016	1036	1042	1053	rVB	433163	979710	48.21%	5.262%
7	8.369	1092	1102	1115	rBV	241189	561046	27.61%	3.013%
8	8.898	1183	1192	1207	rBV	608022	1274213	62.70%	6.843%
9	9.386	1271	1275	1283	rVB4	10443	21625	1.06%	0.116%
10	10.374	1434	1443	1450	rBV	834595	1539176	75.74%	8.266%
11	10.439	1450	1454	1462	rVB	56248	98368	4.84%	0.528%
12	11.680	1656	1665	1676	rBV	928281	1601723	78.82%	8.602%
13	11.780	1676	1682	1692	rVV	549917	914009	44.98%	4.909%
14	11.892	1692	1701	1713	rVB	995752	1952626	96.08%	10.487%
15	12.216	1749	1756	1766	rVB	282852	476068	23.43%	2.557%
16	12.515	1797	1807	1815	rBV	67272	114488	5.63%	0.615%
17	12.668	1826	1833	1842	rBV	767912	1292245	63.59%	6.940%
18	12.857	1859	1865	1870	rBV	117734	183731	9.04%	0.987%
19	12.921	1870	1876	1879	rVV	352901	596923	29.37%	3.206%
20	12.951	1879	1881	1885	rVV	195615	273222	13.44%	1.467%
21	12.998	1885	1889	1897	rVB	245127	388688	19.13%	2.087%
22	13.157	1909	1916	1927	rBV	288840	478268	23.53%	2.569%
23	13.304	1933	1941	1948	rBV	960214	1497221	73.67%	8.041%
24	13.610	1986	1993	2009	rBV2	980444	2032254	100.00%	10.914%
25	13.810	2016	2027	2044	rVB3	286252	642670	31.62%	3.451%
26	14.004	2054	2060	2065	rVV3	16447	26860	1.32%	0.144%
27	14.068	2065	2071	2074	rVV	37877	69842	3.44%	0.375%
28	14.098	2074	2076	2080	rVV	30583	34526	1.70%	0.185%
29	14.151	2080	2085	2091	rVB	63991	98534	4.85%	0.529%
30	14.262	2099	2104	2110	rVB2	44735	75250	3.70%	0.404%
31	14.392	2123	2126	2132	rVB6	13976	21019	1.03%	0.113%
32	14.474	2135	2140	2143	rBV2	30148	49615	2.44%	0.266%
33	14.515	2143	2147	2152	rVB	46402	70183	3.45%	0.377%
34	14.745	2181	2186	2191	rBV2	37324	57990	2.85%	0.311%
35	14.862	2199	2206	2212	rBV3	73367	150287	7.40%	0.807%
36	15.433	2295	2303	2312	rBV	143553	270584	13.31%	1.453%

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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\82N062822W.M
Title : SW846 8260

37	16.527	2481	2489	2496	rBV5	20461	47638	2.34%	0.256%
38	16.727	2517	2523	2530	rBV4	14769	28980	1.43%	0.156%

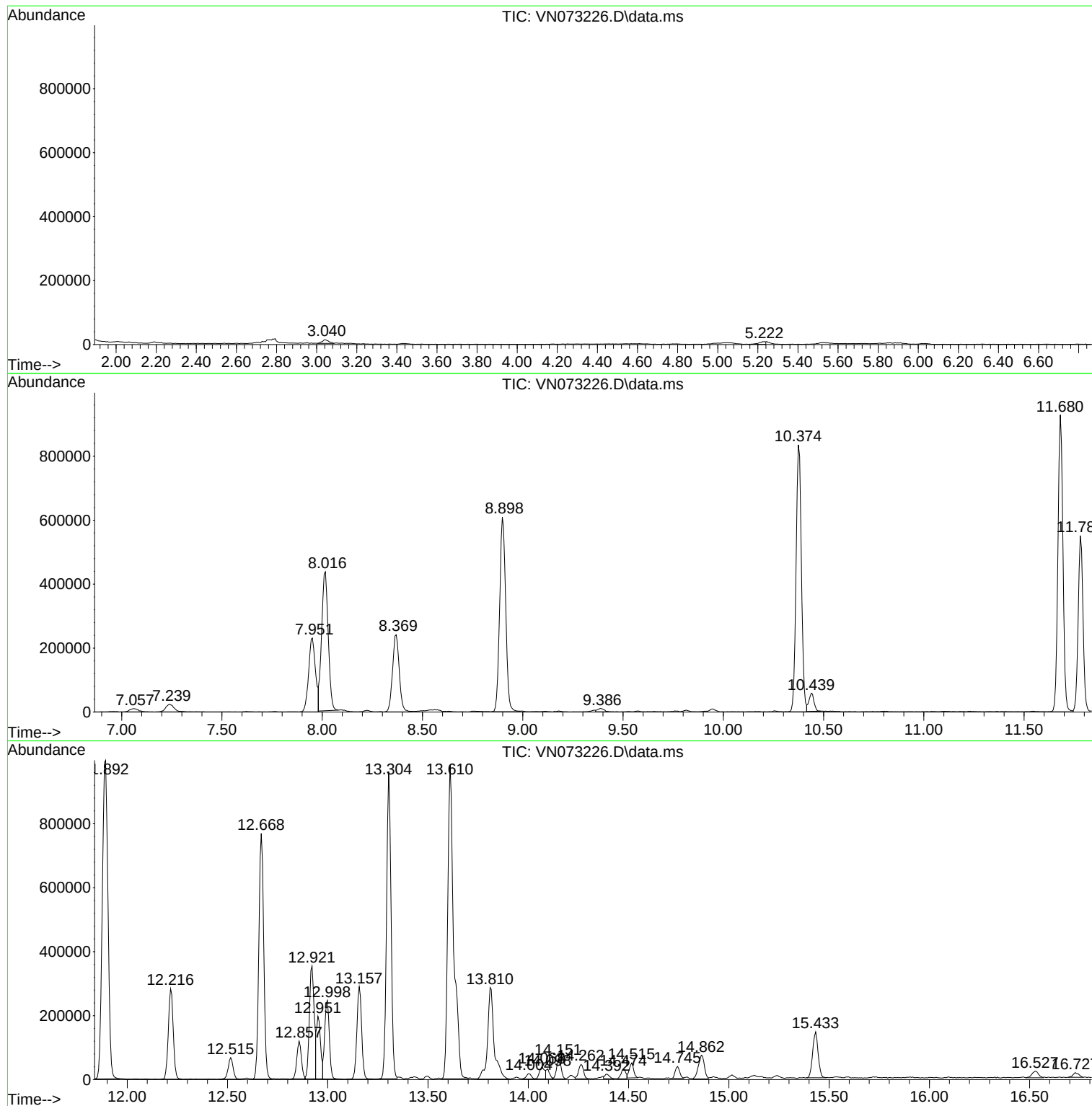
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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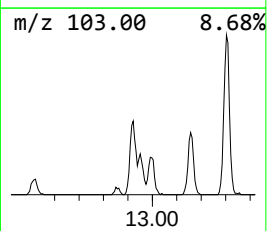
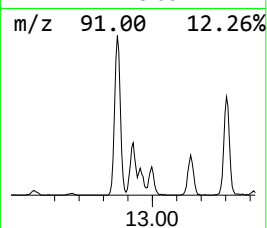
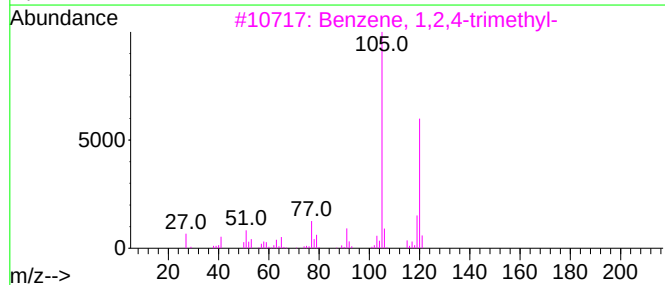
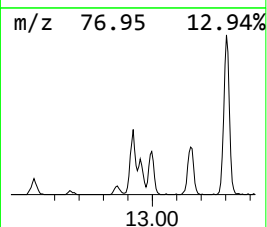
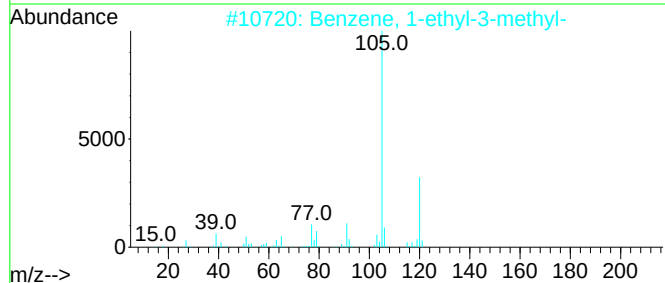
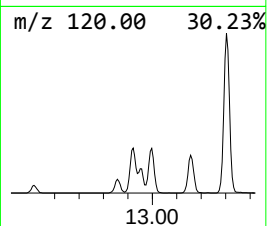
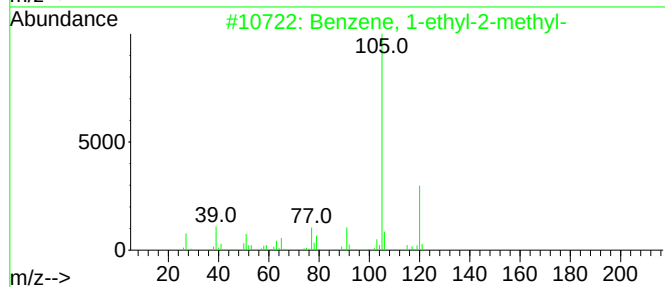
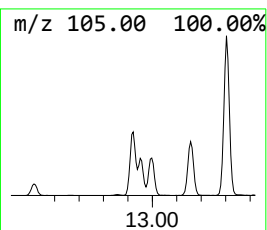
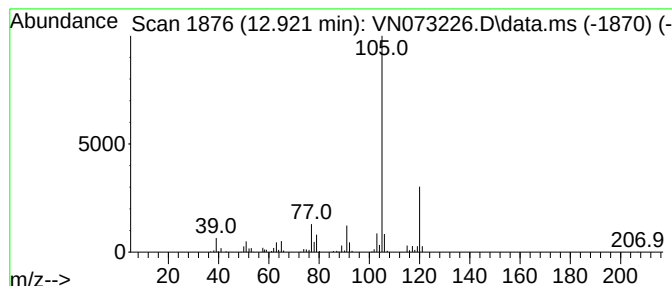
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	14.69 ug/l	596923	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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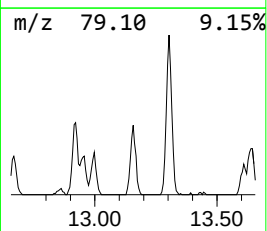
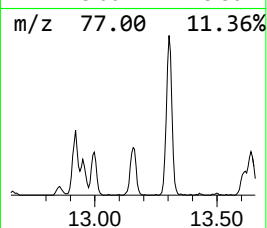
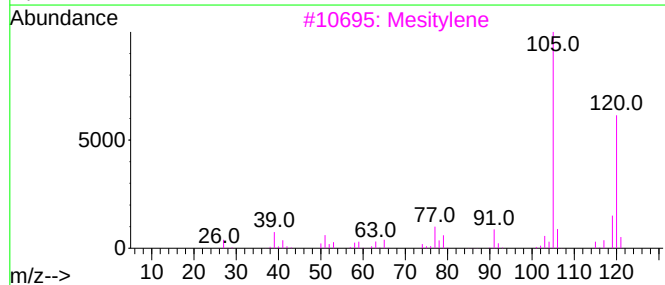
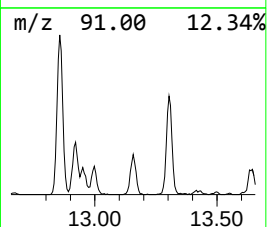
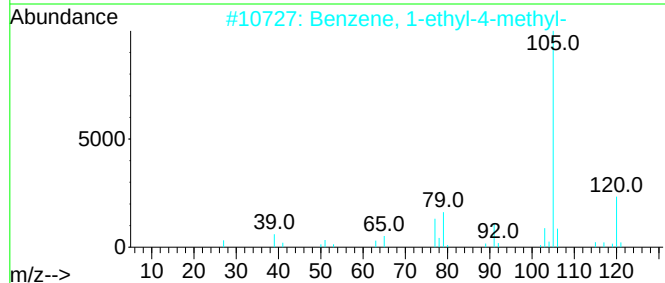
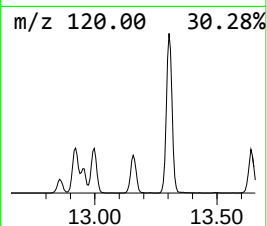
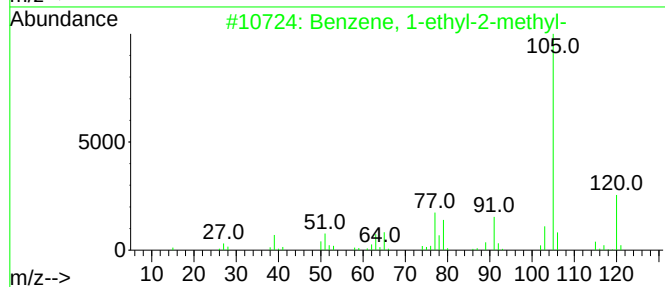
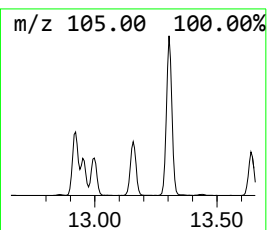
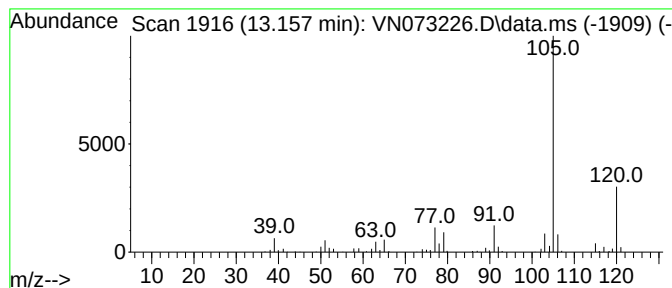
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Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	11.77 ug/l	478268	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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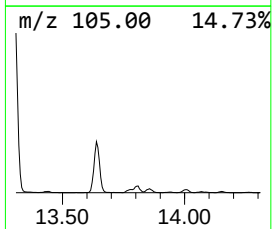
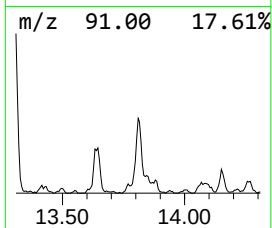
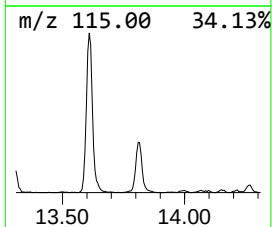
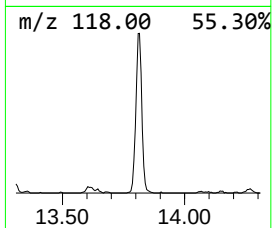
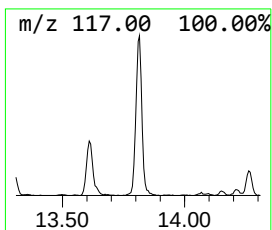
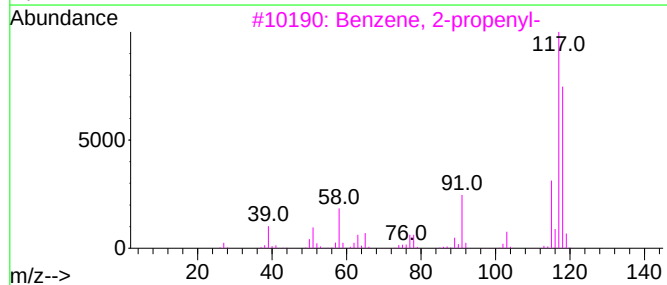
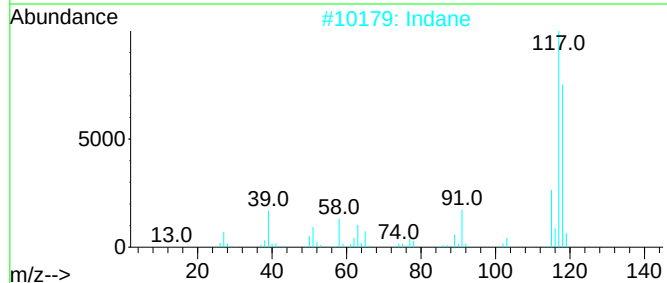
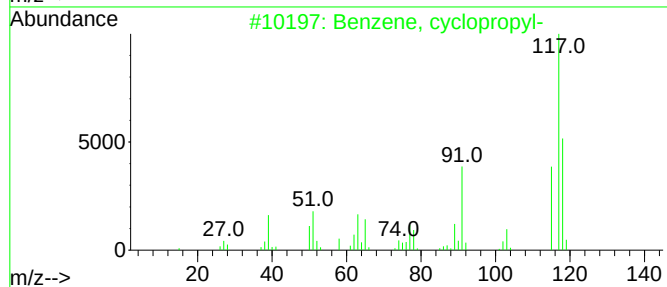
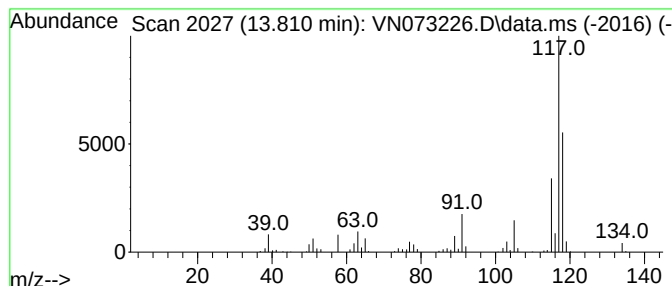
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, cyclopropyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	15.81 ug/l	642670	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	94
2			Indane	118	C9H10	000496-11-7	93
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
5			Deltacyclene	118	C9H10	007785-10-6	68



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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
Benzene, 1-ethy...	12.921	14.7	ug/l	596923	4	13.610	2032250	50.0
Benzene, 1-ethy...	13.157	11.8	ug/l	478268	4	13.610	2032250	50.0
Benzene, cyclop...	13.810	15.8	ug/l	642670	4	13.610	2032250	50.0