

Supplementary Materials

Table S1. Comparison of the finger-print vibrational frequencies obtained theoretically and experimentally for 3-Ishwarone.

Config 1			Config 2		ConFigure 3		ConFigure 4	
Exp. (cm ⁻¹)	Theor. (cm ⁻¹)	$\Delta_{\text{teor-exp}}$ (cm ⁻¹) ^a	Theor. (cm ⁻¹)	$\Delta_{\text{teor-exp}}$ (cm ⁻¹) ^a	Theor. (cm ⁻¹)	$\Delta_{\text{teor-exp}}$ (cm ⁻¹) ^a	Theor. (cm ⁻¹)	$\Delta_{\text{teor-exp}}$ (cm ⁻¹) ^a
828	824	4 [0,5]	839	11 [1,3]	844	16 [1,9]	850	22 [2,6]
858	856	2 [0,2]	881	23 [2,6]	879	21 [2,4]	884	26 [3,0]
905	899	6 [0,6]	899	6 [0,7]	898	7 [0,8]	901	4 [0,4]
931	930	1 [0,1]	927	4 [0,4]	911	20 [2,1]	911	20 [2,1]
1006	997	9 [0,9]	985	21 [2,1]	971	35 [3,5]	998	8 [0,8]
1034	1017	17 [1,6]	1003	31 [3,0]	1001	33 [3,2]	1017	17 [1,6]
1067	1040	27 [2,5]	1061	6 [0,6]	1041	26 [2,4]	1043	24 [2,2]
1092	1078	14 [1,3]	1090	2 [0,2]	1052	40 [3,7]	1074	18 [1,6]
1107	1089	18 [1,6]	1111	4 [0,4]	1066	41 [3,7]	1098	9 [0,8]
1124	1107	17 [1,5]	1134	10 [0,9]	1103	21 [1,9]	1128	4 [0,4]
1168	1148	20 [1,7]	1183	15 [1,3]	1143	25 [2,1]	1159	9 [0,8]
1246	1220	26 [2,1]	1227	19 [1,5]	1226	20 [1,6]	1219	27 [2,2]
MAD=		13 [1,2]	MAD=		13 [1,2]	MAD=		16 [1,5]

^a values in brackets presents the percentage deviation in relation at calculated value.

Figure S1. ¹³C-NMR spectrum of 3-ishwarone in C₆D₆ solution.

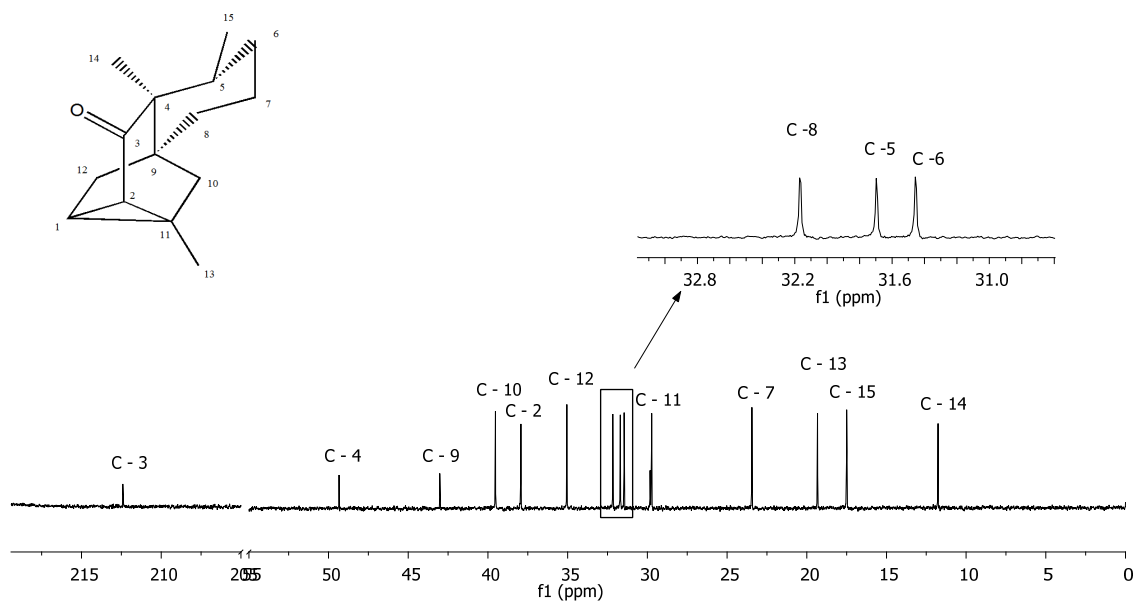


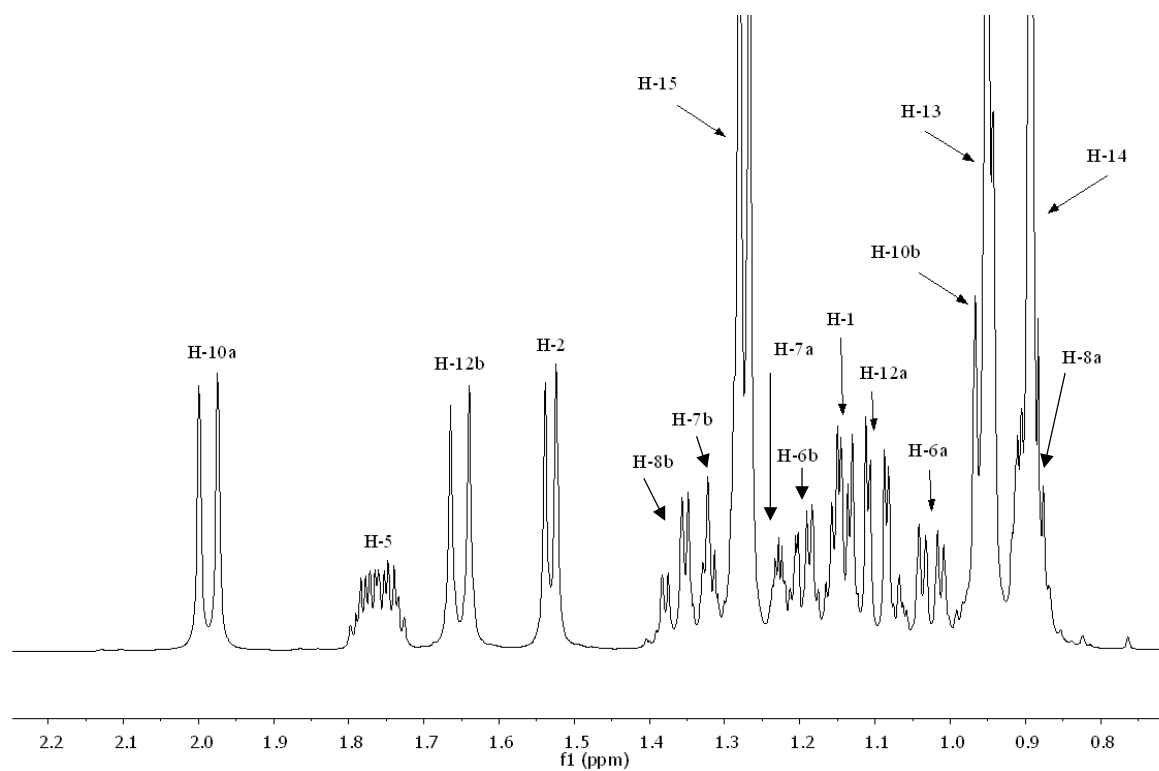
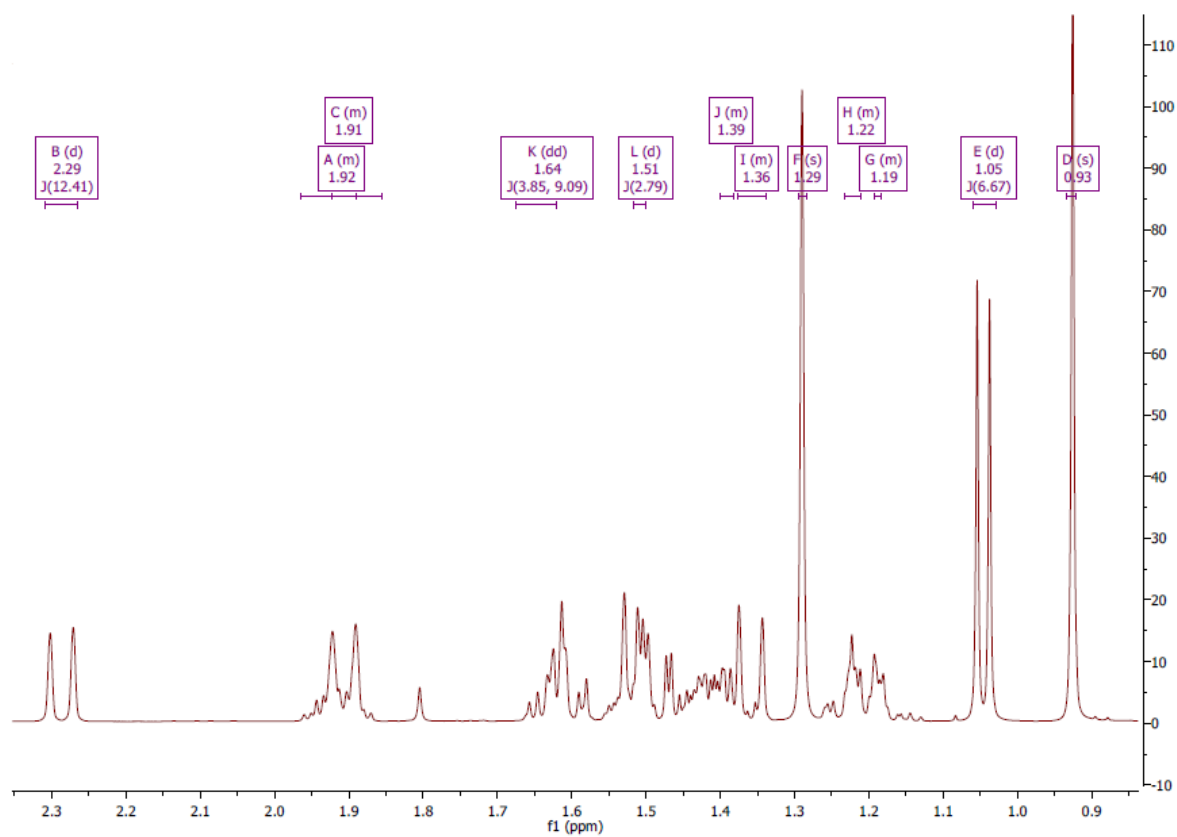
Figure S2. ^1H -NMR spectrum of 3-ishwarone in C_6D_6 solution.**Figure S3.** ^1H -NMR spectrum of 3-ishwarone in CDCl_3 .

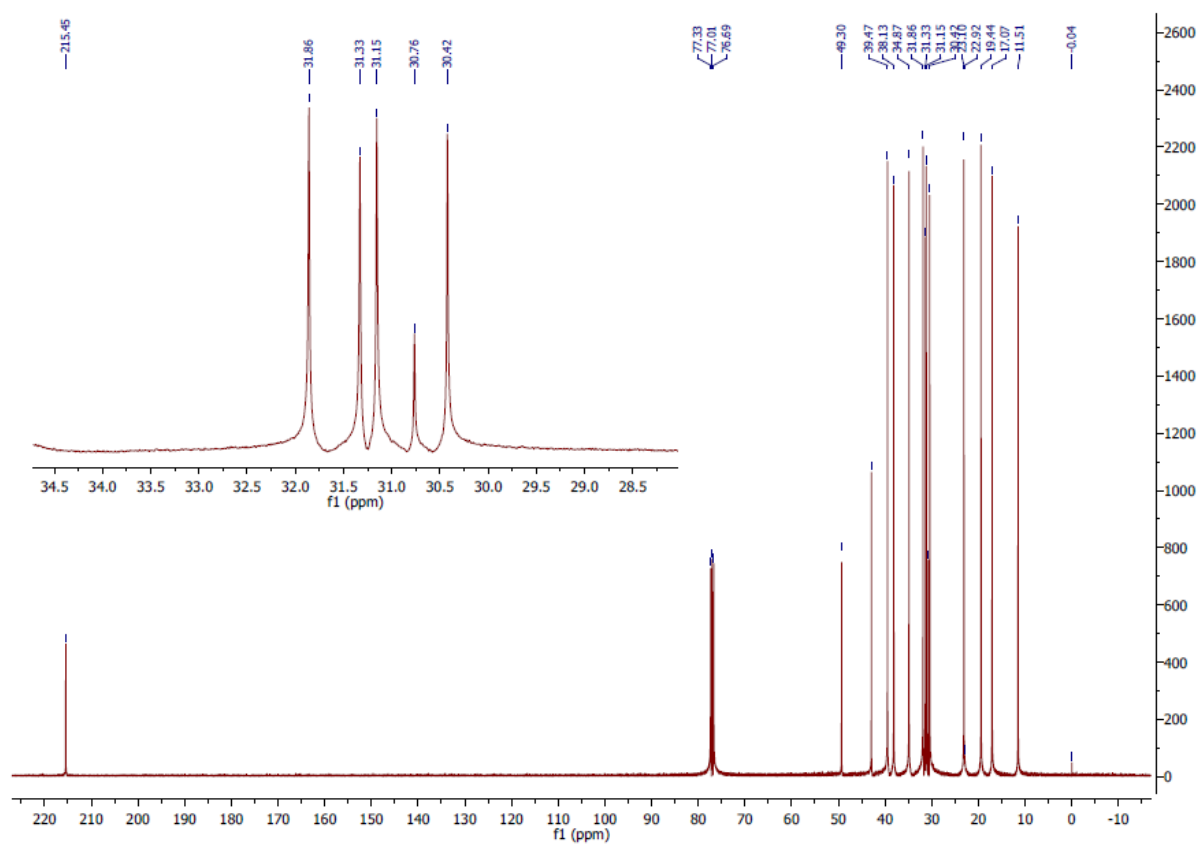
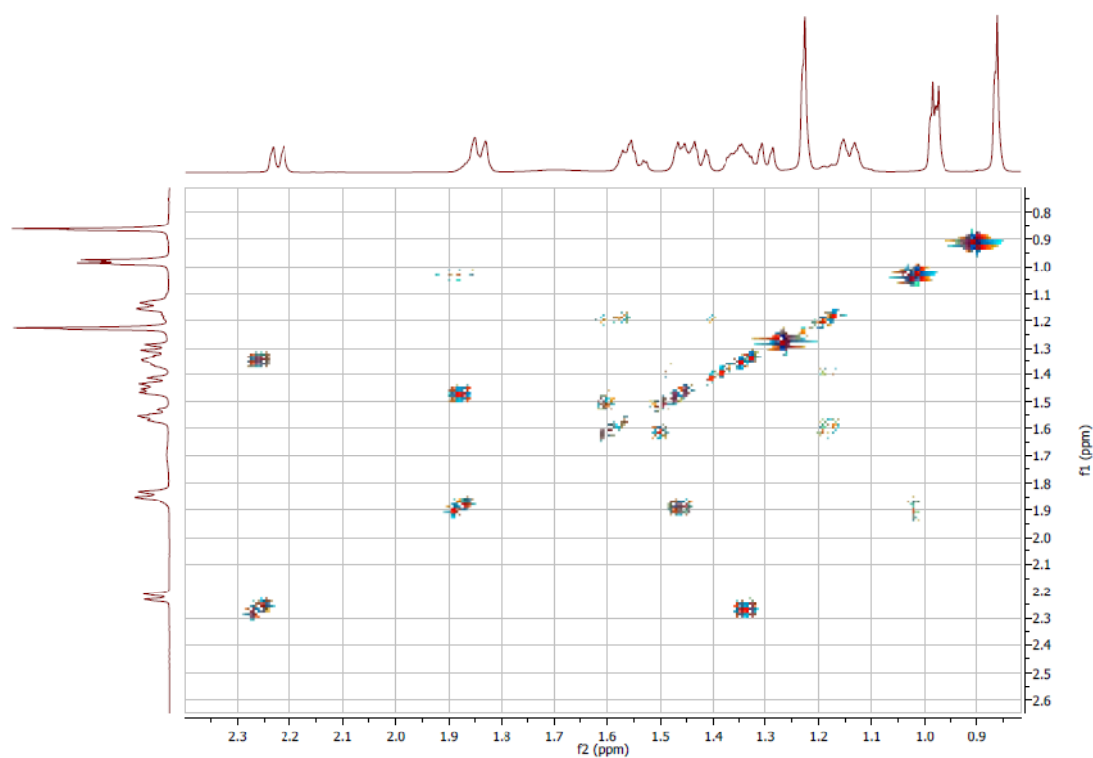
Figure S4. ^{13}C -NMR spectrum of 3-ishwarone in CDCl_3 .**Figure S5.** COSY ^1H - ^1H NMR spectrum 3-ishwarone in CDCl_3 .

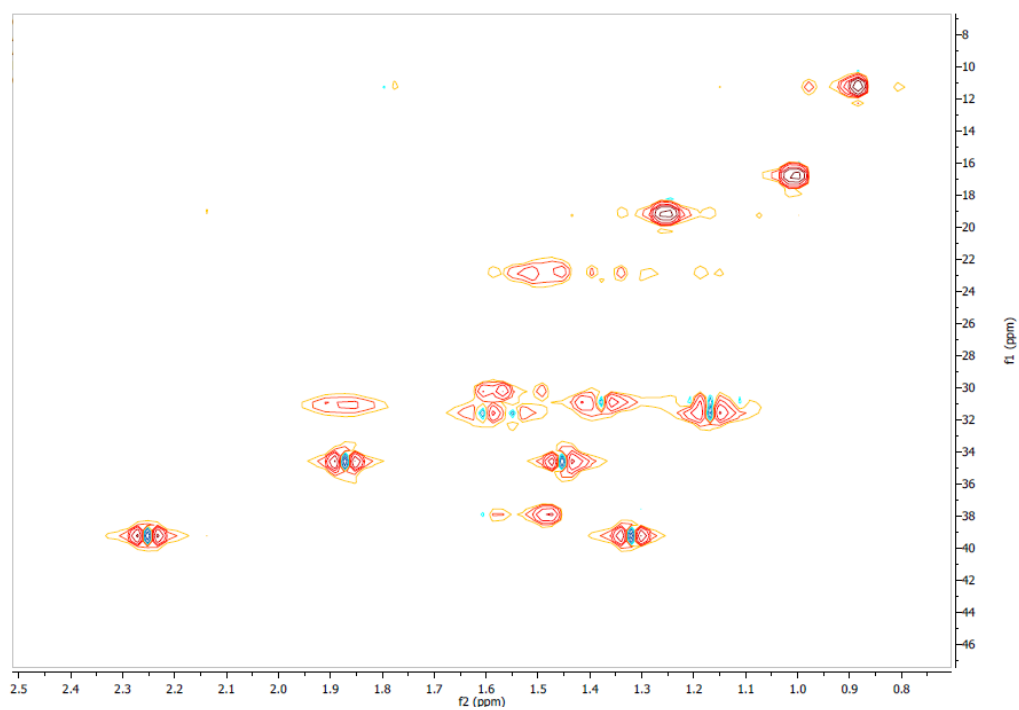
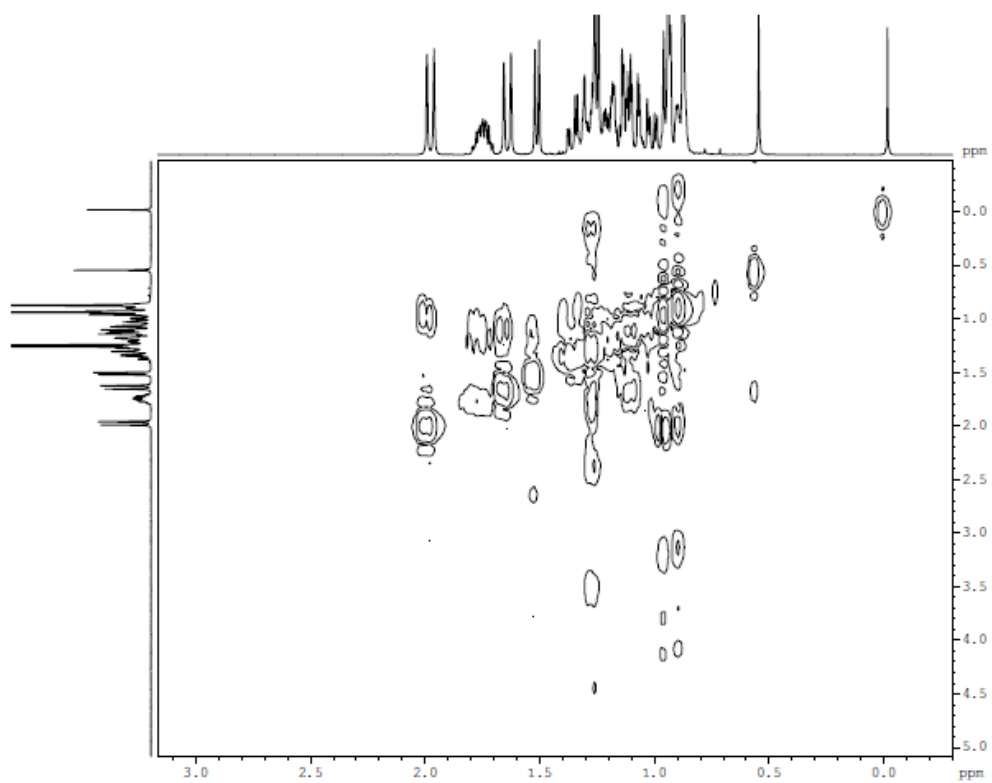
Figure S6. HSQC ^1H - ^{13}C -NMR spectrum of 3-ishwarone in CDCl_3 .**Figure S7.** COSY ^1H - ^1H -NMR spectrum 3-ishwarone in C_6D_6 .

Figure S8. HSQC ^1H - ^{13}C -NMR spectrum of 3-ishwarone in C_6D_6 .

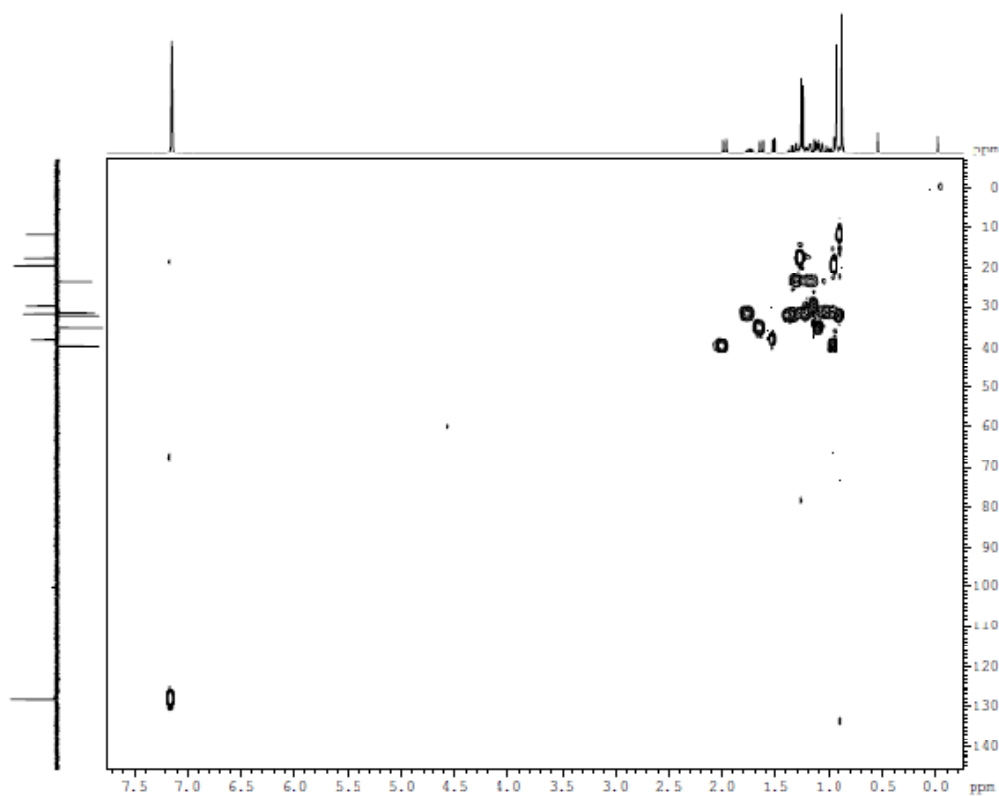


Figure S9. NOESY spectrum of 3-ishwarone in C_6D_6 (symmetrized with COSY-like, Apodization function with TRAF 1 Hz, in MNova program).

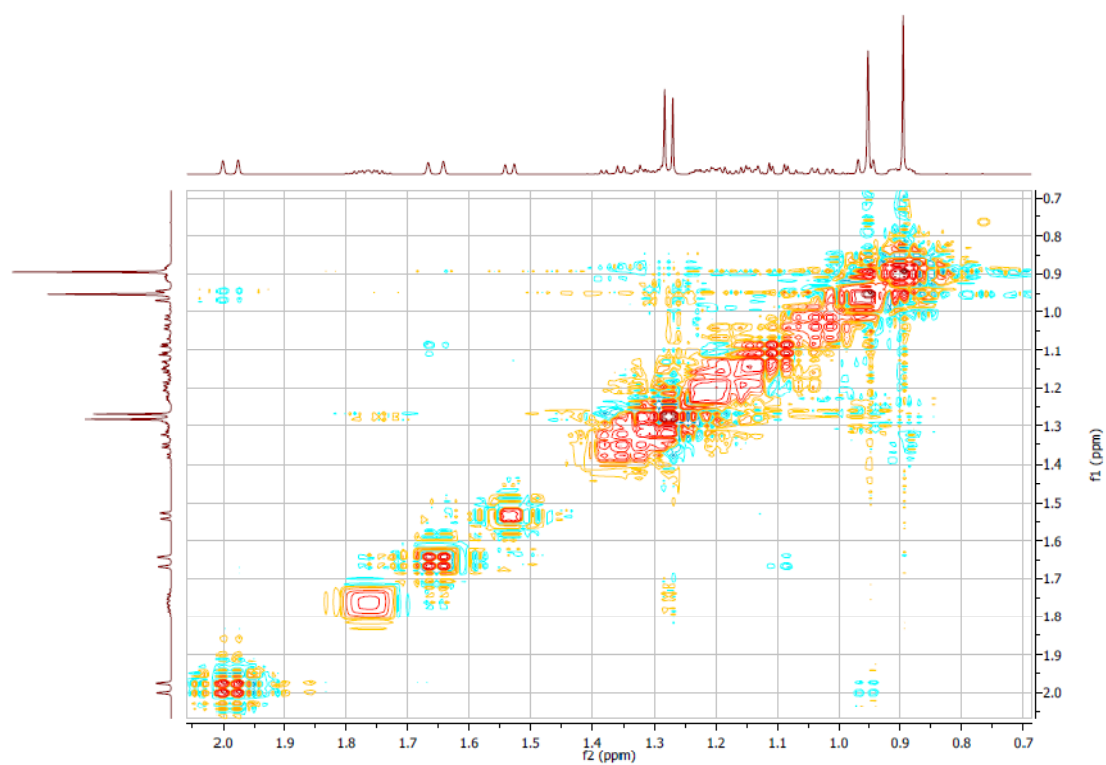
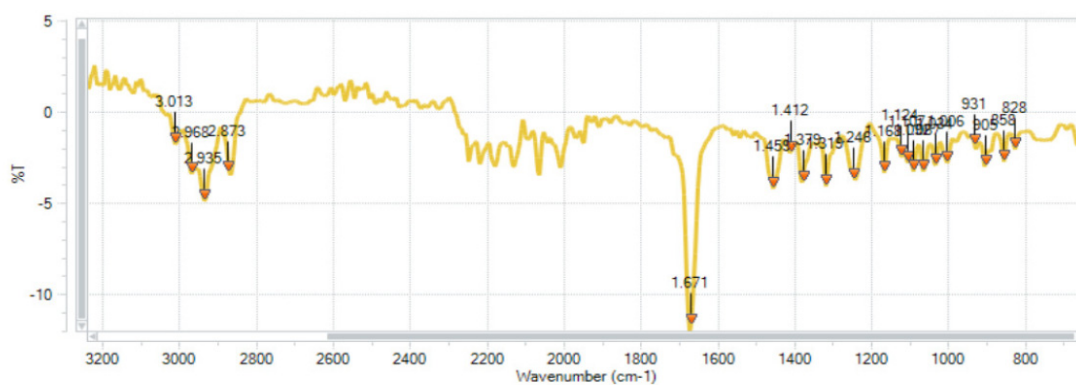
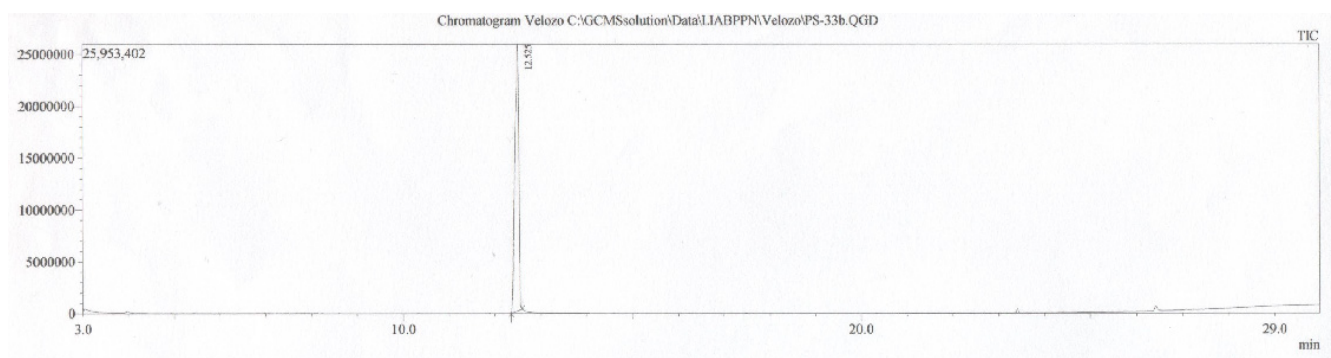


Figure S10. IR spectrum of 3-ishwarone in CHCl_3 .**Figure S11.** Chromatogram of 3-ishwarone under the experimental conditions recorded for GC-MS analysis.**Figure S12.** Mass Spectra of 3-ishwarone under the experimental conditions recorded for GC-MS analysis.