Supporting Information

***Org. Commun.* 14:2 (2021) 133-143**

Discovery of new capsaicin and dihydrocapsaicin derivatives as histone deacetylase inhibitors and molecular docking studies

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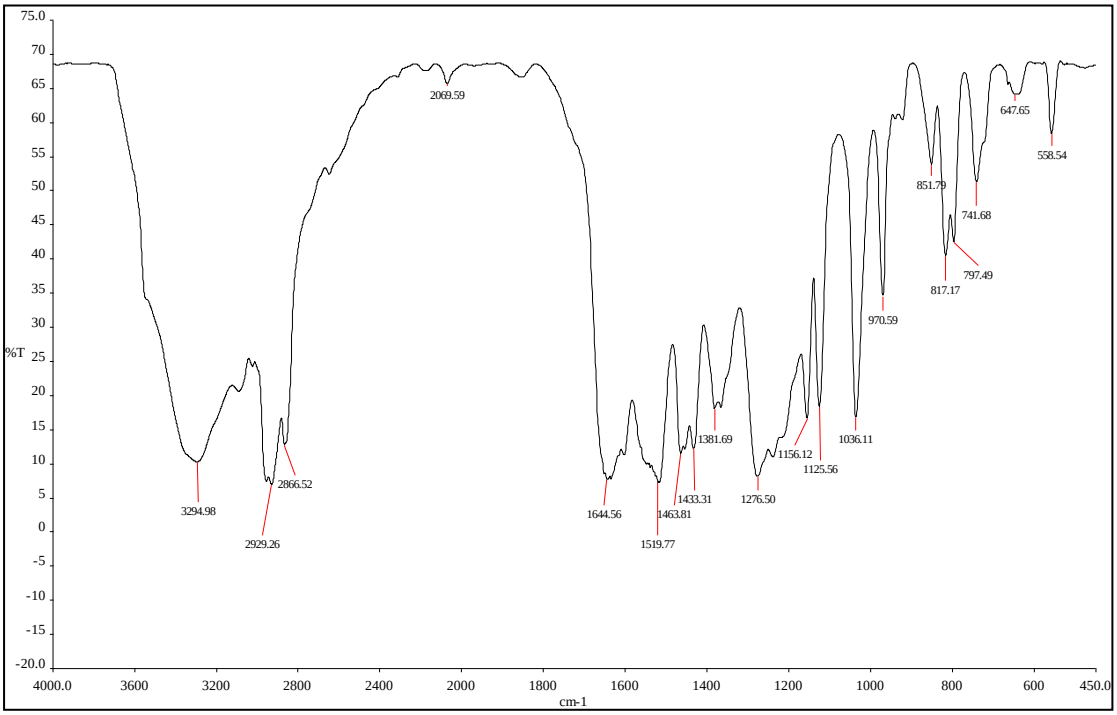

Figure S1: IR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-ena-mide (**1**) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (**2**)

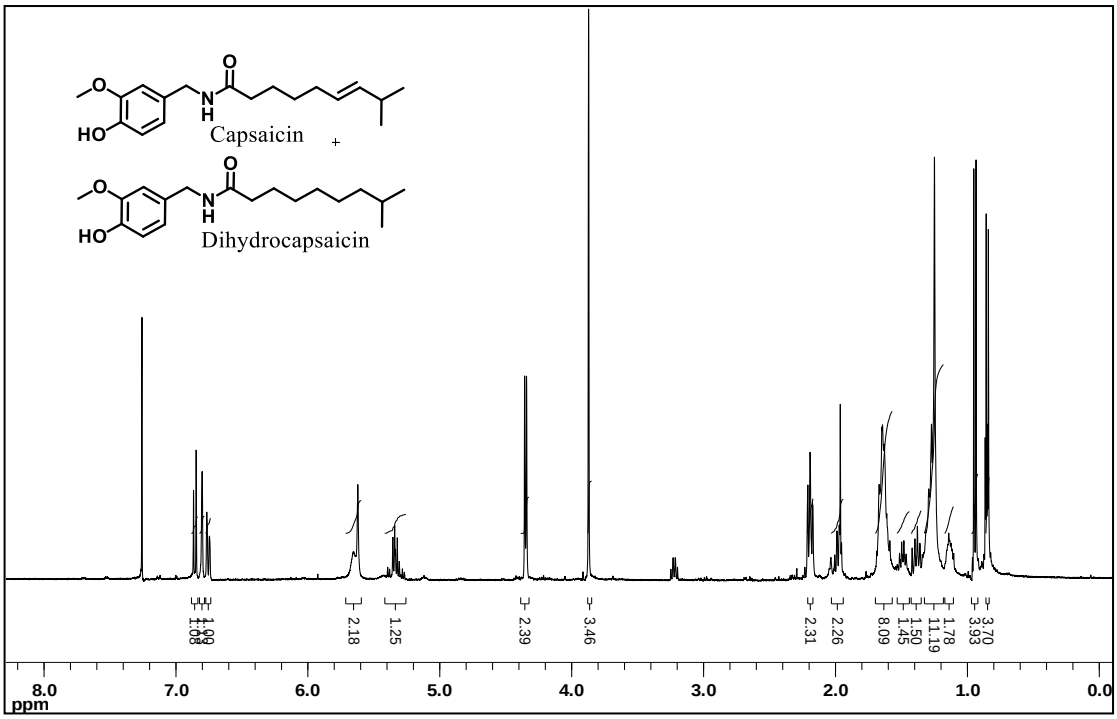

Figure S2: ^{1}H NMR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**1**) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (**2**)

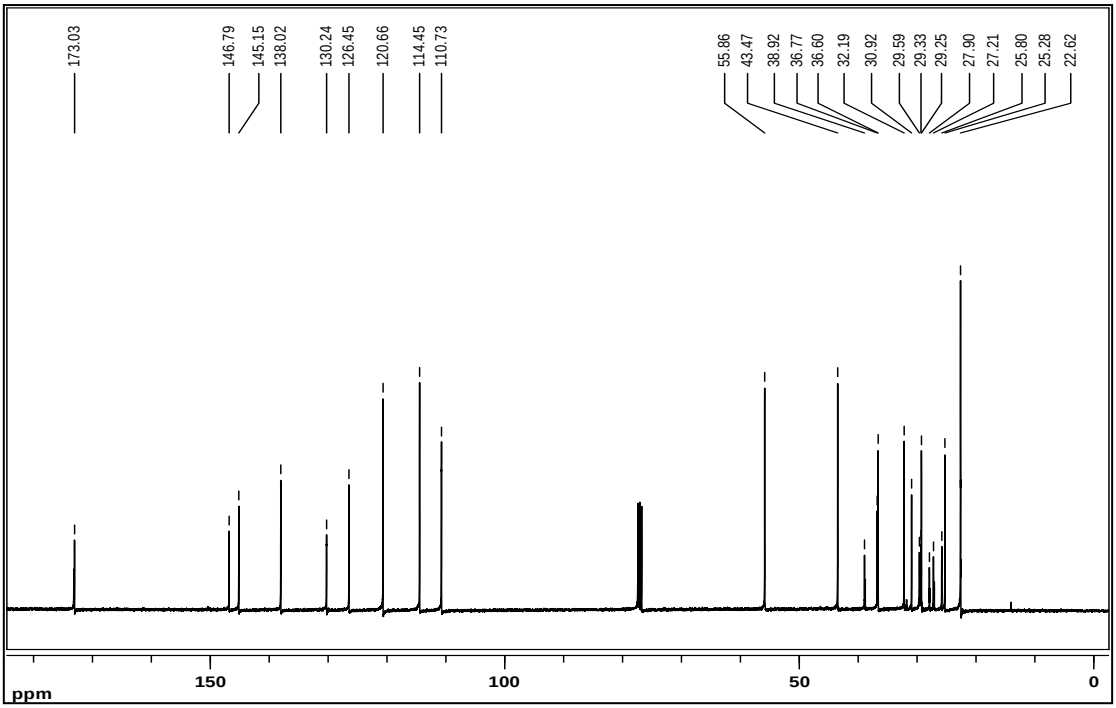

Figure S3: ^{13}C NMR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**1**) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (**2**)

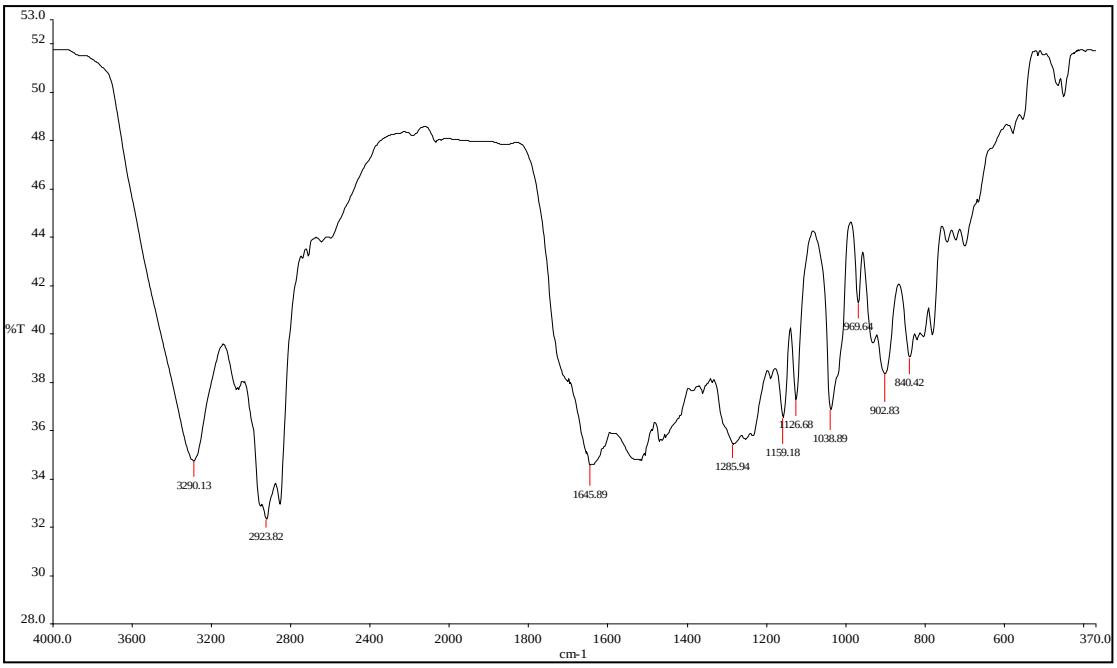

Figure S4: IR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnon-6-enamide (**3)** and *N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (**4**)

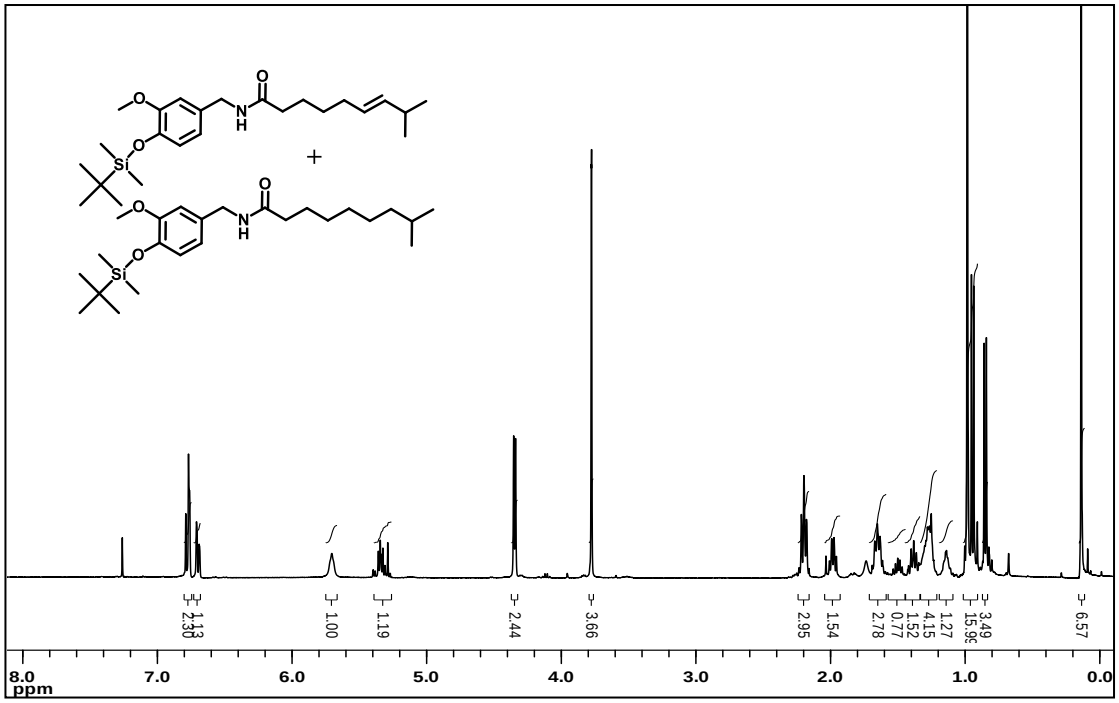

Figure S5: [1]H NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-8-methylnon-6-enamide (**3)** and *N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (**4**)

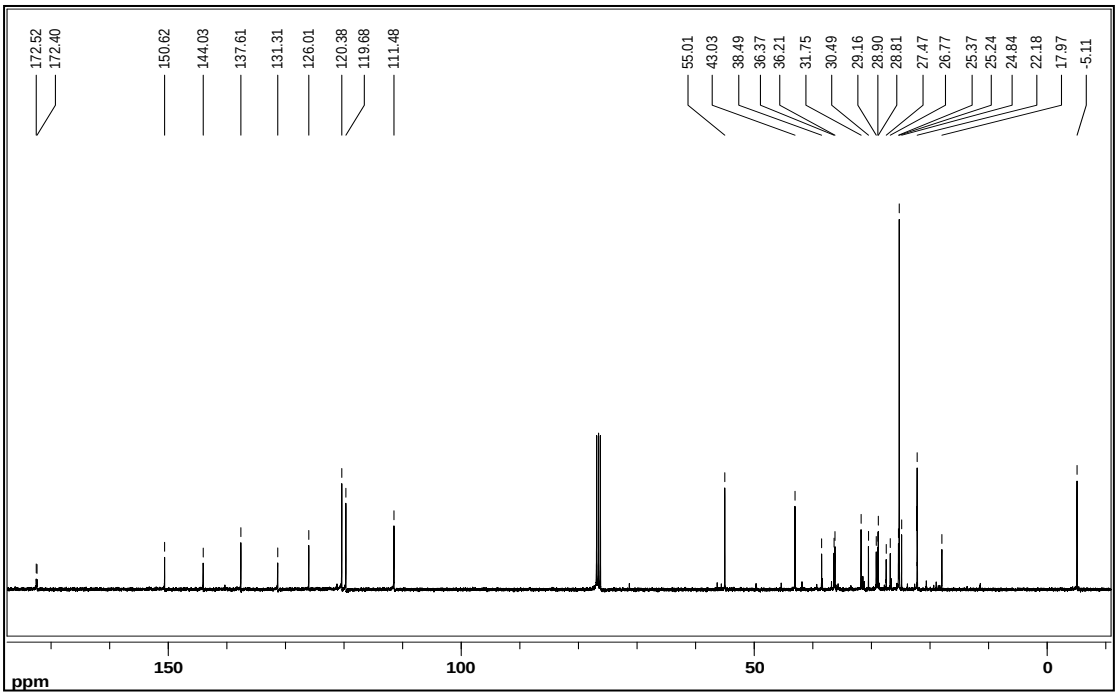

Figure S6: [13]C NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-8-methylnon-6-enamide (**3**) and *N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (**4**)

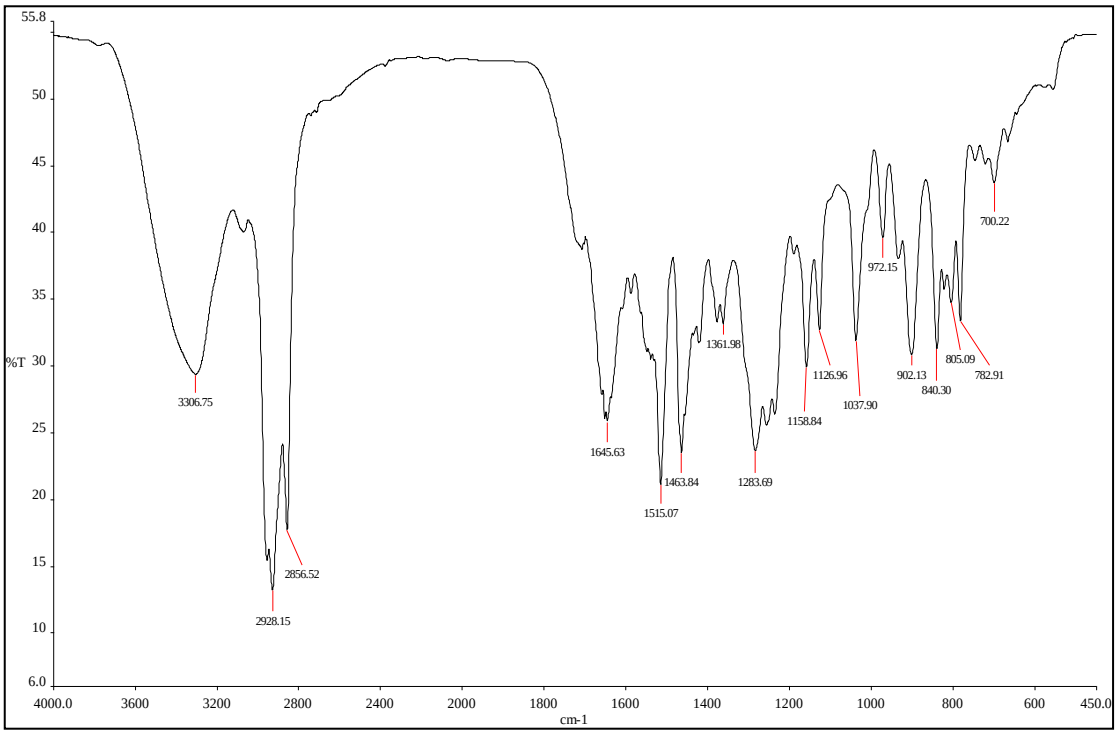

Figure S7: IR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

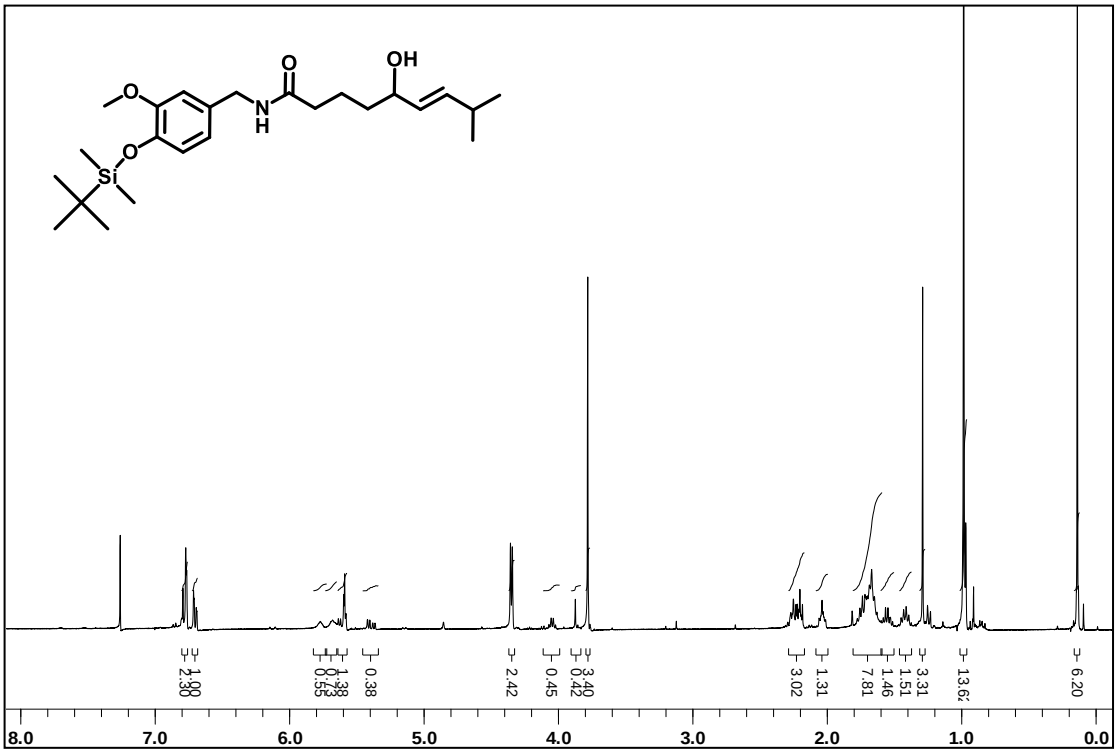

Figure S8: ^{1}H NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

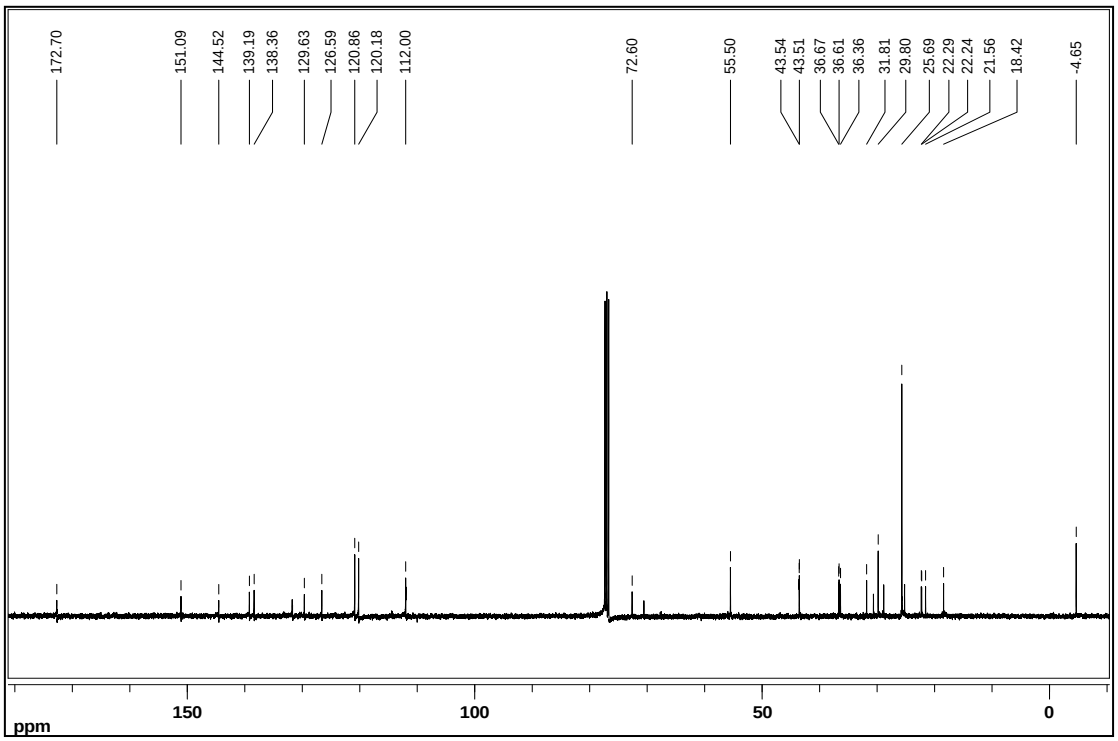

Figure S9: ^{13}C NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

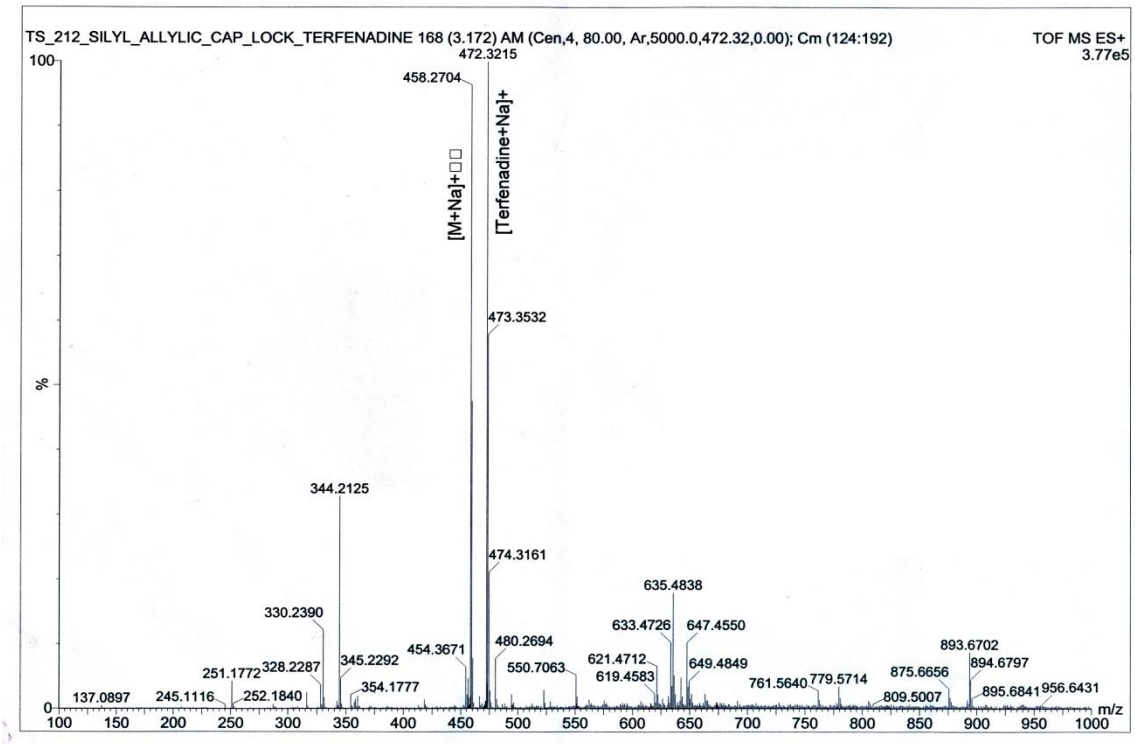

Figure S10: Mass spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

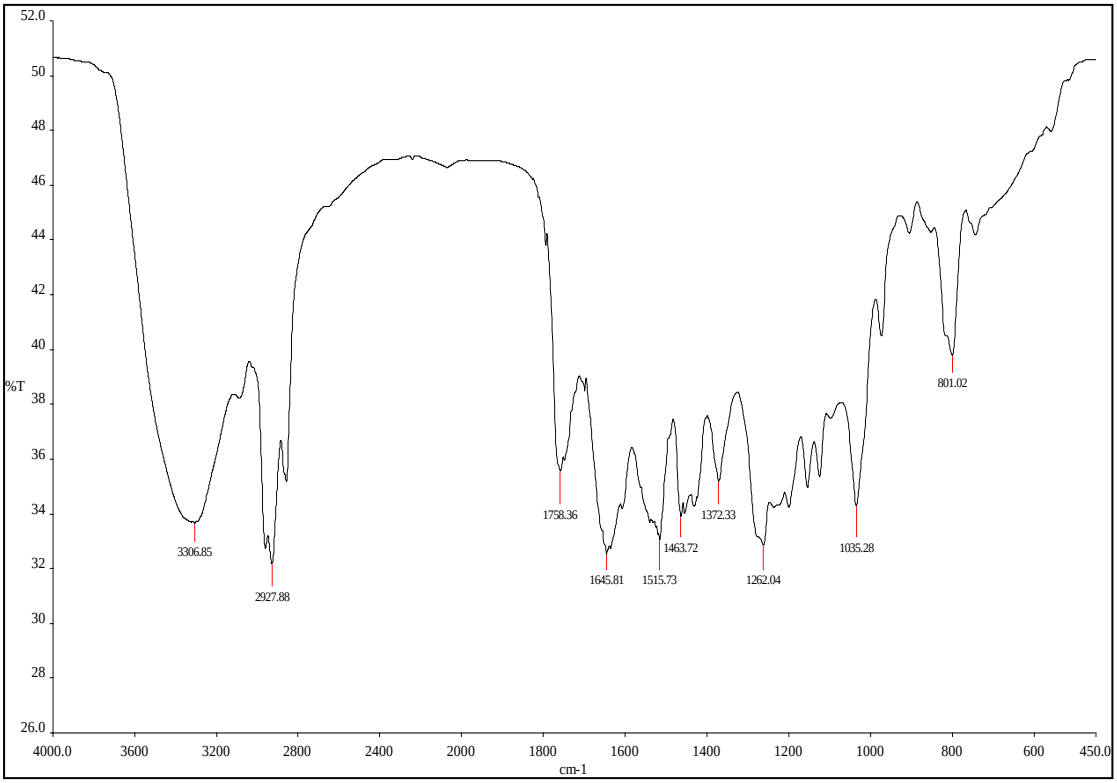

Figure S11: IR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

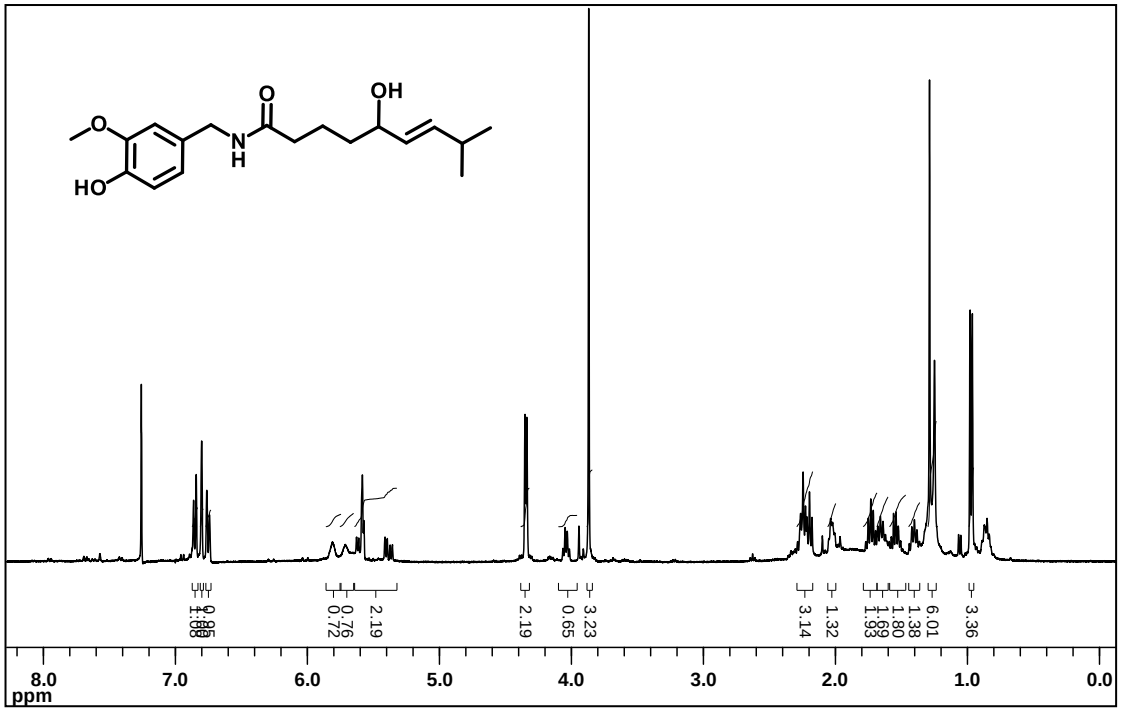

Figure S12: ^{1}H NMR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

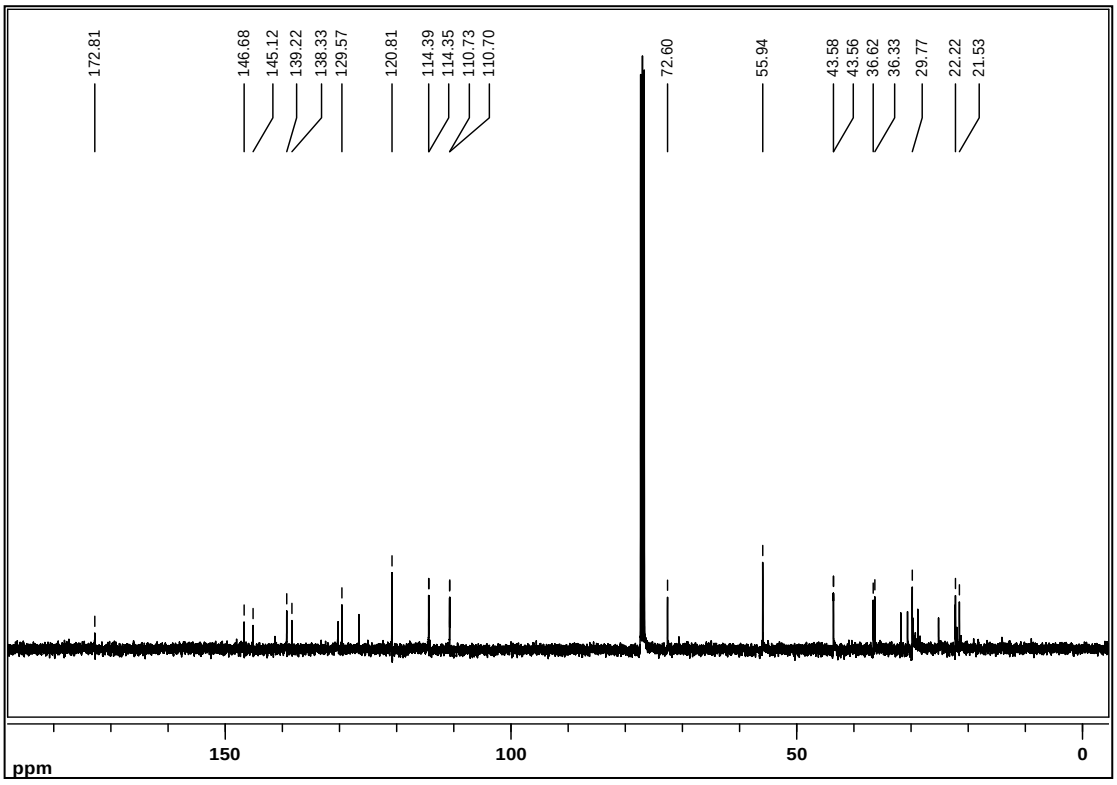

Figure S13: ^{13}C NMR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

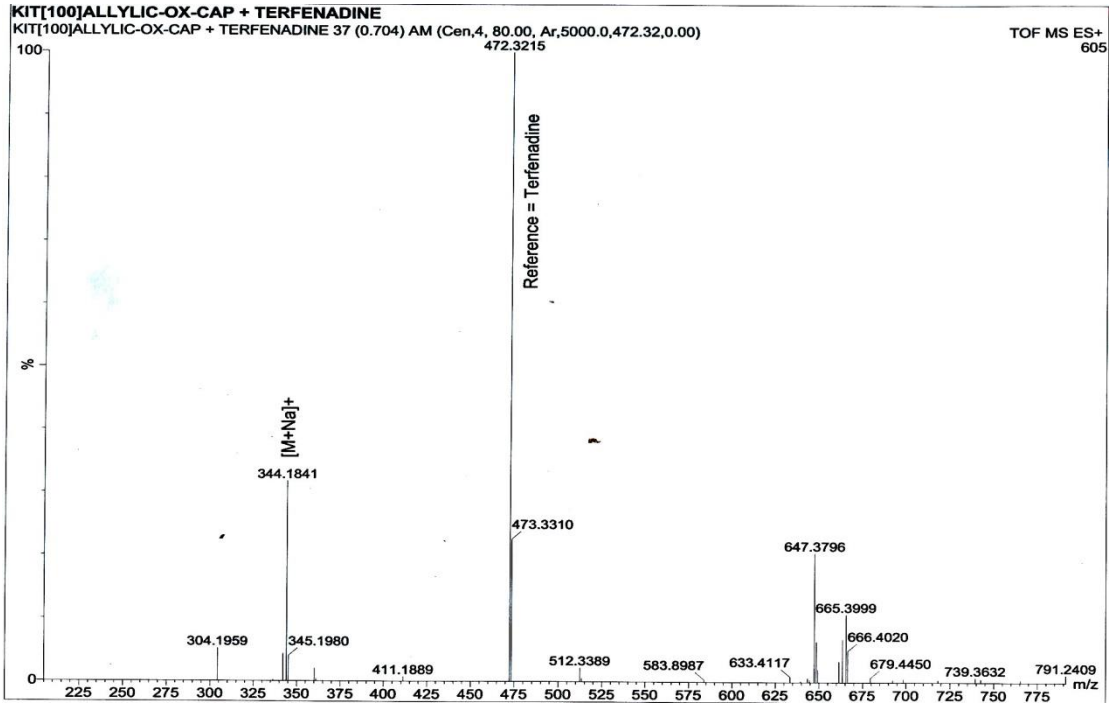

Figure S14: Mass spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

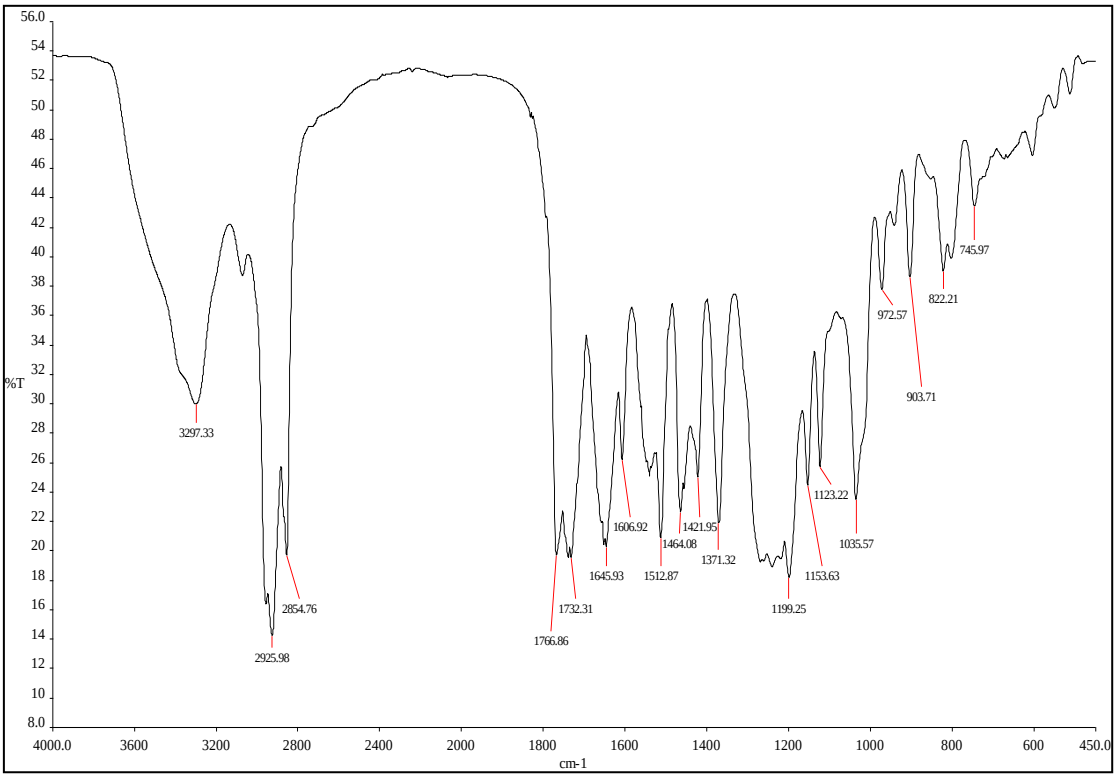

Figure S15: IR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (**7**)

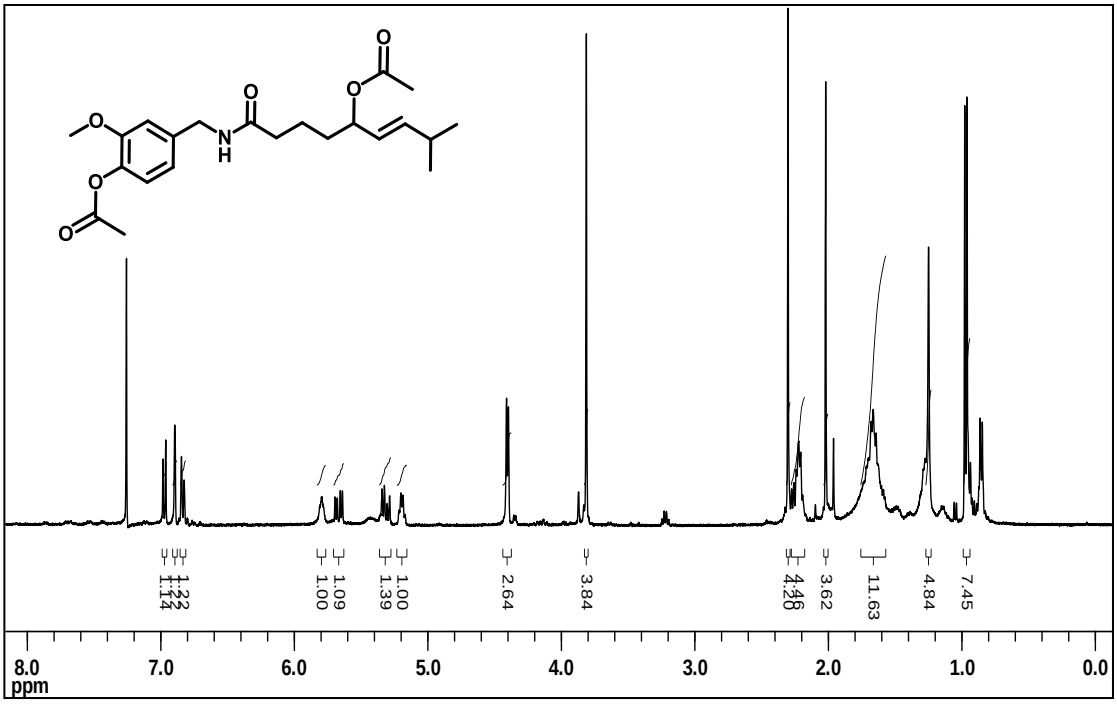

Figure S16: ^{1}H NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (**7**)

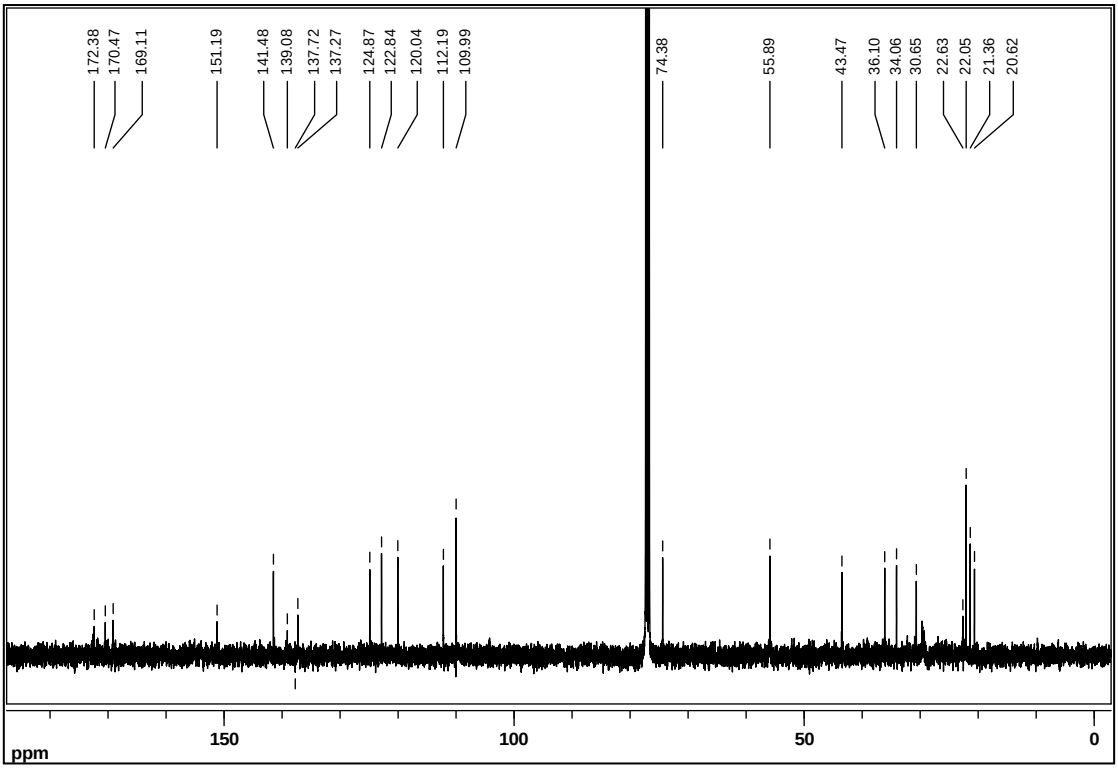

Figure S17: ^{13}C NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (**7**)

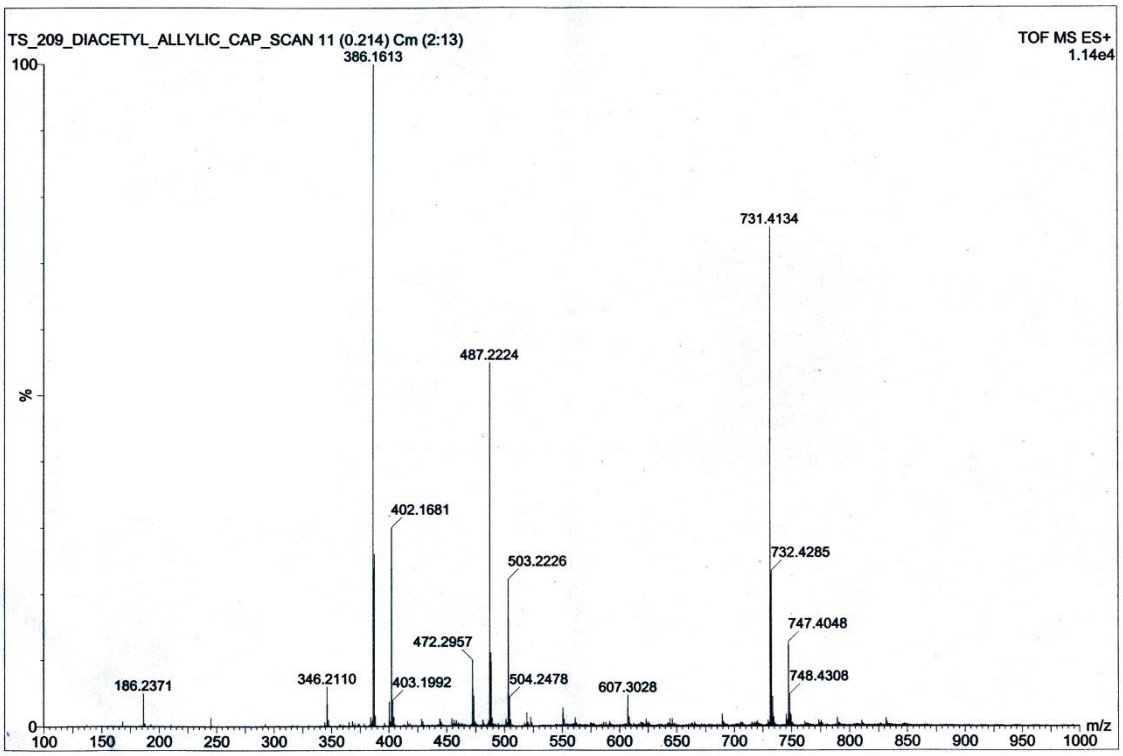

Figure S18: Mass spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (**7**)

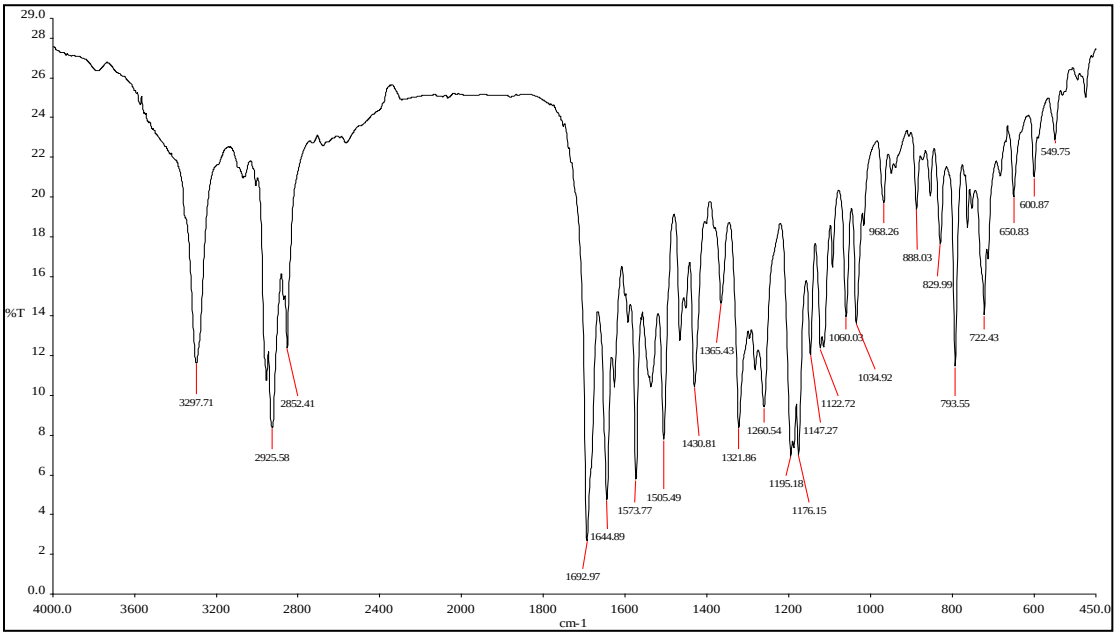

Figure S19: IR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

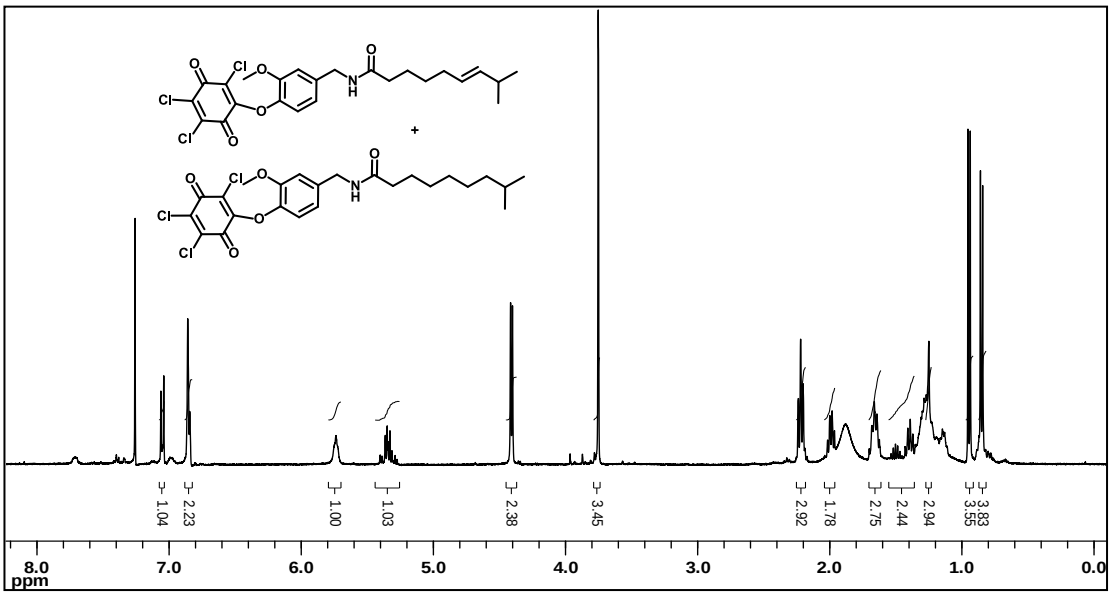

Figure S20: ^{1}H NMR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

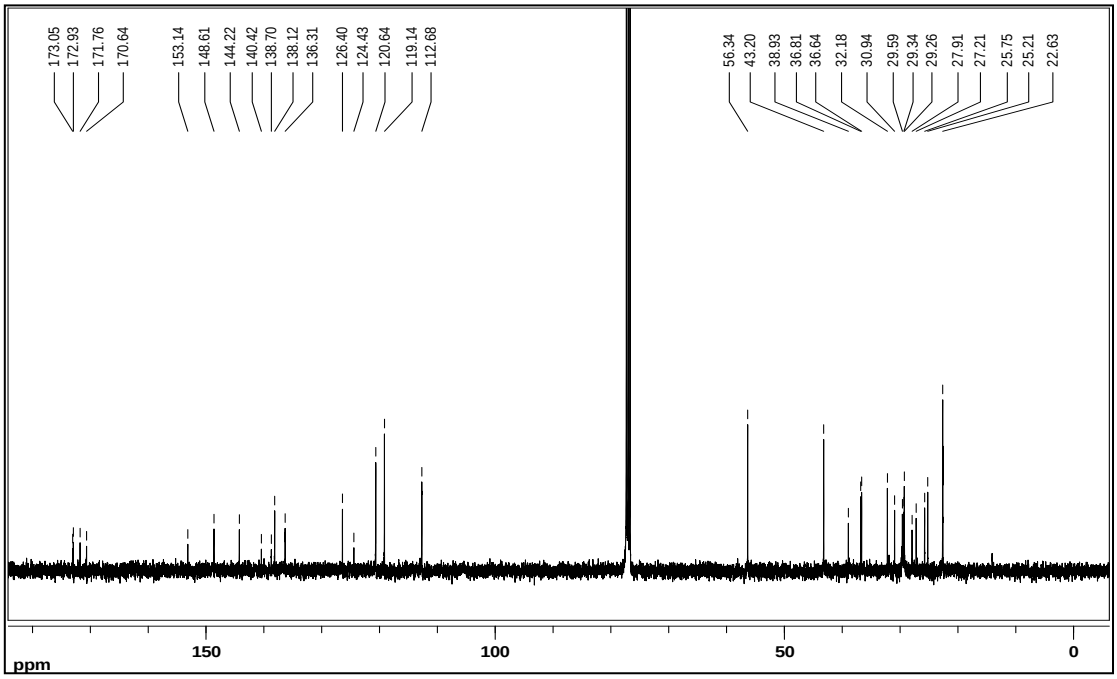

Figure S21: ^{13}C NMR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8)** and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

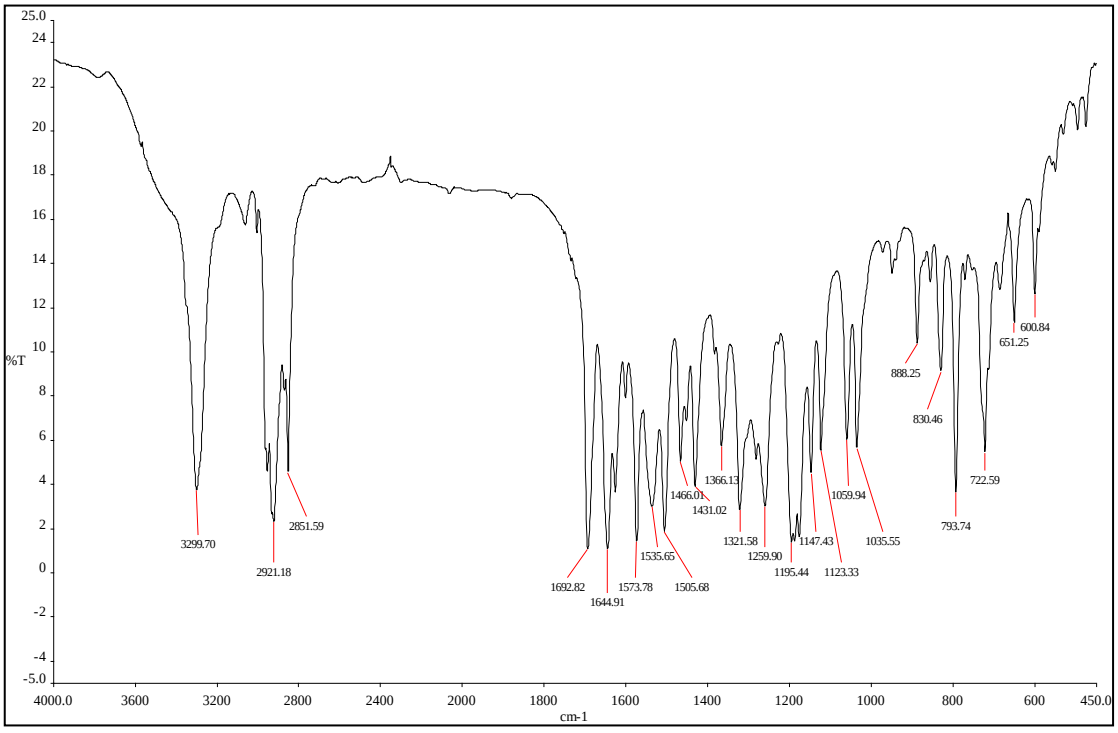

Figure S22: IR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4 dienyloxy)benzyl)-8-methylnonanamide (**9**)

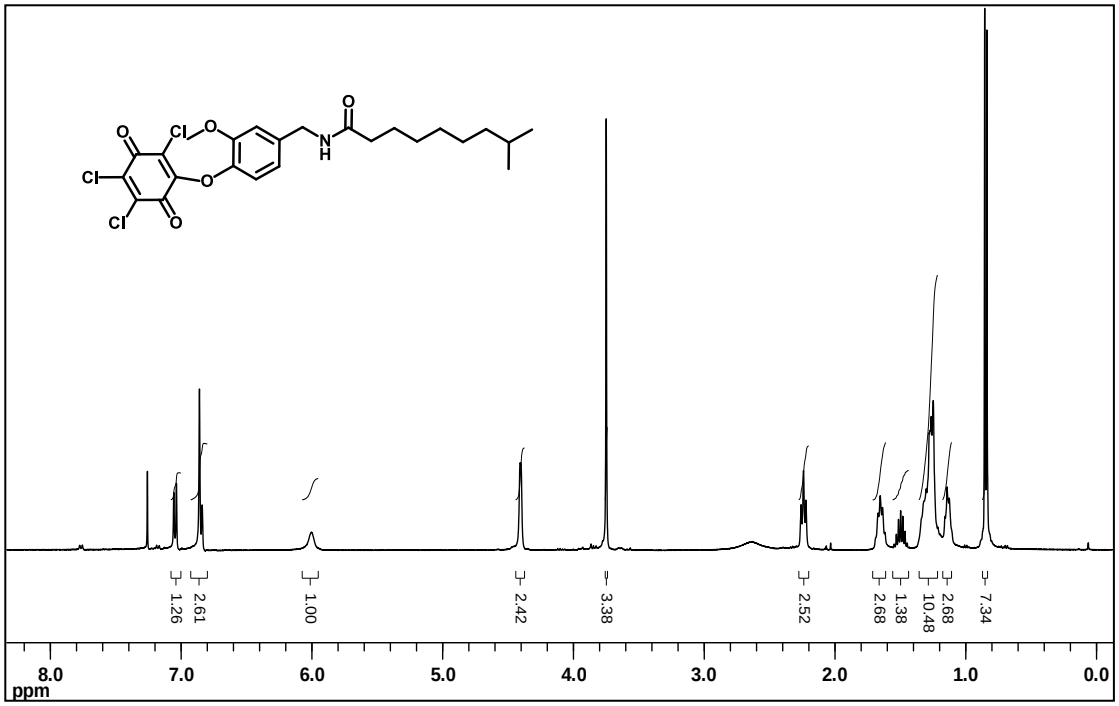

Figure S23: ^{1}H NMR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

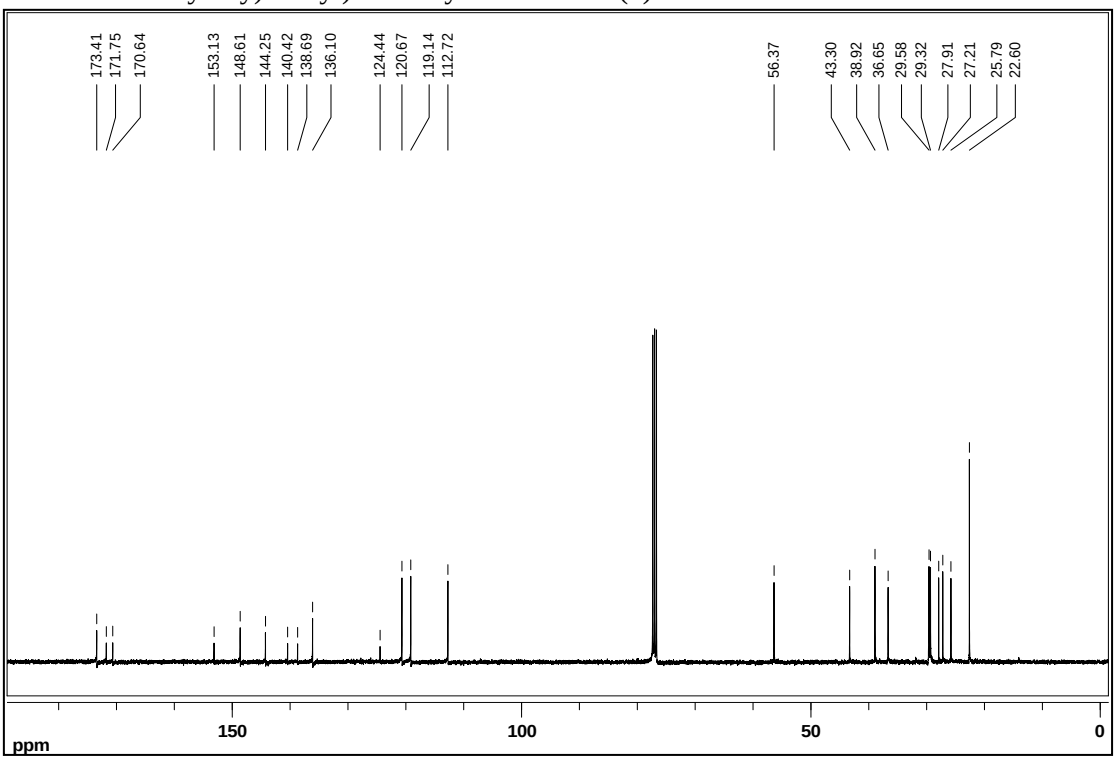

Figure S24: ^{13}C NMR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

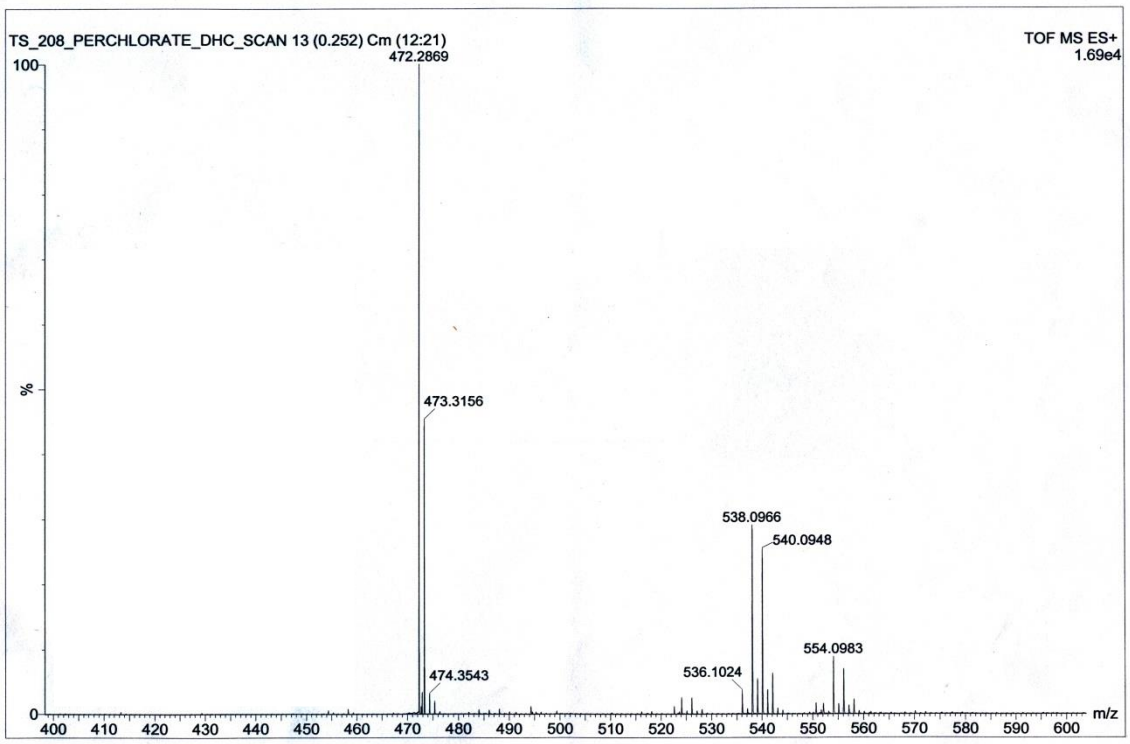

Figure S25: Mass spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)