

Supporting Information

Org. Commun. 14:2 (2021) XX-XX

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

¹Department of Applied Chemistry, Faculty of Science and Liberal Arts,

Rajamangala University of Technology Isan, Nakhon Ratchasima, 30000 Thailand

²Ban Dong Subdistrict Administration Organization, Ubonratana District, Khon Kaen 40250, Thailand

³Natural Products Research Unit, Department of Biochemistry, Faculty of Science, Khon Kaen University, Khon Kaen, 40002 Thailand

⁴Natural Products Research Unit, Center of Excellence for Innovation in Chemistry, Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen, 40002 Thailand

| Table of Contents | Page |
|--|------|
| Figure S1: IR spectrum of (<i>E</i>)- <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (1) and <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (2) | 3 |
| Figure S2: ¹ H NMR spectrum of (<i>E</i>)- <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (1) and <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (2) | 3 |
| Figure S3: ¹³ C NMR spectrum of (<i>E</i>)- <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (1) and <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (2) | 4 |
| Figure S4: IR spectrum of (<i>E</i>)- <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnon-6-enamide (3) and <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (4) | 4 |
| Figure S5: ¹ H NMR spectrum of (<i>E</i>)- <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnon-6-enamide (3) and <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (4) | 5 |
| Figure S6: ¹³ C NMR spectrum of (<i>E</i>)- <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnon-6-enamide (3) and <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (4) | 5 |
| Figure S7: IR spectrum of (<i>E</i>)- <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-5-hydroxy-8-methylnon-6-enamide (5) | 6 |
| Figure S8: ¹ H NMR spectrum of (<i>E</i>)- <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-5-hydroxy-8-methylnon-6-enamide (5) | 6 |
| Figure S9: ¹³ C NMR spectrum of (<i>E</i>)- <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-5-hydroxy-8-methylnon-6-enamide (5) | 7 |
| Figure S10: Mass spectrum of (<i>E</i>)- <i>N</i> -(4-(<i>tert</i> -butyldimethylsilyloxy)-3-methoxybenzyl)-5-hydroxy-8-methylnon-6-enamide (5) | 7 |
| Figure S11: IR spectrum of (<i>E</i>)-5-hydroxy- <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (6) | 8 |

| | |
|---|----|
| Figure S12: ^1H NMR spectrum of (<i>E</i>)-5-hydroxy- <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (6) | 8 |
| Figure S13: ^{13}C NMR spectrum of (<i>E</i>)-5-hydroxy- <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (6) | 9 |
| Figure S14: Mass spectrum of (<i>E</i>)-5-hydroxy- <i>N</i> -(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (6) | 9 |
| Figure S15: IR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (7) | 10 |
| Figure S16: ^1H NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (7) | 10 |
| Figure S17: ^{13}C NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (7) | 11 |
| Figure S18: Mass spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (7) | 11 |
| Figure S19: IR spectrum of (<i>E</i>)- <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (8) and <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (9) | 12 |
| Figure S20: ^1H NMR spectrum of (<i>E</i>)- <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (8) and <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (9) | 12 |
| Figure S21: ^{13}C NMR spectrum of (<i>E</i>)- <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (8) and <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (9) | 13 |
| Figure S22: IR spectrum of <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (9) | 13 |
| Figure S23: ^1H NMR spectrum of <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (9) | 14 |
| Figure S24: ^{13}C NMR spectrum of <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (9) | 14 |
| Figure S25: Mass spectrum of <i>N</i> -(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (9) | 15 |

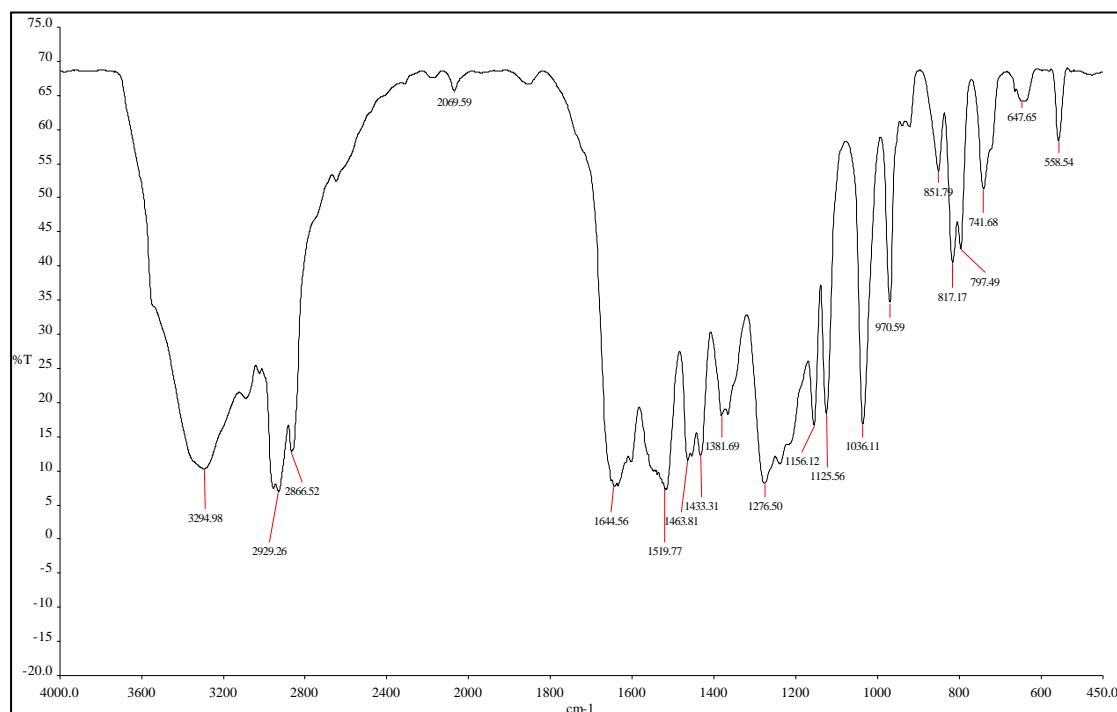


Figure S1: IR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-ena-mide (**1**) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (**2**)

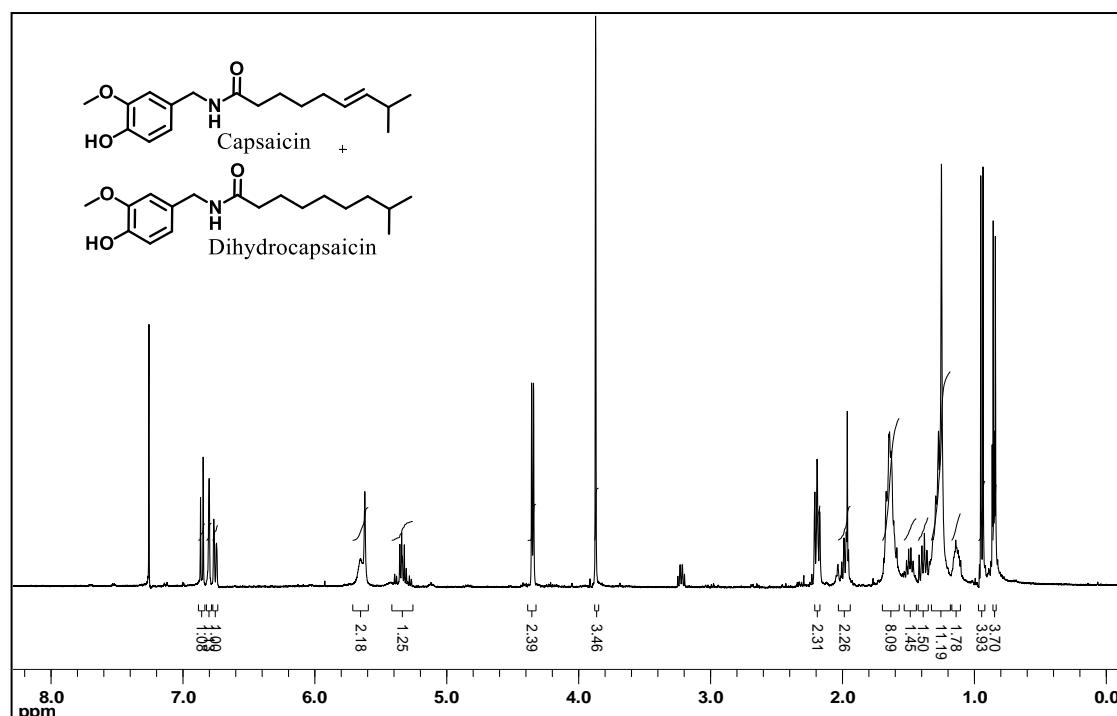


Figure S2: ^1H NMR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-ena-mide (**1**) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (**2**)

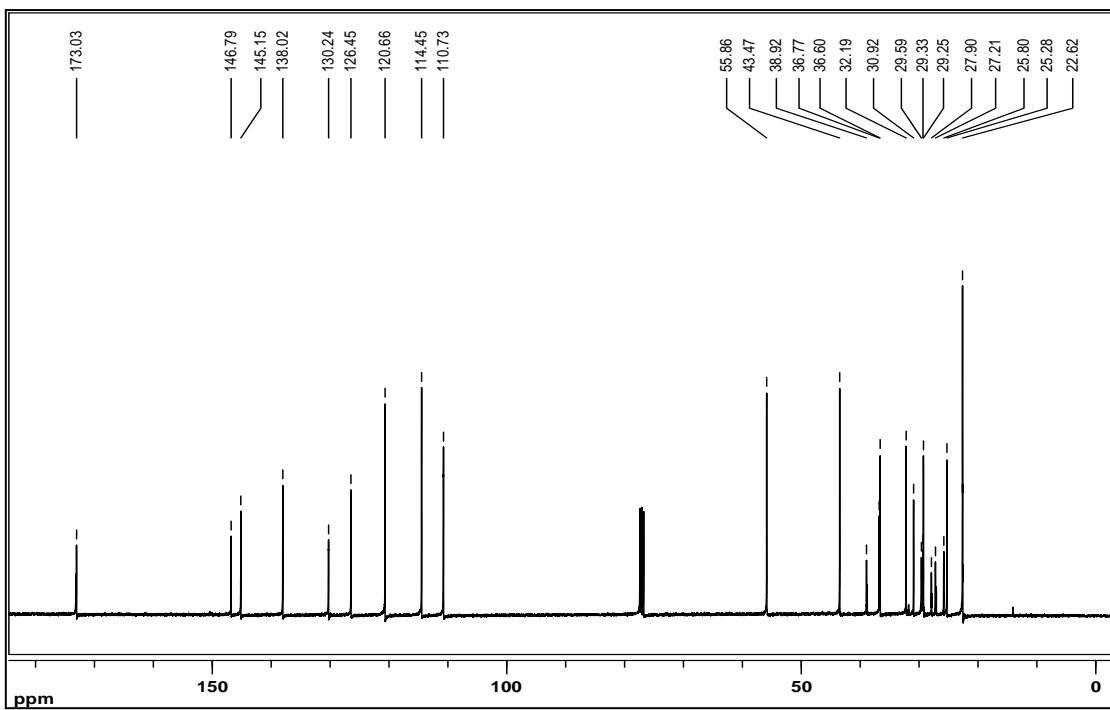


Figure S3: ^{13}C NMR spectrum of (*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**1**) and *N*-(4-hydroxy-3-methoxybenzyl)-8-methylnonanamide (**2**)

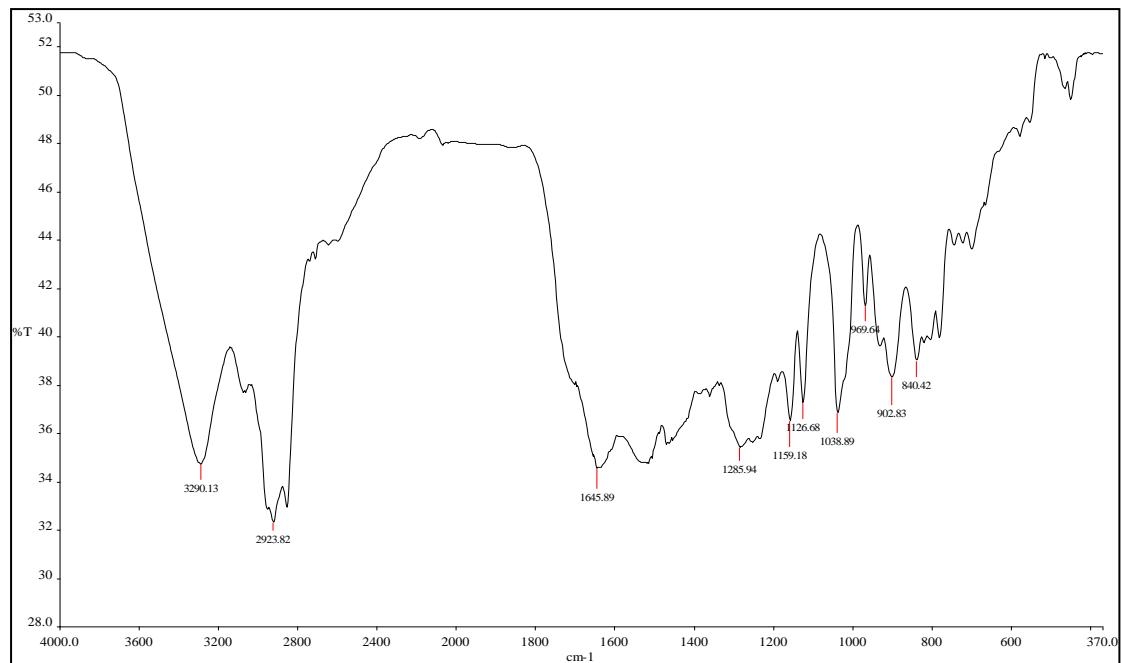


Figure S4: IR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnon-6-enamide (**3**) and *N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (**4**)

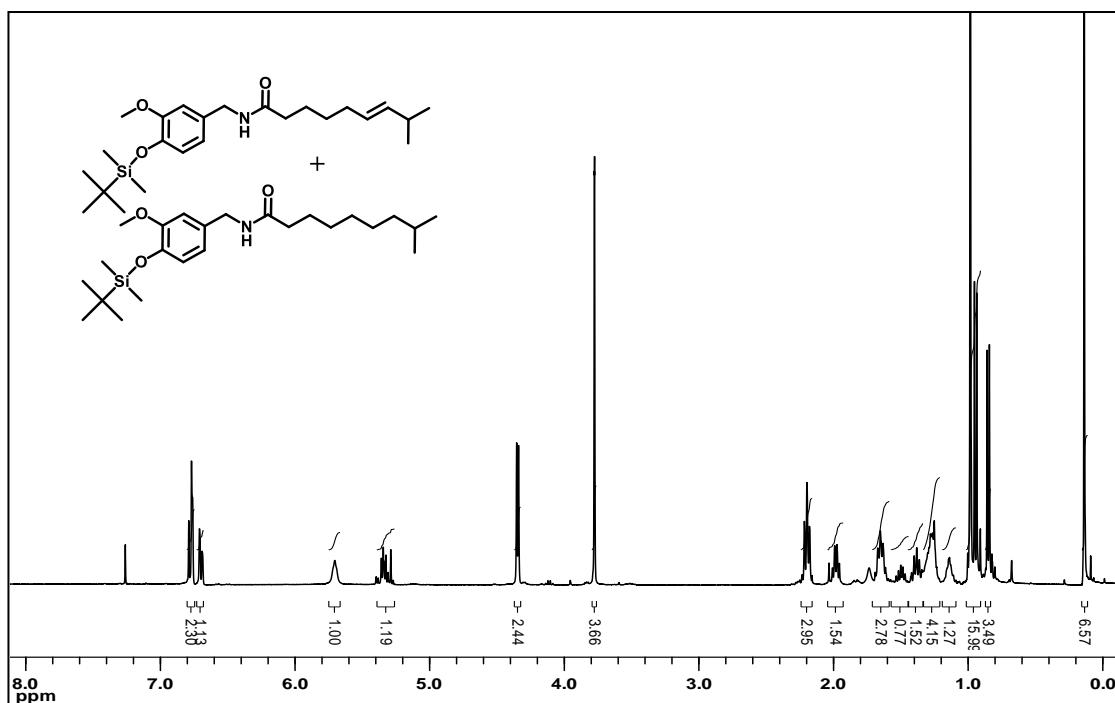


Figure S5: ^1H NMR spectrum of *(E)-N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnon-6-enamide (**3**) and *N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (**4**)

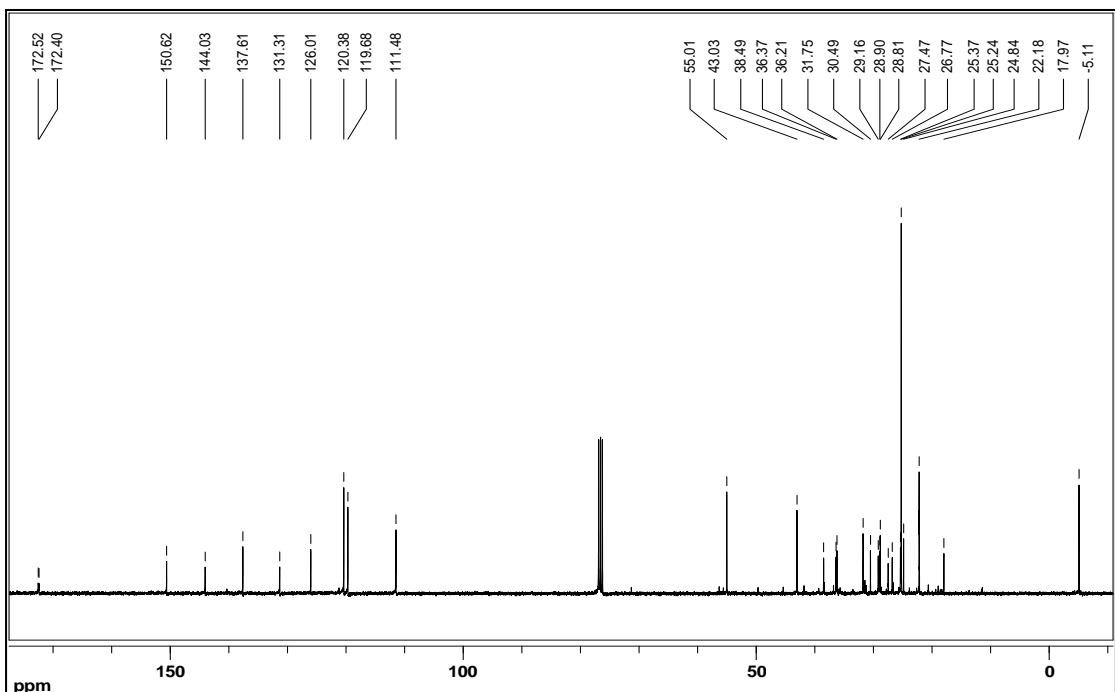


Figure S6: ^{13}C NMR spectrum of *(E)-N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnon-6-enamide (**3**) and *N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-8-methylnonanamide (**4**)

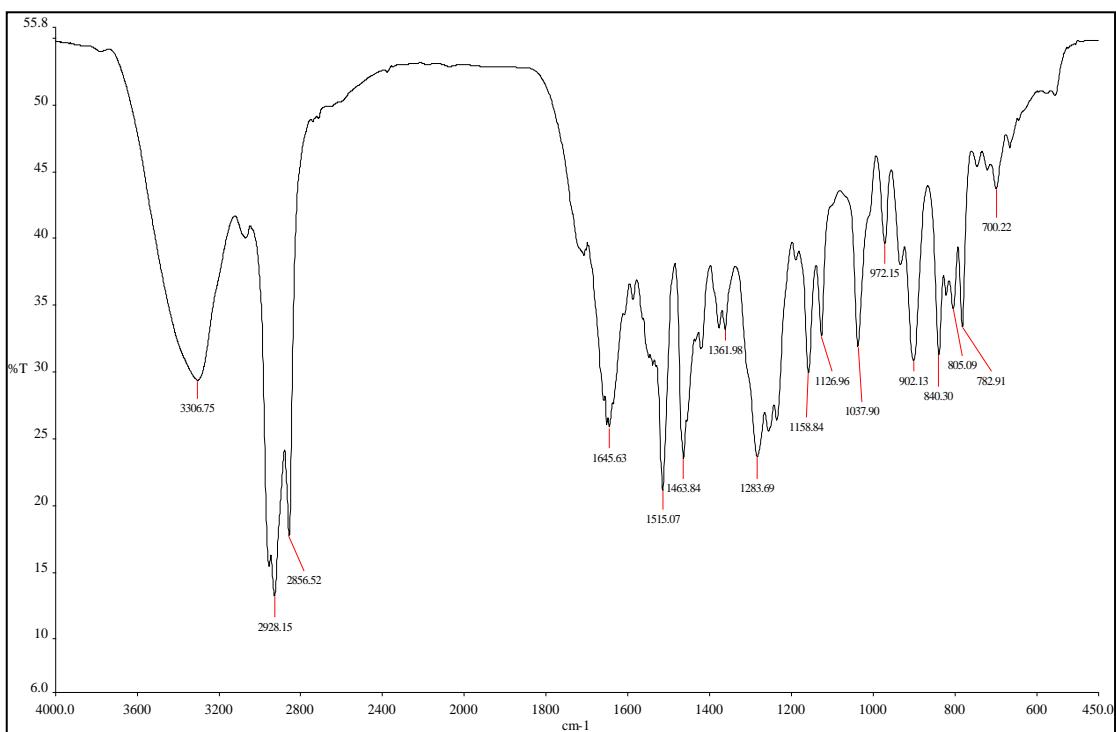


Figure S7: IR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

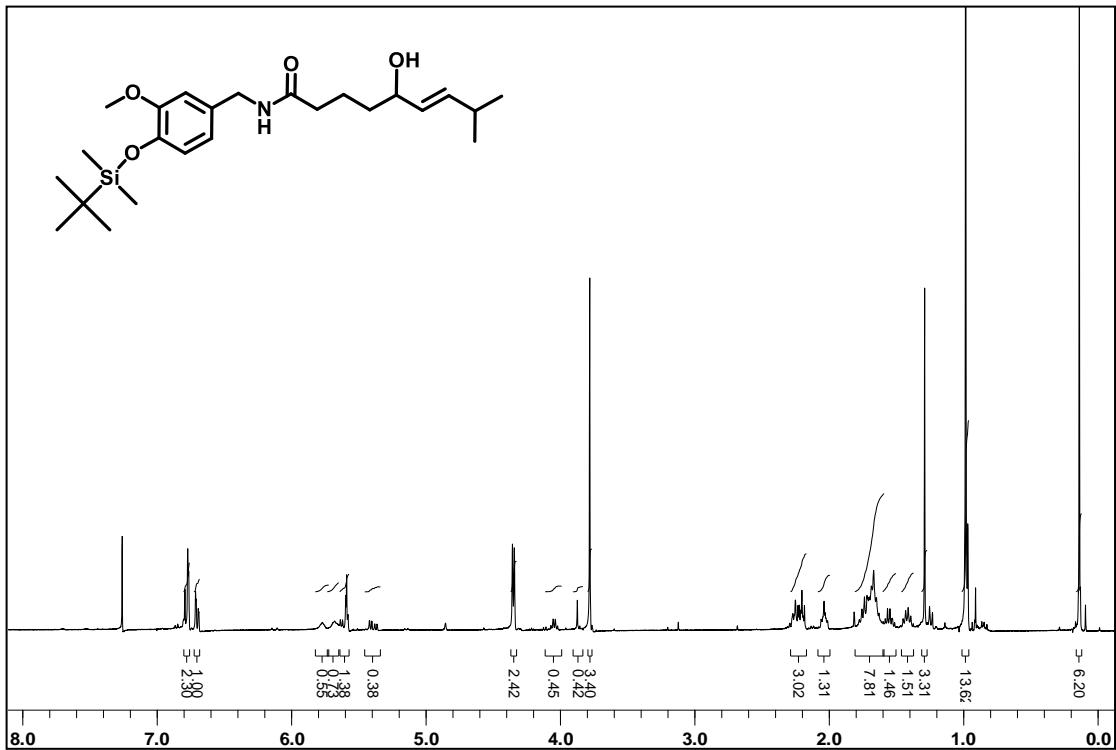


Figure S8: ^1H NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxybenzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

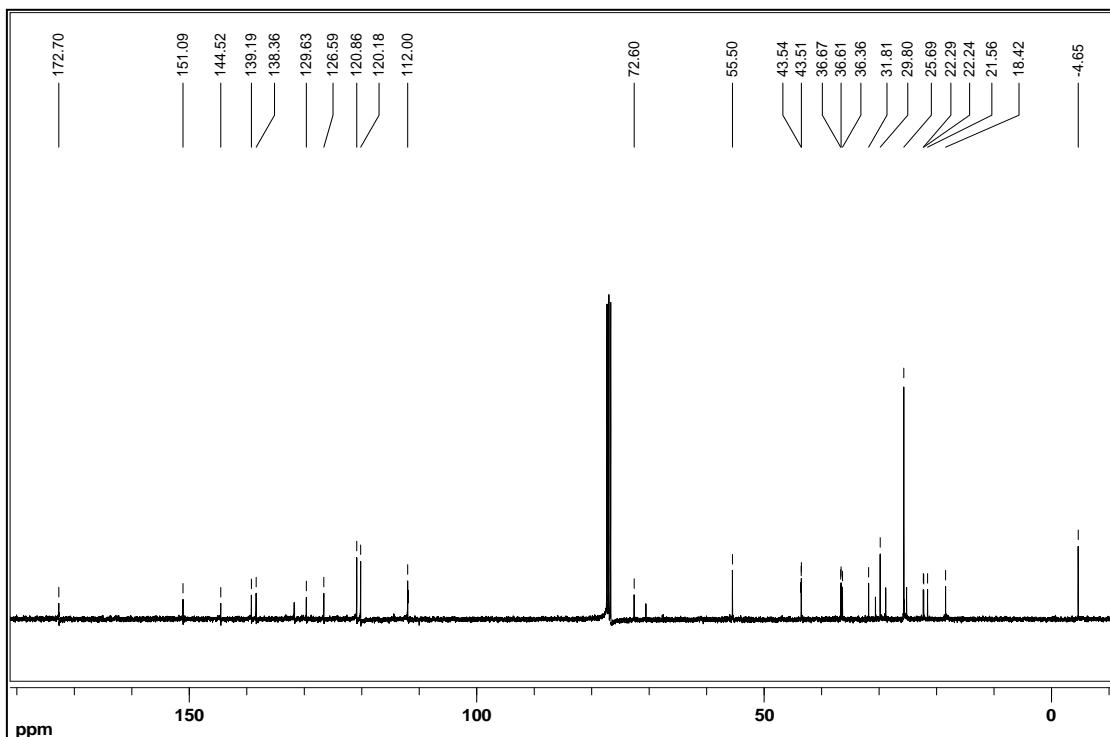


Figure S9: ^{13}C NMR spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

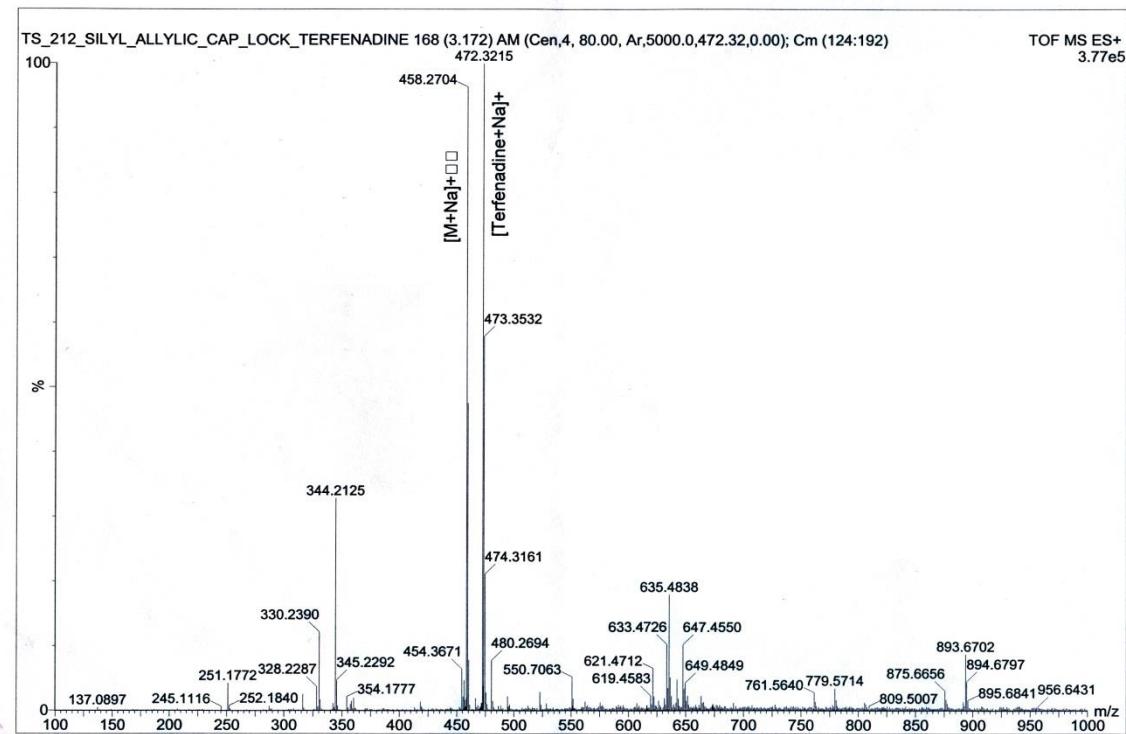


Figure S10: Mass spectrum of (*E*)-*N*-(4-(*tert*-butyldimethylsilyloxy)-3-methoxy-benzyl)-5-hydroxy-8-methylnon-6-enamide (**5**)

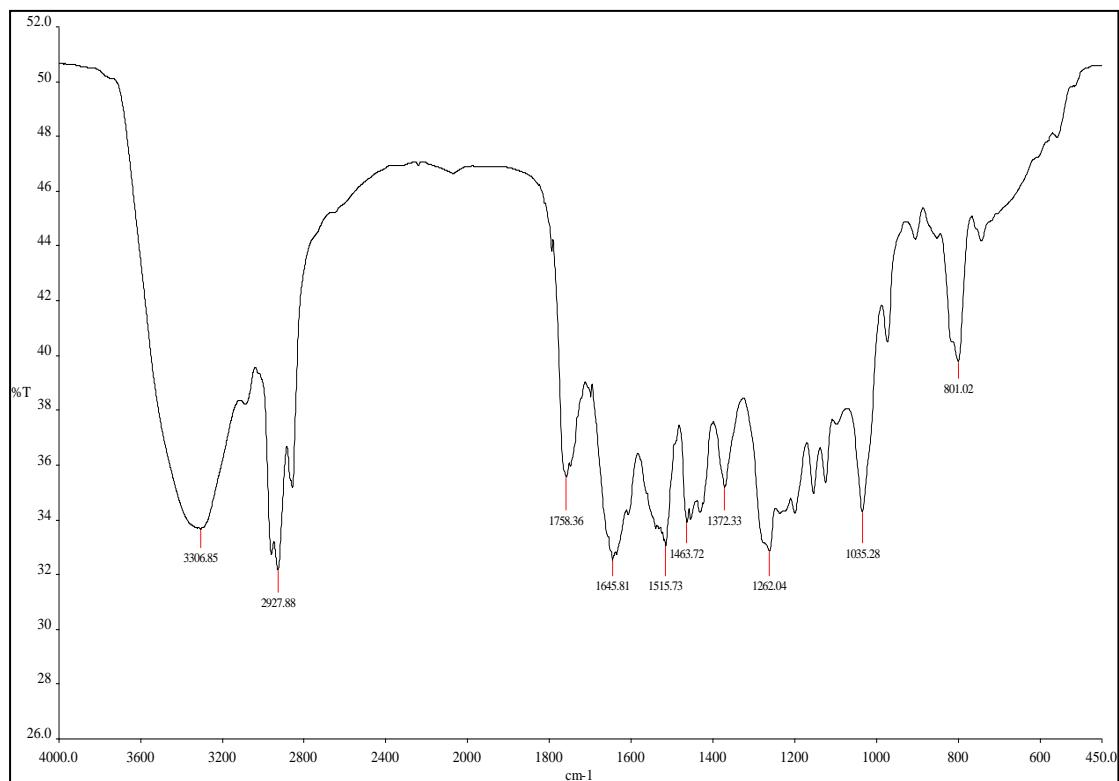


Figure S11: IR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

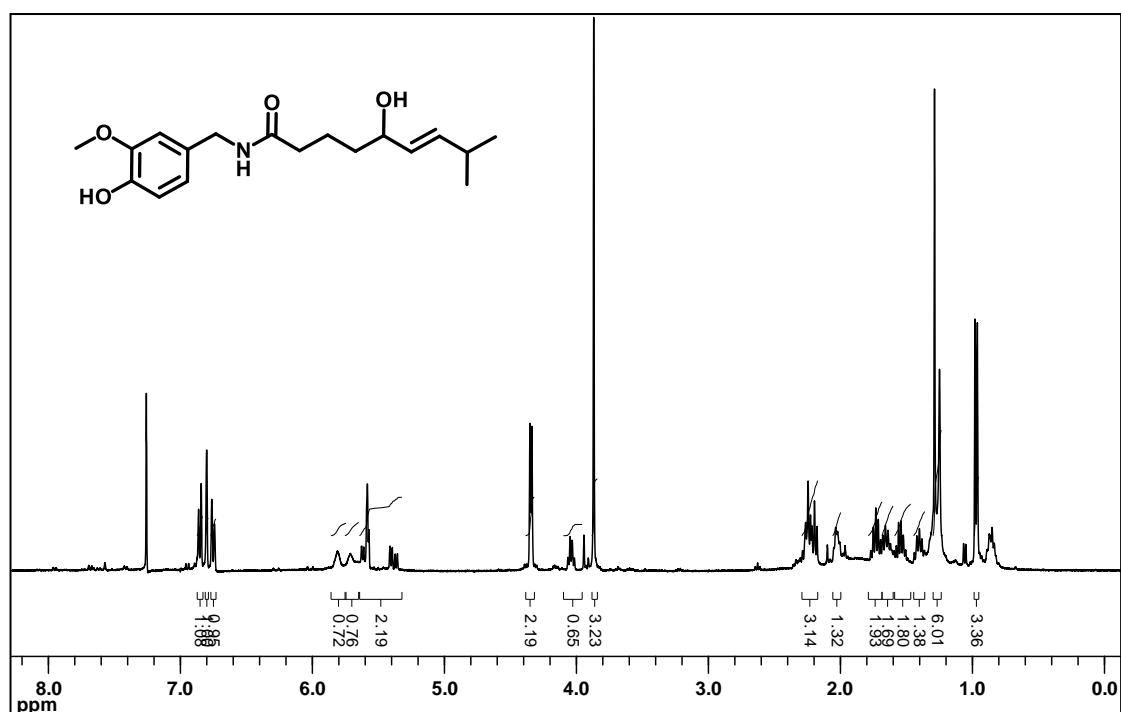


Figure S12: ¹H NMR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

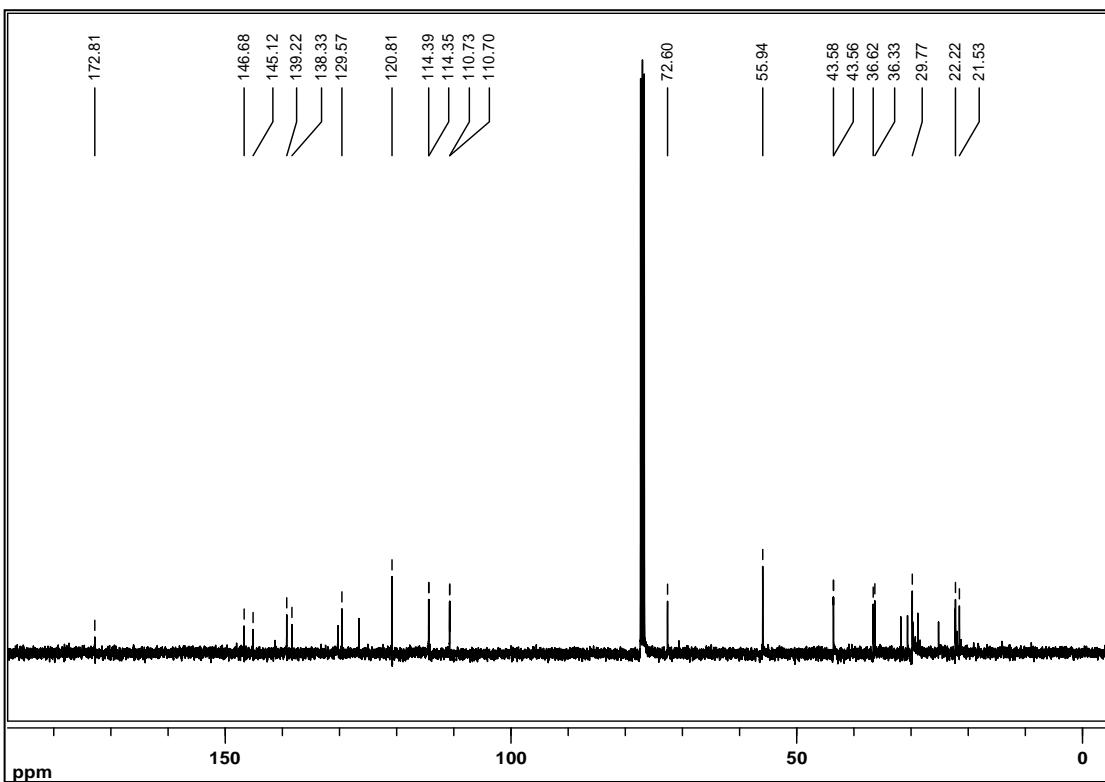


Figure S13: ^{13}C NMR spectrum of (*E*)-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

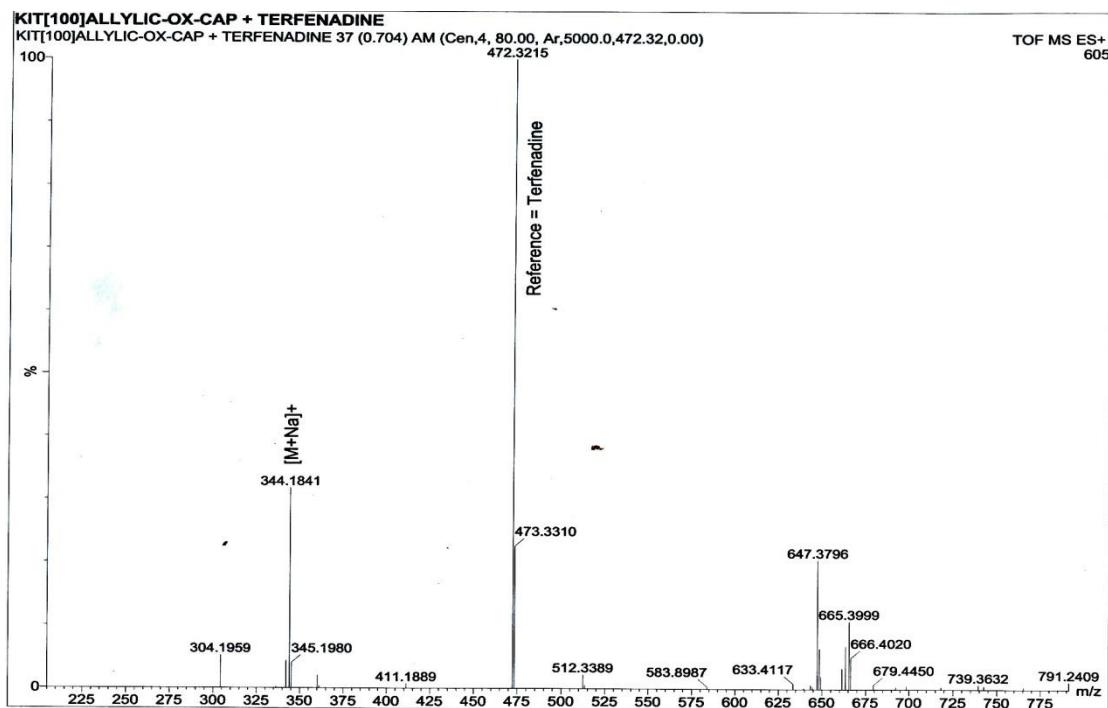


Figure S14: Mass spectrum of (*E*-5-hydroxy-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide (**6**)

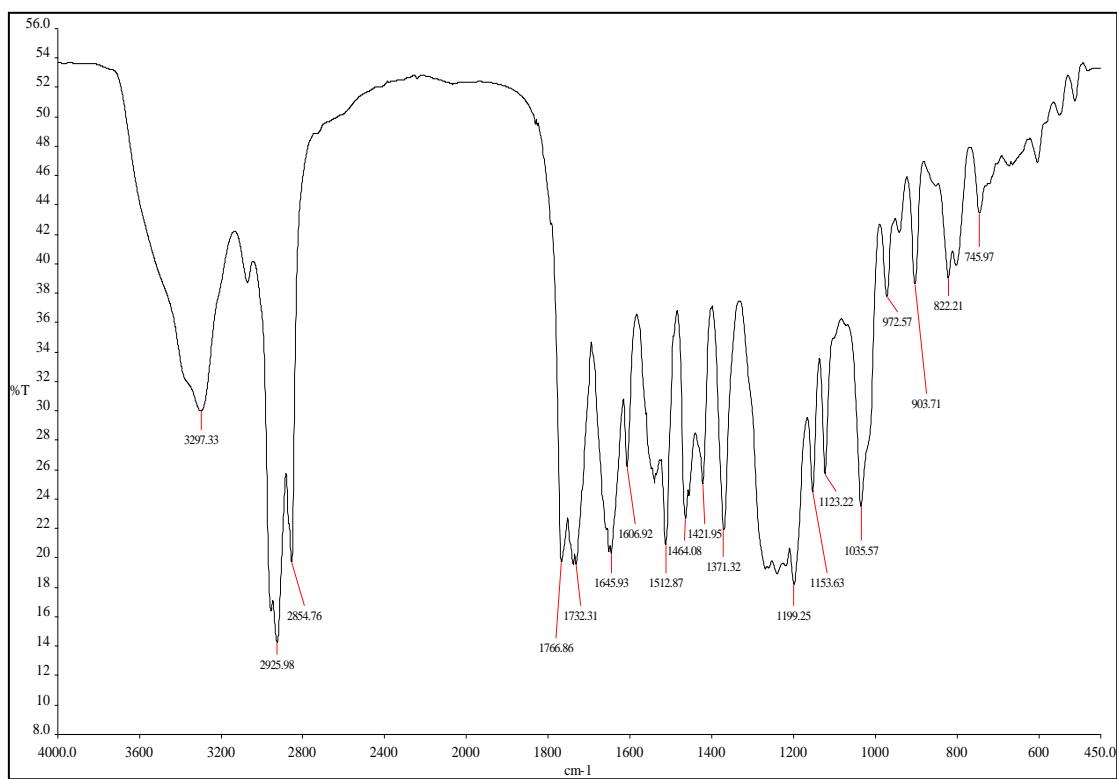


Figure S15: IR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (**7**)

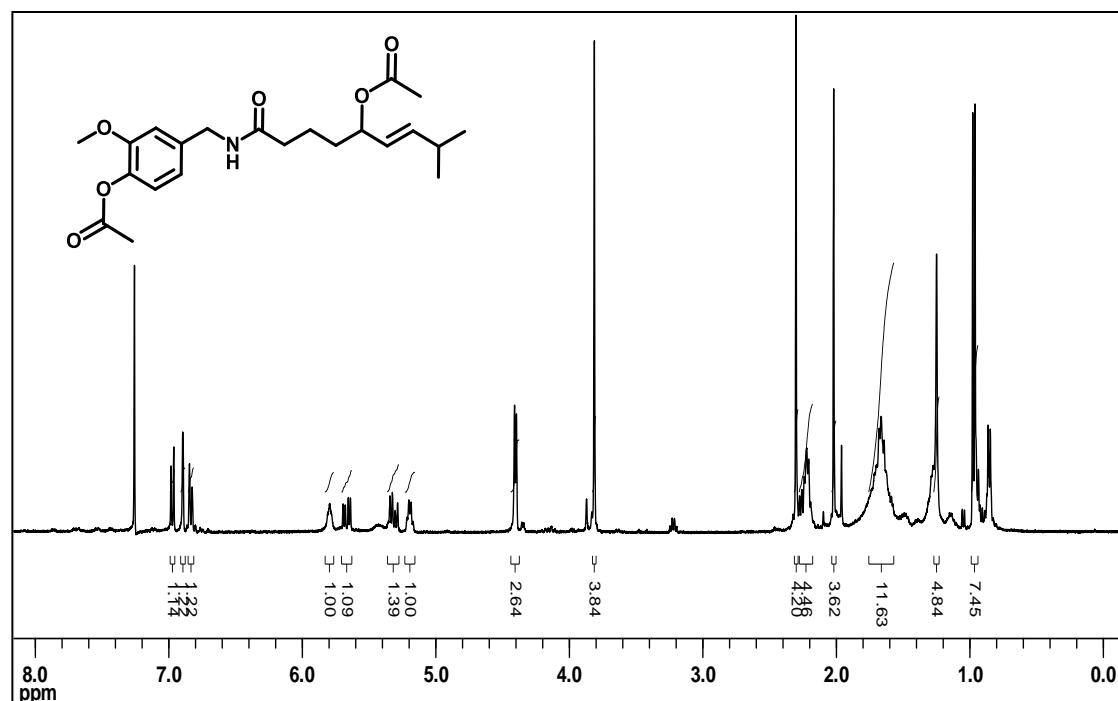


Figure S16: ¹H NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxononan-4-yl acetate (**7**)

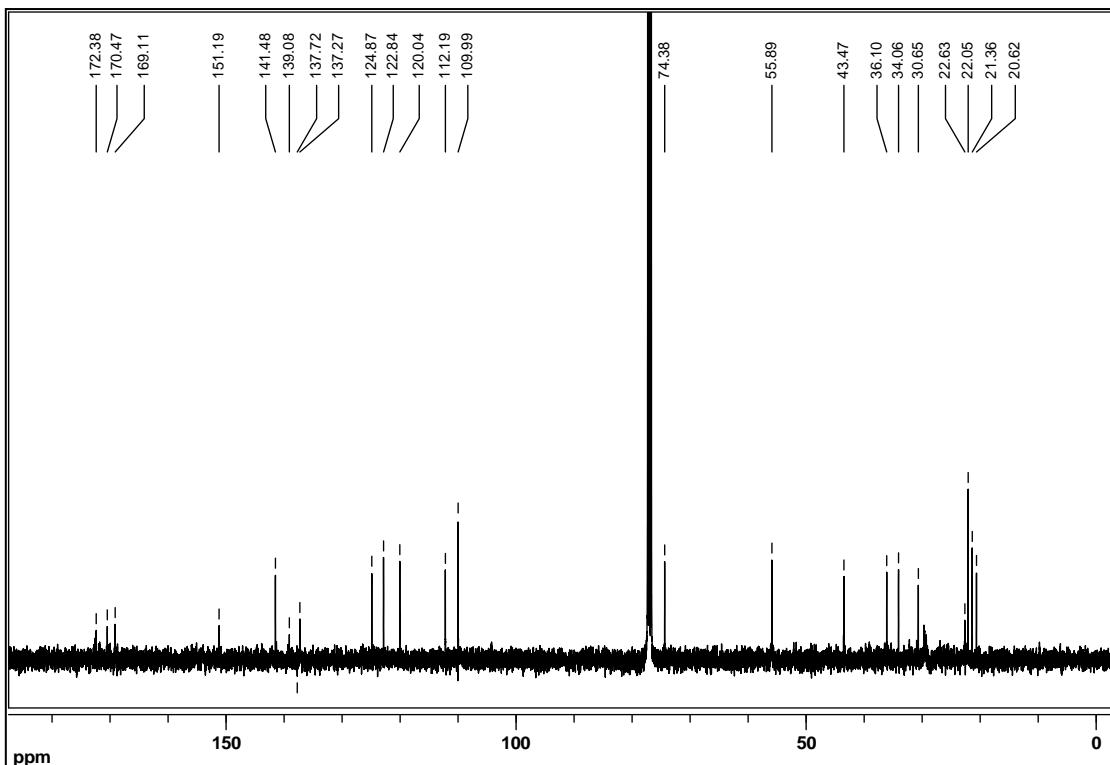


Figure S17: ^{13}C NMR spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxonanonan-4-yl acetate (**7**)

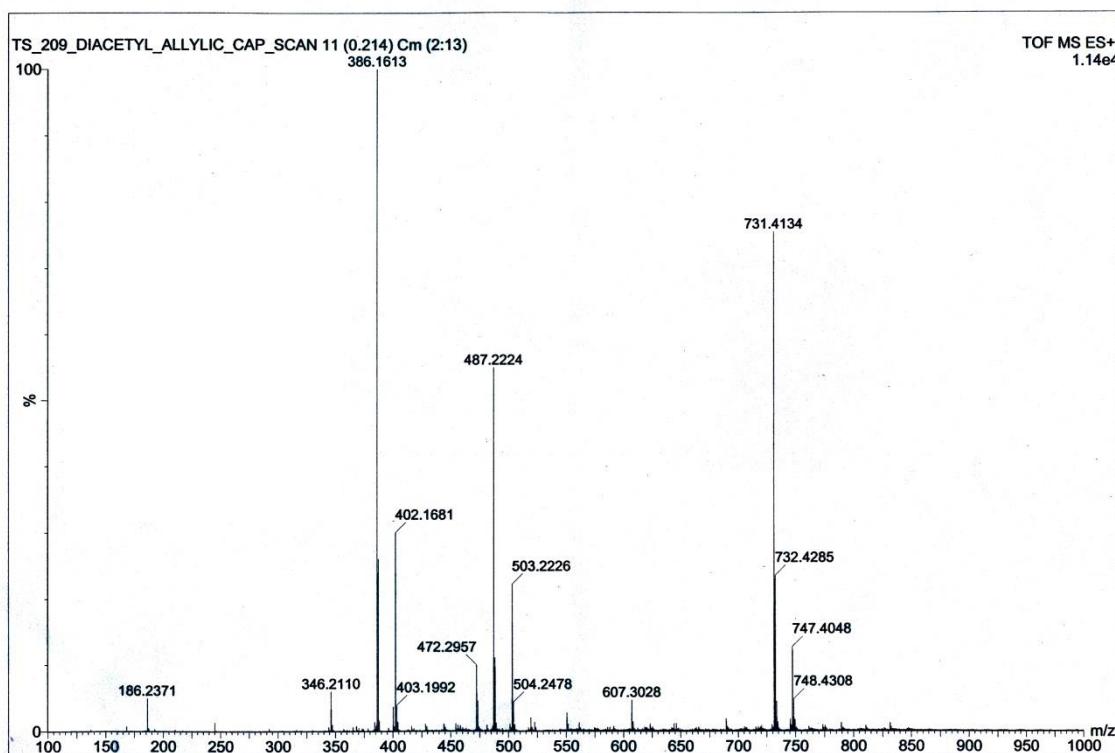


Figure S18: Mass spectrum of 9-(4-acetoxy-3-methoxybenzylamino)-2-methyl-9-oxonanonan-4-yl acetate (**7**)

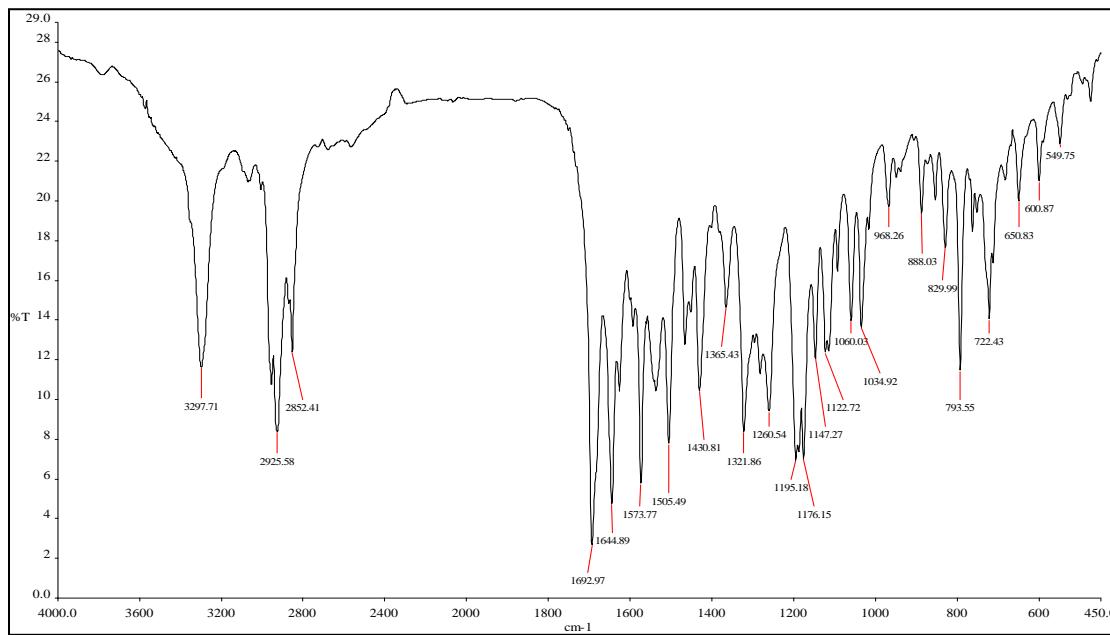


Figure S19: IR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

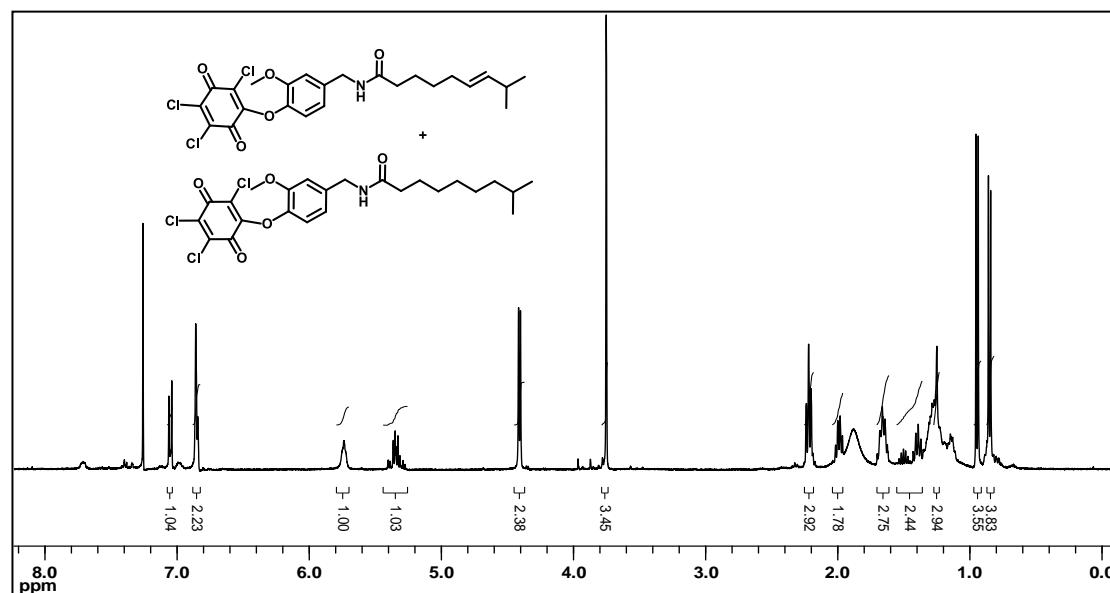


Figure S20: ¹H NMR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

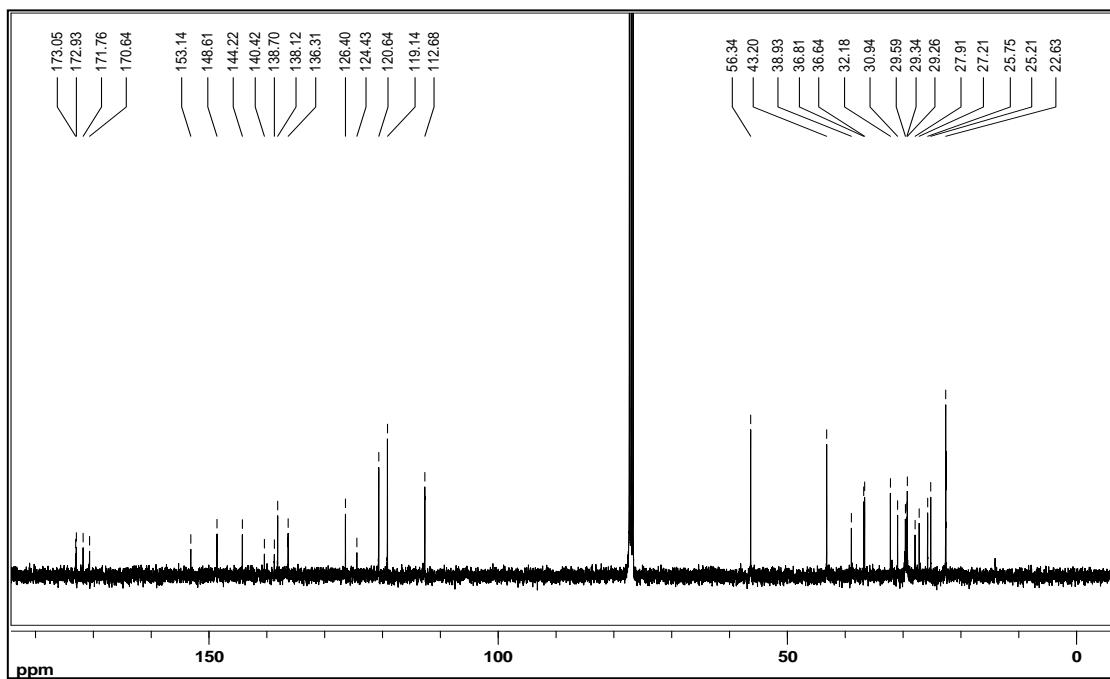


Figure S21: ^{13}C NMR spectrum of (*E*)-*N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnon-6-enamide (**8**) and *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

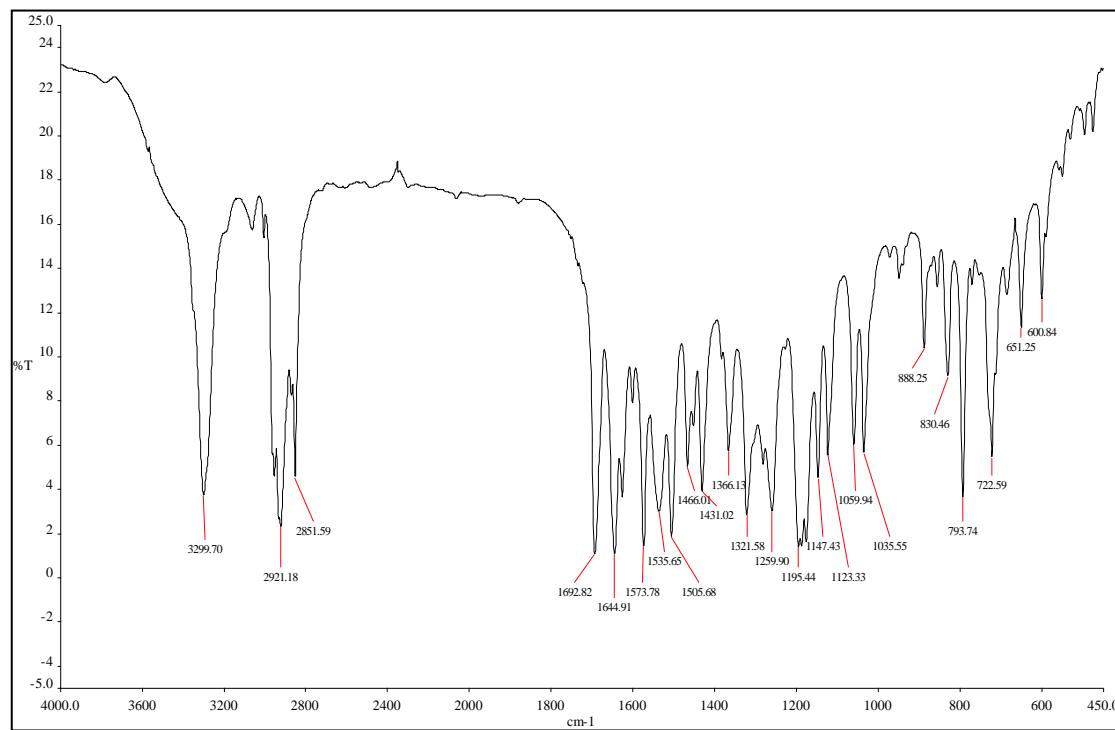


Figure S22: IR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

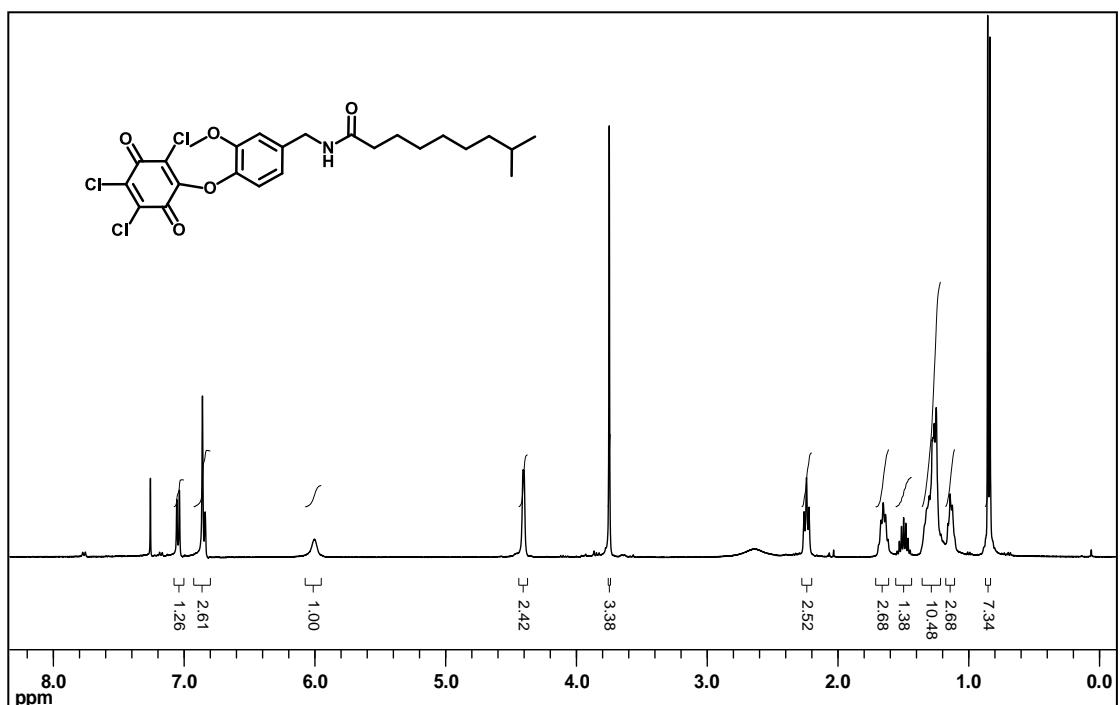


Figure S23: ¹H NMR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

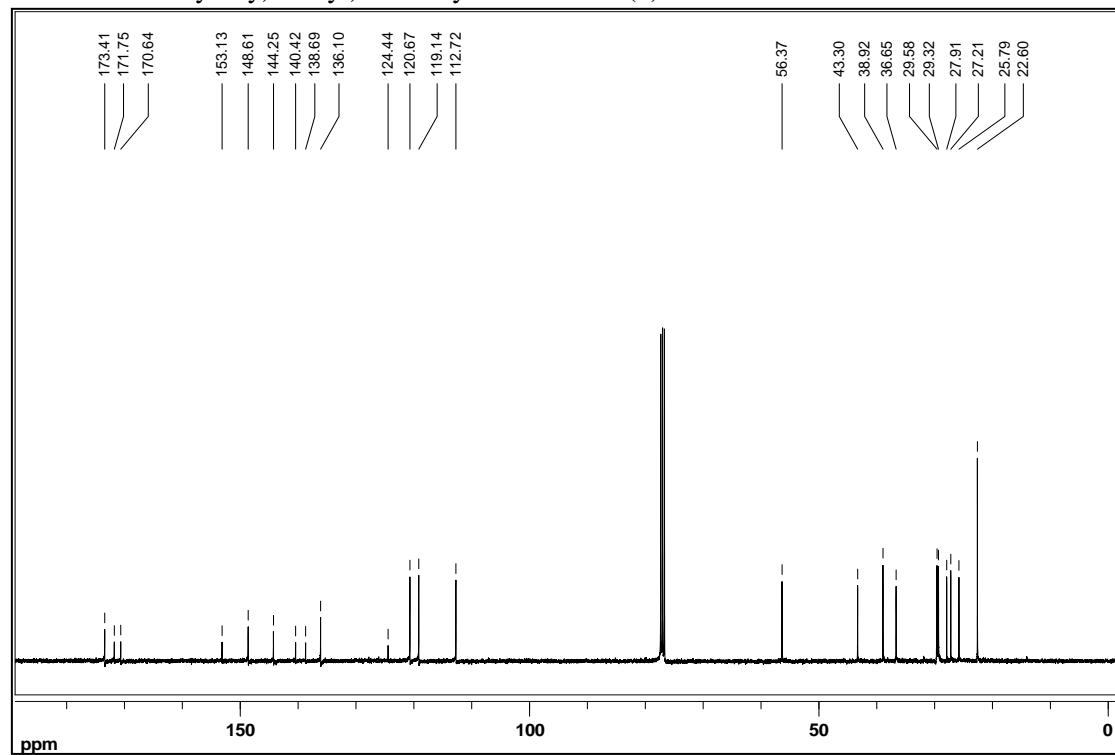


Figure S24: ¹³C NMR spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)

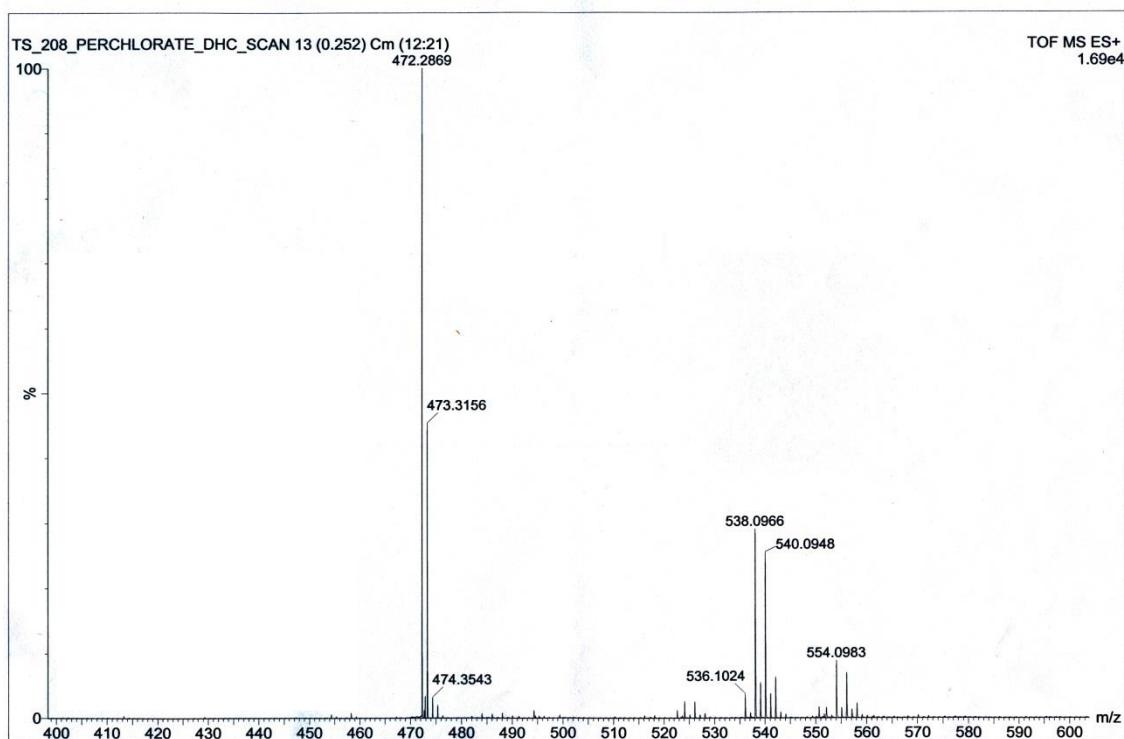


Figure S25: Mass spectrum of *N*-(3-methoxy-4-(2,4,5-trichloro-3,6-dioxocyclohexa-1,4-dienyloxy)benzyl)-8-methylnonanamide (**9**)