Supporting Information

Design, synthesis, antibacterial and antiviral evaluation of chalcone derivatives containing benzoxazole

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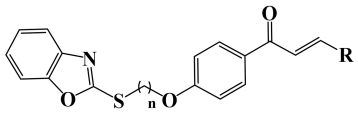
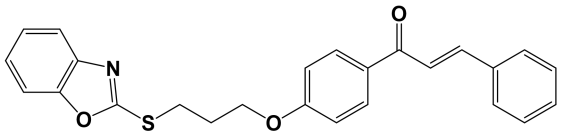
Abbreviation

	abbreviation	full name
1	^{1}H NMR	^{1}H nuclear magnetic resonance
2	^{13}C NMR	^{13}C nuclear magnetic resonance
3	^{19}F NMR	^{19}F nuclear magnetic resonance
4	HRMS	High-resolution mass spectrometry
5	*Xac*	*Xanthomonas axonopodis pv. Citri*
6	*Xoo*	*Xanthomonas oryzae pv.oryzae*
7	*Psa*	*pseudomonas syringae pv.actinidiae*
8	*Ac*	*Acidovorax citrulli*
9	*Rs*	*Ralstonia solanacearum*
10	*Pcb*	*Pectobacterium carotovorum subsp. brasiliense*
11	*Xcm*	*Xanthomonas campestris pv. mangiferae indicae*
12	TMV	Tobacco mosaic virus
13	TMV-CP	Tobacco mosaic virus coat protein
14	NNM	Ningnanmycin
15	EC_{50}	Median effective concentration
16	SEM	Scanning electron microscopy
17	EPS	Exopolysaccharide
18	m.p.	Melting point
19	DMSO	Dimethylsulfoxide
20	SAR	Structure–activity relationship

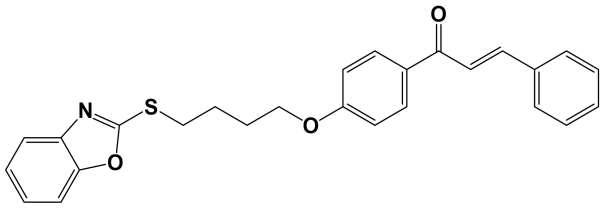
Structure and physical property of Z1-Z24

Compounds					
	n	R	Physical	m.p.(℃)	Yelid(%)
Z1	3	Ph	Yellow solid	79.2-80.9	53
Z2	4	Ph	Yellow solid	96.6-98.2	57
Z3	3	4-CH_3-Ph	White solid	85.7-87.1	62
Z4	4	4-CH_3-Ph	White solid	104.8-106.2	74
Z5	3	4-OCH_3-Ph	White solid	85.2-86.8	33
Z6	3	4-F-Ph	Yellow solid	110.3-112.1	63
Z7	4	4-F-Ph	Yellow solid	127.2-128.5	67
Z8	3	4-Br-Ph	Yellow solid	92.6-93.9	65
Z9	3	3-CH_3-Ph	Yellow solid	59.4-61.1	50
Z10	4	3-CH_3-Ph	Yellow solid	72.6-74.1	56
Z11	3	3-OCH_3-Ph	Yellow solid	88.8-90.6	82
Z12	4	3-OCH_3-Ph	White solid	80.7-82.4	78
Z13	4	3-F-Ph	Yellow solid	78.4-79.6	71
Z14	4	3-NO_2-Ph	Red solid	133.1-134.9	93
Z15	3	3-Cl-Ph	Yellow solid	80.1-80.5	71
Z16	4	3-Cl-Ph	Yellow solid	98.1-99.7	85
Z17	3	3-Br-Ph	Yellow solid	85.2-87.1	72
Z18	4	3-Br-Ph	Yellow solid	93.9-95.1	62
Z19	3	2-CH_3-Ph	White solid	82.5-84.2	48
Z20	4	2-CH_3-Ph	White solid	112.3-113.6	47
Z21	3	2-Fruan	Brown solid	81.6-82.8	64
Z22	4	2-Fruan	Brown solid	94.9-96.8	85
Z23	3	2-Thioen	Yellow solid	71.9-73.8	58
Z24	4	2-Thioen	Yellow solid	95.7-96.4	52

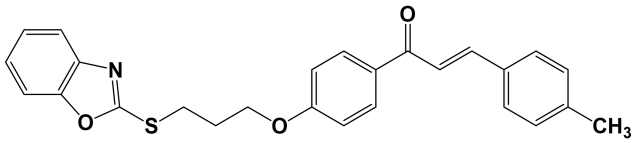
1. Spectra data of target compounds Z1-Z24



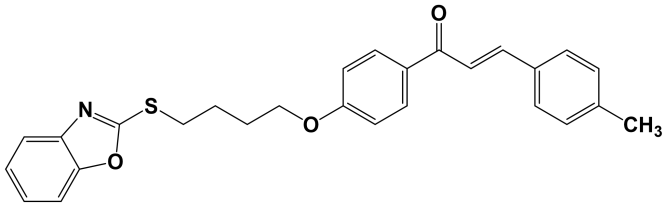
(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-phenylprop-2-en-1-one (Z1).Yellow solid, m.p.79.2-80.9℃; yelid53%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.14 – 8.11 (m, 2H, Ph-H), 7.91 (d, *J* = 15.6 Hz,1H, Ph-CH=), 7.86 – 7.82 (m,1H, Ph-H), 7.67 (d, *J* = 15.6 Hz, 1H, =CH-CO-Ph), 7.60 – 7.56 (m, 2H, Ph-H), 7.41 (dt, *J* = 3.5, 1.7 Hz, 3H, Ph-H), 7.30 – 7.23 (m, 2H, Ph-H), 7.08 – 7.04 (m, 2H, Ph-H), 4.20 (t, *J* = 6.0 Hz, 2H, -O-CH_2-), 3.46 (t, *J* = 7.1 Hz, 2H, -CH_2-S-), 2.29 – 2.22 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126MHz, DMSO-d_6) δ 187.8 (s), 164.7 (s), 162.9 (s), 151.7 (s), 143.7 (s), 141.8 (s), 135.3 (s), 131.4 (s), 130.9 (s), 129.4 (s), 129.3 (s),125.1 (s), 124.7 (s), 122.4 (s), 118.7 (s), 115.0 (s), 110.6 (s), 66.7 (s), 29.1 (s), 29.0 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{25}H_{21}NO_3S$: 416.13149, found: 416.13065.



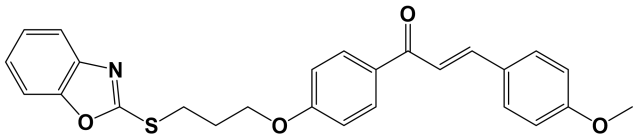
(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-phenylprop-2-en-1-one (Z2); Yellow solid; m.p.96.6-98.2; Yelid%: 54%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 – 8.10 (m, 2H, Ph=H), 7.91 (d, *J* = 15.6 Hz, 1H, Ph-Ch=), 7.84 (dd, *J* = 7.2, 2.2 Hz, 2H, Ph-H), 7.67 (d, *J* = 15.6 Hz, 1H, =CH-CO-Ph), 7.61 – 7.57 (m, 2H, Ph-H), 7.41 (dd, *J* = 5.2, 1.9 Hz, 3H, Ph-H), 7.30 – 7.25 (m, 2H, Ph-H), 7.03 (d, *J* = 8.9 Hz, 2H, Ph-H), 4.11 (t, *J* = 6.0 Hz, 2H, Ph-O-CH_2-), 3.38 (t, *J* = 6.9 Hz, 2H, -CH_2-S-Ph), 1.95 – 1.86 (m, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.9 (s), 163.1 (s), 151.7 (s), 143.6 (s), 141.8 (s), 135.3 (s), 131.4 (s), 130.9 (d, *J* = 14.2 Hz), 129.3 (d, *J* = 10.8 Hz), 125.1 (s), 124.7 (s), 122.5 (s), 118.7(s), 114.9 (s), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s), 26.2 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}NO_3S$; HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{26}H_{23}NO_3S$: 430.14714, found: 430.14655.



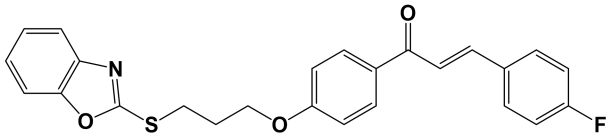
(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(p-tolyl)prop-2-en-1-one (Z3); White solid; m.p. 85.7-87.1℃; yelid: 64%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.11 (d, J = 8.8 Hz, 2H, Ph-H), 7.85 (d, J = 15.5 Hz, 1H, Ph-CH=), 7.73 (d, J = 8.1 Hz, 2H, Ph-H), 7.64 (d, J = 15.5 Hz, 1H, =CH-CO-Ph), 7.58 (dt, J = 4.4, 1.6 Hz,2H, Ph-H), 7.30 – 7.25 (m, 2H, Ph-H), 7.22 (d, J = 8.0 Hz, 2H, Ph-H), 7.05 (d, J = 8.9 Hz, 2H, Ph-H), 4.20 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph),2.30 (s, 3H, Ph-CH_3), 2.28 – 2.23 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.7 (s), 162.8 (s), 151.7 (s), 143.7 (s), 141.8 (s), 141.0 (s), 132.6 (s), 131.4 (s), 131.1 (s), 130.0 (s), 129.3 (s), 125.1 (s), 124.7 (s), 121.4 (s), 118.7 (s), 114. (s), 110.6 (s), 66.7 (s), 29.1 (s), 29.0 (s), 21.6 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}NO_3S$; HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{26}H_{23}NO_3S$: 430.14714, found: 430.20483.



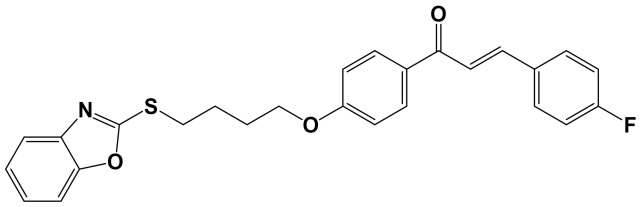
(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(p-tolyl)prop-2-en-1-one (Z4);White solid; m.p. 104.8-106.2℃; Yelid: 74%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.10 (d, J = 8.9 Hz, 2H, Ph-H), 7.85 (d, J = 15.5 Hz, 1H, Ph-CH=), 7.73 (d, J = 8.1 Hz, 2H, Ph-H), 7.64 (d, J = 15.5 Hz, 1H, =CH-CO-Ph), 7.60 – 7.57 (m, 2H, Ph-H), 7.27 (ddd, J = 11.2, 6.3, 3.6 Hz, 2H, Ph-H), 7.02 (d, J = 8.9 Hz, 2H, Ph-H), 4.10 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.38 (t, J = 6.9 Hz, 2H, -CH_2-S-Ph), 2.30 (s, 3H, Ph-CH_3), 1.90 (tdd, J = 13.6, 8.5, 5.4 Hz, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.9 (s), 163.0 (s), 151.7 (s), 143.7 (s), 141.8 (s), 141.0 (s), 132.6 (s), 131.4 (s), 130.9 (s), 130.0 (s), 129.3 (s), 125.1 (s), 124.7 (s), 121.4 (s), 118.7 (s), 114.9 (s), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s), 26.1 (s), 21.6 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{27}H_{25}NO_3S$; 444.16279, found:444.16107.



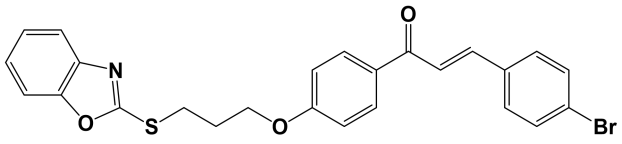
(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Z5); White solid; m.p. 85.2-86.8℃; Yelid: 33%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.11 – 8.09 (m, 2H, Ph-H), 7.82 – 7.78 (m, 3H, Ph-H), 7.75 (s, 1H, Ph-CH=), 7.64 (d, J = 15.5 Hz, 1H, =CH-CO-Ph), 7.58 (ddd, J = 6.3, 2.8, 1.6 Hz, 2H, Ph-H), 7.30 – 7.24 (m, 2H, Ph-H), 7.05 (d, J = 8.9 Hz, 2H, Ph-H), 6.98 – 6.96 (m, 2H, Ph-H), 4.20 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.77 (s, 3H, Ph-O-CH_3), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.25 (dd, J = 13.3, 6.6 Hz, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.7 (s), 164.7 (s), 162.7 (s), 161.7 (s), 151.7 (s), 143.7 (s), 141.8 (s), 131.3 (s), 131.2 (s), 127.9 (s), 125.1 (s), 124.7 (s), 119.9 (s), 118.7 (s), 114.9 (d, J = 6.4 Hz), 110.7 (s), 66.7 (s), 55.8 (s), 29.1 (s), 29.0 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}NO_4S$; 446.23619, found: 446.14206.



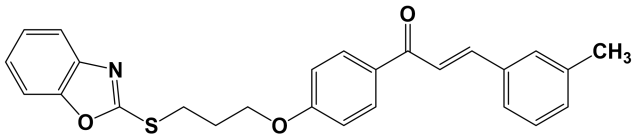
(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(4-fluorophenyl)prop-2-en-1-one (Z6);Yellow solid; m.p. 110.3-112.1℃; Yelid: 63%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 – 8.11 (m, 2H, Ph-H), 7.94 – 7.91 (m, 2H, Ph-H), 7.88 (d, J = 15.6 Hz, 1H, PH=CH-), 7.67 (d, J = 15.6 Hz, 1H, =CH-CO-Ph), 7.60 – 7.56 (m, 2H, Ph-H), 7.28 – 7.24 (m, 4H, Ph-H), 7.06 (d, J = 8.8 Hz, 2H, Ph-H), 4.20 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.25 (dd, J = 13.3, 6.6 Hz, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.7 (s), 164.8 (s), 164.7 (s),163.0 (s), 162.9 (s), 162.8 (s),151.7 (s), 142.4 (s), 141.8 (s), 132.0 (s), 131.7 (s),131.65(s),131.5 (s),130.9 (s), 125.1 (s), 124.7 (s), 122.3 (s), 118.7 (s), 116.5 (s), 116.3 (s), 115.0 (s), 110.6 (s), 66.7 (s), 29.1 (s), 28.9 (s); ^{19}F NMR (471 MHz, DMSO-d_6) δ -109.80 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{25}H_{20}FNO_3S$; 434.12207, found: 432.12189.



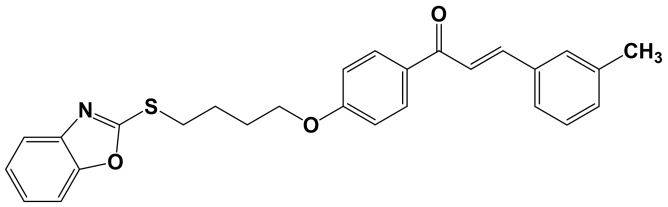
(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(4-fluorophenyl)prop-2-en-1-one (Z7); Yellow solid; m.p.127.2-128.5℃; Yelid: 67%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.11 (d, J = 8.9 Hz, 2H, Ph-H), 7.92 (dd, J = 8.7, 5.7 Hz, 2H, Ph-H), 7.87 (d, J = 15.6 Hz,1H, Ph-CH=), 7.66 (d, J = 15.6 Hz, 1H, =CH-CO), 7.58 (dd, J = 6.8, 2.1 Hz, 2H, Ph-H), 7.26 (dt, J = 12.7, 5.5 Hz, 4H, Ph-H), 7.03 (d, J = 8.9 Hz, 2H, Ph-H), 4.10 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.37 (d, J = 7.1 Hz, 2H, -CH_2-S-Ph), 1.93 – 1.86 (m, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.7 (s), 164.9 (s), 163.1 (s), 162.8 (s), 151.7 (s), 142.4 (s), 141.8 (s), 132.0 (s), 132.0 (s),131.9 – 131.3 (m), 130.8 (s), 125.1 (s), 124.7 (s),122.3 (s), 118.7 (s), 116.51 (s), 116.3 (s), 114.9 (s), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s), 26.1 (s); ^{19}F NMR (471 MHz, DMSO-d_6) δ -109.8(s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{22}FNO_3S$; 448.13772, found: 448.13635.



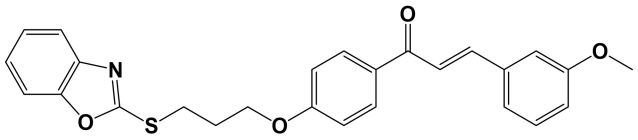
(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(4-bromophenyl)prop-2-en-1-one (Z8); Yellow solid; m.p. 92.6-93.9℃; Yelid: 65%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.12 (d, J = 8.9 Hz, 2H, Ph-H), 7.95 (d, J = 15.6 Hz, 1H, Ph-CH=), 7.82 – 7.80 (m, 2H, Ph-H), 7.65 (s, 1H, =CH-CO-Ph), 7.62 – 7.60 (m, 2H, Ph-H), 7.59 – 7.57 (m, 2H, Ph-H), 7.29 – 7.25 (m, 2H, Ph-H), 7.06 (d, J = 8.9 Hz, 2H, Ph-H), 4.21 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.28 – 2.23 (m, 2h, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.7 (s), 164.7 (s), 163.0 (s), 151.7 (s), 142.3 (s), 141.8 (s), 134.6 (s), 132.3 (s), 131.5 (s), 131.2 (s), 130.9 (s), 125.1 (s), 124.7 (s), 124.3 (s), 123.2 (s), 118.7 (s), 115.0 (s), 110.7 (s), 66.7 (s), 29.1 (s), 28.9 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{25}H_{20}BrNO_3S$; 494.04200, found: 494.04205.



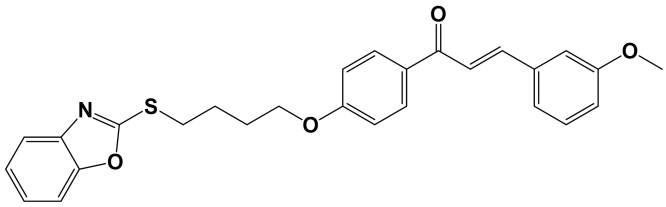
(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(m-tolyl)prop-2-en-1-one (Z9); Yellow solid; m.p. 59.4-61.1℃; Yelid: 50%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 – 8.11 (m, 2H, Ph-H), 7.89 (d, J = 15.6 Hz,1H, Ph-CH=), 7.66 (d, J = 17.1 Hz, 2H, Ph-H), 7.62 (s, 1H, =CH-CO), 7.58 (dt, J = 4.5, 1.7 Hz, 2H, Ph-H), 7.28 (ddd, J = 10.3, 7.5, 5.7 Hz, 3H, Ph-H), 7.21 (d, J = 7.5 Hz, 1H, Ph-H), 7.06 (d, J = 8.9 Hz, 2H, Ph-H), 4.20 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.28 – 2.23 (m,2H,-O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.7 (s), 162.9 (s), 151.7 (s), 143.8 (s), 141.8 (s), 138.6 (s), 135.2 (s), 131.7 (s), 131.4 (s), 131.0 (s), 129.6 (s), 129.3 (s), 126.7 (s), 125.1 (s), 124.7 (s), 122.2 (s), 118.7 (s), 115.0 (s), 110.6 (s), 66.7 (s), 29.1 (s), 29.0 (s), 21.4 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{24}NO_3S$; 430.14714, found: 430.14597.



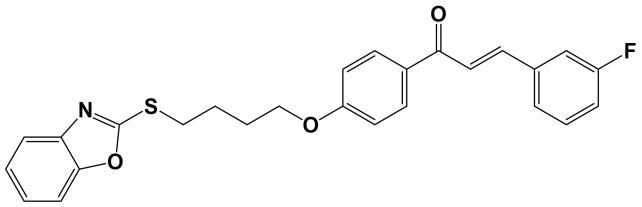
(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(m-tolyl)prop-2-en-1-one (Z10); Yellow solid; m.p. 72.6-74.1℃; Yelid: 62%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.11 (d, J = 8.9 Hz, 2H, -Ph-H), 7.88 (d, J = 15.6 Hz, 1H, Ph-CH=), 7.66 (d, J = 16.9 Hz, 2H, Ph-H), 7.61 (s, 1H, =CH-CO-Ph), 7.58 (dd, J = 7.0, 2.2 Hz, 2H, Ph-H), 7.27 (ddd, J = 9.4, 5.3, 2.5 Hz, 3H, Ph-H), 7.21 (d, J = 7.6 Hz, 1H, Ph-H), 7.02 (d, J = 8.9 Hz, 2H, Ph-H), 4.10 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.39 – 3.37 (m, 2H, -CH_2-S-Ph), 2.31 (s, 3H, Ph-CH_3), 1.93 – 1.86 (m, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.9 (s), 163.1 (s), 151.7 (s), 143.8 (s), 141.8 (s), 138.6 (s), 135.2 (s), 131.6 (s), 131.4 (s), 130.9 (s), 129.5 (s), 129.3 (s), 126.7 (s), 125.1 (s), 124.7 (s), 122.2 (s), 118.7 (s), 114.9 (s), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s), 26.1 (s), 21.4 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{27}H_{26}NO_3S$; 444.16279, found: 444.16116.



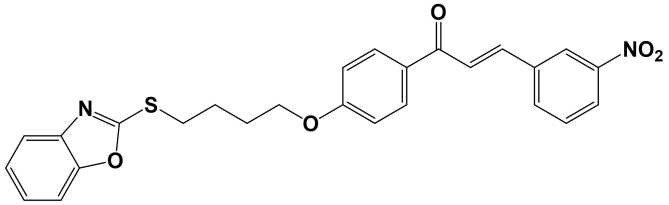
(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (Z11); Yellow solid; m.p. 88.8-90.6℃; Yelid: 82%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 – 8.10 (m, 2H, Ph-H), 7.89 (d, J = 15.6 Hz, 1H, Ph-CH=), 7.68 (s, 1H, =CH-CO-Ph), 7.65 – 7.57 (m, 4H, Ph-H), 7.31 – 7.21 (m, 4H, Ph-H), 7.06 (d, J = 8.9 Hz, 2H, Ph-H), 4.20 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.31 (s, 3H, Ph-O-CH_3), 2.29 – 2.23 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.7 (s), 162.9 (s), 151.7 (s), 143.8 (s), 141.8 (s), 138.6 (s), 135.2 (s), 131.7 (s), 131.4 (s), 131.0 (s), 129.6 (s), 129.3 (s), 126.7 (s), 125.1 (s), 124.7 (s), 122.2 (s), 118.7 (s), 115.0 (s), 110.6 (s), 66.7 (s), 29.1 (s), 29.0 (s), 21.4 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}NO_4S$; 445.13423, found: 445.14804.



(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(3-methoxyphenyl)prop-2-en-1-one (Z12); White solid; m.p. 80.7-82.4℃; Yelid: 78%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.12 (d, J = 8.9 Hz, 2H, Ph-H), 7.91 (d, J = 15.6 Hz, 1H, Ph-CH=), 7.64 (d, J = 15.6 Hz, 1H, =CH-CO-Ph), 7.58 (dd, J = 6.5, 1.9 Hz, 2H, Ph-H), 7.43 (d, J = 2.0 Hz, 1H, Ph-H), 7.39 (d, J = 7.7 Hz, 1H, Ph-H), 7.32 (d, J = 8.0 Hz, 1H, Ph-H), 7.29 – 7.24 (m, 2H, Ph-H), 7.03 (d, J = 8.9 Hz, 2H, Ph-H), 6.97 (dd, J = 7.9, 2.1 Hz, 1H, Ph-H), 4.10 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.78 (s, 3H, Ph-O-CH_3), 3.37 (d, J = 7.2 Hz, 2H, -CH_2-S-Ph), 1.89 (ddd, J = 20.2, 8.1, 5.1 Hz, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.9 (s), 163.1 (s), 160.1 (s), 151.7 (s), 143.6 (s), 141.8 (s), 136.7 (s), 131.5 (s), 130.84(s), 130.4 (s), 125.1 (s), 124.7 (s), 122.7 (s), 122.1 (s), 118.7 (s), 117.0 (s), 114.9 (s), 113.8 (s), 110.6 (s), 67.8 (s), 55.8 (s), 31.9 (s), 27.9 (s), 26.1 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{27}H_{26}NO_4S$; 460.15771, found: 460.15570.

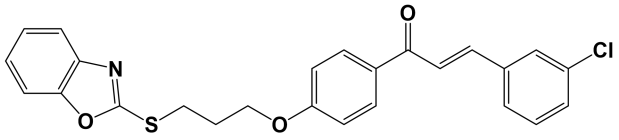


(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(3-fluorophenyl)prop-2-en-1-one (Z13); Yellow solid; m.p. 78.4-79.6℃; Yelid: 71%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.14 – 8.12 (m, 2H, Ph-H), 7.99 – 7.96 (m, 1H, Ph-CH=), 7.81 (d, J = 10.4 Hz, 1H, =CH-CO-PH), 7.64 (d, J = 6.5 Hz, 2H, Ph-H), 7.58 (dd, J = 6.7, 2.1 Hz, 2H, Ph-H), 7.44 (dd, J = 7.9, 1.7 Hz, 2H, Ph-H), 7.28 – 7.25 (m, 2H, Ph-H), 7.24 – 7.21 (m, 1H, Ph-H), 7.04 – 7.02 (m, 2H, Ph-H), 4.11 (t, J = 6.1 Hz, 2H, Ph-O-CH_2-), 3.39 – 3.36 (m, 2H, -CH_2-S-Ph), 1.93 – 1.86 (m, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.7 (s), 164.9 (s), 164.0 (s), 163.2 (s), 162.0 (s), 151.7 (s), 142.2 (s), 141.8 (s), 137.9 (d, J = 8.0 Hz), 131.5 (s), 131.3 (d, J = 8.3 Hz), 130.7 (s), 126.0 (s), 125.1 (s), 124.7 (s), 123.9 (s), 118.7 (s), 117.6 (d, J = 21.4 Hz), 115.4 – 115.2 (m), 115.0 (d, J = 22.1 Hz), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s), 26.2 (s); ^{19}F NMR (471 MHz, DMSO-d_6) δ -112.84 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}FNO_3S$; 448.13772, found: 448.13608.

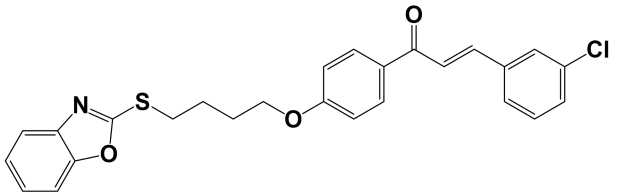


(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one (Z14); Yellow solid; m.p. 133.1-134.9℃; Yelid: 93%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.74 (s, 1H, Ph-H), 8.29 (d, J = 7.7 Hz, 1H, Ph-H), 8.21 (dd, J = 8.2, 1.2 Hz, 1H, Ph-H), 8.14 (d, J = 16.7 Hz, 3H, Ph-H), 7.77 (d, J = 15.6 Hz, 1H, Ph-CH=), 7.69 (d, J = 8.0 Hz, 1H,=CH-CO-Ph), 7.60 – 7.57 (m, 2H, Ph-H), 7.29 – 7.25 (m, 2H, Ph-H), 7.04 (d, J = 8.9 Hz, 2H, Ph-H), 4.12 (t, J = 5.9 Hz, 2H, Ph-O-CH_2-), 3.38 (t, J = 6.9 Hz, 2H, -S-CH_2-Ph), 1.94 – 1.87 (m, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.6 (s), 164.9 (s), 163.3 (s), 151.7(s), 148.9 (s), 141.8 (s), 141.1 (s), 137.2 (s), 135.6 (s), 131.7 (s), 130.8 (s), 130.5 (s), 125.2 (s), 125.0 (d, J = 8.3 Hz), 124.7 (s), 123.4 (s), 118.7 (s), 115.0 (s), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s),

26.1 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}N_2O_5S$; 475.13222, found: 475.13184.

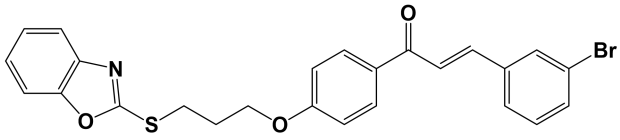


(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(3-chlorophenyl)prop-2-en-1-one (Z15); Yellow solid; m.p. 80.1-80.5℃; Yelid: 75%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.16 – 8.14 (m, 2H, Ph-H), 8.03 (d, J = 10.8 Hz, 2H, Ph-H), 7.78 – 7.76 (m, 1H, Ph-CH=), 7.62 (s, 1H, =CH-CO-Ph), 7.59 – 7.56 (m, 2H, Ph-H), 7.43 (d, J = 7.0 Hz, 2H, Ph-H), 7.28 – 7.25 (m, 2H, Ph-H), 7.06 (d, J = 8.9 Hz, 2H, Ph-H), 4.21 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.28 – 2.24 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.6 (s), 164.7 (s), 163.0 (s), 151.7 (s), 141.9 (s), 141.8 (s), 137.6 (s), 134.3 (s), 131.6 (s), 131.1 (s), 130.84 (s), 130.5 (s), 128.4 (s), 125.1 (s), 124.7 (s), 124.0 (s), 118.7 (s), 115.0 (s), 110.6 (s), 66.7 (s), 29.1 (s), 28.9 (s). HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{25}H_{21}ClNO_3S$; 450.09252, found: 450.09204.

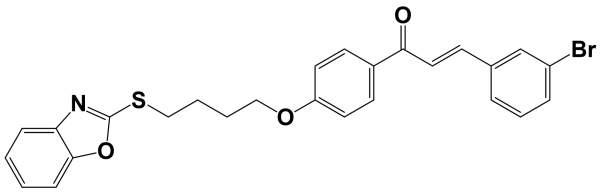


(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(3-chlorophenyl)prop-2-en-1-one (Z16); Yellow solid; m.p. 98.1-99.7℃; Yelid: 85%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.14 (d, J = 8.9 Hz, 2H, Ph-H), 8.04 – 7.98 (m, 2H, Ph-H), 7.77 (d, J = 6.7 Hz, 1H, Ph-CH=), 7.63 (d, J = 15.6 Hz, 1H, =CH-CO-Ph), 7.58 (dd, J = 6.4, 1.9 Hz, 2H, Ph-H), 7.43 (d, J = 7.0 Hz, 2H, Ph-H), 7.30 – 7.24 (m, 2H, Ph-H), 7.03 (d, J = 8.9 Hz, 2H, Ph-H), 4.11 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.38 (d, J = 6.7 Hz, 2H, -CH_2-S-Ph), 1.90 (tdd, J = 13.5, 8.5, 5.4 Hz, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.6 (s), 164.9 (s), 163.2 (s), 141.8 (d, J = 15.1 Hz), 137.6 (s), 134.3 (s), 131.6 (s), 131.1 (s), 130.6 (s), 130.4 (s), 128.3 (d, J = 3.7 Hz), 125.1 (s), 124.7 (s), 124.0 (s), 118.7 (s), 114.9 (s), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s),

26.1 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}ClNO_3S$; 464.10817, found: 464.10773.

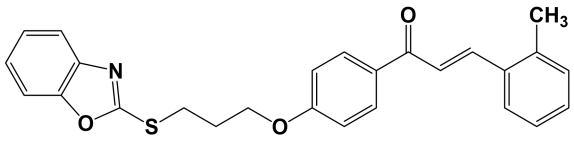


(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(3-bromophenyl)prop-2-en-1-one (Z17); Yellow solid; m.p. 85.2-87.1℃; Yelid: 72%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.17 (d, J = 1.6 Hz, 2H, Ph-H), 8.16 – 8.14 (m, 2H, Ph-H), 8.00 (d, J = 15.6 Hz, 1H, Ph-H), 7.81 (d, J = 7.8 Hz, 1H, Ph-CH=), 7.62 (d, J = 15.6 Hz, 1H, =CH-CO-Ph), 7.59 – 7.57 (m, 2H, Ph-H), 7.35 (d, J = 7.8 Hz, 1H, Ph-H), 7.28 – 7.25 (m, 2H, Ph-H), 7.06 (d, J = 8.9 Hz, 2H, Ph-H), 4.21 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.46 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.28 – 2.24 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.6 (s), 164.7 (s), 163.0 (s), 151.7 (s), 141.8 (d, J = 18.0 Hz), 137.8 (s), 133.3 (s), 131.5 (d, J = 24.8 Hz), 131.2 (s), 130.8 (s), 128.7 (s), 125.1 (s), 124.7 (s), 123.9 (s), 122.9 (s), 118.7 (s), 115.0 (s), 110.6 (s), 66.7 (s), 29.11(s), 29.0 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{25}H_{21}BrNO_3S$; 494.04200, found: 494.04156.

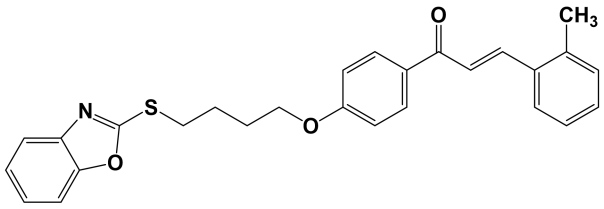


(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(3-bromophenyl)prop-2-en-1-one (Z18); Yellow solid; m.p. 93.9-95.1℃; Yelid: 62%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.18 – 8.13 (m, 3H, Ph-H), 8.00 (d, J = 15.6 Hz, 1H, Ph-H), 7.81 (d, J = 7.8 Hz, 1H, Ph-CH=), 7.62 (d, J = 15.6 Hz, 1H, =CH-CO-Ph), 7.59 – 7.56 (m, 3H, Ph-H), 7.36 (t, J = 7.9 Hz, 1H, Ph-H), 7.27 (ddd, J = 11.3, 6.3, 3.6 Hz, 2H, Ph-H), 7.03 (d, J = 8.9 Hz, 2H, Ph-H), 4.11 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.37 (t, J = 6.9 Hz, 2H, -CH_2-S-Ph), 1.89 (ddd, J = 13.7, 8.1, 5.0 Hz, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.6 (s), 164.9 (s), 163.2 (s), 151.7 (s), 141.8 (d, J = 4.7 Hz), 137.8 (s), 133.3 (s), 131.6 (s), 131.4 (s), 131.2 (s), 130.7 (s), 128.7 (s), 125.0 (s), 124.7 (s), 124.0 (s), 122.9 (s), 118.7 (s), 114.9 (s), 110.6 (s), 67.8 (s), 31.9

(s), 27.9 (s), 26.1 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{23}BrNO_3S$; 508.05765, found: 508.05719.

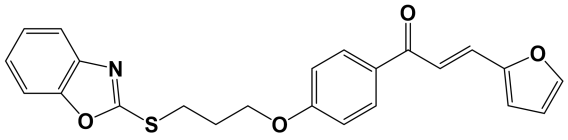


(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(o-tolyl)prop-2-en-1-one (Z19); White solid; m.p. 82.5-84.2℃; Yelid: 28%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.13 – 8.10 (m, 2H, Ph-H), 7.95 (d, J = 7.7 Hz, 1H, Ph-CH=), 7.90 (s,1 H, Ph-H), 7.78 (d, J = 15.4 Hz, 1H, =CH-CO-Ph), 7.59 – 7.56 (m, 2H, Ph-H), 7.28 – 7.26 (m, 2H, Ph-H), 7.24 (dd, J = 11.4, 4.5 Hz, 3H, Ph-H), 7.06 – 7.04 (m, 2H, Ph-H), 4.19 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.45 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.38 (s, 3H, Ph-CH_3), 2.27 – 2.22 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.7 (s), 162.9 (s), 151.7 (s), 141.8 (s), 140.7 (s), 138.4 (s), 133.9 (s), 131.4 (s), 131.3 (d, J = 23.7 Hz), 131.0 (s), 130.7 (s), 127.3 (s), 126.8 (s), 125.1 (s), 124.74 (s), 123.3 (s), 118.7 (s), 115.0 (s), 110.6 (s), 66.7 (s), 29.1 (s), 29.0 (s),19.8 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{26}H_{24}NO_3S$; 430.14714, found: 430.14670.

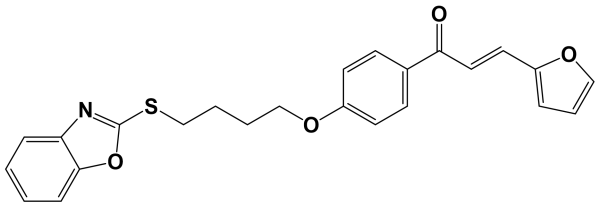


(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(o-tolyl)prop-2-en-1-one (Z20); White solid; m.p. 112.3-113.6℃; Yelid: 47%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.11 (d, J = 8.7 Hz, 2H, Ph-H), 7.95 (d, J = 7.5 Hz,1H,Ph-CH=), 7.90 (s, 1H, Ph-H), 7.79 (d, J = 15.4 Hz, 1H, =CH-CO-Ph), 7.58 (d, J = 8.2 Hz, 2H, Ph-H), 7.28 (d, J = 6.8 Hz, 3H, Ph-H), 7.24 (d, J = 6.2 Hz, 2H, Ph-H), 7.03 (d, J = 8.8 Hz, 2H, Ph-H), 4.10 (t, J = 5.9 Hz, 2H, Ph-O-CH_2-), 3.37 (t, J = 6.8 Hz, 2H, -CH_2-S-Ph), 2.46 (s, 3H, Ph-CH_3), 1.94 – 1.86 (m, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.8 (s), 164.9 (s), 163.1 (s), 151.7 (s), 141.8 (s), 140.6 (s), 138.3 (s), 133.9 (s), 131.4 (s), 131.2 (s), 130.7 (d, J = 16.3 Hz), 127.3 (s), 126.8 (s), 125.10 (s), 124.7 (s), 123.3 (s), 118.7 (s), 115.0 (s), 110.6 (s), 67.8 (s), 31.9 (s), 27.9 (s), 26.1 (s),

19.8 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{27}H_{26}NO_3S$; 444.16279, found: 444.16223.

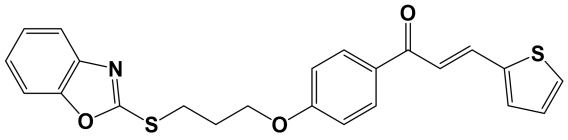


(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(furan-2-yl)prop-2-en-1-one (Z21); Yellow solid; m.p. 81.6-82.8℃; Yelid: 64%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.03 – 7.99 (m, 3H, -Ph-H, Fruan-H), 7.86 (d, J = 1.6 Hz,1H, Fruan-CH=), 7.59 – 7.55 (m, 2H, Ph-H), 7.50 (s, 3H, Ph-H, Fruan-H), 7.25 (ddd, J = 11.6, 6.5, 3.8 Hz, 2H, Ph-H, =CH-CO-Ph), 7.03 (dd, J = 5.8, 2.8 Hz, 4H, Ph-H, Fruan-H), 6.64 (dd, J = 3.4, 1.8 Hz, 1H, Ph-H), 4.17 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.44 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.25 (dd, J = 13.1, 6.5 Hz, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.3 (s), 164.7 (s), 162.9 (d, J = 9.2 Hz), 151.7 (s), 146.5 (s), 141.8 (s), 131.2 (s), 130.9 (s), 130.3 (s), 125.10 (s), 124.7 (s), 119.2 (s), 118.7 (s), 117.0 (s), 115.0 (s), 113.5 (s), 110.6 (s), 66.7 (s), 29.1 (s), 29.0 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{23}H_{20}NO_4S$; 406.11076, found: 406.10913.

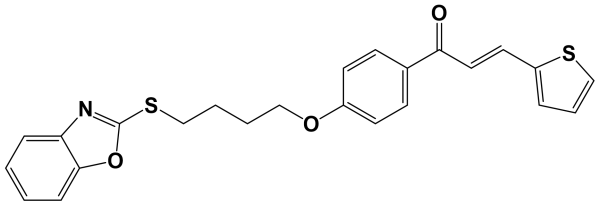


(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(furan-2-yl)prop-2-en-1-one (Z22); Yellow solid; m.p. 94.9-96.8℃; Yelid: 85%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.01 (d, J = 8.7 Hz, 2H, Ph-H), 7.86 (s, 1H, Ph-CH=), 7.58 (dd, J = 6.7, 1.8 Hz, 2H, Ph-H, Fruan-H), 7.50 (d, J = 1.2 Hz, 2H, =CH-CO-Ph, Fruan-H), 7.26 (td, J = 7.1, 5.7 Hz, 2H, Ph-H), 7.04 (d, J = 3.3 Hz, 2H, Ph-H), 7.01 (d, J = 8.8 Hz, 3H, Ph-H, Fruan-H), 6.64 (dd, J = 3.1, 1.7 Hz, 1H, Fruan-H), 4.09 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.37 (t, J = 6.9 Hz, 2H,-CH_2-S-Ph), 1.93 – 1.85 (m, 4H, -O-CH_2-$\underline{CH_2}$-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.2 (s), 164.9 (s), 163.0 (s), 151.7 (s), 146.4 (s), 141.8 (s), 131.1 (s), 130.8 (s), 130.2 (s), 125.0 (s), 124.6 (s), 119.2 (s), 118.7 (s), 117.0 (s), 115.0 (s), 113.5 (s), 110.6 (s), 67.8 (s), 31.9

(s), 27.9 (s), 26.1 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{24}H_{22}NO_4S$; 420.12641, found: 420.12601.



(*E*)-1-(4-(3-(benzo[*d*]oxazol-2-ylthio)propoxy)phenyl)-3-(thiophen-2-yl)prop-2-en-1-one (Z23); Yellow solid; m.p. 71.9-73.8℃; Yelid: 58%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.06 – 8.04 (m, 2H, Ph-H), 7.84 (d, J = 15.3 Hz, 1H, Ph-CH=), 7.73 (d, J = 5.0 Hz, 1H, Thioen-H), 7.63 (d, J = 3.2 Hz, 1H, =CH-CO-), 7.59 – 7.57 (m, 2H, Ph-H), 7.53 (d, J = 15.3 Hz, 1H, Thioen-H), 7.27 (ddd, J = 7.1, 5.2, 1.5 Hz, 2H, Ph-H), 7.14 (dd, J = 4.9, 3.7 Hz, 1H, Thioen-H), 7.05 (d, J = 8.8 Hz, 2H, Thioen-H, Ph-H), 4.19 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.45 (t, J = 7.1 Hz, 2H, -CH_2-S-Ph), 2.27 – 2.23 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}CNMR (126 MHz, DMSO-d_6) δ 187.3 (s), 164.7 (s), 162.8 (s), 151.7 (s), 141.8 (s), 140.3 (s), 136.4 (s), 133.0 (s), 131.3 (s), 130.9 (s), 130.6 (s), 129.2 (s), 125.1 (s), 124.7 (s), 120.8 (s), 118.7 (s), 115.0 (s), 110.6 (s), 66.75 (s), 29.1 (s), 28.9 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{23}H_{20}NO_3S_2$; 422.08791, found: 422.08731.



(*E*)-1-(4-(4-(benzo[*d*]oxazol-2-ylthio)butoxy)phenyl)-3-(thiophen-2-yl)prop-2-en-1-one (Z24); Yellow solid; m.p. 95.7-96.4℃; Yelid: 52%; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.04 (d, J = 8.8 Hz, 2H, Ph-H), 7.83 (d, J = 15.3 Hz, 1H, Thioen-H), 7.73 (d, J = 5.0 Hz,1H, Ph-CH=), 7.63 (d, J = 3.4 Hz, 1H,=CH-Ph), 7.58 (dd, J = 6.7, 1.9 Hz, 1H, Thioen-H), 7.53 (d, J = 15.3 Hz, 2H, Ph-H), 7.29 – 7.24 (m, 2H, Ph-H), 7.16 – 7.13 (m, 1H, Thioen-H), 7.01 (d, J = 8.8 Hz, 2H, Ph-H, Thioen-H), 4.09 (t, J = 6.0 Hz, 2H, Ph-O-CH_2-), 3.37 (t, J = 6.9 Hz, 2H, -CH_2-S-Ph), 1.93 – 1.85 (m, 2H, -O-CH_2-$\underline{CH_2}$-CH_2-S-); ^{13}C NMR (126 MHz, DMSO-d_6) δ 187.2 (s), 164.9 (s), 163.0 (s), 151.7 (s), 141.8 (s), 140.3 (s), 136.4 (s), 133.0 (s), 131.2 (s), 130.7 (d, J = 11.7 Hz), 129.2 (s), 125.0 (s), 124.7 (s), 120.8 (s), 118.7 (s), 114.9 (s), 110.6 (s), 67.8 (s),

31.9 (s), 27.9 (s), 26.1 (s); HRMS (ESI) m/z $[M+H]^+$ calcd for: $C_{24}H_{22}NO_3S_2$; 436.10356, found: 436.10327.

2. Spectra of target compounds Z1-Z24

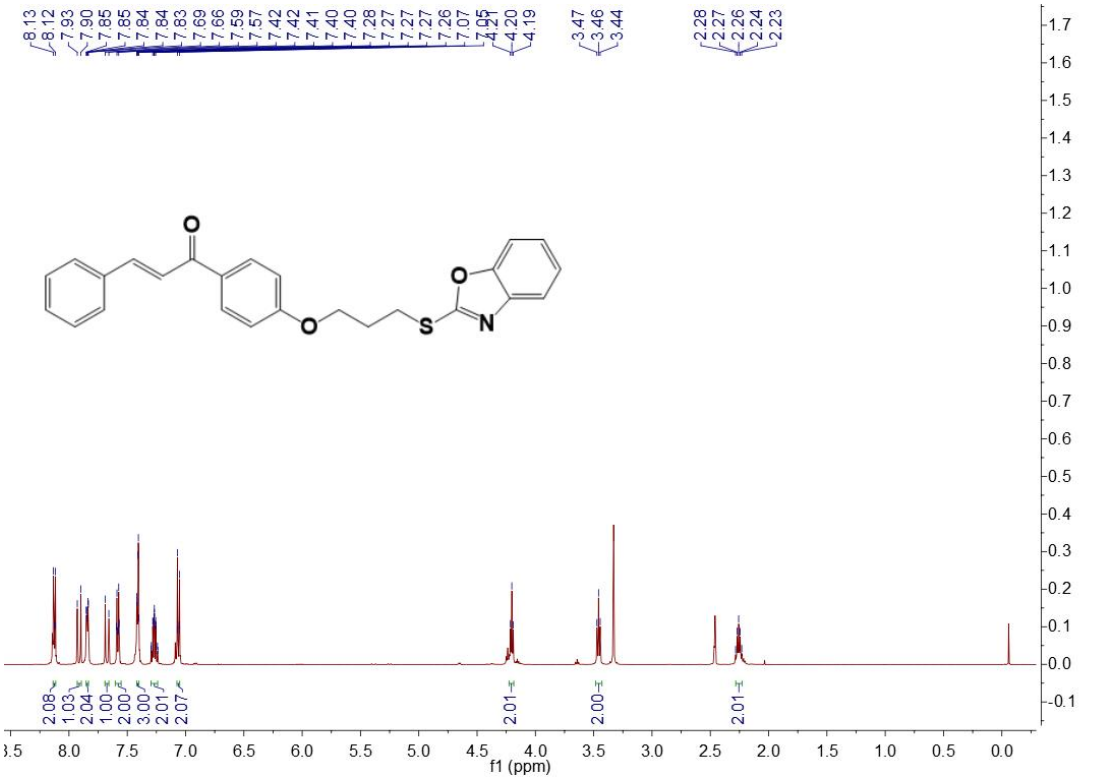


Fig. S1 ^{1}H NMR spectra of compound Z1

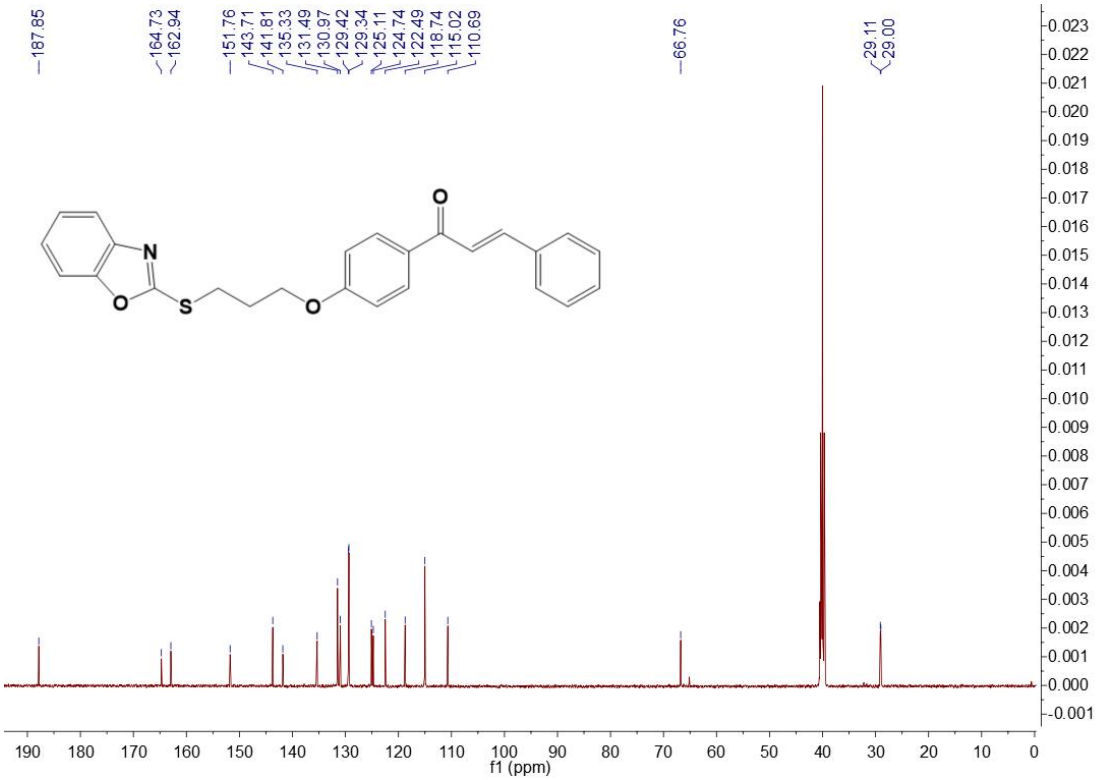


Fig. S1 ^{13}C NMR spectra of compound Z1

156 #69 RT: 0.68 AV: 1 NL: 1.33E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

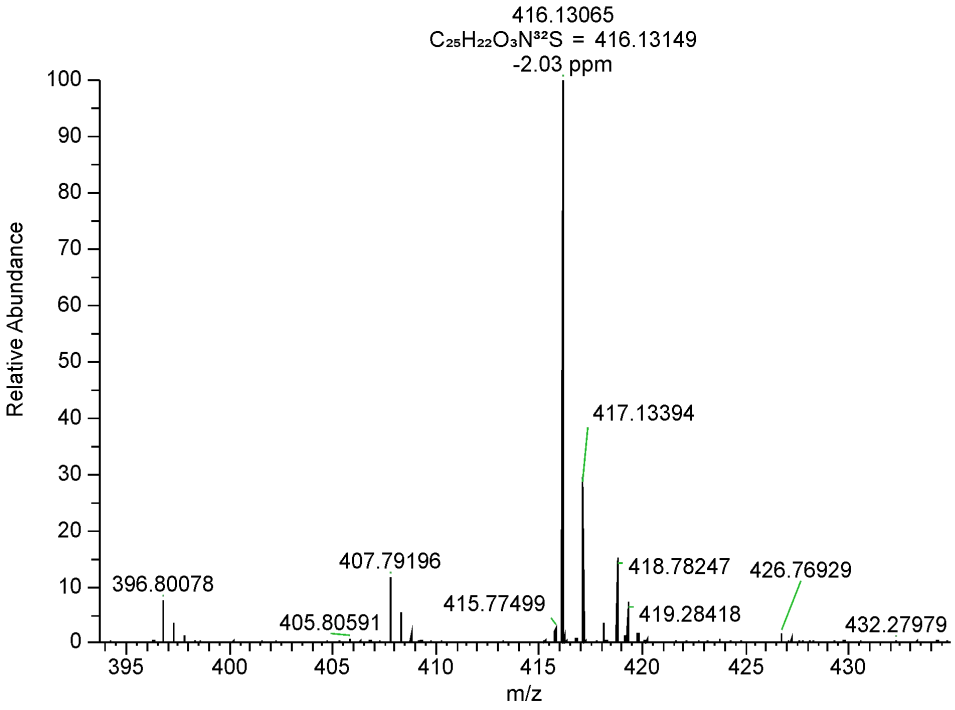


Fig. S1 HRMS spectra of compound Z1

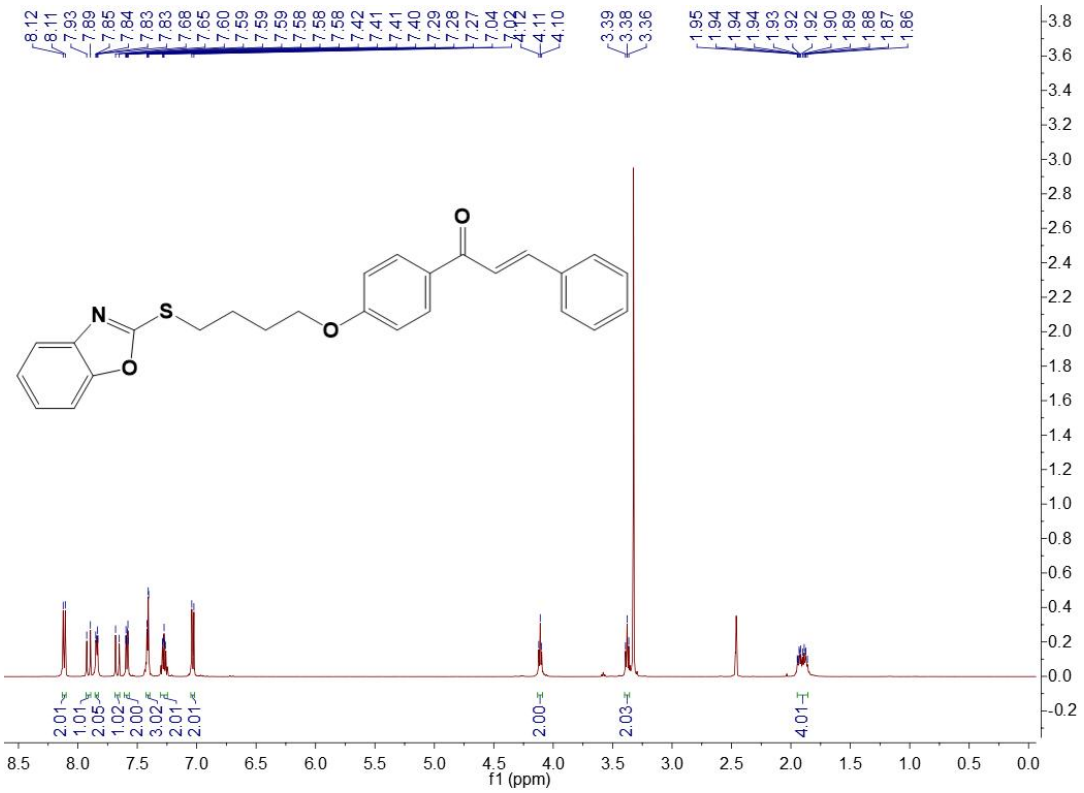


Fig. S2 ^{1}H NMR spectra of compound Z2

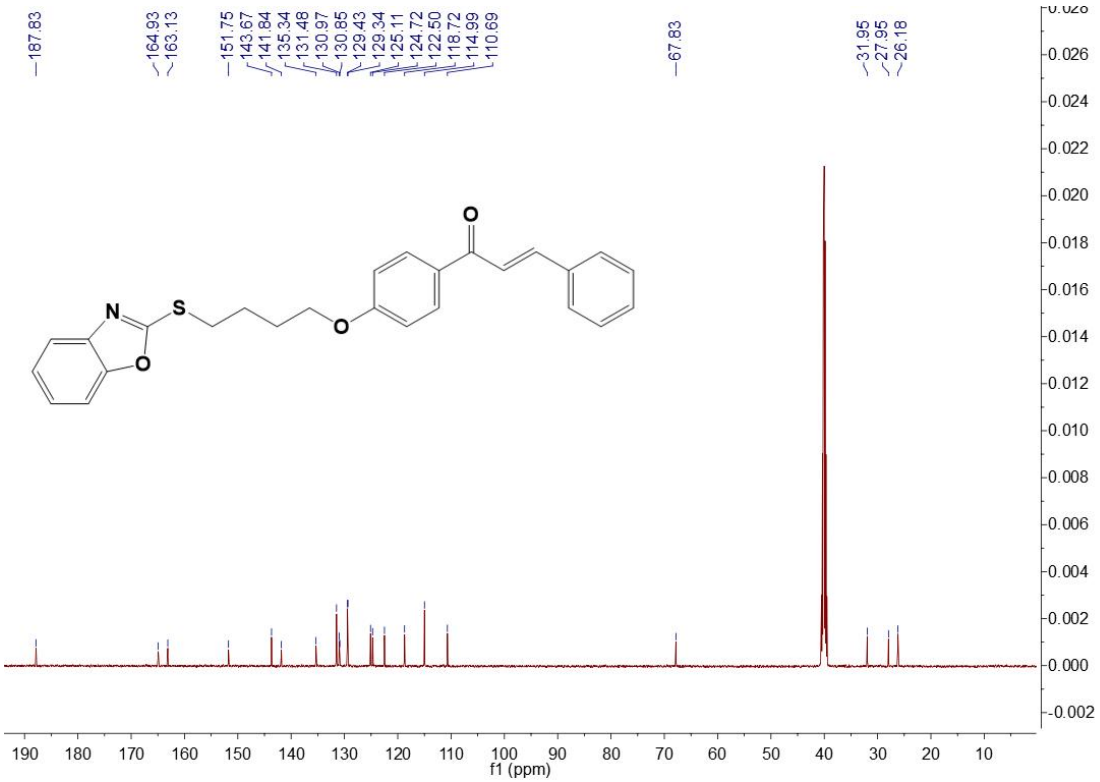


Fig. S2 ^{13}C NMR spectra of compound Z2

154 #79 RT: 0.77 AV: 1 NL: 1.34E+008
T: FTMS + p ESI Full ms [100.0000-1300.0000]

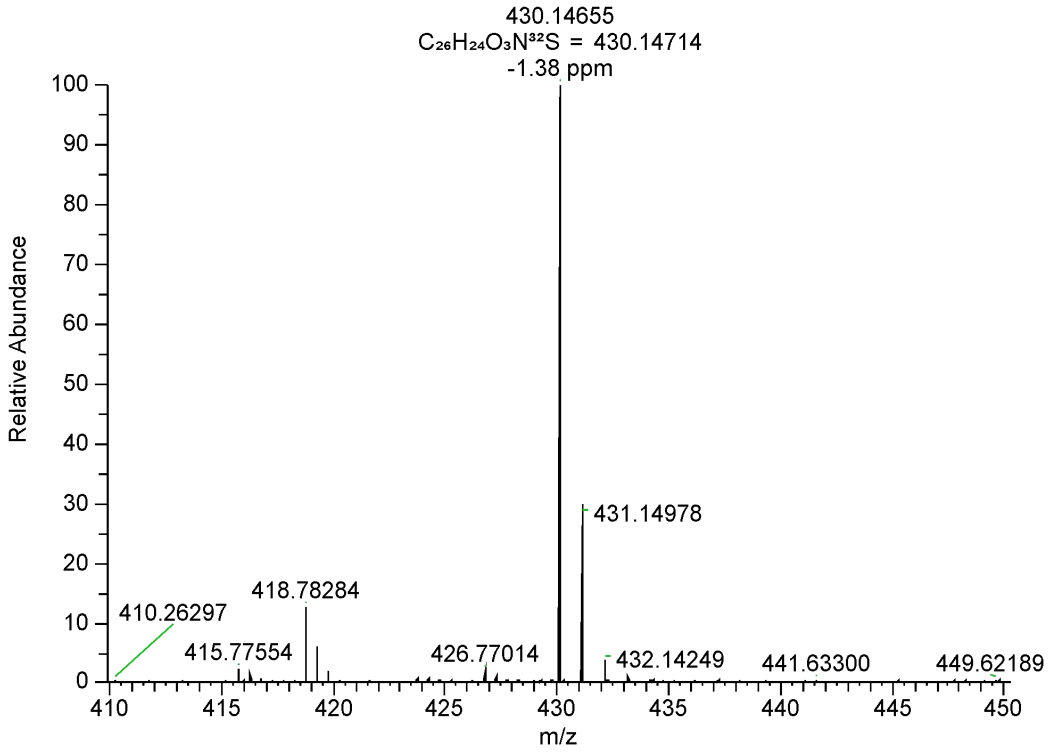


Fig. S2 HRMS spectra of compound Z2

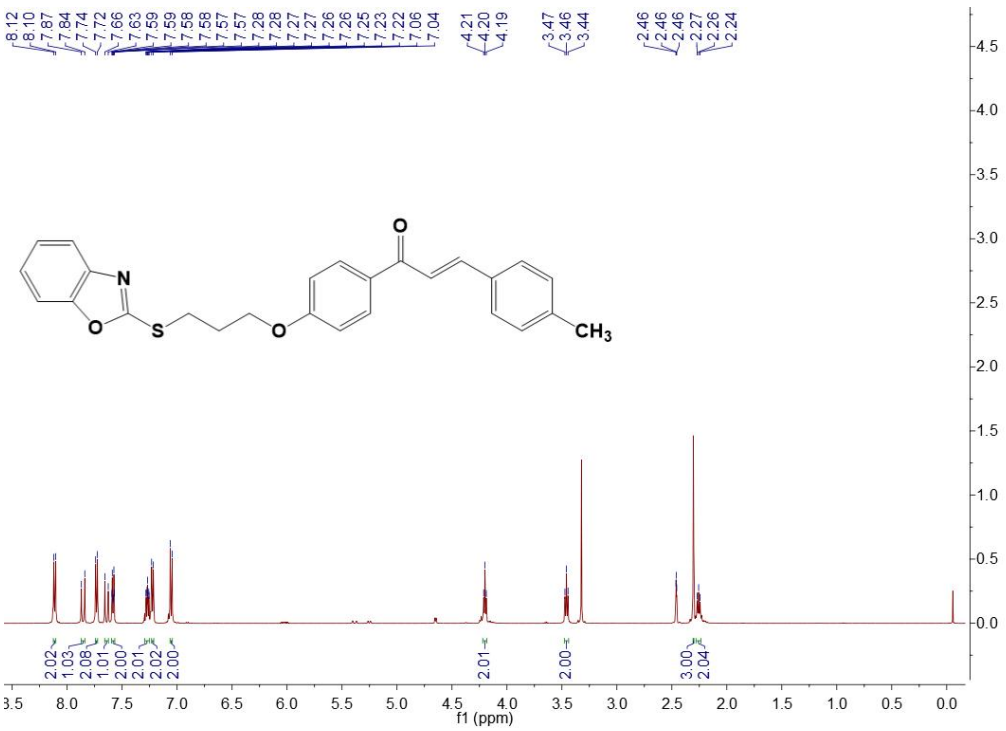


Fig. S3 ^{1}H NMR spectra of compound Z3

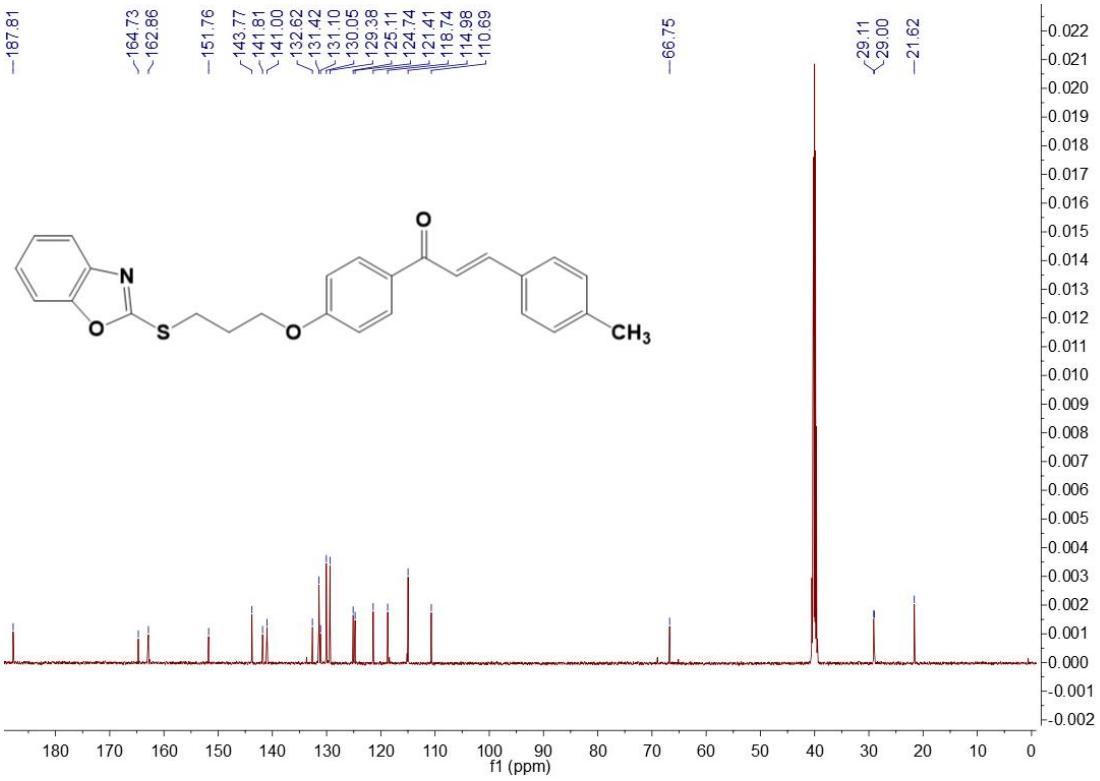


Fig. S3 ^{13}C NMR spectra of compound Z3

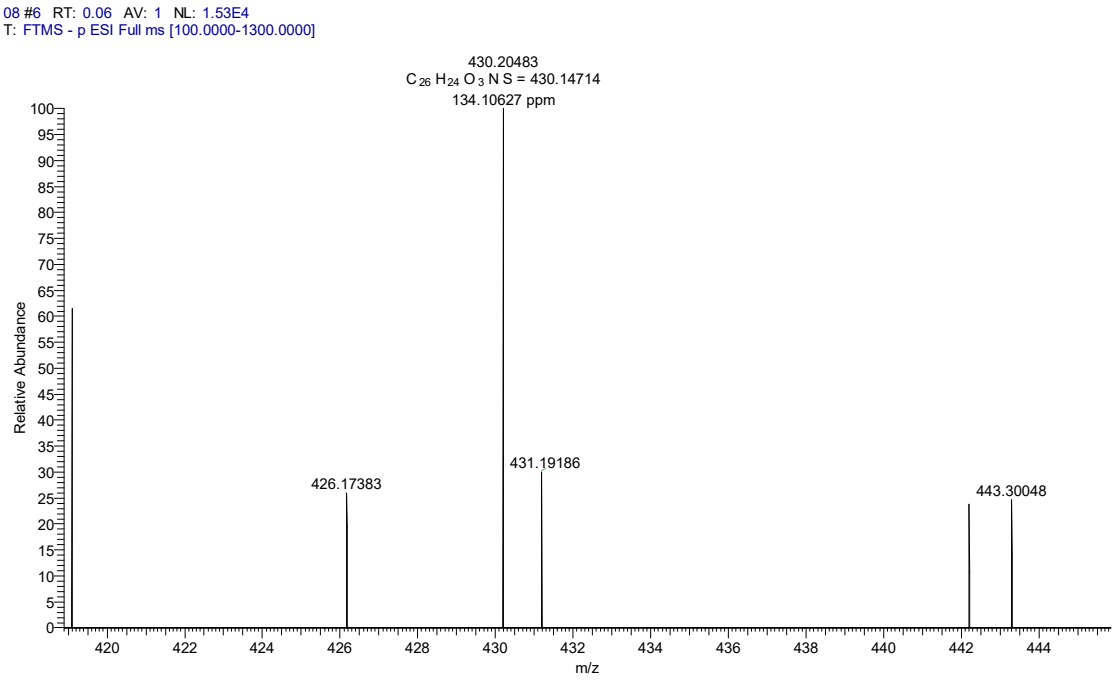


Fig. S3 HRMS spectra of compound Z3

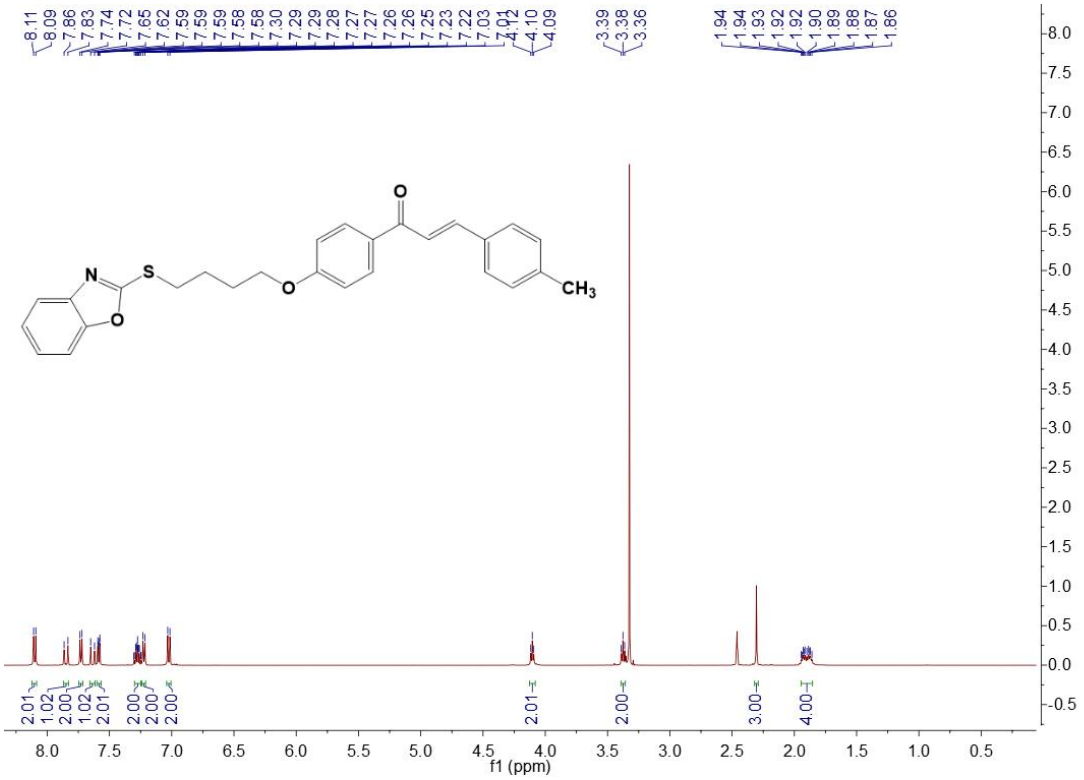


Fig. S4 ^{1}H NMR spectra of compound Z4

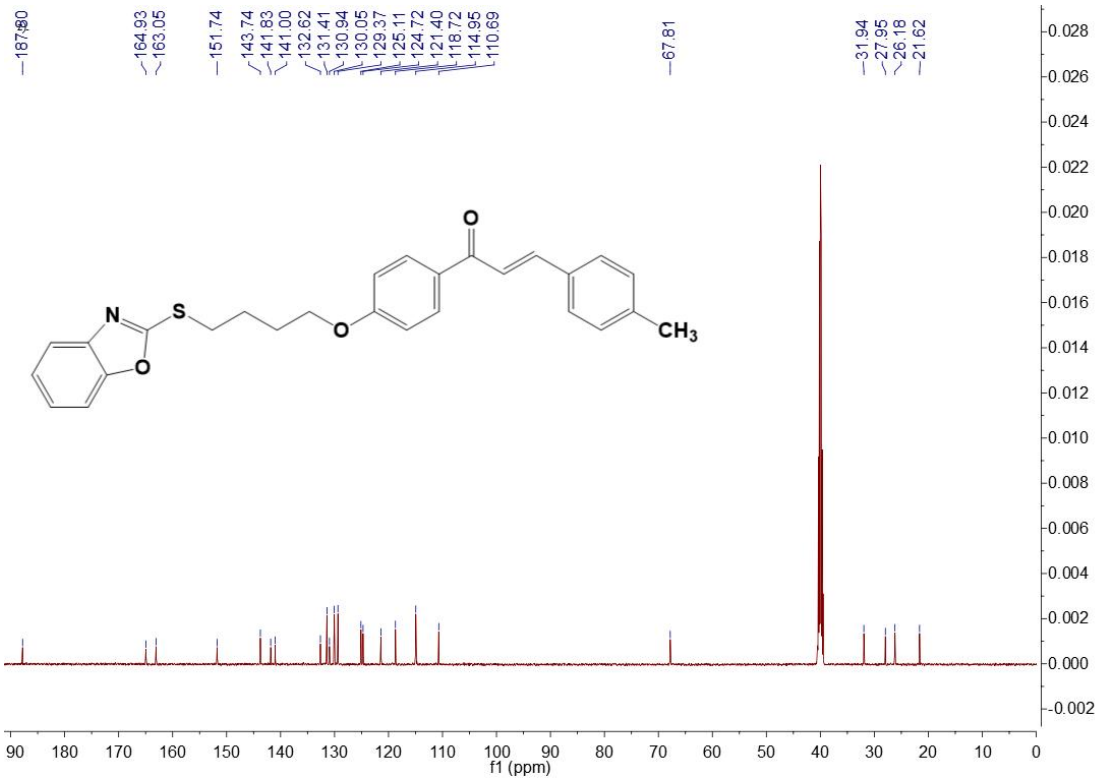


Fig. S4 ^{13}C NMR spectra of compound Z4

10 #89 RT: 0.86 AV: 1 NL: 7.16E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

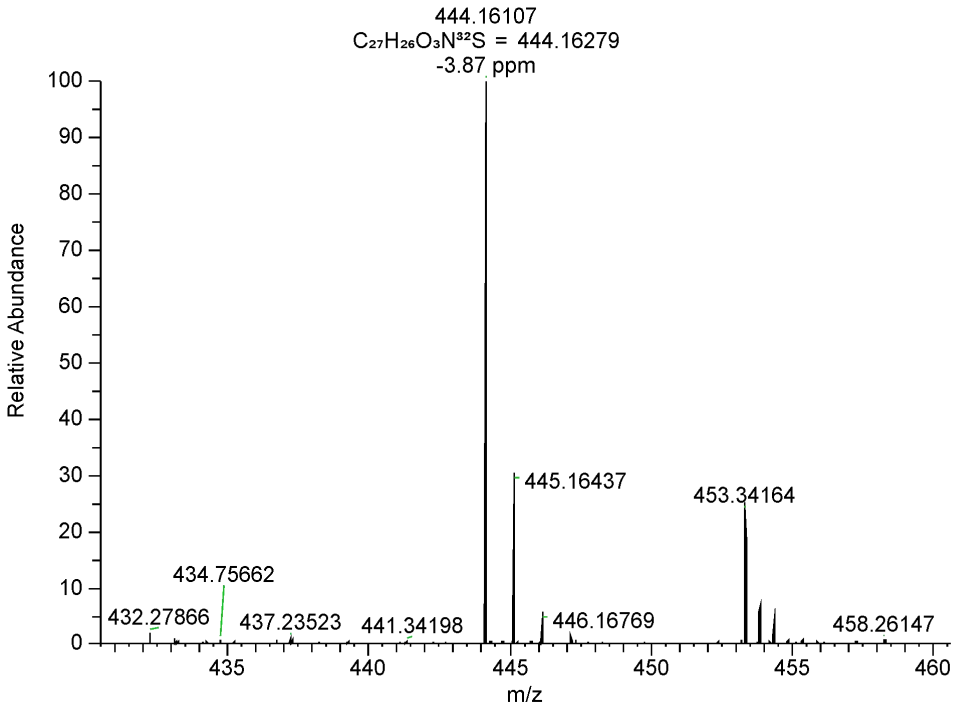


Fig. S4 HRMS spectra of compound Z4

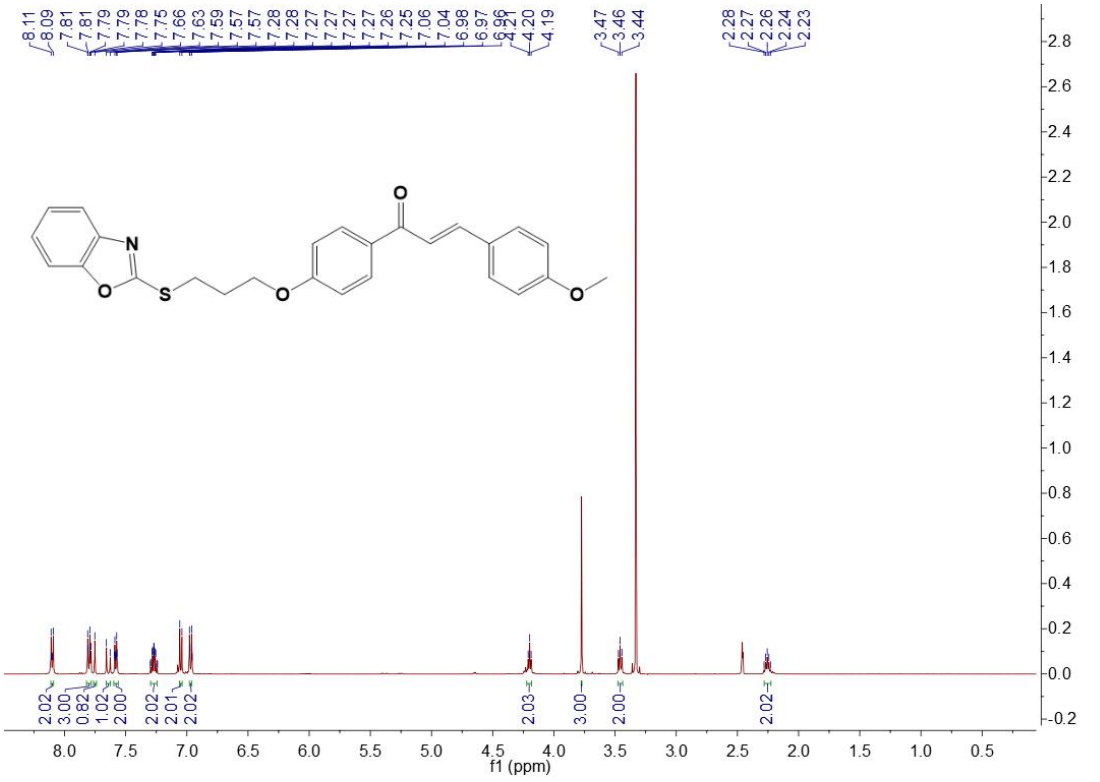


Fig. S5 ^{1}H NMR spectra of compound Z5

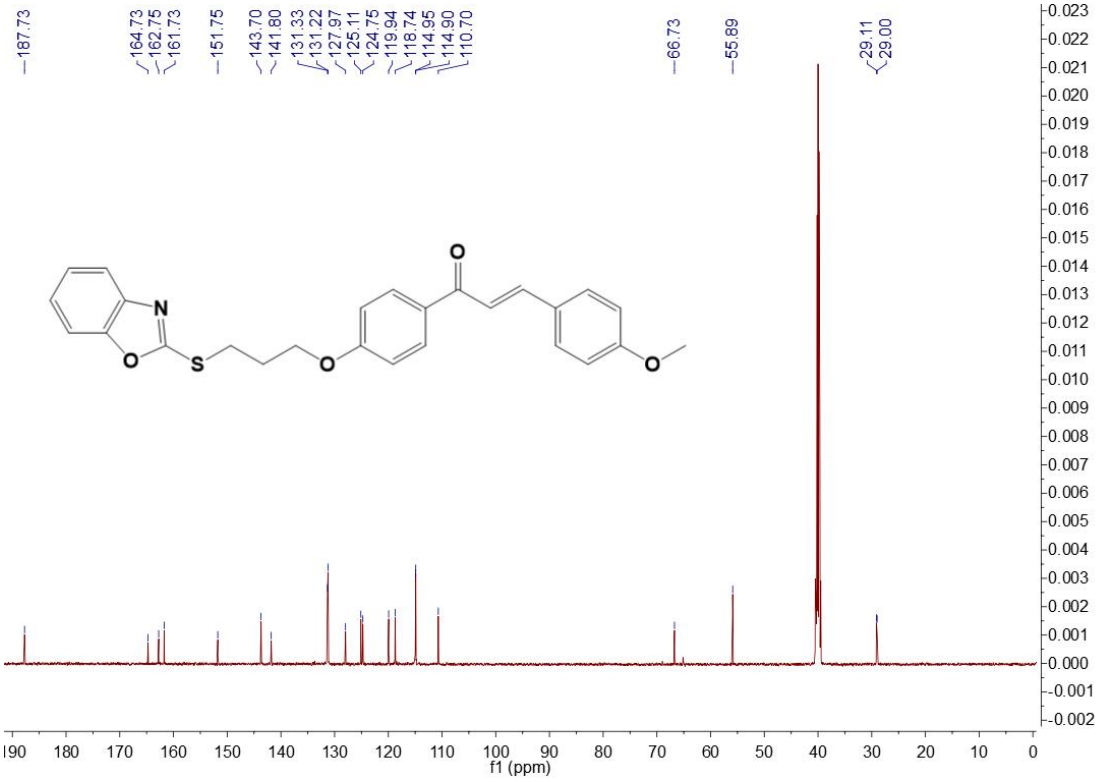


Fig. S5 ^{13}C NMR spectra of compound Z5

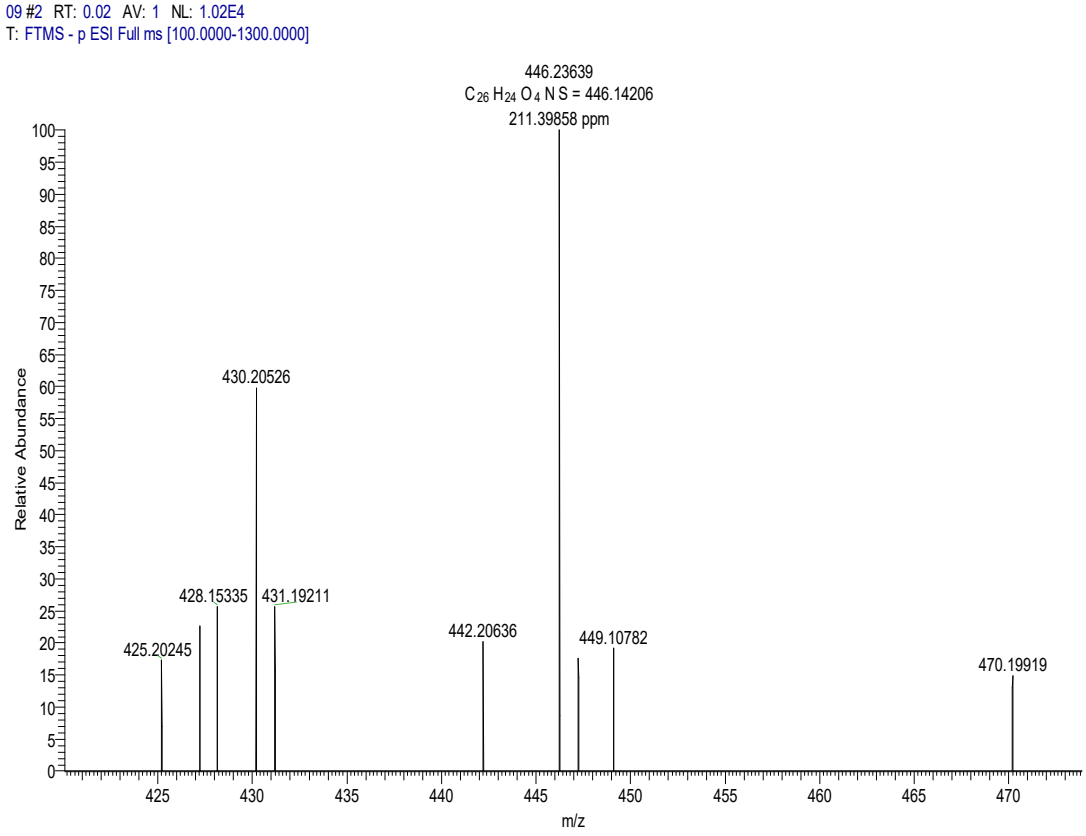


Fig. S5 HRMS spectra of compound Z5

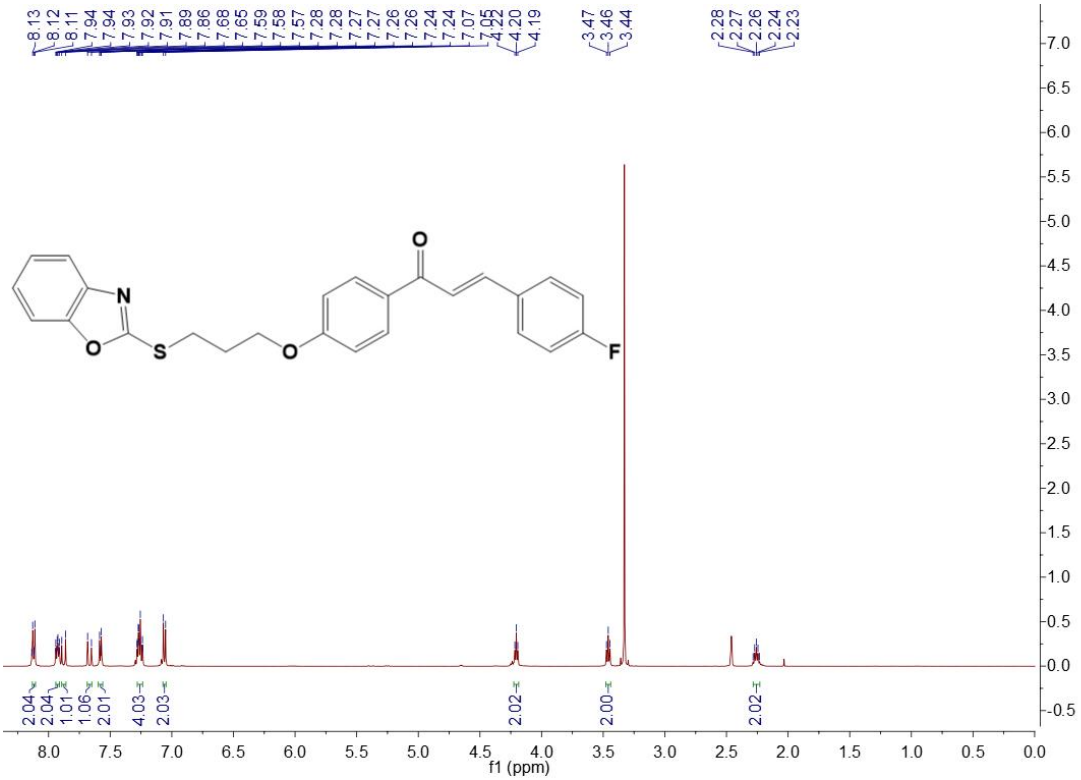


Fig. S6 ^{1}H NMR spectra of compound Z6

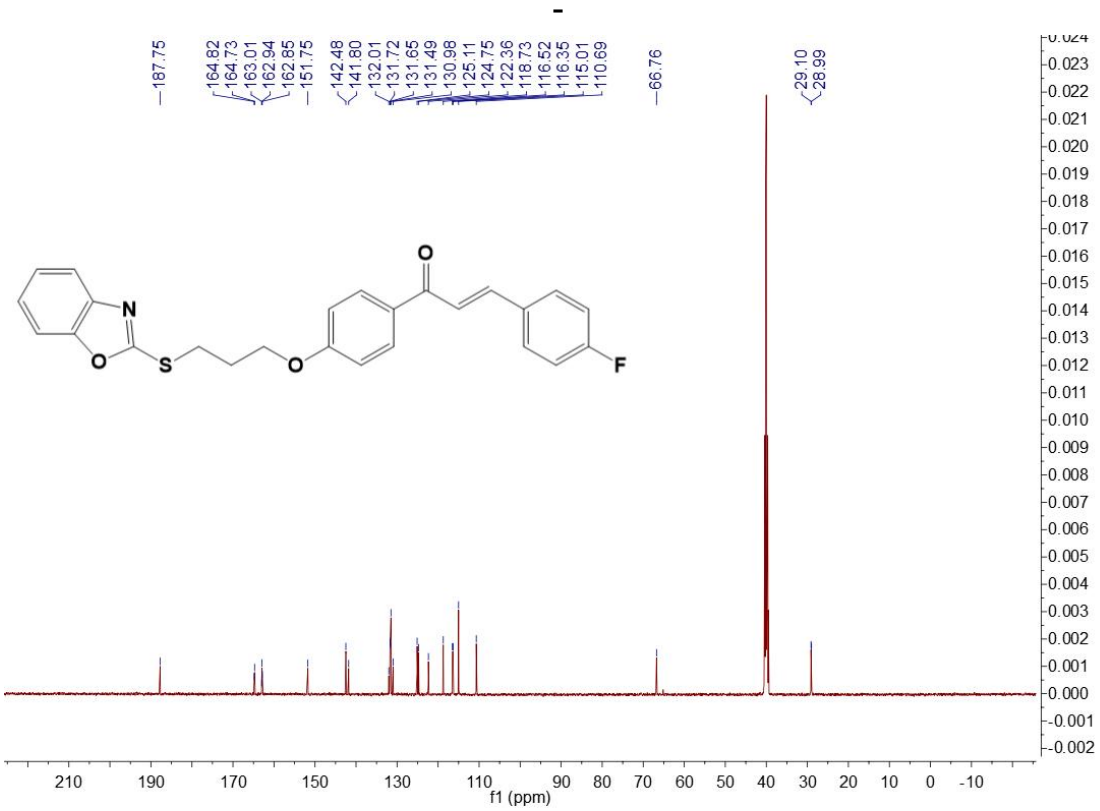


Fig. S6 ^{13}C NMR spectra of compound Z6

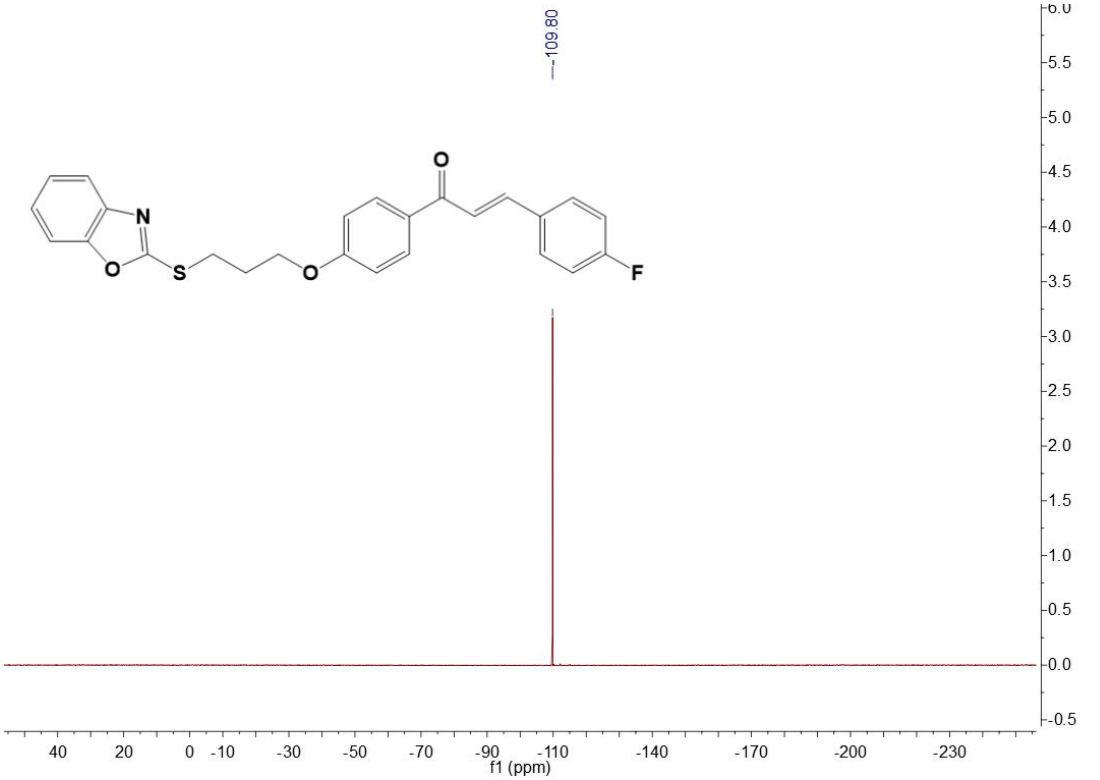


Fig. S6 ^{19}F NMR spectra of compound Z6

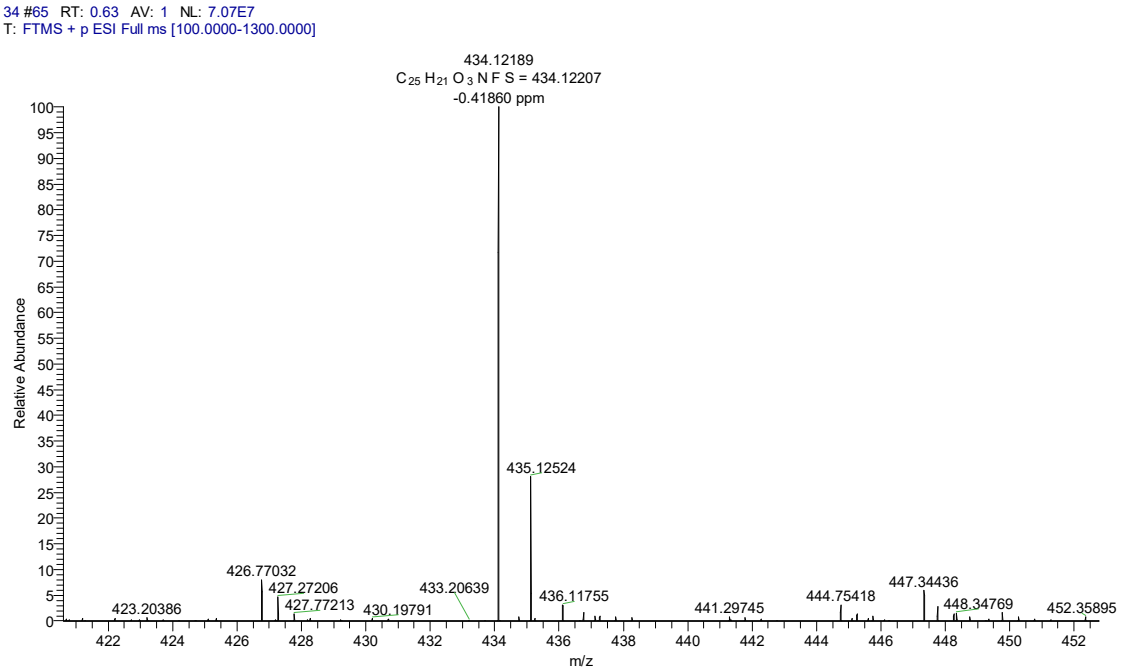


Fig. S6 HRMS spectra of compound Z6

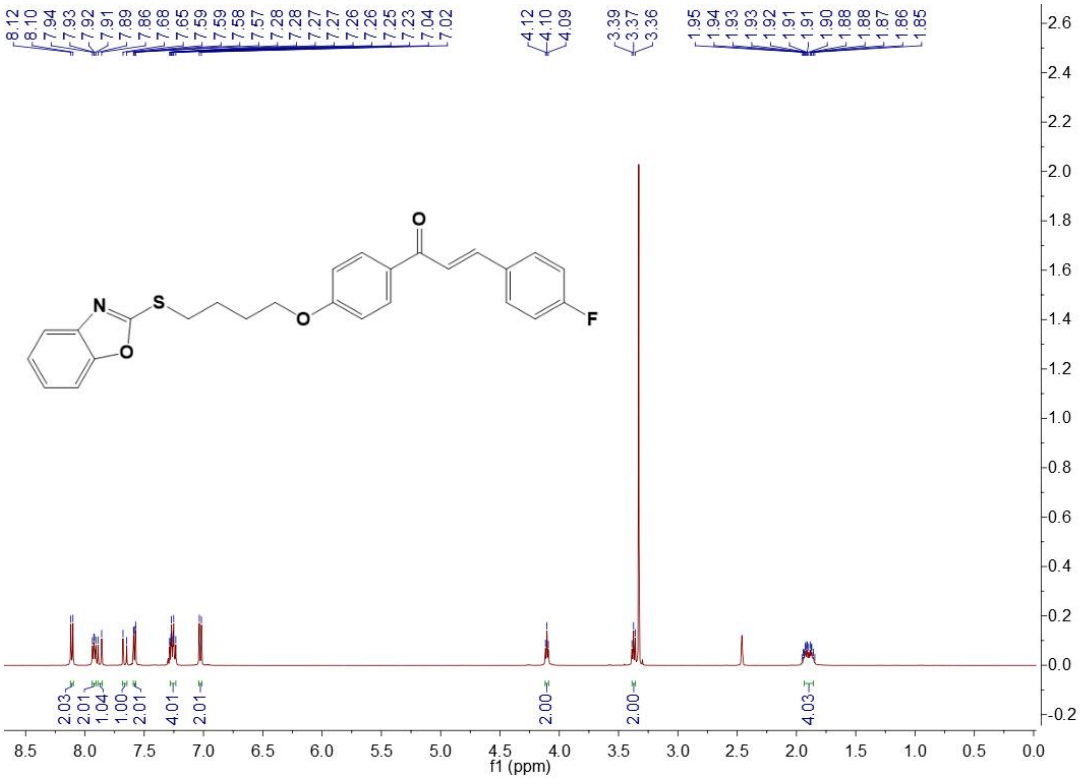


Fig. S7 1H NMR spectra of compound Z7

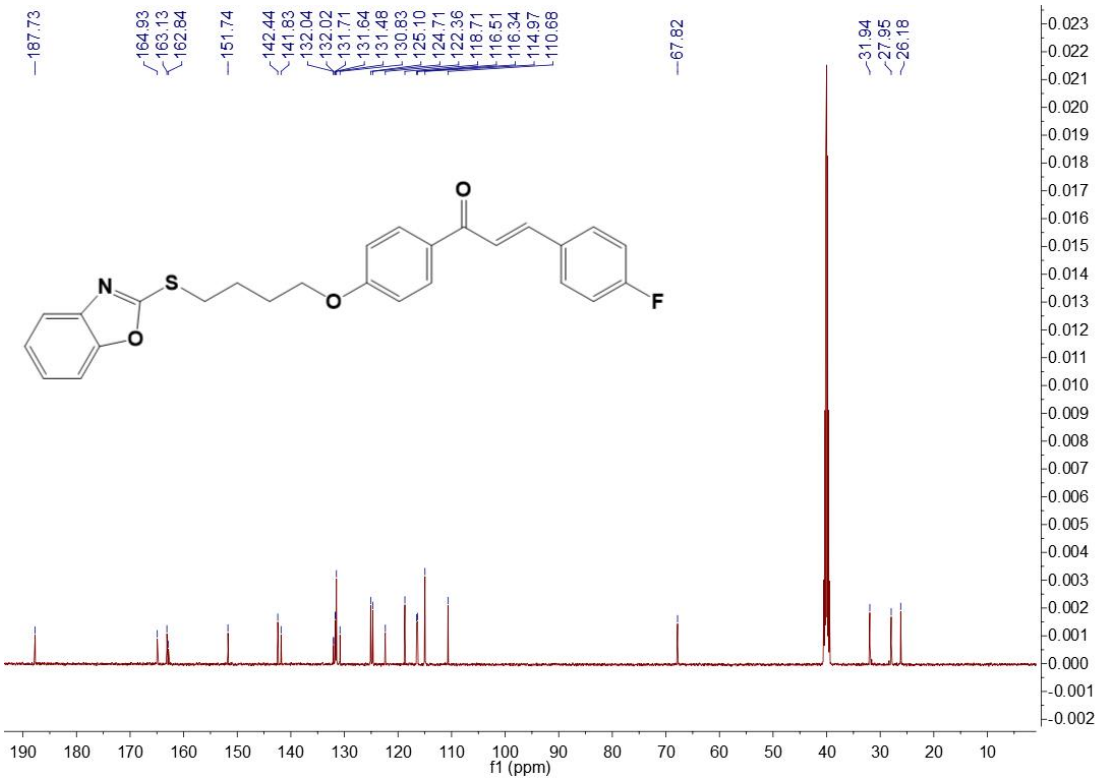


Fig. S7 ^{13}C NMR spectra of compound Z7

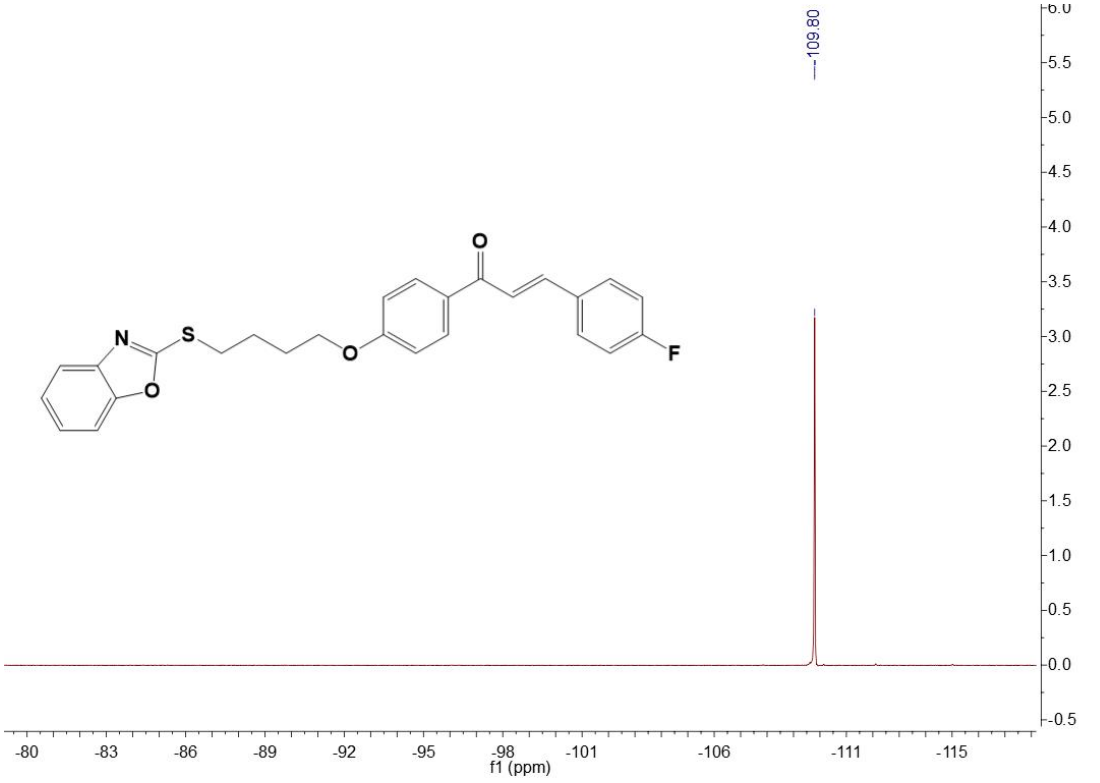


Fig. S7 ^{19}F NMR spectra of compound Z7

51 #79 RT: 0.77 AV: 1 NL: 3.10E+005
T: FTMS + p ESI Full ms [100.0000-1300.0000]

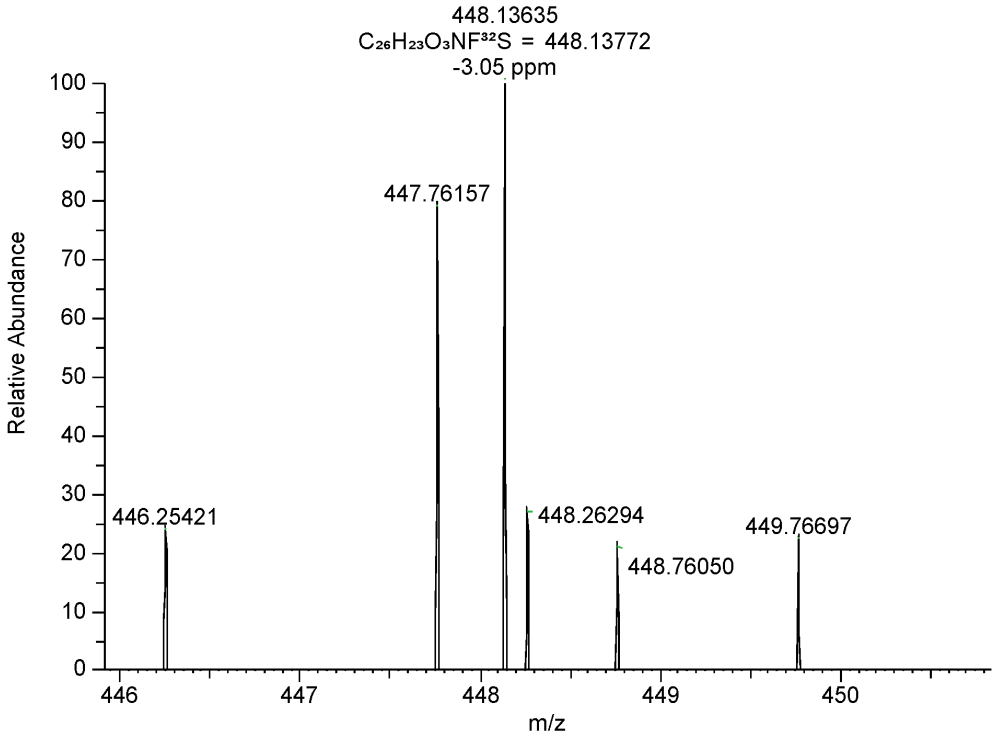


Fig. S7 HRMS spectra of compound Z7

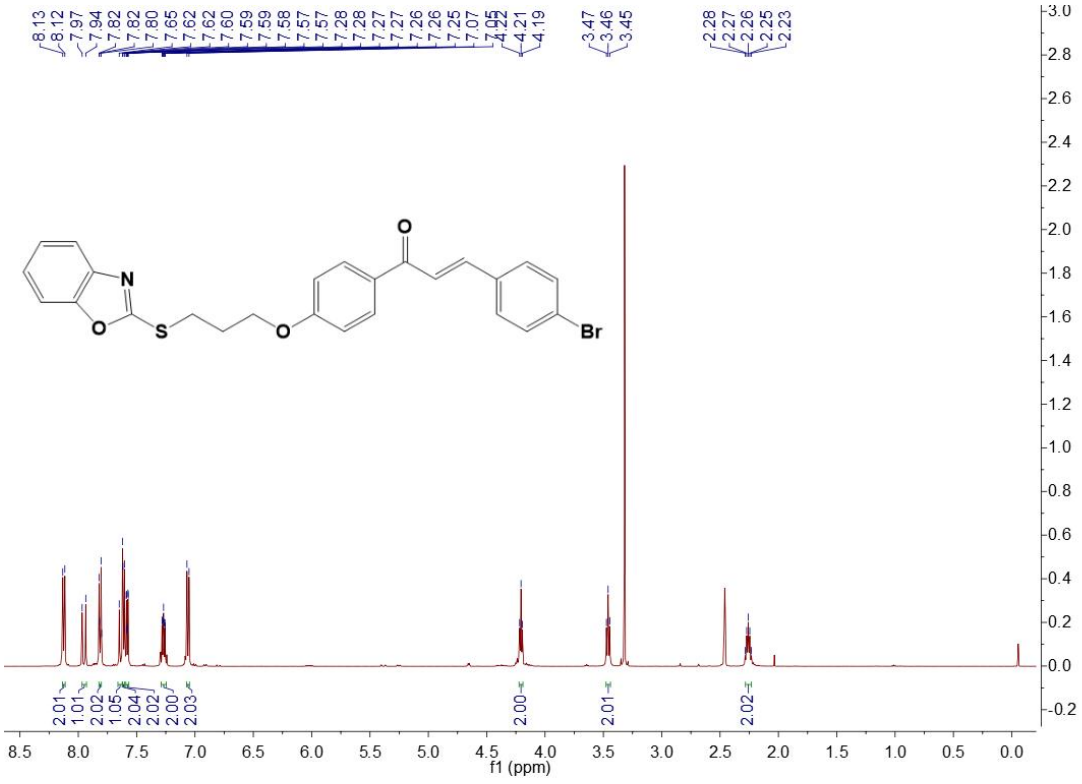


Fig. S8 ^{1}H NMR spectra of compound Z8

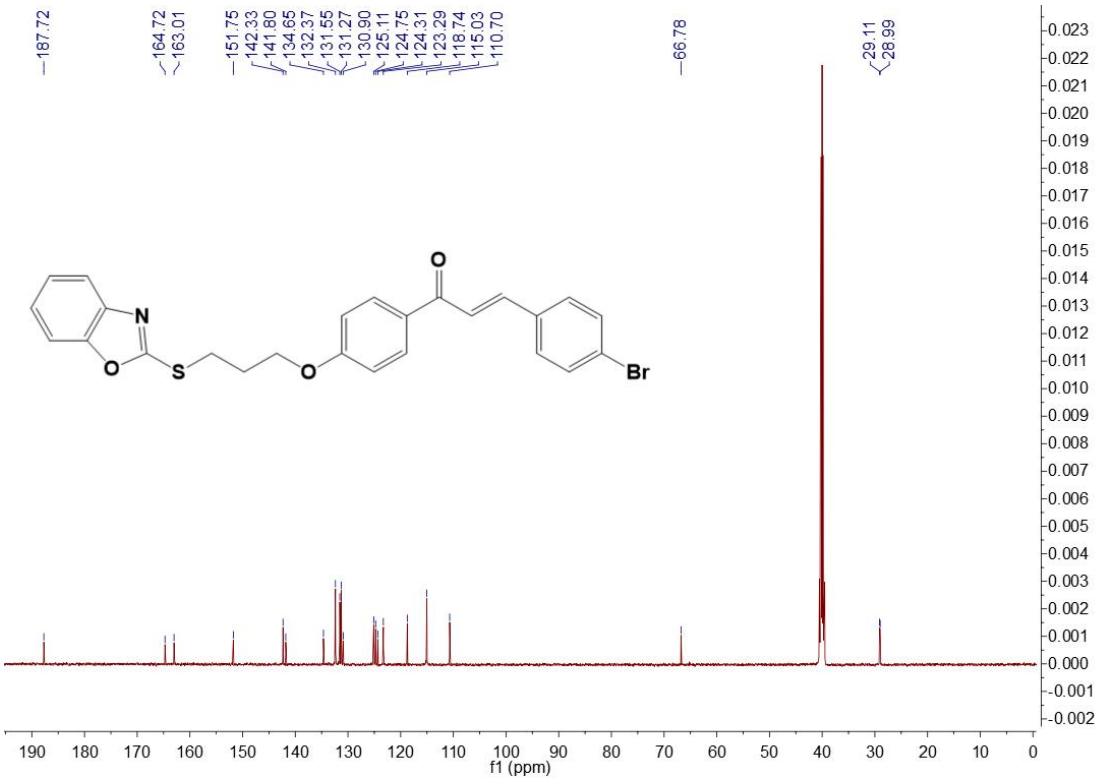


Fig. S8 ^{13}C NMR spectra of compound Z8

52 #7 RT: 0.08 AV: 1 NL: 1.83E+005
T: FTMS + p ESI Full ms [100.0000-1300.0000]

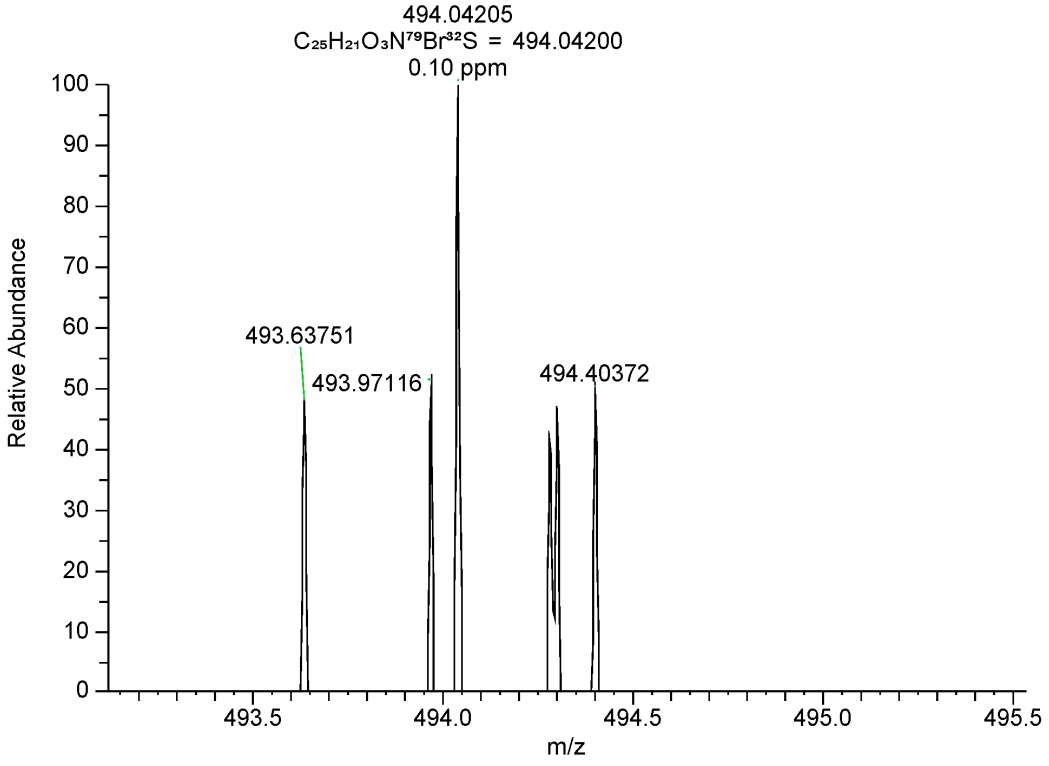


Fig. S8 HRMS spectra of compound Z8

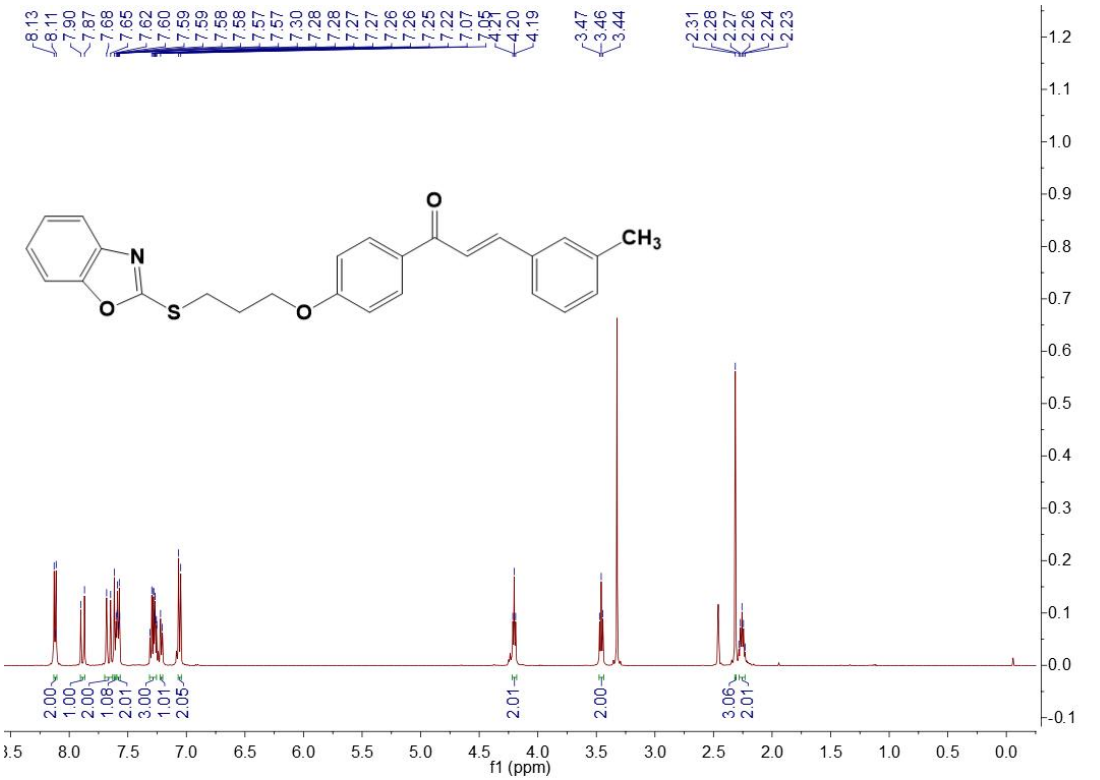


Fig. S9 ^{1}H NMR spectra of compound Z9

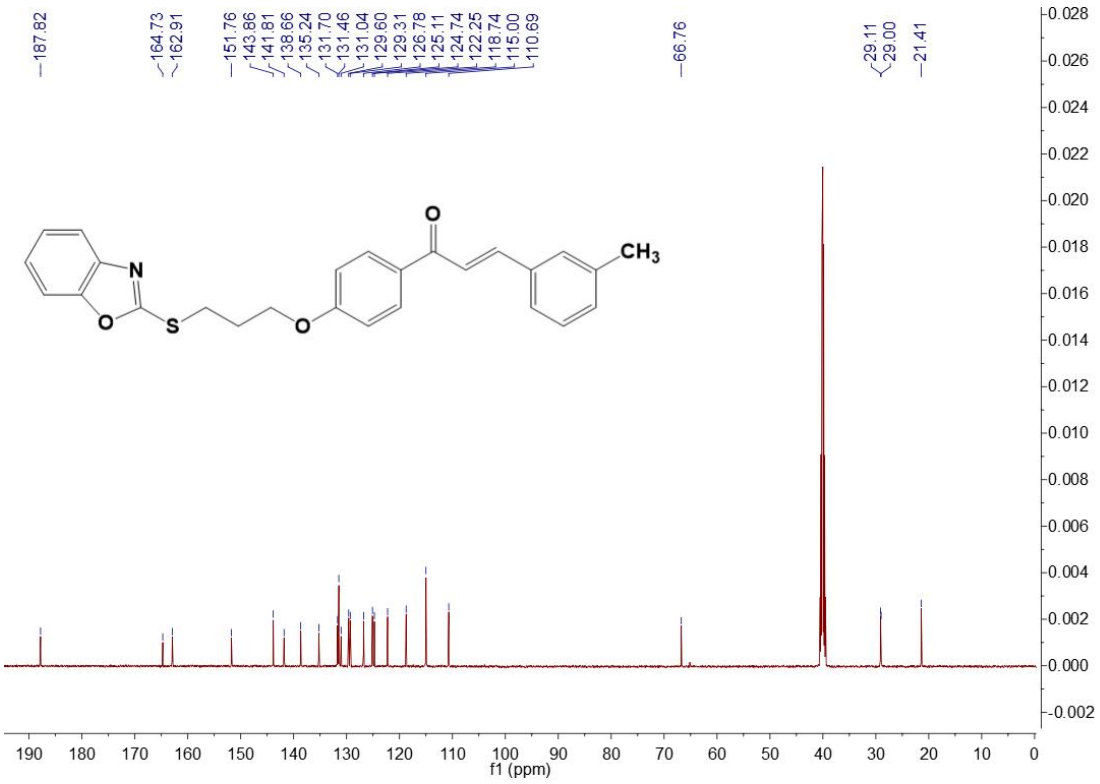


Fig. S9 ^{13}C NMR spectra of compound Z9

15 #79 RT: 0.76 AV: 1 NL: 1.33E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

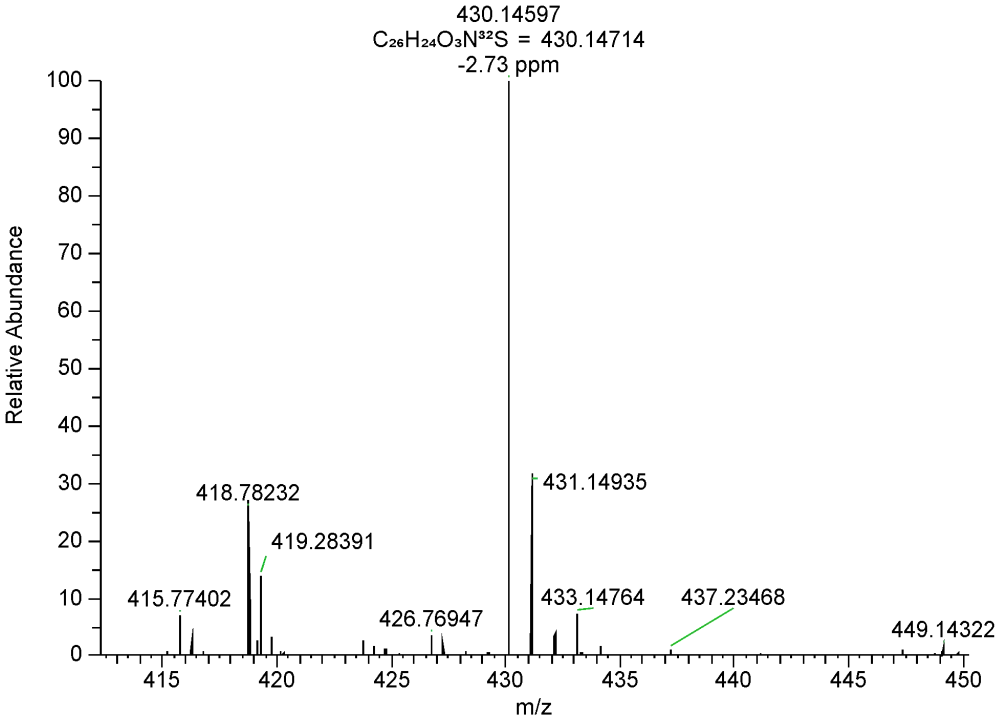


Fig. S9 HRMS spectra of compound Z9

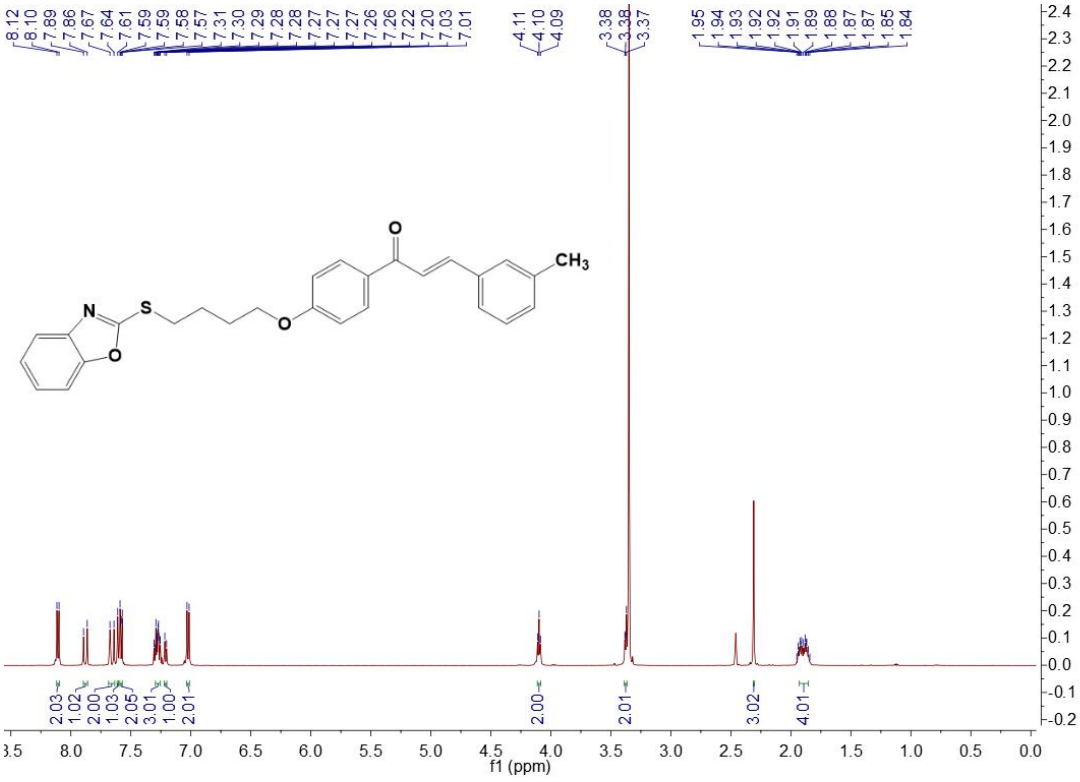


Fig. S10 ^{1}H NMR spectra of compound Z10

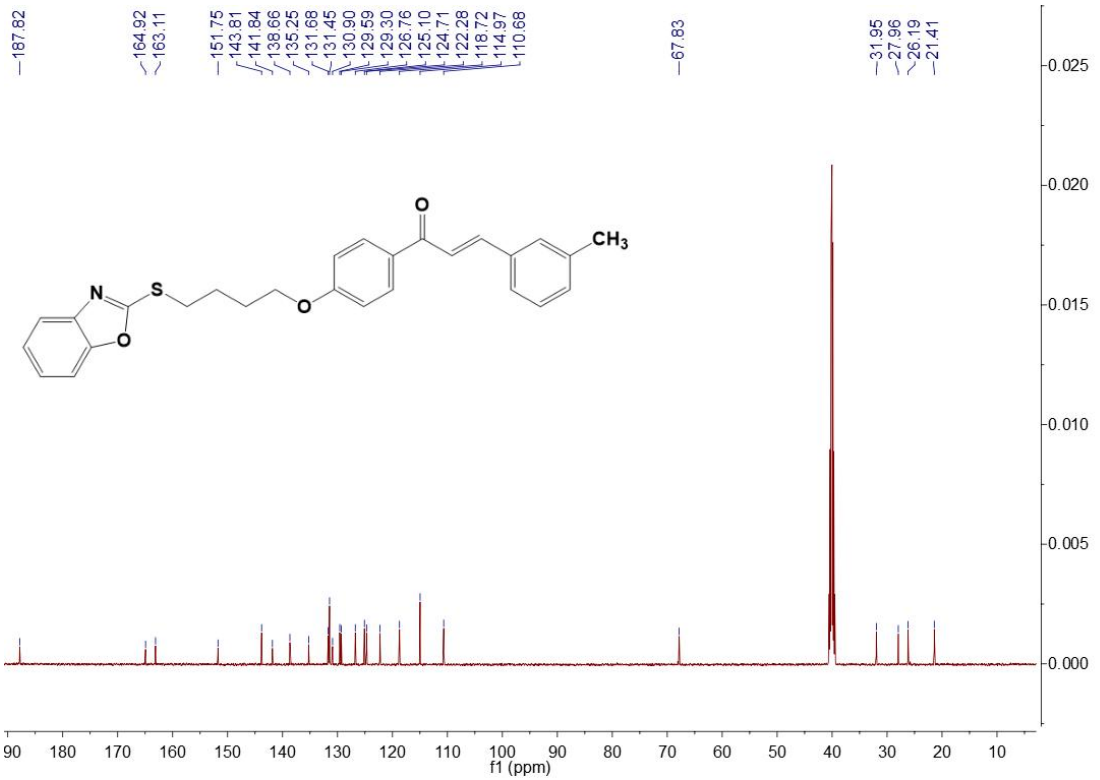


Fig. S10 ^{13}C NMR spectra of compound Z10

19 #97 RT: 0.94 AV: 1 NL: 3.30E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

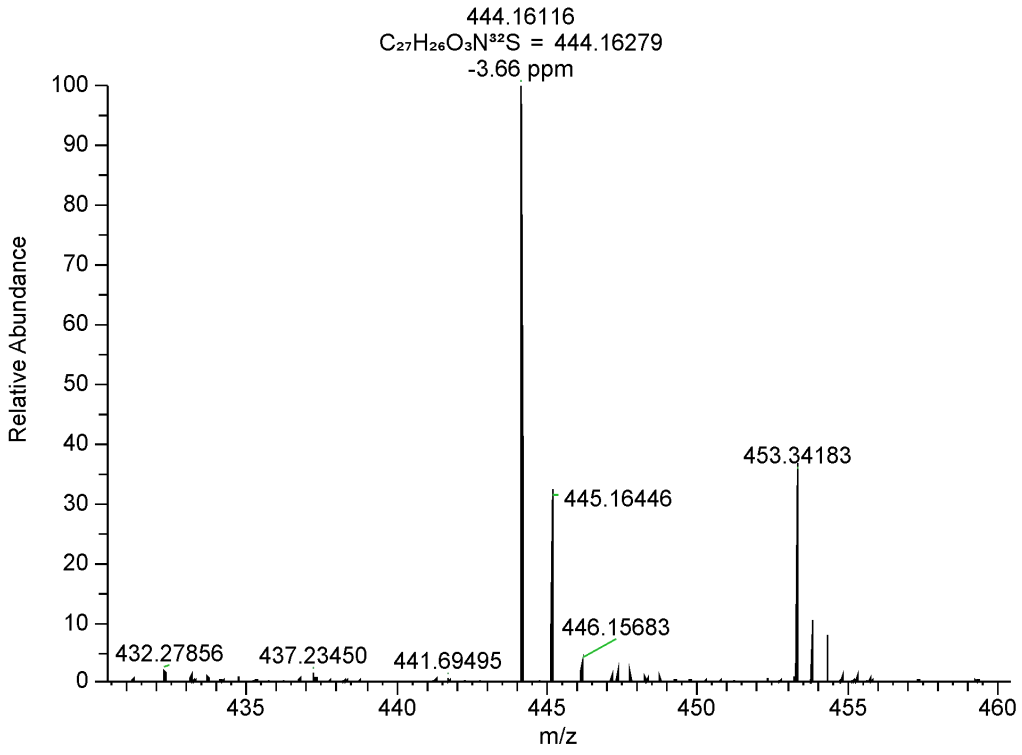


Fig. S10 HRMS spectra of compound Z10

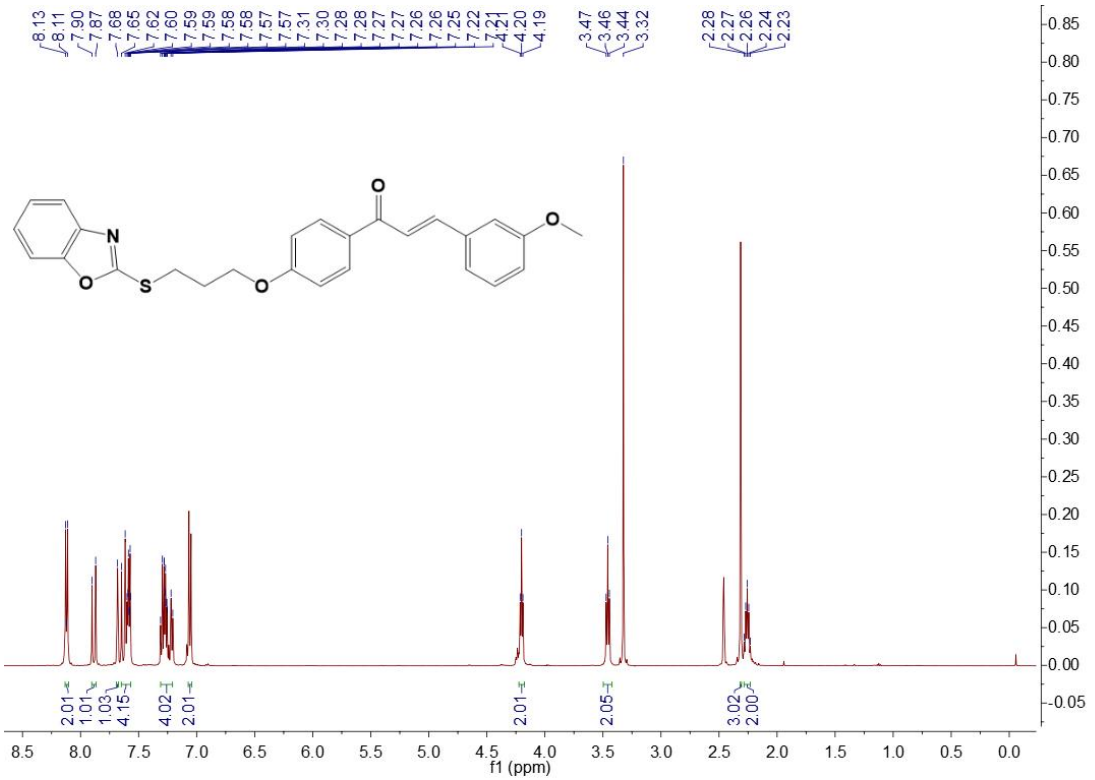


Fig. S11 ^{1}H NMR spectra of compound Z11

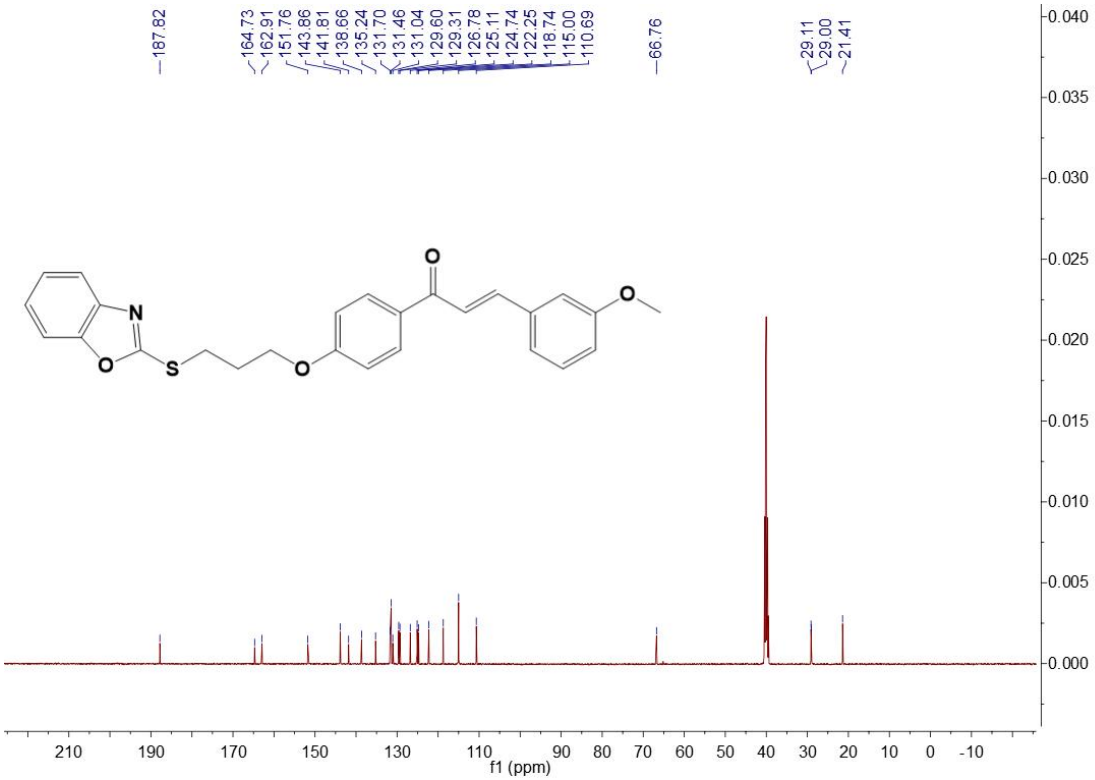


Fig. S11 ^{13}C NMR spectra of compound Z11

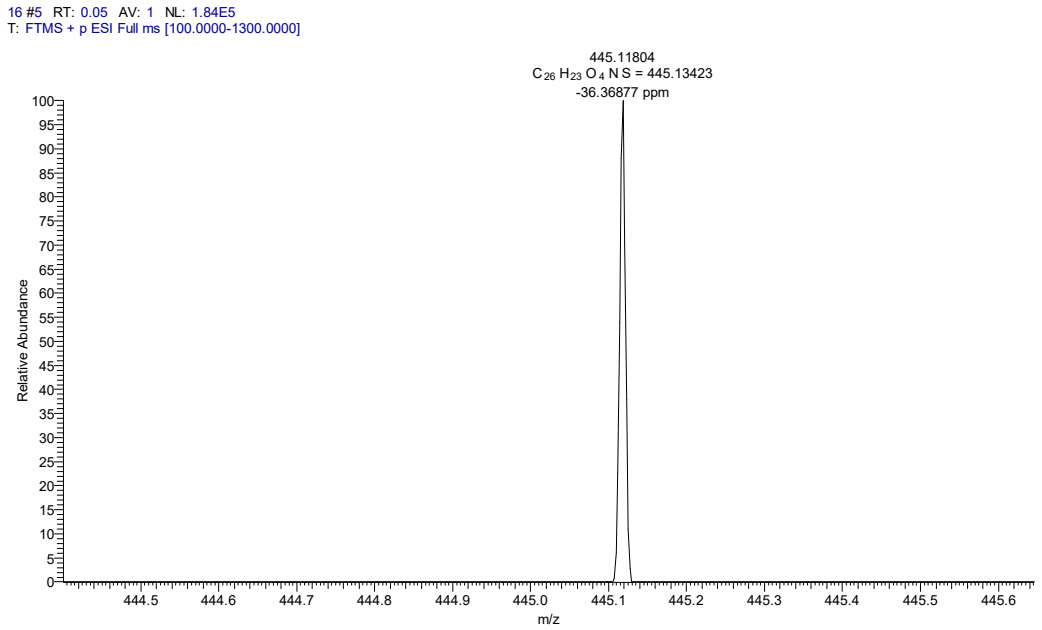


Fig. S11 HRMS spectra of compound Z11

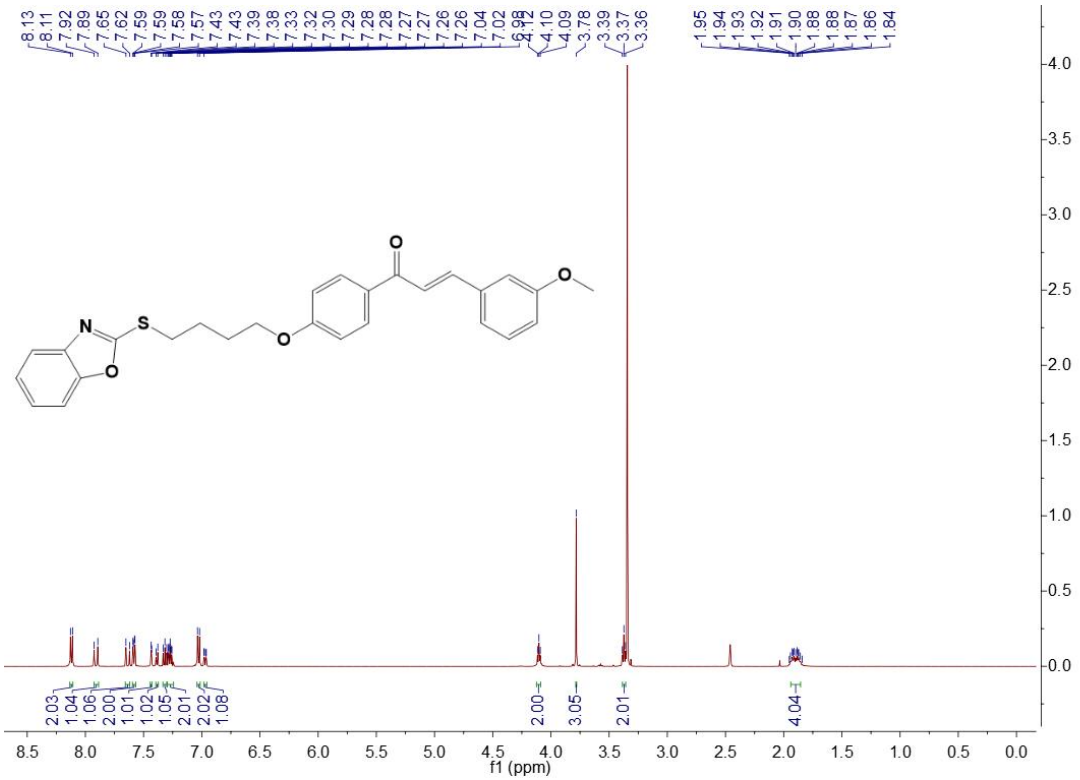


Fig. S12 ^{1}H NMR spectra of compound Z12

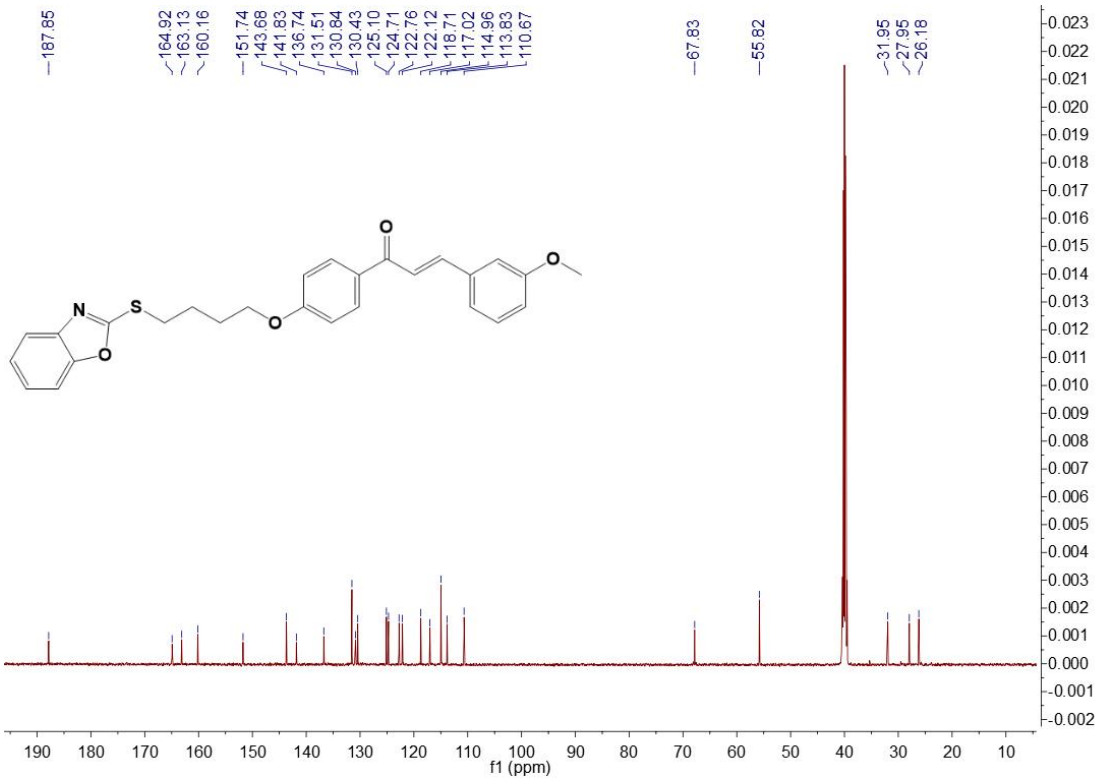


Fig. S12 ^{13}C NMR spectra of compound Z12

20 #83 RT: 0.80 AV: 1 NL: 3.99E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

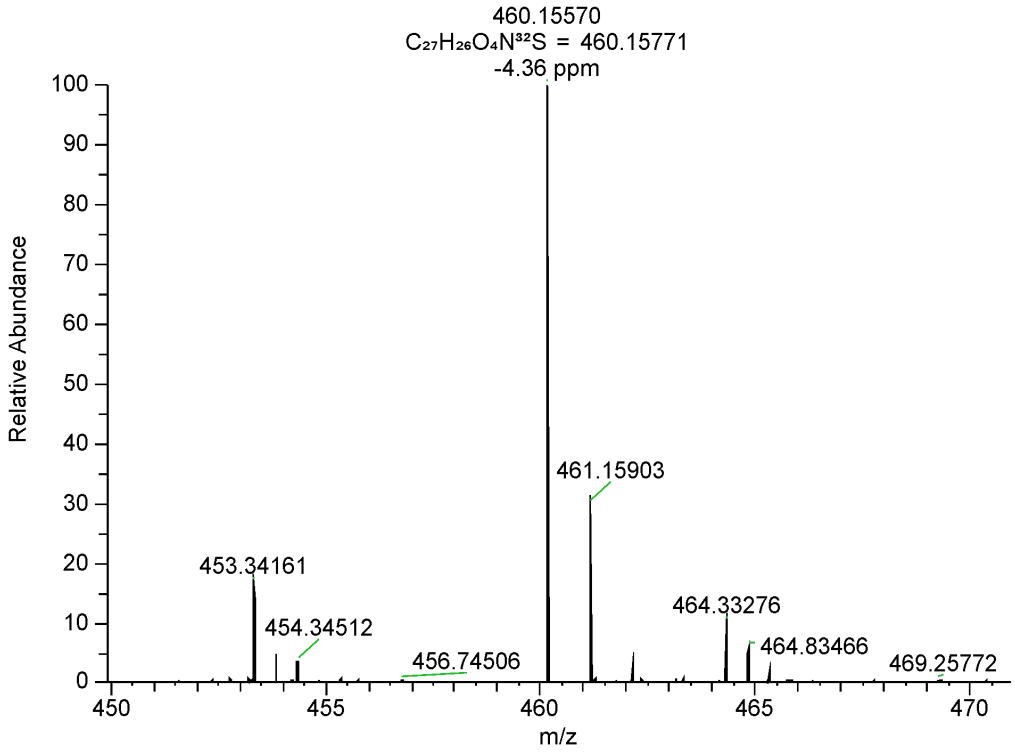


Fig. S12 HRMS spectra of compound Z12

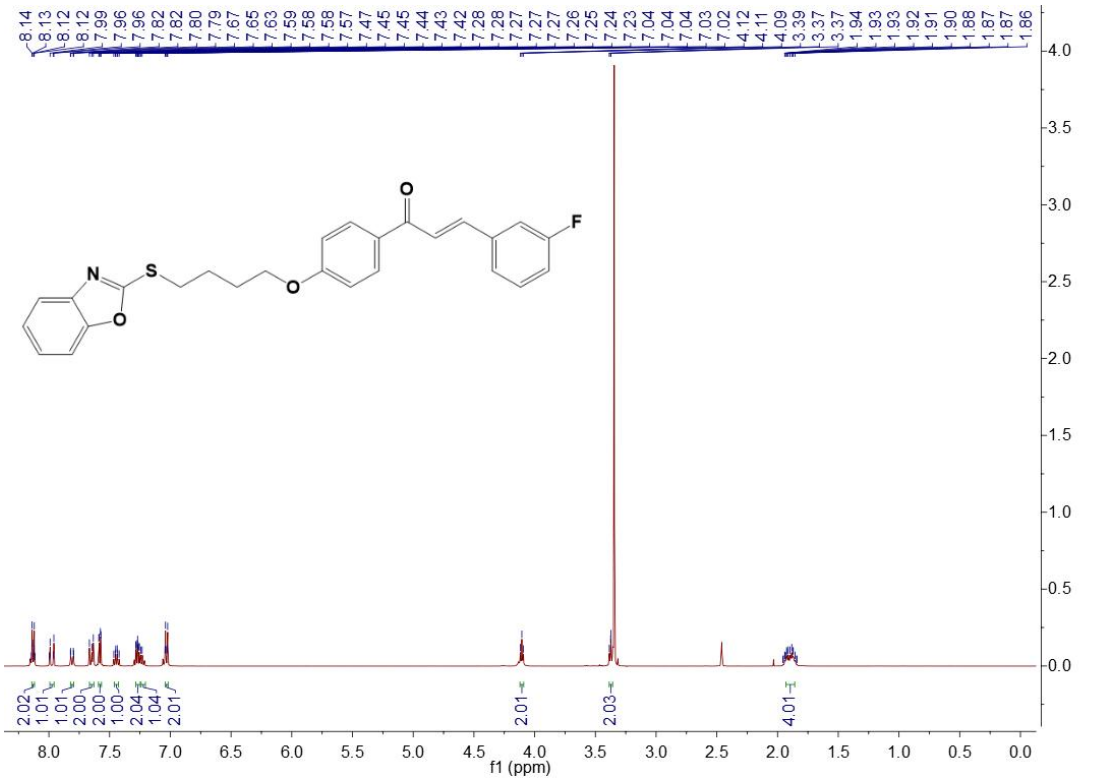


Fig. S13 ^{1}H NMR spectra of compound Z13

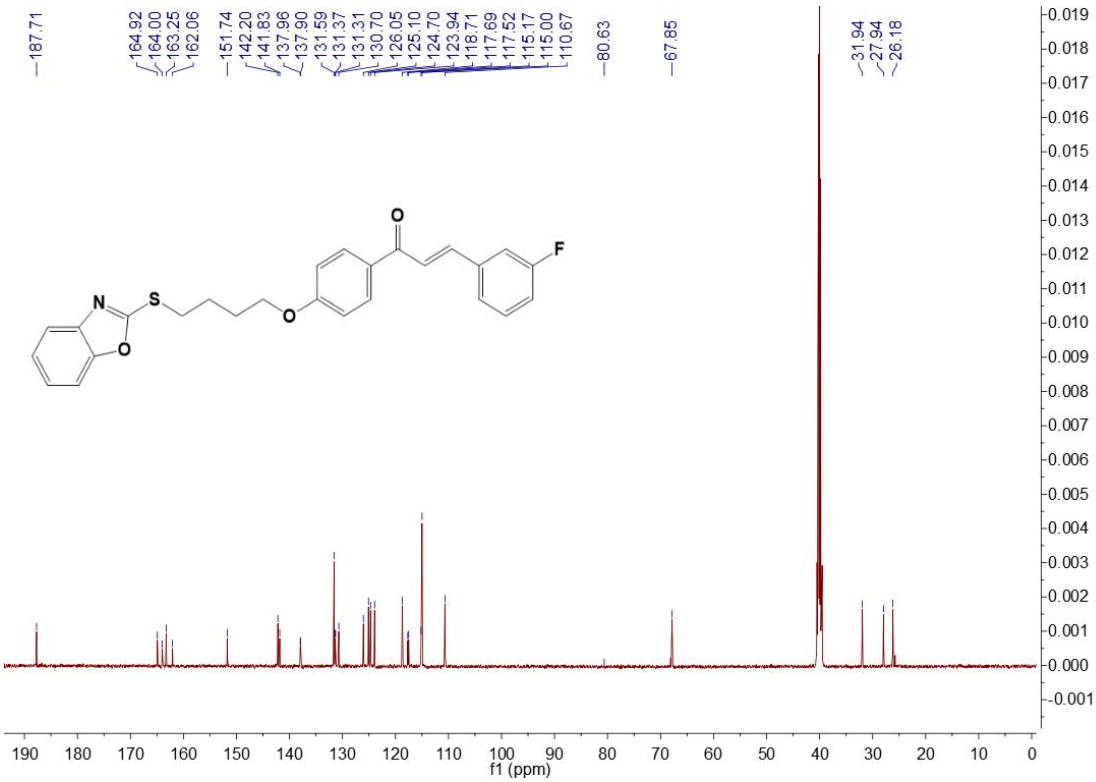


Fig. S13 ^{13}C NMR spectra of compound Z13

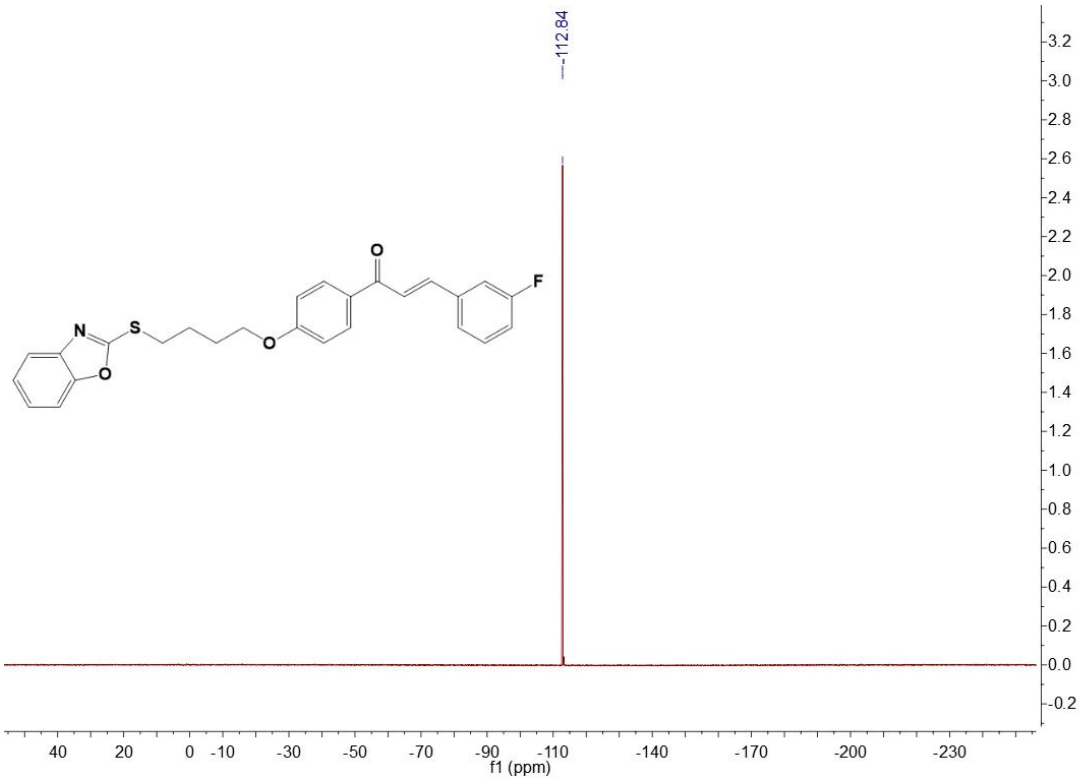


Fig. S13 ^{19}F NMR spectra of compound Z13

11 #79 RT: 0.76 AV: 1 NL: 5.71E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

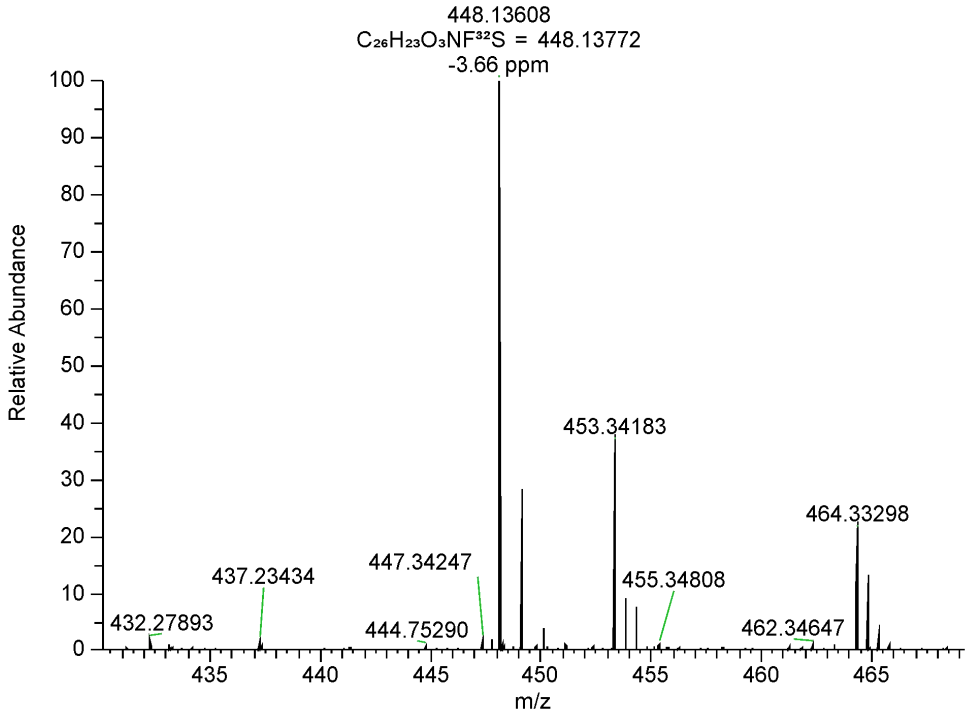


Fig. S13 HRMS spectra of compound Z13

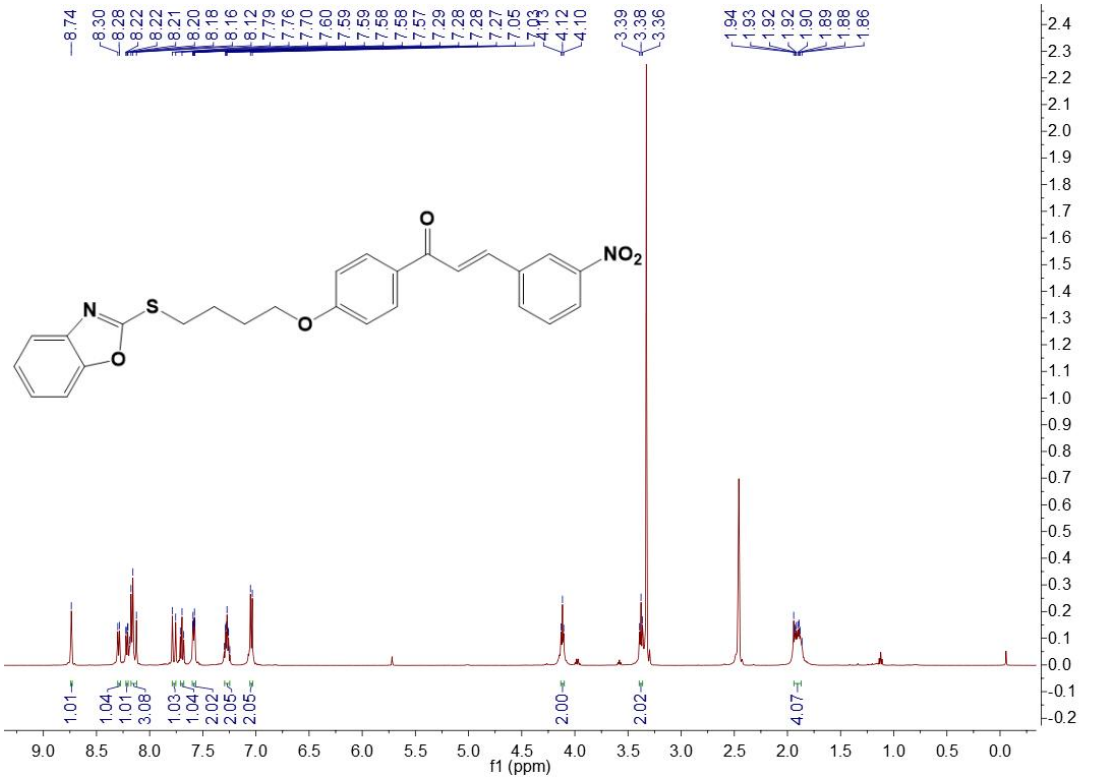


Fig. S14 ^{1}H NMR spectra of compound Z14

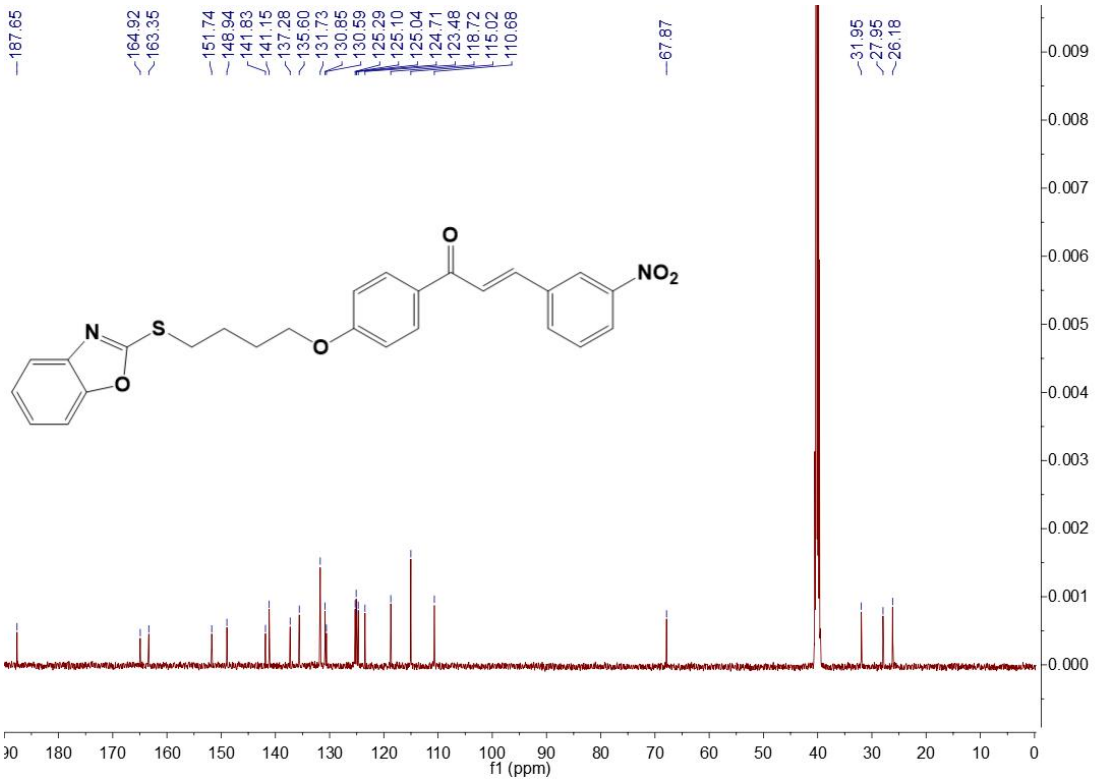


Fig. S14 ^{13}C NMR spectra of compound Z14

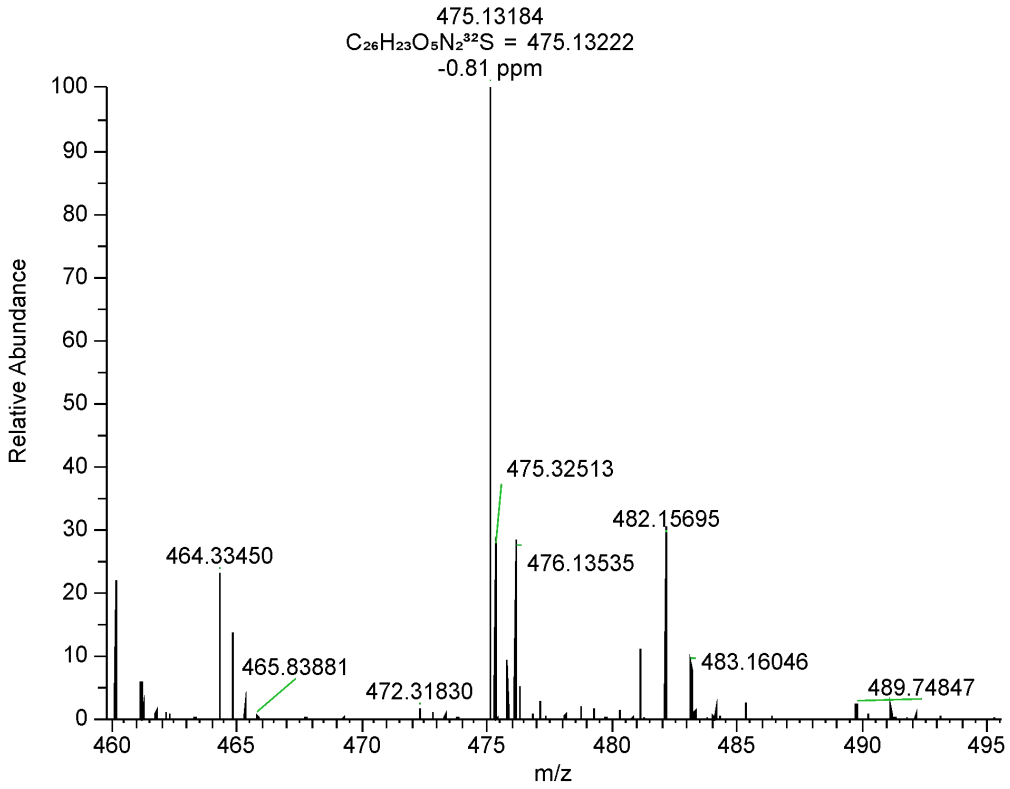


Fig. S14 HRMS spectra of compound Z14

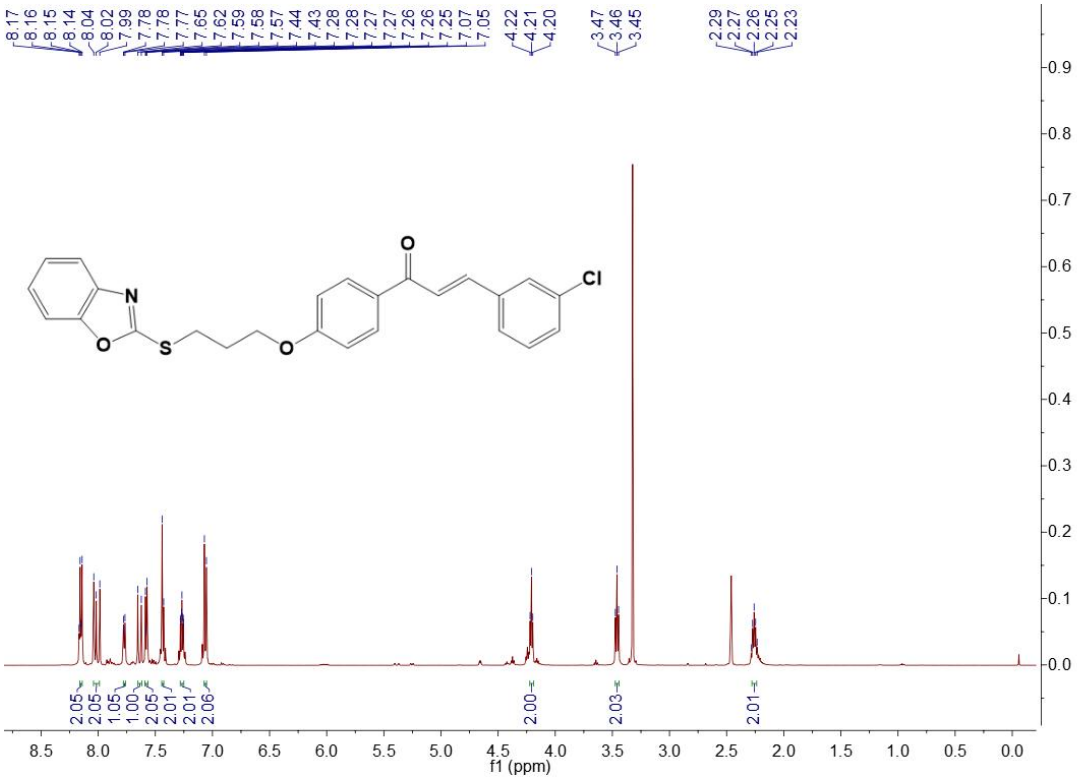


Fig. S15 ^{1}H NMR spectra of compound Z15

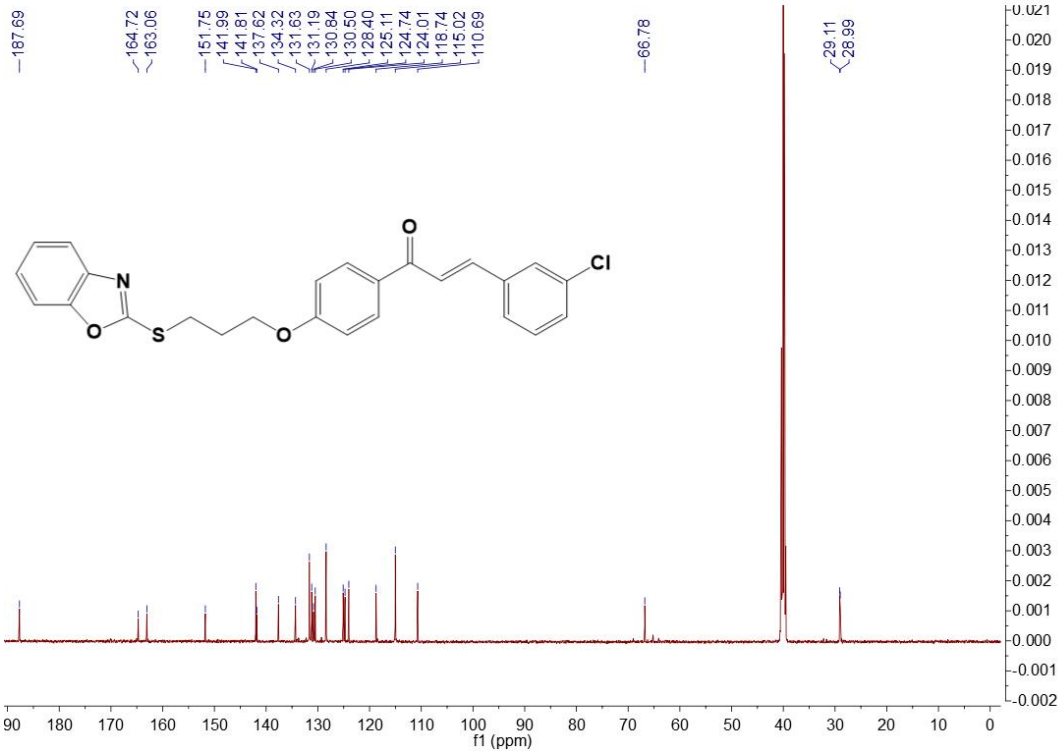


Fig. S15 ^{13}C NMR spectra of compound Z15

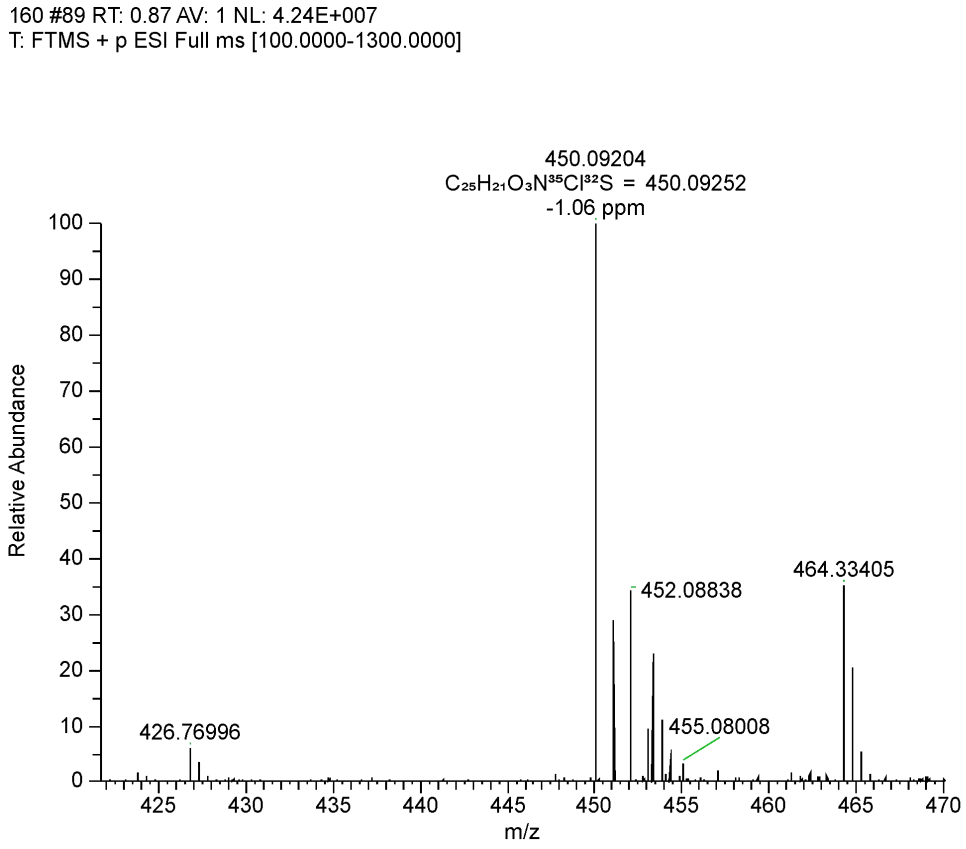


Fig. S15 HRMS spectra of compound Z15

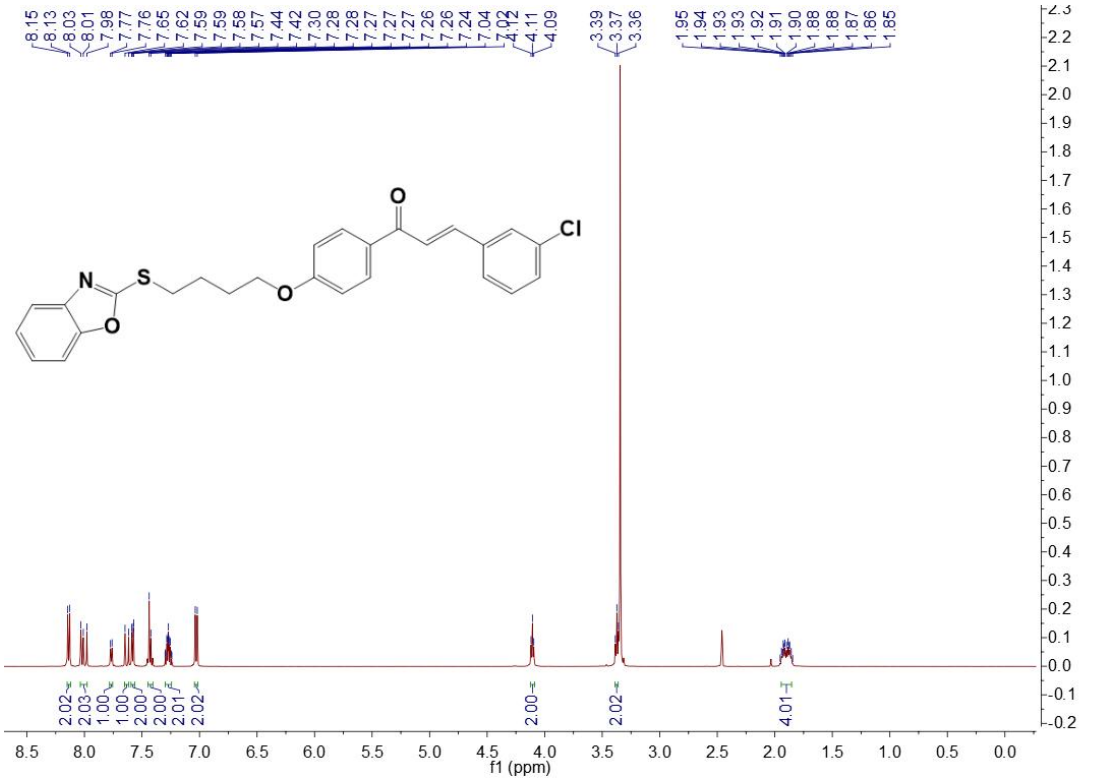


Fig. S16 ^{1}H NMR spectra of compound Z16

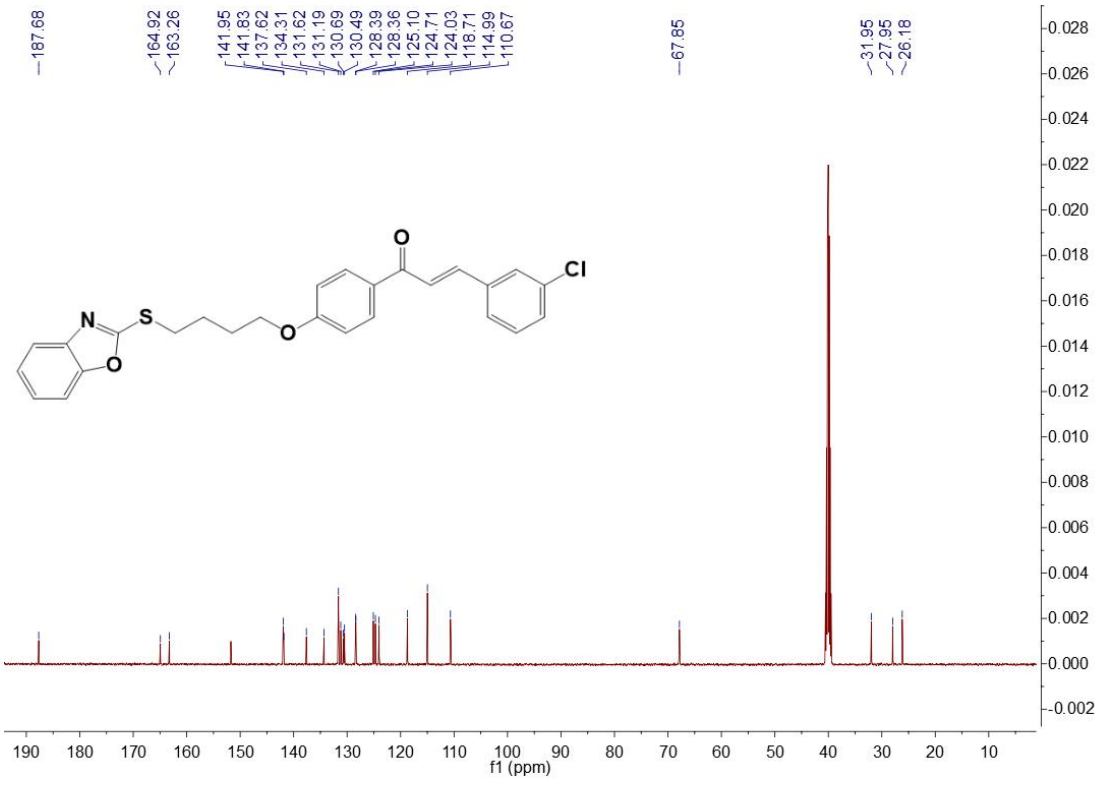


Fig. S16 ^{13}C NMR spectra of compound Z16

157 #101 RT: 0.99 AV: 1 NL: 2.63E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

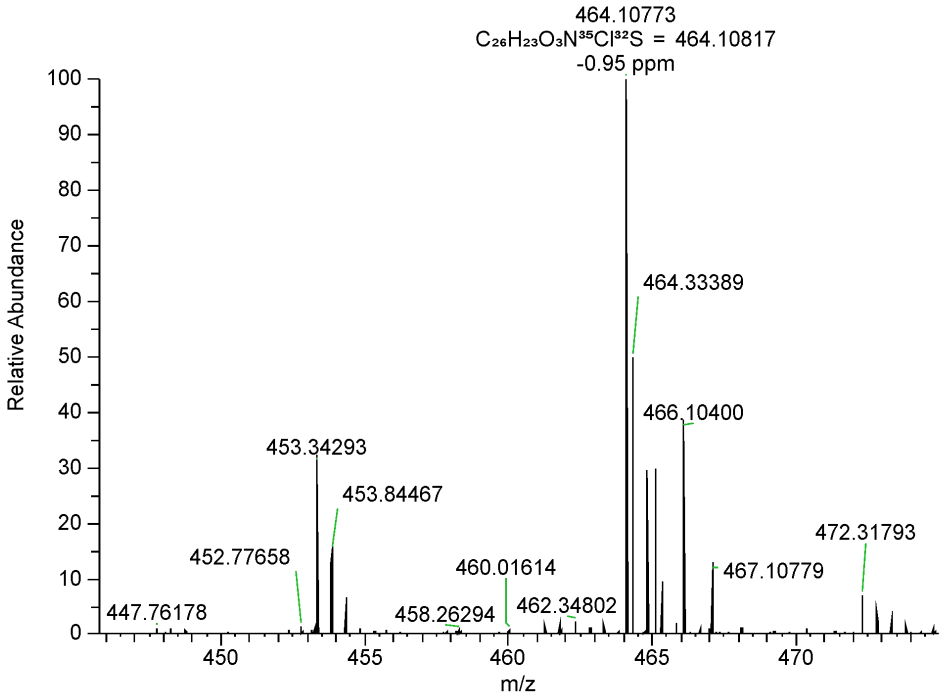


Fig. S16 HRMS spectra of compound Z16

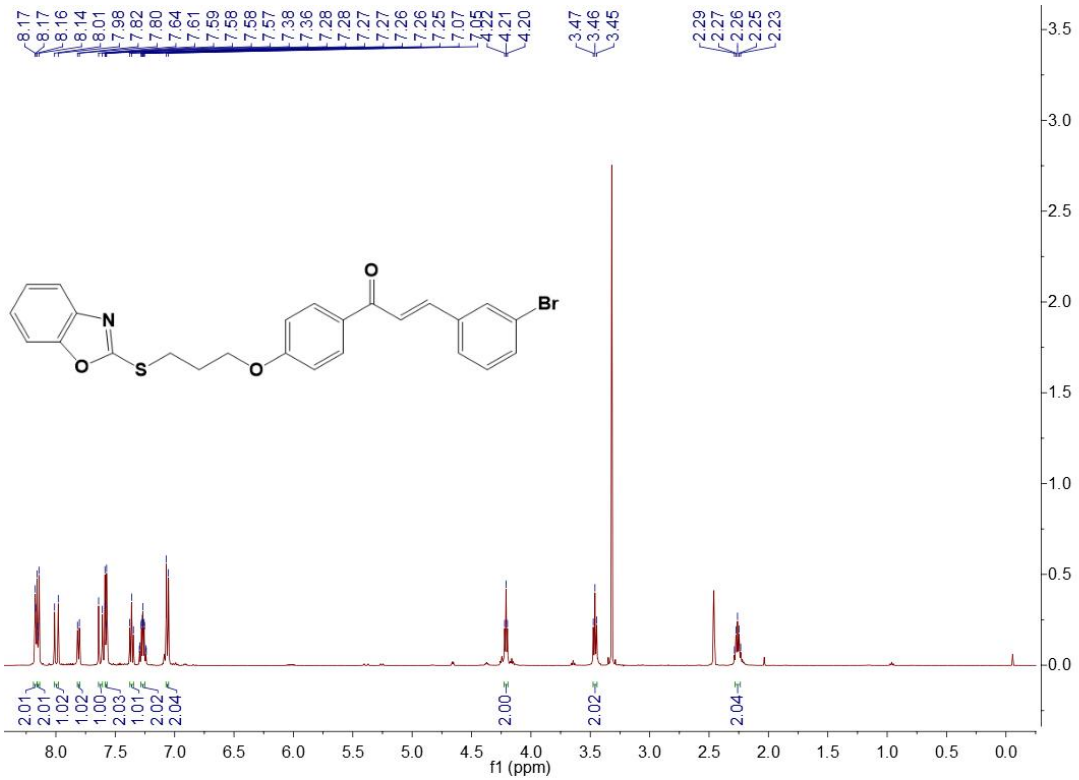


Fig. S17 ^{1}H NMR spectra of compound Z17

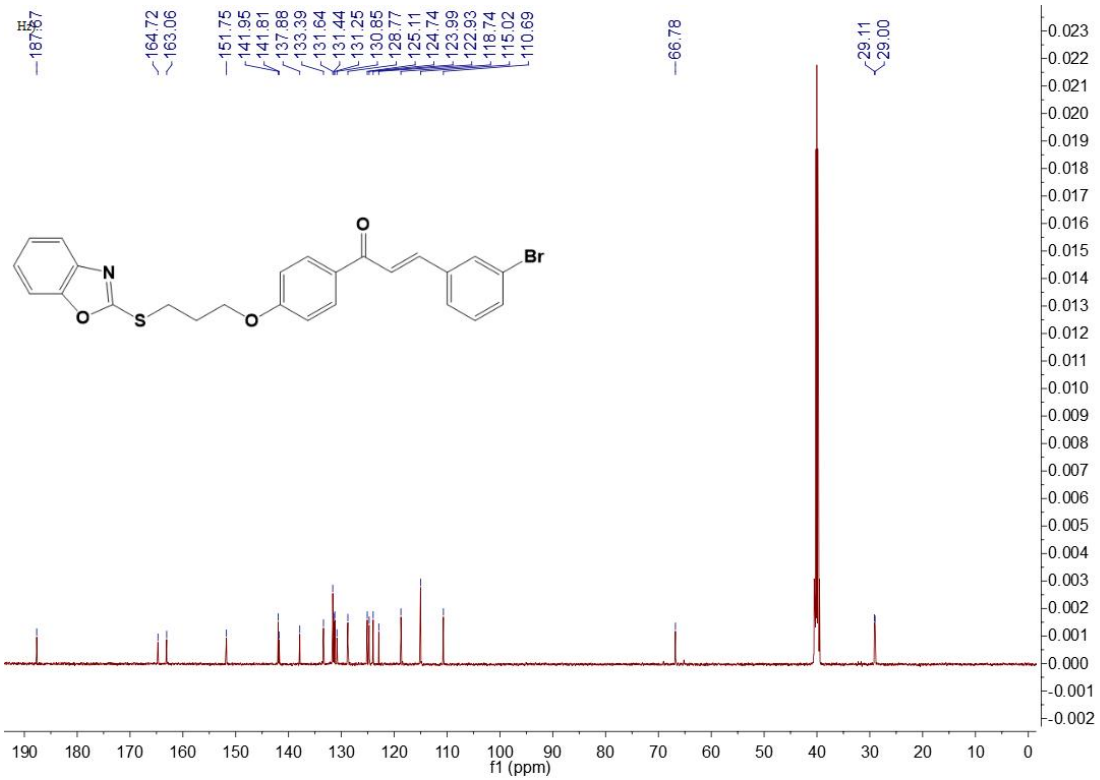


Fig. S17 ^{13}C NMR spectra of compound Z17

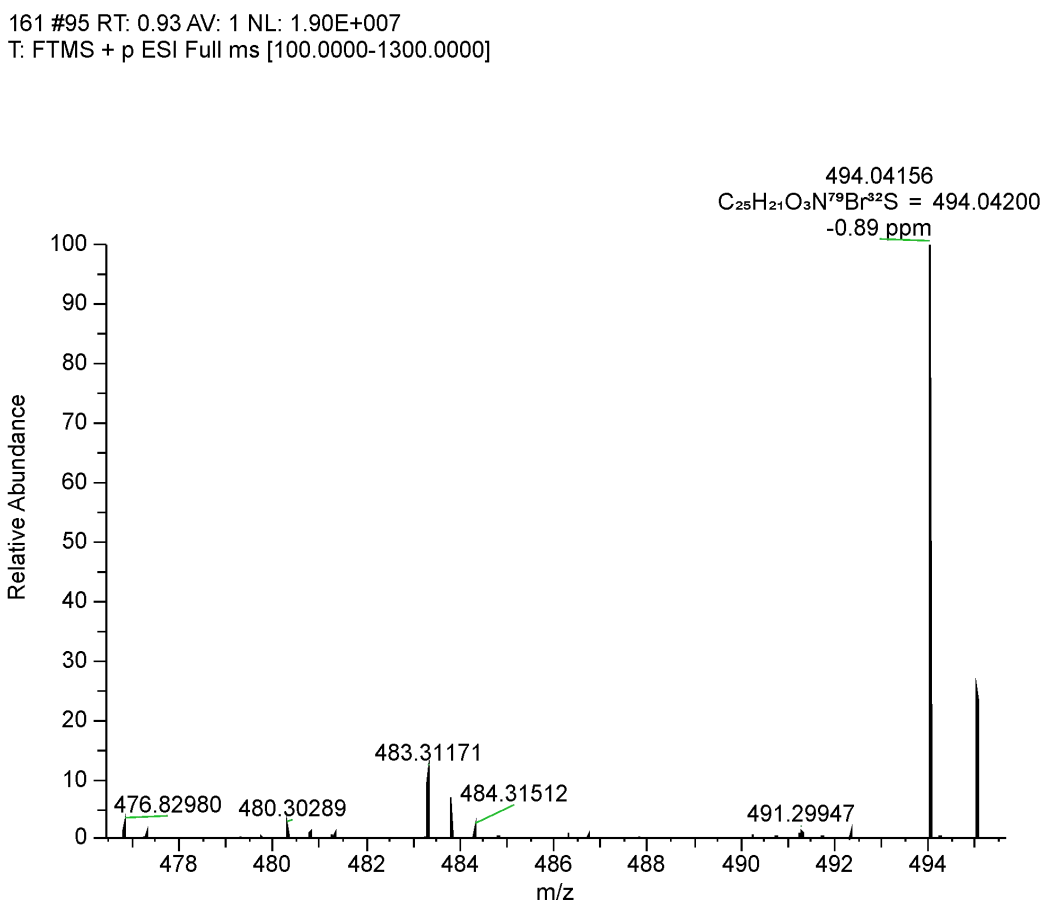


Fig. S17 HRMS spectra of compound Z17

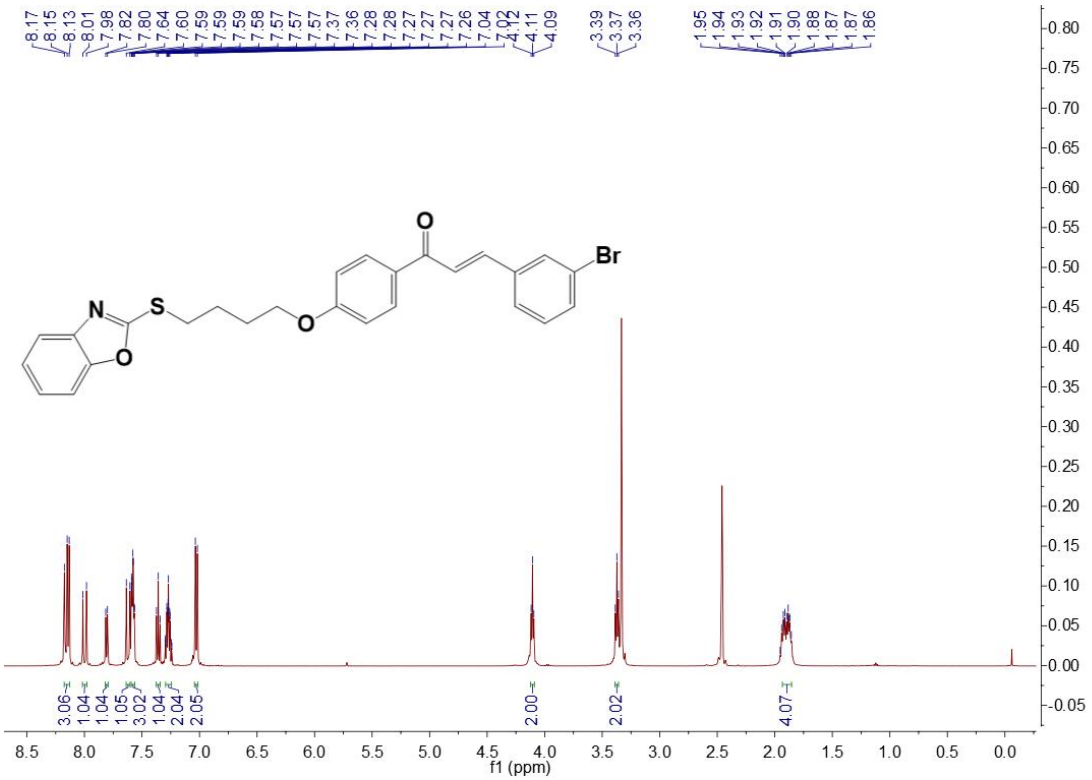


Fig. S18 ^{1}H NMR spectra of compound Z18

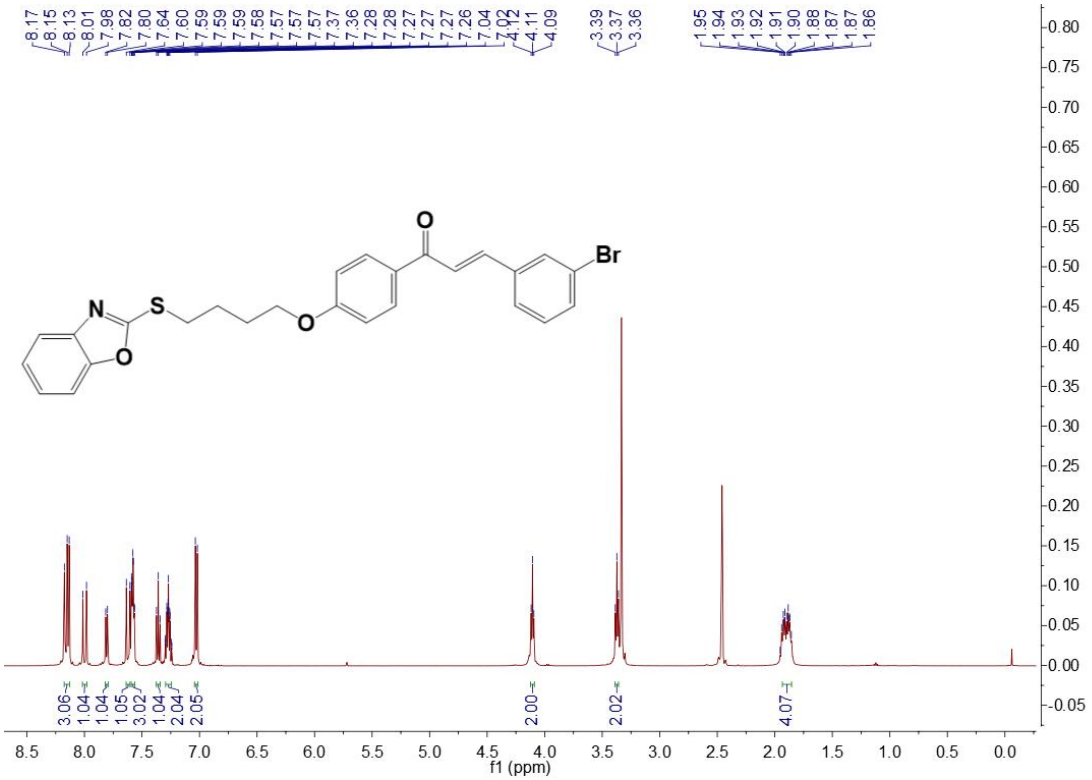


Fig. S18 ^{13}C NMR spectra of compound Z18

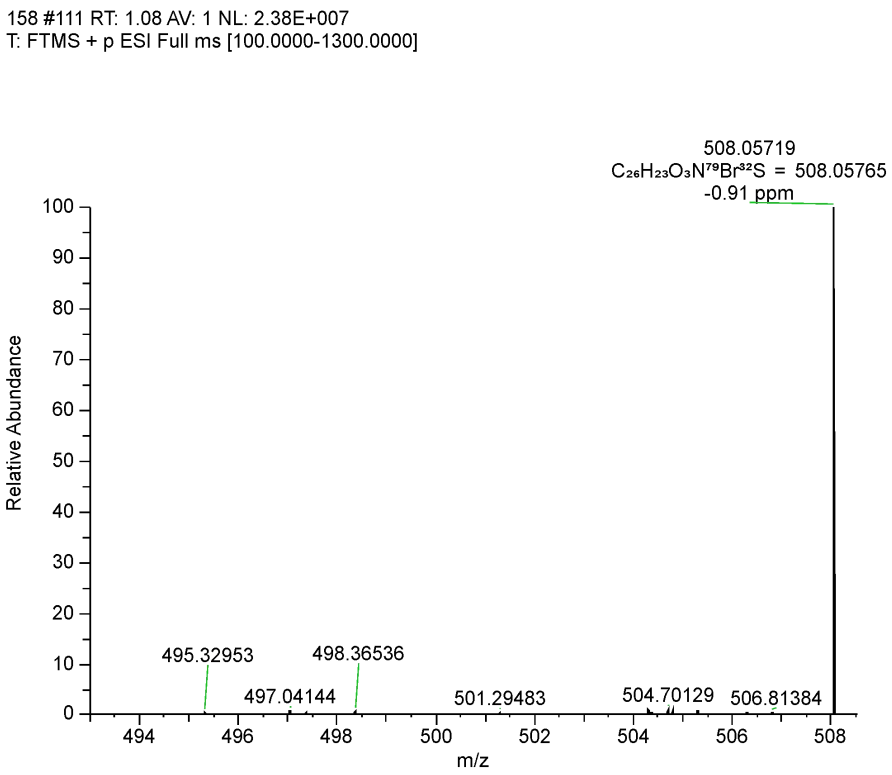


Fig. S18 HRMS spectra of compound Z18

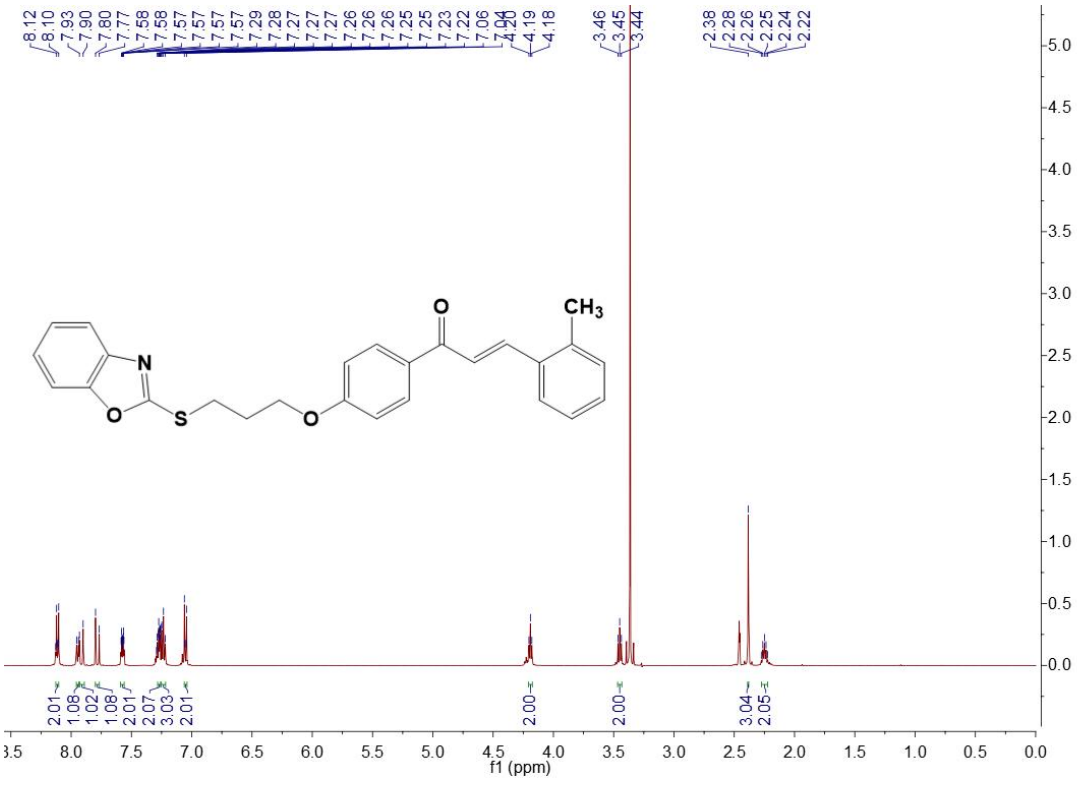


Fig. S19 ^{1}H NMR spectra of compound Z19

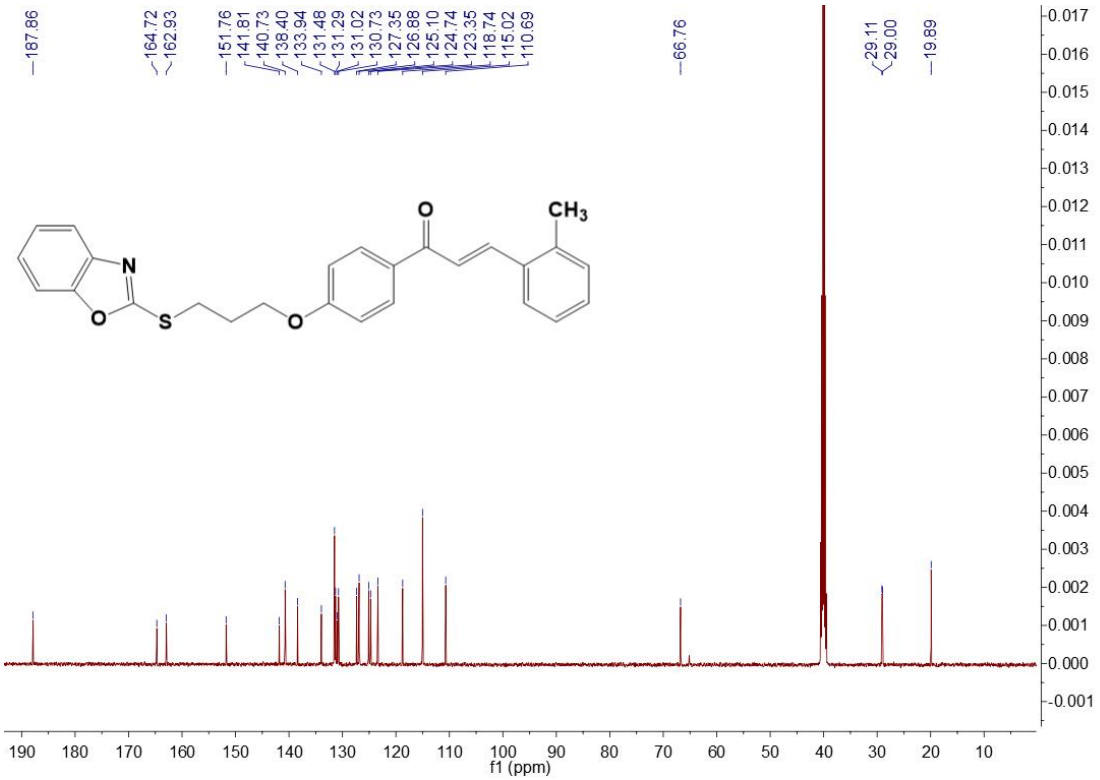


Fig. S19 ^{13}C NMR spectra of compound Z19

60_220709044745 #87 RT: 0.84 AV: 1 NL: 1.17E+00 ...

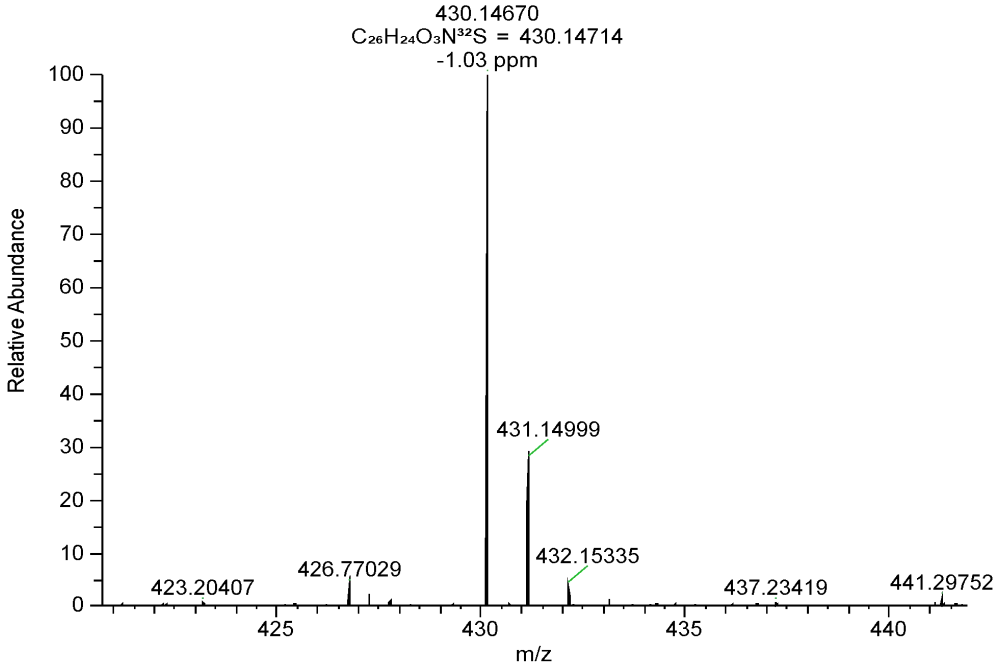


Fig. S19 ^{13}C NMR spectra of compound Z19

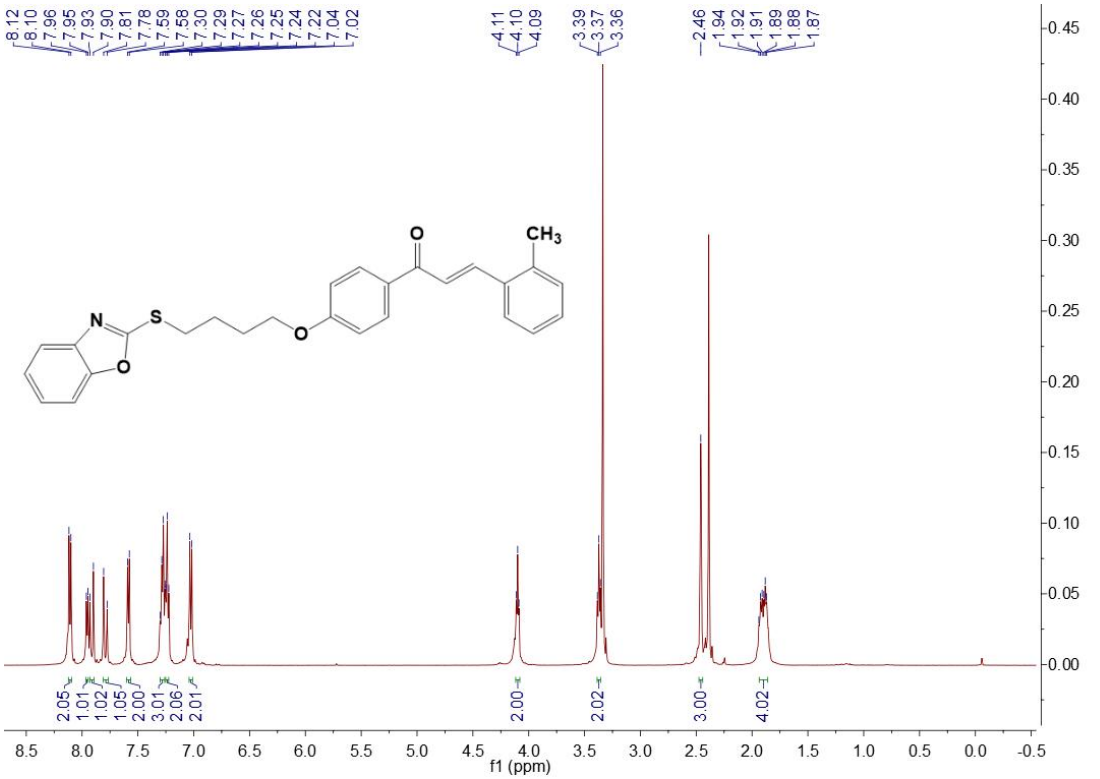


Fig. S20 ^{1}H NMR spectra of compound Z20

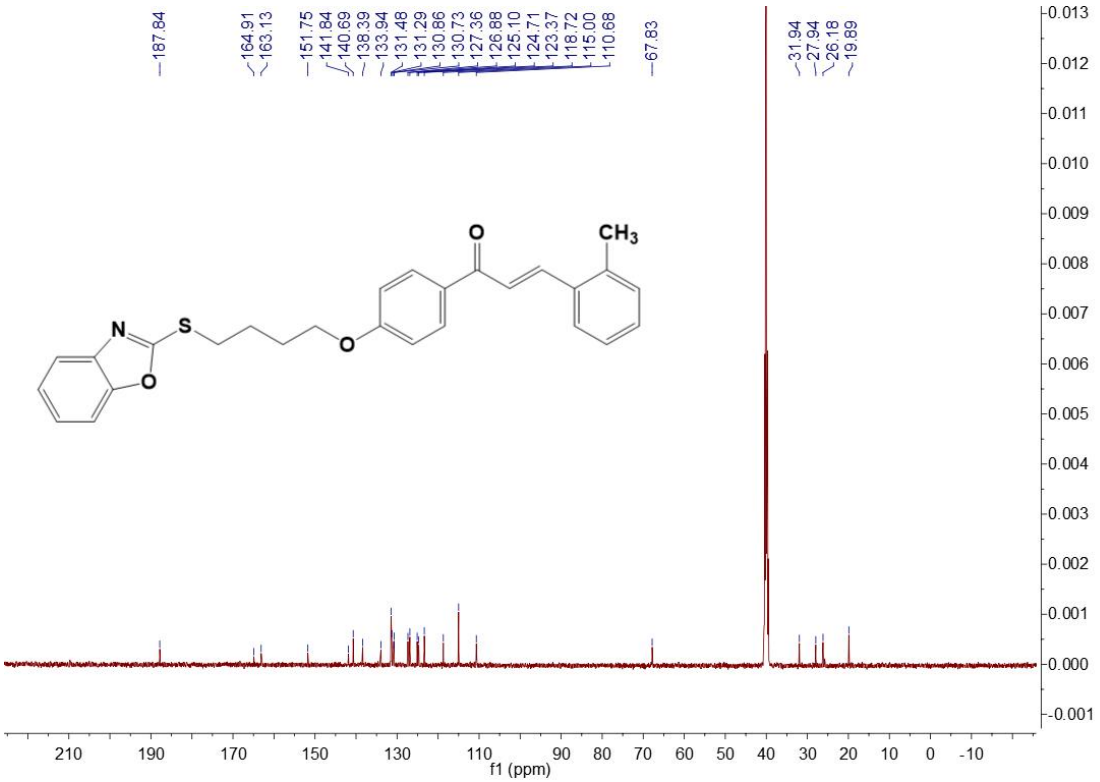


Fig. S20 ^{13}C NMR spectra of compound Z20

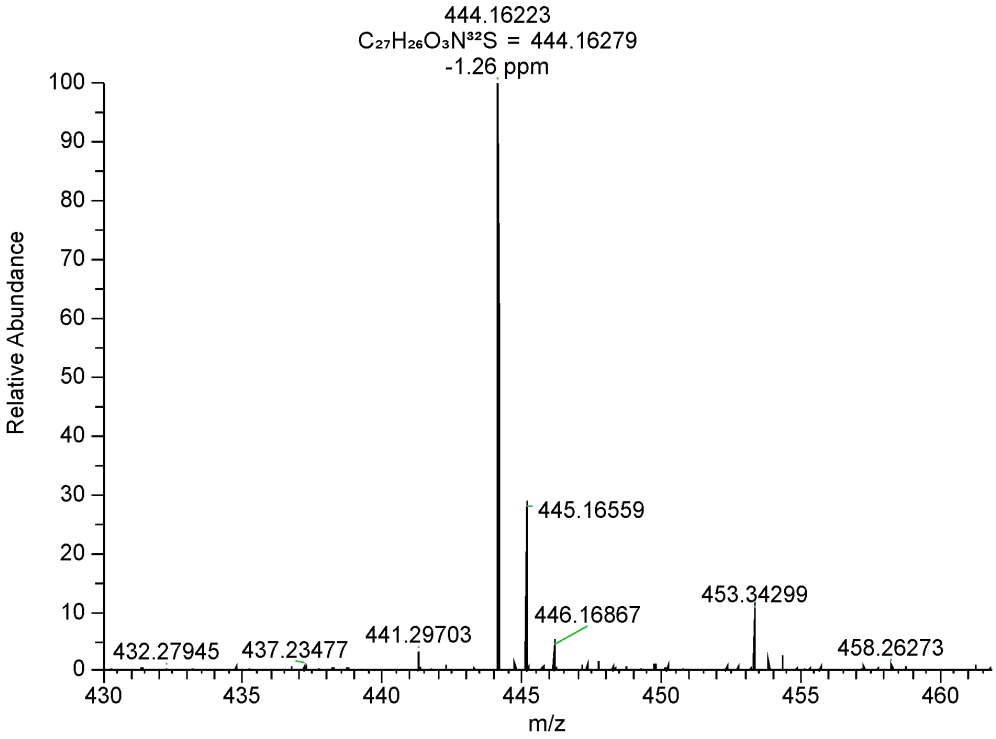


Fig. S20 HRMS spectra of compound Z20

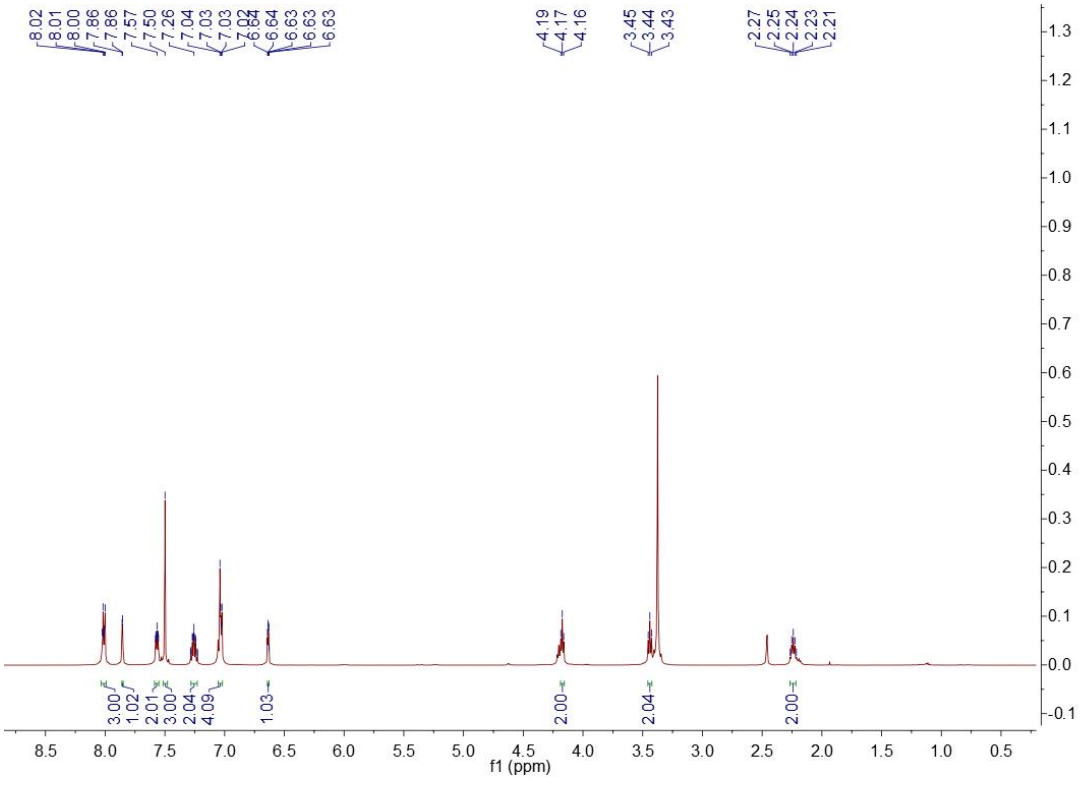


Fig. S21 ^{1}H NMR spectra of compound Z21

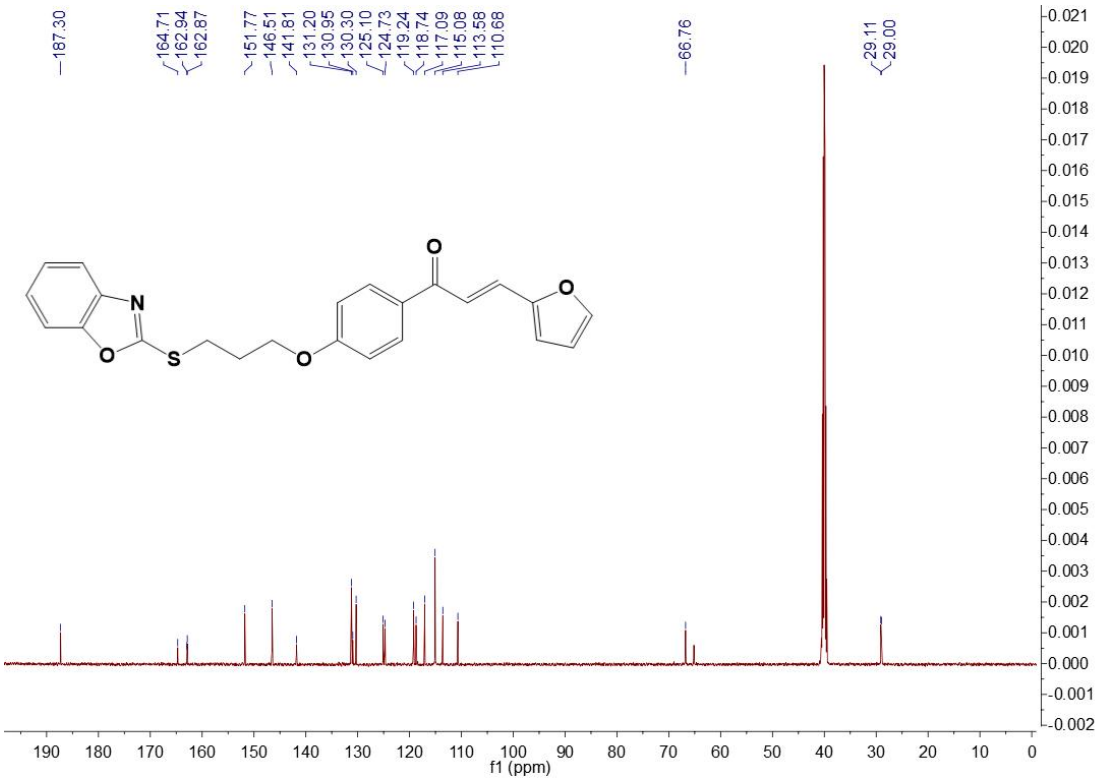


Fig. S21 ^{13}C NMR spectra of compound Z21

21 #61 RT: 0.59 AV: 1 NL: 5.75E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

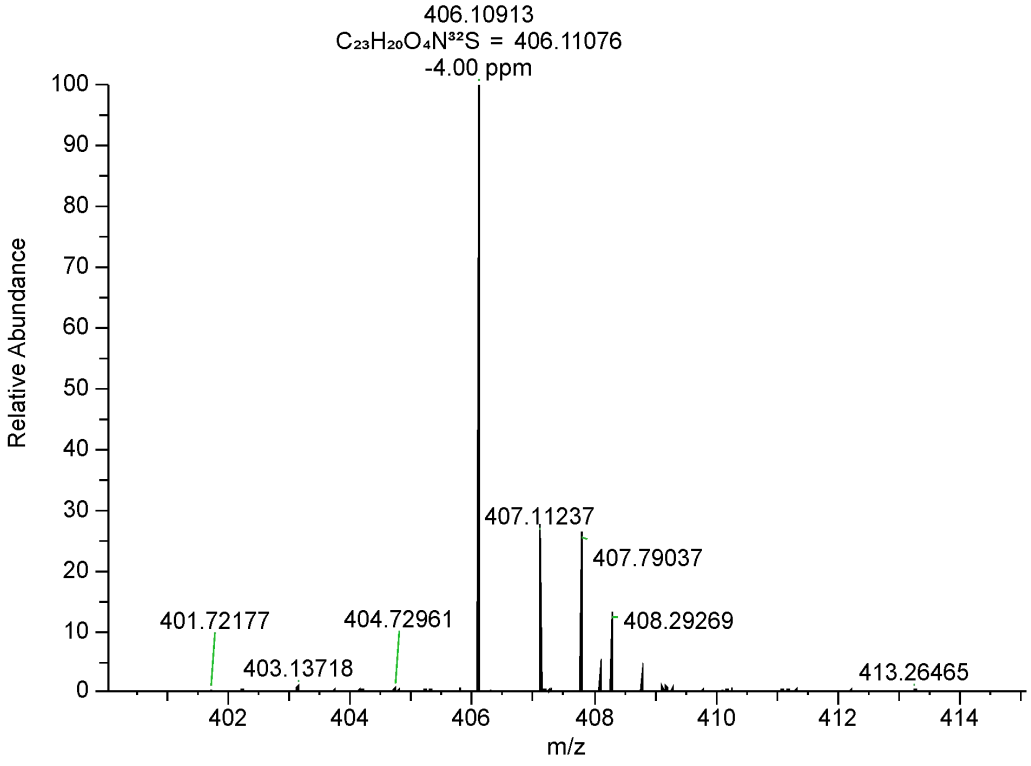


Fig. S21 HRMS spectra of compound Z21

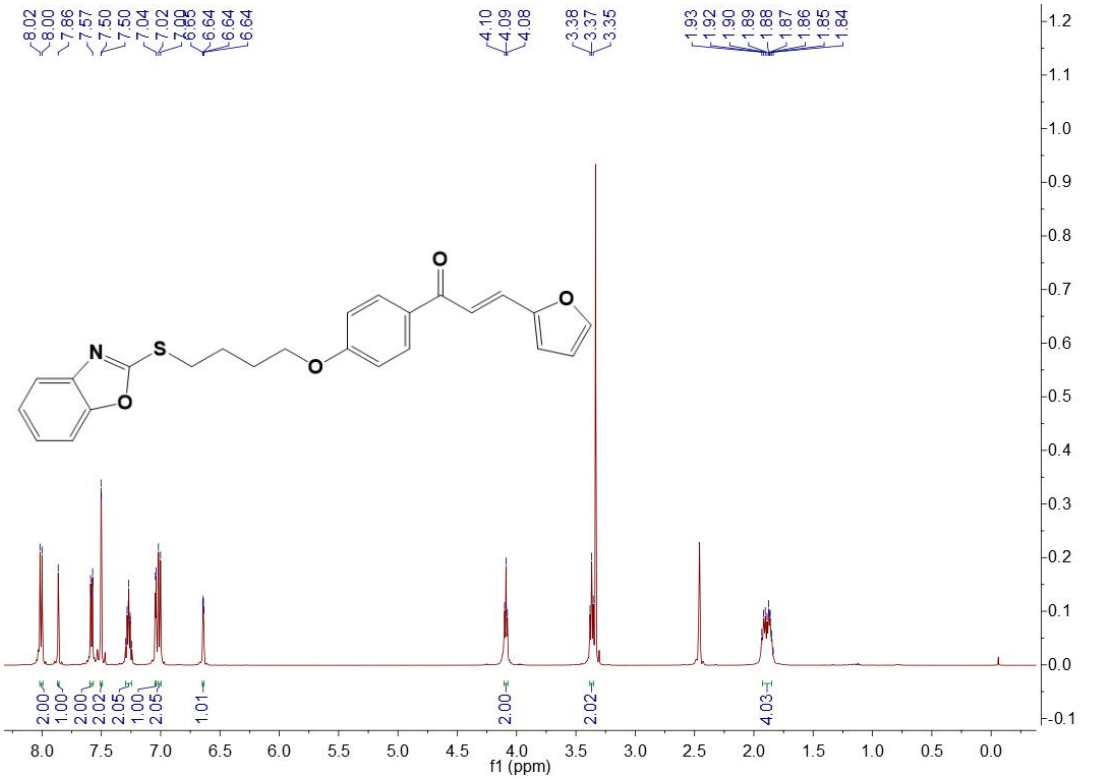


Fig. S22 ^{1}H NMR spectra of compound Z22

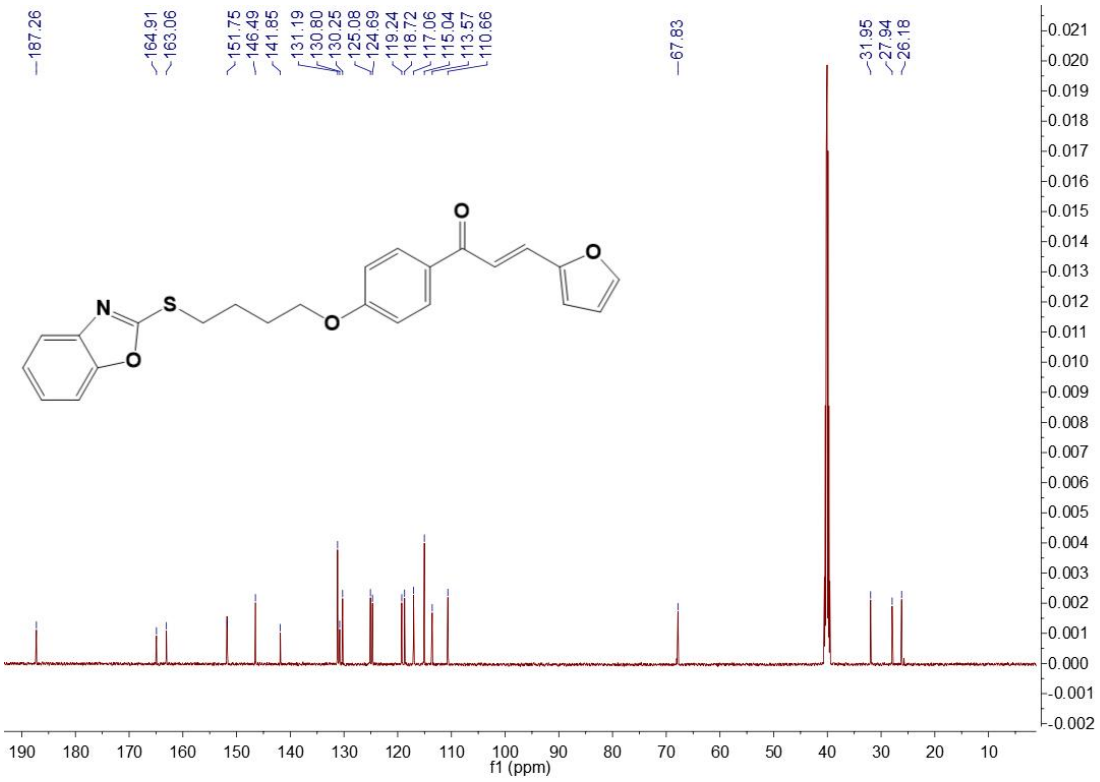


Fig. S22 ^{13}C NMR spectra of compound Z22

162 #57 RT: 0.56 AV: 1 NL: 8.07E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

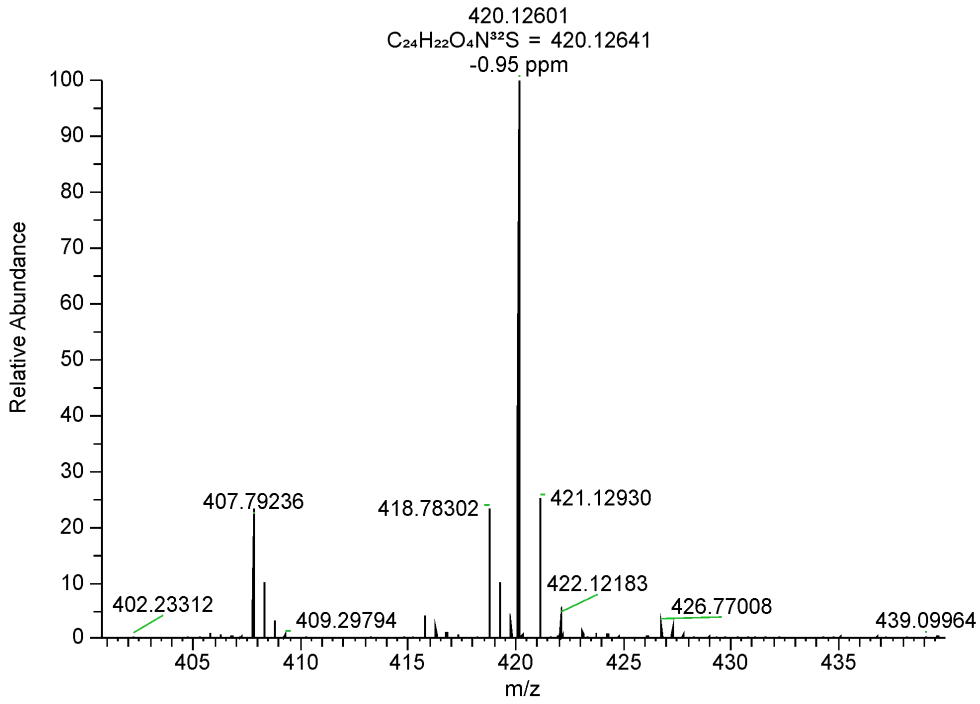


Fig. S22 HRMS spectra of compound Z22

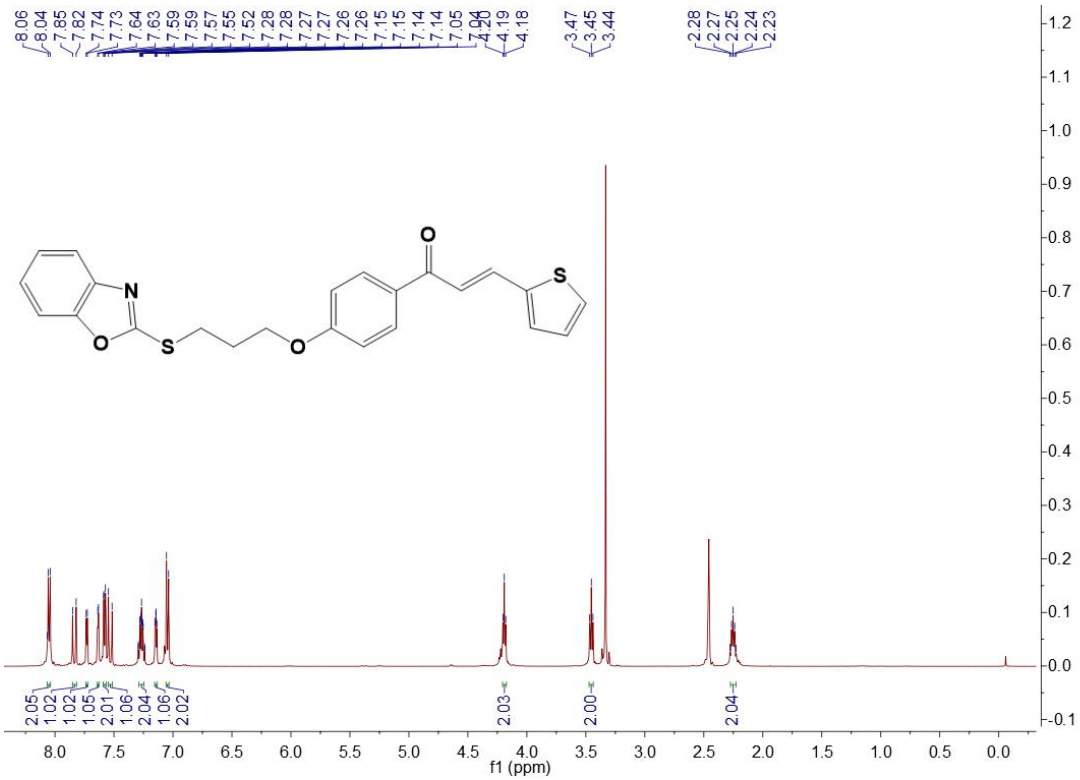


Fig. S23 ^{1}H NMR spectra of compound Z23

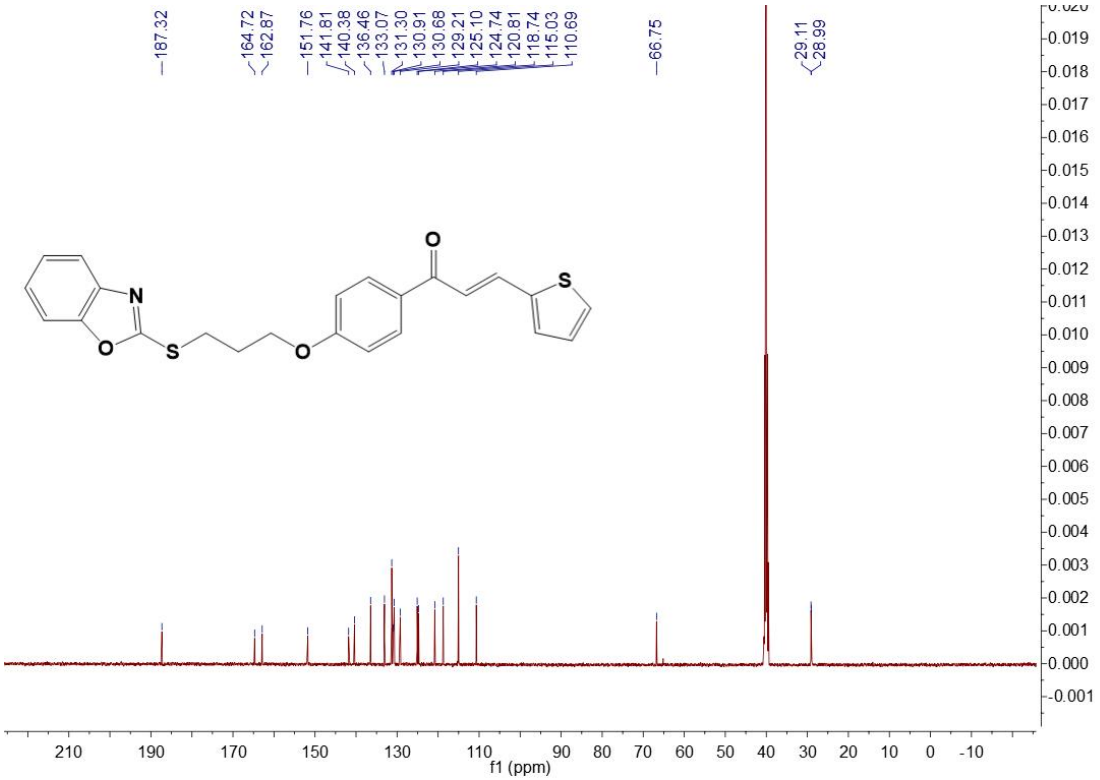


Fig. S23 ^{13}C NMR spectra of compound Z23

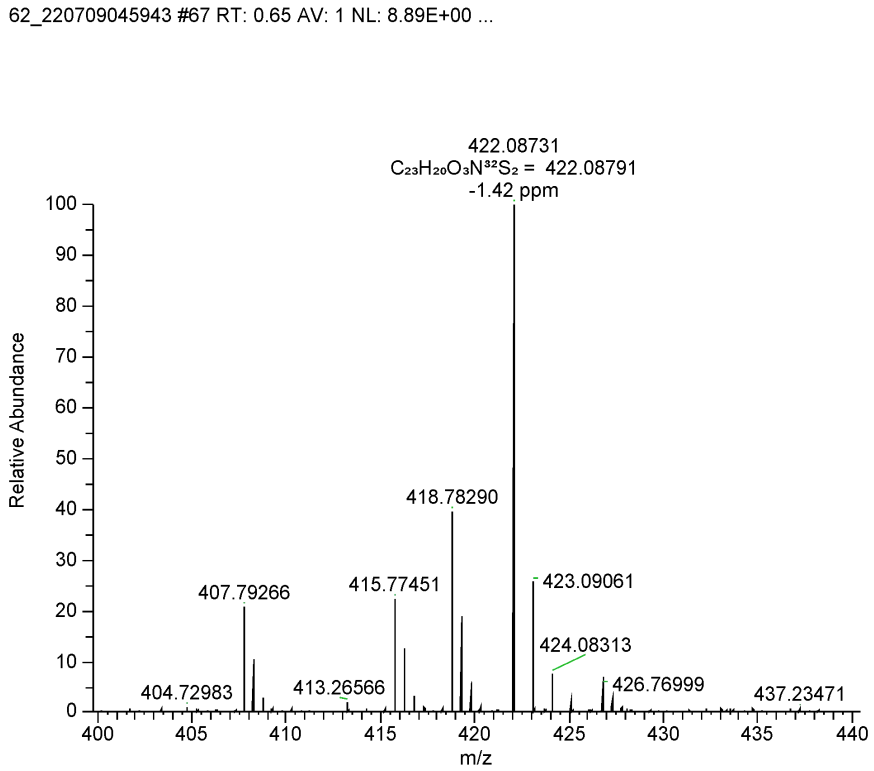


Fig. S23 HRMS spectra of compound Z23

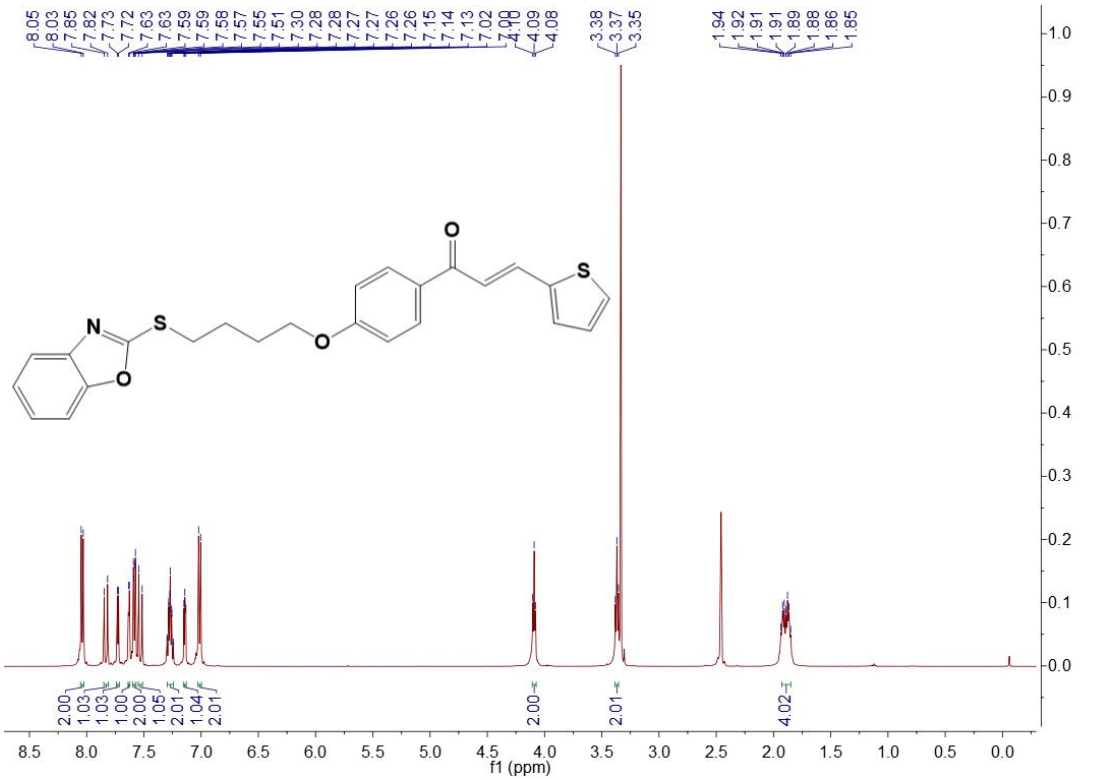


Fig. S24 ^{1}H NMR spectra of compound Z24

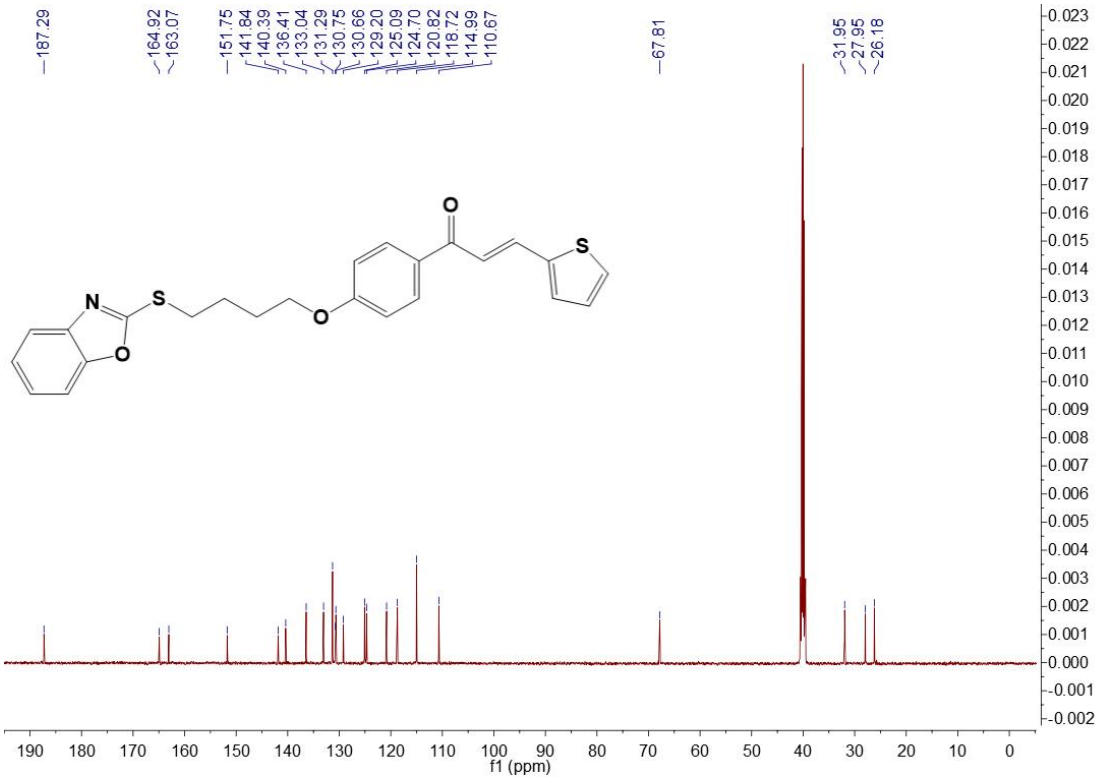


Fig. S24 ^{13}C NMR spectra of compound Z24

163 #61 RT: 0.60 AV: 1 NL: 2.09E+007
T: FTMS + p ESI Full ms [100.0000-1300.0000]

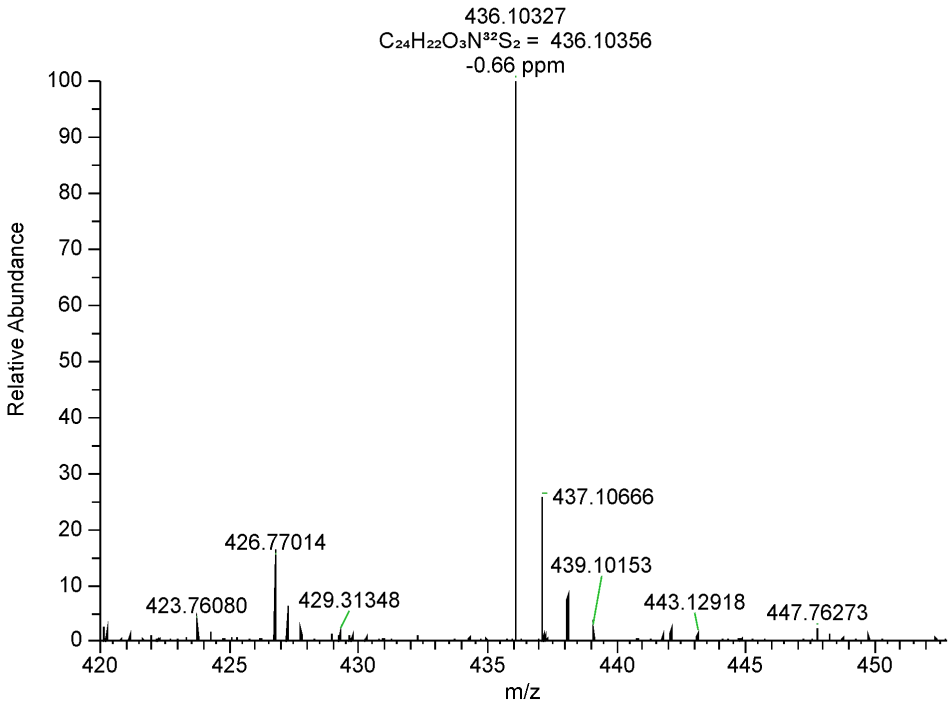


Fig. S24 HRMS spectra of compound Z24