Supporting Information

Synthesis, antibacterial, and antiviral activity of myricetin derivatives containing a 1,2,4-triazole Schiff base

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Content

1. Experimental section

Bruker ASCEND 400 (400 MHz) NMR spectrometer [tetramethylsilane (TMS) for internal standard, Bruker, Switzerland] and JEOL-ECX 500 (500 MHz) NMR (TMS for internal standard, Japan JEOL); Thermo Scientic Q Exactive High Resolution Mass Spectrometer (HRMS, Thermo Fisher Scientific); X-4 Digital Micro Melting Point Tester (Beijing Tektronix Instrument Co., Ltd.); Sartorius Electronic Balance (German Sartorius Group); QY-20 three-purpose ultraviolet analyzer (Shanghai Anting Electronic Instrument Factory). All reagents and solvents were purchased from Chinese Chemical Reagent Company.

2. Biological activities tests

2.1 *In vitro* Antibacterial Activity Test

In this study, a series of myricetin derivatives containing 1,2,4-triazole Schiff bases were synthesized and their antibacterial activity against *Xanthomonas axonopodis pv.citri* (*Xac*), *Ralstonia solanacearum* (*Rs*) and *Xanthomonas oryzae pv. oryzae* (*Xoo*) *in vitro* were investigated using turbidity tests.[33] The solvent nutrient broth (NB; 40 μL) medium (1.5 g beef extract, 2.5 g peptone, 0.5 g yeast powder, 5.0 g glucose, and 500 mL distilled water, pH 7.0-7.2) was added to *Xac*, *Rs*, or *Xoo.*

After adding 5 mL of the solvent NB medium, containing the test compound and commercial fungicide, the inoculated tubes were incubated at 28±1 °C and continuously shaken at 180 rpm for 24–48 h until the bacteria were incubated in the logarithmic growth phase. The growth of the culture was monitored by measuring the optical density (OD_{595}) at 595 nm using a 680 type plate reader (BIO-RAD, Hercules, CA, USA). The inhibition rate I was then calculated by the following formula:

Inhibition rate I (%) = (C-T)/C×100

Where C is the corrected turbidity value (OD_{595}) of bacterial growth on untreated NB, T is the corrected turbidity value (OD_{595}) of bacterial growth on treated NB, and I represents inhibition rate.

2.2 Antiviral activities *in vitro*

2.2.1 Purification of TMV

The virus was propagated in tobacco using the Gooding method. Tabacum (N. tabacum) cv. K326 was purified. The absorbance at 260 nm was estimated using an ultraviolet spectrophotometer.

Virus concentration (mg/mL) = (A_{260}×dilution ratio)/$E^{0.1\%}_{1\ cm}{}^{260\ nm}$, where E represents the extinction coefficient of TMV, $E^{0.1\%}_{1\ cm}{}^{260\ nm}$ is 3.1.

2.2.2. Curative activity of the target compounds against TMV *in vivo*

To determine curative activity, growing *Nicotiana tabacum* L. (*N. tabacum* L.) leaves of the same age were selected, which were then inoculated with TMV (concentration of 6×10^{-3} mg/mL) by dipping and brushing the entire leaves after they had been spread with silicon carbide. After inoculation, the leaves were then washed with water for 0.5 h. The compound solution was applied to the left side of the leaves, and the solvent was applied to the right side as a control. Then, after 3–4 d of inoculation, the number of local lesions was counted with three replicates being set for each compound.

2.2.3. Inactivation activity of the target compounds against TMV *in vivo*

The virus was inhibited by mixing it with the same volume of the compound solution for 30 min. Note that the right side of the leaves was inoculated with a mixture of solvent and virus as control. All the leaves had been previously spread with silicon carbide. Then, after 3–4 d of inoculation, the number of local lesions was counted with three replicates being set for each compound.

2.2.4. Protection activity of the target compounds against TMV *in vivo*

The compound solution was applied to the left side of the tobacco L leaf. The solvent was applied to the right side as a control for growing the tobacco leaves. After 12 h, crude TMV (concentration 6×10^{-3} mg/mL) was seeded at the same concentration on the entire leaves on either side of the leaves, which had previously been spread with silicon carbide. After 0.5 h, the leaves were washed with water and dried. Then, after 3–4 d of inoculation, the number of local lesions was recorded with three replicates being set for each compound.

The inhibition rate of the compound was calculated according to the following formula ("av" represents the average value):

Inhibition rate (%) = [(av local lesion no. of control (not treated with compd)−av local lesion no. smeared with drugs)/av local lesion no. of control (not treated with compd)]×100%

2.3 Scanning electron microscopy[33]

In this assay, 1.5 mL Xanthomonas axonopodis pv.citri (*Xac*) cells incubated at the logarithmic phase were centrifuged and washed with PBS (pH = 7.1), and re-suspended in 1.5 mL of PBS buffer (pH = 7.1). After that, bacteria Xanthomonas axonopodis pv.citri (*Xac*) was incubated with compound **6q** at concentration of 12.5 μg/mL, 25.0 μg/mL, and an equivalent volume of DMSO (solvent control) for 4 h at room temperature. After incubation, these samples were washed 3 times with PBS (pH = 7.1). Subsequently, the bacterial cells were fixed for 8 h at 4 °C with 2.5% glutaraldehyde, and then dehydrated with graded ethanol series and pure tert-butanol (2 times with 10 min/time). Following dehydration, samples were freezing dried and coated with gold, and

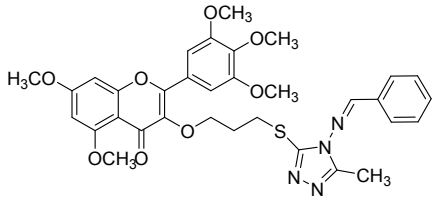
visualized using Nova Nano SEM 450.

2.4 Molecular docking[33]

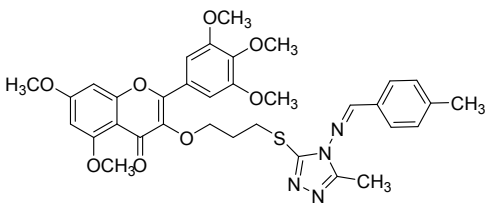
Molecular docking. The molecular docking was performed by using DS-CDocker implemented in Discovery Studio (version 4.5). The coat protein subunit amino acid sequence of tobacco mosaic virus (TMV) was searched by the UniProt database. The Protein BLAST server was used to search the template protein and the homologies of TMV-CP sequences were aligned. Homology modeling of TMV-CP was carried out using Create Homology Models, which is a module integrated in Discovery Studio. The obtained models were evaluated by Ramachandran plots. The 3D structures of the compounds were constructed using the Sketching module and optimized by the Full Minimization module. All parameters are default during the docking process.

2.5 ^{1}H NMR, ^{13}C NMR, and HRMS spectrum of the title compounds

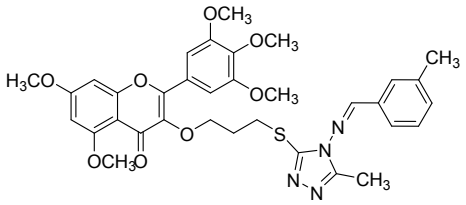
The physical characteristics, HRMS, ^{1}H NMR, ^{13}C NMR data for all the target compounds were shown in below.



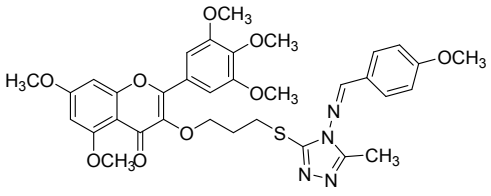
*3-(3-((4-(benzylideneamino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6a**)*: White solid, yield: 53.2%, m.p: 82-84 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.83 (s, 1H, CH=N), 7.91 (d, J = 2.2 Hz, 2H, Ar-2,6-H), 7.60 (ddd, J = 12.6, 9.5, 5.1 Hz, 3H, Ar-3,4,5-H), 7.34 (s, 2H, Myr-2',6'-H), 6.82 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 3.99 (t, J = 6.2 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.84 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.22 (t, J = 7.0 Hz, 2H, CH_2), 2.44 (s, 3H, triazole-CH_3), 2.08 – 2.02 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.56, 164.23, 160.75, 158.64, 153.17, 152.22, 149.49, 146.66, 140.17, 139.88, 133.43, 132.30, 129.63, 129.31, 129.08, 125.96, 108.89, 106.15, 96.38, 93.56, 70.50, 60.63, 56.53, 56.50, 30.27, 29.57, 11.44; HRMS Calcd for $C_{33}H_{35}O_8N_4S$ $[M+H]^+$: 647.21701, Found: 647.21680.



*3-(3-((4-((4-methylbenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6b**)*: White solid, yield: 61.0%, m.p: 76-78 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.77 (s, 1H, CH=N), 7.80 (d, J = 8.0 Hz, 2H, Ar-2,6-H), 7.36 (d, J = 8.0 Hz, 2H, Ar-3,5-H), 7.33 (s, 2H, Myr-2',6'-H), 6.83 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 4.00 (t, J = 6.0 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.84 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.21 (t, J = 6.0 Hz, 2H, CH_2), 2.41 (s, 3H, triazole-CH_3), 2.39 (s, 3H, Ar-4-CH_3), 2.08 – 1.99 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.56, 165.79, 164.22, 160.73, 158.64, 153.16, 152.20, 149.46, 146.54, 143.88, 140.17, 139.84, 130.21, 129.61, 129.34, 125.96, 108.87, 106.10, 96.38, 93.56, 70.49, 60.63, 56.54, 56.51, 30.25, 29.57, 21.75, 11.40; HRMS Calcd for $C_{34}H_{37}O_8N_4S$ $[M+H]^+$: 661.23266, Found: 661.23224.

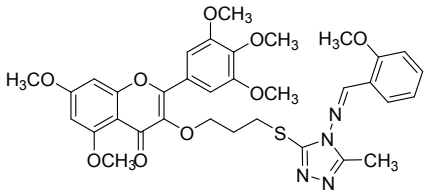


*3-(3-((4-((3-methylbenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6c**)*: Yellow solid, yield: 69.4%, m.p: 78-80 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.78 (s, 1H, CH=N), 7.73 (s, 1H, Ar-2-H), 7.71 (d, J = 4.6 Hz, 1H, Ar-6-H), 7.44 (d, J = 5.0 Hz, 1H, Ar-4-H), 7.37 (t, J = 6.2 Hz, 1H, Ar-5-H), 7.33 (s, 2H, Myr-2',6'-H), 6.82 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 4.00 (t, J = 5.6 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.86 (s, 3H, Myr-7-OCH_3), 3.84 (s, 6H, Myr-3',5'-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.22 (t, J = 7.1 Hz, 2H, CH_2), 2.43 (s, 3H, triazole-CH_3), 2.38 (s, 3H, Ar-3-CH_3), 2.07 – 2.03 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.55, 165.87, 164.23, 160.75, 158.64, 153.17, 152.21, 149.48, 146.58, 140.17, 139.88, 139.06, 134.12, 132.25, 129.52, 126.72, 126.41, 125.96, 108.89, 106.15, 96.38, 93.57, 70.50, 60.63, 56.53, 56.50, 30.27, 29.58, 21.23, 11.42; HRMS Calcd for $C_{34}H_{37}O_8N_4S$ $[M+H]^+$: 661.23266, Found: 661.23212.

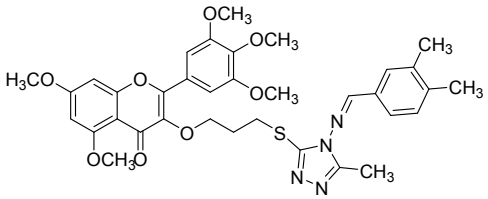


*3-(3-((4-((4-methoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6d**)*: Brown solid, yield: 75.1%, m.p: 76-78 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.72 (s, 1H, CH=N), 7.87 (d, J = 8.7 Hz, 2H, Ar-2,6-H), 7.34 (s, 2H, Myr-2',6'-H), 7.10 (d, J = 8.7 Hz, 2H,

Ar-3,5-H), 6.82 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 4.00 (t, *J* = 5.9 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 9H, Myr-3',5'-OCH_3 and Ar-4-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.20 (t, *J* = 6.9 Hz, 2H, CH_2), 2.40 (s, 3H, triazole-CH_3), 2.07 – 1.99 (m, 2H, CH_2); ^{13}C NMR (125MHz, DMSO-d_6) δ 172.61, 165.93, 164.27, 163.62, 160.78, 158.69, 153.22, 152.24, 149.49, 146.46, 140.24, 139.88, 131.44, 126.02, 124.79, 115.18, 108.93, 106.15, 96.43, 93.60, 70.55, 60.69, 56.57, 56.11, 30.35, 29.61, 11.38; HRMS Calcd for $C_{34}H_{37}O_9N_4S$ $[M+H]^+$: 677.22758, Found: 677.22681.

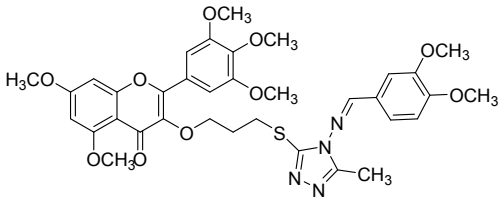


3-(3-((4-((2-methoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one ***(6e)***: White solid, yield: 66.3%, m.p: 74-76 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.95 (s, 1H, CH=N), 7.94 (d, *J* = 9.5 Hz, 1H, Ar-6-H), 7.60 (t, *J* = 7.4 Hz, 1H, Ar-4-H), 7.33 (s, 2H, Myr-2',6'-H), 7.20 (d, *J* = 8.3 Hz, 1H, Ar-3-H), 7.09 (t, *J* = 7.5 Hz, 1H, Ar-5-H), 6.82 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 4.01 (t, *J* = 6.1 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.88 (s, 3H, Myr-7-OCH_3), 3.84 (s, 9H, Myr-3',5'-OCH_3 and Ar-2-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.22 (t, *J* = 7.0 Hz, 2H, CH_2), 2.40 (s, 3H, triazole-CH_3), 2.13 – 2.00 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.55, 164.23, 160.77, 160.34, 159.77, 158.64, 153.18, 152.18, 150.00, 145.81, 140.19, 139.92, 135.30, 127.24, 125.96, 121.40, 120.20, 112.82, 108.91, 106.18, 96.39, 93.58, 70.53, 60.63, 56.54, 56.51, 30.28, 29.82, 11.36. HRMS Calcd for $C_{34}H_{37}O_9N_4S$ $[M+H]^+$: 677.22758, Found: 677.22681.

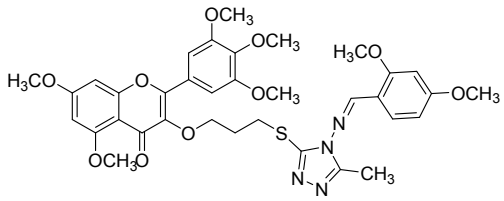


3-(3-((4-((3,4-dimethylbenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one ***(6f)***: Yellow solid, yield: 51.5%, m.p: 81-83 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.72 (s, 1H, CH=N), 7.67 (s, 1H, Ar-2-H), 7.62 (d, *J* = 8.1 Hz, 1H, Ar-6-H), 7.36 (d, *J* = 8.3 Hz, 1H, Ar-5-H), 7.33 (s, 2H, Myr-2',6'-H), 6.83 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 4.00 (t, *J* = 6.2 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.84 (s, 6H, Myr-3',5'-OCH_3), 3.76 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.20 (t, *J* = 7.0 Hz, 2H, CH_2), 2.40 (s, 3H, triazole-CH_3), 2.30 (s, 3H, Ar-4-CH_3), 2.28 (s, 3H, Ar-3-CH_3), 2.05 – 2.02 (m, 2H, CH_2); ^{13}C NMR

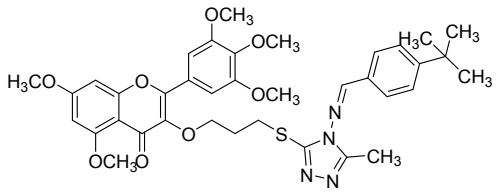
(100 MHz, DMSO-d_6) δ 172.55, 166.20, 164.25, 160.79, 158.65, 153.19, 152.21, 146.40, 142.77, 140.19, 139.95, 137.79, 130.67, 129.96, 129.91, 127.17, 125.96, 108.92, 106.23, 96.41, 93.61, 70.52, 60.64, 56.61, 56.57, 56.52, 30.27, 29.64, 20.14, 19.69, 11.35; HRMS Calcd for $C_{35}H_{39}O_8N_4S$ $[M+H]^+$: 675.24831, Found: 675.24750.



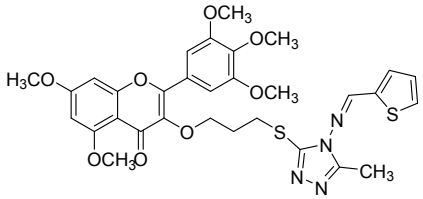
*3-(3-((4-((3,4-dimethoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6g**)*: White solid, yield: 64.9%, m.p: 85-87 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.69 (s, 1H, CH=N), 7.48 (d, J = 1.8 Hz, 1H, Ar-6-H), 7.45 (d, J = 1.9 Hz, 1H, Ar-5-H), 7.33 (s, 2H, Myr-2',6'-H), 7.13 (s, 1H, Ar-2-H), 6.83 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 4.00 (t, J = 6.1 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 3H, Ar-3-OCH_3), 3.84 (s, 9H, Myr-3',5'-OCH_3 and Ar-4-OCH_3), 3.82 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.20 (t, J = 7.0 Hz, 2H, CH_2), 2.39 (s, 3H, triazole-CH_3), 2.07 – 1.99 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.56, 166.32, 164.26, 160.78, 158.65, 153.60, 153.19, 152.23, 149.62, 149.46, 146.30, 140.19, 139.94, 125.96, 125.23, 124.77, 112.01, 109.96, 108.92, 106.23, 96.42, 93.61, 70.54, 60.65, 56.57, 56.11, 30.31, 29.61, 11.29; HRMS Calcd for $C_{35}H_{39}O_{10}N_4S$ $[M+H]^+$: 707.23814, Found: 707.23749.



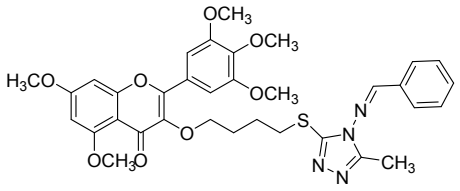
*3-(3-((4-((2,4-dimethoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6h**)*: White solid, yield: 56.7%, m.p: 74-76 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.79 (s, 1H, CH=N), 7.89 (d, J = 8.6 Hz, 1H, Ar-6-H), 7.33 (s, 2H, Myr-2',6'-H), 6.80 (s, 1H, Myr-6-H), 6.67 (d, J = 9.8 Hz, 2H, Ar-3,5-H), 6.47 (s, 1H, Myr-8-H), 4.00 (t, J = 6.1 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.87 (s, 9H, Myr-3',5'-OCH_3 and Ar-4-OCH_3), 3.84 (s, 6H, Myr-7-OCH_3 and Ar-2-OCH_3), 3.75 (s, 3H, Myr-4'-OCH_3), 3.20 (t, J = 7.0 Hz, 2H, CH_2), 2.36 (s, 3H, triazole-CH_3), 2.16 – 2.00 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.54, 165.54, 164.21, 161.60, 160.84, 160.75, 158.61, 153.16, 152.11, 147.78, 145.65, 140.20, 139.91, 128.82, 125.96, 112.91, 108.89, 107.63, 106.15, 98.65, 96.34, 93.55, 70.51, 60.62, 56.52, 56.20, 30.29, 29.81, 11.21; HRMS Calcd for $C_{35}H_{39}O_{10}N_4S$ $[M+H]^+$: 707.23814, Found: 707.23773.



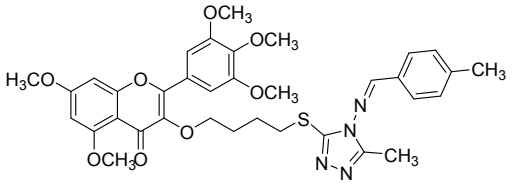
3-(3-((4-((4-(tert-butyl)benzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one ***(6i)***: White solid, yield: 44.6%, m.p: 75-77 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.78 (s, 1H, CH=N), 7.83 (d, J = 8.2 Hz, 2H, Ar-2,6-H), 7.57 (d, J = 8.1 Hz, 2H, Ar-3,5-H), 7.36 (s, 2H, Myr-2',6'-H), 6.83 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 4.01 (t, J = 6.0 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.84 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.21 (t, J = 6.9 Hz, 2H, CH_2), 2.41 (s, 3H, triazole-CH_3), 2.07 – 2.00 (m, 2H, CH_2),1.31 (s, 9H, Ar-4-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6) δ 172.61, 165.93, 164.29, 160.79, 158.70, 156.72, 153.22, 152.23, 149.50, 146.54, 140.25, 139.90, 129.70, 129.31, 129.06, 126.54, 126.02, 108.93, 106.15, 96.45, 93.62, 70.56, 60.69, 56.57, 35.45, 31.31, 30.33, 29.65, 11.42; HRMS Calcd for $C_{37}H_{43}O_8N_4S$ $[M+H]^+$: 703.27961, Found: 703.27643.



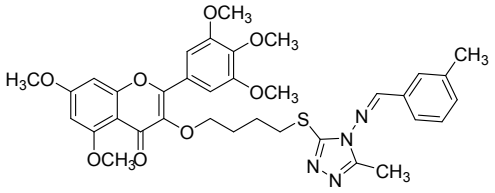
3-(3-((4-((thiophen-2-ylmethylene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)propoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one ***(6j)***: Yellow solid, yield: 40.8%, m.p: 98-100 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.01 (s, 1H, CH=N), 7.98 (d, J = 5.1 Hz, 1H, thiophene-5-H), 7.82 (d, J = 3.6 Hz, 1H, thiophene-3-H), 7.34 (s, 2H, Myr-2',6'-H), 7.29 (t, J = 4.9, 3.7 Hz, 1H, thiophene-4-H), 6.82 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 4.00 (t, J = 6.2 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.75 (s, 3H, Myr-4'-OCH_3), 3.21 (t, J = 7.0 Hz, 2H, CH_2), 2.40 (s, 3H, triazole-CH_3), 2.08 – 2.02 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.56, 164.22, 160.74, 160.26, 158.63, 153.17, 152.21, 149.42, 146.56, 140.17, 139.88, 137.09, 136.26, 133.99, 129.12, 125.96, 108.89, 106.15, 96.37, 93.56, 70.49, 60.64, 56.53, 56.49, 30.30, 29.55, 11.33; HRMS Calcd for $C_{31}H_{33}O_8N_4S_2$ $[M+H]^+$: 653.17343, Found: 653.17279.



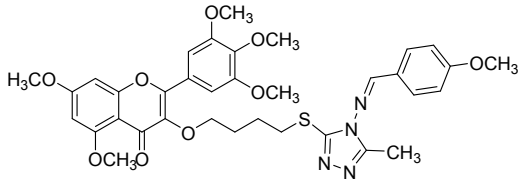
*3-(4-((4-(benzylideneamino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6k**)*: Yellow solid, yield: 52.3%, m.p: 73-75 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.71 (s, 1H, CH=N), 7.86 (d, J = 8.8 Hz, 2H, Ar-2,6-H), 7.38 (t, J = 8.0 Hz, 1H, Ar-4-H), 7.33 (s, 2H, Myr-2',6'-H), 7.10 (t, J = 8.8 Hz, 2H, Ar-3,5-H), 6.83 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 4.00 (t, J = 7.2 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 3H, Myr-7-OCH_3), 3.84 (s, 6H, Myr-3',5'-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.19 (t, J = 7.0 Hz, 2H, CH_2), 2.39 (s, 3H, triazole-CH_3), 2.07 – 2.00 (m, 2H, CH_2), 1.29 – 1.11 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.65, 163.90, 159.51, 157.89, 155.06, 151.88, 150.73, 148.95, 143.11, 141.05, 135.93, 133.83, 129.47, 128.31, 127.70, 127.12, 107.57, 106.18, 95.83, 93.72, 72.65, 60.70, 56.83, 56.08, 33.71, 27.91, 26.55, 10.55; HRMS Calcd for $C_{34}H_{37}O_8N_4S$ $[M+H]^+$: 661.23266, Found: 661.23199.



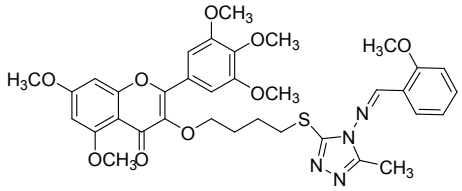
*3-(4-((4-((4-methylbenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6l**)*: Yellow solid, yield: 46.6%, m.p: 82-84 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.79 (s, 1H, CH=N), 7.82 (d, J = 8.2 Hz, 2H, Ar-2,6-H), 7.37 (d, J = 7.6 Hz, 2H, Ar-3,5-H), 7.35 (s, 2H, Myr-2',6'-H), 6.80 (s, 1H, Myr-6-H), 6.47 (s, 1H, Myr-8-H), 3.95 (t, J = 6.0 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.75 (s, 3H, Myr-4'-OCH_3), 3.18 (t, J = 6.3 Hz, 2H, CH_2), 2.42 (s, 3H, triazole-CH_3), 2.39 (s, 3H, Myr-4-CH_3), 1.77 (s, 4H, 2×CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.61, 165.64, 164.18, 160.72, 158.59, 153.13, 151.99, 146.64, 143.86, 140.29, 139.85, 130.21, 129.65, 129.32, 129.08, 126.02, 108.89, 106.09, 96.31, 93.51, 71.32, 60.61, 56.51, 56.46, 32.32, 28.91, 26.21, 21.73, 11.39; HRMS Calcd for $C_{35}H_{39}O_8N_4S$ $[M+H]^+$: 675.24831, Found: 675.24792.



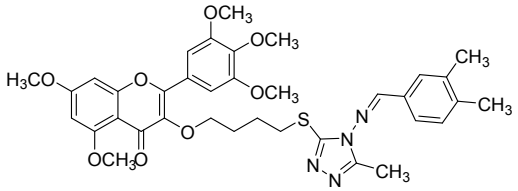
*3-(4-((4-((3-methylbenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6m**)*: Yellow solid, yield: 43.5%, m.p: 73-75 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.86 (s, 1H, CH=N), 7.73 (s, 1H, Ar-2-H), 7.71 (d, J = 4.9 Hz, 1H, Ar-6-H), 7.47 (t, J = 6.0 Hz, 1H, Ar-5-H), 7.45 (d, J = 5.3 Hz, 1H, Ar-4-H), 7.37 (s, 2H, Myr-2',6'-H), 6.86 (s, 1H, Myr-6-H), 6.50 (s, 1H, Myr-8-H), 4.14 (t, J = 6.8 Hz, 2H, CH_2), 3.96 (t, J = 6.3 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.86 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 2.40 (s, 3H, triazole-CH_3), 2.38 (s, 3H, Ar-3-CH_3), 1.92 – 1.84 (m, 2H, CH_2), 1.73 – 1.66 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.66, 164.67, 164.24, 160.75, 158.65, 153.16, 152.13, 147.74, 140.33, 139.84, 139.07, 135.39, 133.91, 132.50, 129.55, 129.36, 126.47, 126.05, 108.91, 106.15, 96.42, 93.60, 71.51, 60.66, 56.54, 48.01, 27.18, 27.06, 24.86, 21.29, 11.07; HRMS Calcd for $C_{35}H_{39}O_8N_4S$ $[M+H]^+$: 675.24831, Found: 675.24768.



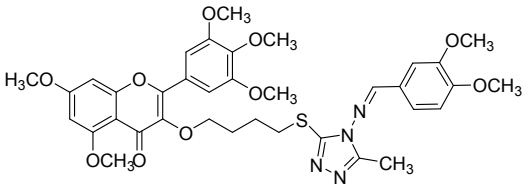
*3-(4-((4-((4-methoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6n**)*: White solid, yield: 65.7%, m.p: 68-70 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (s, 1H, CH=N), 7.88 (d, J = 8.8 Hz, 2H, Ar-2,6-H), 7.35 (s, 2H, Myr-2',6'-H), 7.11 (d, J = 8.8 Hz, 2H, Ar-3,5-H), 6.82 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 3.98 (t, J = 6.4 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 6H, Myr-7-OCH_3 and Ar-4-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.15 (t, J = 6.4 Hz, 2H, CH_2), 2.40 (s, 3H, triazole-CH_3), 1.87 – 1.77 (m, 2H, CH_2), 1.76 – 1.69 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.62, 165.85, 164.21, 163.59, 160.76, 158.62, 153.15, 152.04, 149.40, 146.47, 140.31, 139.91, 131.38, 126.04, 124.78, 115.16, 108.93, 106.18, 96.37, 93.57, 71.37, 60.64, 56.56, 56.05, 32.34, 28.90, 26.24, 11.31.; HRMS Calcd for $C_{35}H_{39}O_9N_4S$ $[M+H]^+$: 691.24323, Found: 691.24255.



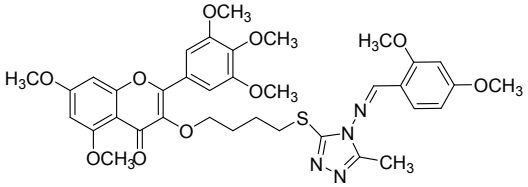
*3-(4-((4-((2-methoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6o**)*: Yellow solid, yield: 58.1%, m.p: 62-64 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.97 (s, 1H, CH=N), 7.97 (d, J = 7.6 Hz, 1H, Ar-6-H), 7.61 (t, J = 7.1 Hz, 1H, Ar-4-H), 7.35 (s, 2H, Myr-2',6'-H), 7.20 (d, J = 8.4 Hz, 1H, Ar-3-H), 7.10 (t, J = 7.5 Hz, 1H, Ar-5-H), 6.80 (s, 1H, Myr-6-H), 6.47 (s, 1H, Myr-8-H), 4.03 (t, J = 6.5 Hz, 2H, CH_2), 3.89 (s, 3H, Myr-5-OCH_3), 3.87 (s, 3H, Myr-7-OCH_3), 3.85 (s, 9H, Myr-3',5'-OCH_3 and Ar-2-OCH_3), 3.75 (s, 3H, Myr-4'-OCH_3), 3.18 (s, 2H, CH_2), 2.41 (s, 3H, triazole-CH_3), 1.79 – 1.57 (m, 2H, CH_2), 1.24 – 0.85 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.60, 164.17, 160.75, 160.10, 159.77, 158.59, 153.14, 151.98, 149.99, 145.94, 140.30, 139.92, 135.26, 127.23, 126.02, 121.40, 120.23, 112.81, 108.92, 106.16, 96.31, 93.53, 71.35, 60.62, 56.54, 56.45, 32.56, 31.42, 28.93, 26.23; HRMS Calcd for $C_{35}H_{39}O_9N_4S$ $[M+H]^+$: 691.24323, Found: 691.24286.



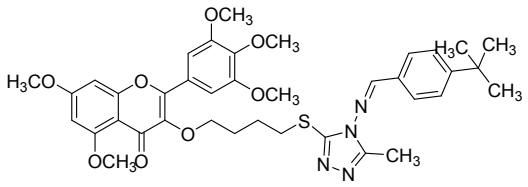
*3-(4-((4-((3,4-dimethylbenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6p**)*: Yellow solid, yield: 42.3%, m.p: 64-66 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (s, 1H, CH=N), 7.70 (s, 1H, Ar-2-H), 7.64 (d, J = 7.6 Hz, 1H, Ar-6-H), 7.35 (s, 2H, Myr-2',6'-H), 7.32 (d, J = 7.9 Hz, 1H, Ar-5-H), 6.83 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 3.98 (t, J = 6.4 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.19 (t, J = 6.7 Hz, 2H, CH_2), 2.41 (s, 3H, triazole-CH_3), 2.30 (s, 3H, Ar-4-CH_3), 2.29 (s, 3H, Ar-3-CH_3), 1.76 – 1.72 (m, 4H, 2×CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.62, 166.09, 164.21, 160.75, 158.62, 153.15, 152.04, 149.47, 146.55, 142.78, 140.30, 139.86, 137.82, 130.69, 129.93, 127.19, 126.85, 126.03, 108.91, 106.12, 96.37, 93.56, 71.36, 60.63, 56.54, 56.50, 32.35, 28.89, 26.22, 20.15, 19.70, 11.37; HRMS Calcd for $C_{36}H_{41}O_8N_4S$ $[M+H]^+$: 689.26396. Found: 689.26196.



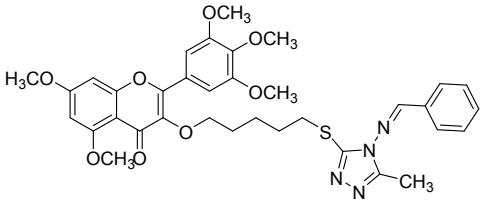
3-(4-((4-((3,4-dimethoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (***6q***): Brown solid, yield: 61.8%, m.p: 65-67°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.71 (s, 1H, CH=N), 7.50 (d, J = 7.8 Hz, 1H, Ar-6-H), 7.47 (s, 1H, Ar-2-H), 7.35 (s, 2H, Myr-2',6'-H), 7.13 (d, J = 8.3 Hz, 1H, Ar-5-H), 6.83 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 3.98 (t, J = 6.1 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.87 (s, 3H, Ar-3-OCH_3), 3.85 (s, 9H, Myr-3',5'-OCH_3 and Ar-4-OCH_3), 3.83 (s, 3H, Myr-7-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.22 (t, J = 6.3 Hz, 2H, CH_2), 2.40 (s, 3H, triazole-CH_3), 1.79 – 1.64 (m, 4H, 2×CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.63, 166.19, 164.22, 160.75, 158.62, 153.57, 153.15, 152.05, 149.61, 149.42, 146.46, 140.30, 139.86, 126.03, 125.24, 124.78, 112.01, 109.88, 108.90, 106.12, 96.37, 93.57, 71.38, 60.64, 56.55, 55.98, 32.32, 28.90, 26.24, 11.31; HRMS Calcd for $C_{36}H_{41}O_{10}N_4S$ $[M+H]^+$: 721.25379, Found: 721.25275.



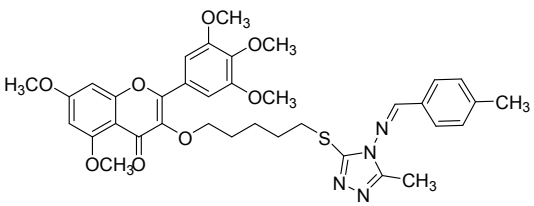
3-(4-((4-((2,4-dimethoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (***6r***): Yellow solid, yield: 67.5%, m.p: 72-74 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H, CH=N), 7.77 (s, 1H, Ar-3-H), 7.74 (d, J = 3.7 Hz, 1H, Ar-6-H), 7.32 (d, J = 3.8 Hz,, 1H, Ar-5-H), 7.29 (s, 2H, Myr-2',6'-H), 6.49 (s, 1H, Myr-6-H), 6.36 (s, 1H, Myr-8-H), 4.11 (t, J = 6.9 Hz, 2H, CH_2), 3.96 (s, 3H, Myr-5-OCH_3), 3.96 (s, 3H, Myr-7-OCH_3), 3.93 (s, 3H, Ar-2-OCH_3), 3.91 (s, 9H, Myr-3',5'-OCH_3 and Ar-4-OCH_3), 3.90 (s, 3H, Myr-4'-OCH_3), 3.37 (t, J = 7.0 Hz, 2H, CH_2), 2.45 (s, 3H, triazole-CH_3), 2.24 – 2.16 (m, 2H, CH_2), 1.95 – 1.83(m, 2H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.93, 164.01, 162.87, 160.99, 158.81, 153.02, 152.85, 150.97, 145.83, 143.83, 140.37, 139.89, 129.86, 129.65, 129.15, 128.98, 128.69, 125.95, 109.38, 105.80, 95.85, 92.43, 70.58, 61.03, 56.37, 55.86, 30.31, 30.03, 21.83, 11.21; HRMS Calcd for $C_{36}H_{41}O_{10}N_4S$ $[M+H]^+$: 721.25379, Found: 721.25287.



*3-(4-((4-((4-(tert-butyl)benzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)butoxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6s**)*: Yellow solid, yield: 45.0%, m.p: 89-91 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.80 (s, 1H, CH=N), 7.86 (d, J = 8.4 Hz, 2H, Ar-2,6-H), 7.57 (d, J = 8.3 Hz, 2H, Ar-3,5-H), 7.35 (s, 2H, Myr-2',6'-H), 6.79 (s, 1H, Myr-6-H), 6.46 (s, 1H, Myr-8-H), 3.94 (t, J = 6.5 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.88 (s, 6H, Myr-3',5'-OCH_3), 3.86 (s, 3H, Myr-7-OCH_3), 3.78 (s, 3H, Myr-4'-OCH_3), 3.14 (t, J = 6.7 Hz, 2H, CH_2), 2.43 (s, 3H, triazole-CH_3), 2.34 – 2.29 (m, 2H, CH_2), 1.78 – 1.73 (m, 2H, CH_2), 1.32 (s, 9H, Ar-4-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.62, 165.70, 164.17, 160.74, 158.58, 156.66, 153.14, 151.96, 140.34, 140.31, 139.93, 129.66, 129.23, 128.95, 126.46, 126.04, 108.92, 106.15, 96.29, 93.51, 71.41, 60.64, 56.53, 56.43, 35.34, 32.39, 31.21, 29.12, 26.54, 22.52; HRMS Calcd for $C_{38}H_{45}O_8N_4S$ $[M+H]^+$: 717.29526, Found: 717.29498.

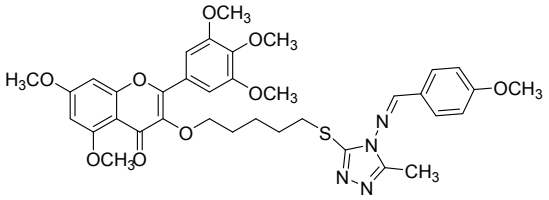


*3-((5-((4-(benzylideneamino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)pentyl)oxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6t**)*: Brown solid, yield: 51.6%, m.p: 88-90 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.92 (s, 1H, CH=N), 7.93 (d, J = 2.2 Hz, 1H, Ar-6-H), 7.91 (d, J = 1.5 Hz, 1H, Ar-2-H), 7.63 (t, J = 6.7 Hz, 1H, Ar-4-H), 7.59 (t, J = 6.5 Hz, 1H, Ar-5-H), 7.55 (t, J = 6.6 Hz, 1H, Ar-3-H), 7.39 (s, 2H, Myr-2',6'-H), 6.85 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 4.08 (t, J = 7.0 Hz, 2H, CH_2), 3.94 (t, J = 6.8 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.88 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.75 (s, 3H, Myr-4'-OCH_3), 2.38 (s, 3H, triazole-CH_3), 1.82 – 1.75 (m, 2H, CH_2), 1.73 – 1.66 (m, 2H, CH_2), 1.45 – 1.38 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.70, 164.42, 164.22, 160.74, 160.54, 153.15, 152.00, 147.75, 140.55, 140.45, 139.83, 133.20, 132.56, 129.65, 129.11, 126.10, 108.92, 106.18, 96.40, 93.58, 71.91, 60.67, 56.57, 56.53, 29.65, 27.62, 27.60, 22.84, 11.09; HRMS Calcd for $C_{35}H_{39}O_8N_4S$ $[M+H]^+$: 675.24831, Found: 675.24719.

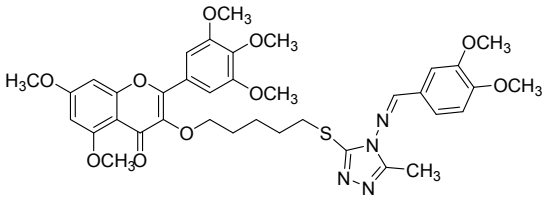


*3-((5-((4-((4-methylbenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)pentyl)oxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6u**)*: Yellow solid, yield: 64.4%, m.p: 57-59 °C; ^{1}H NMR (400 MHz,

DMSO-d_6) δ 8.79 (s, 1H, CH=N), 7.81 (d, J = 2.0 Hz, 2H, Ar-2,6-H), 7.38 (d, J = 1.6 Hz, 2H, Ar-3,5-H), 7.36 (s, 2H, Myr-2',6'-H), 6.82 (s, 1H, Myr-6-H), 6.48 (s, 1H, Myr-8-H), 3.95 (t, J = 6.8 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.86 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 3H, Myr-7-OCH_3), 3.75 (s, 3H, Myr-4'-OCH_3), 3.07 (t, J = 7.1 Hz, 2H, CH_2), 2.42 (s, 3H, triazole-CH_3), 2.38 (s, 3H, Ar-4-CH_3), 1.67 – 1.61 (m, 4H, 2×CH_2), 1.47 – 1.42 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.64, 165.78, 164.17, 160.73, 158.59, 153.12, 151.93, 149.46, 146.60, 143.85, 140.43, 139.83, 130.21, 129.65, 129.33, 126.09, 108.91, 106.16, 96.32, 93.52, 71.83, 60.64, 56.52, 56.47, 32.75, 29.60, 29.11, 24.95, 21.72, 11.37; HRMS Calcd for $C_{36}H_{41}O_8N_4S$ $[M+H]^+$: 689.26396, Found: 689.26233.



*3-((5-((4-((4-methoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)pentyl)oxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6v**)*: Yellow solid, yield: 66.8%, m.p: 54-56 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (s, 1H, CH=N), 7.88 (d, J = 8.8 Hz, 2H, Ar-2,6-H), 7.36 (s, 2H, Myr-2',6'-H), 7.10 (d, J = 8.8 Hz, 2H, Ar-3,5-H), 6.84 (s, 1H, Myr-6-H), 6.49 (s, 1H, Myr-8-H), 3.99 (t, J = 7.2 Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.85 (s, 6H, Myr-3',5'-OCH_3), 3.84 (s, 6H, Myr-7-OCH_3 and Ar-4-OCH_3), 3.74 (s, 3H, Myr-4'-OCH_3), 3.05 (t, J = 7.1 Hz, 2H, CH_2), 2.39 (s, 3H, triazole-CH_3), 1.64 – 1.56 (m, 4H, 2×CH_2), 1.46 – 1.41 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.67, 166.00, 164.21, 163.57, 160.75, 158.63, 153.14, 152.01, 149.43, 146.46, 140.43, 139.84, 131.40, 126.10, 124.76, 115.16, 108.92, 106.20, 96.38, 93.57, 71.88, 60.66, 56.56, 56.04, 32.73, 29.59, 29.11, 24.93, 11.30; HRMS Calcd for $C_{36}H_{41}O_9N_4S$ $[M+H]^+$: 705.25888, Found: 705.25720.



*3-((5-((4-((3,4-dimethoxybenzylidene)amino)-5-methyl-4H-1,2,4-triazol-3-yl)thio)pentyl)oxy)-5,7-dimethoxy-2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one (**6w**)*: Yellow solid, yield: 69.7%, m.p: 86-88 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.71 (s, 1H, CH=N), 7.50 (d, J = 7.7 Hz, 1H, Ar-6-H), 7.47 (s, 1H, Ar-2-H), 7.36 (s, 2H, Myr-2',6'-H), 7.12 (d, J = 8.3 Hz, 1H, Ar-5-H), 6.81 (s, 1H, Myr-6-H), 6.47 (s, 1H, Myr-8-H), 3.94 (t, J = 7.6Hz, 2H, CH_2), 3.90 (s, 3H, Myr-5-OCH_3), 3.89 (s, 3H, Ar-3-OCH_3), 3.86 (s, 9H, Myr-3',5'-OCH_3 and Ar-4-OCH_3), 3.83 (s, 3H, Myr-7-OCH_3), 3.75

(s, 3H, Myr-4'-OCH_3), 3.08 (t, J = 7.1 Hz, 2H, CH_2), 2.41 (s, 3H, triazole-CH_3), 1.68 – 1.62 (m, 4H, 2×CH_2), 1.49 – 1.43 (m, 2H, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.64, 166.14, 164.16, 160.72, 158.59, 153.55, 153.12, 151.92, 149.60, 149.43, 146.45, 140.42, 139.83, 126.09, 125.18, 124.78, 111.97, 109.90, 108.91, 106.16, 96.31, 93.51, 71.83, 60.64, 56.53, 55.97, 32.65, 29.62, 29.14, 24.98, 11.28; HRMS Calcd for $C_{37}H_{43}O_{10}N_4S$ $[M+H]^+$: 735.26944, Found: 735.26782.

^{1}H NMR, ^{13}C NMR, ^{19}F NMR and HRMS spectrum of the title compounds

Figure S1. ^{1}H NMR spectrum of compound **6a**

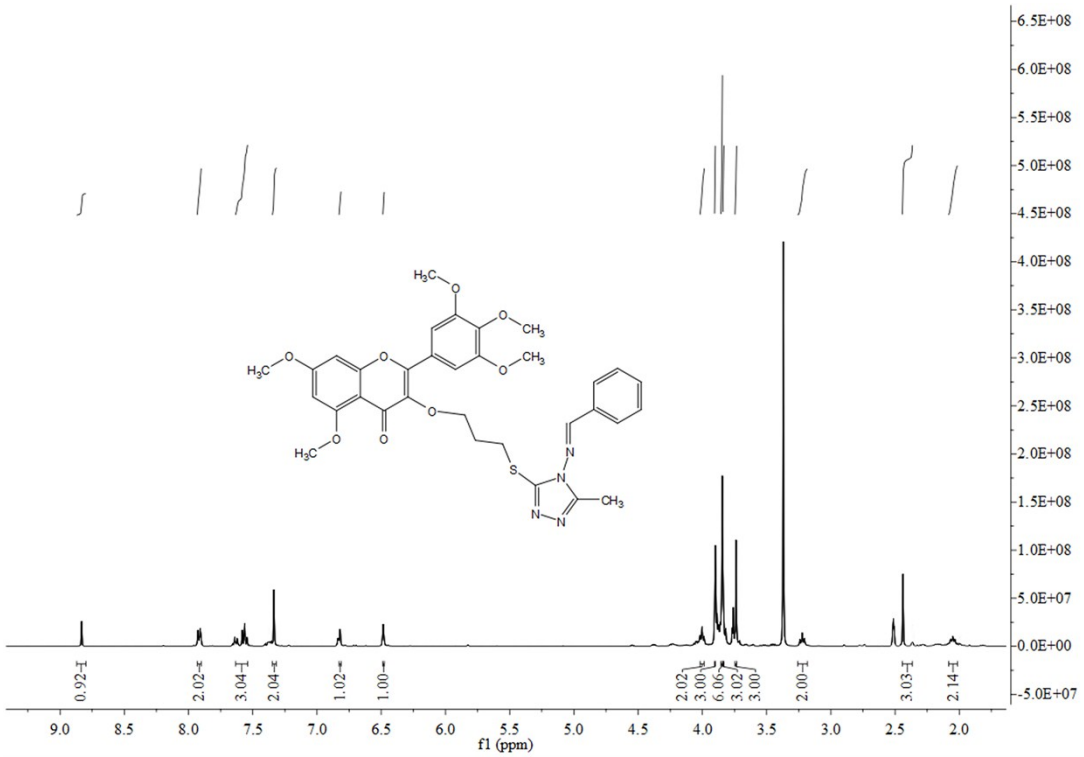


Figure S2. ^{13}C NMR spectrum of compound **6a**

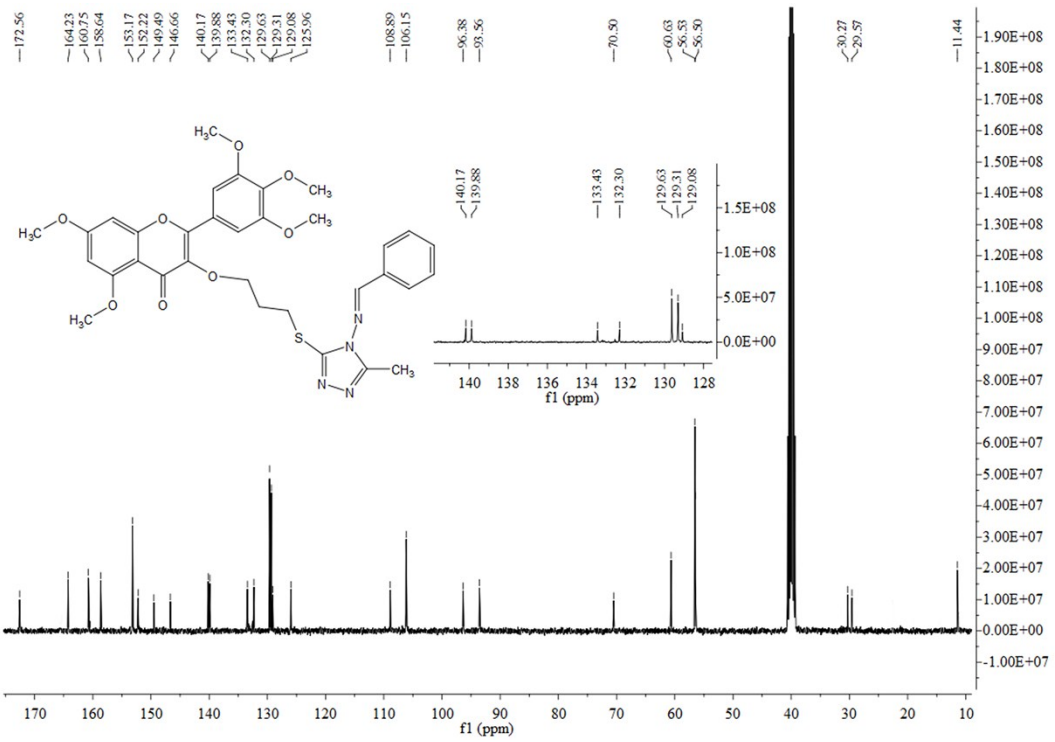


Figure S3. HRMS spectrum of compound **6a**

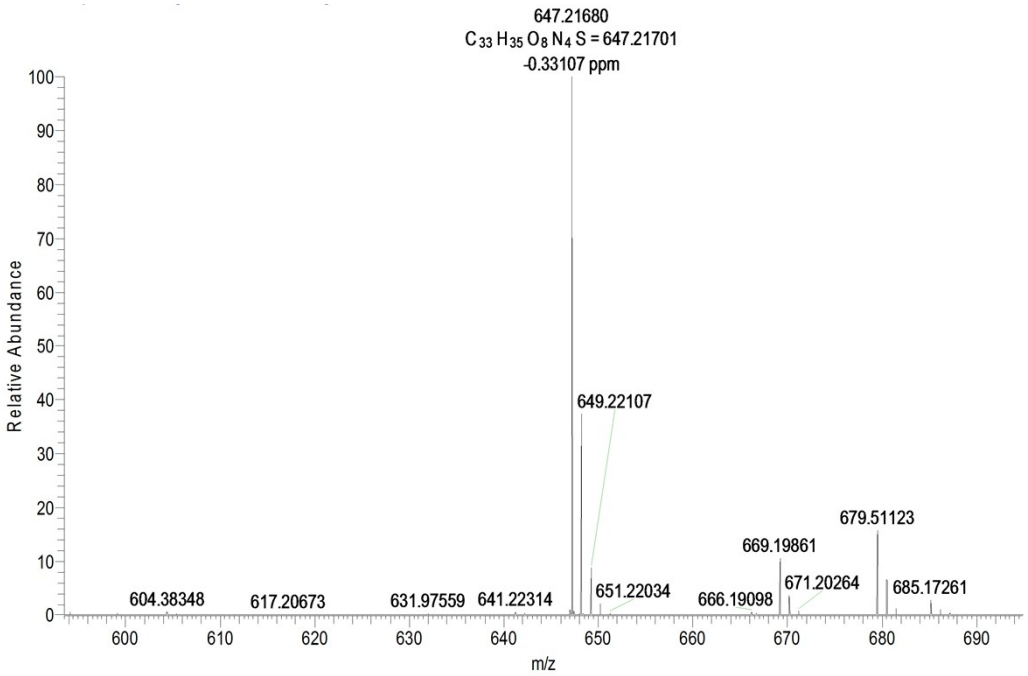


Figure S4. ^{1}H NMR spectrum of compound **6b**

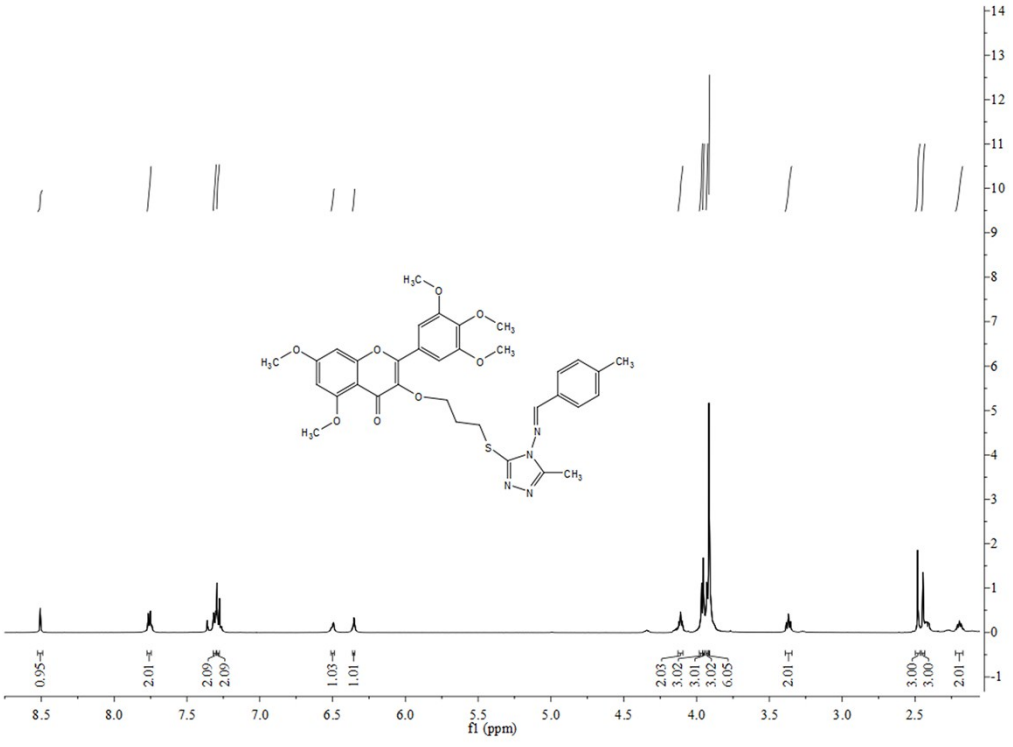


Figure S5. ^{13}C NMR spectrum of compound **6b**

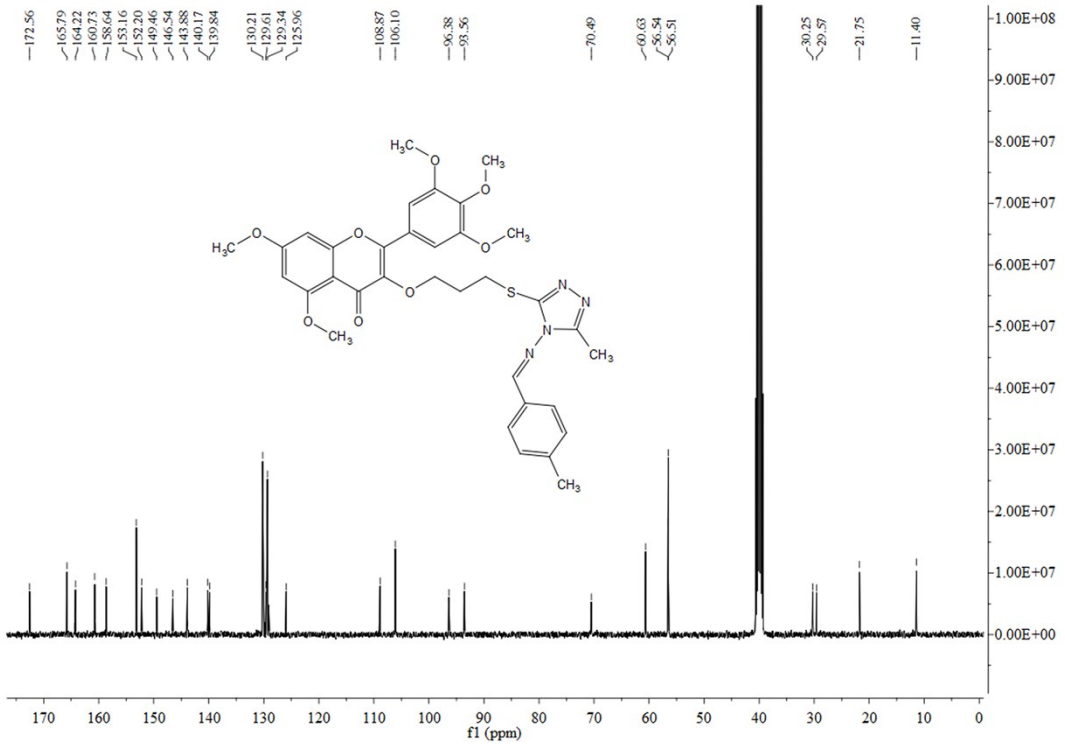


Figure S6. HRMS spectrum of compound **6b**

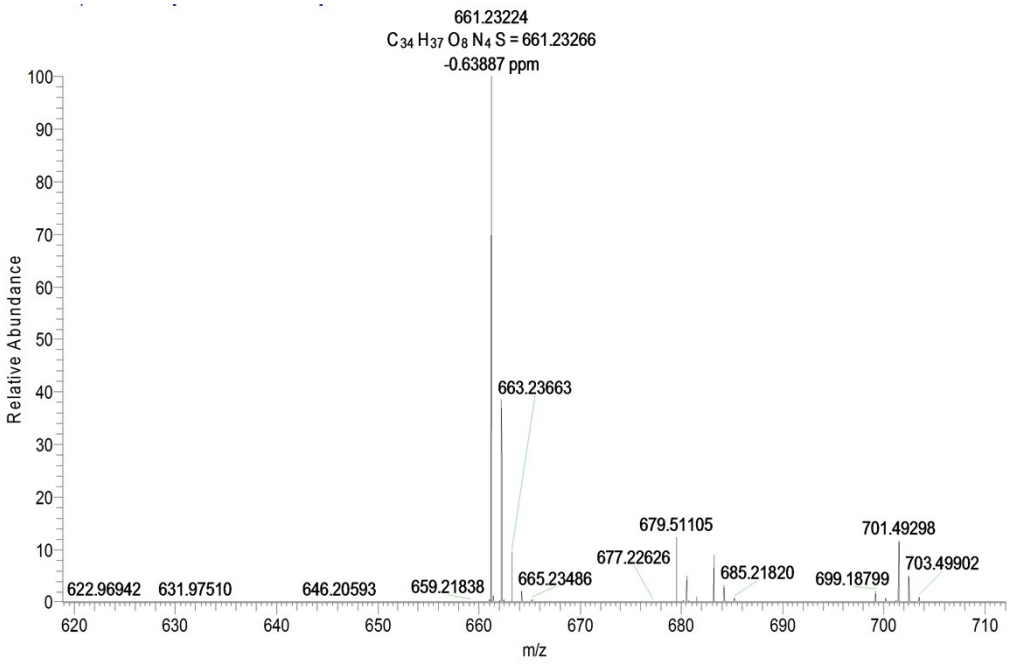


Figure S7. ^{1}H NMR spectrum of compound **6c**

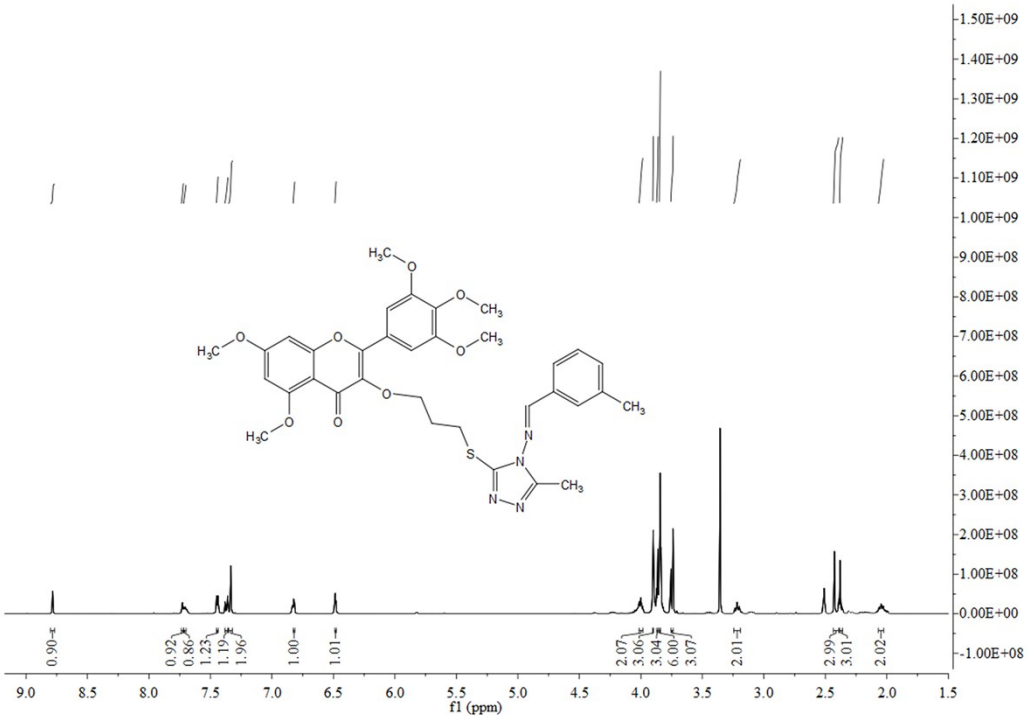


Figure S8. ^{13}C NMR spectrum of compound **6c**

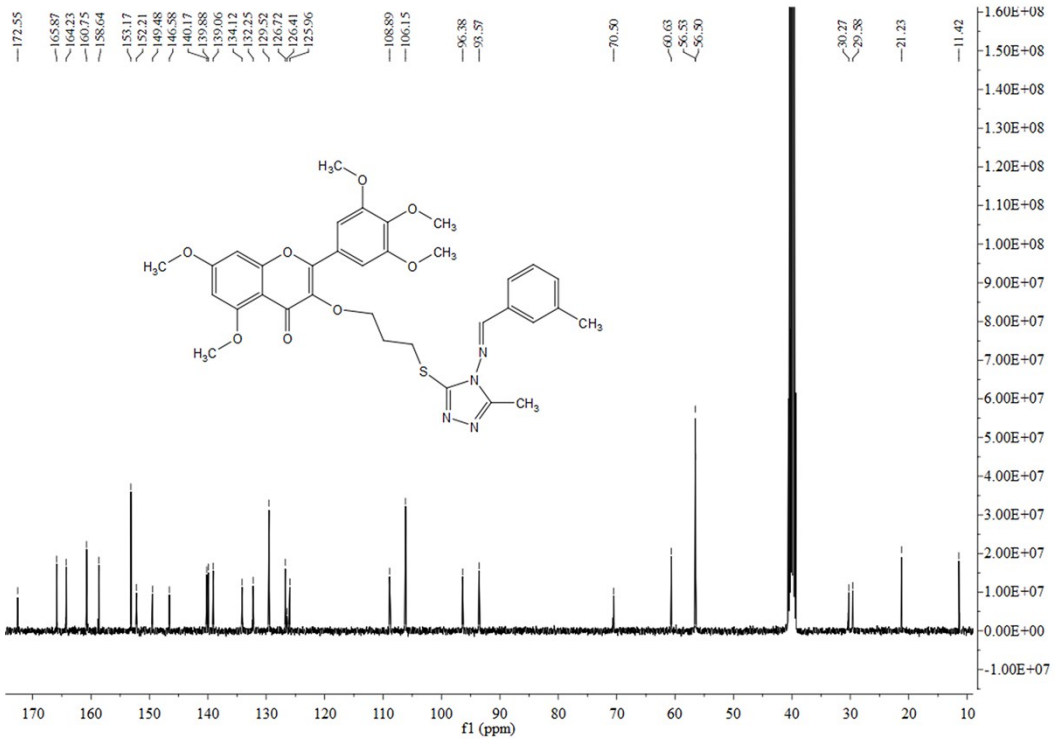


Figure S9. HRMS spectrum of compound **6c**

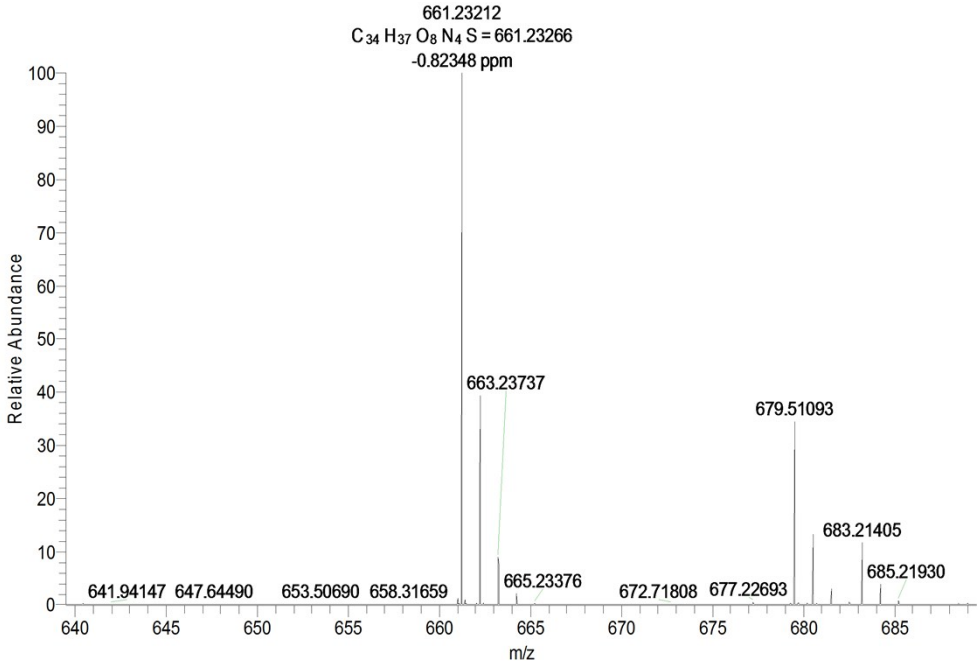


Figure S10. ^{1}H NMR spectrum of compound **6d**

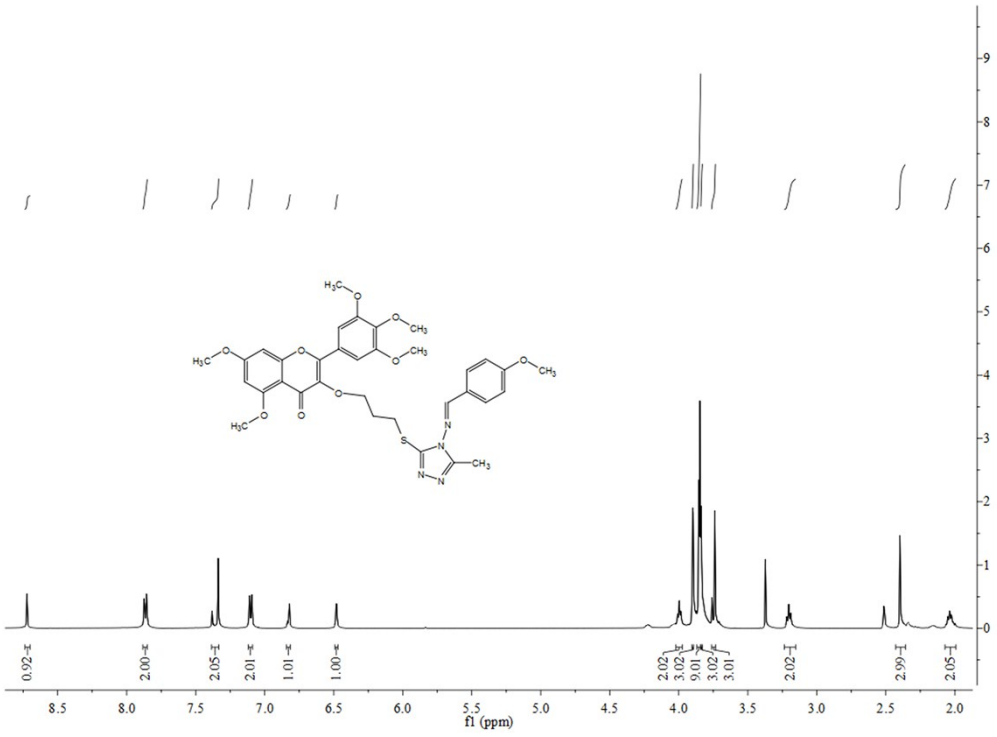


Figure S11. ^{13}C NMR spectrum of compound **6d**

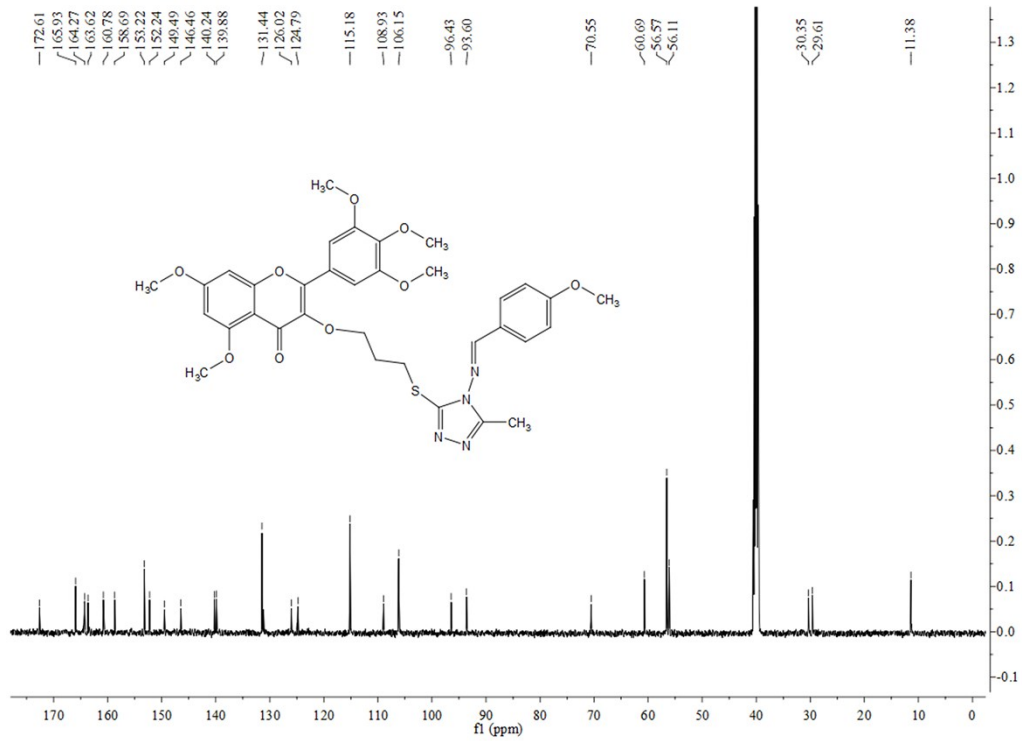


Figure S12. HRMS spectrum of compound **6d**

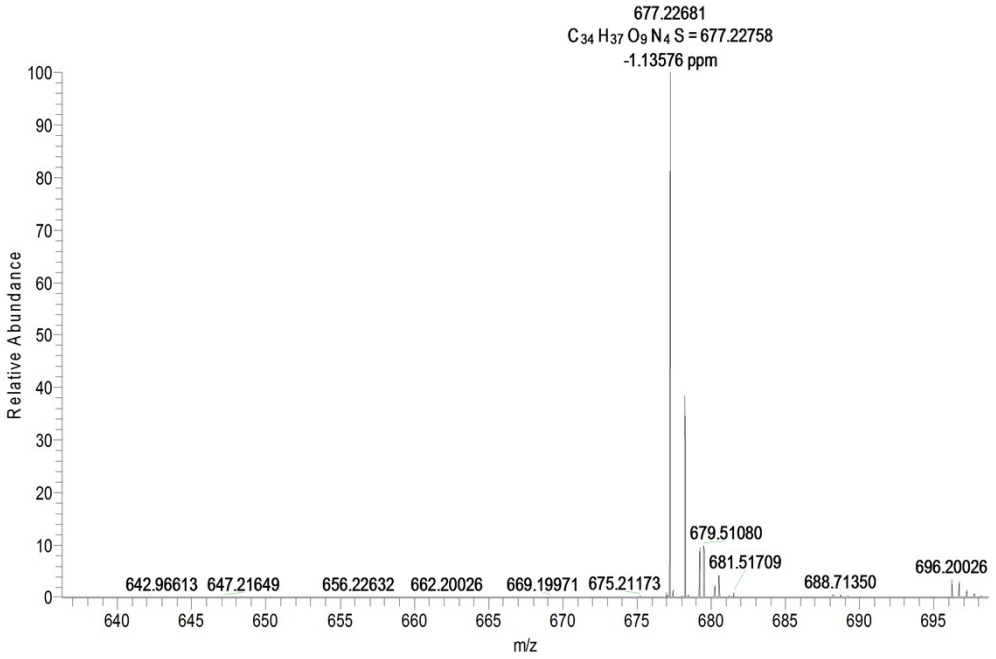


Figure S13. ^{1}H NMR spectrum of compound **6e**

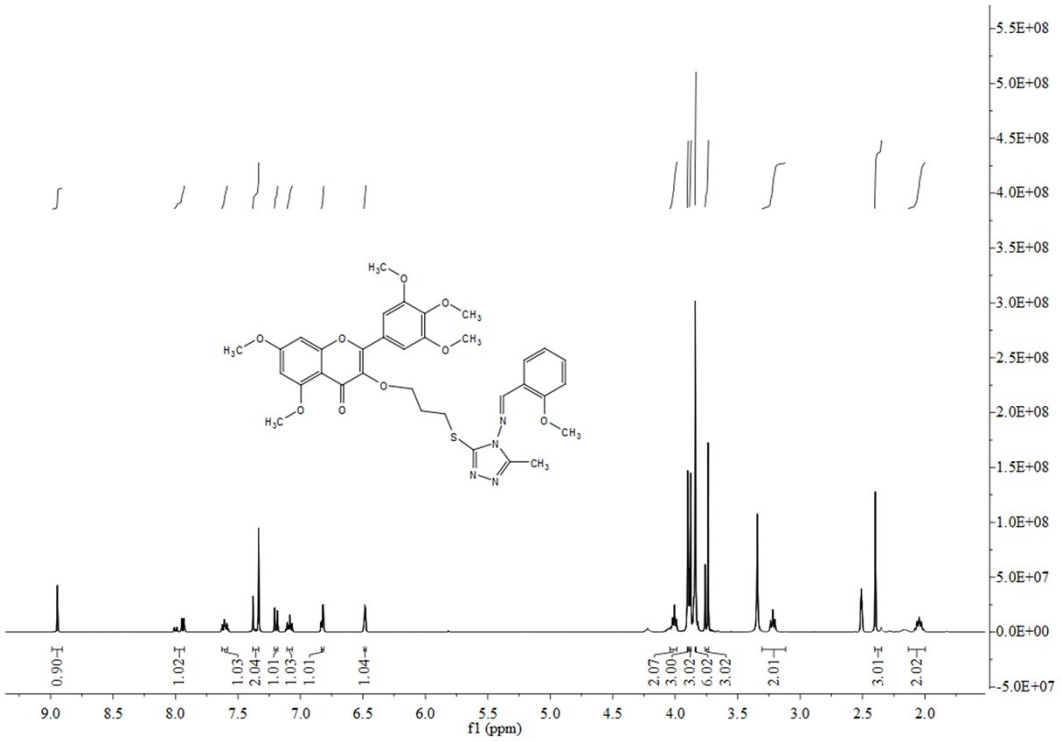


Figure S14. ^{13}C NMR spectrum of compound **6e**

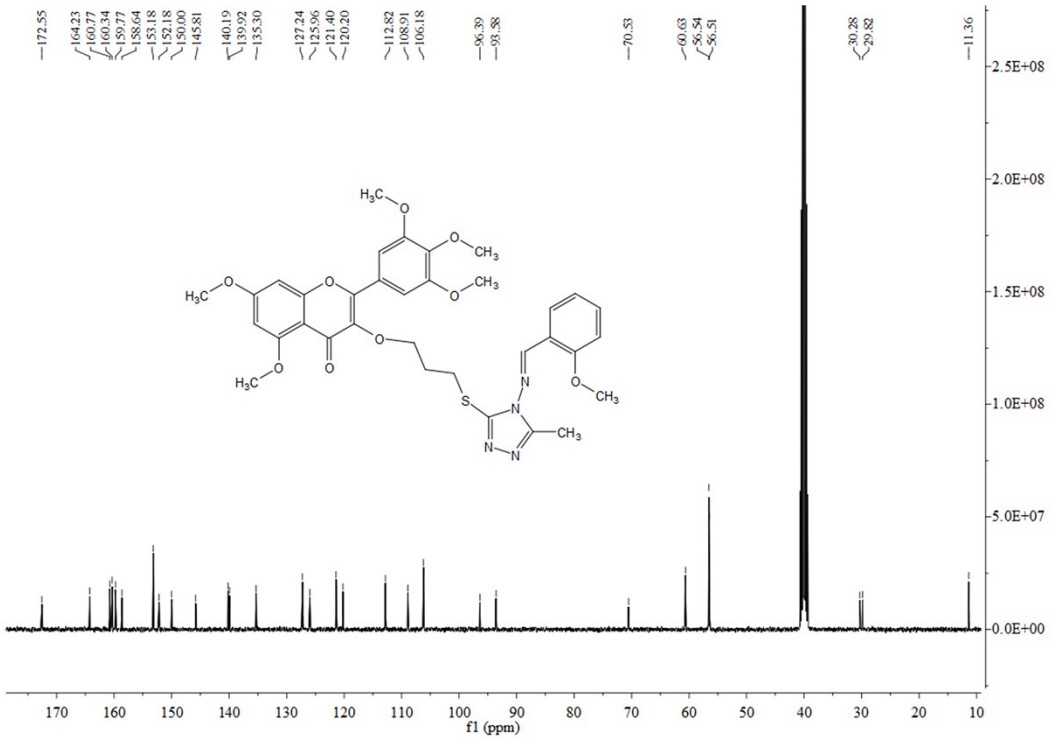


Figure S15. HRMS spectrum of compound **6e**

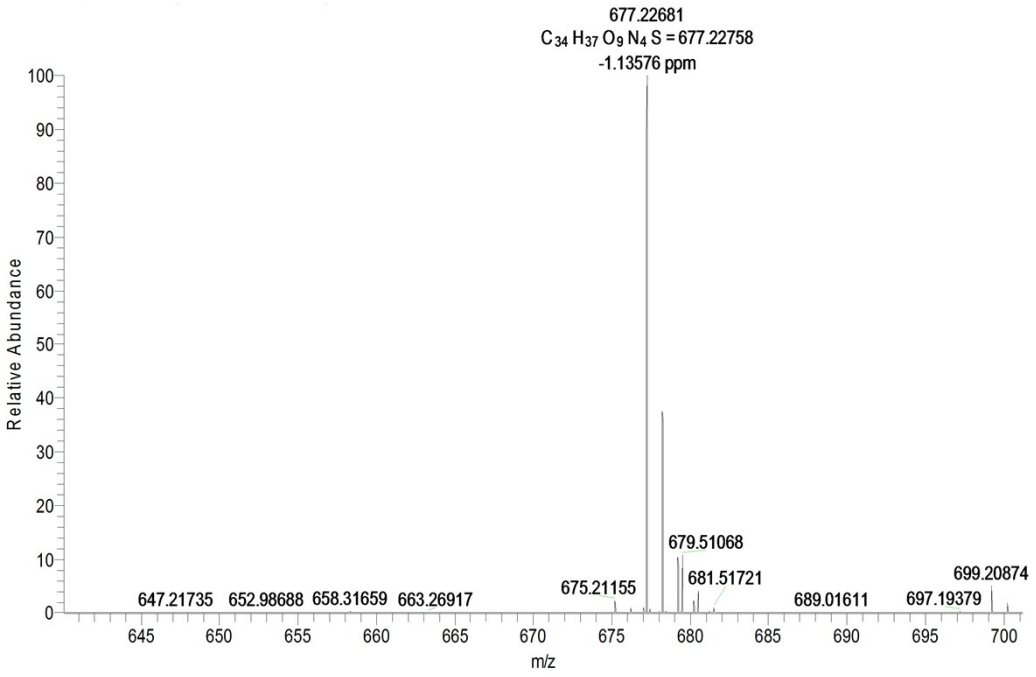


Figure S16. ^{1}H NMR spectrum of compound **6f**

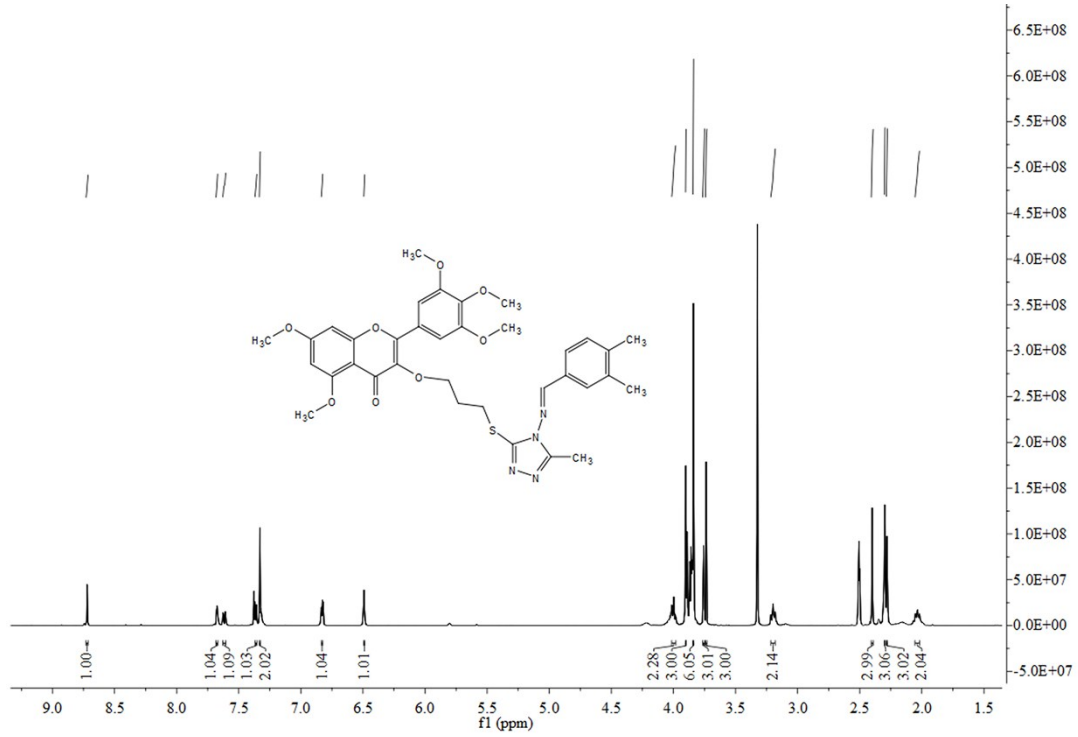


Figure S17. ^{13}C NMR spectrum of compound **6f**

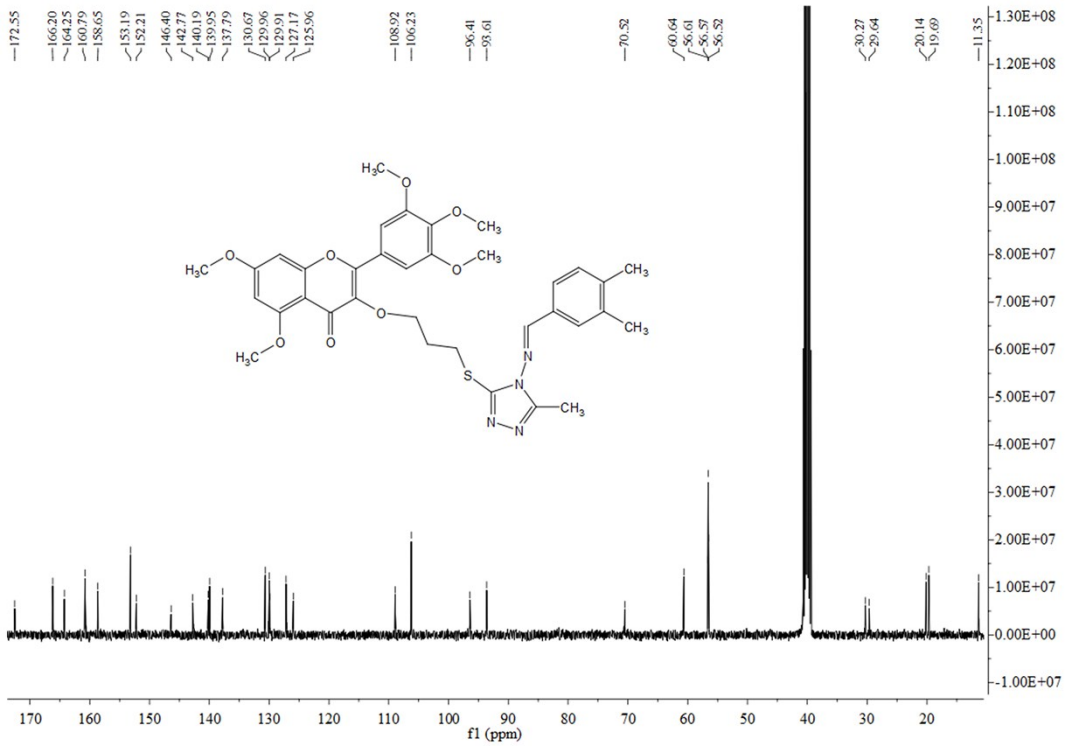


Figure S18. HRMS spectrum of compound **6f**

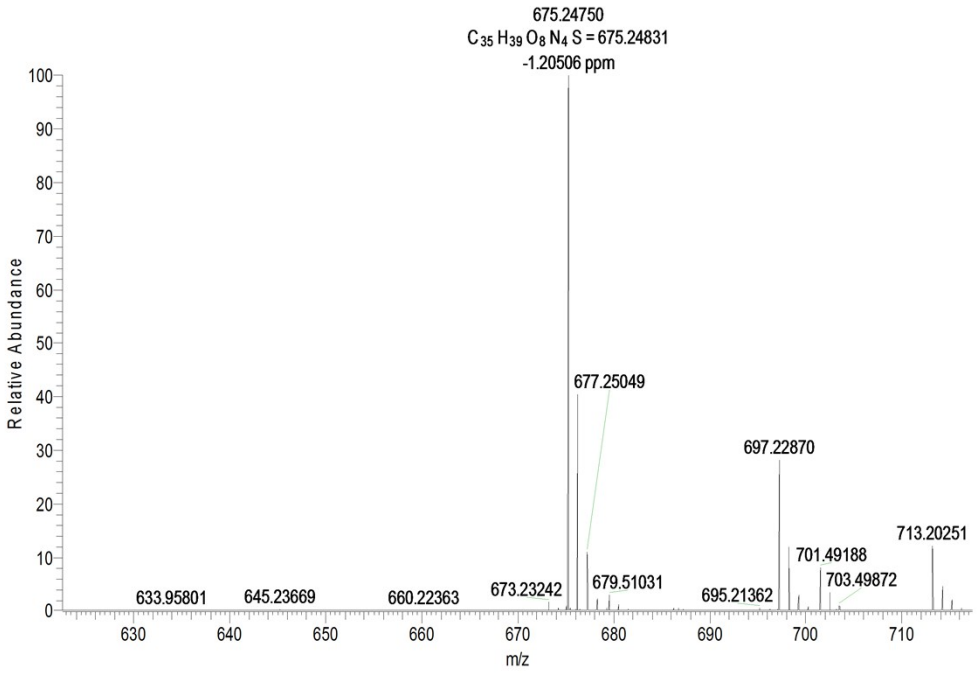


Figure S19. ^{1}H NMR spectrum of compound **6g**

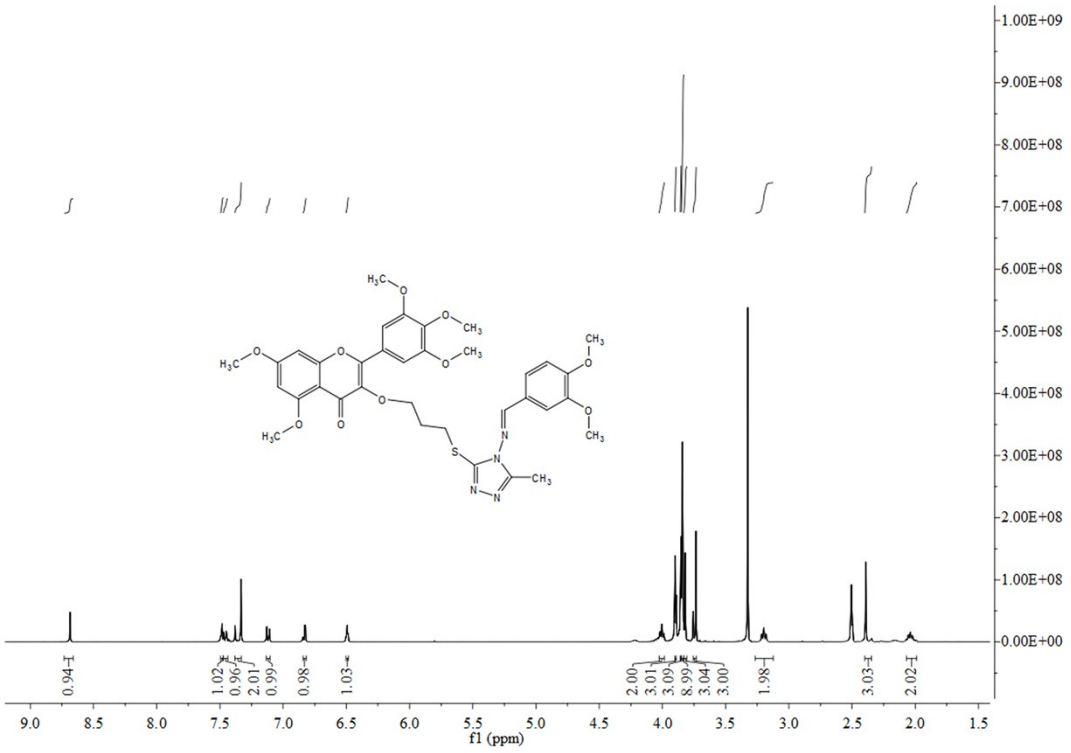


Figure S20. ^{13}C NMR spectrum of compound **6g**

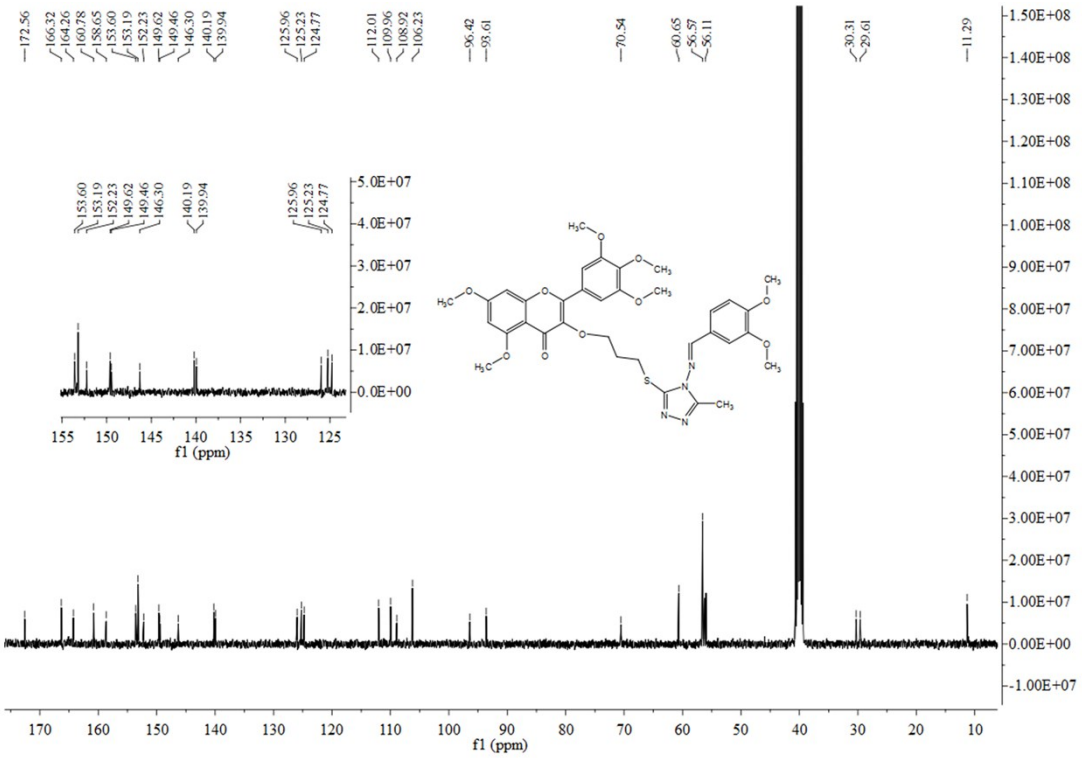


Figure S21. HRMS spectrum of compound **6g**

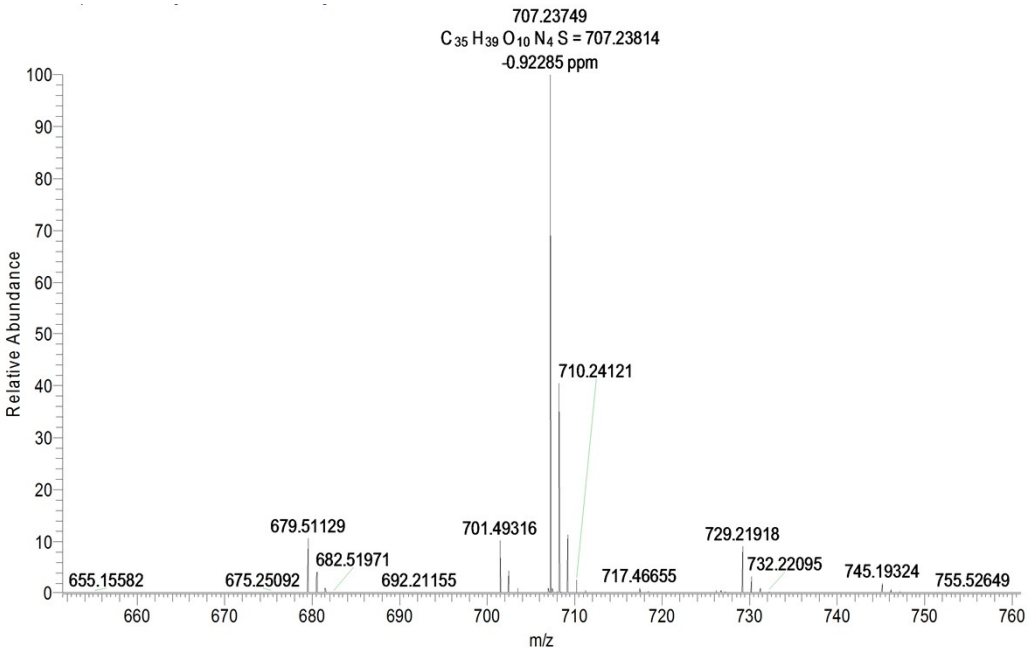


Figure S22. ^{1}H NMR spectrum of compound **6h**

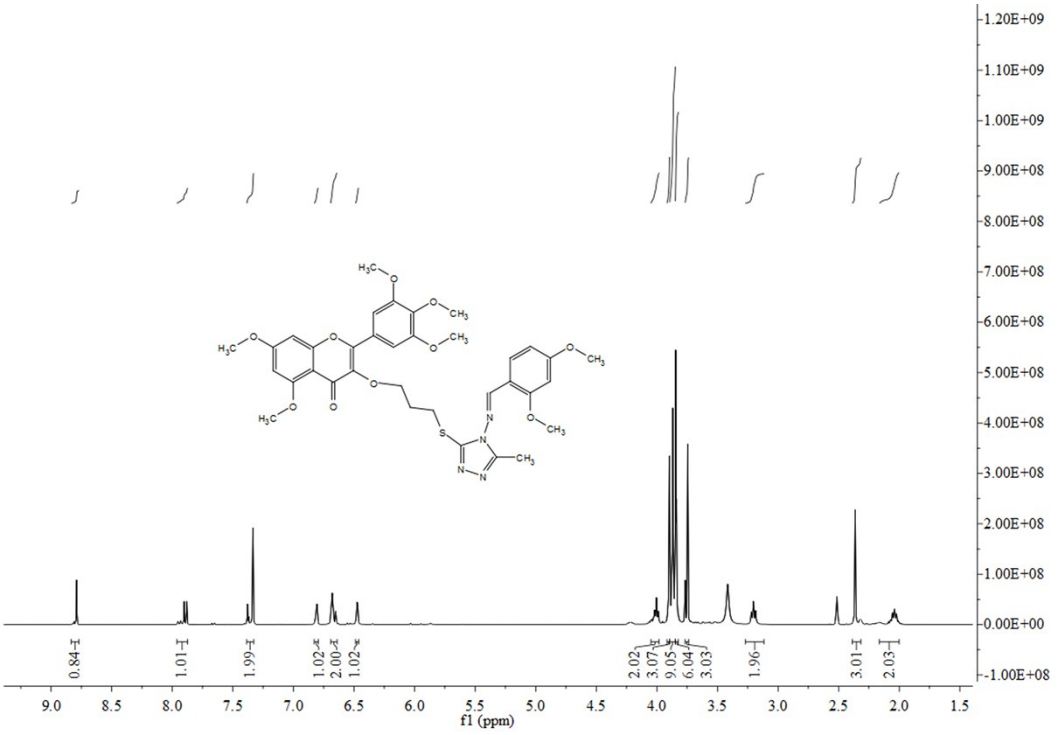


Figure S23. ^{13}C NMR spectrum of compound **6h**

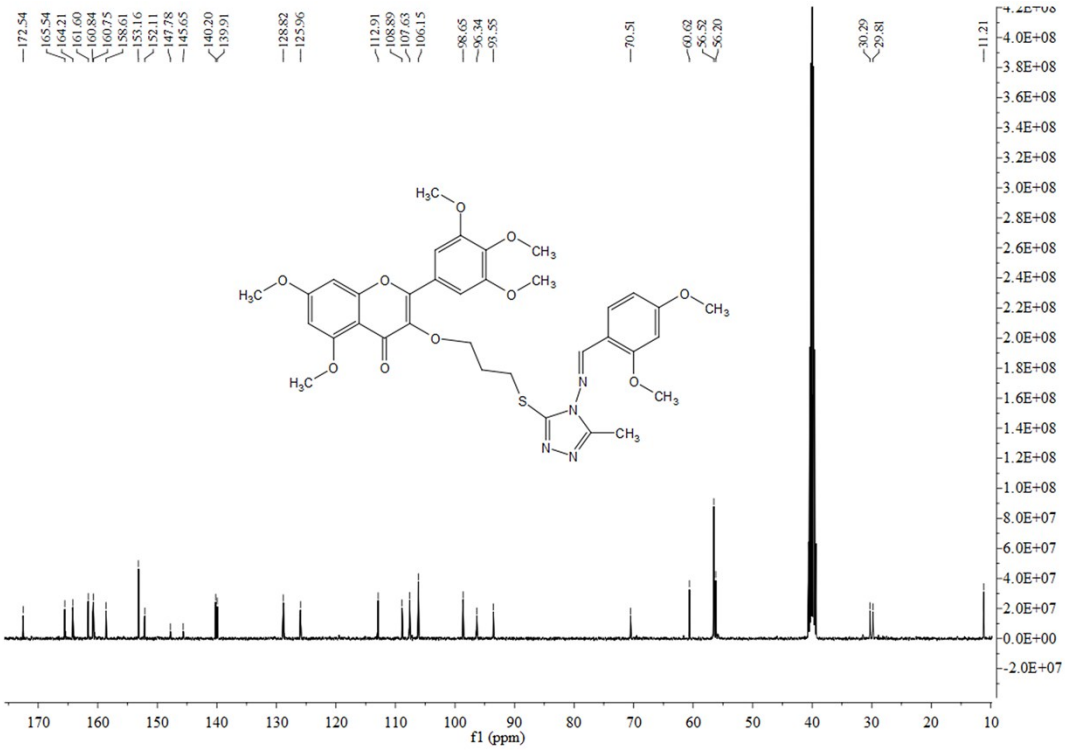


Figure S24. HRMS spectrum of compound **6h**

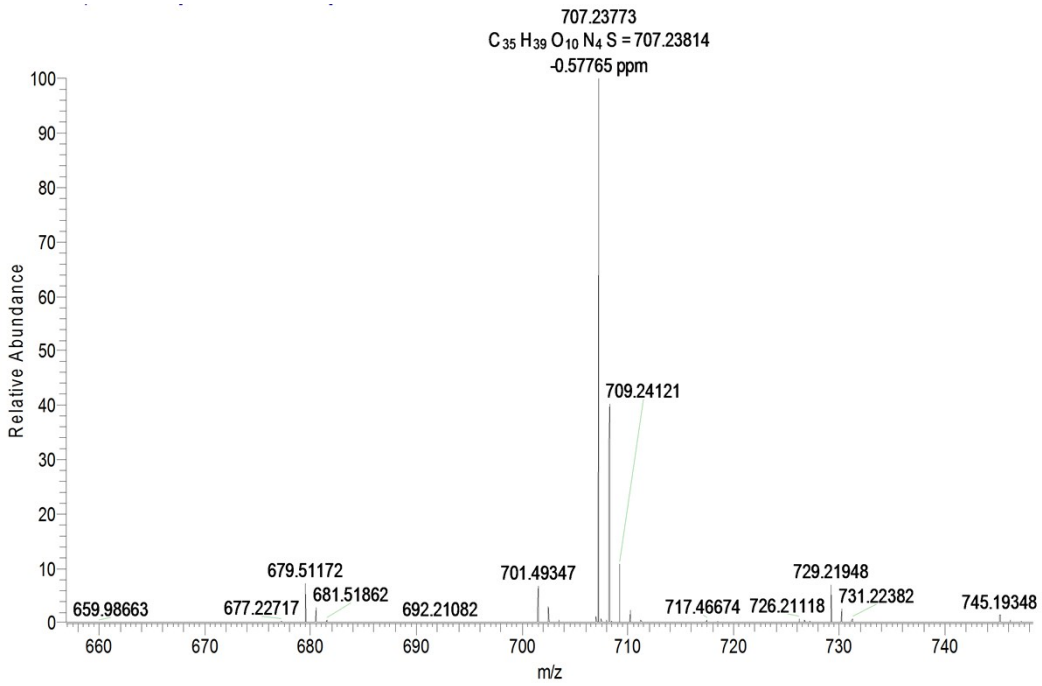


Figure S25. ^{1}H NMR spectrum of compound **6i**

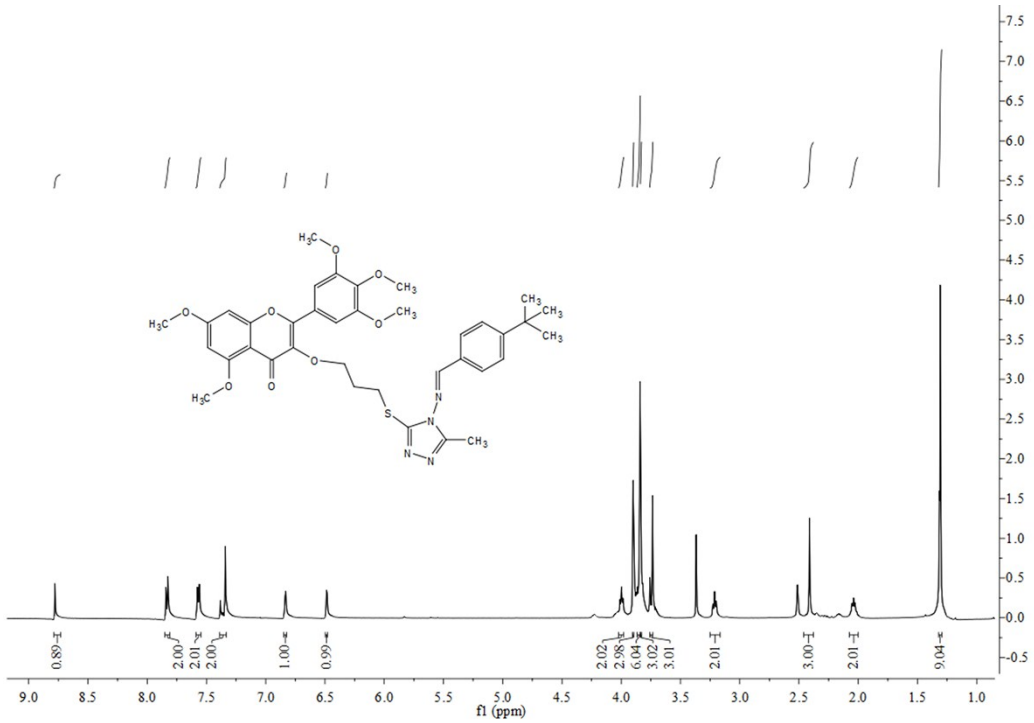


Figure S26. ^{13}C NMR spectrum of compound **6i**

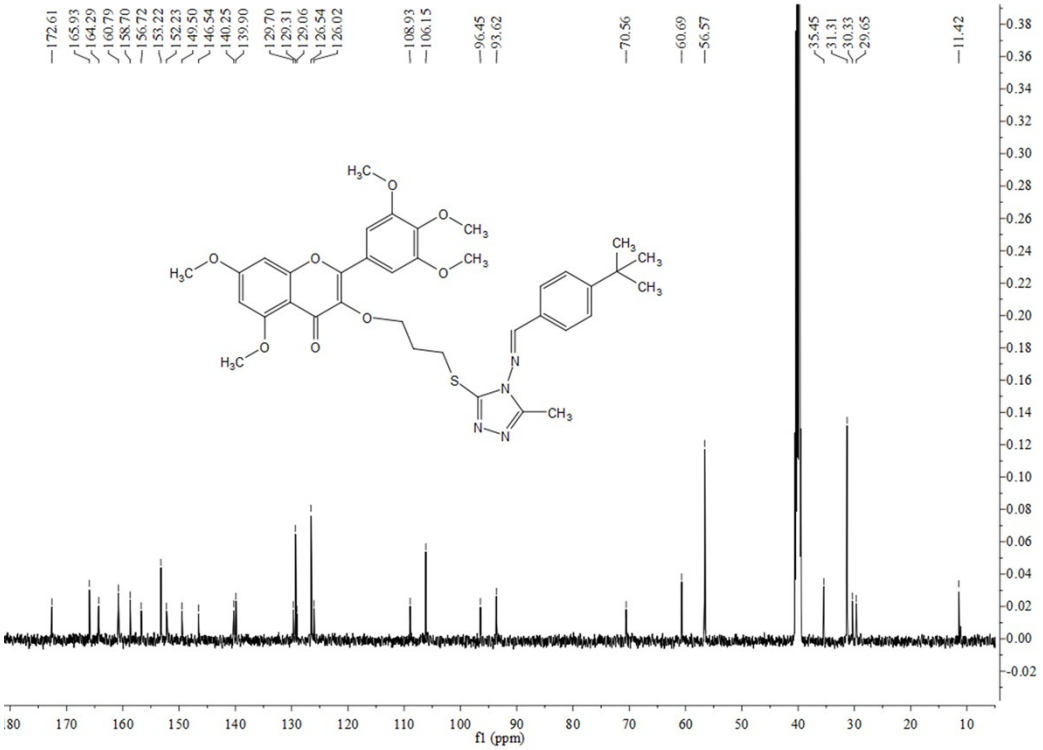


Figure S27. HRMS spectrum of compound **6i**

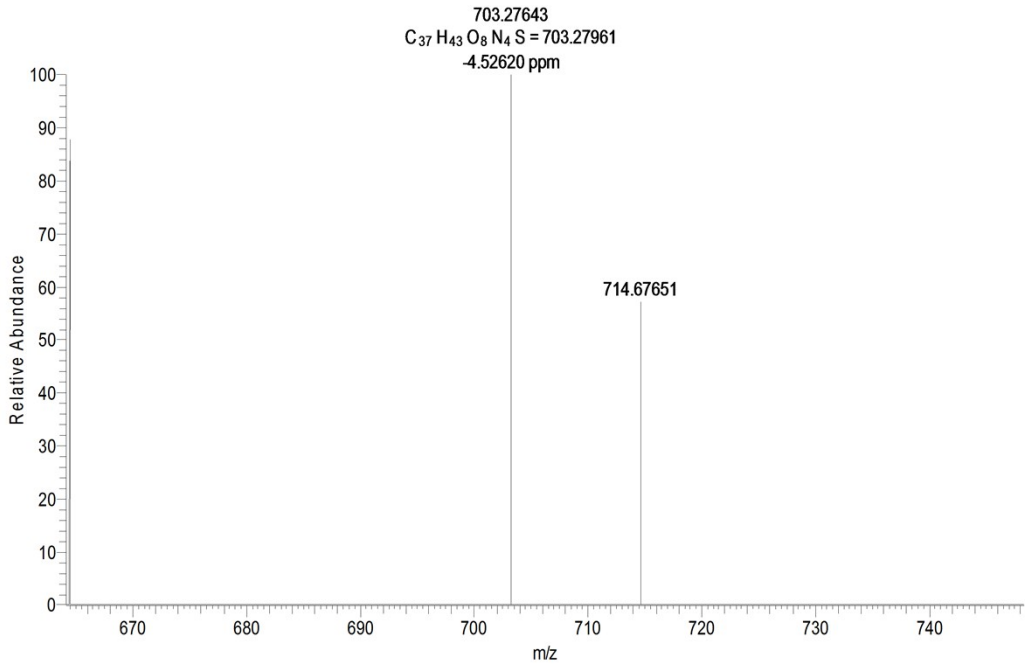


Figure S28. ^{1}H NMR spectrum of compound **6j**

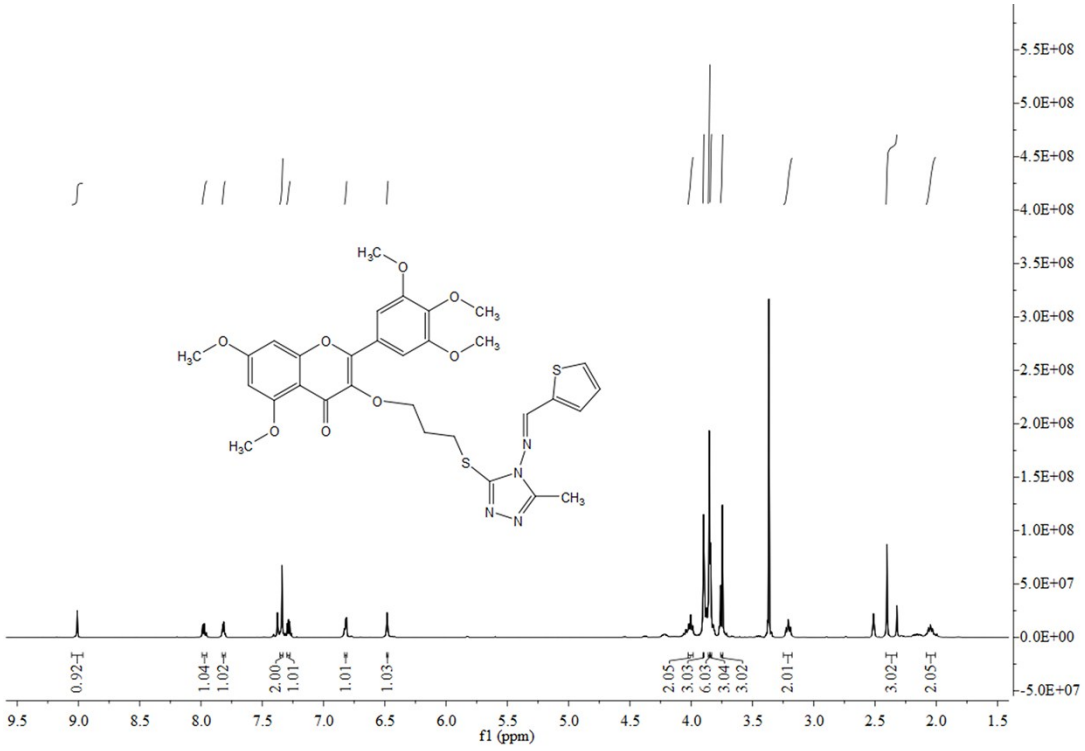


Figure S29. ^{13}C NMR spectrum of compound **6j**

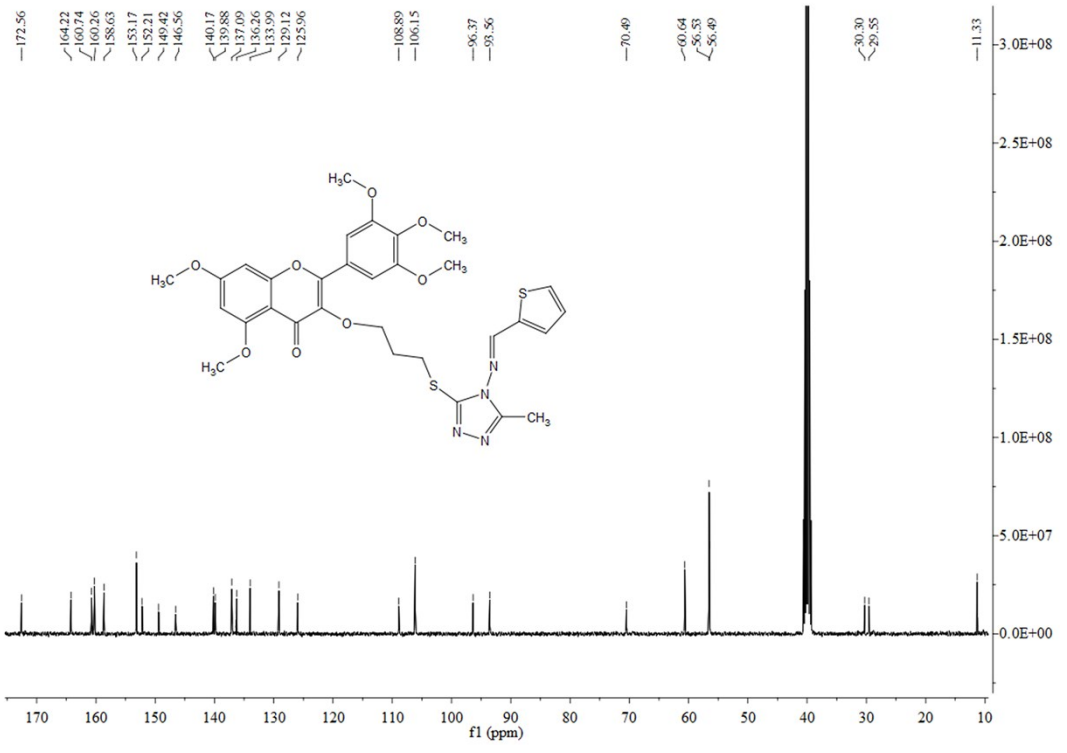


Figure S30. HRMS spectrum of compound **6j**

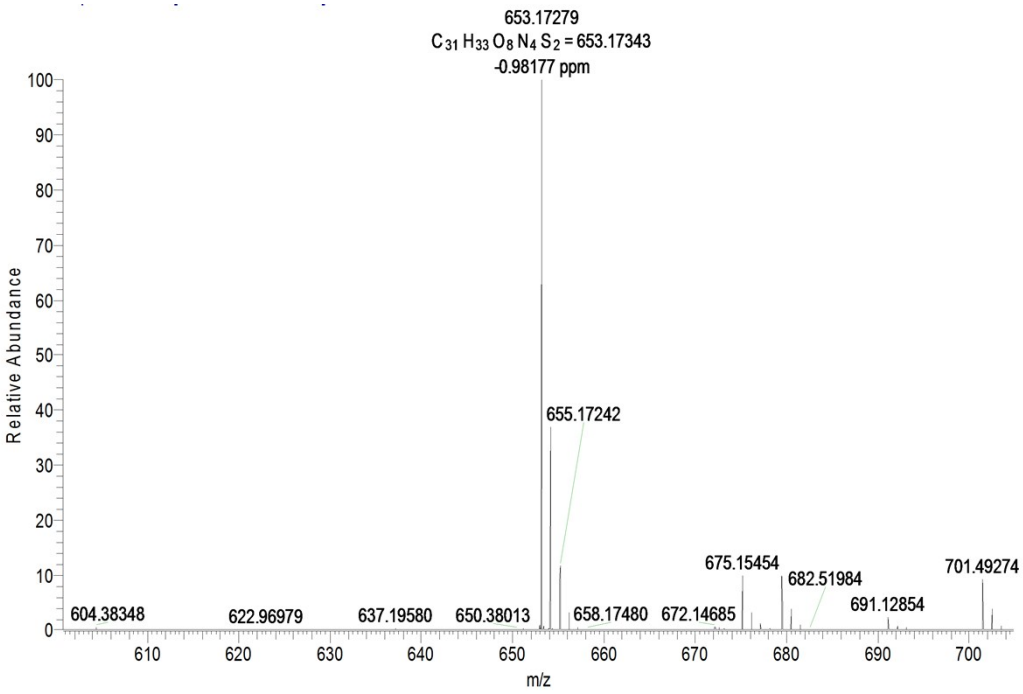


Figure S31. ^{1}H NMR spectrum of compound **6k**

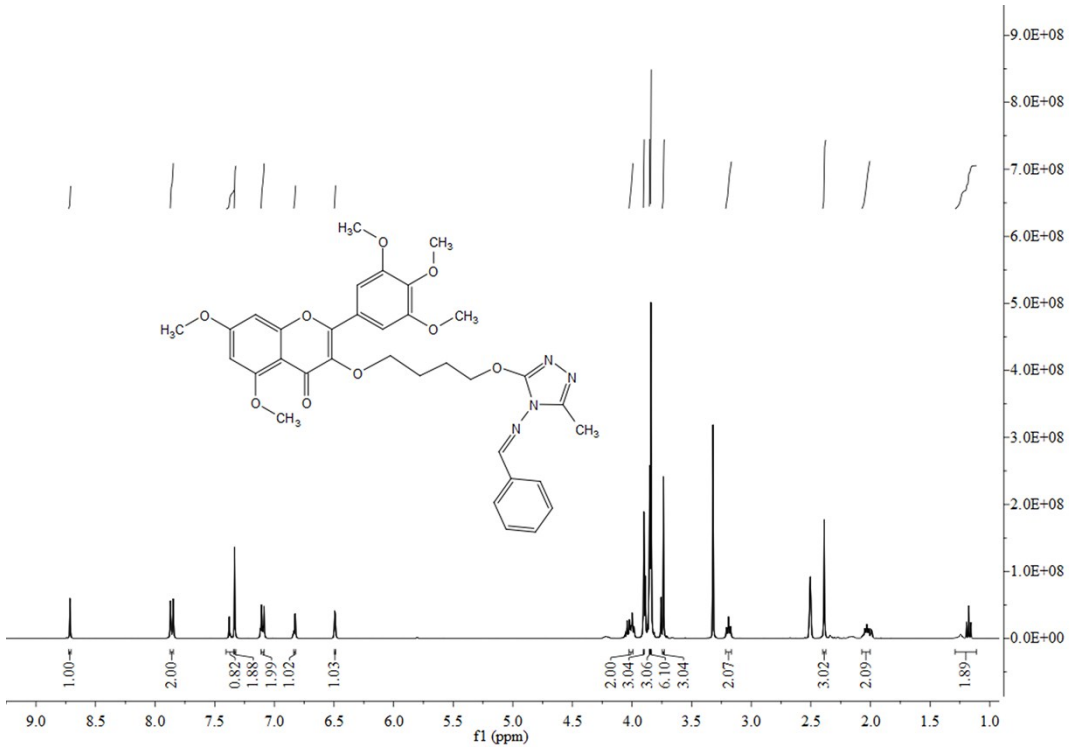


Figure S32. ^{13}C NMR spectrum of compound **6k**

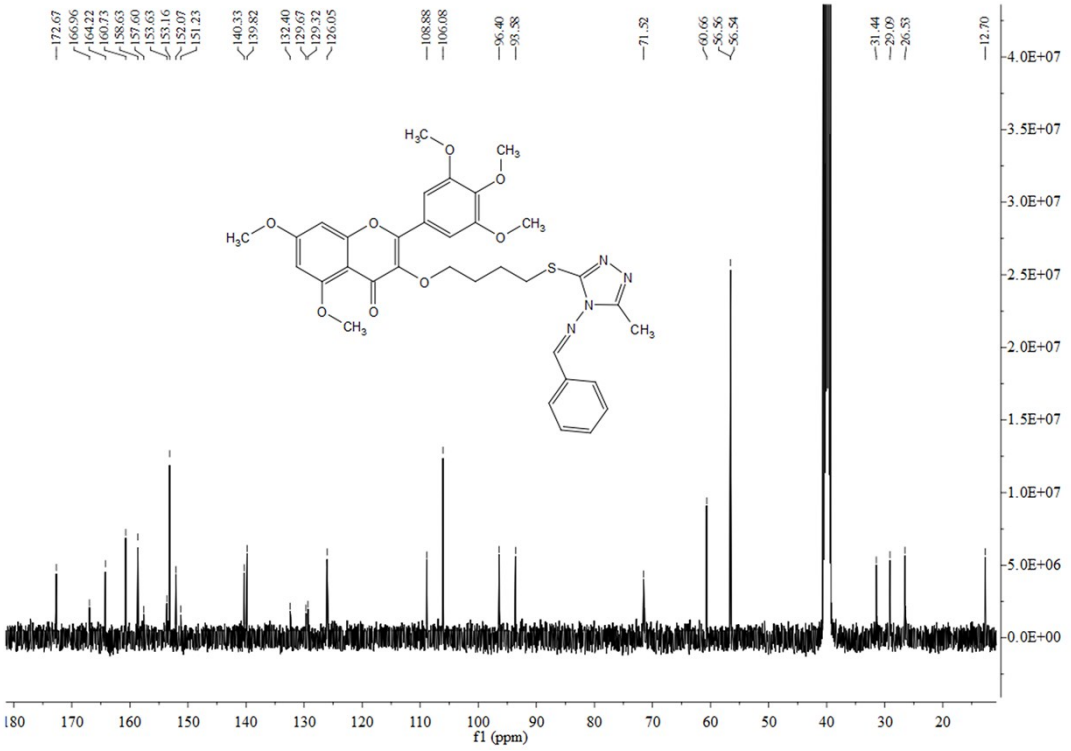


Figure S33. HRMS spectrum of compound **6k**

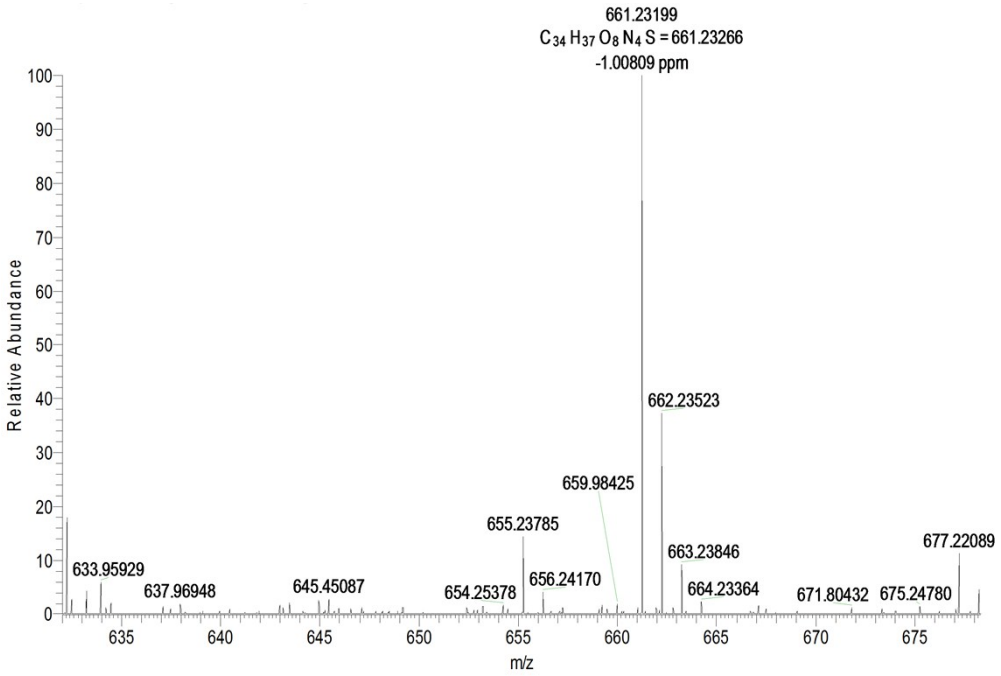


Figure S34. ^{1}H NMR spectrum of compound **6l**

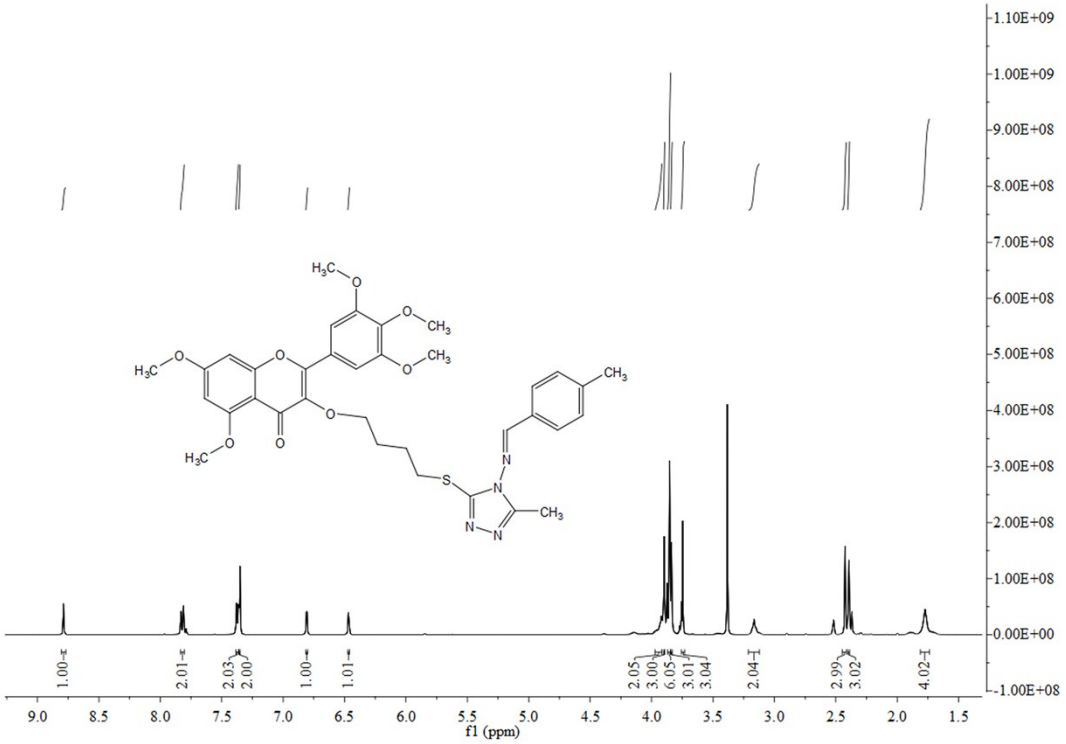


Figure S35. ^{13}C NMR spectrum of compound **6l**

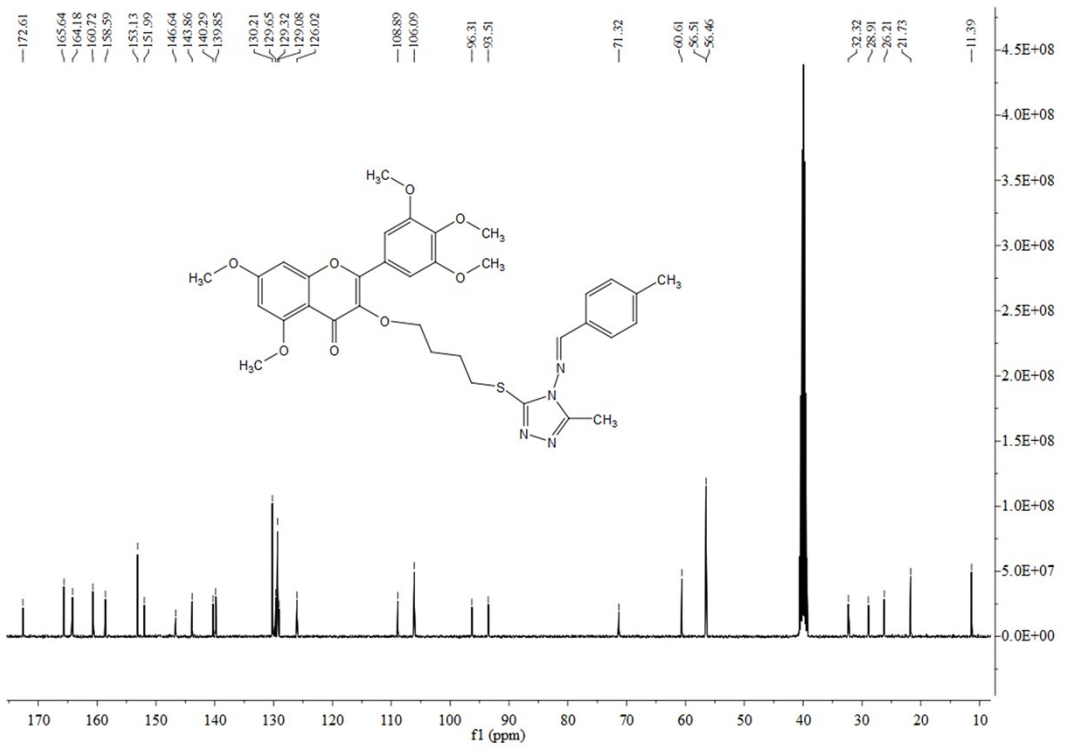


Figure S36. HRMS spectrum of compound **6l**

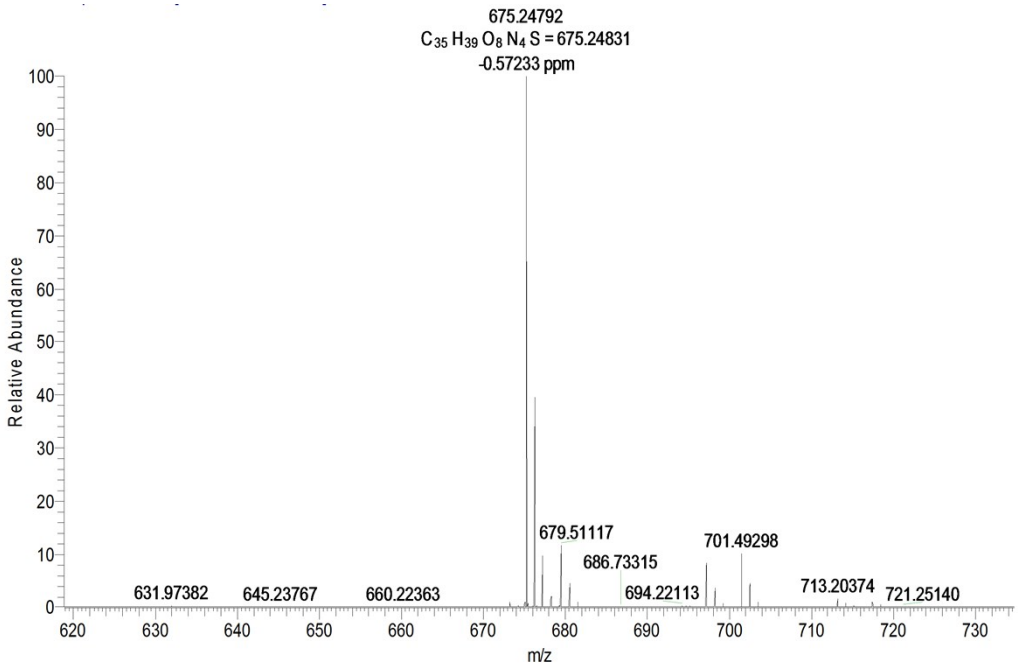


Figure S37. ^{1}H NMR spectrum of compound **6m**

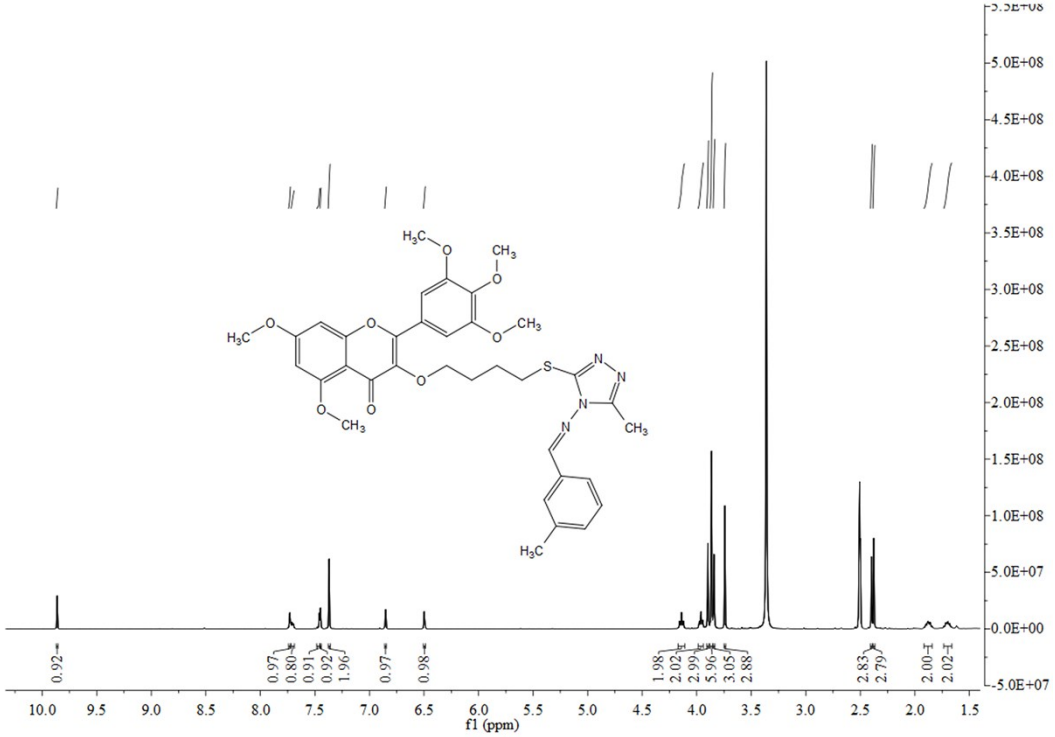


Figure S38. ^{13}C NMR spectrum of compound **6m**

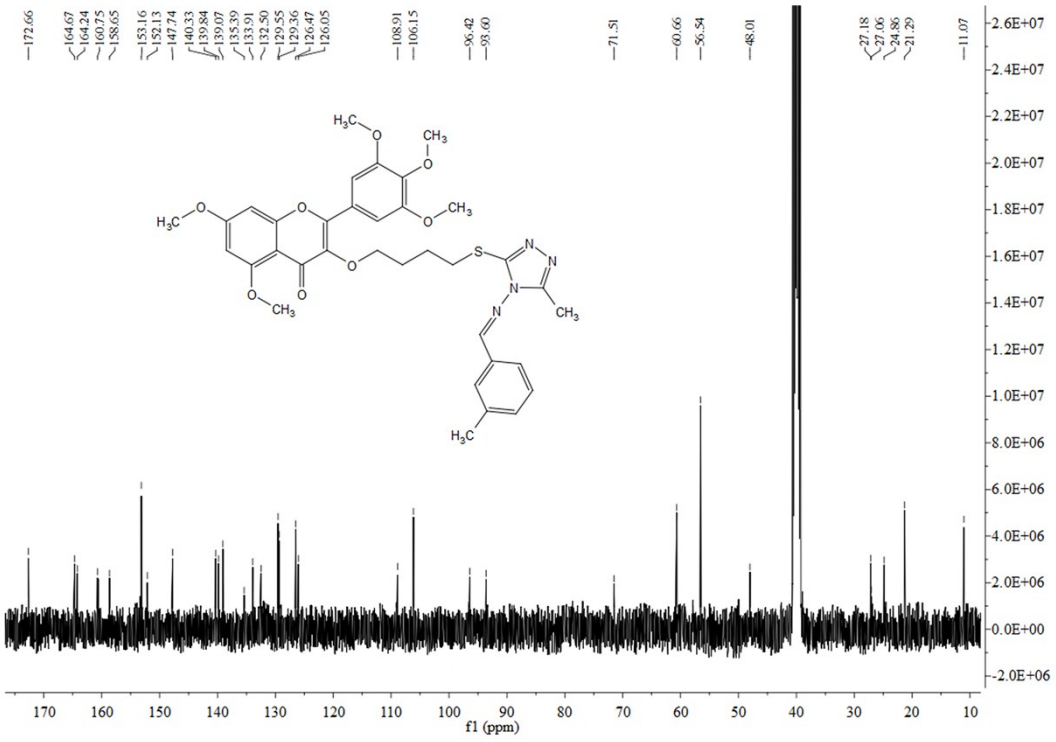


Figure S39. HRMS spectrum of compound **6m**

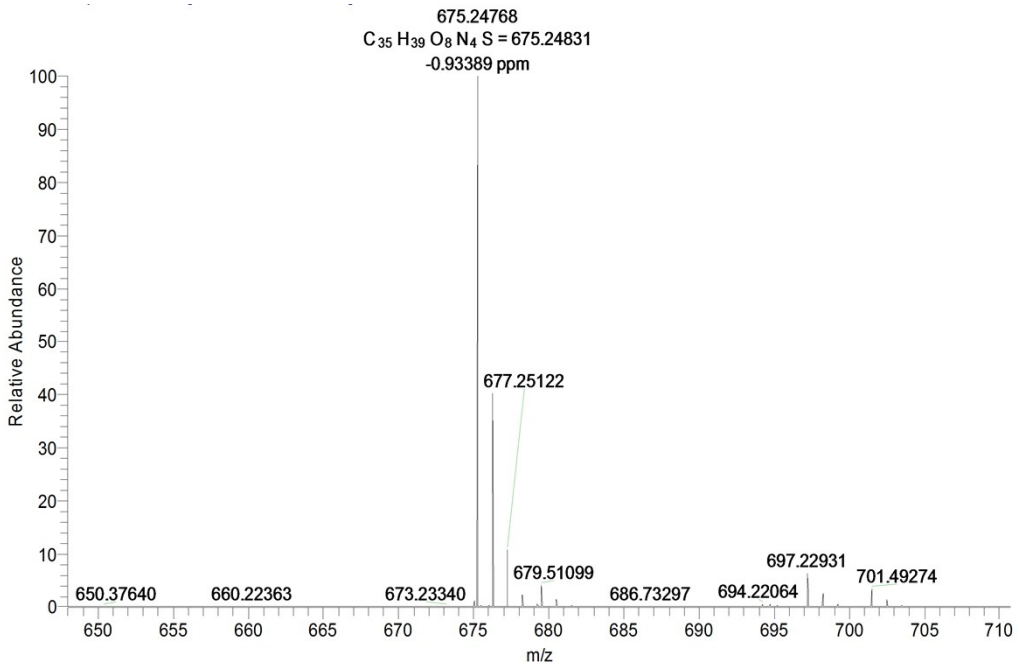


Figure S40. ^{1}H NMR spectrum of compound **6n**

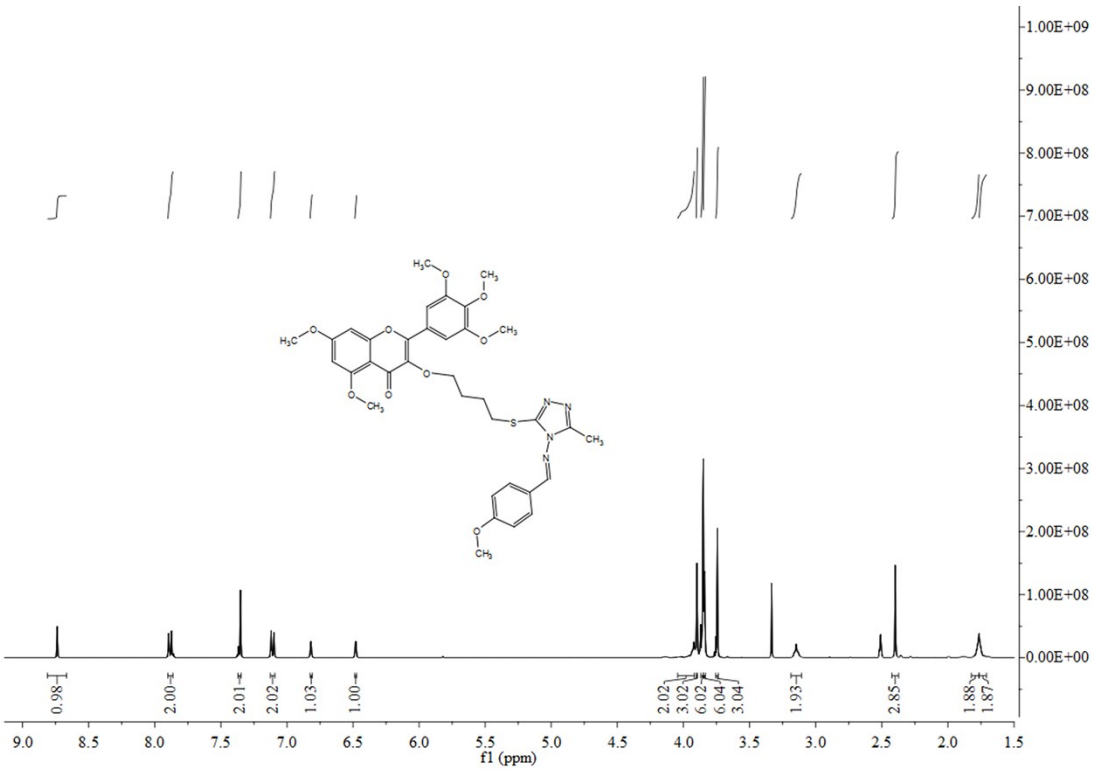


Figure S41. ^{13}C NMR spectrum of compound **6n**

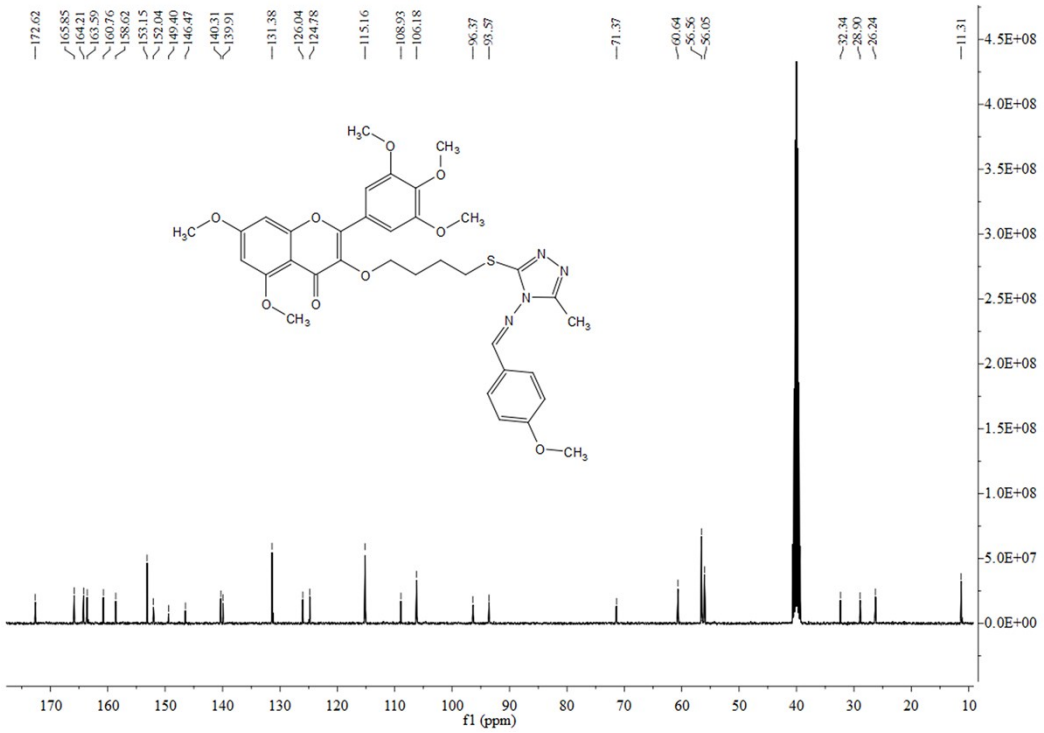


Figure S42. HRMS spectrum of compound **6n**

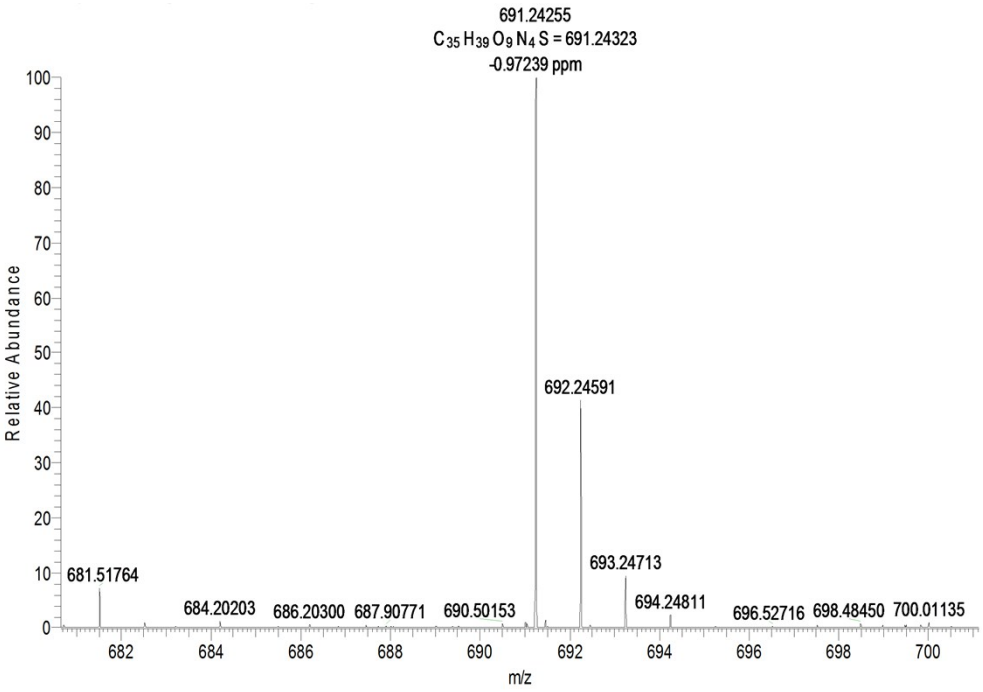


Figure S43. ^{1}H NMR spectrum of compound **6o**

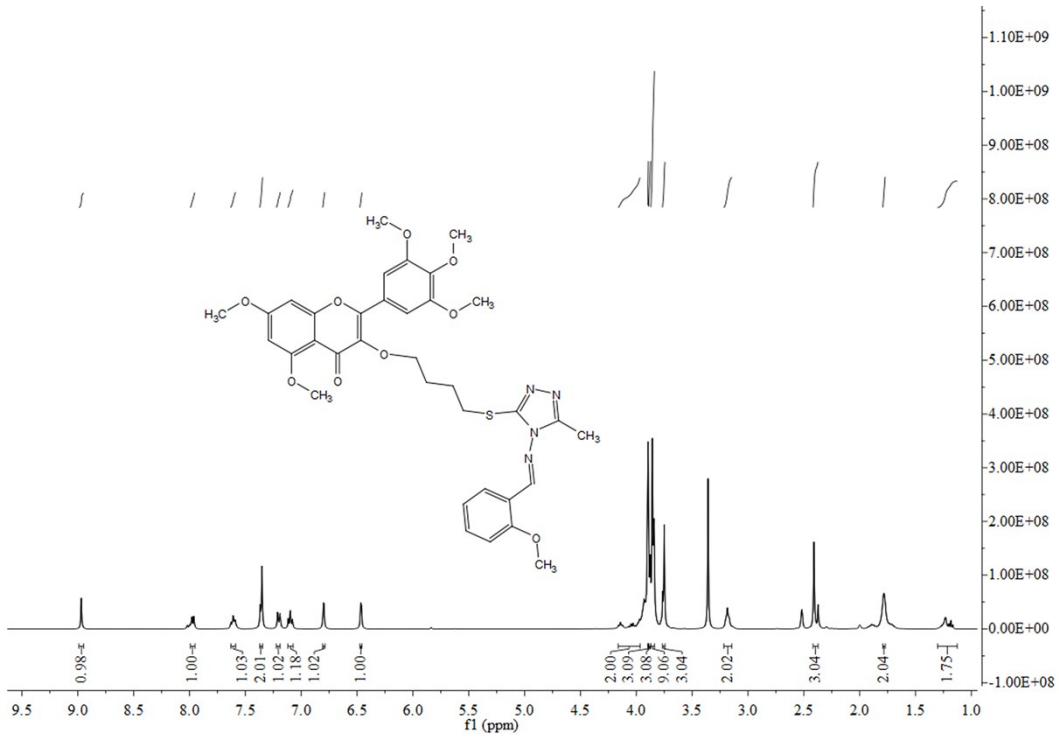


Figure S44. ^{13}C NMR spectrum of compound **6o**

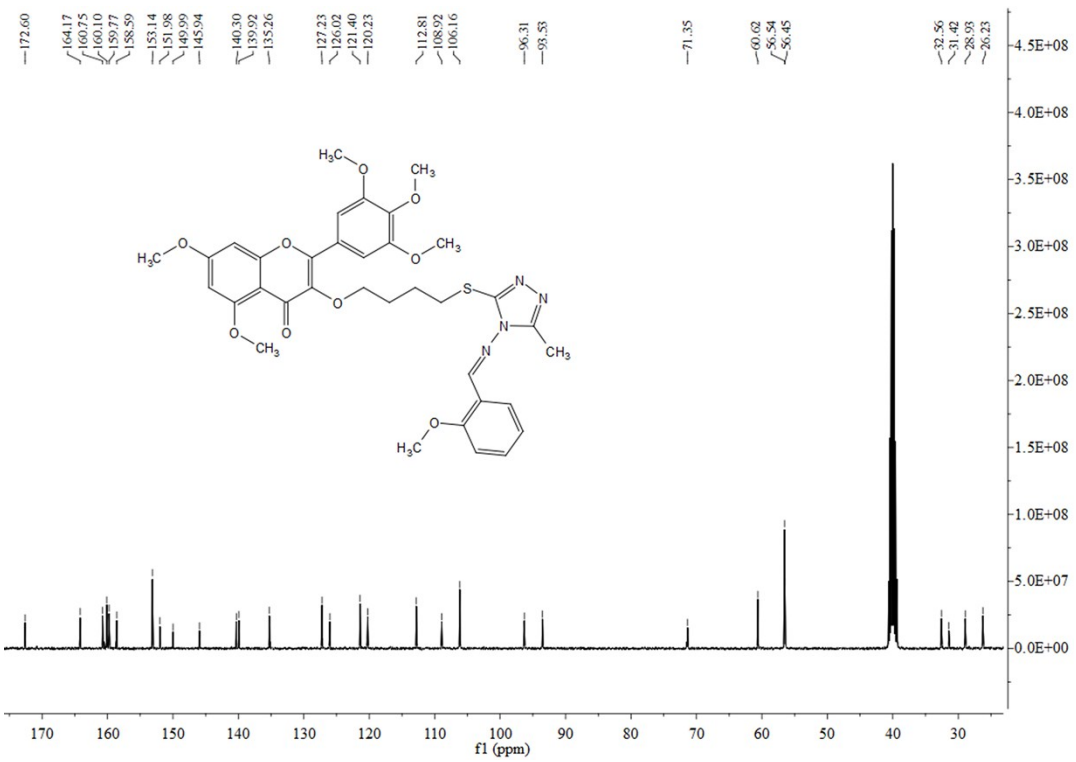


Figure S45. HRMS spectrum of compound **6o**

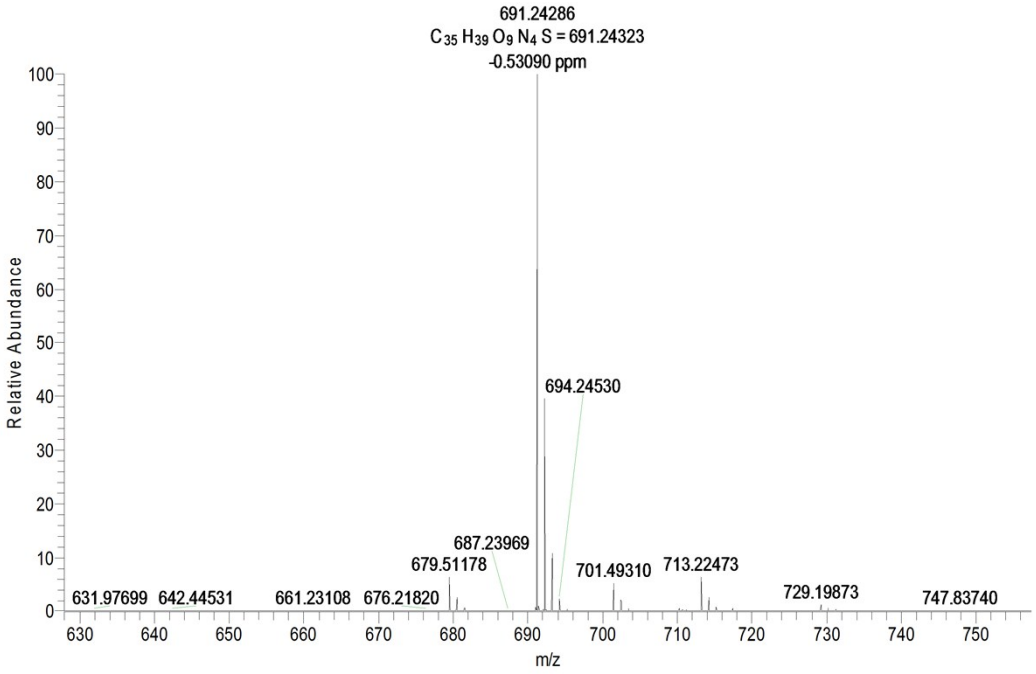


Figure S46. ^{1}H NMR spectrum of compound **6p**

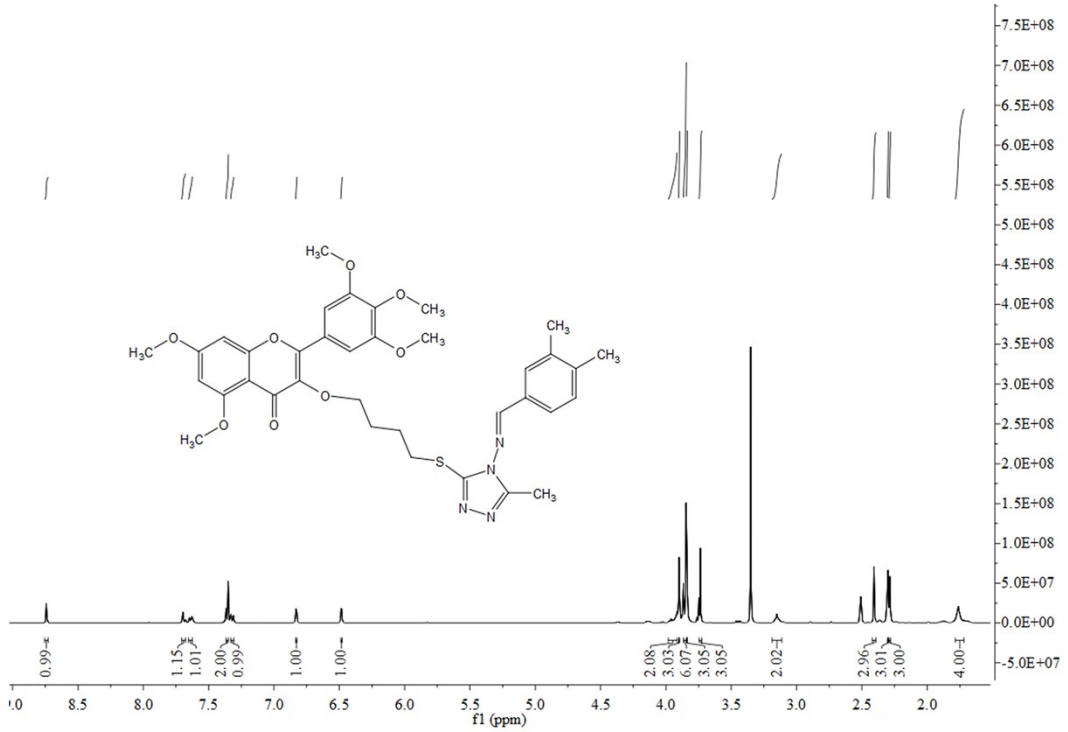


Figure S47. ^{13}C NMR spectrum of compound **6p**

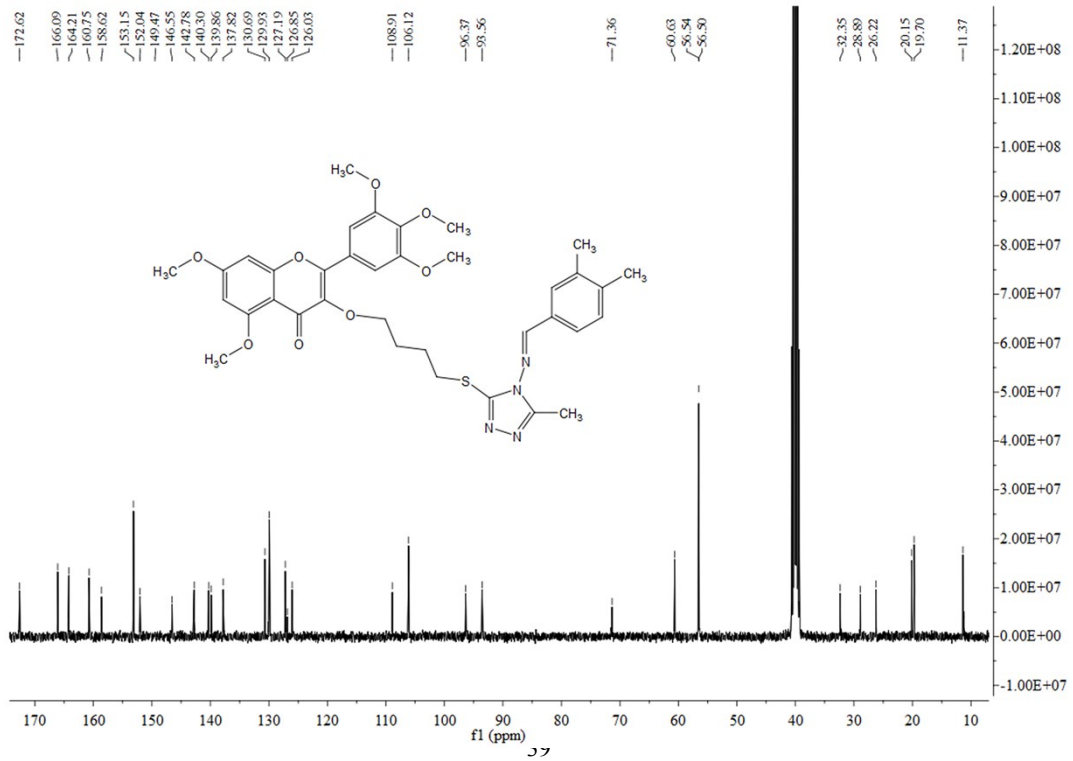


Figure S48. HRMS spectrum of compound **6p**

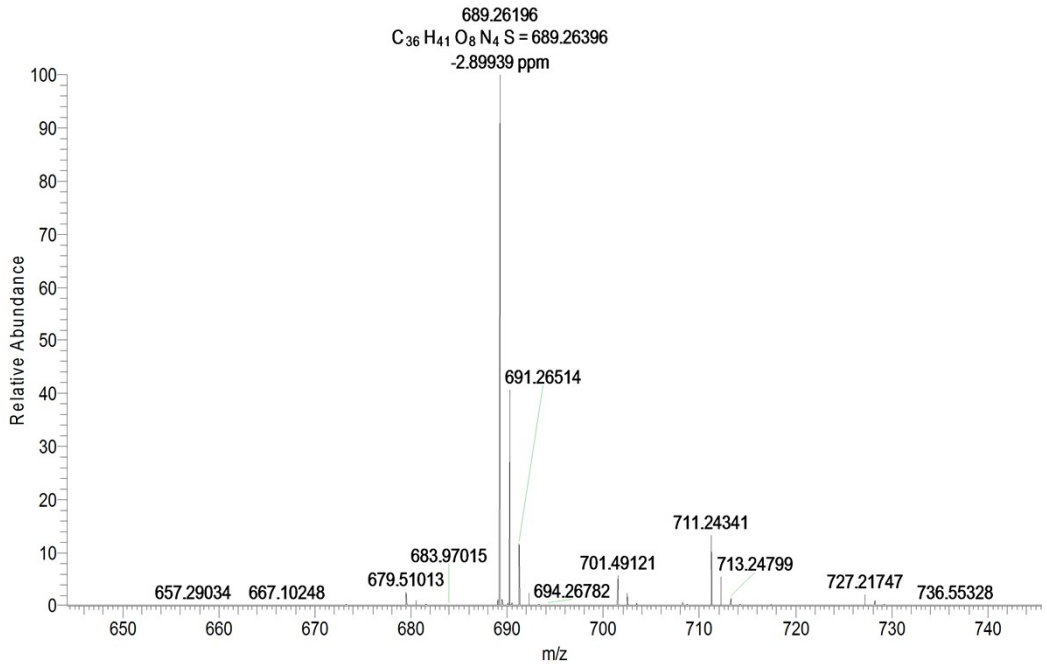


Figure S49. ^{1}H NMR spectrum of compound **6q**

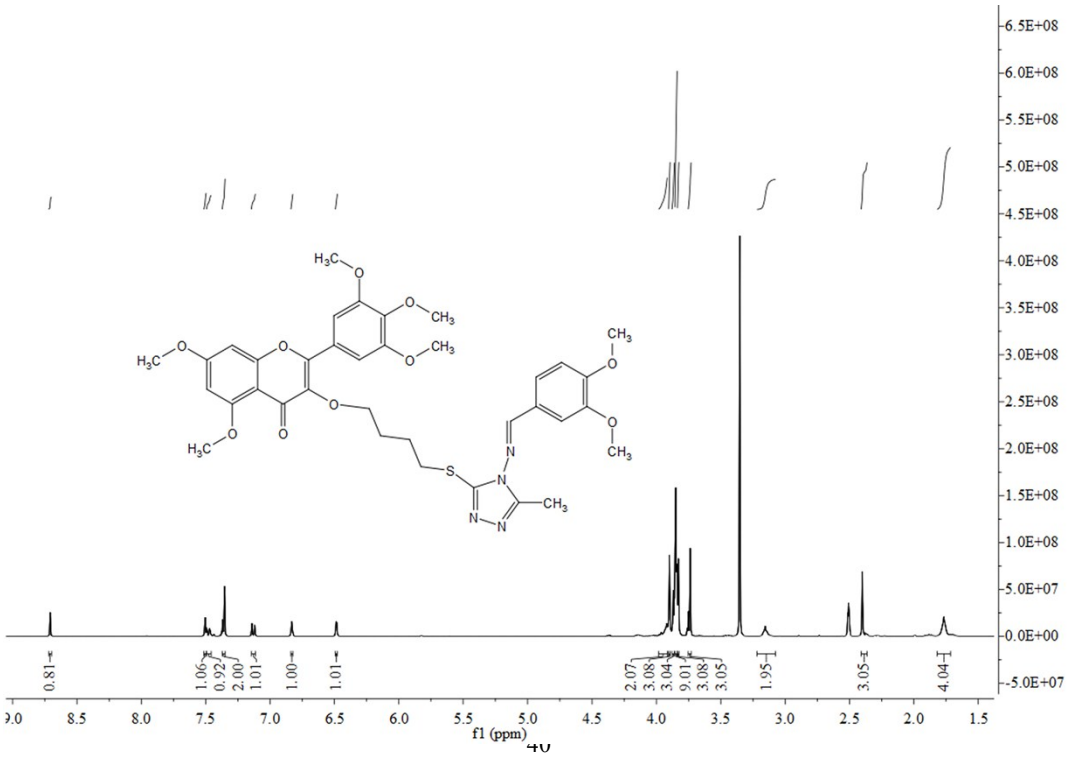


Figure S50. ^{13}C NMR spectrum of compound **6q**

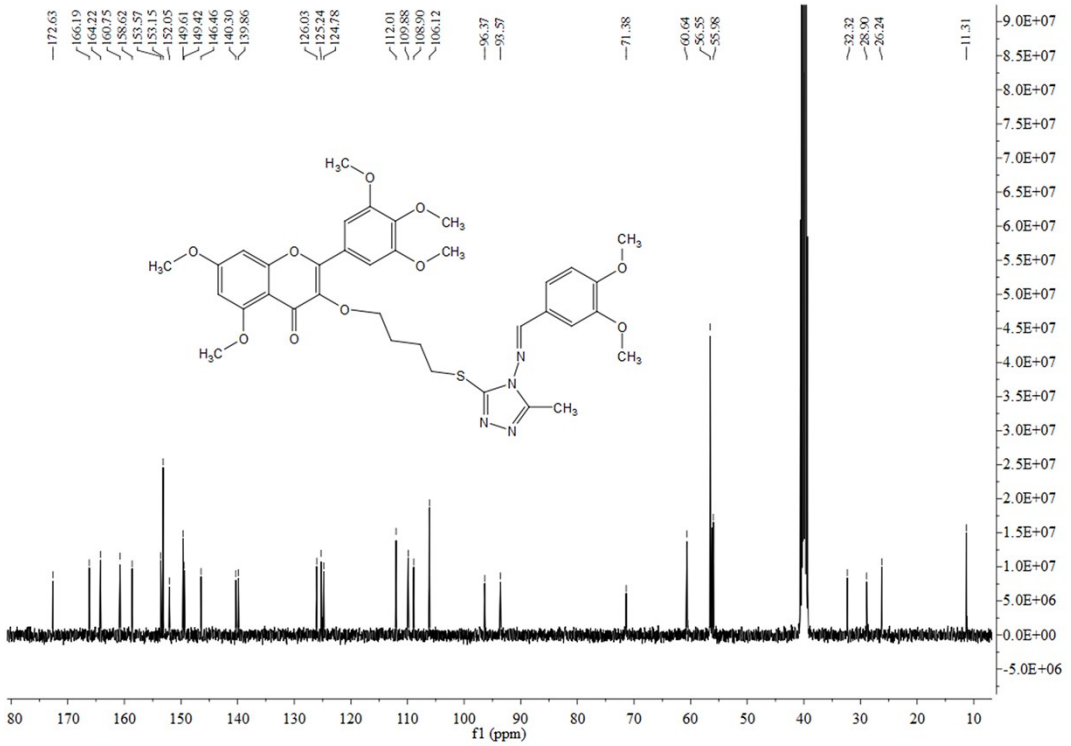


Figure S51. HRMS spectrum of compound **6q**

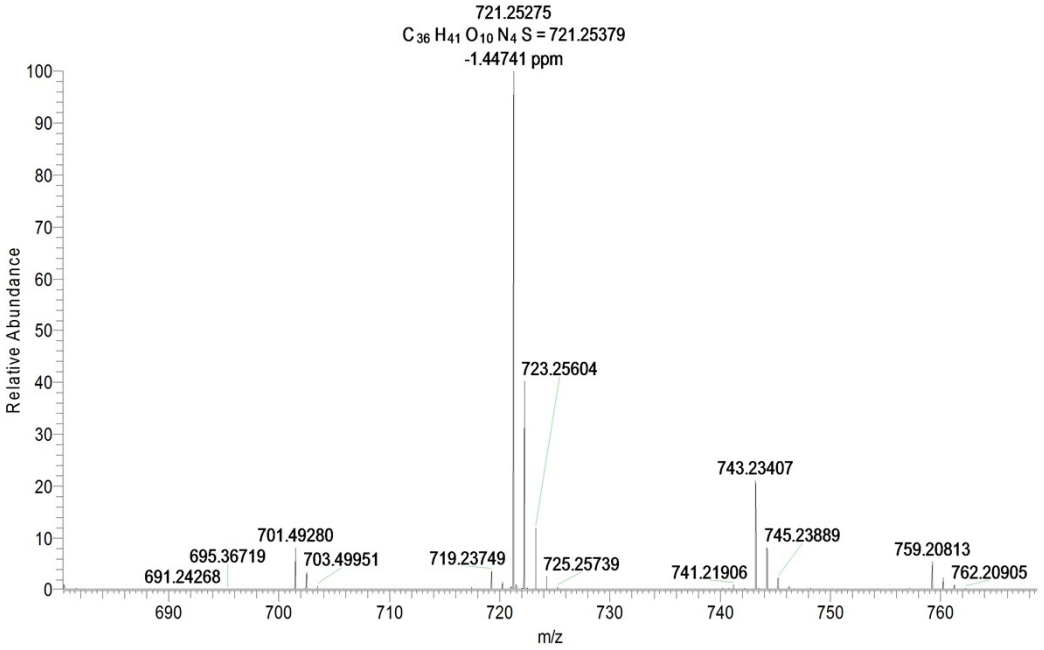


Figure S52. ^{1}H NMR spectrum of compound **6r**

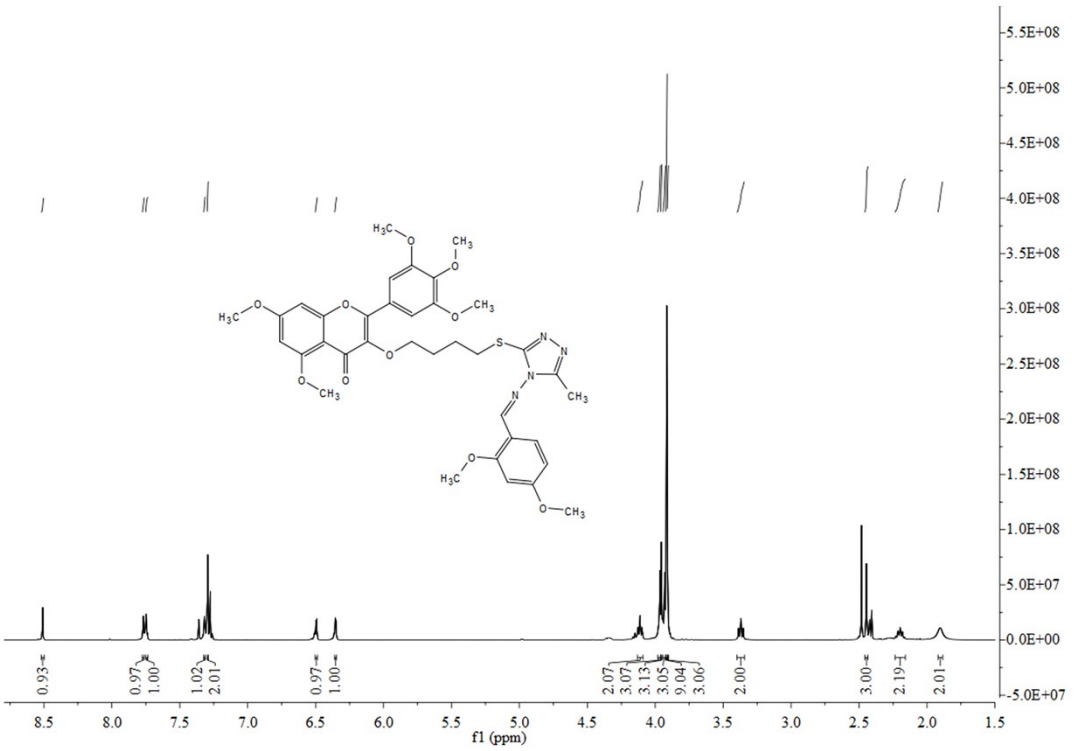


Figure S53. ^{13}C NMR spectrum of compound **6r**

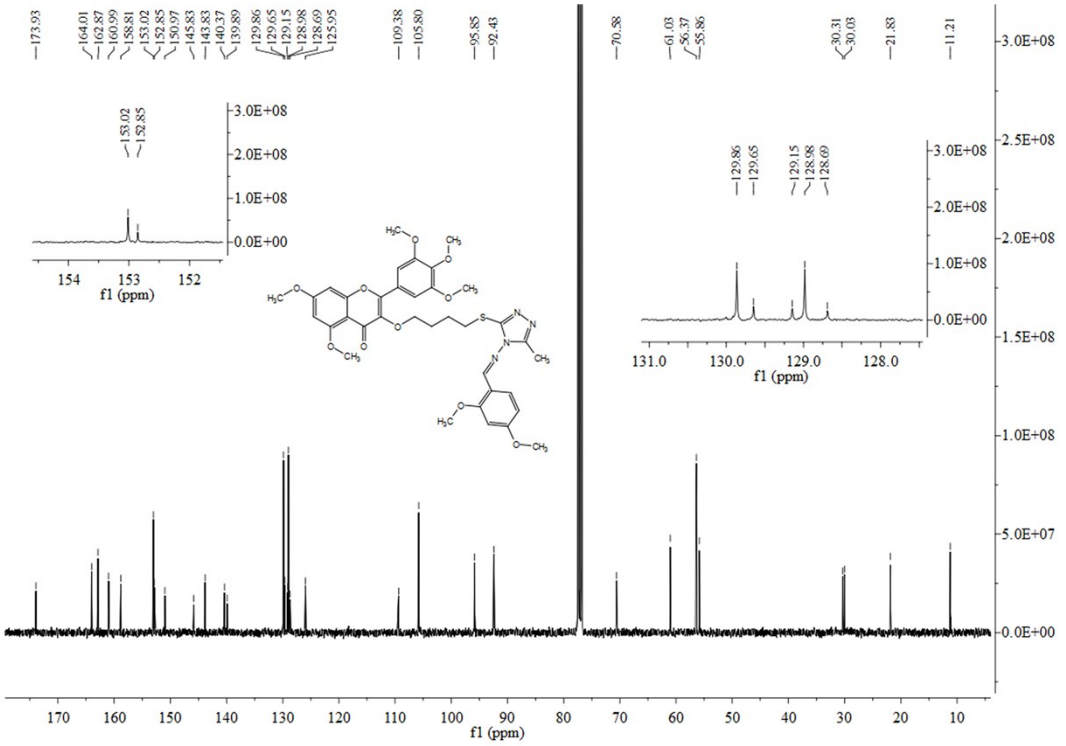


Figure S54. HRMS spectrum of compound **6r**

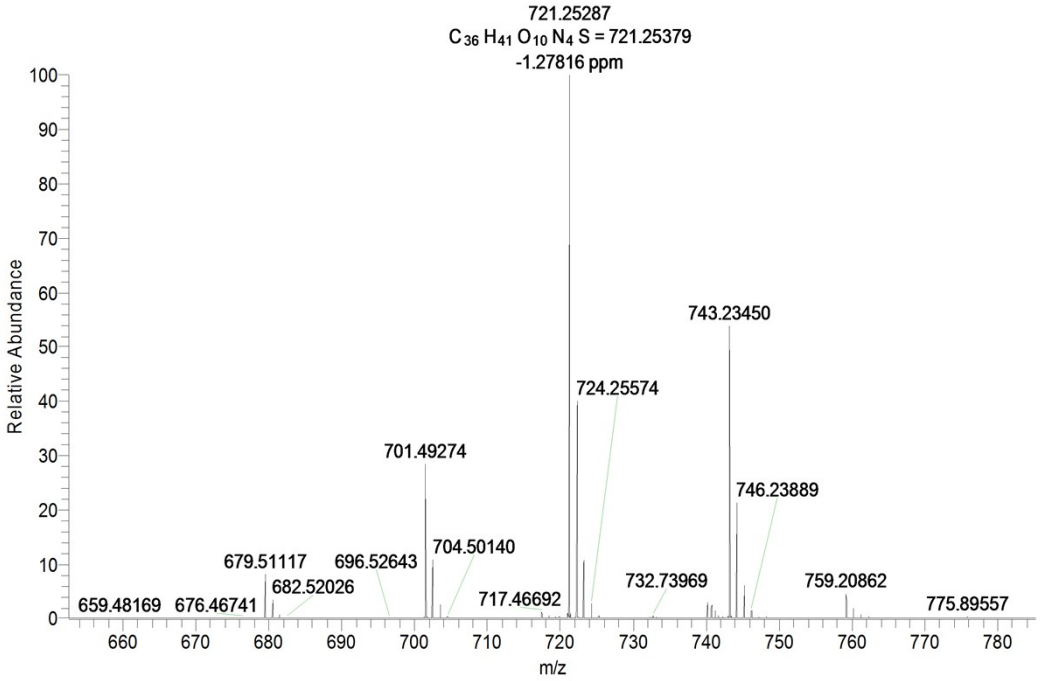


Figure S55. ^{1}H NMR spectrum of compound **6s**

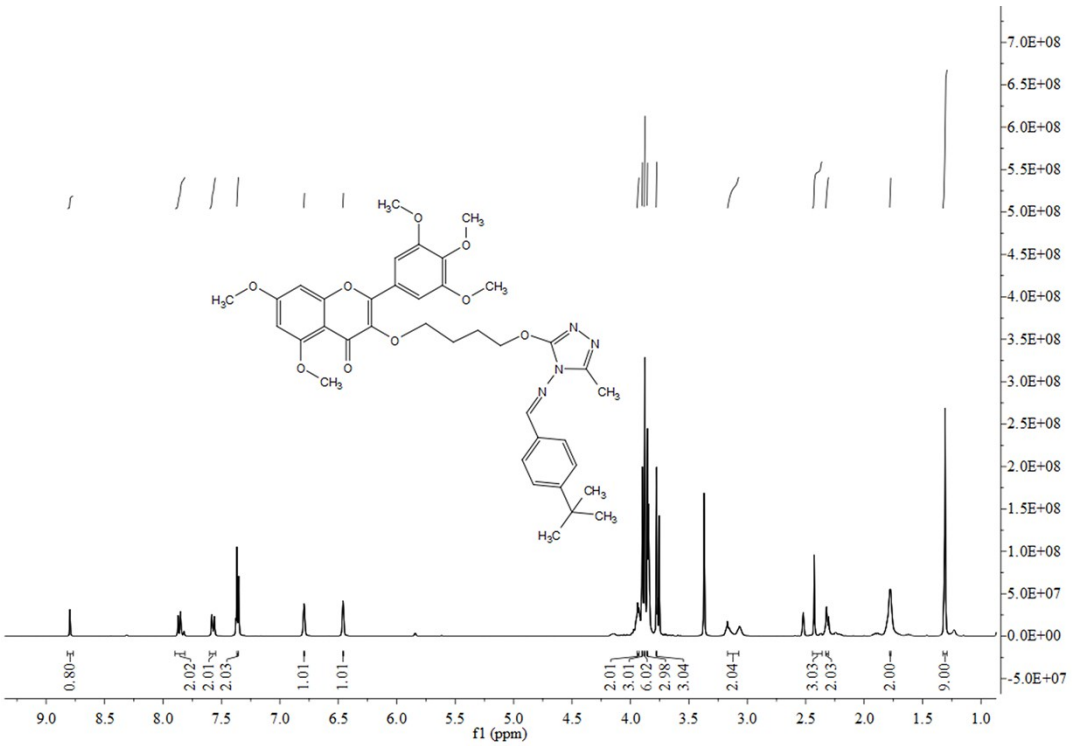


Figure S56. ^{13}C NMR spectrum of compound **6s**

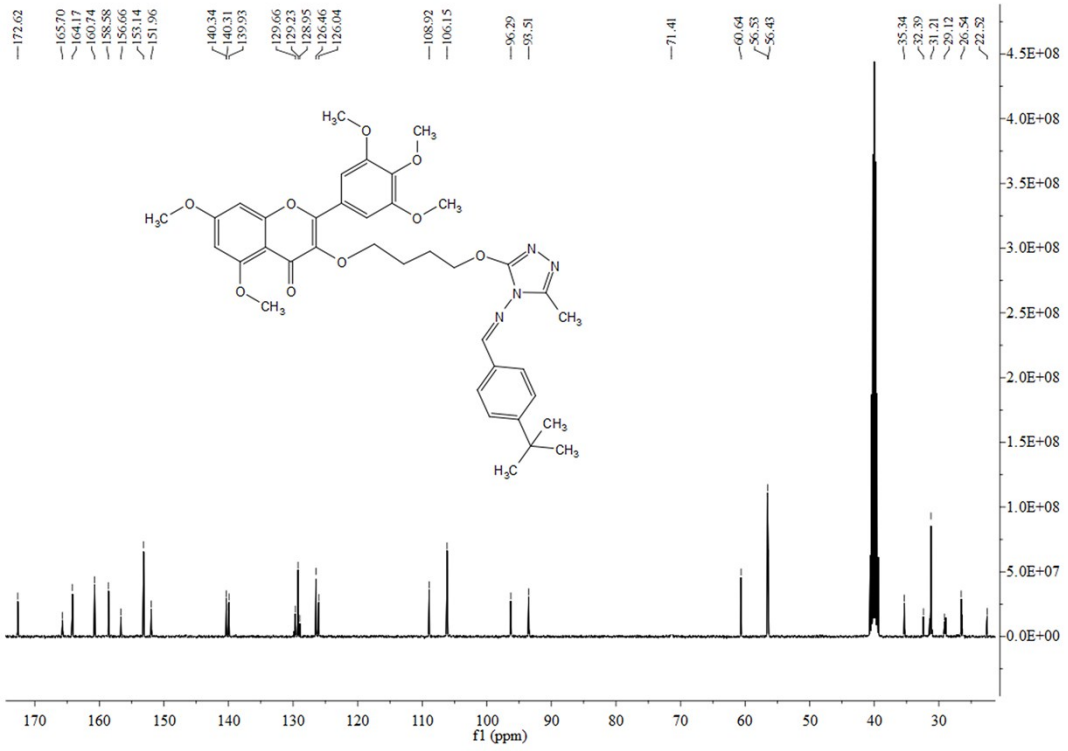


Figure S57. HRMS spectrum of compound **6s**

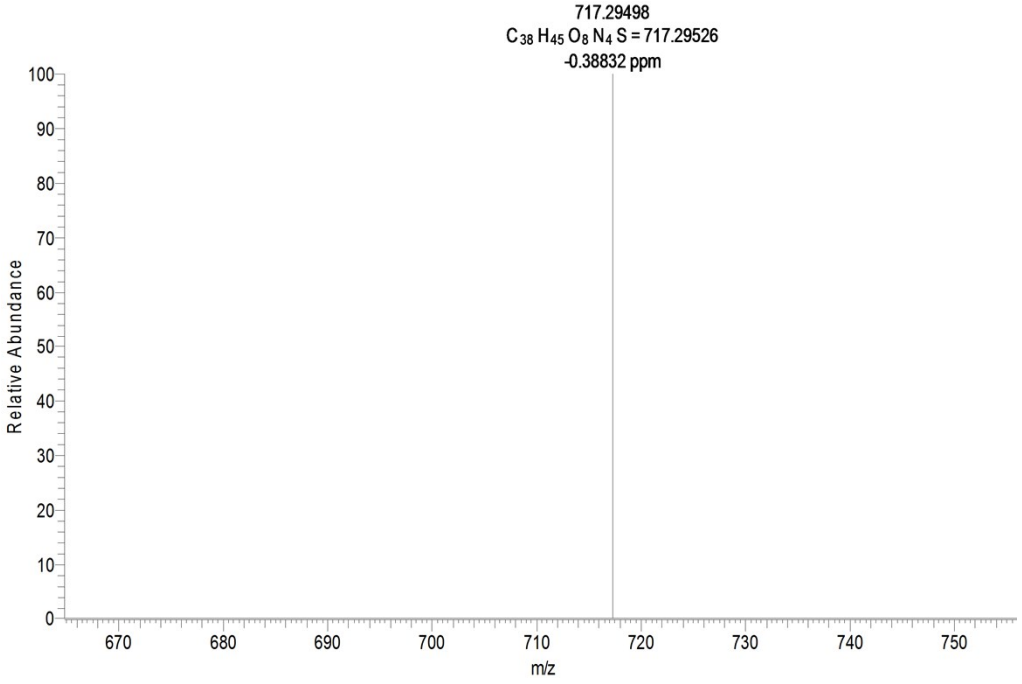


Figure S58. ^{1}H NMR spectrum of compound **6t**

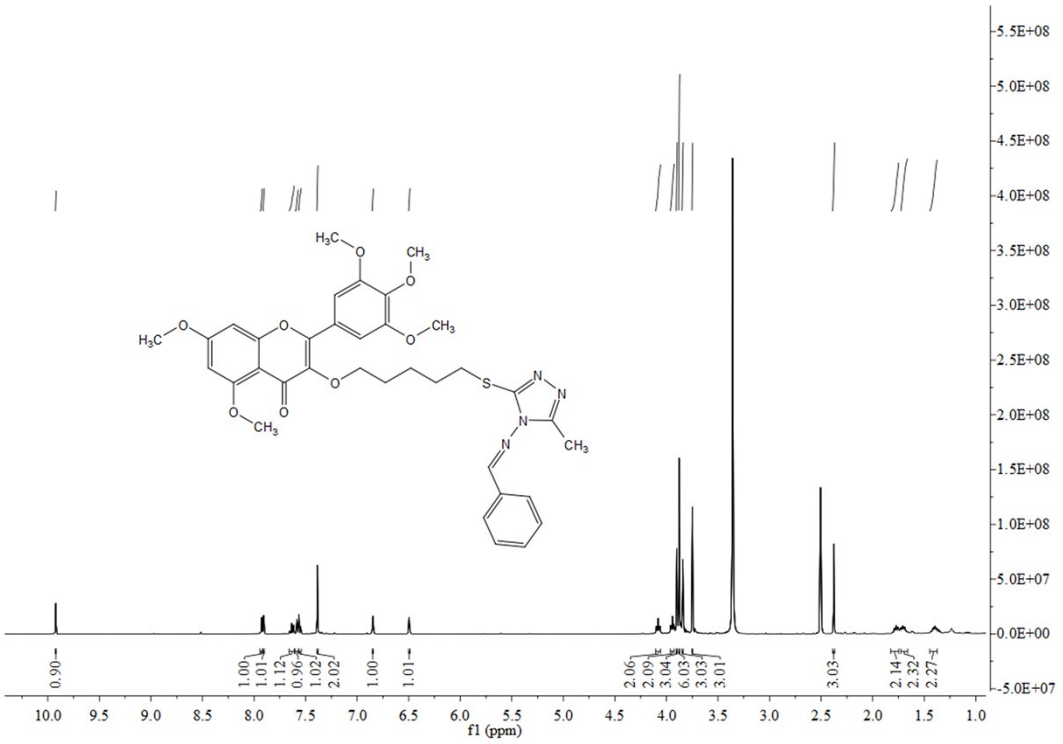


Figure S59. ^{13}C NMR spectrum of compound **6t**

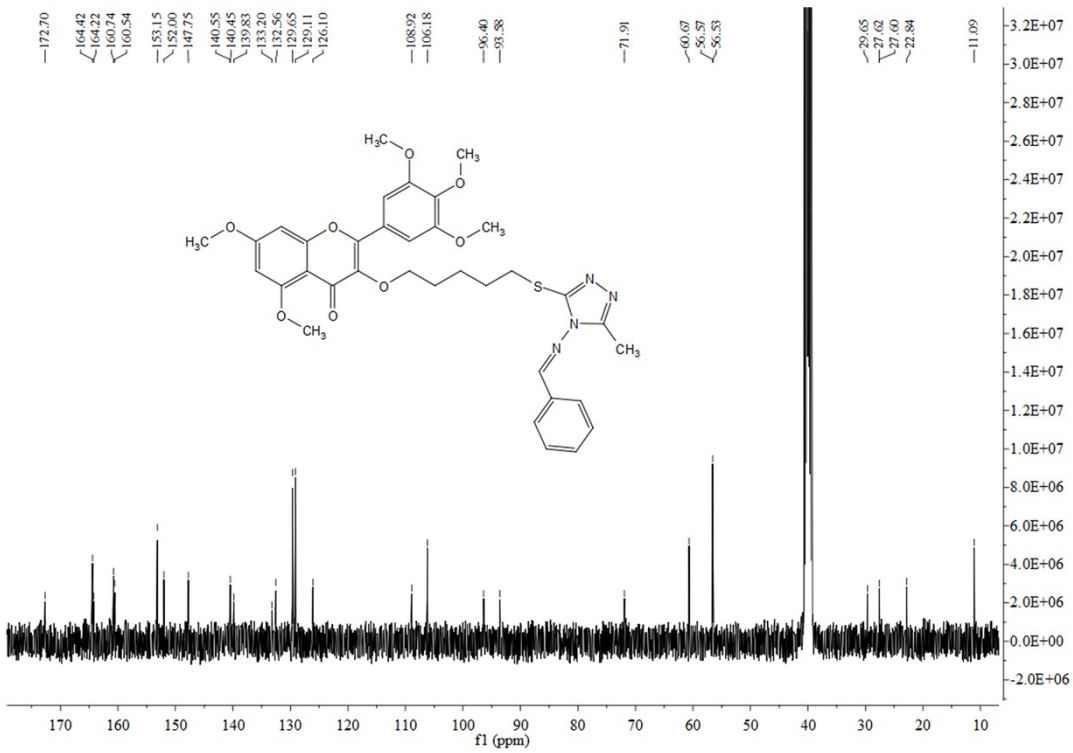


Figure S60. HRMS spectrum of compound **6t**

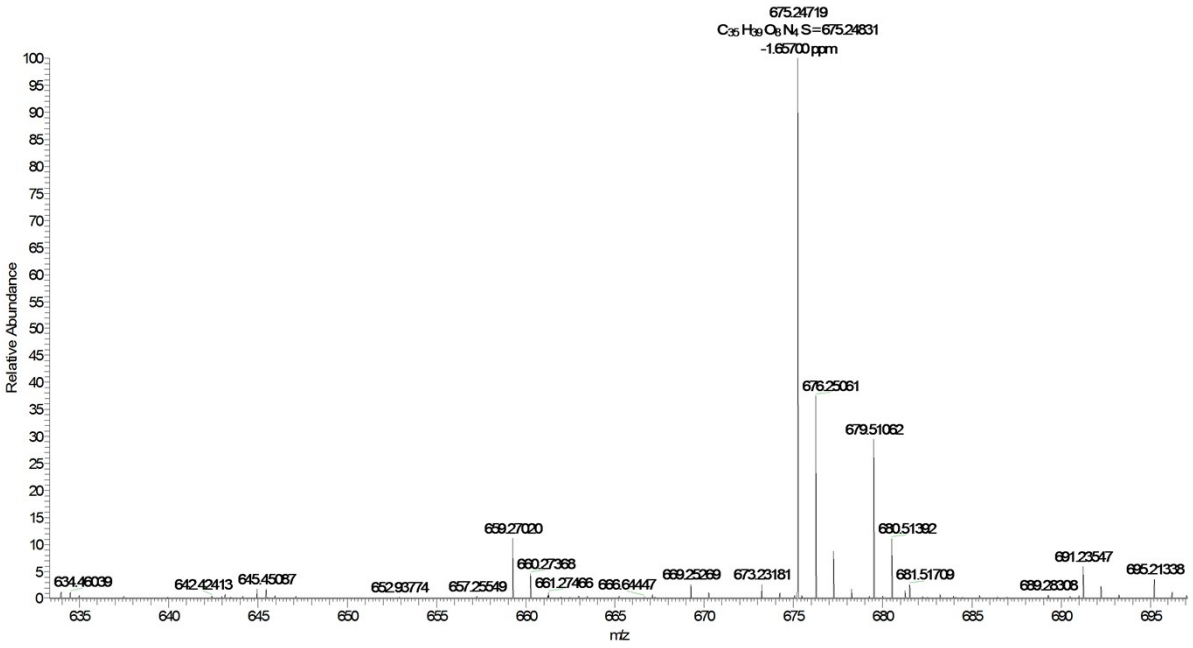


Figure S61. ^{1}H NMR spectrum of compound **6u**

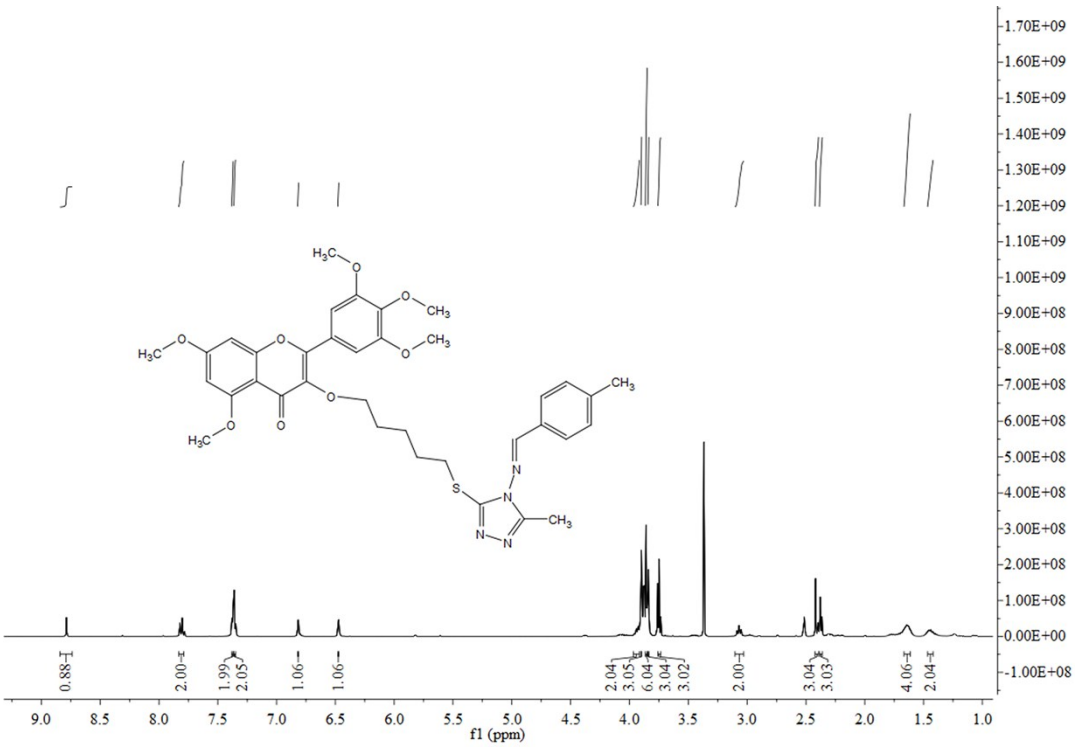


Figure S62. ^{13}C NMR spectrum of compound **6u**

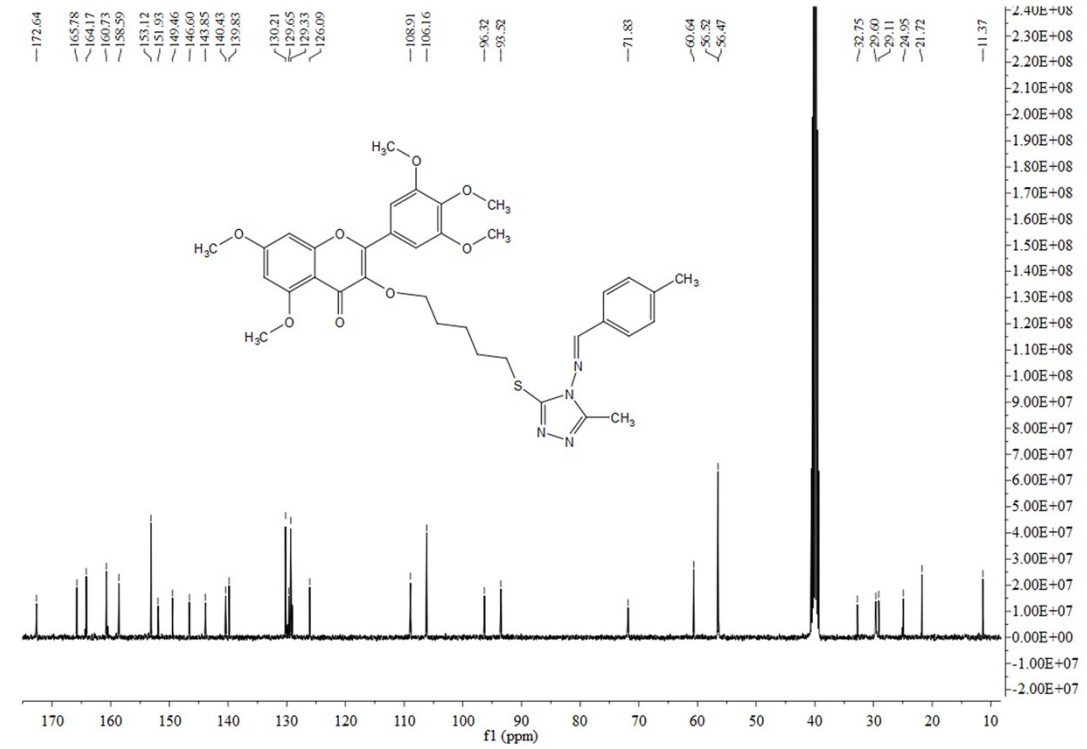


Figure S63. HRMS spectrum of compound **6u**

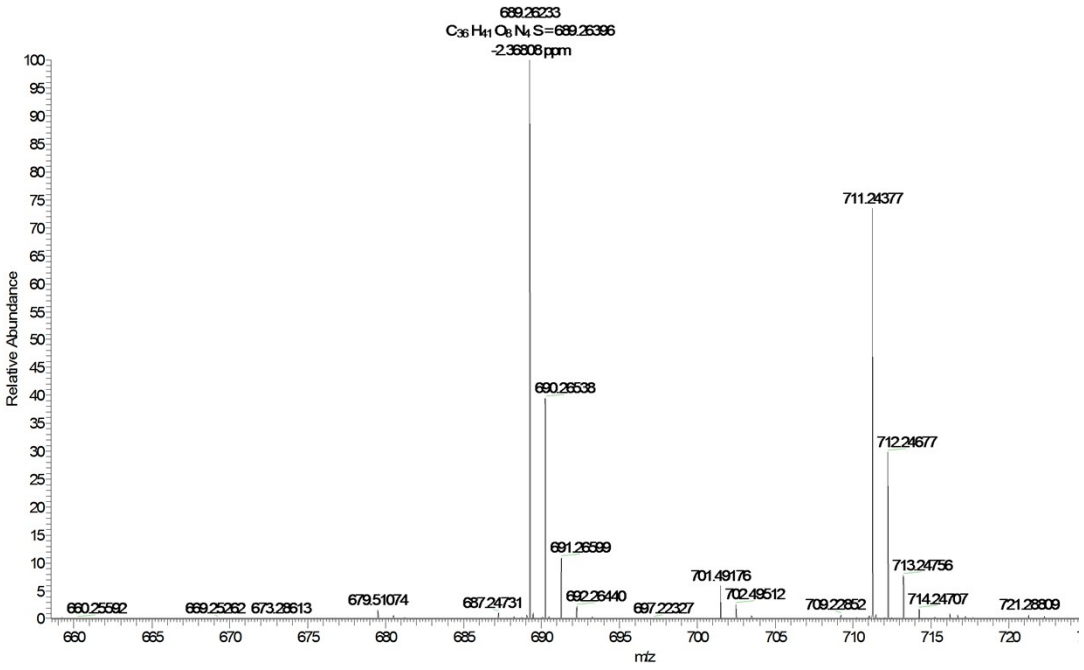


Figure S64. ^{1}H NMR spectrum of compound **6v**

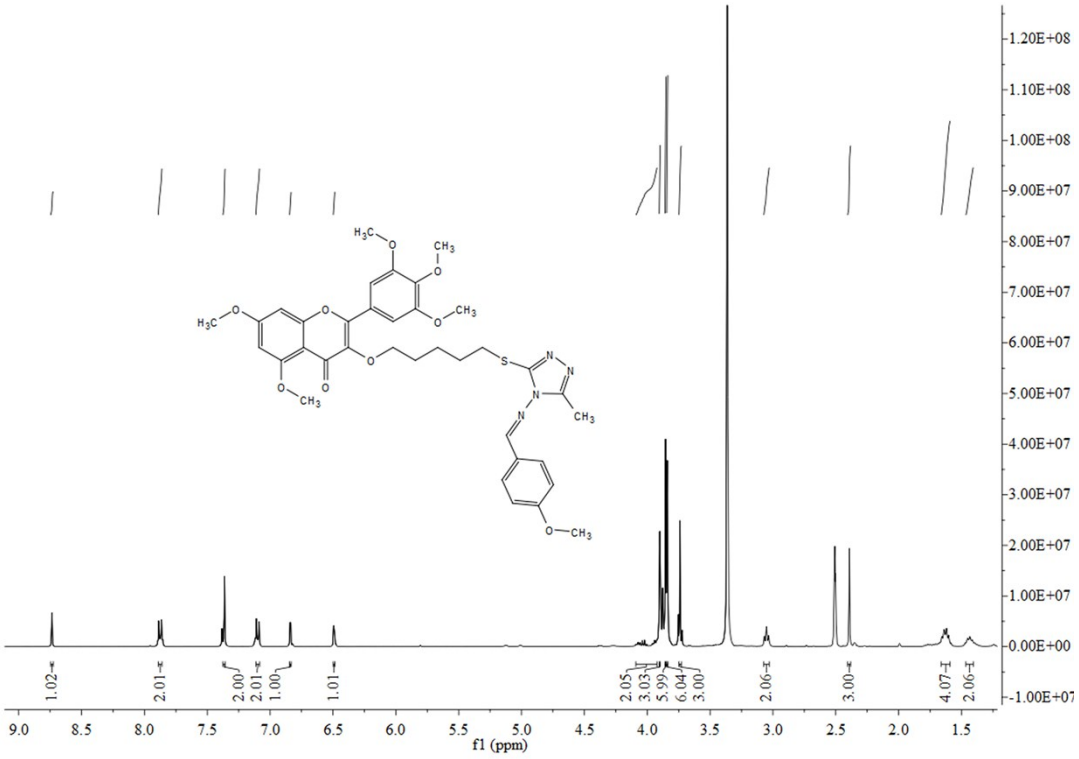


Figure S65. ^{13}C NMR spectrum of compound **6v**

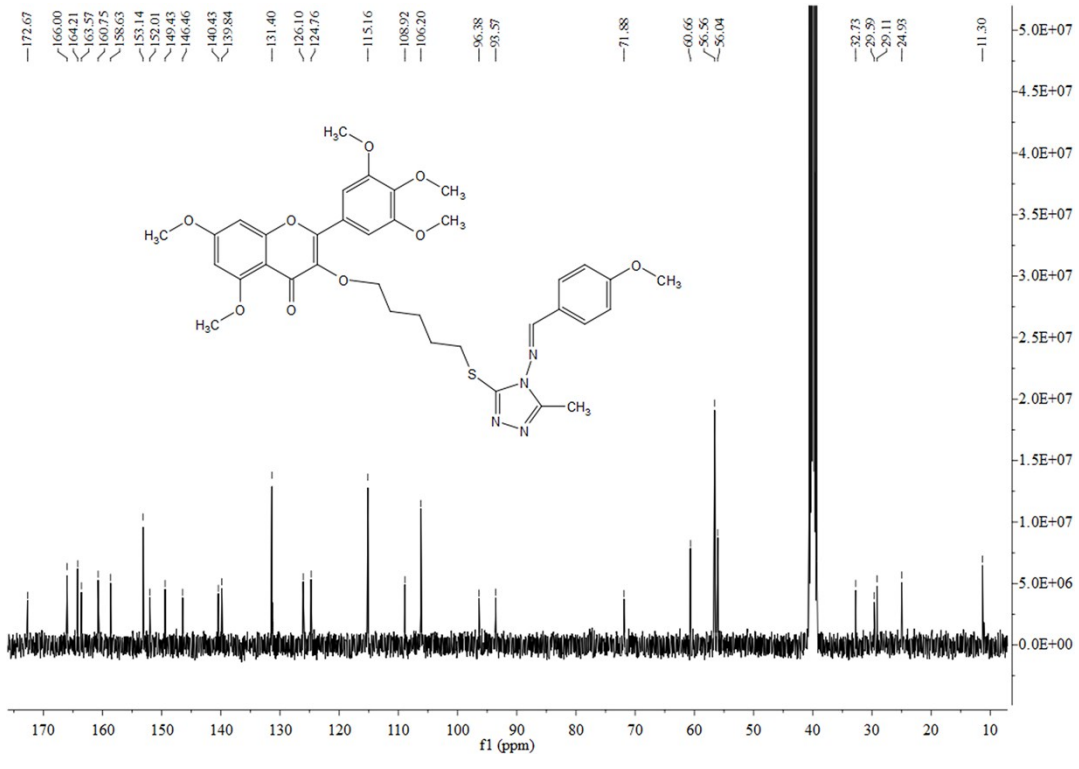


Figure S66. HRMS spectrum of compound **6v**

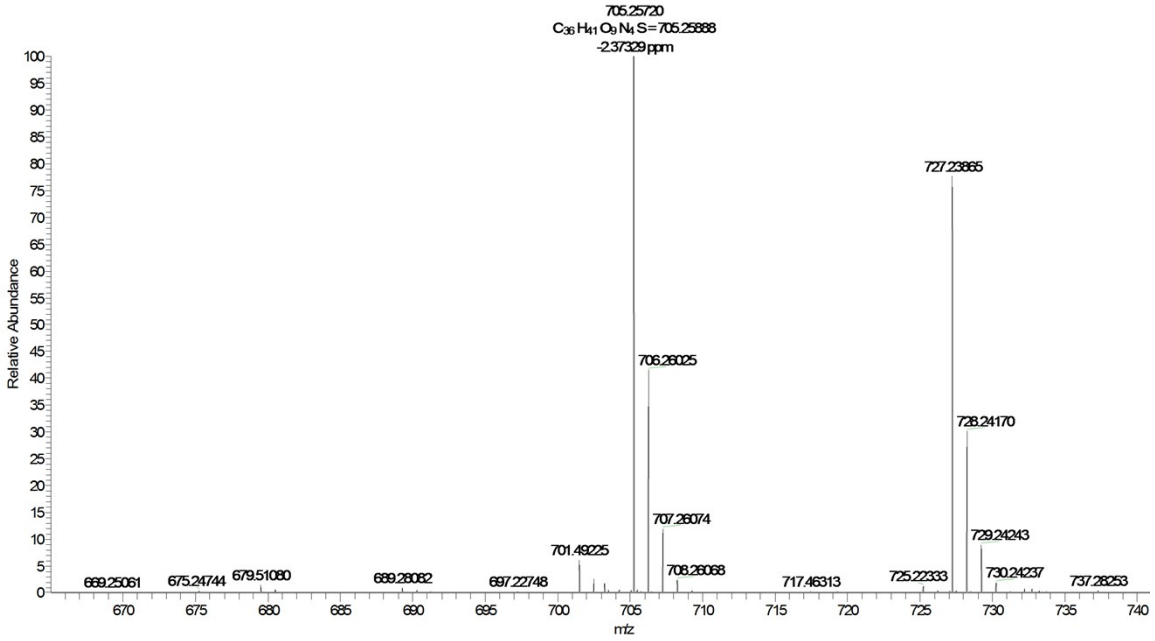


Figure S67. ^{1}H NMR spectrum of compound **6w**

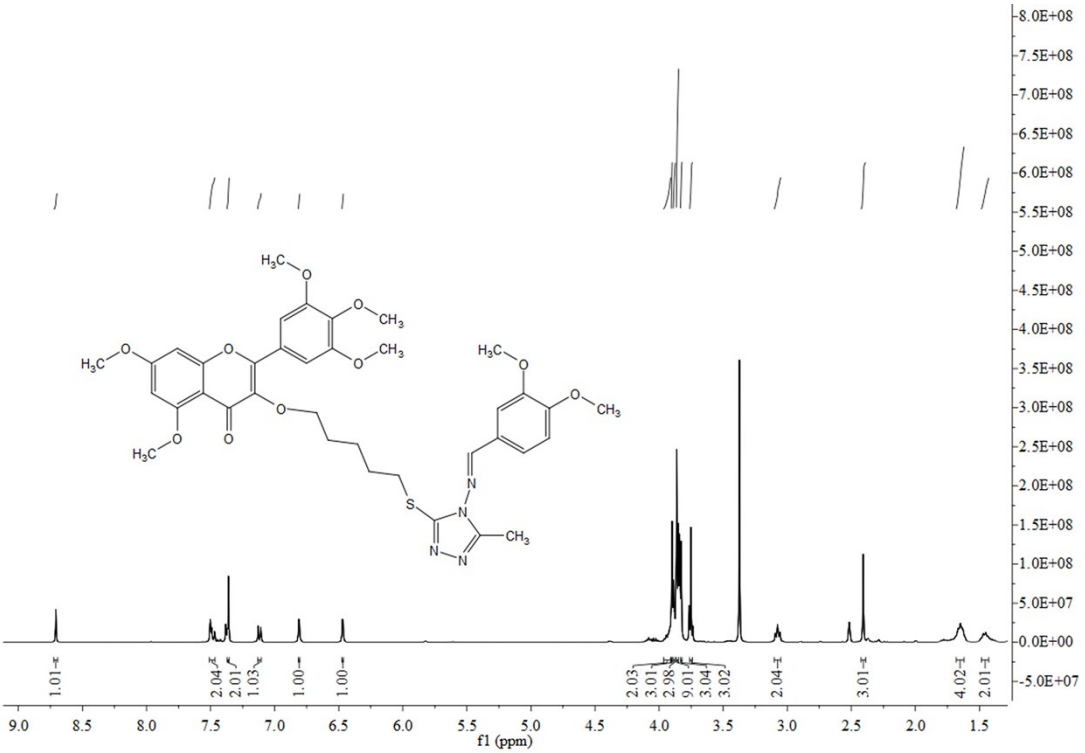


Figure S68. ^{13}C NMR spectrum of compound **6w**

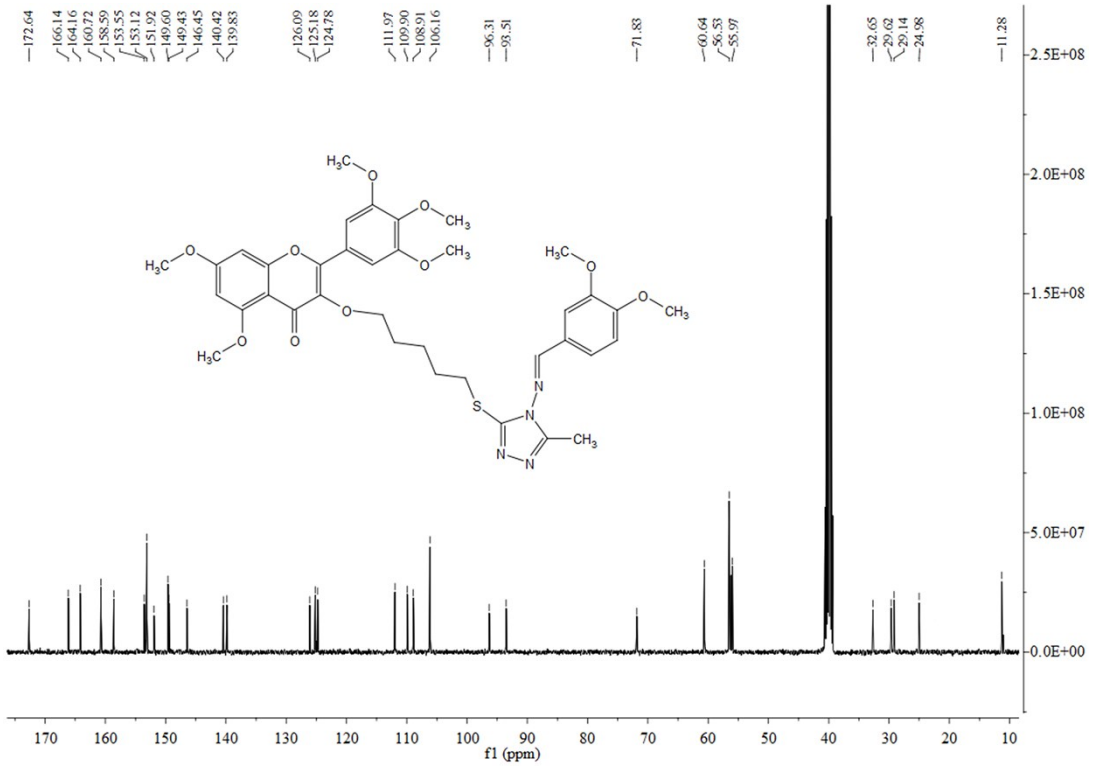


Figure S69. HRMS spectrum of compound **6w**