Supporting Information

Antioxidant, antibacterial, and cytotoxic activities of Cimemoxin derivatives and their molecular docking studies

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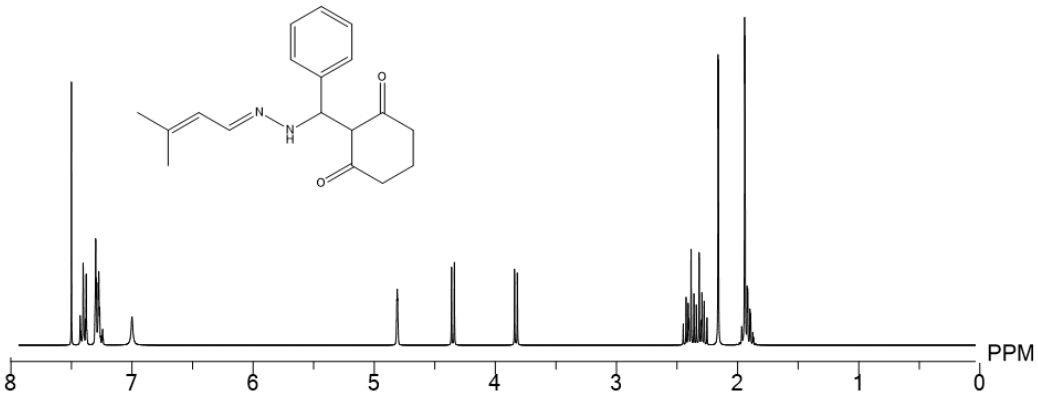


Figure S1 ^{1}H NMR spectrum of the compound **1a**

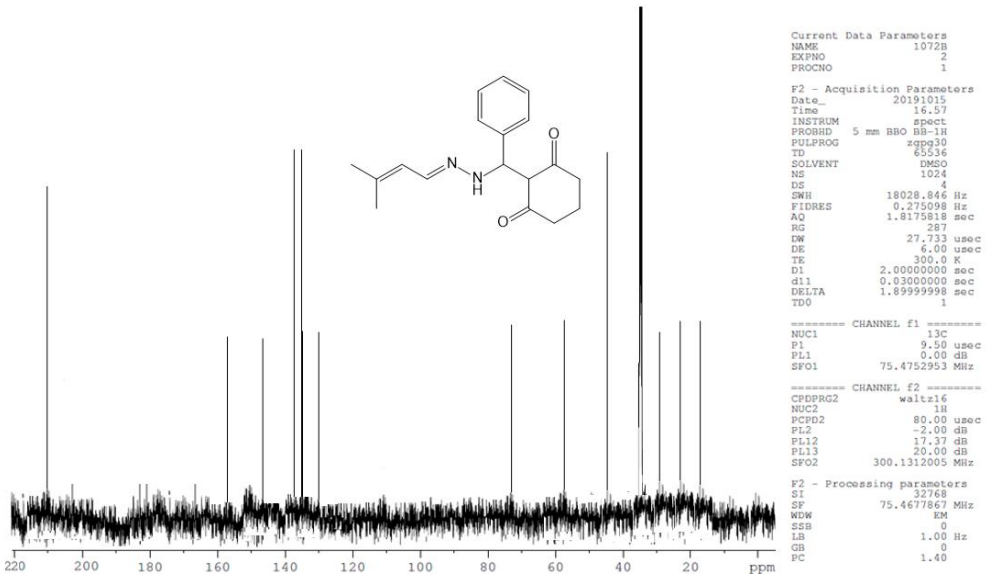


Figure S2 ^{13}C NMR spectrum of the compound **1a**

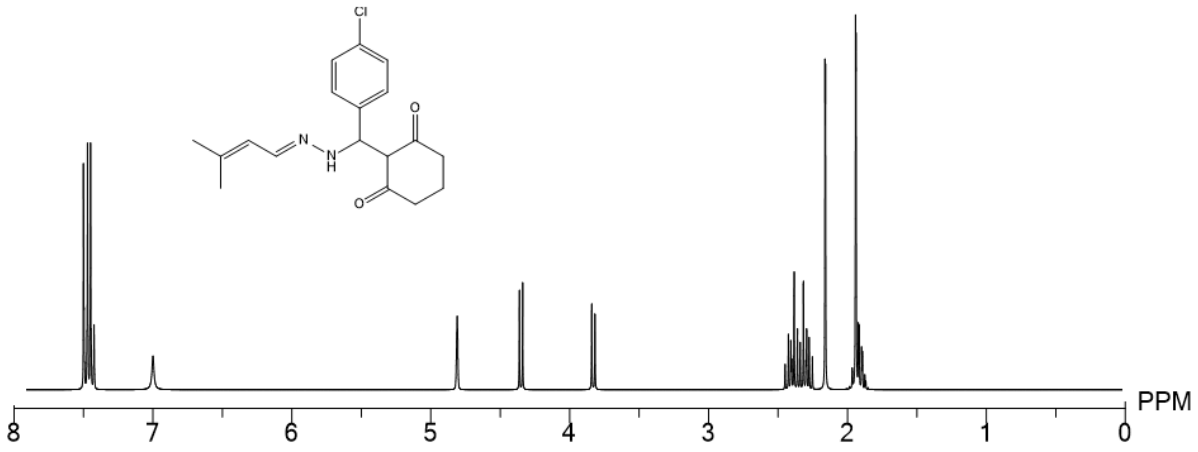


Figure S3 ^{1}H NMR spectrum of the compound **1b**

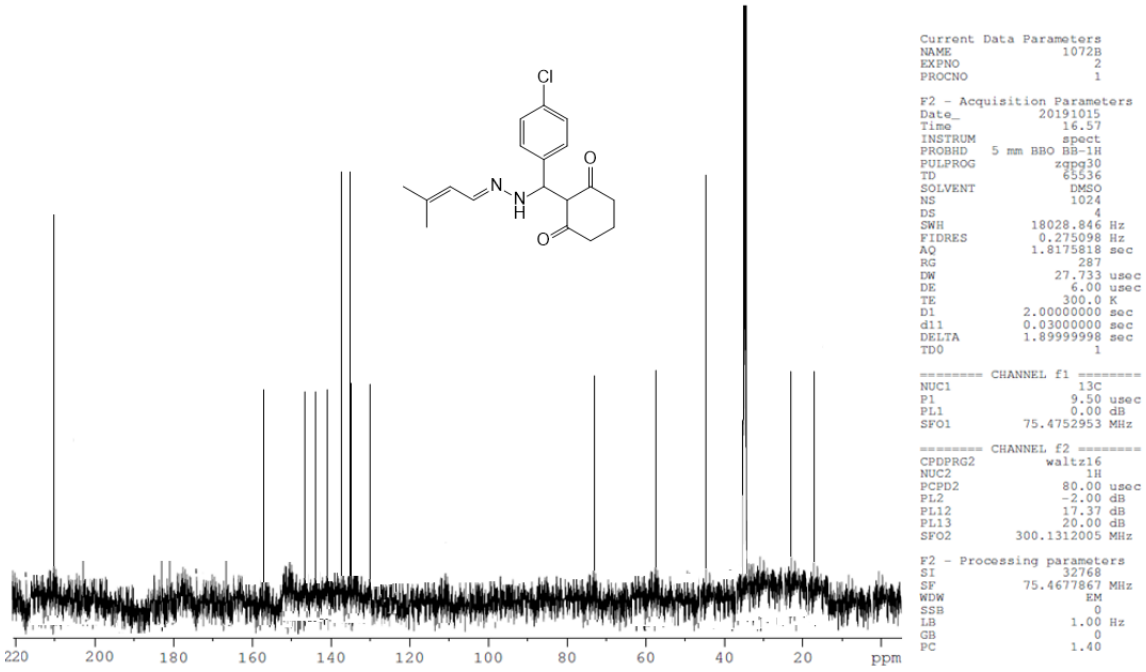


Figure S4 ^{13}C NMR spectrum of the compound **1b**

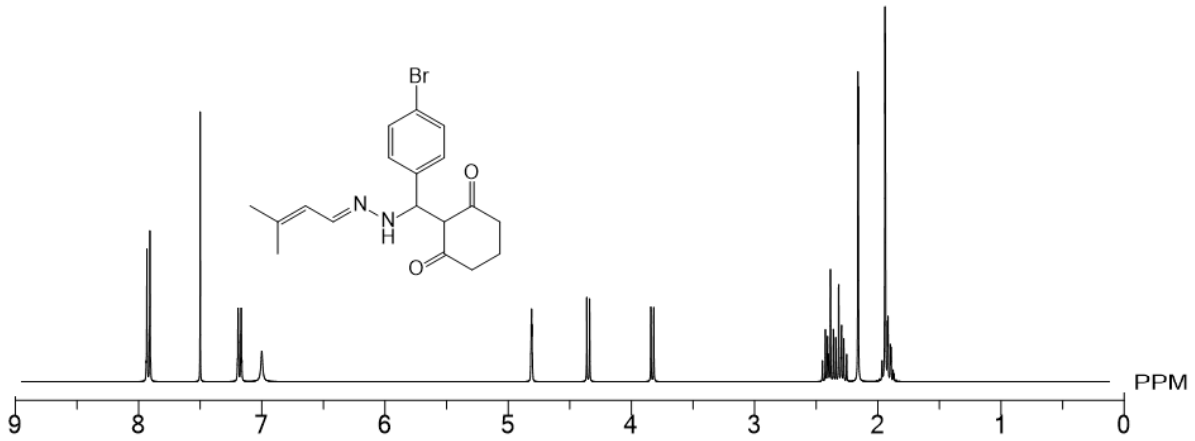


Figure S5 ^{1}H NMR spectrum of the compound **1c**

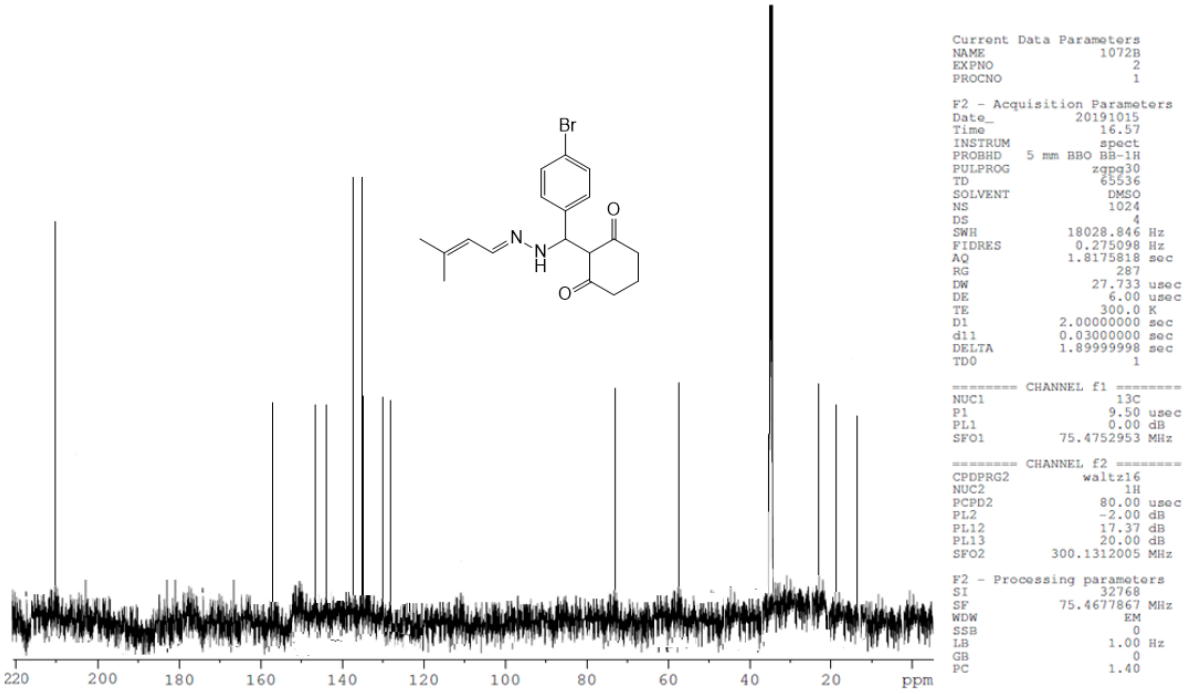


Figure S6 ^{13}C NMR spectrum of the compound **1c**

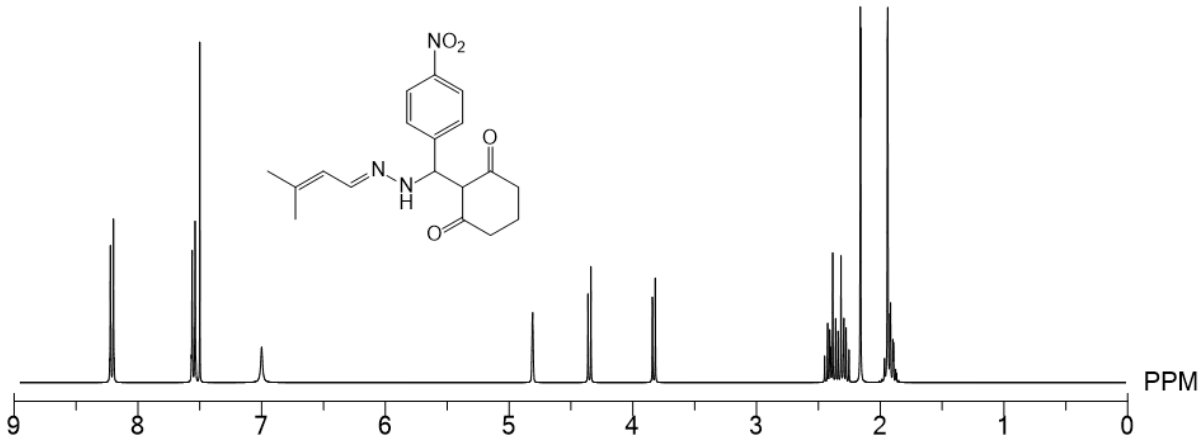


Figure S7 ^{1}H NMR spectrum of the compound **1d**

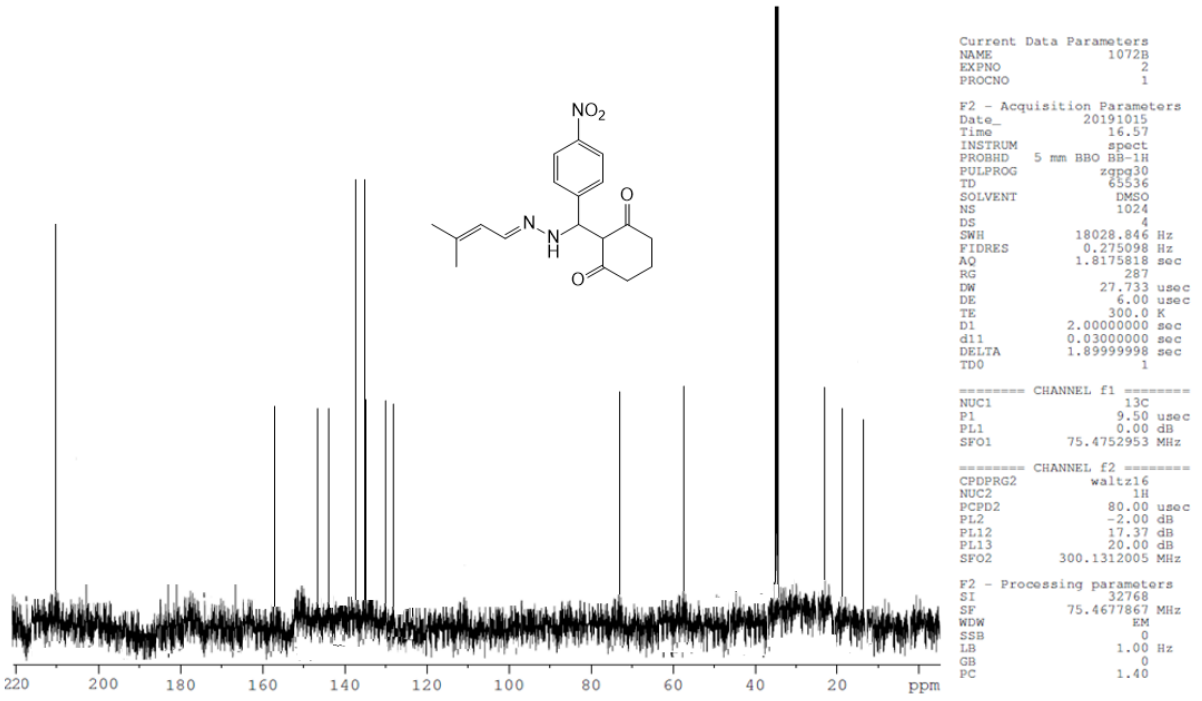


Figure S8 ^{13}C NMR spectrum of the compound **1d**

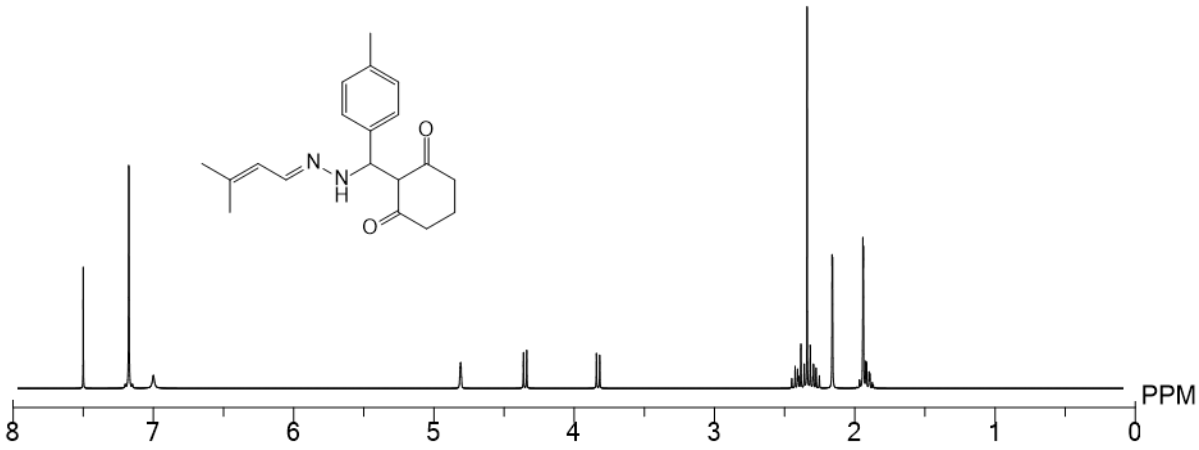


Figure S9 [1]H NMR spectrum of the compound **1e**

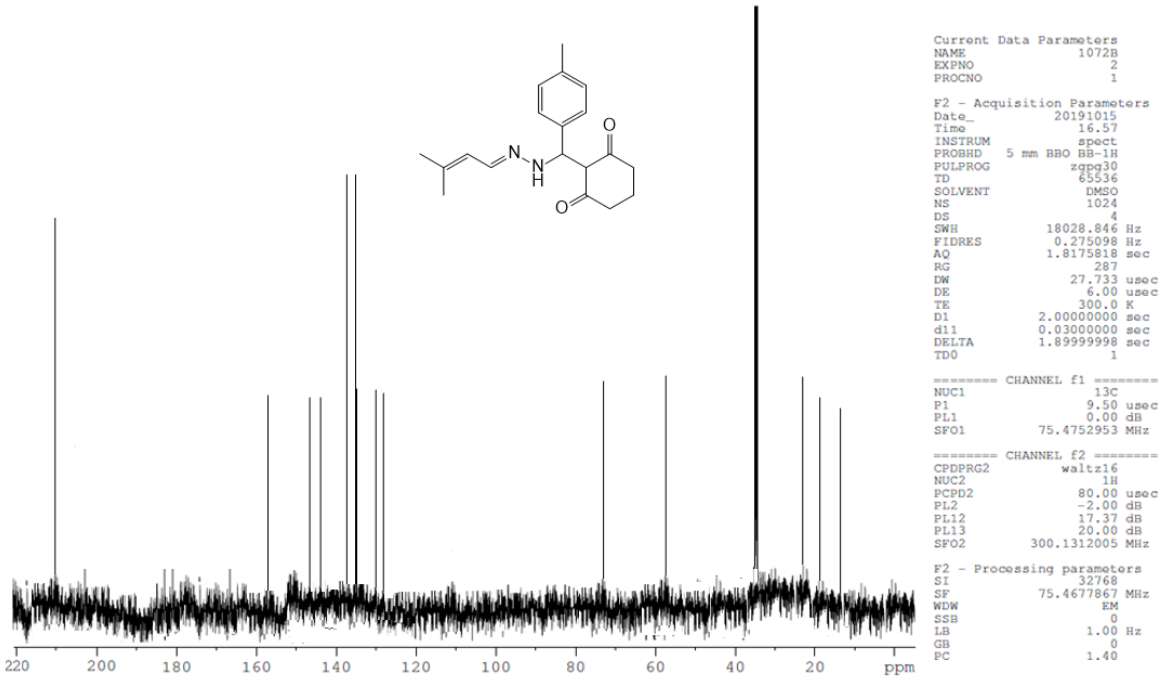


Figure S10 [13]C NMR spectrum of the compound **1e**

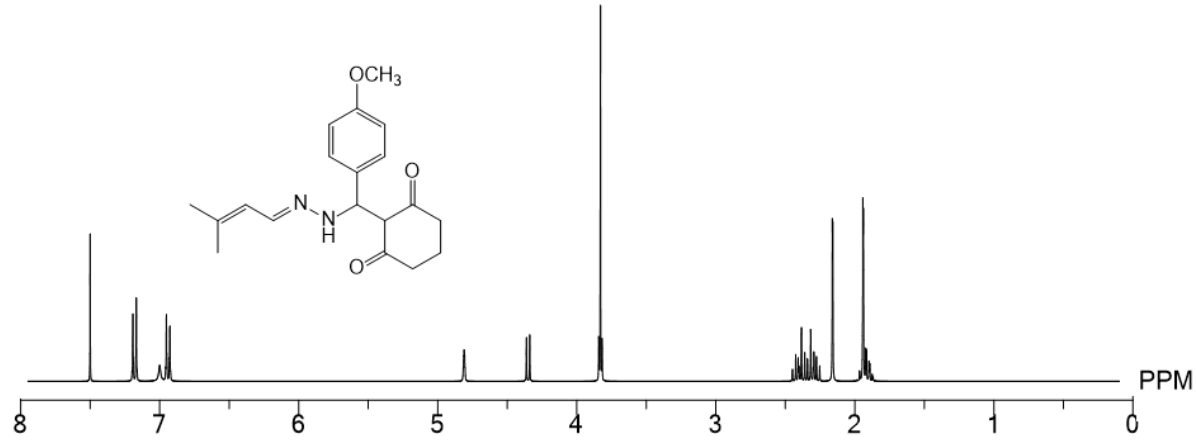


Figure S11 ^{1}H NMR spectrum of the compound **1f**

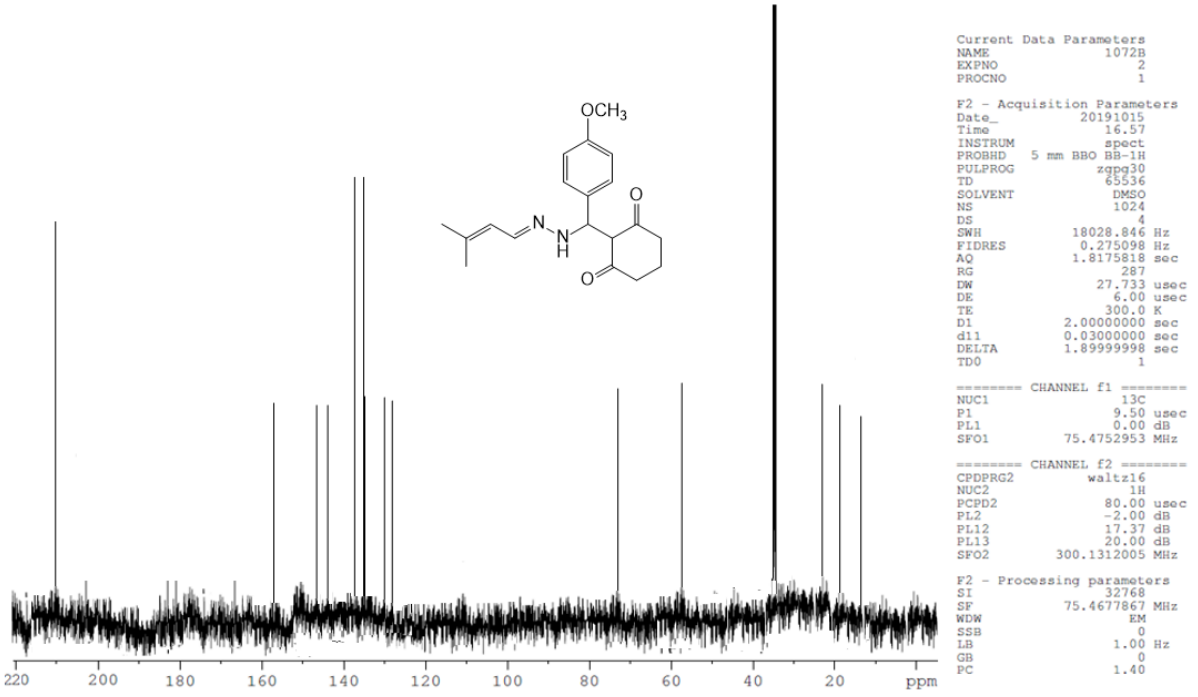


Figure S12 ^{13}C NMR spectrum of the compound **1f**

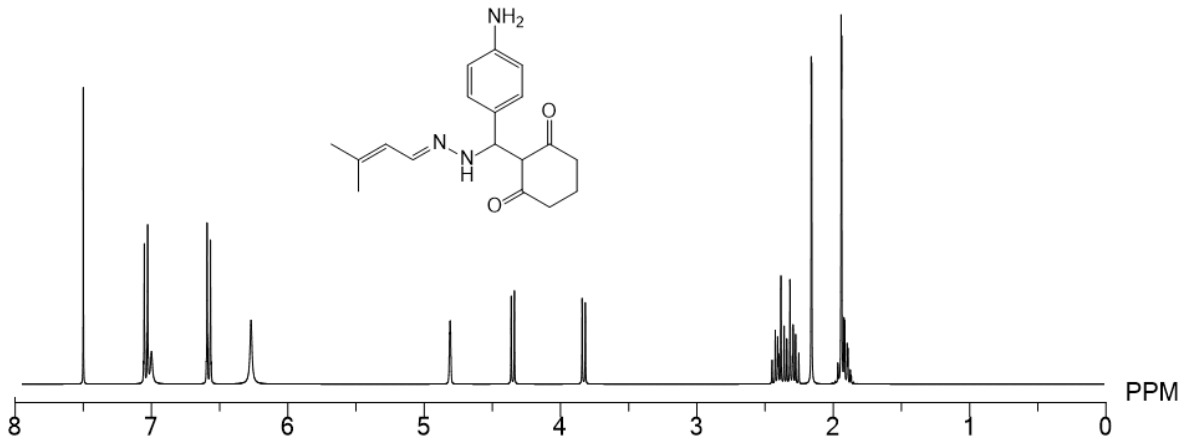


Figure S13 ^{1}H NMR spectrum of the compound **1g**

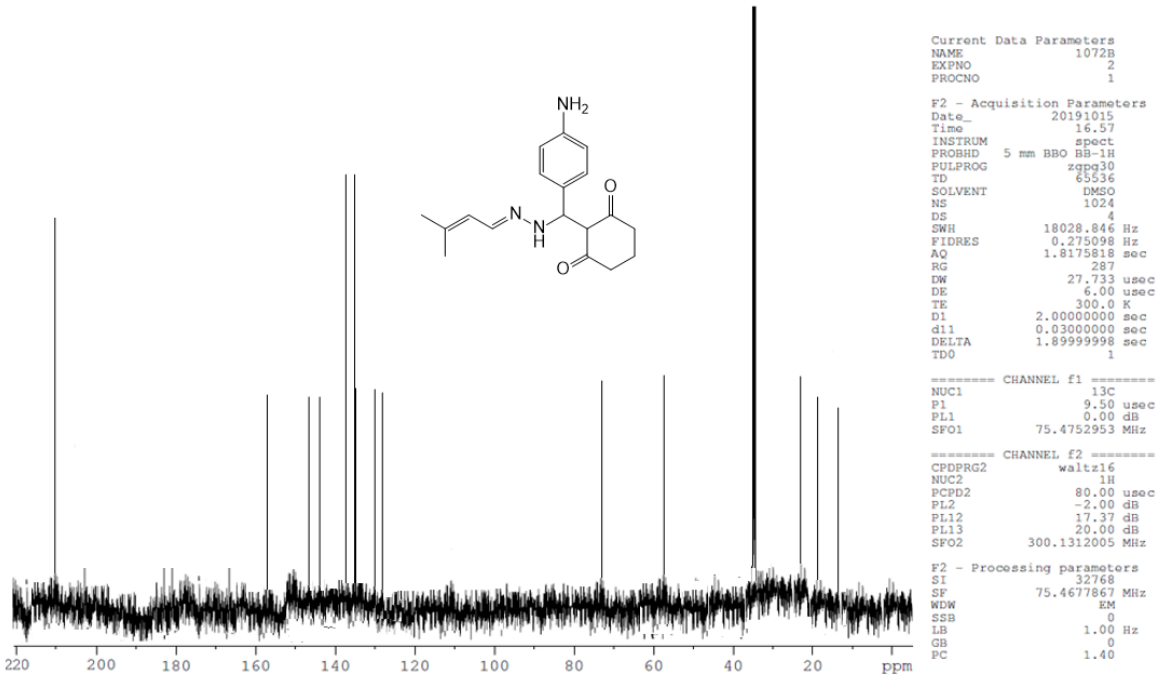


Figure S14 ^{13}C NMR spectrum of the compound **1g**

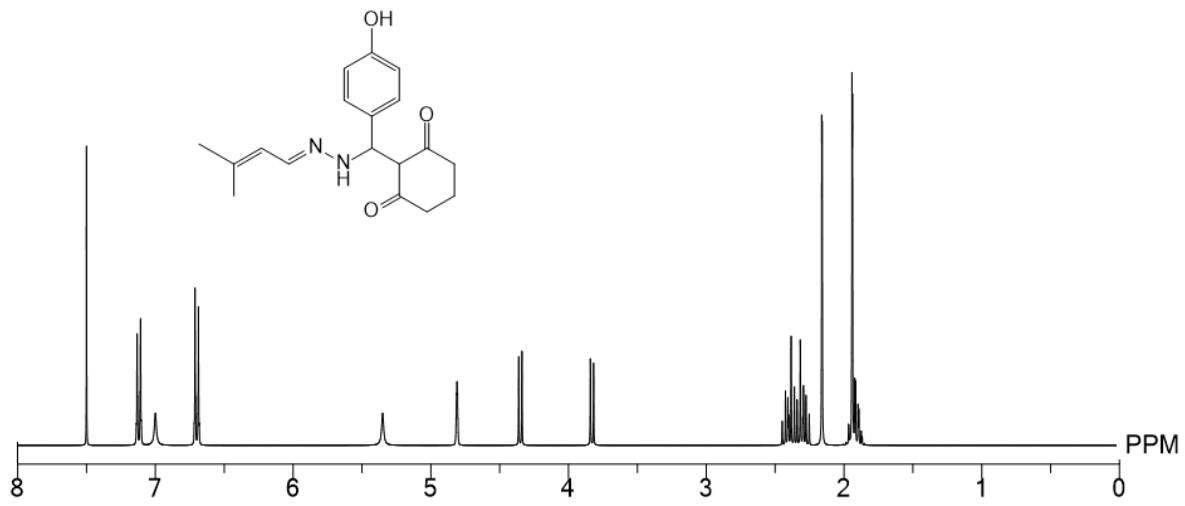


Figure S15 ^{1}H NMR spectrum of the compound **1h**

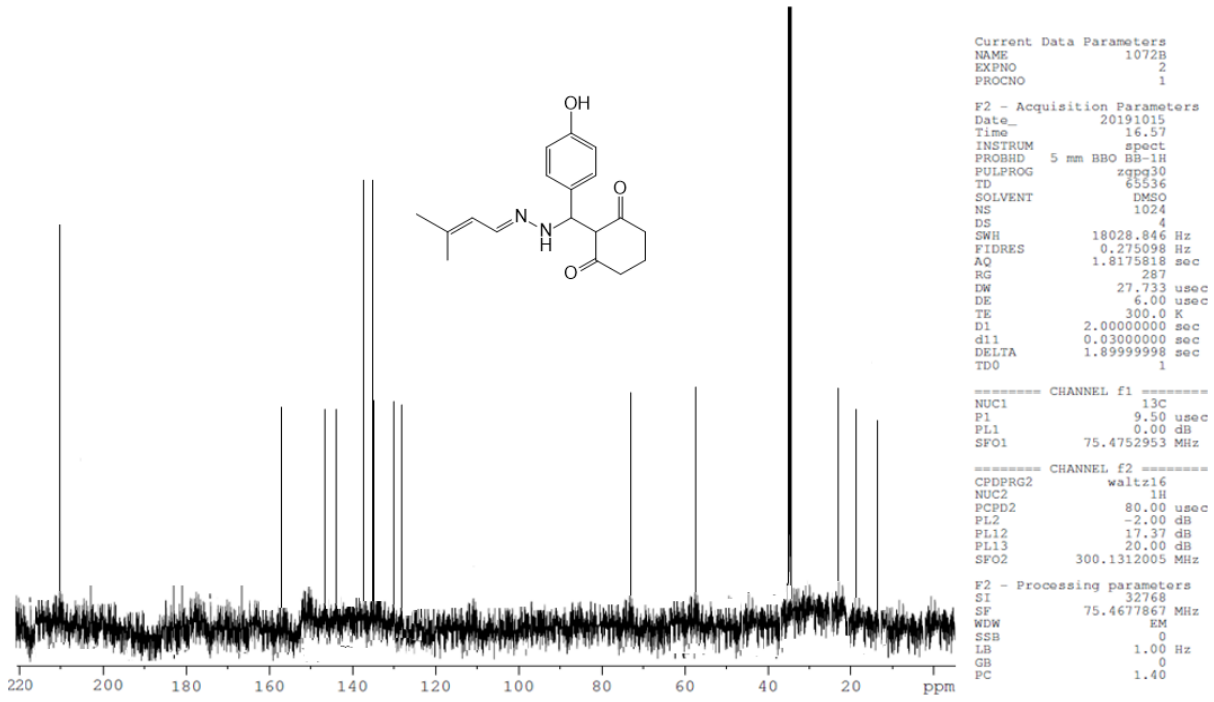


Figure S16 ^{13}C NMR spectrum of the compound **1h**

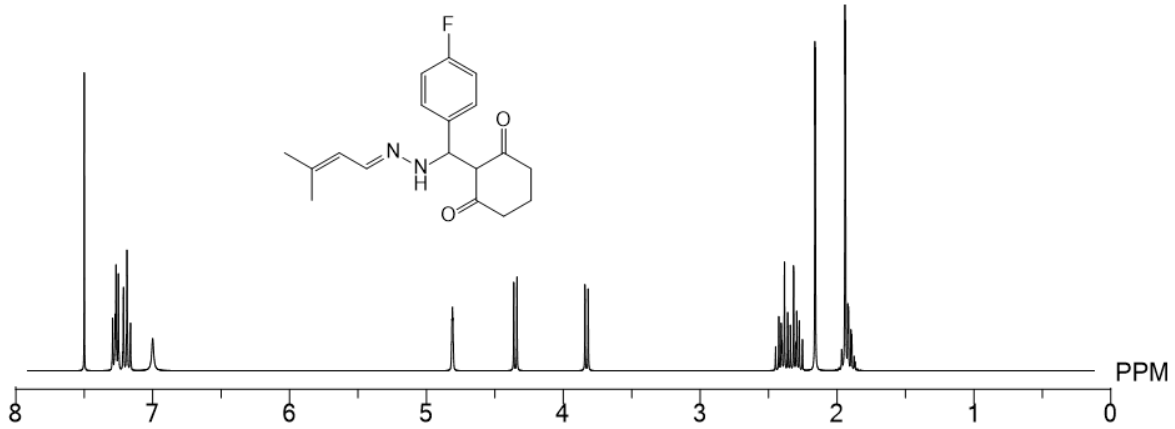


Figure S17 ^{1}H NMR spectrum of the compound **1i**

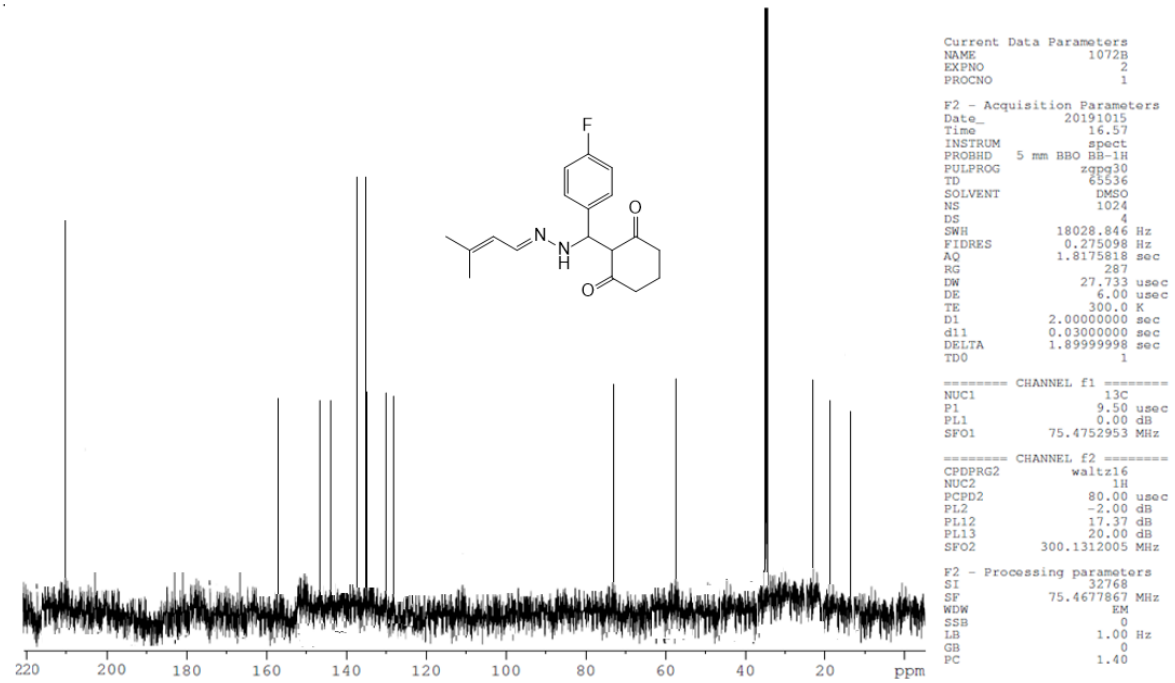


Figure S18 ^{13}C NMR spectrum of the compound **1i**

(*E*)-2-((2-(3-methylbut-2-en-1-ylidene)hydrazinyl)(phenyl)methyl)cyclohexane-1,3-dione (1a)

Yield 78%, mp.145^{o}C; IR(KBr, cm^{-1}): 3395 (-NH), 1815 (CO), 1685 (C=N). ^{1}H NMR (DMSO-d$_6$), δ(ppm): 7.50 (1H, N=CH, s), 7.40-7.27 (5H, Ph-ring, dd), 7.0 (1H, -NH, s), 4.80 (1H, -CH=, s), 4.35 (1H, Ph-CH, d, *J*=4.32Hz), 3.83 (1H, CO-CH-, d, *J*=4.22Hz), 2.40 (4H, CO-CH$_2$, 1,3-cyclohexadione, s), 2.18 (3H, -CH$_3$, s), 1.94 (3H, -CH$_3$, s), 1.93 (2H, -CH$_2$-, s). ^{13}C NMR (DMSO-d$_6$), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 151.1 (1C, =C-(CH$_3$)$_2$), 143.5, 128.5, 126.9, 126.7 (6C, Ph ring), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH$_2$-, 1,3-cyclohexadione), 26.9 (1C, -CH$_3$), 20.7 (1C, -CH$_3$), 16.4 (1C, -CH$_2$-). EI-Ms; *m/z*: 298.38 (M$^+$, 20.5%). Anal. $C_{18}H_{22}N_2O_2$: C, 72.45; H, 7.34; N, 9.36%, Found: C, 72.44; H, 7.36; N, 9.37%.

(*E*)-2-((4-chlorophenyl)(2-(3-methylbut-2-en-1-ylidene)hydrazinyl)methyl)cyclohexane-1,3-dione (1b)

Yield 82%, mp.135^{o}C; IR(KBr, cm^{-1}): 3380 (-NH), 1790 (CO), 1670 (C=N). ^{1}H NMR (DMSO-d$_6$), δ(ppm): 7.50 (1H, N=CH, s), 7.48-7.44 (4H, -Cl-Ph-, s), 7.0 (1H, -NH, s), 4.81 (1H, -CH=, s), 4.33 (1H, Ph-CH, *J*=4.20Hz), 3.81 (1H, CO-CH-, *J*=4.12Hz), 2.40-2.30 (4H, CO-CH$_2$, 1,3-cyclohexadione, s), 2.16 (3H, -CH$_3$, s), 1.94 (3H, -CH$_3$, s), 1.93-1.91 (2H, -CH$_2$-, dd). ^{13}C NMR (DMSO-d$_6$), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 151.1 (1C, =C-(CH$_3$)$_2$), 141.6, 132.3, 128.6, 127.2 (6C, Cl-Ph-), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH$_2$-, 1,3-cyclohexadione), 26.9 (1C, -CH$_3$), 20.7 (1C, -CH$_3$), 16.4 (1C, -CH$_2$-). EI-Ms; *m/z*: 332.13 (M$^+$, 20.3%). Anal. $C_{18}H_{21}ClN_2O_2$: C, 64.97; H, 6.33; N, 8.43%, Found: C, 64.99; H, 6.34; N, 8.44%.

(*E*)-2-((4-bromophenyl)(2-(3-methylbut-2-en-1-ylidene)hydrazinyl)methyl)cyclohexane-1,3-dione (1c)

Yield 86%, mp.132^{o}C; IR(KBr, cm^{-1}): 3384 (-NH), 1780 (CO), 1680 (C=N). ^{1}H NMR (DMSO-d$_6$), δ(ppm): 7.92-7.18 (4H, -Br-Ph-, s), 7.50 (1H, N=CH, s), 7.0 (1H, -NH, s), 4.81 (1H, -CH=, s), 4.31 (1H, Ph-CH, 4.73Hz), 3.84 (1H, CO-CH-, *J*=4.67Hz), 2.40-2.30 (4H, CO-CH$_2$, 1,3-cyclohexadione, s), 2.16 (3H, -CH$_3$, s), 1.94 (3H, -CH$_3$,s), 1.93-1.91 (2H, -CH$_2$-, dd). ^{13}C NMR (DMSO-d$_6$), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 151.1 (1C, =C-(CH$_3$)$_2$), 142.5, 131.4, 127.2, 121.1 (6C, Br-Ph-), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH$_2$-, 1,3-cyclohexadione), 26.9 (1C, -CH$_3$),

20.5 (1C, -CH_3), 16.4 (1C, -CH_2-). EI-Ms; *m/z*: 377.28 (M^+, 20.5%). Anal. $C_{18}H_{21}BrN_2O_2$: C, 57.31; H, 5.60; N, 7.45%, Found: C, 57.33; H, 5.59; N, 7.44%.

(*E*)-2-((2-(3-methylbut-2-en-1-ylidene)hydrazinyl)(4-nitrophenyl)methyl)cyclohexane-1,3-dione (1d)

Yield 83%, mp.147ºC; IR(KBr, cm^{-1}): 3338 (-NH), 1795 (CO), 1675 (C=N). ^{1}H NMR (DMSO-d_6), δ(ppm): 8.21-7.55 (4H, NO_2-Ph-, s), 7.50 (1H, N=CH, s), 7.0 (1H, -NH, s), 4.81 (1H, -CH=, s), 4.35 (1H, Ph-CH, *J*=4.61Hz), 3.83 (1H, CO-CH-, *J*=4.45Hz), 2.40-2.30 (4H, CO-CH_2, 1,3-cyclohexadione, s), 2.16 (3H, -CH_3, s), 1.94 (3H, -CH_3, s), 1.93-1.91 (2H, -CH_2-, dd). ^{13}C NMR (DMSO-d_6), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 151.1 (1C, =C-$(CH_3)_2$), 149.6, 145.9, 123.7, 123.4 (6C, NO_2-Ph-), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH_2-, 1,3-cyclohexadione), 26.9 (1C, -CH_3), 20.9 (1C, -CH_3), 16.4 (1C, -CH_2-). EI-Ms; *m/z*: 343.38 (M^+, 19.9%). Anal. $C_{18}H_{21}N_3O_4$: C, 62.95; H, 6.17; N, 12.27%, Found: C, 62.94; H, 6.15; N, 12.25%.

(*E*)-2-((2-(3-methylbut-2-en-1-ylidene)hydrazinyl)(p-tolyl)methyl)cyclohexane-1,3-dione (1e)

Yield 80%, mp.150ºC; IR(KBr, cm^{-1}): 3325 (-NH), 1810 (CO), 1660 (C=N). ¹H NMR (DMSO-d_6), δ(ppm): 7.50 (1H, N=CH, s), 7.18-7.17 (4H, Ph-ring, s), 7.0 (1H, -NH, s), 4.81 (1H, -CH=, s), 4.25(1H, Ph-CH, *J*=4.21Hz), 3.80 (1H, CO-CH-, *J*=4.23Hz), 2.40-2.30 (4H, CO-CH_2, 1,3-cyclohexadione, s), 2.34 (3H, CH_3-Ph, s), 2.16 (3H, -CH_3, s), 1.94 (3H, -CH_3, s), 1.93-1.91 (2H, -CH_2-, dd). ^{13}C NMR (DMSO-d_6), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 151.1 (1C, =C-$(CH_3)_2$), 140.5, 136.4, 128.8, 125.3 (6C, Ph-ring), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH_2-, 1,3-cyclohexadione), 26.9 (1C, -CH_3), 21.3 (1C, -CH_3), 20.6 (1C, -CH_3), 16.4 (1C, -CH_2-). EI-Ms; *m/z*: 312.41 (M^+, 20.9%). Anal. $C_{19}H_{24}N_2O_2$: C, 73.06; H, 7.75; N, 8.98%, Found: C, 73.08; H, 7.72; N, 8.96%.

(*E*)-2-((4-methoxyphenyl)(2-(3-methylbut-2-en-1-ylidene)hydrazinyl)methyl) cyclohexane-1,3-dione (1f)

Yield 86%, mp.159ºC; IR(KBr, cm^{-1}): 3315 (-NH), 1780 (CO), 1665 (C=N). ¹H NMR (DMSO-d_6), δ(ppm): 7.50 (1H, N=CH, s), 7.18-6.94 (4H, Ph-ring, s), 7.0 (1H, -NH, s), 4.81 (1H, -CH=, s), 4.19 (1H, Ph-CH, *J*=4.11Hz, s), 3.76 (1H, CO-CH-, *J*=4.09Hz, s), 3.83 (3H, -OCH_3, s), 2.40-2.30 (4H, CO-CH_2, s), 2.16 (3H, -CH_3, s), 1.94 (3H, -CH_3, s), 1.93-1.91 (2H, -

CH_2-, dd). ^{13}C NMR (DMSO-d_6), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 151.1 (1C, =C-$(CH_3)_2$), 158.6, 135.8, 126.6, 114.1 (6C, Ph-ring), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 55.8 (1C, -OCH_3), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH_2-, 1,3-cyclohexadione), 26.9 (1C, -CH_3), 20.7 (1C, -CH_3), 16.4 (1C, -CH_2-). EI-Ms; *m/z*: 328.41 (M^+, 21.7%). Anal. $C_{19}H_{24}N_2O_3$: C, 69.49; H, 7.37; N, 8.55%, Found: C, 69.51; H, 7.35; N, 8.54%.

(*E*)-2-((4-aminophenyl)(2-(3-methylbut-2-en-1-ylidene)hydrazinyl)methyl)cyclohexane-1,3-dione (1g)

Yield 82%, mp.156ºC; IR(KBr, cm^{-1}): 3390 (-NH), 1799 (CO), 1654 (C=N). ¹H NMR (DMSO-d_6), δ(ppm): 7.50 (1H, N=CH, s), 7.04-6.58 (4H, NH_2-Ph-, s), 7.0 (1H, -NH, s), 6.27 (2H, -Ph-NH_2, s), 4. (1H, -CH=, s), 4.28 (1H, Ph-CH, *J*=4.56Hz), 3.11 (1H, CO-CH-, *J*=4.23Hz), 2.40-2.30 (4H, CO-CH_2, 1,3-cyclohexadione, s), 2.16 (3H, -CH_3, s), 1.94 (3H, -CH_3, s), 1.93-1.91 (2H, -CH_2-, dd). ^{13}C NMR (DMSO-d_6), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 151.1 (1C, =C-$(CH_3)_2$), 146.4, 133.5, 129.1, 115.0 (6C, NH_2-Ph-), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH_2-, 1,3-cyclohexadione), 26.9 (1C, -CH_3), 20.9 (1C, -CH_3), 16.4 (1C, -CH_2-). EI-Ms; *m/z*: 313.39 (M^+, 20.7%). Anal. $C_{18}H_{23}N_3O_2$: C, 68.94; H, 7.43; N, 13.43%, Found: C, 68.97; H, 7.41; N, 13.40%.

(*E*)-2-((4-hydroxyphenyl)(2-(3-methylbut-2-en-1-ylidene)hydrazinyl)methyl) cyclohexane-1,3-dione (1h)

Yield 86%, mp.140ºC; IR(KBr, cm^{-1}): 3367 (-NH), 1680 (CO), 1650 (C=N). ¹H NMR (DMSO-d_6), δ(ppm): 7.50 (1H, N=CH, s), 7.12-6.70 (4H, Ph-ring, s), 7.0 (1H, -NH, s), 5.35 (1H, -OH, s), 4.81 (1H, -CH=, s), 4.45(1H, Ph-CH, *J*=4.34Hz), 3.76 (1H, CO-CH-, *J*=4.21Hz), 2.40-2.30 (4H, CO-CH_2, 1,3-cyclohexadione, s), 2.16 (3H, -CH_3, s), 1.94 (3H, -CH_3, s), 1.93-1.91 (2H, -CH_2-, dd); ^{13}C NMR (DMSO-d_6), δ(ppm): 208.3 (2C, CO, 1,3-cyclohexadione), 156.5, 136.1, 127.0, 115.7 (6C, Ph-ring), 151.1 (1C, =C-$(CH_3)_2$), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH_2-, 1,3-cyclohexadione), 26.9 (1C, -CH_3), 20.6 (1C, -CH_3), 16.4 (1C, -CH_2-). EI-Ms; *m/z*: 314.38 (M^+, 19.8%). Anal. $C_{18}H_{22}N_2O_3$: C, 68.76; H, 7.06; N, 8.95%, Found: C, 68.79; H, 7.03; N, 8.93%.

(*E*)-2-((4-fluorophenyl)(2-(3-methylbut-2-en-1-ylidene)hydrazinyl)methyl)cyclohexane-1,3-dione (1i)

Yield 82%, mp.149^{o}C; IR(KBr, cm^{-1}): 3354 (-NH), 1695 (CO), 1644 (C=N). ^{1}H NMR (DMSO-d$_6$), δ(ppm): 7.50 (1H, N=CH, s), 7.27-7.19 (4H, F-Ph-, s), 7.0 (1H, -NH, s), 4.81 (1H, -CH=, s), 4.31 (1H, Ph-CH, *J*=4.86Hz), 3.80 (1H, CO-CH-, *J*=4.78Hz), 2.40-2.30 (4H, CO-CH$_2$, 1,3-cyclohexadione, s), 2.16 (3H, -CH$_3$, s), 1.94 (3H, -CH$_3$, s), 1.93-1.91 (2H, -CH$_2$-, dd). ^{13}C NMR (DMSO-d$_6$), δ(ppm): 208.3 (2C, C=O, 1,3-cyclohexadione), 151.1 (1C, =C-(CH$_3$)$_2$), 160.9, 139.1, 128.5, 115.3 (6C, Ph-ring), 137.2 (1C, N=CH-), 123.2 (1C, -CH=), 70.4 (1C, CO-CH-), 52.0 (1C, Ph-CH), 40.8 (2C, CO-CH$_2$-, 1,3-cyclohexadione), 26.9 (1C, -CH$_3$), 20.5 (1C, -CH$_3$), 16.4 (1C, -CH$_2$-). EI-Ms; *m/z*: 316.37 (M^{+}, 20.5%). Anal. C$_{18}$H$_{21}$FN$_2$O$_2$: C, 68.37; H, 6.68; N, 8.88%, Found: C, 68.35; H, 6.67; N, 8.86%.

Experimental Section

Biological activity

Antibacterial activity

Antibacterial activity was carried out for all synthesised compounds (**2a-j**) via disc diffusion method, and activity was assessed from following bacterial strain such as gram-positive of *Staphylococcus aureus* (ATCC-25923), *Enterococcus faecalis* (recultured) and gram-negative bacteria of *Escherichia coli* (ATCC-25922), *Pseudomonas aeruginosa* (ATCC-27853), and *K. pneumonia* (recultured) by using Mueller– Hinton agar (Hi-Media) medium. Each compound and standard was tested at a concentration of 64 µg/mL in DMSO the zone of inhibition was measured after 24h incubation at 37ºC. After the incubation period the diameter of the clear zone of inhibition was measured in mm. Ciprofloxacin was chosen as a standard for antibacterial activity screening.

Determination of the minimum inhibitory concentration (MIC)

To determine the minimal inhibitory concentrations (MICs) of **2a–j,** their 64 µg/mL solutions were subjected to successive twofold dilutions, furnishing samples with concentrations of 64, 32, and 0.25 µg/mL. Microbial suspensions of 106 CFU/mL (CFU = colony forming unit) were inoculated in the corresponding wells, and the plates were incubated at 36 °C for 24 h. The MICs were determined as the lowest concentrations completely inhibiting the visible growth of microorganisms.

Cytotoxic activity

The newly synthesized compounds (**2a-2j**) were screened for cytotoxic activity according to a previously described procedure. Three cell lines were treated with these compounds at one primary cytotoxic assay dose of 100µM for 48 h (MTT anticancer assay). Doxorubicin was used as a standard. The present investigation was MCF-7(breast) used to screen the censer cell line. In the current protocol, all cell lines were pre-incubated on a microtiter plate. The results of each test were reported as the growth percentage of treated cells compared to untreated control cells. Compounds reducing the growth of any one of the cell lines to approximately 32% or less were described as having cytotoxic activity. A 0.1mL aliquot of the cell suspension (5 × 106 cells/100 µL) and 0.1 mL of the test solution (6.25–100 µg in 1% DMSO, with the final DMSO concentration in media less than 1%) were added

to the wells, with the plates kept in an incubator (5% CO2) at 37 °C for 72 h. The blank sample contained only the cell suspension, and the control wells contained 1% DMSO and the cell suspension. After 72 h, 20 µL of MTT was added, and the plates were kept in the CO2 incubator for 2 h, followed by the addition of propanol (100 µL). The plates were covered withaluminum foil to protect them from light and subsequently agitated in a rotary shaker for 10–20 min. Afterwards, the 27-well plates were processed on an ELISA reader to obtain absorption data at 562 nm.

Results and Discussion

Table S1. DPPH scavenging activity of compounds (**1a-1i)**

Compounds	**Concentration(µg/mL)[a], % activity**				**IC_{50} (µg/mL)**
	10 µg/mL	**25 µg/mL**	**50 µg/mL**	**100 µg/mL**	
1a	26.20 ± 0.10	45.15 ± 0.01	63.13 ± 0.05	72.11 ± 0.17	42.57
1b	32.44 ± 0.13	48.02 ± 0.31	65.01 ± 0.19	82.01 ± 0.02	33.18
1c	12.46 ± 0.45	28.21 ± 0.07	44.10 ± 0.02	52.62 ± 0.09	83.86
1d	19.10 ± 0.51	24.09 ± 0.05	49.12 ± 0.01	56.06 ± 0.11	76.48
1e	21.01 ± 0.03	44.1 ± 0.03	62.02 ± 0.11	78.20 ± 0.00	43.97
1f	30.13 ± 0.03	45.63 ± 0.02	63.04 ± 0.05	100 ± 0.00	33.49
1g	9.32 ± 0.02	18.20 ± 0.02	28.20 ± 0.09	32.66 ± 0.27	> 100
1h	38.10 ± 0.27	56.21 ± 0.07	76.04 ± 0.21	100 ± 0.00	19.62
1i	28.10 ± 0.12	43.01 ± 0.10	66.10 ± 0.11	81.21 ± 0.20	38.22
BHT	22.08 ± 0.01	54.27 ± 0.22	70.30 ± 0.34	82.31 ± 0.25	33.88

[a] Value expressed are means ± SD of three different experiments

Table S2. Hydrogen peroxide (H_2O_2) scavenging activity of compounds (**1a-1i)**

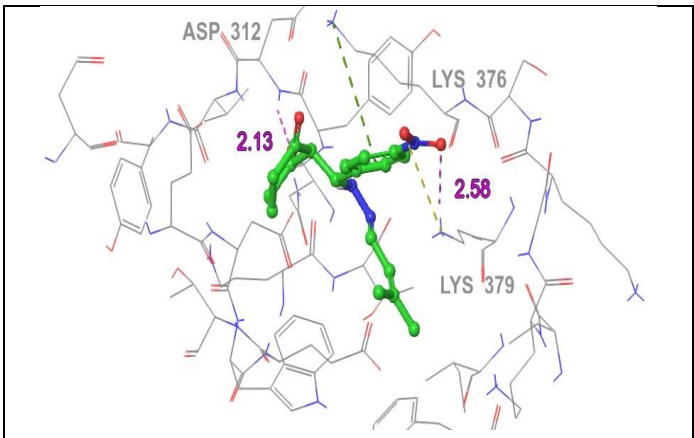
Compounds	**Concentration (µg/mL)[a], % activity**				**IC_{50} (µg/mL)**
	10	**25**	**50**	**100**	
1a	25.20 ± 0.03	42.12± 0.02	63.20 ± 0.02	72.10 ± 0.02	44.19
1b	33.01 ± 0.24	61.25 ± 0.51	72.09 ± 0.13	83.16 ± 0.10	20.47
1c	21.07 ± 0.10	43.07 ± 0.22	62.10 ± 0.01	72.13 ± 0.03	47.02
1d	33.22 ± 0.06	46.09 ± 0.05	53.10 ± 0.01	66.01 ± 0.03	47.42
1e	19.01 ± 0.01	28.10 ± 0.03	49.62 ± 0.02	51.62 ± 0.00	82.26
1f	32.12 ± 0.26	44.10 ± 0.03	61.01 ± 0.06	72.01 ± 0.02	40.85
1g	13.44 ± 0.19	29.22 ± 0.10	35.60 ± 0.22	44.25 ± 0.21	>100
1h	42.10 ± 0.27	54.10 ± 0.07	88.03 ± 0.01	100 ± 0.00	13.79
1i	18.04 ± 0.12	29.10 ± 0.02	34.02 ± 0.14	49.38 ± 0.00	>100
BHT	29.02 ± 0.03	59.01 ± 1.02	68.51 ± 0.02	82.17 ± 0.77	27.16

[a] Value expressed are means ± SD of three different experiments

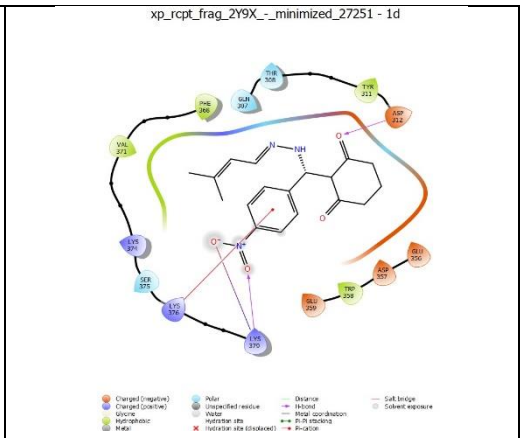
Table S3. NO scavenging activity of compounds (**1a-1i)**

Compounds	**Concentration (µg/mL)[a], % activity**				**IC_{50} (µg/mL)**
	10	**25**	**50**	**100**	
1a	17.90 ± 0.01	32.29 ± 0.12	47.23 ± 0.07	51.41 ± 0.04	83.44
1b	26.61 ± 0.01	52.51 ± 0.21	67.16 ± 0.10	78.12 ± 0.16	34.23
1c	32.30 ± 0.55	58.01 ± 0.03	72.02 ± 0.04	86.10 ± 0.08	23.58
1d	22.10 ± 0.02	46.17 ± 0.11	59.40 ± 0.31	69.10 ± 0.02	48.00
1e	18.02 ± 0.01	39.12 ± 0.02	60.03 ± 0.01	76.10 ± 0.02	49.02
1f	22.20 ± 0.01	47.36 ± 0.20	60.07 ± 0.16	72.04 ± 0.10	45.39
1g	10.01 ± 0.02	22.21 ± 0.06	36.12 ± 0.02	44.21 ± 0.20	>100
1h	29.6 ± 0.07	39.11 ± 0.03	47.13 ± 0.19	58.23 ± 0.00	67.82
1i	19.40 ± 0.01	25.10 ± 0.10	33.02 ± 0.04	49.36 ± 0.00	>100
BHT	28.03 ± 0.02	53.16 ± 0.02	67.65 ±0.01	83.32 ± 0.51	31.73

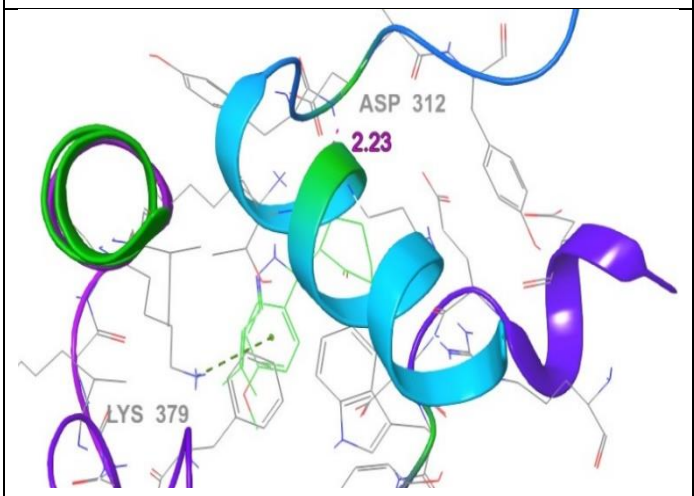
[a] Value expressed are means ± SD of three different experiments



(a) Compound **1d** (3d structure)



(a) Compound **1d** (2d structure)



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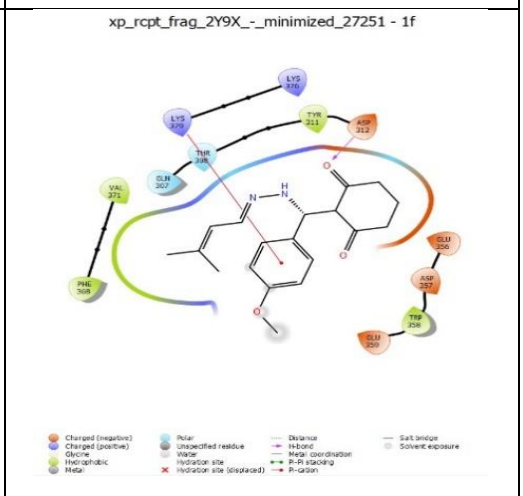
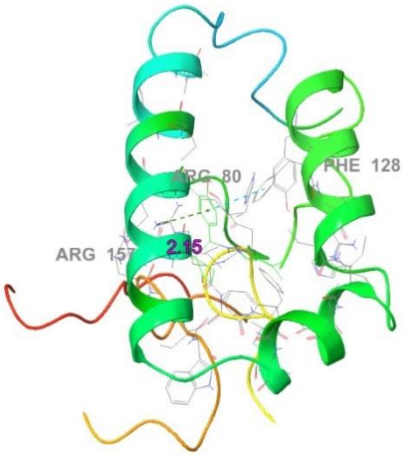
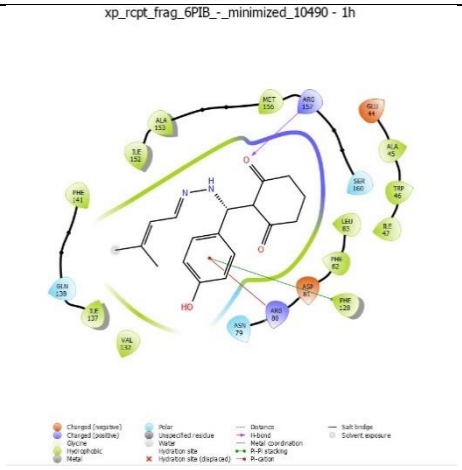


(b) Compound **1f** (2d structure)

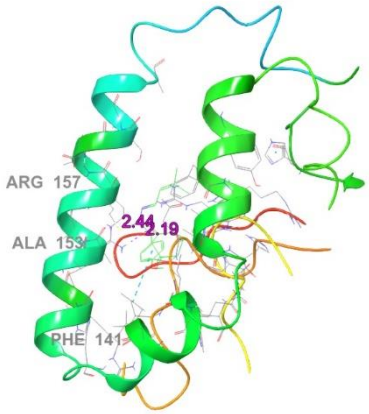
Figure S19. Molecular docking studies of 2d and 3d structure of compound **1d** (a), and **1f** (b) with protein **2Y9X**



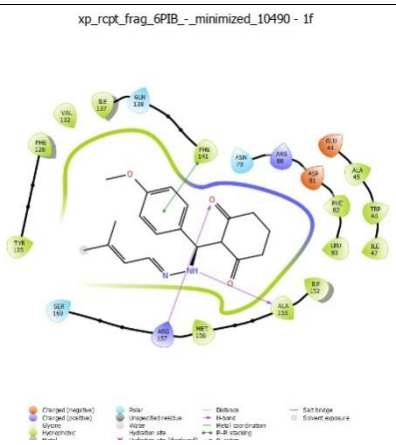
(a) Compound **1h** (3d structure)



(a) Compound **1h**(2d structure)



(b) Compound **1f** (3d structure)



(b) Compound **1f** (2d structure)

Figure S20. Molecular docking studies of 2d and 3d structure of compound **1h** (a), and **1f** (b) with protein **6B1P**