

## SUPPLEMENTARY DATA

### Synthesis of *N'*-(4-/3-/2-/non-substituted benzylidene)-4-[(4-methylphenyl)sulfonyloxy] Benzohydrazides and Evaluation of their Inhibitory Activities against Monoamine Oxidases and $\beta$ -Secretase

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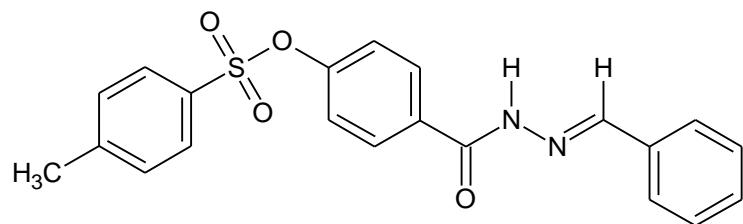
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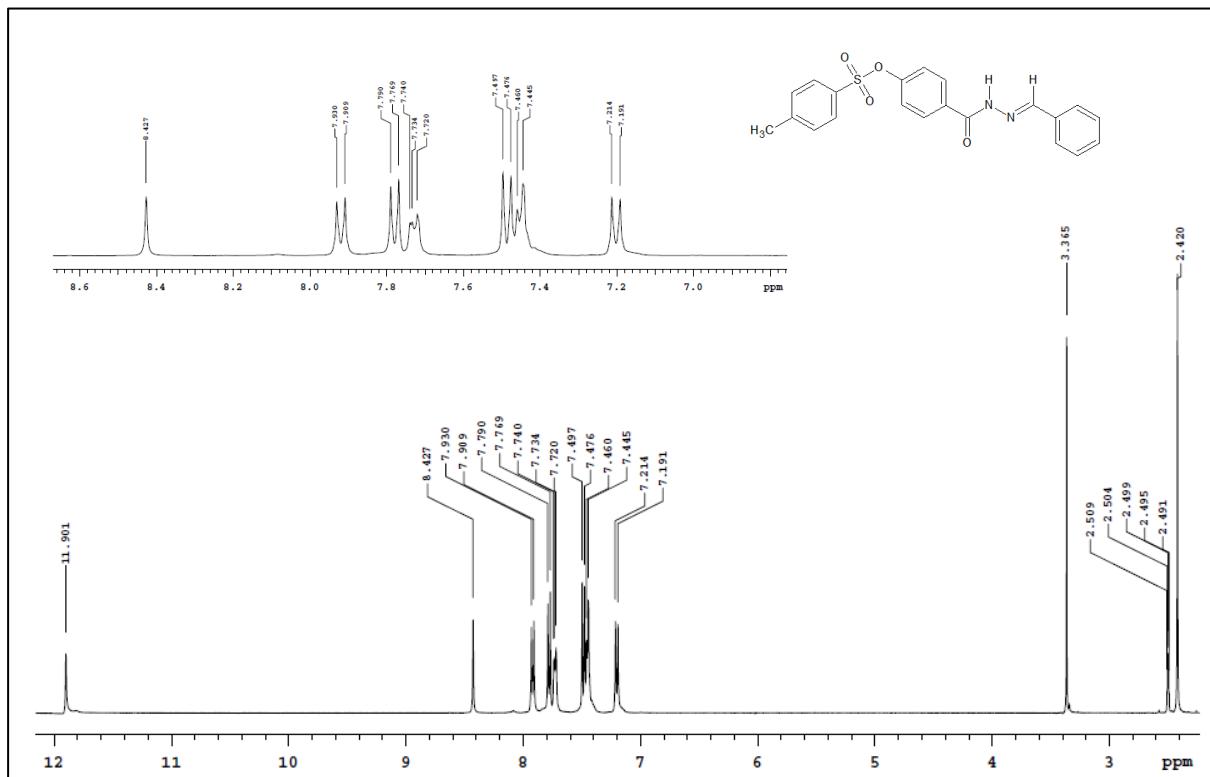
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*(E)-N'*-(Phenylmethylidene)-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3a**)



Lab Code: EP-T-H



**Figure S1.** Compound **3a**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).

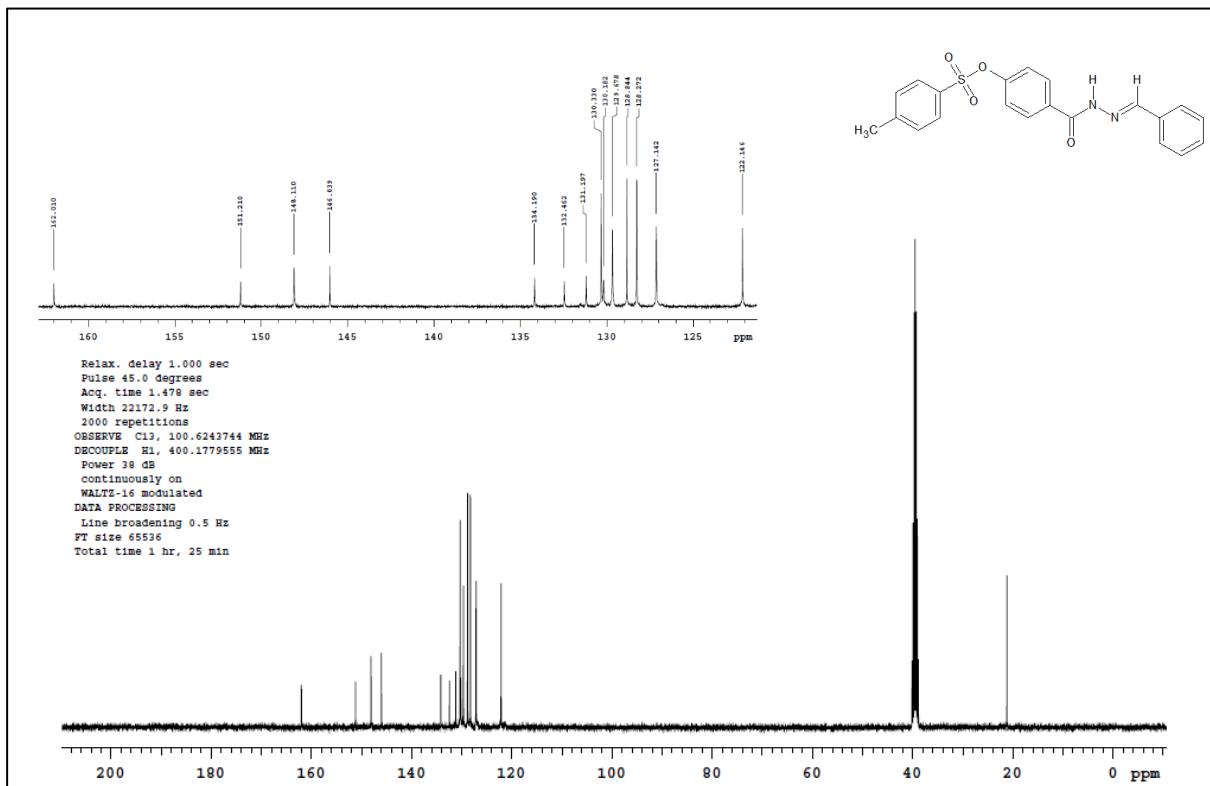


Figure S2. Compound 3a  $^{13}\text{C}$ -NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

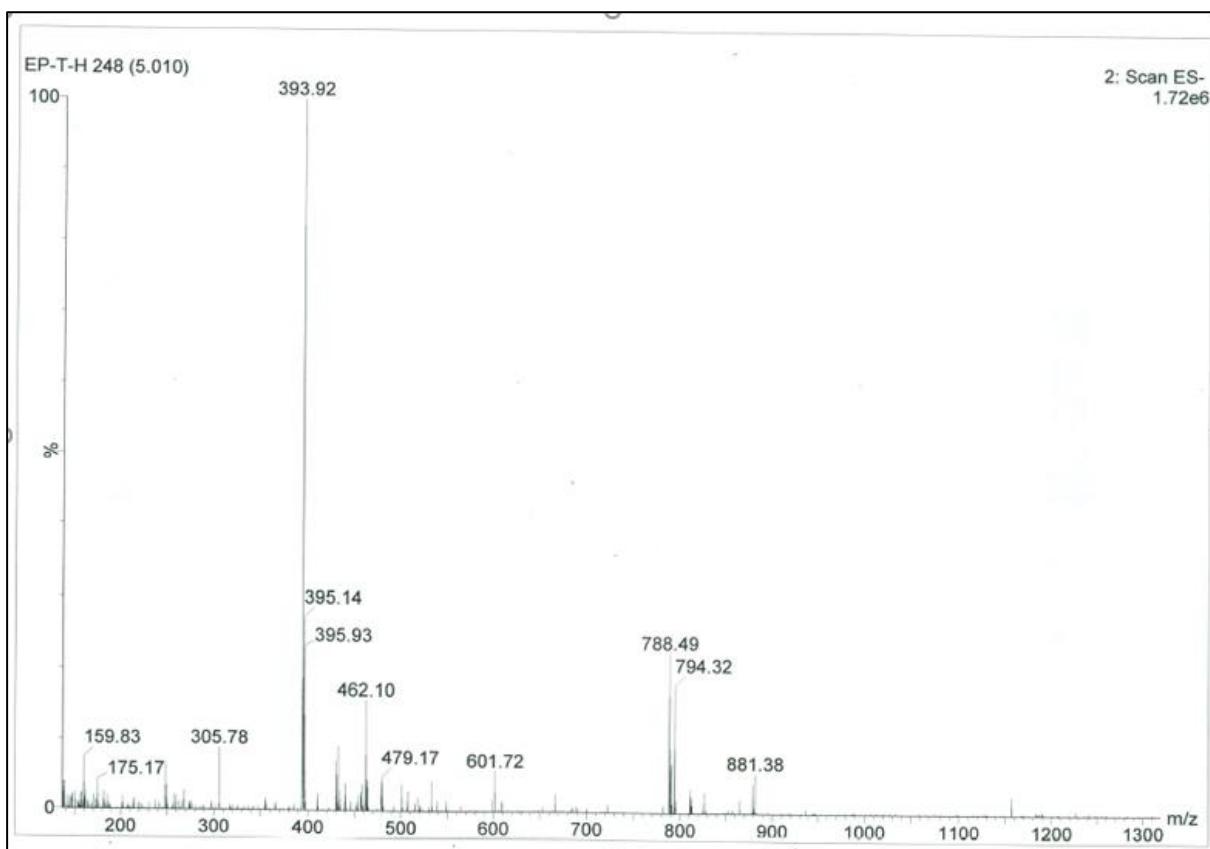
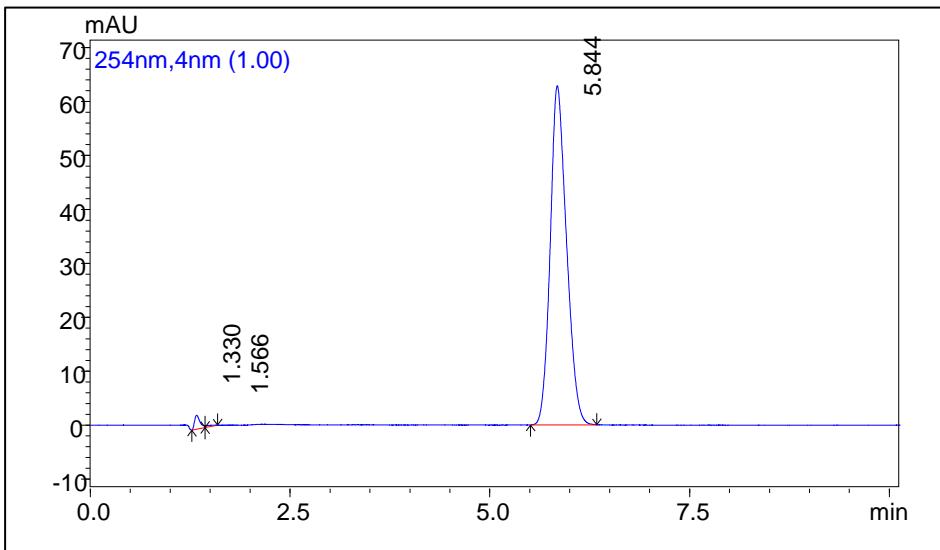
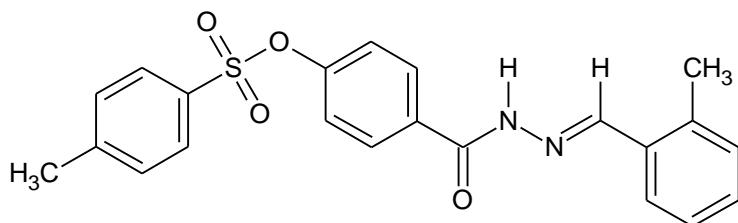


Figure S3. Compound 3a ESI MS spectrum.

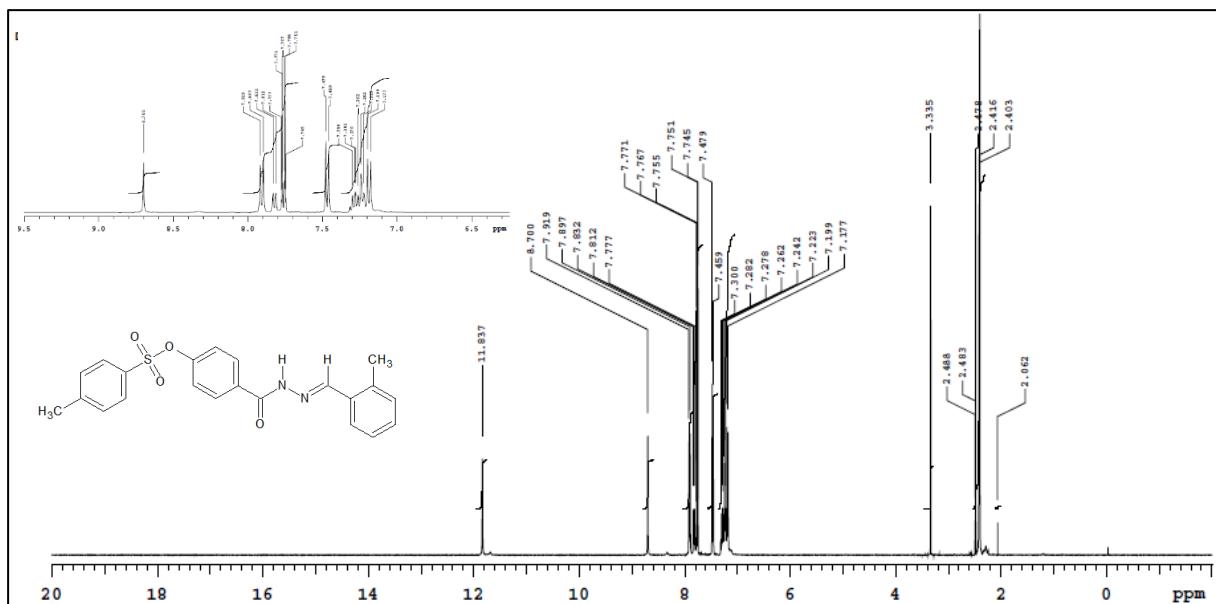


**Figure S4.** Chromatogram of compound **3a** (28 µg/mL) recorded under optimized conditions.

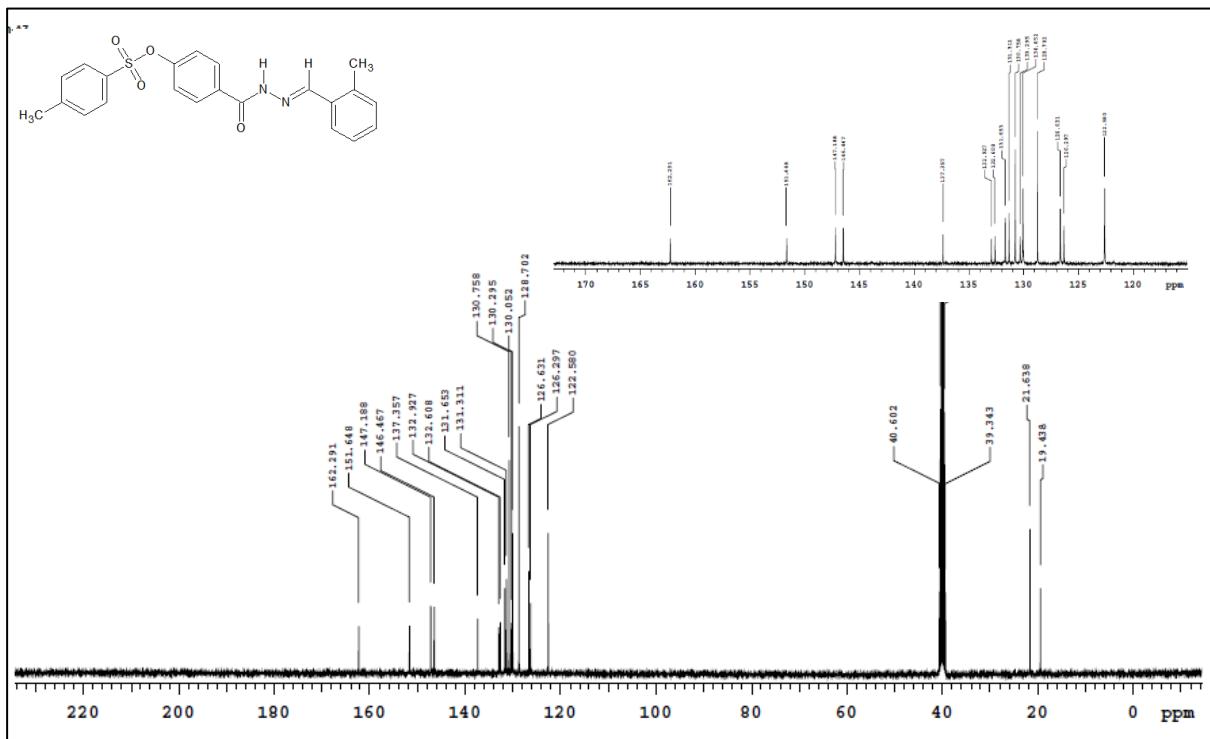
(*E*)-*N'*-[(2-Methylphenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3b**)



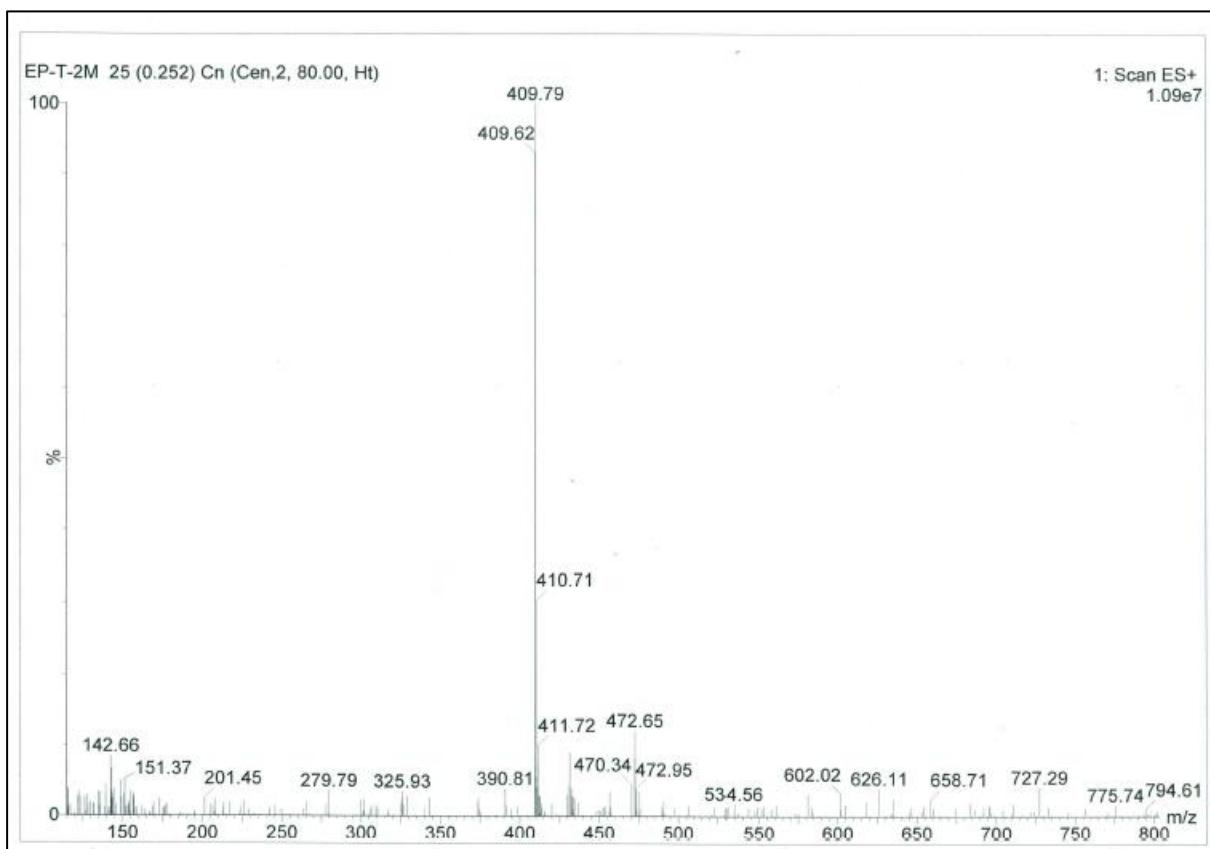
Lab Code: EP-T-2M



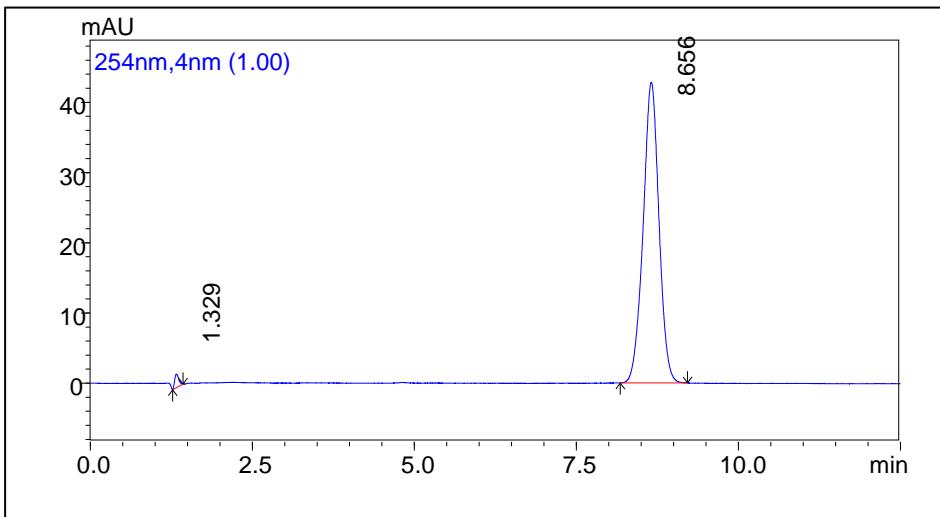
**Figure S5.** Compound **3b**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



**Figure S6.** Compound **3b**  $^{13}\text{C}$ -NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

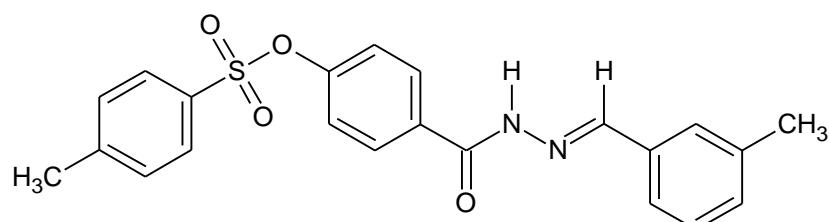


**Figure S7.** Compound **3b** ESI MS spectrum.

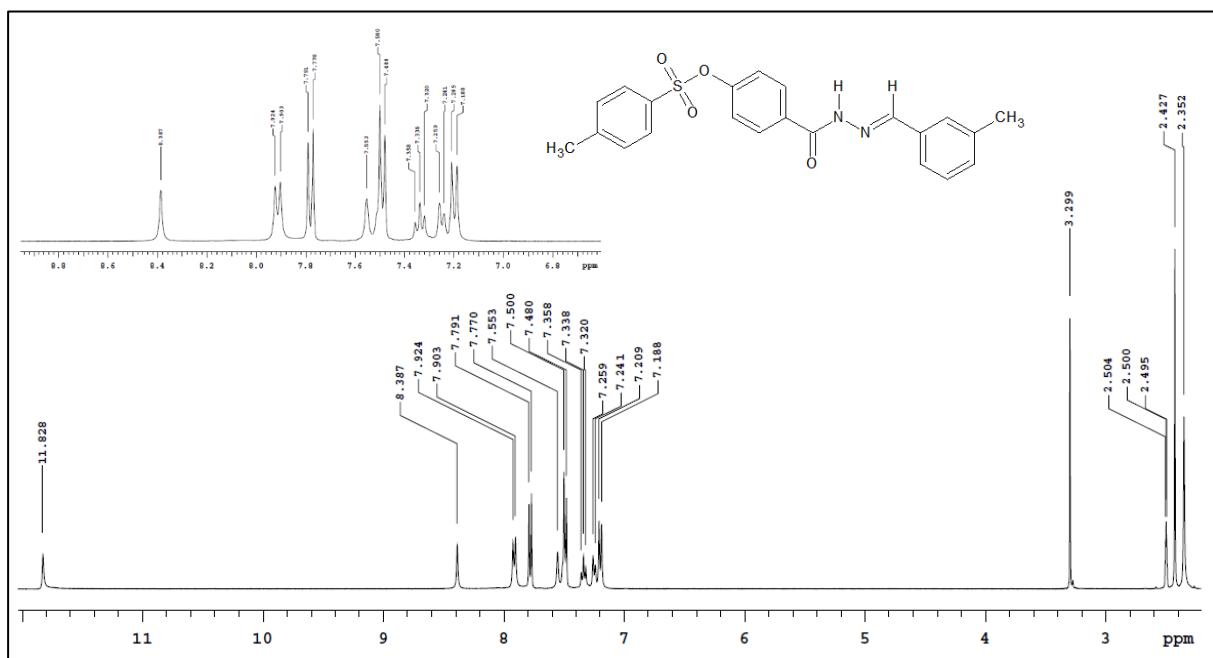


**Figure S8.** Chromatogram of compound **3b** (52 µg/mL) recorded under optimized conditions.

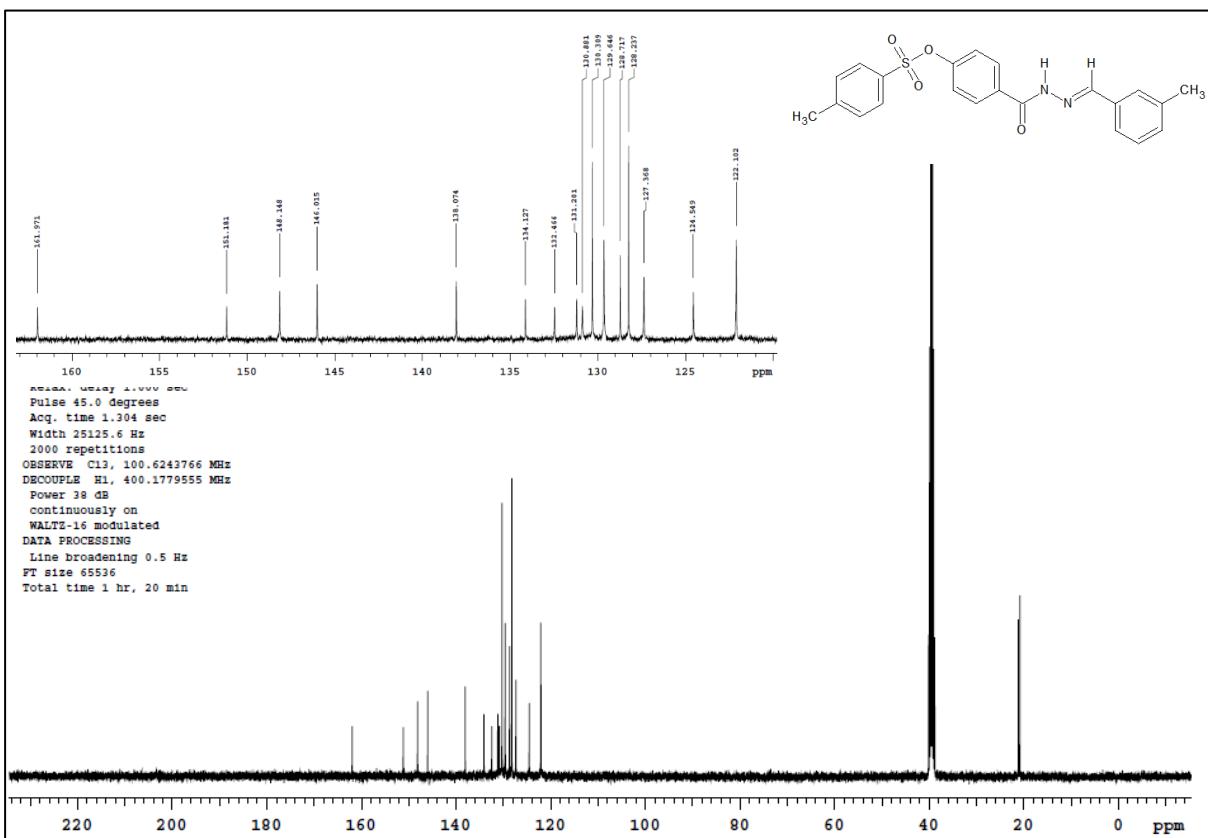
(*E*)-*N'*-[(3-Methylphenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3c**)



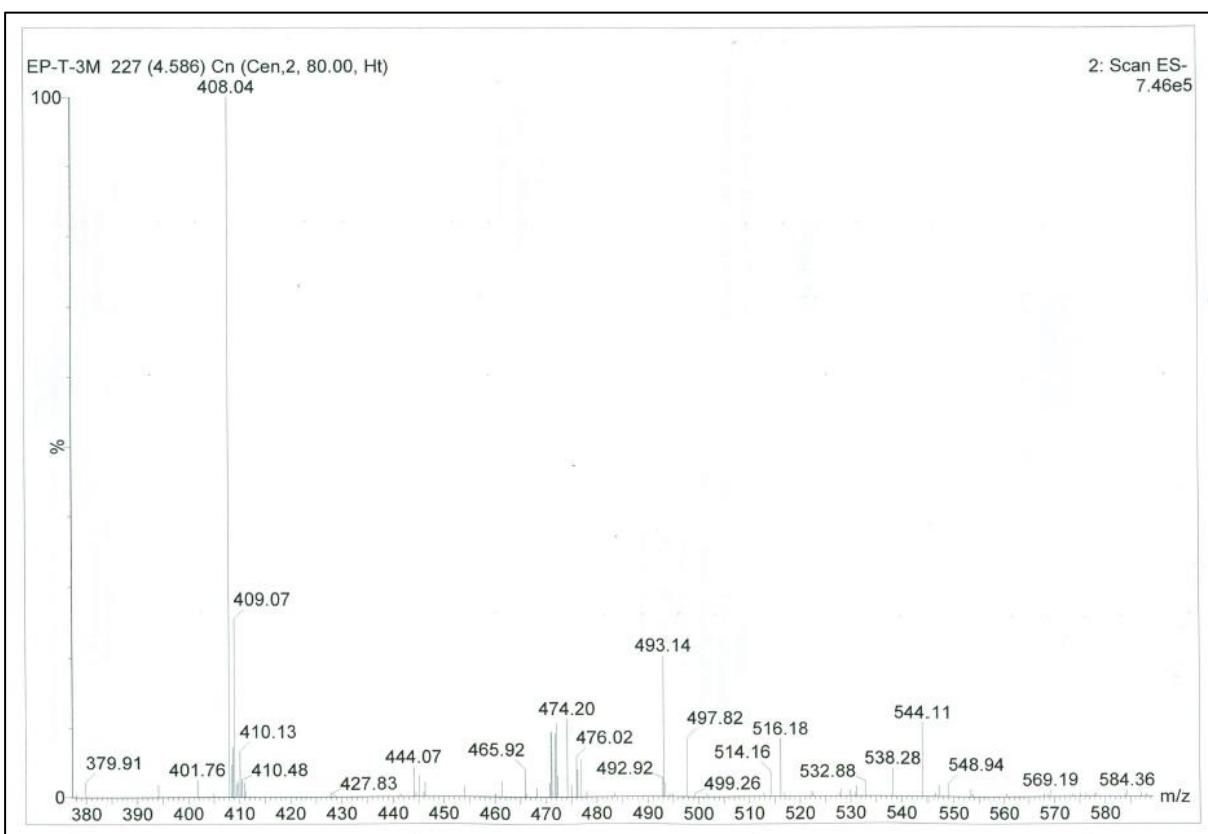
**Lab Code:** EP-T-3M



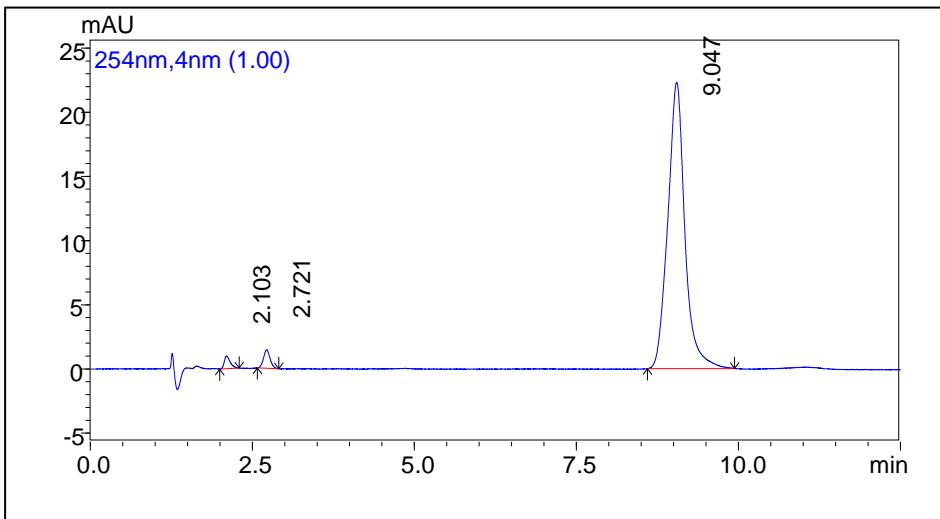
**Figure S9.** Compound **3c**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



**Figure S10.** Compound **3c**  $^{13}\text{C}$ -NMR spectrum (DMSO- $\text{d}_6$ , 100 MHz).

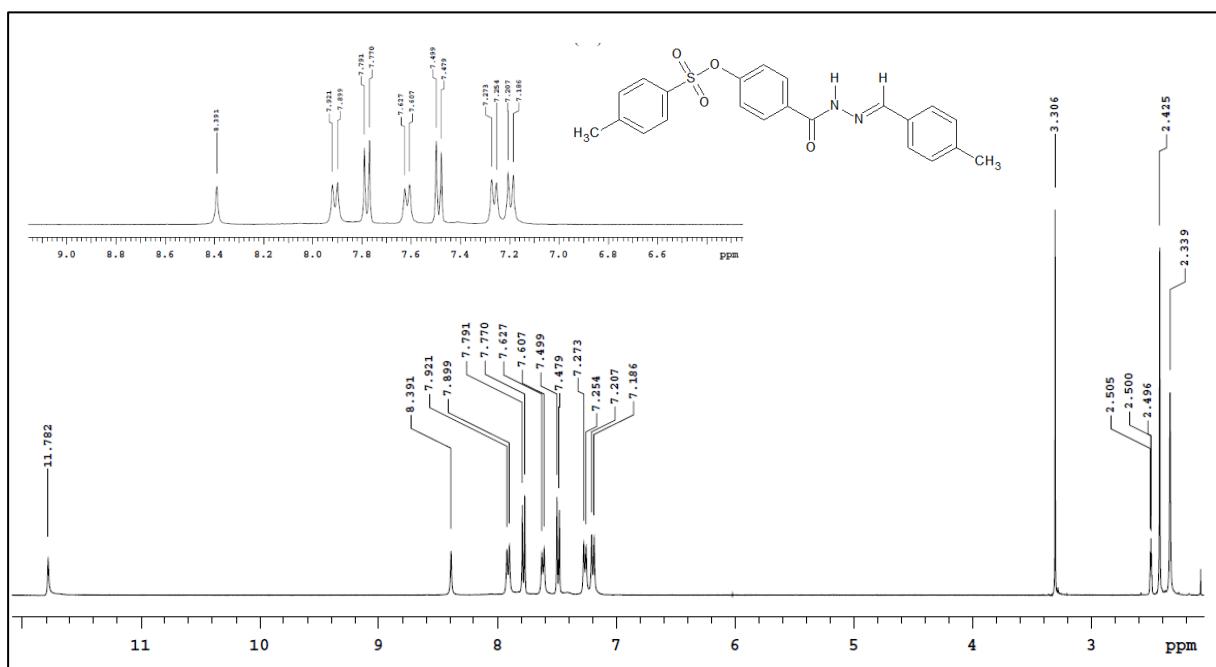
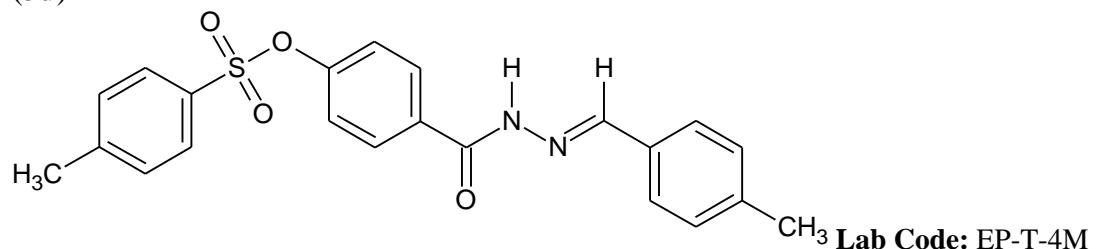


**Figure S11.** Compound 3c ESI MS spectrum.



**Figure S12.** Chromatogram of compound 3c (24 µg/mL) recorded under optimized conditions.

(*E*)-*N'*-[(4-Methylphenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3d**)



**Figure S13.** Compound **3d** <sup>1</sup>H-NMR spectrum (DMSO-d<sub>6</sub>, 400 MHz).

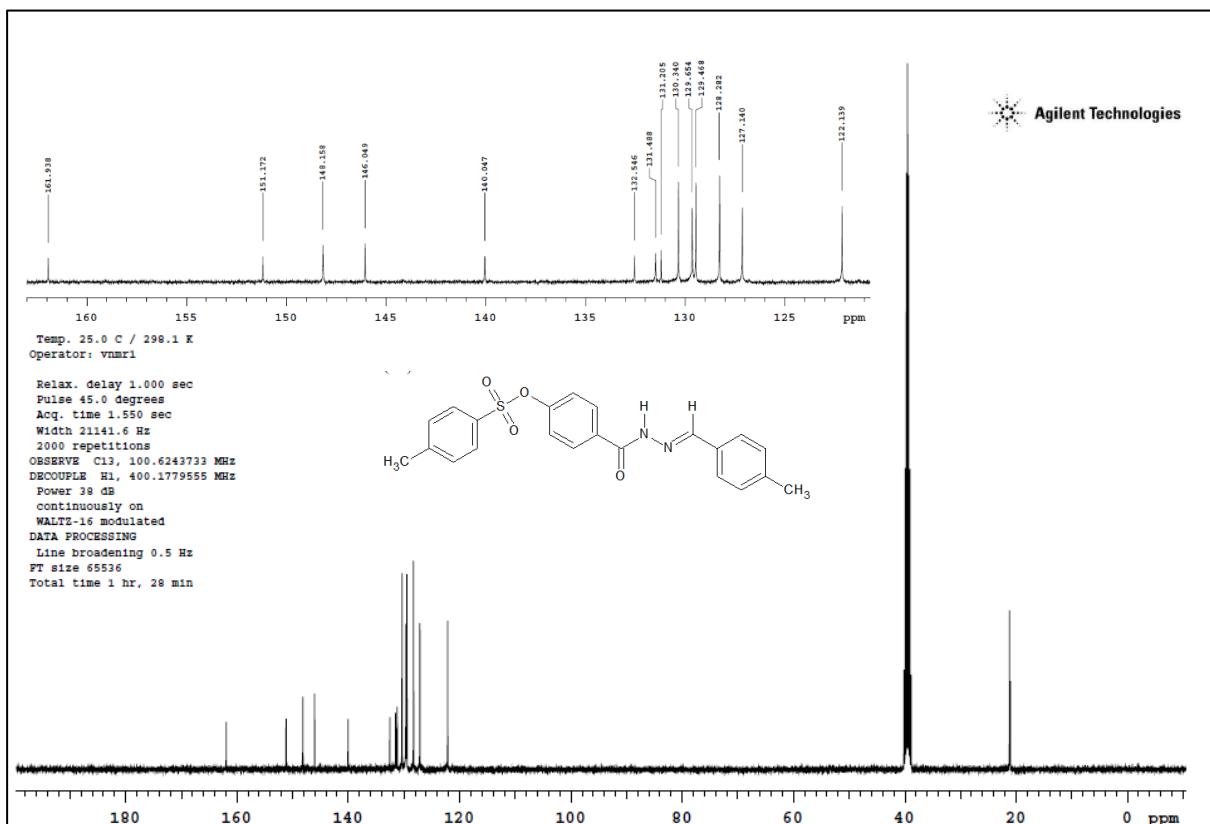


Figure S14. Compound 3d  $^{13}\text{C}$ -NMR spectrum (DMSO- $d_6$ , 100 MHz).

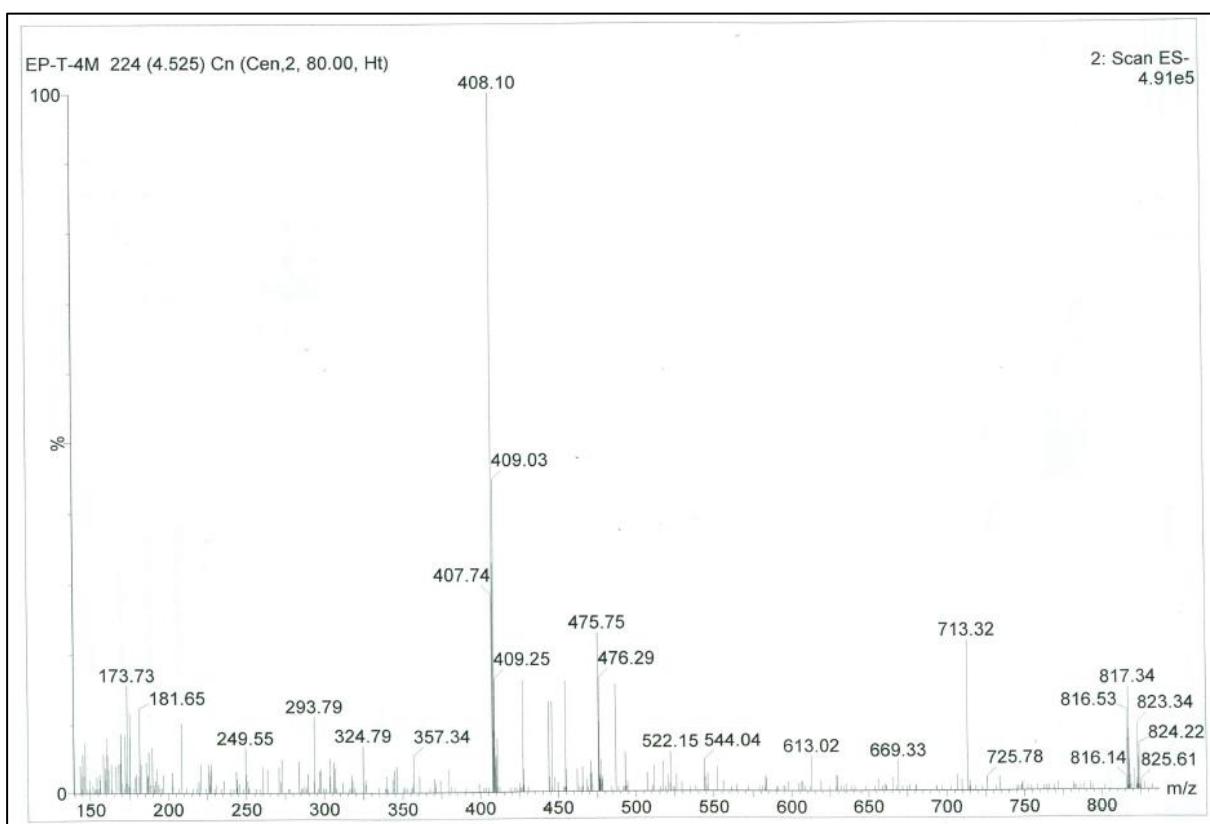
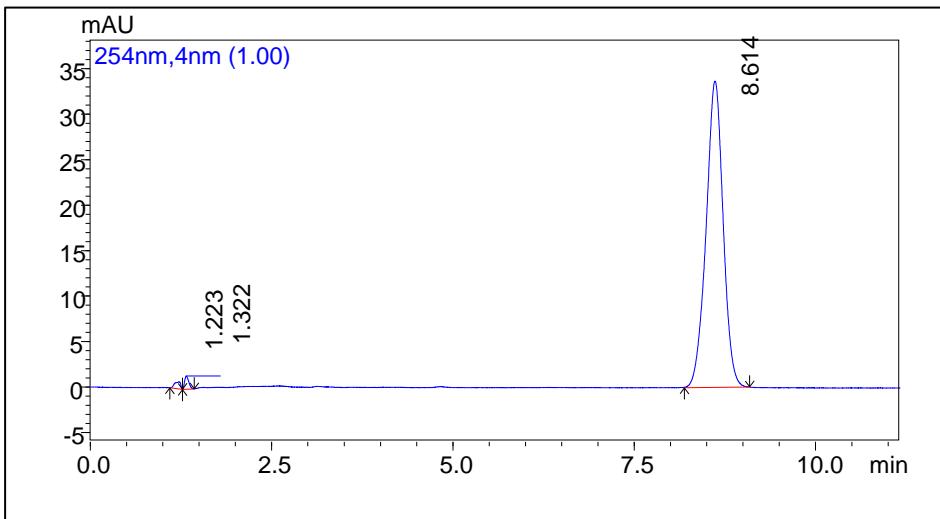
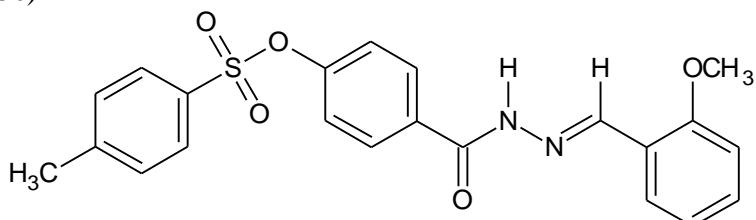


Figure S15. Compound 3d ESI MS spectrum.

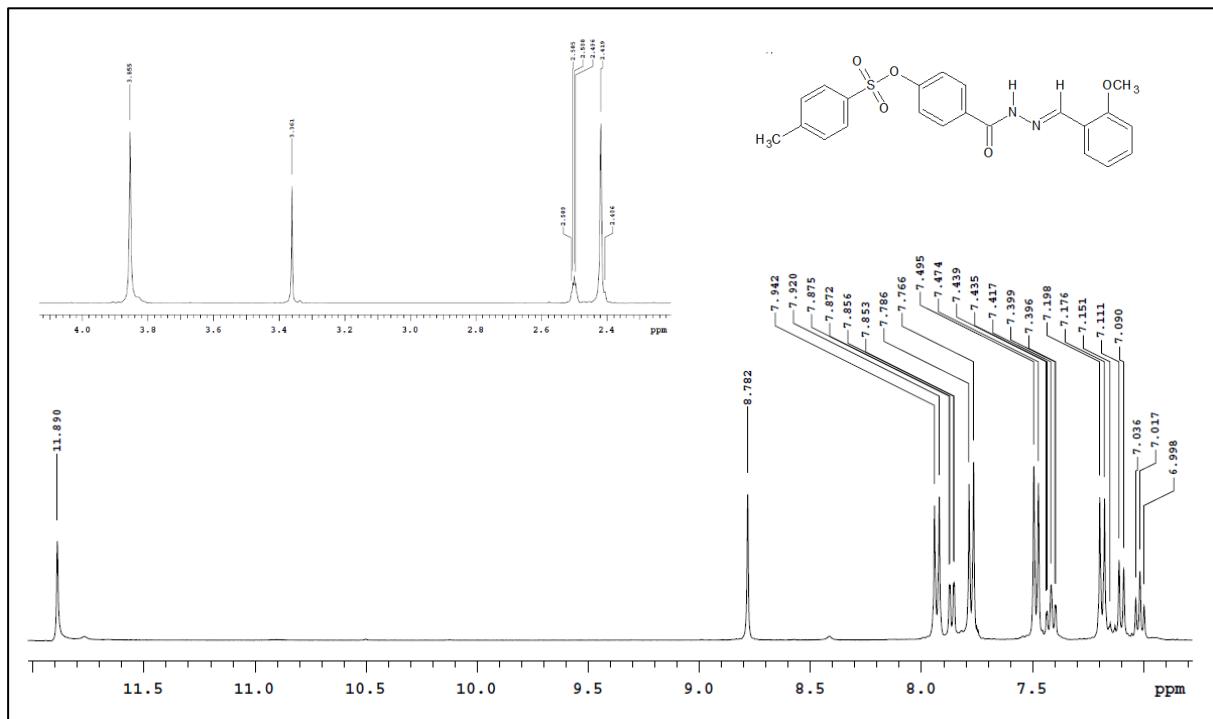


**Figure S16.** Chromatogram of compound **3d** (56 µg/mL) recorded under optimized conditions.

(*E*)-*N'*-[(2-Methoxyphenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3e**)



**Lab Code:** EP-T-2O



**Figure S17.** Compound **3e**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).

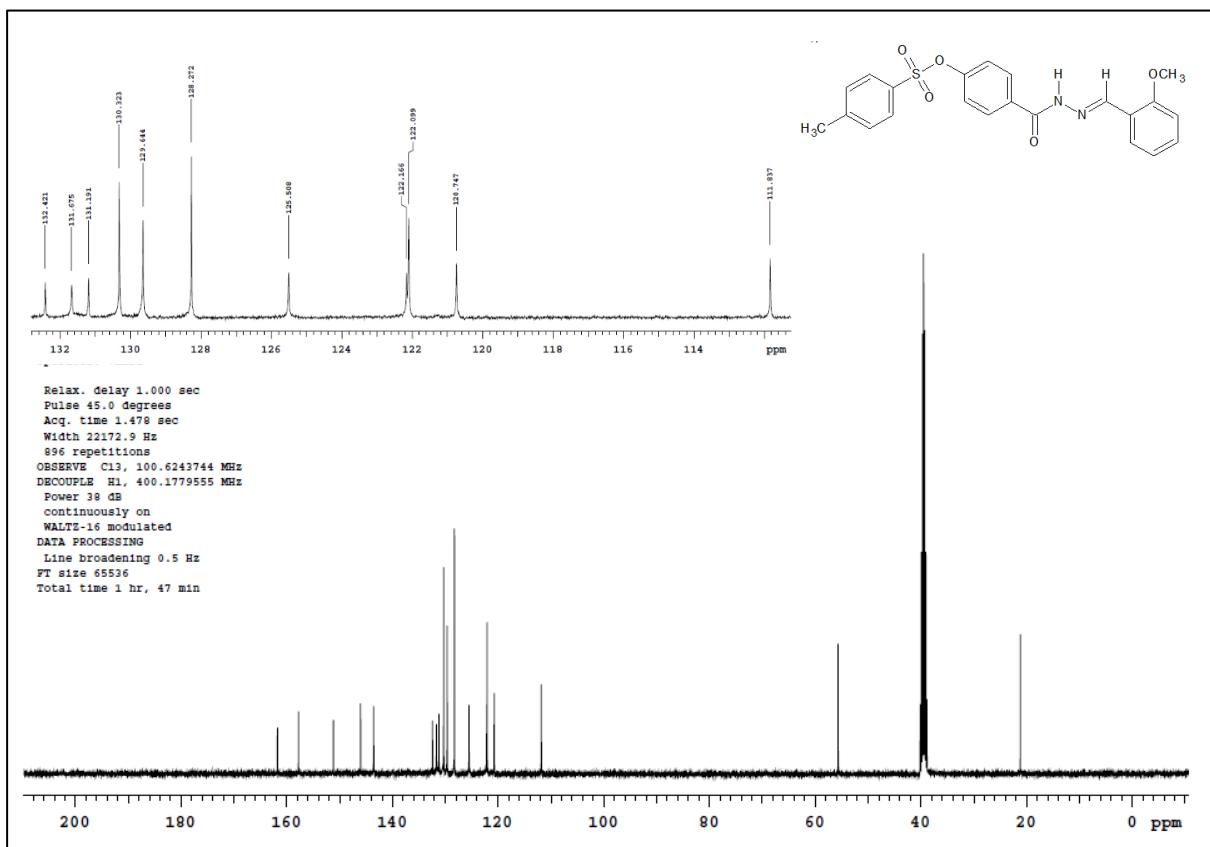


Figure S18. Compound 3e <sup>13</sup>C-NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

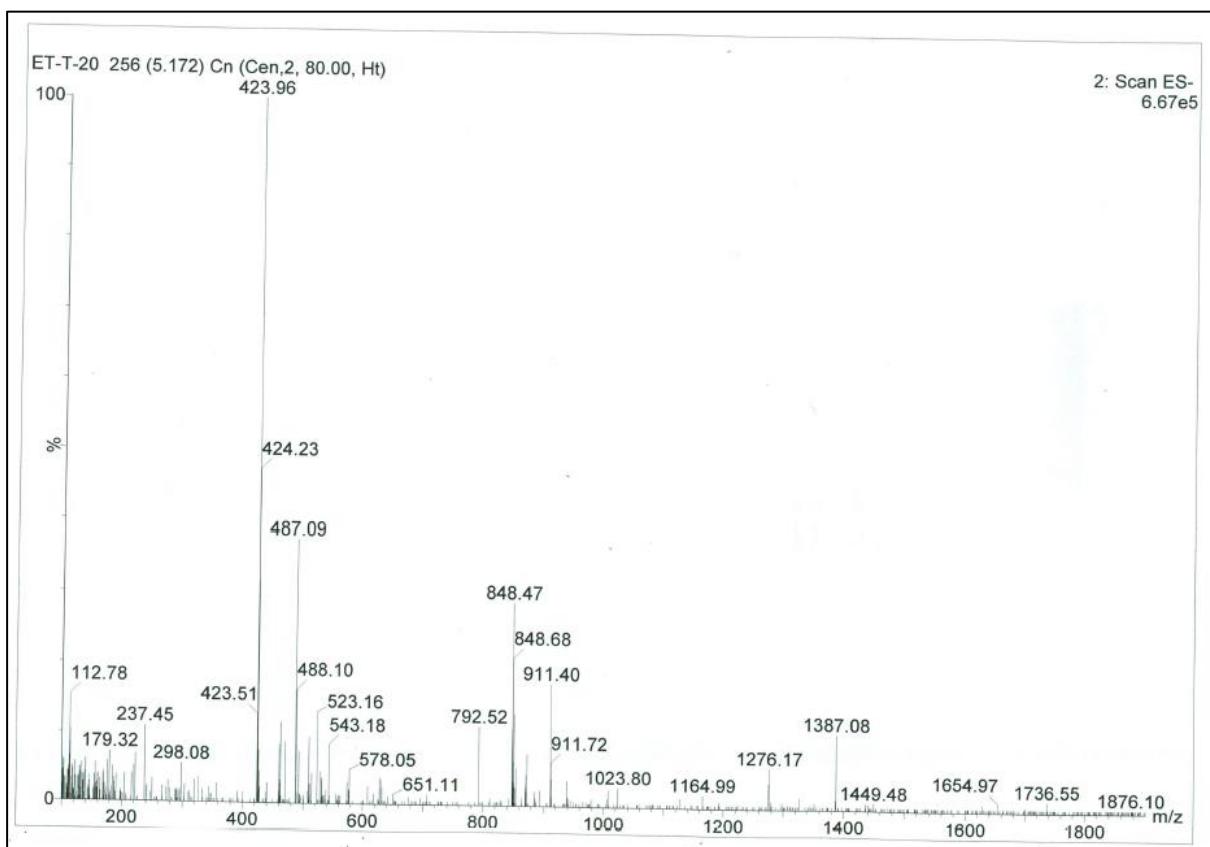
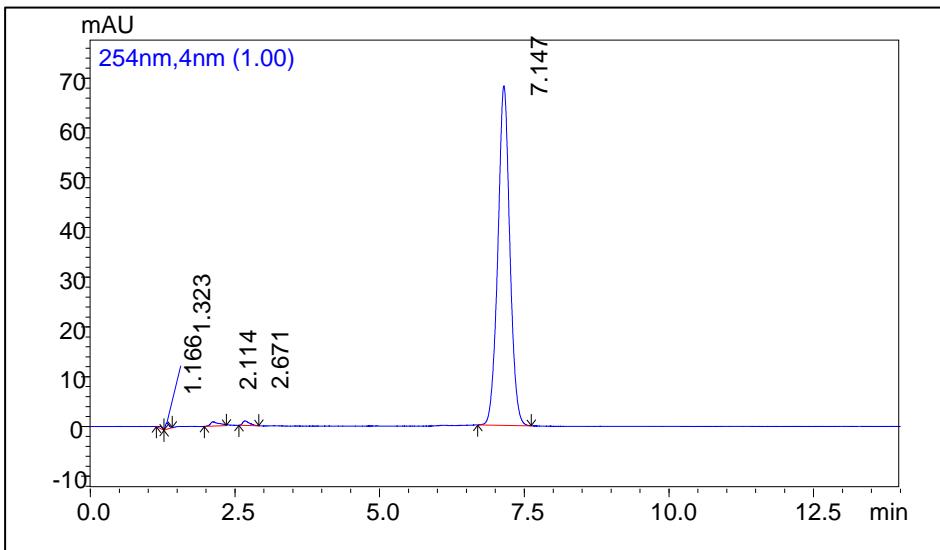
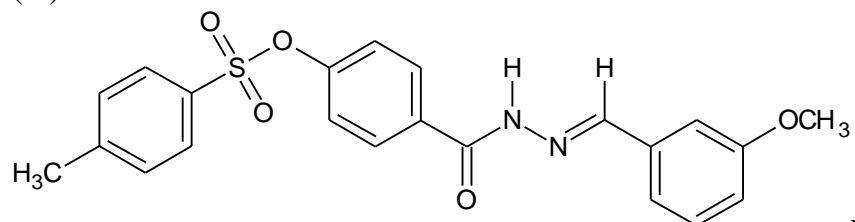


Figure S19. Compound 3e ESI MS spectrum.

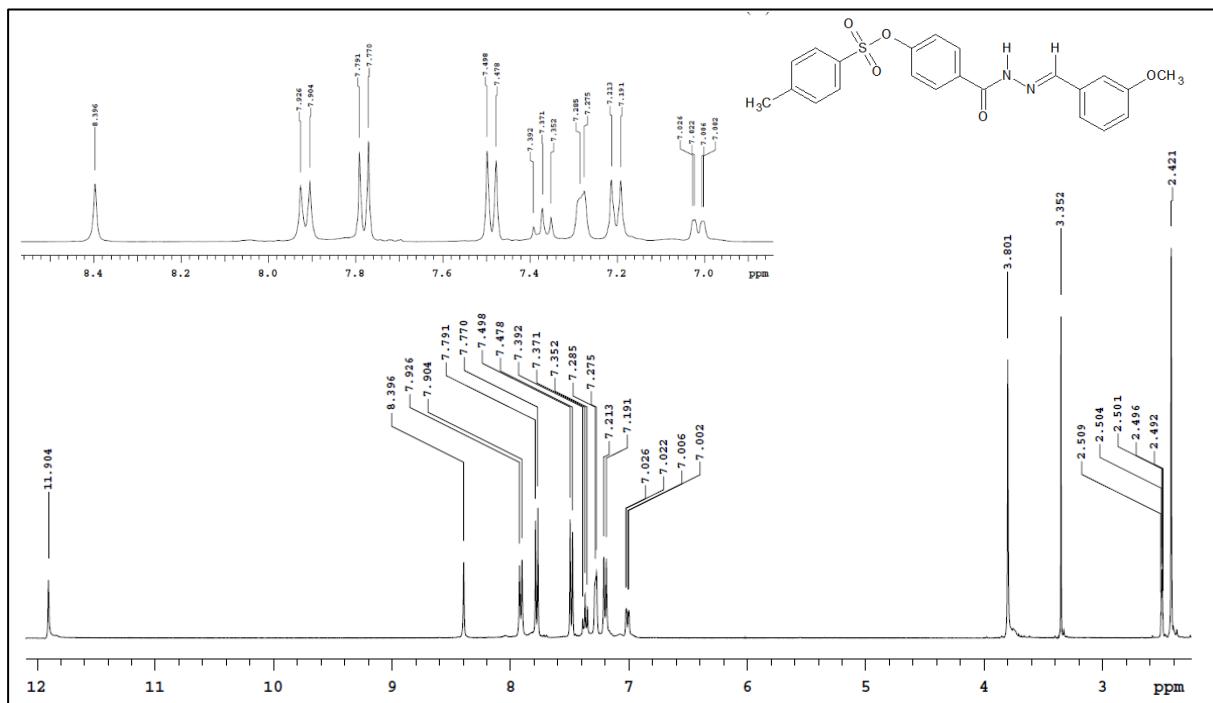


**Figure S20.** Chromatogram of compound **3e** (28 µg/mL) recorded under optimized conditions.

(*E*)-*N'*-[(3-Methoxyphenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3f**)



**Lab Code:** EP-T-3O



**Figure S21.** Compound **3f**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).

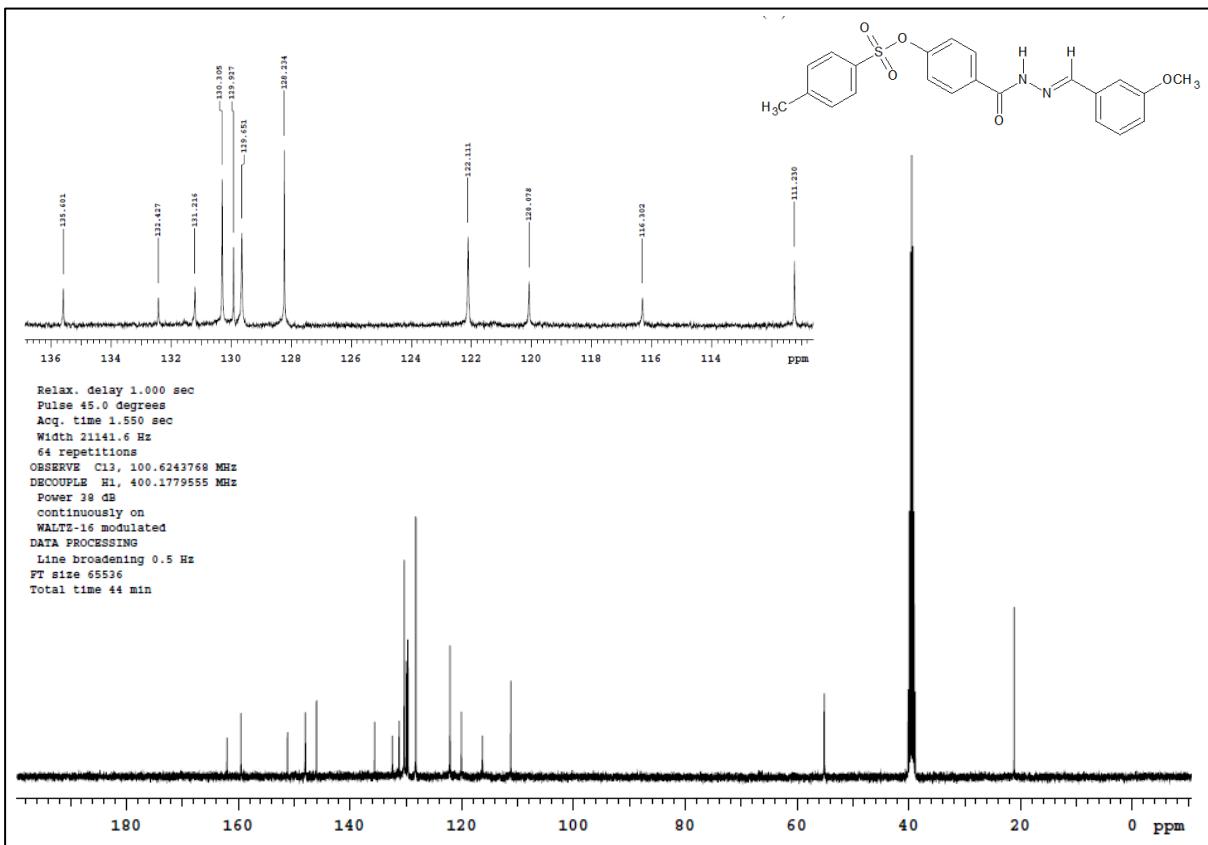


Figure S22. Compound 3f <sup>13</sup>C-NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

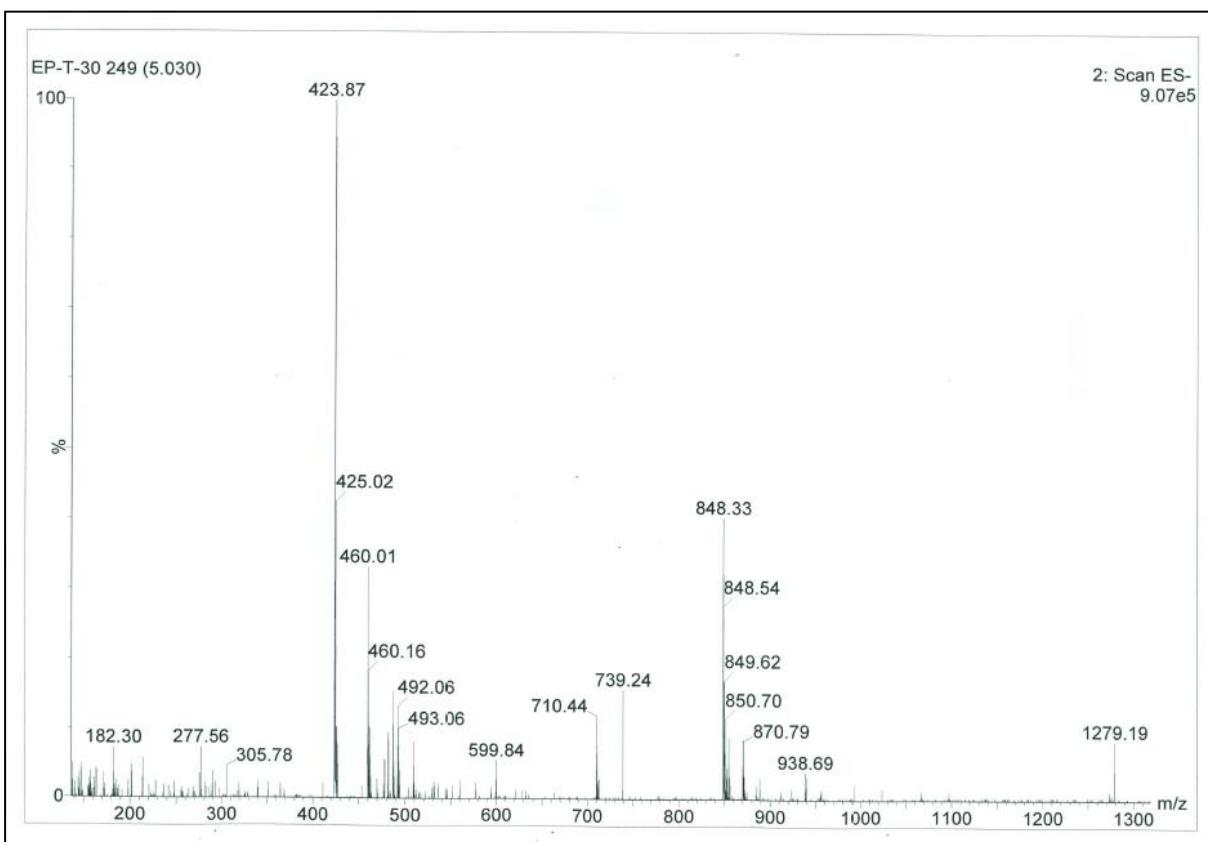
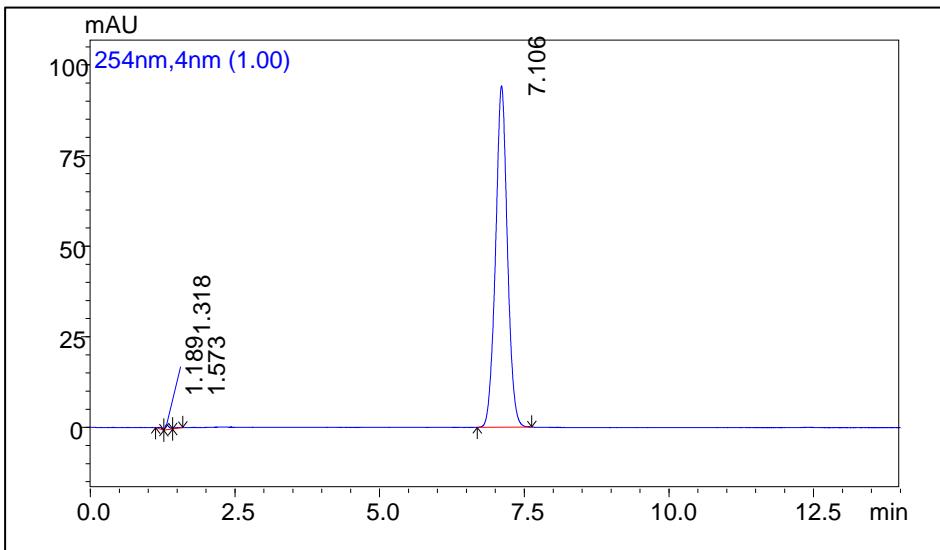
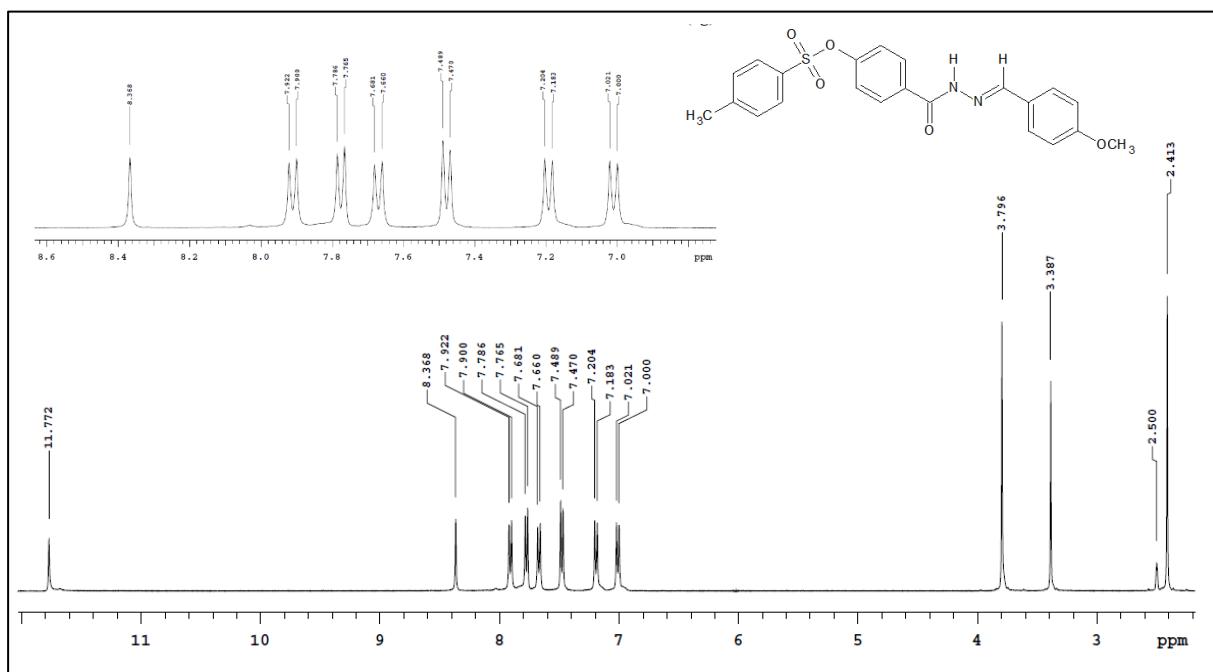
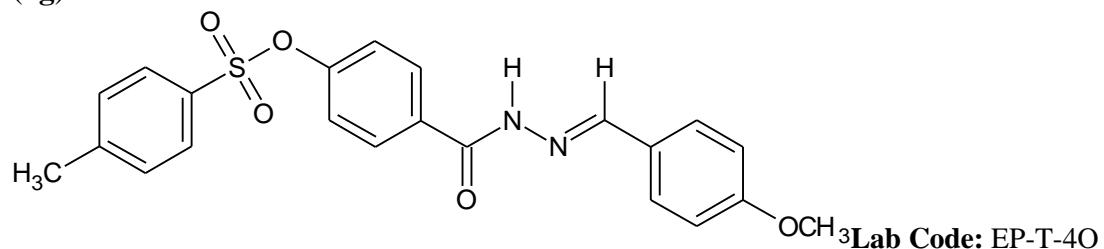


Figure S23. Compound 3f ESI MS spectrum.

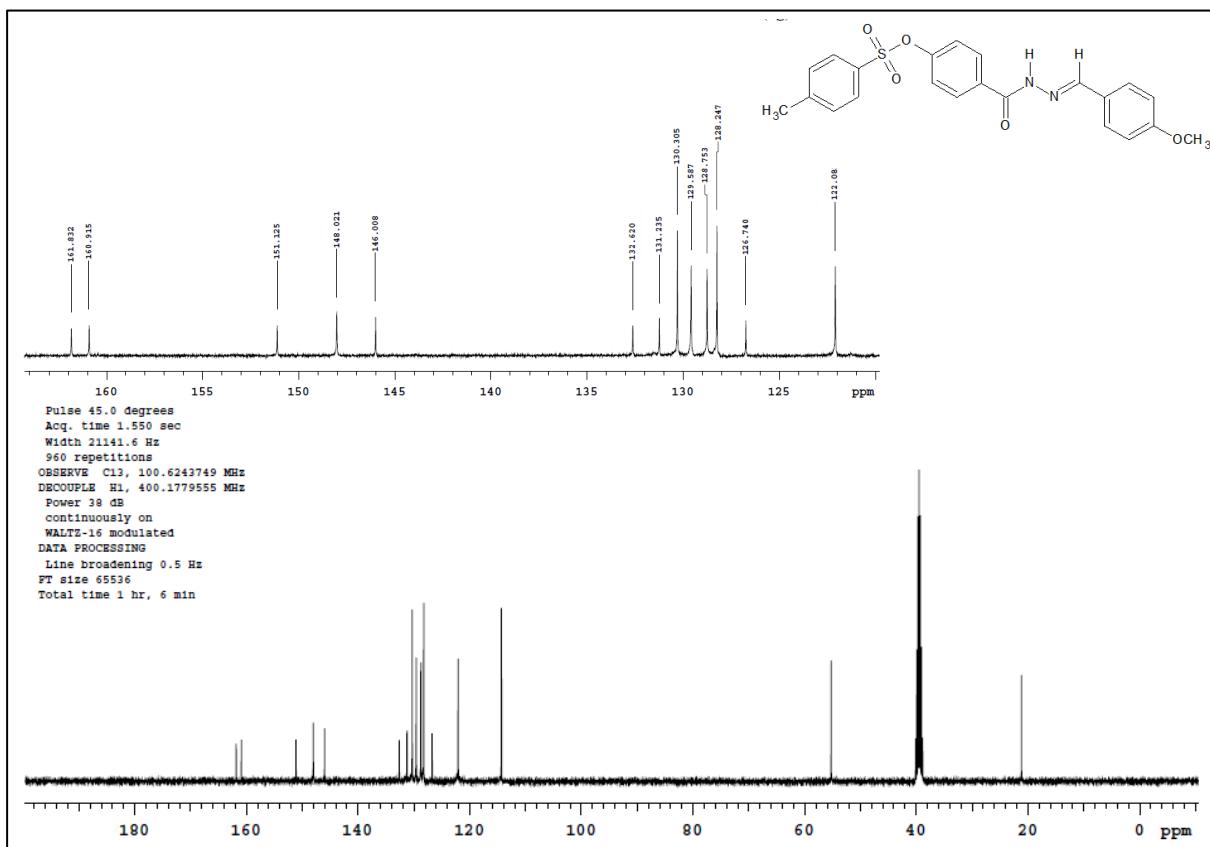


**Figure S24.** Chromatogram of compound **3f** (48 µg/mL) recorded under optimized conditions.

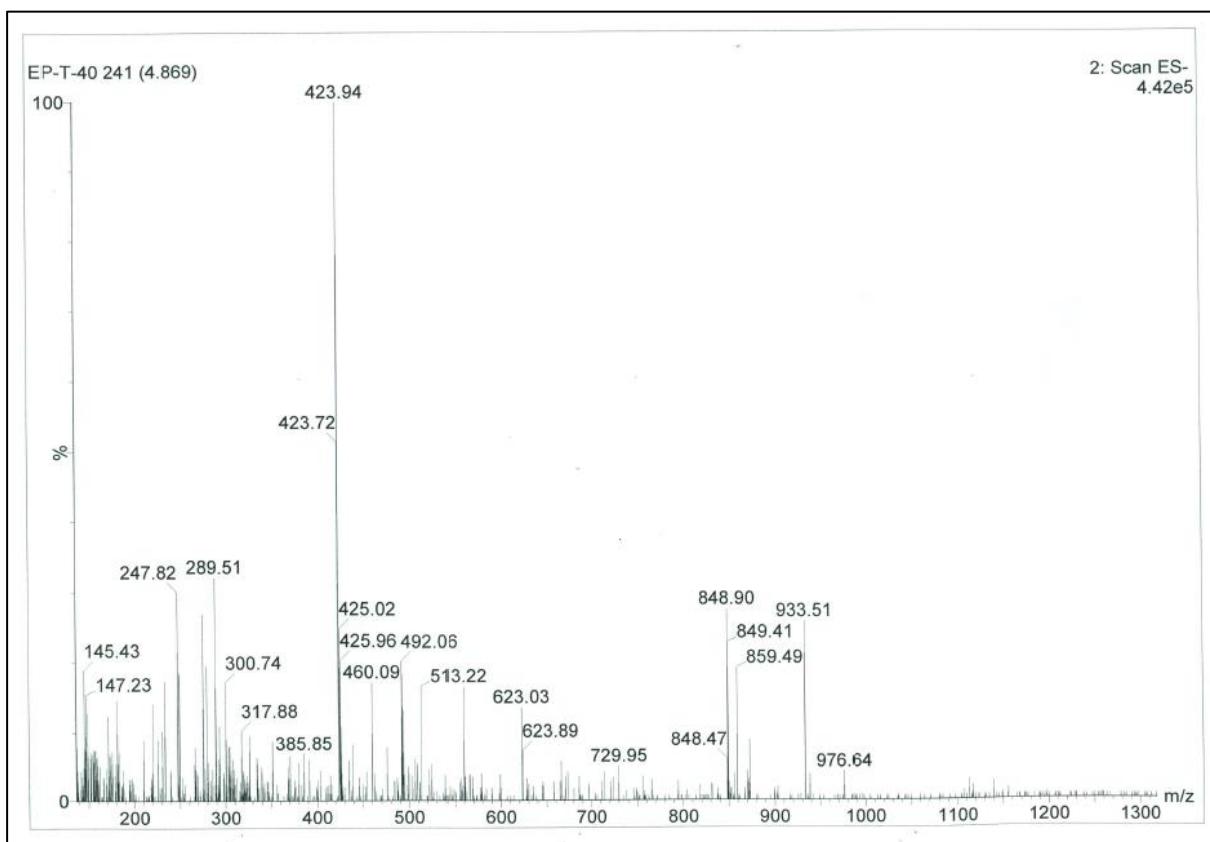
(*E*)-*N'*-[(4-Methoxyphenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3g**)



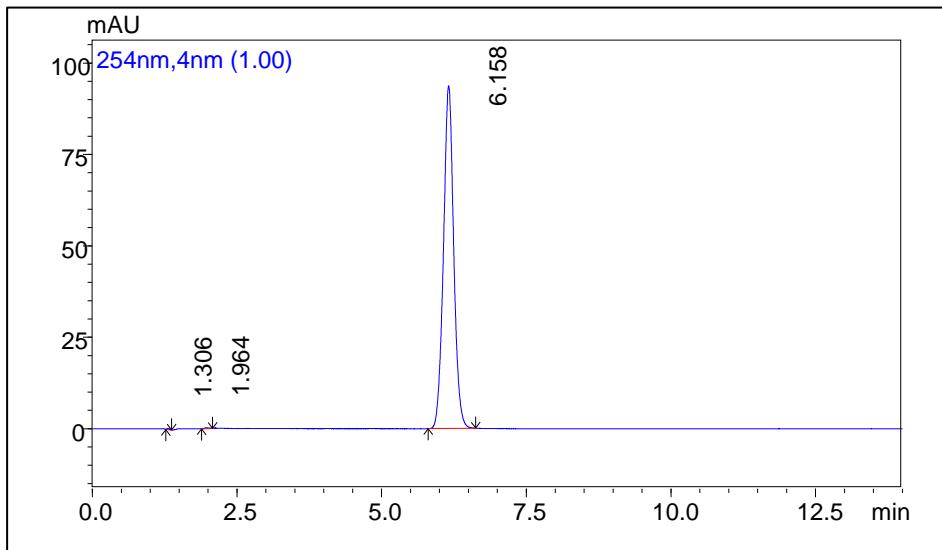
**Figure S25.** Compound **3g**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



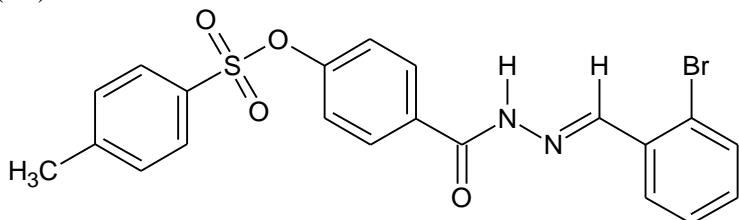
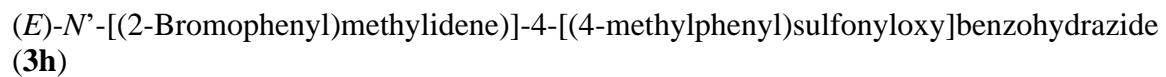
**Figure S26.** Compound **3g**  $^{13}\text{C}$ -NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).



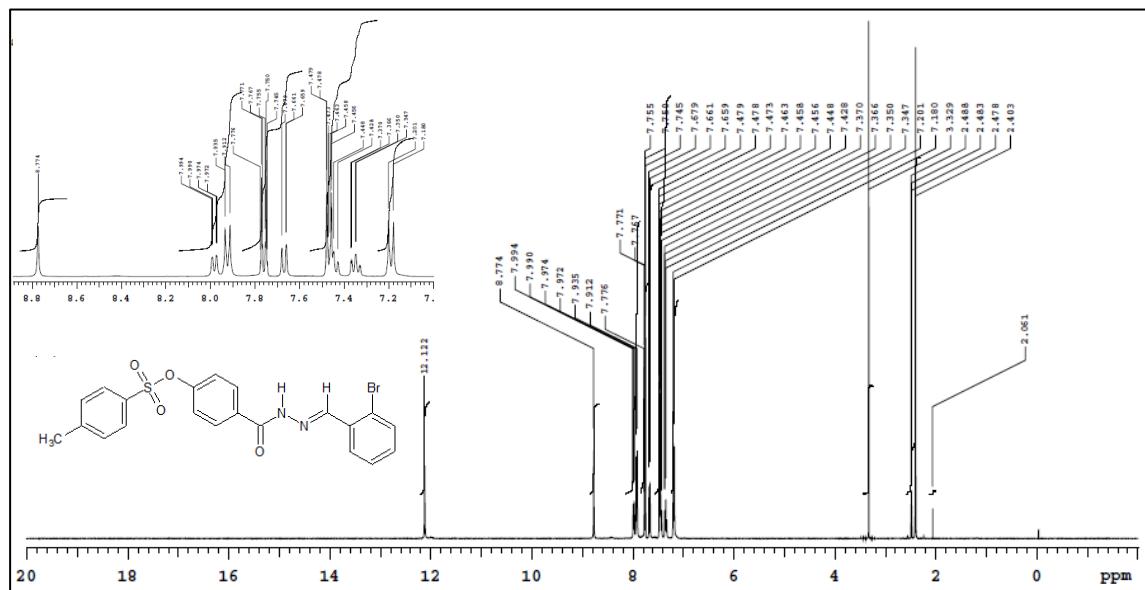
**Figure S27.** Compound **3g** ESI MS spectrum.



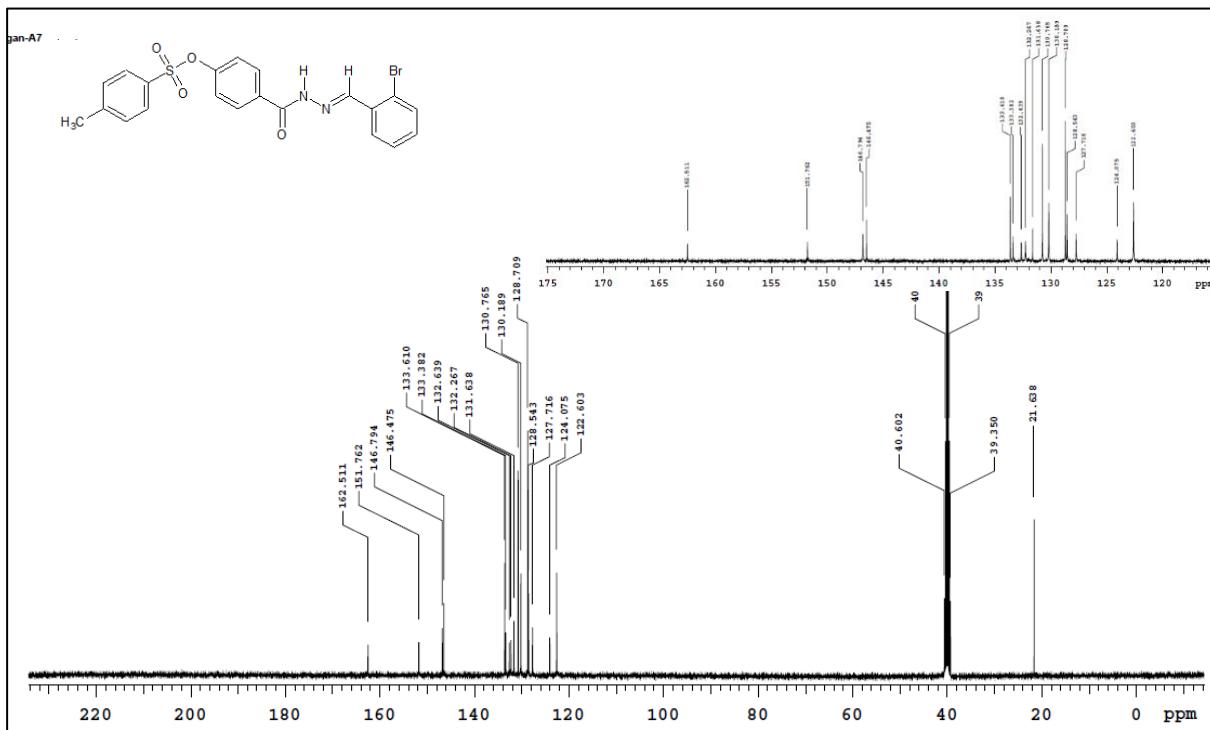
**Figure S28.** Chromatogram of compound **3g** (40 µg/mL) recorded under optimized conditions.



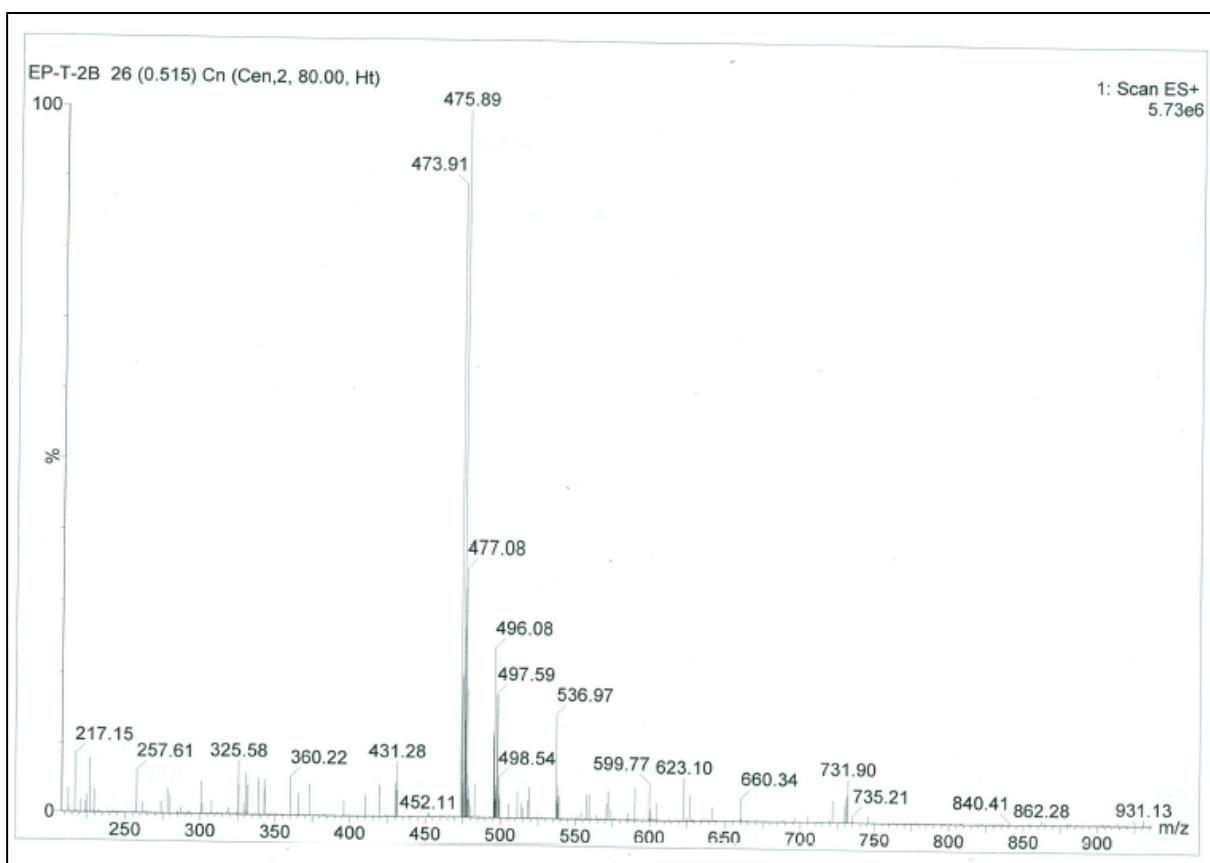
Lab Code: EP-T-2B



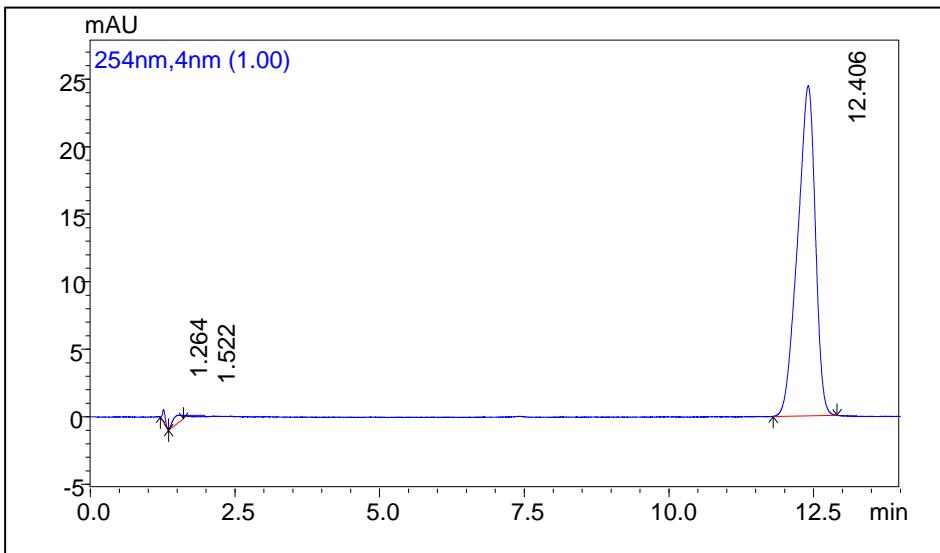
**Figure S29.** Compound **3h**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



**Figure S30.** Compound 3h  $^{13}\text{C}$ -NMR spectrum (DMSO- $\text{d}_6$ , 100 MHz).

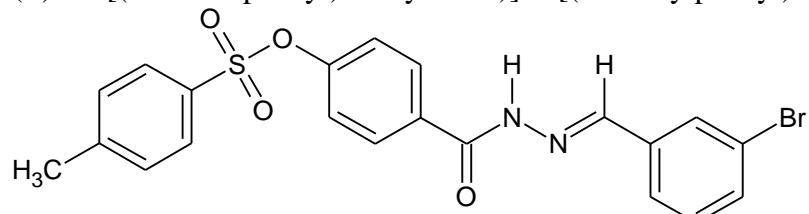


**Figure S31.** Compound 3h ESI MS spectrum.

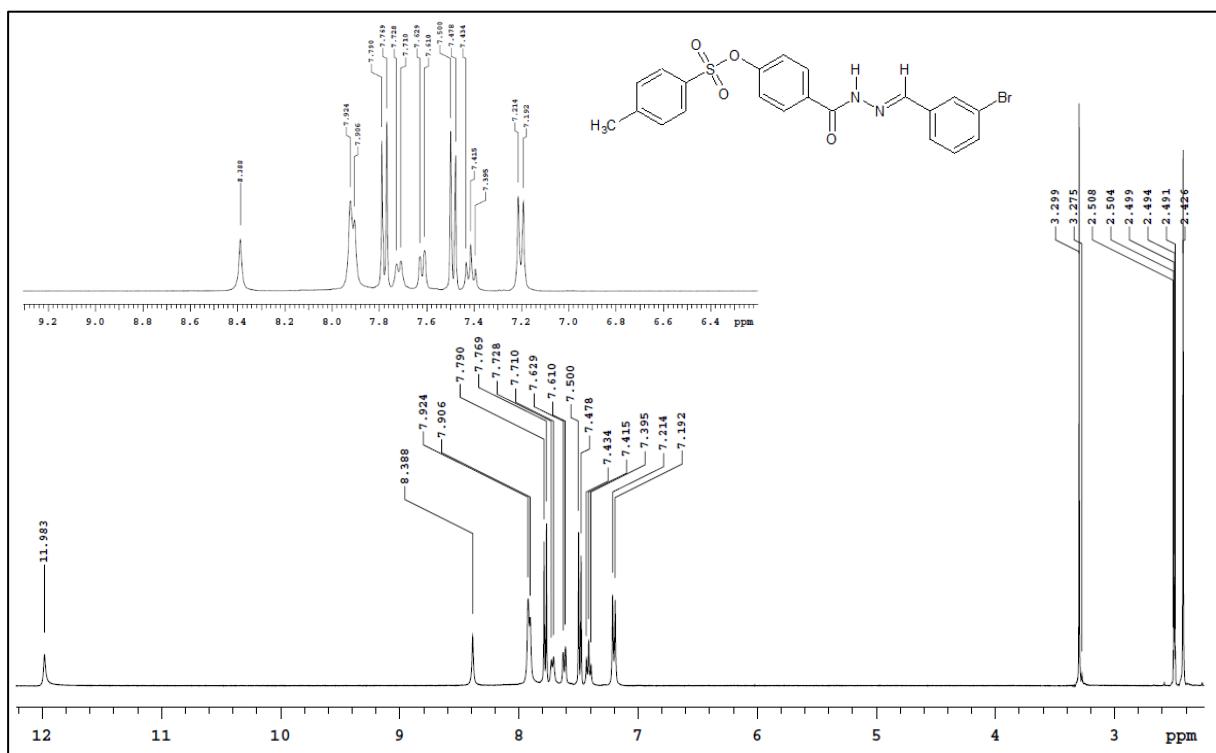


**Figure S32.** Chromatogram of compound **3h** (28 µg/mL) recorded under optimized conditions.

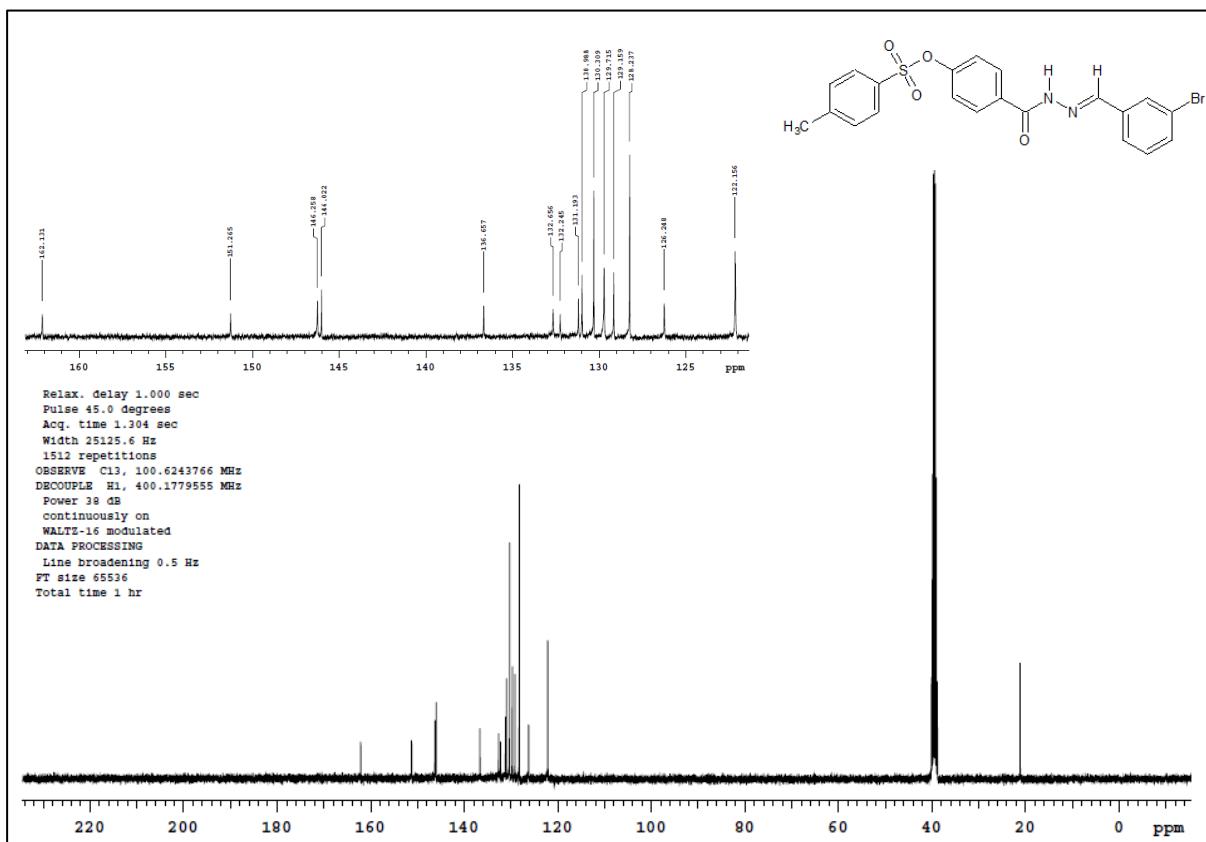
(*E*)-*N'*-[(3-Bromophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3i**)



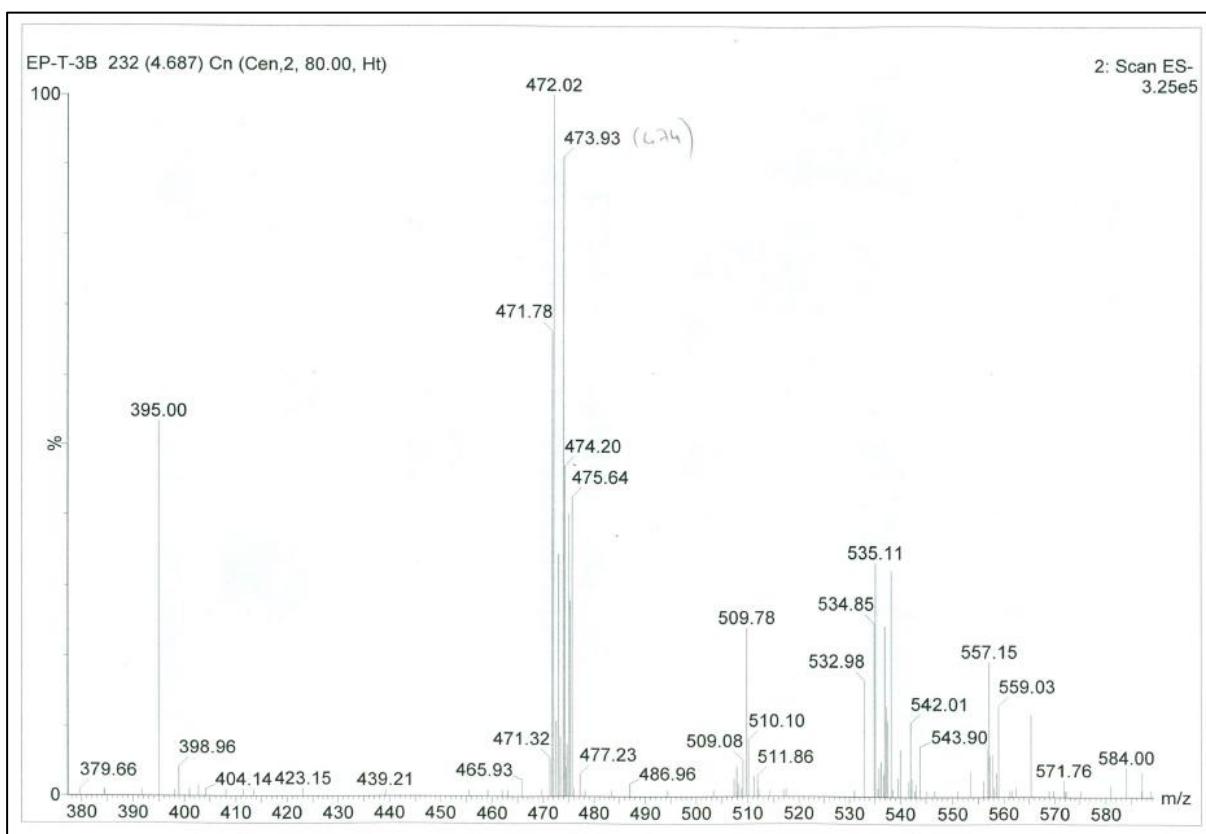
Lab Code: EP-T-3B



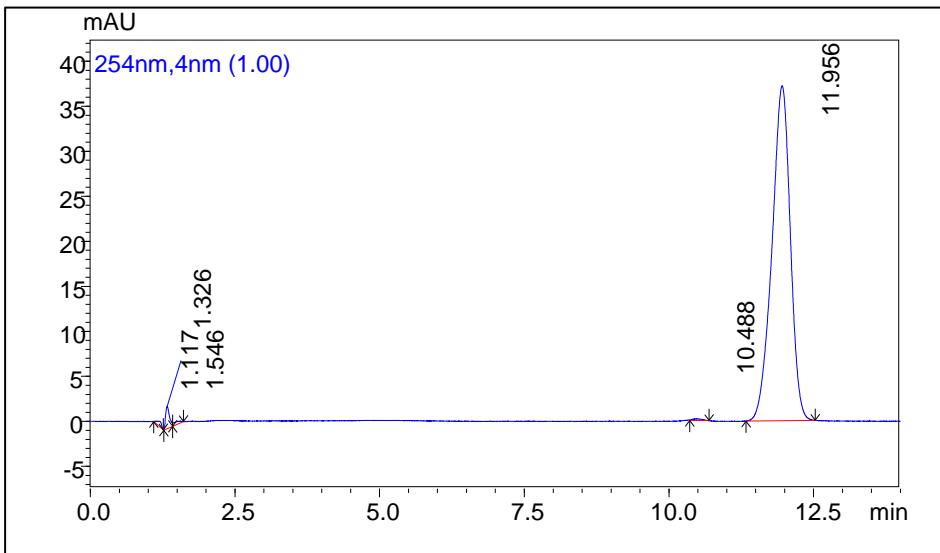
**Figure S33.** Compound **3i**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



**Figure S34.** Compound **3i**  $^{13}\text{C}$ -NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

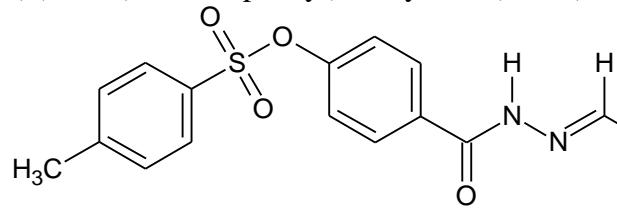


**Figure S35.** Compound **3i** ESI MS spectrum.

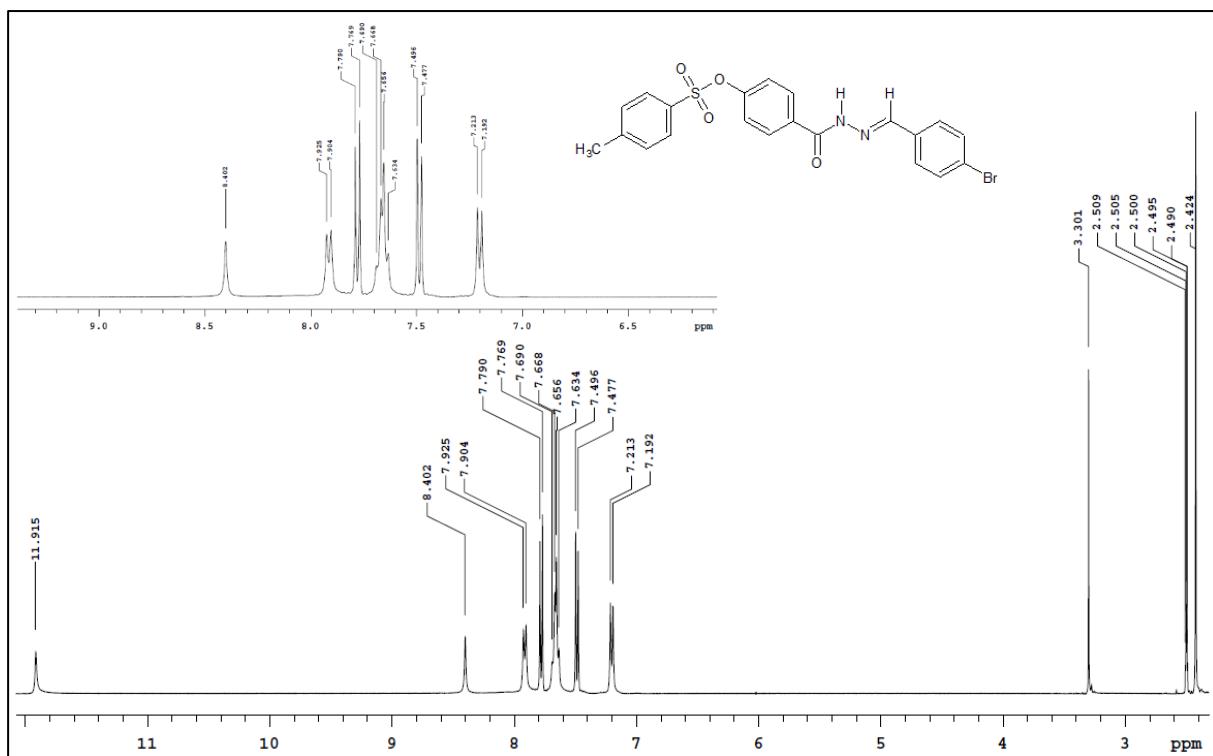


**Figure S36.** Chromatogram of compound **3i** (28 µg/mL) recorded under optimized conditions.

(*E*)-*N'*-[(4-Bromophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3j**)



Lab Code: EP-T-4B



**Figure S37.** Compound **3j** <sup>1</sup>H-NMR spectrum (DMSO-d<sub>6</sub>, 400 MHz).

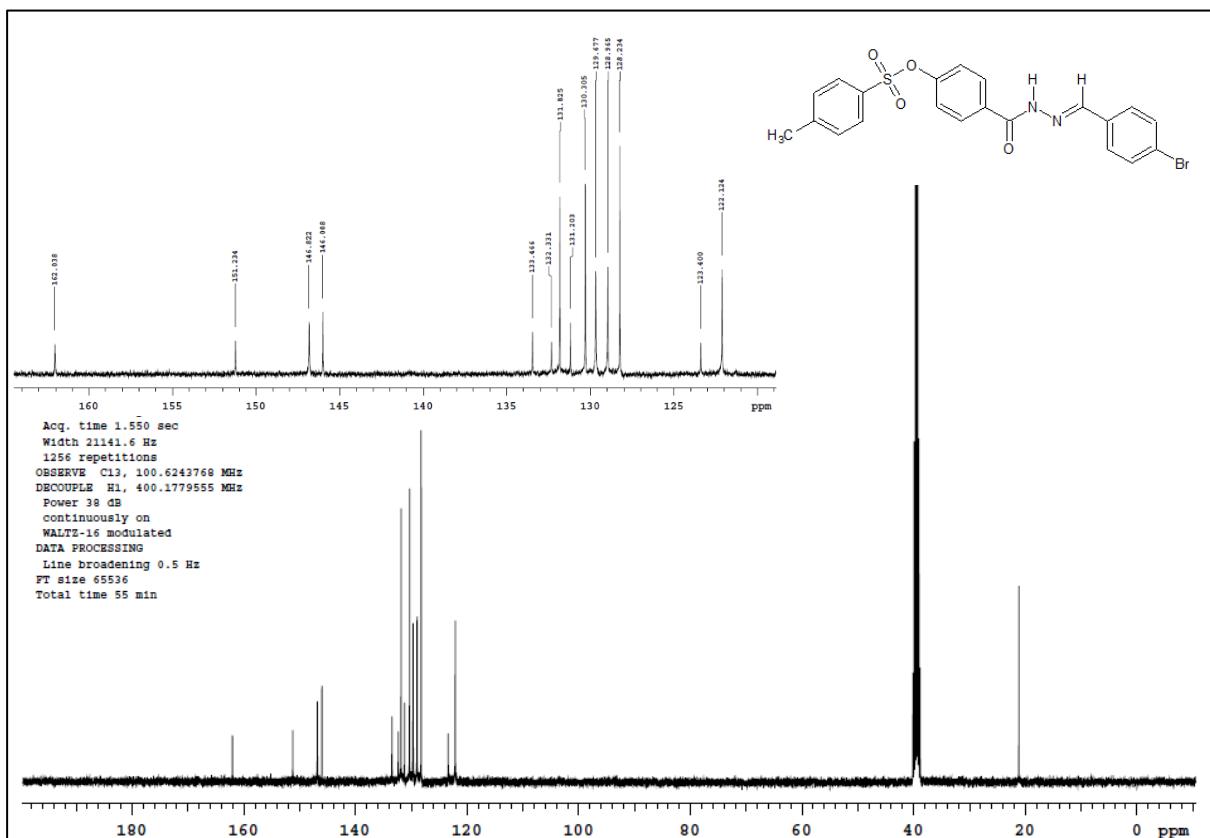


Figure S38. Compound 3j <sup>13</sup>C-NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

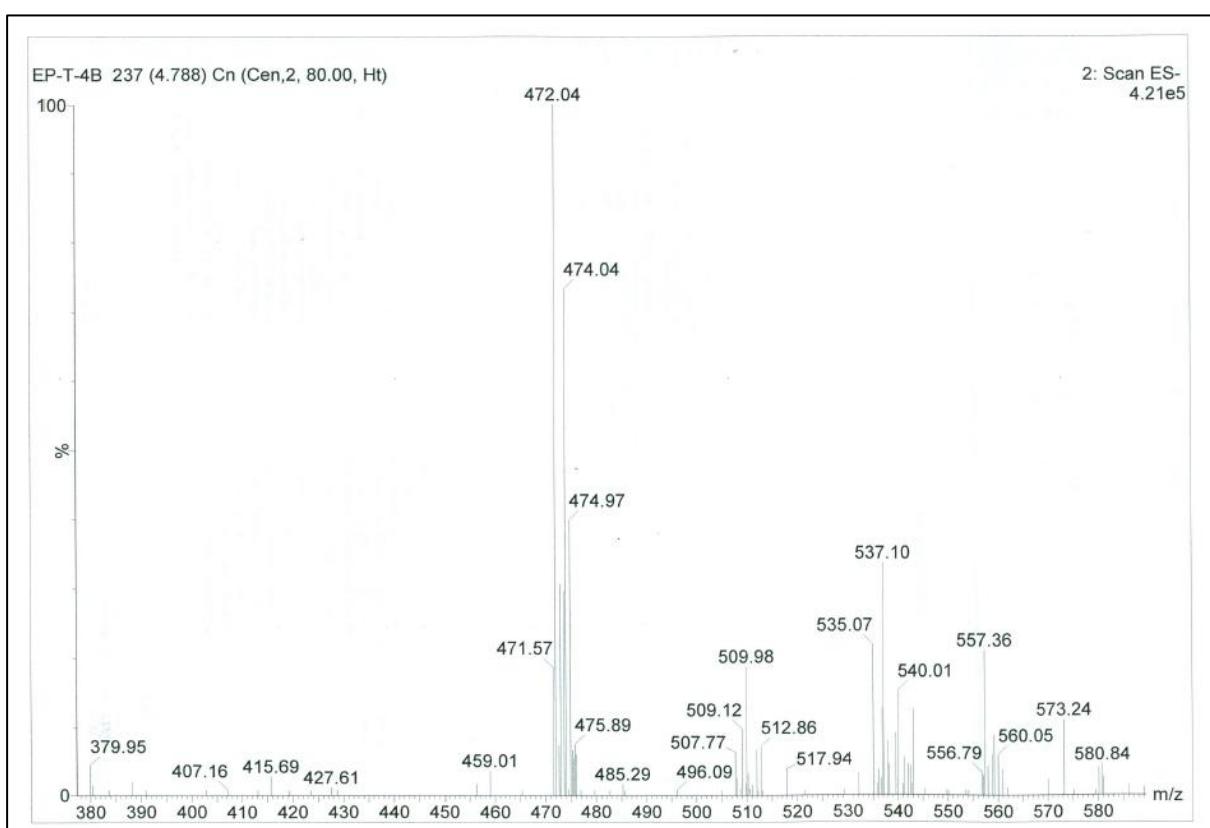
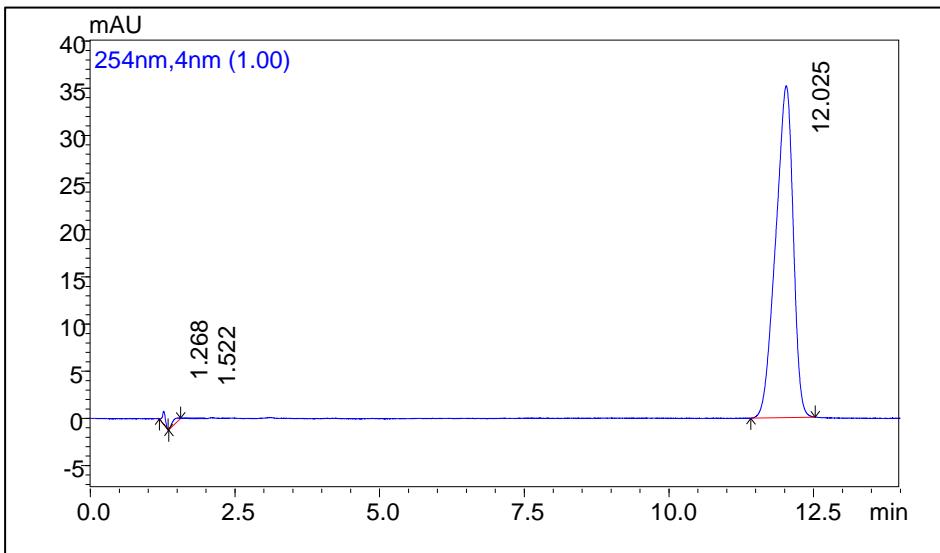
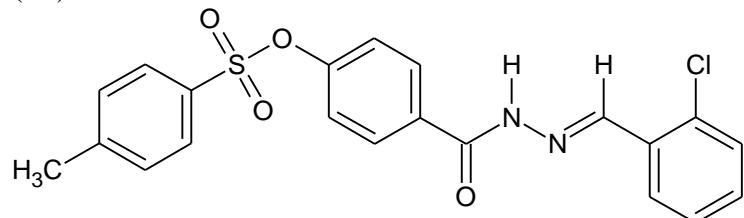


Figure S39. Compound 3j ESI MS spectrum.

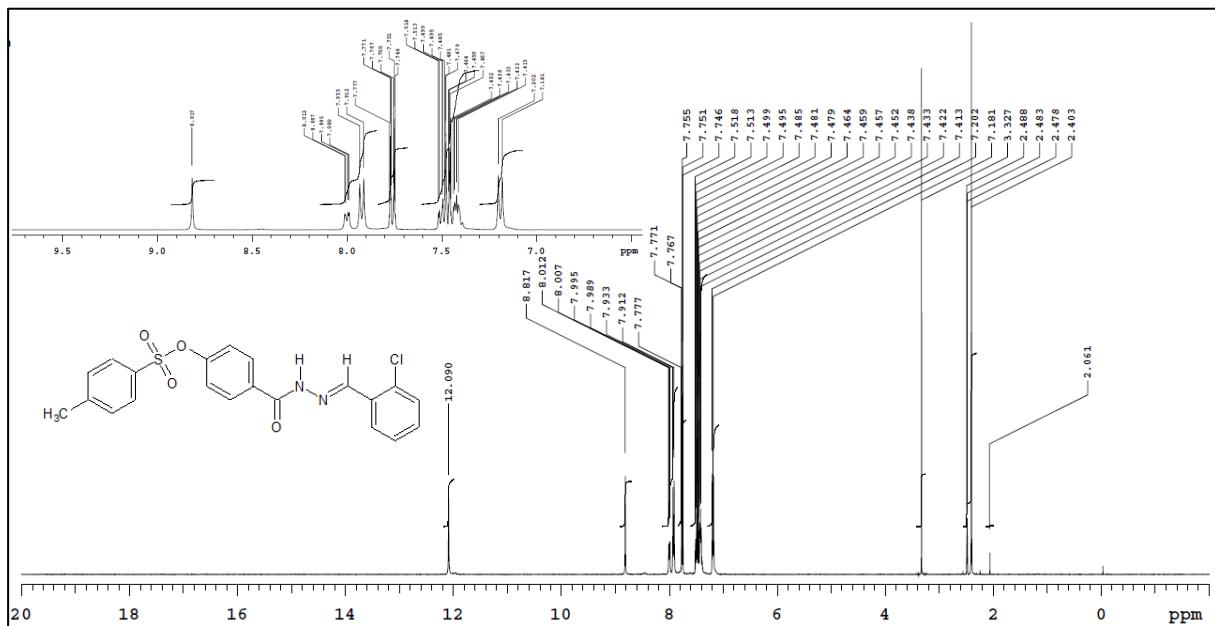


**Figure S40.** Chromatogram of compound **3j** (44 µg/mL) recorded under optimized conditions.

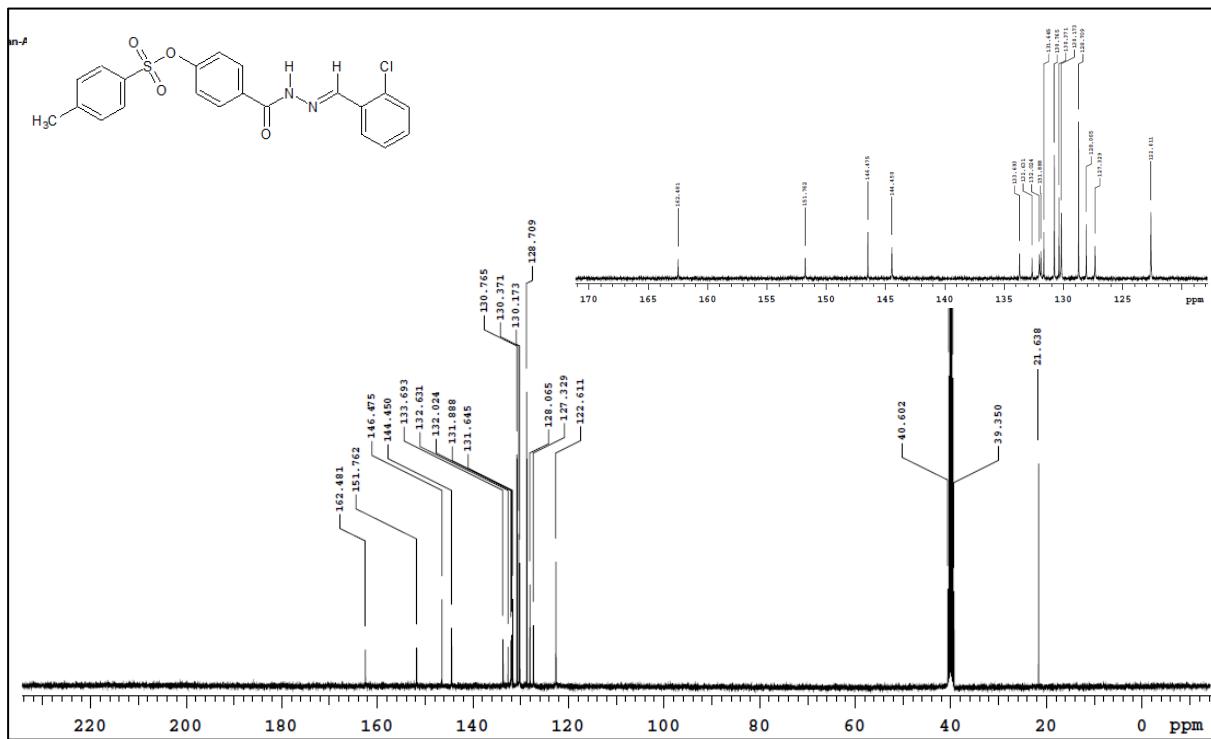
(*E*)-*N'*-[(2-Chlorophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3k**)



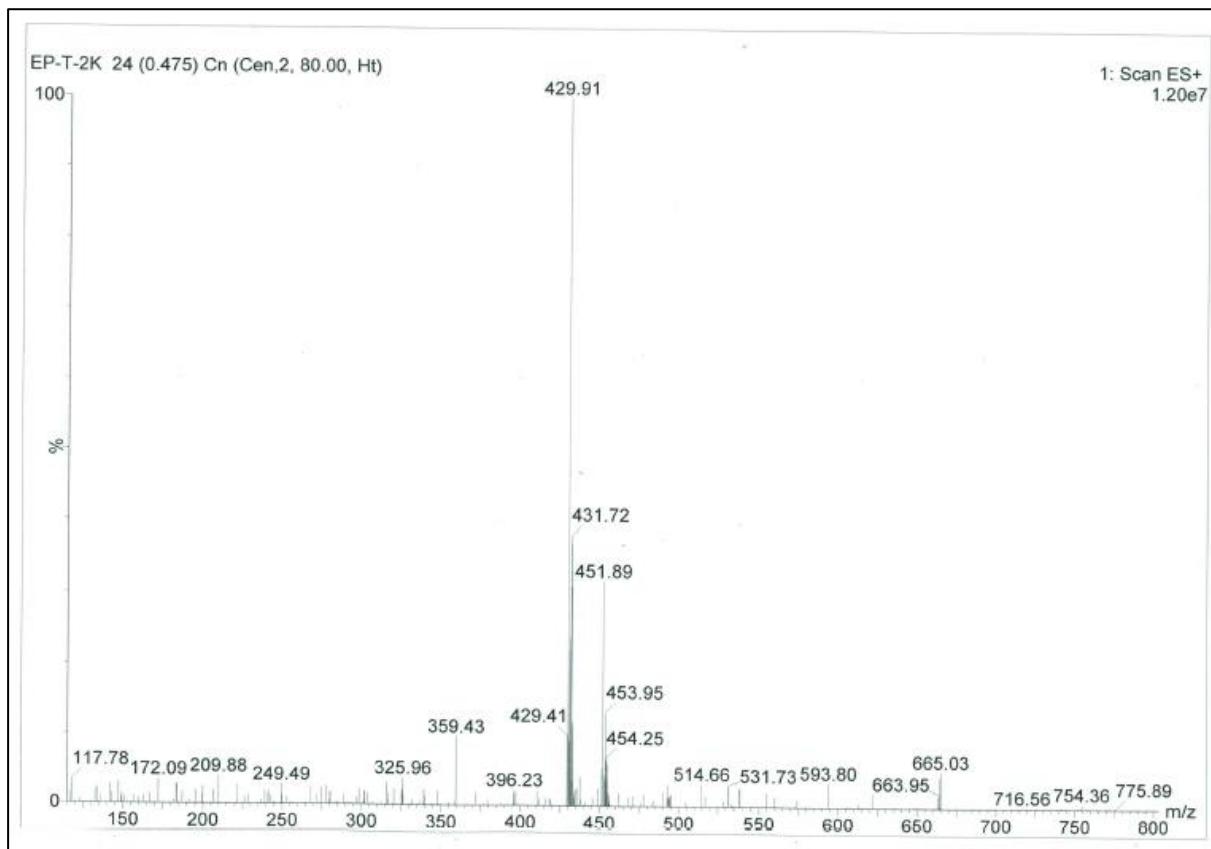
Lab Code: EP-T-2K



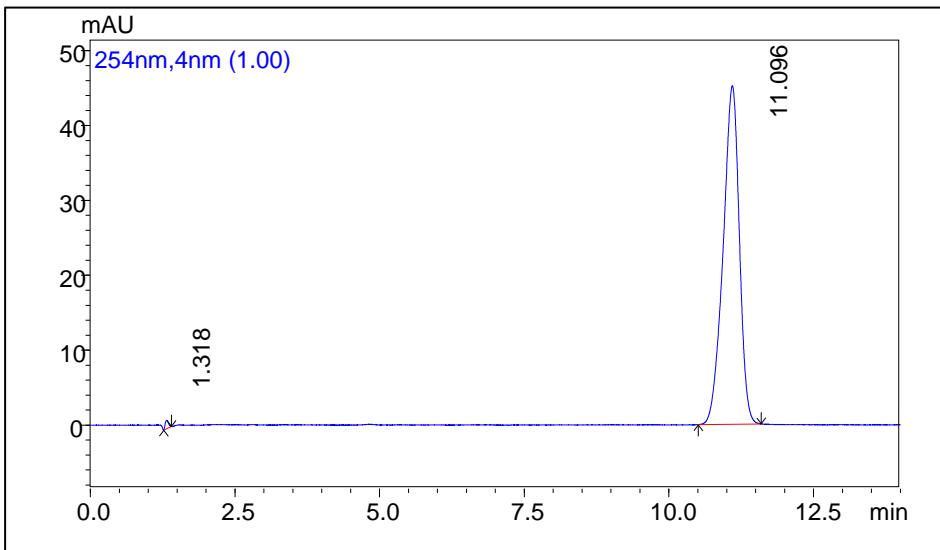
**Figure S41.** Compound **3k** <sup>1</sup>H-NMR spectrum (DMSO-d<sub>6</sub>, 400 MHz).



**Figure S42.** Compound **3k**  $^{13}\text{C}$ -NMR spectrum (DMSO- $\text{d}_6$ , 100 MHz).

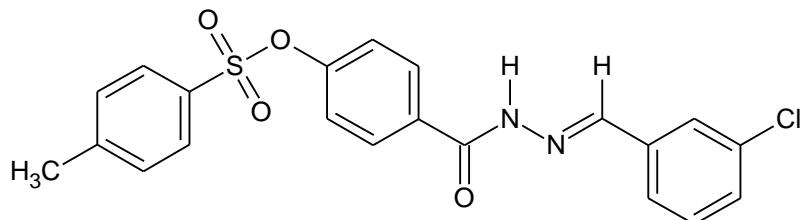


**Figure S43.** Compound **3k** ESI MS spectrum.

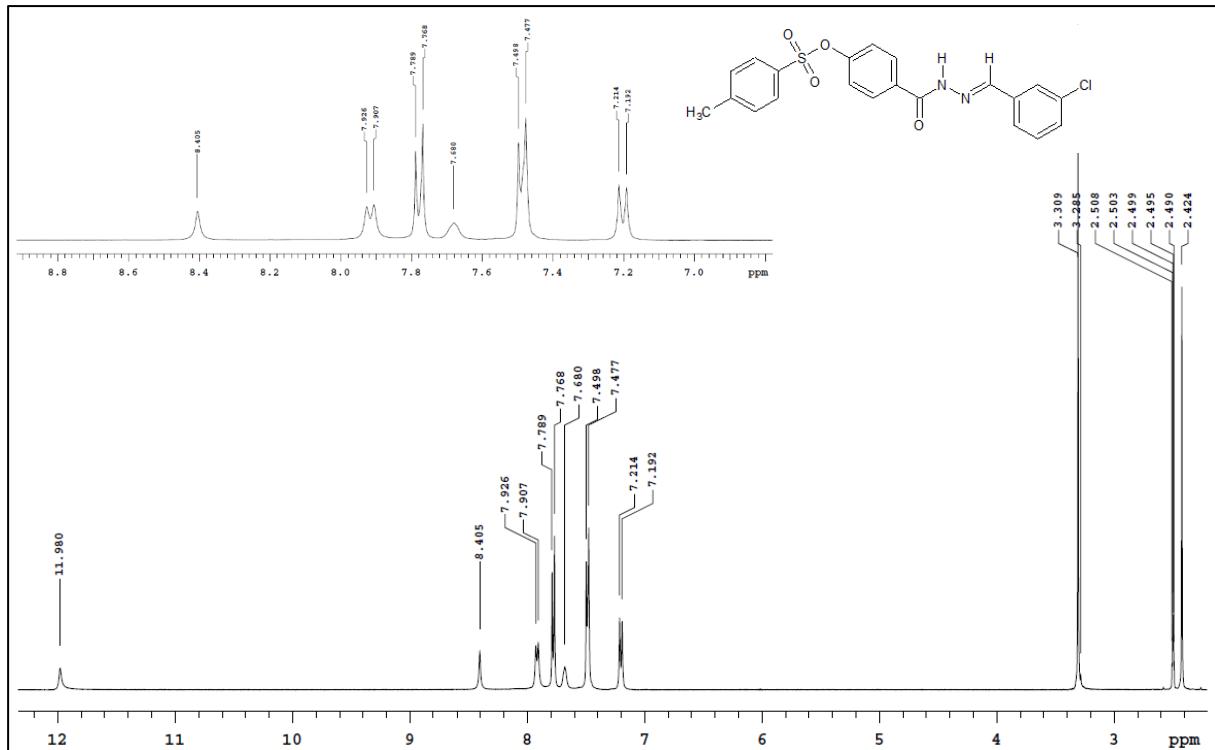


**Figure S44.** Chromatogram of compound **3k** (56 µg/mL) recorded under optimized conditions.

(*E*)-*N'*-[(3-Chlorophenyl)methylidene)]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3l**)



Lab Code: EP-T-3K



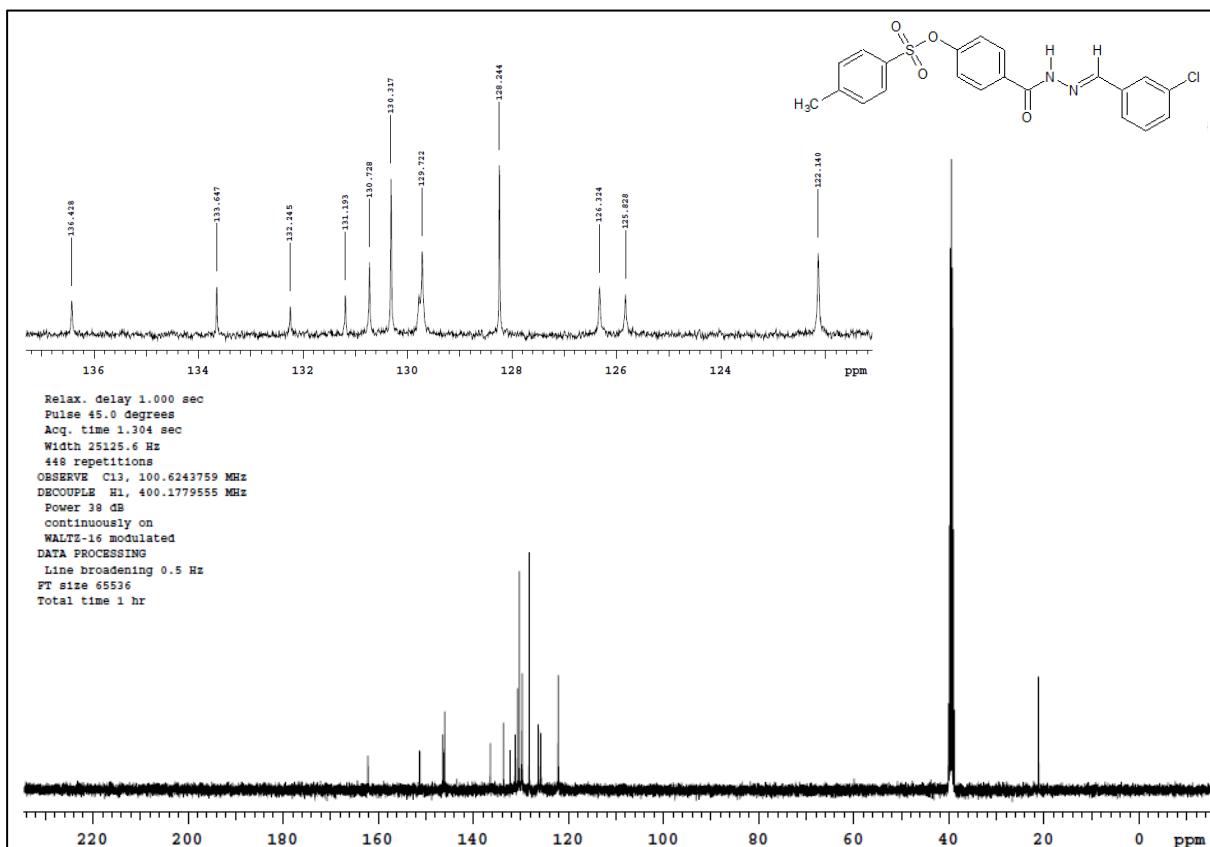


Figure S46. Compound 3l <sup>13</sup>C-NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

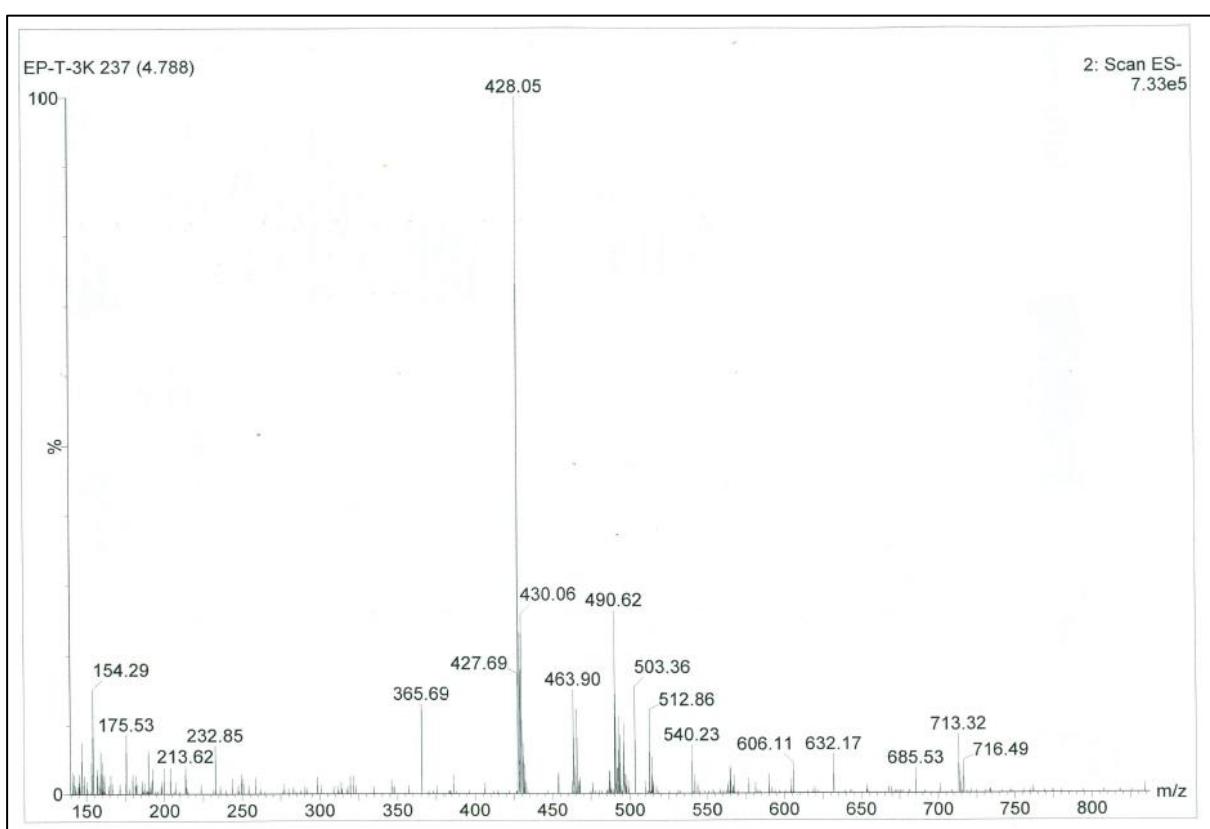
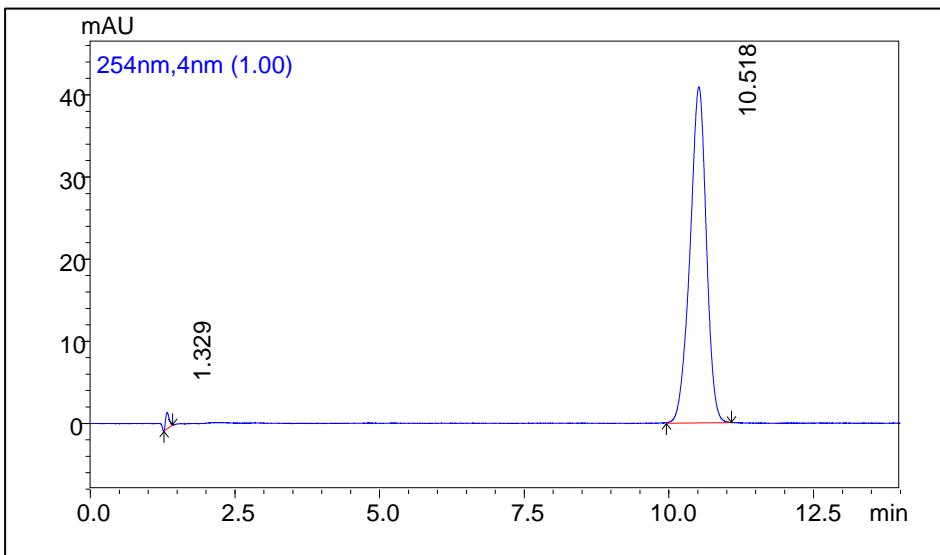
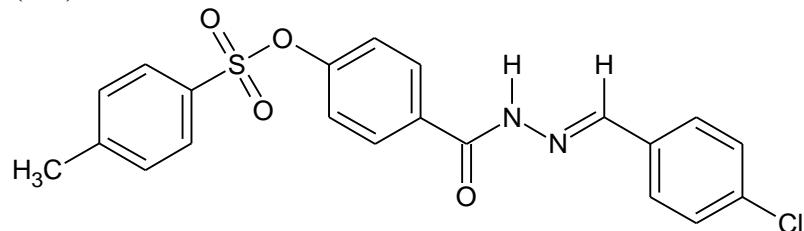


Figure S47. Compound 3l ESI MS spectrum.

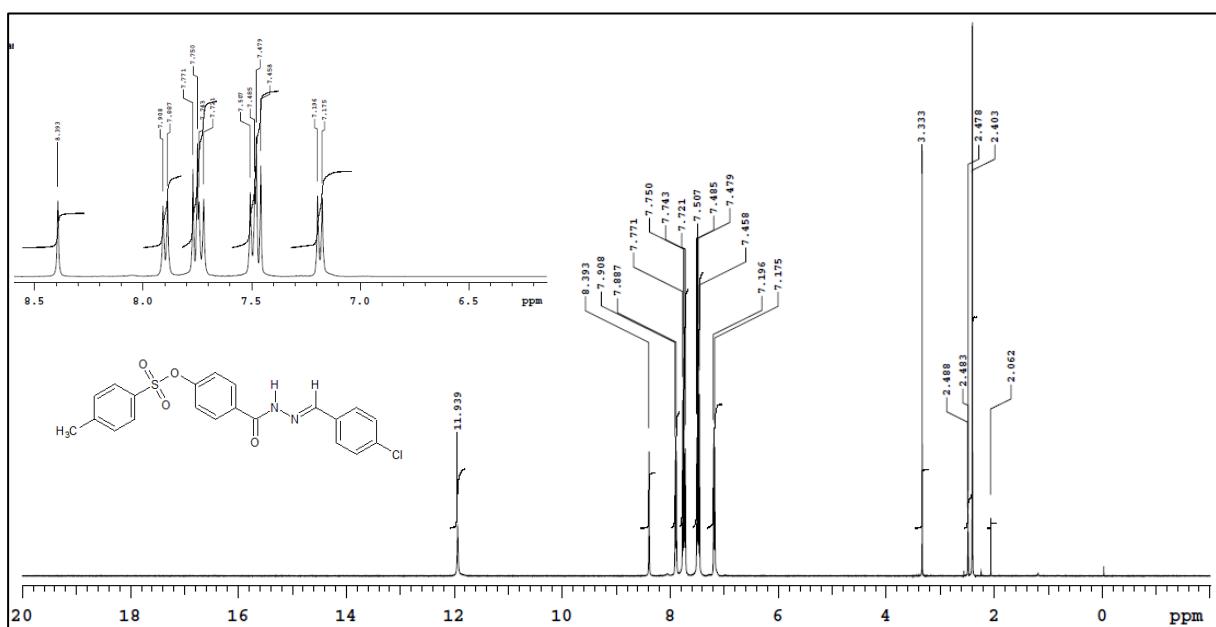


**Figure S48.** Chromatogram of compound **3l** (64  $\mu$ g/mL) recorded under optimized conditions.

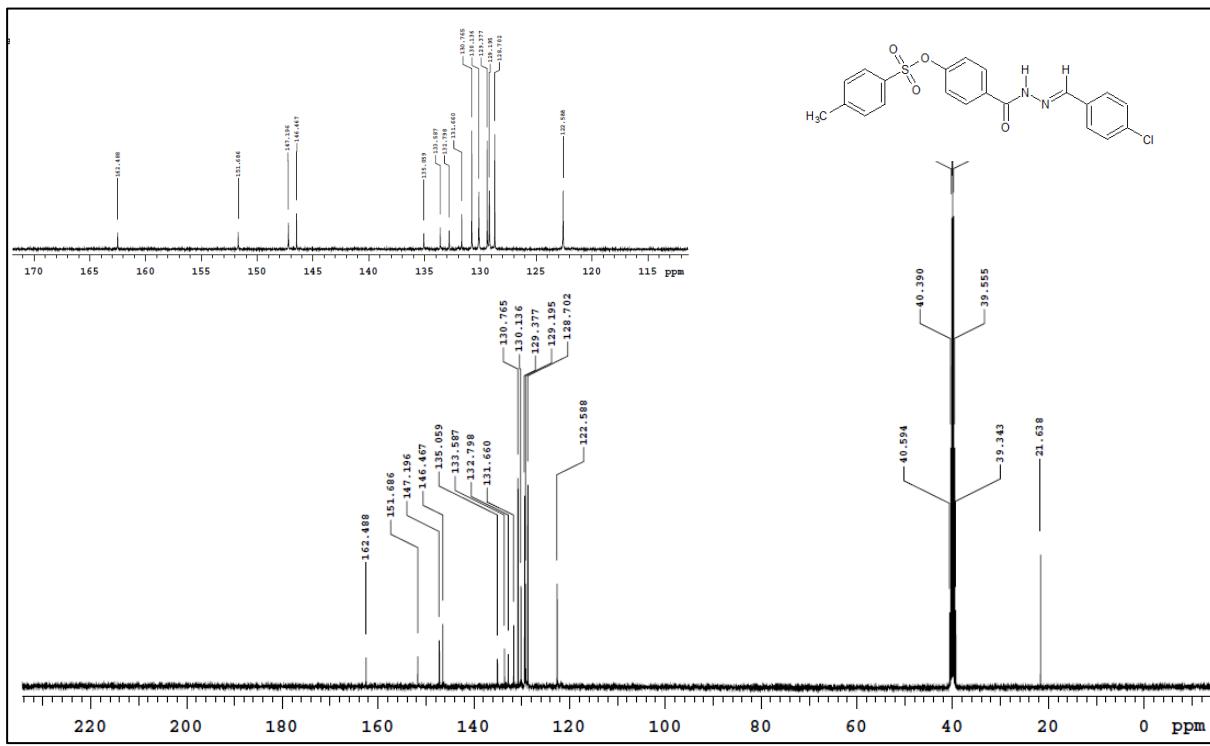
(*E*)-*N'*-[(4-Chlorophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3m**)



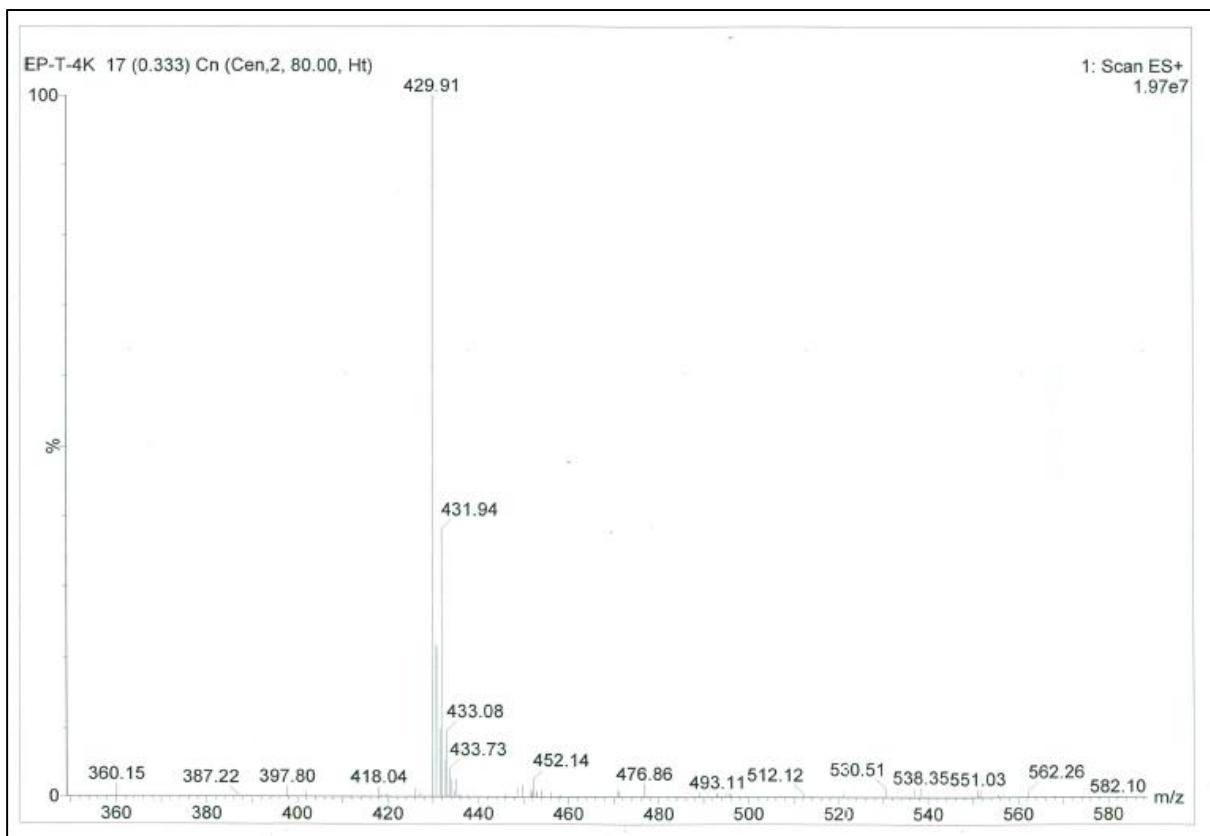
Lab Code: EP-T-4K



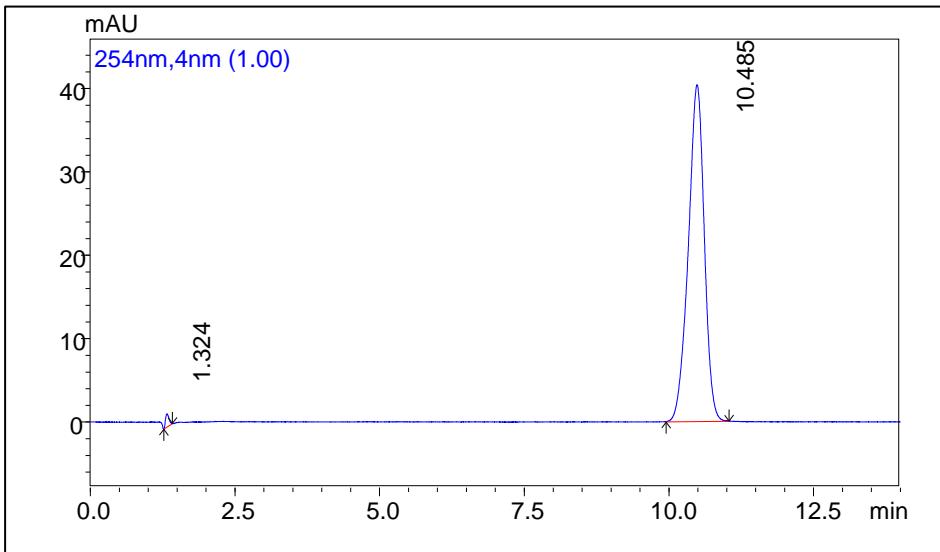
**Figure S49.** Compound **3m**  $^1\text{H}$ -NMR spectrum (DMSO- $d_6$ , 400 MHz).



**Figure S50.** Compound **3m**  $^{13}\text{C}$ -NMR spectrum (DMSO- $\text{d}_6$ , 100 MHz).

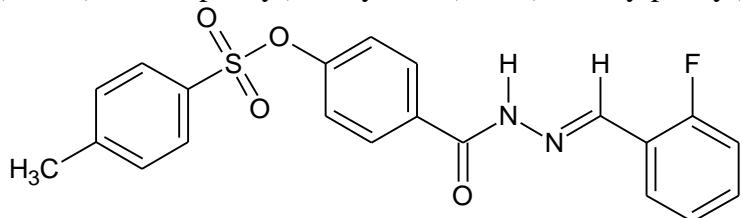


**Figure S51.** Compound **3m** ESI MS spectrum.

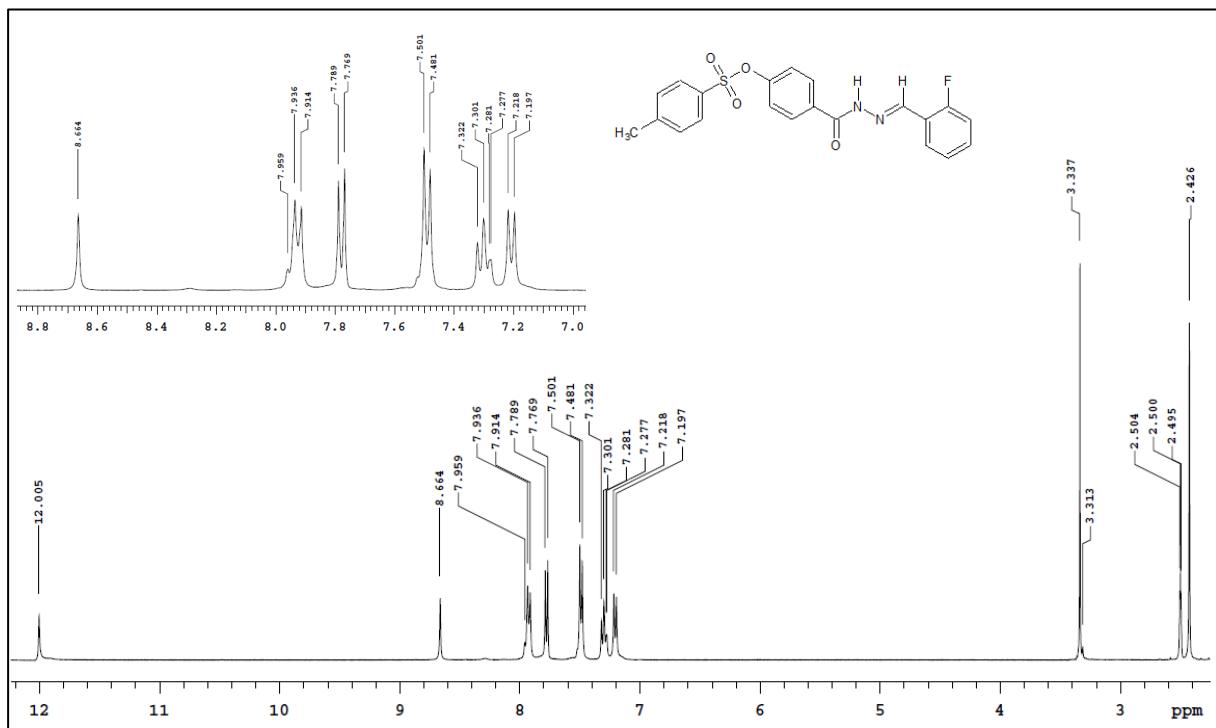


**Figure S52.** Chromatogram of compound **3m** (40 µg/mL) recorded under optimized conditions.

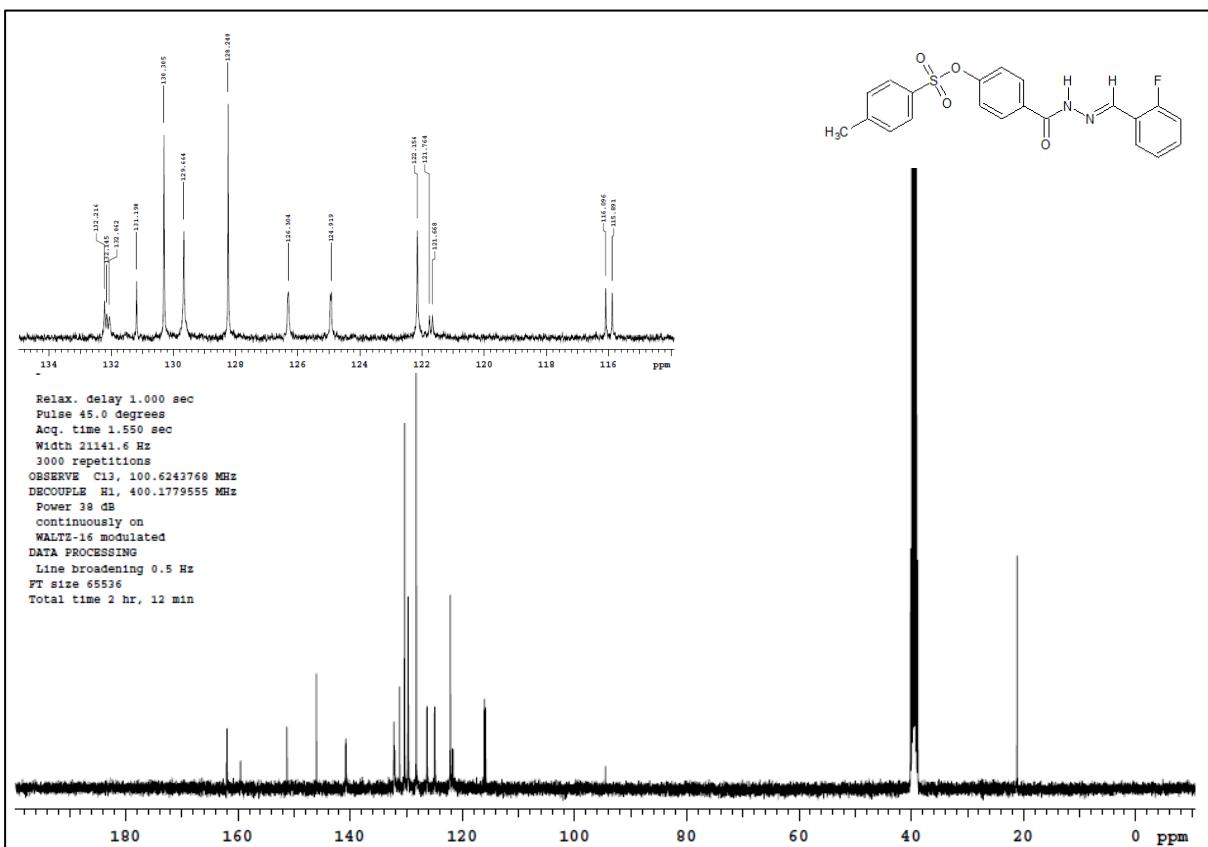
(*E*)-*N'*-[(2-Fluorophenyl)methyldene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3n**)



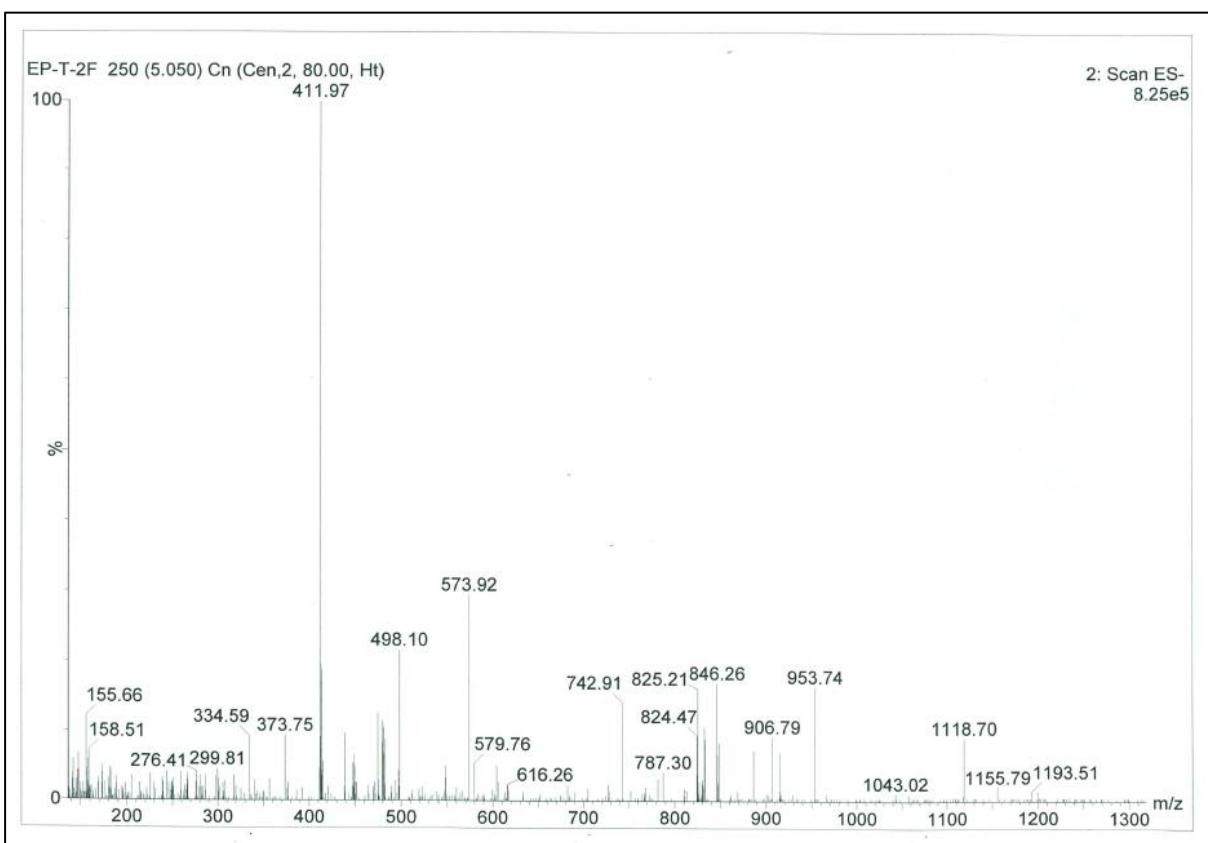
Lab Code: EP-T-2F



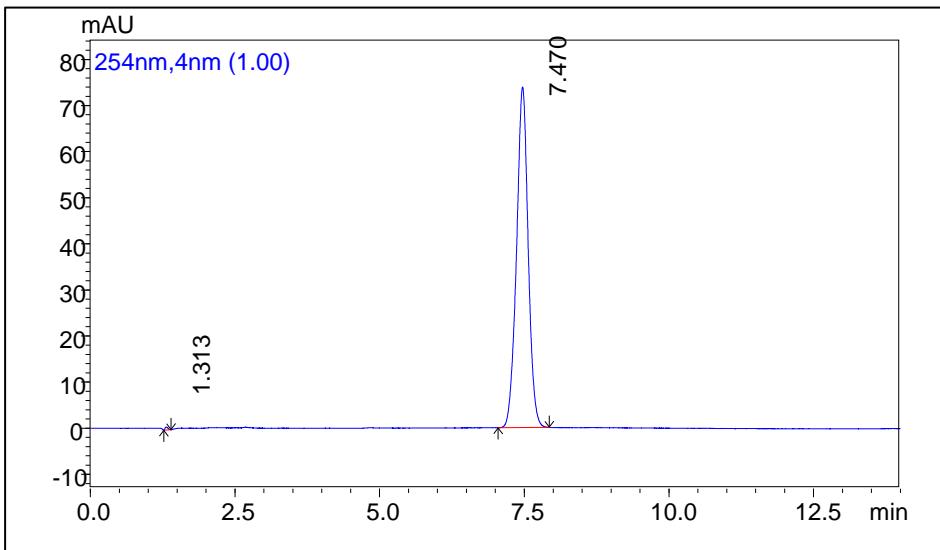
**Figure S53.** Compound **3n**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



**Figure S54.** Compound **3n**  $^{13}\text{C}$ -NMR spectrum (DMSO- $\text{d}_6$ , 100 MHz).

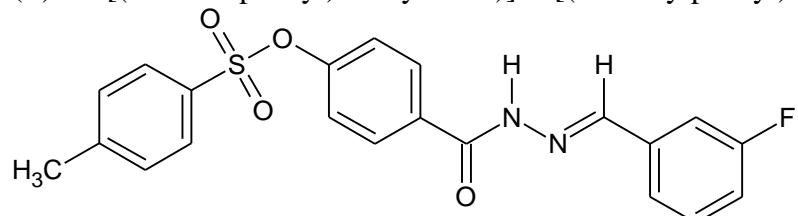


**Figure S55.** Compound **3n** ESI MS spectrum.

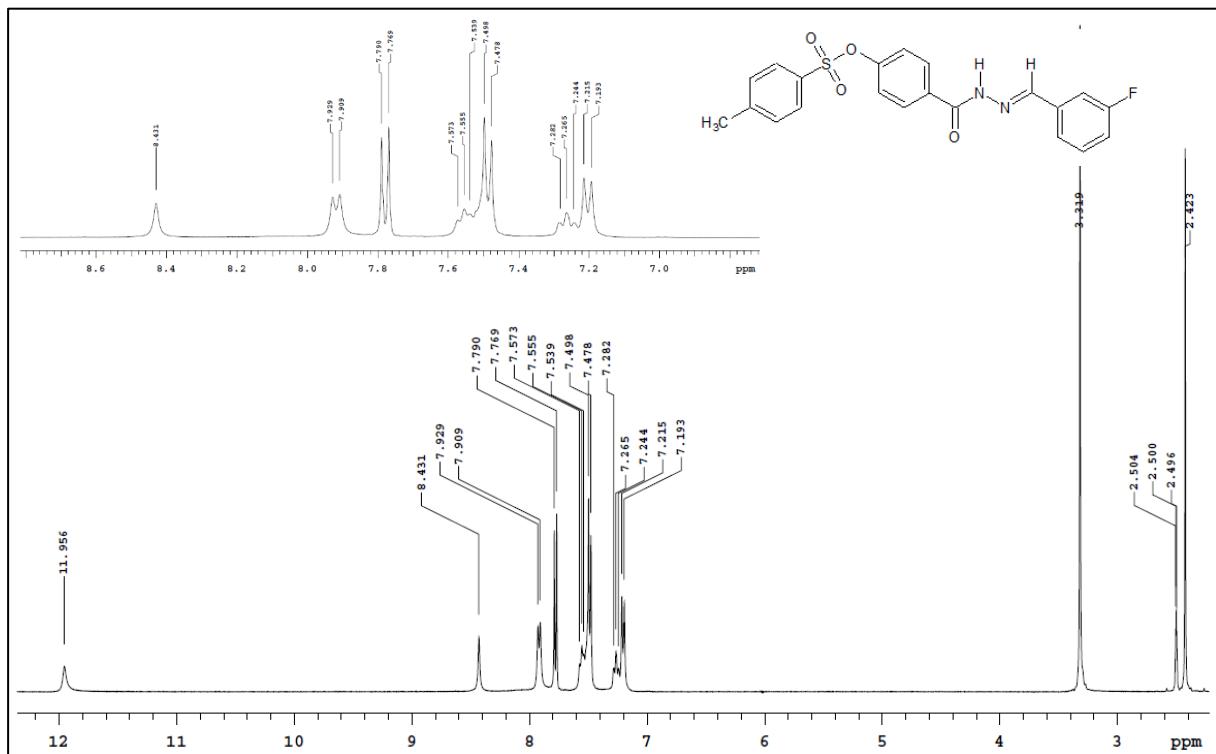


**Figure S56.** Chromatogram of compound **3n** (36 µg/mL) recorded under optimized conditions.

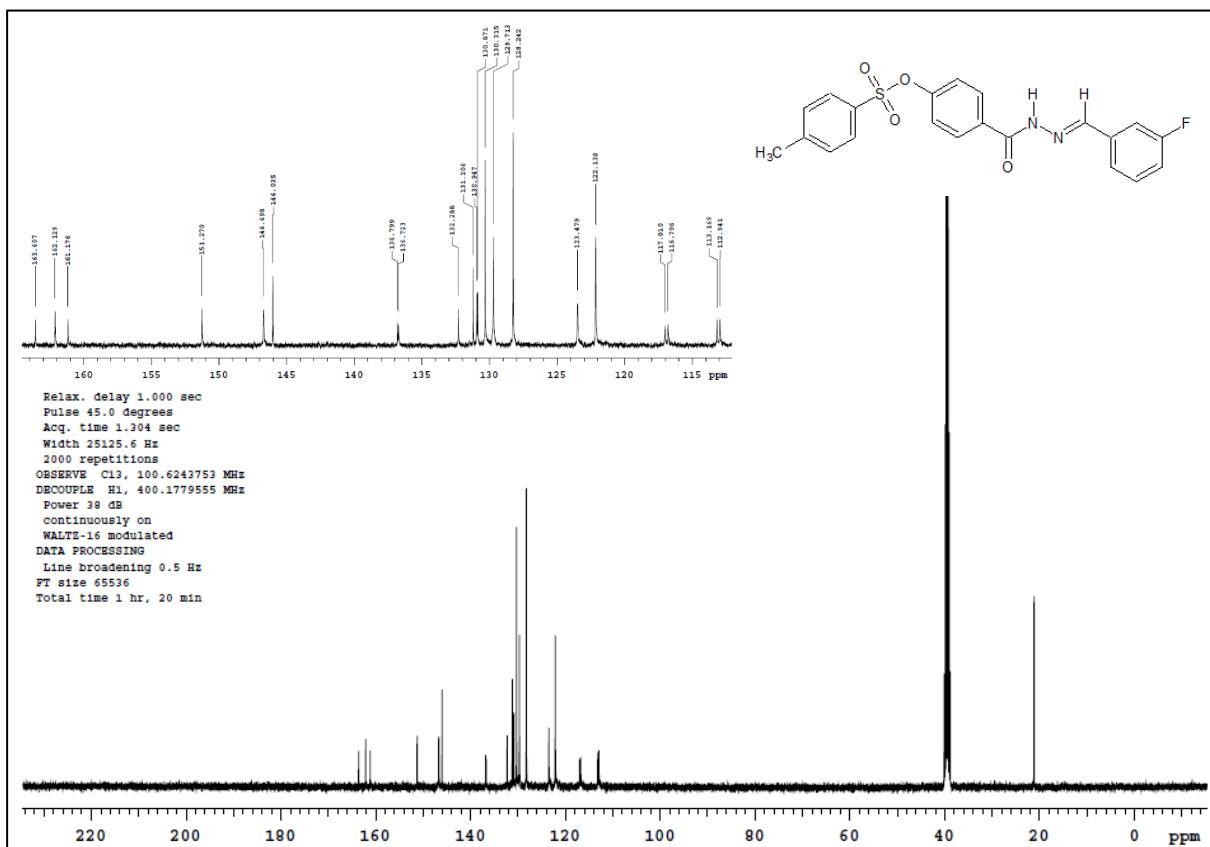
(*E*)-*N'*-[(3-Fluorophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3o**)



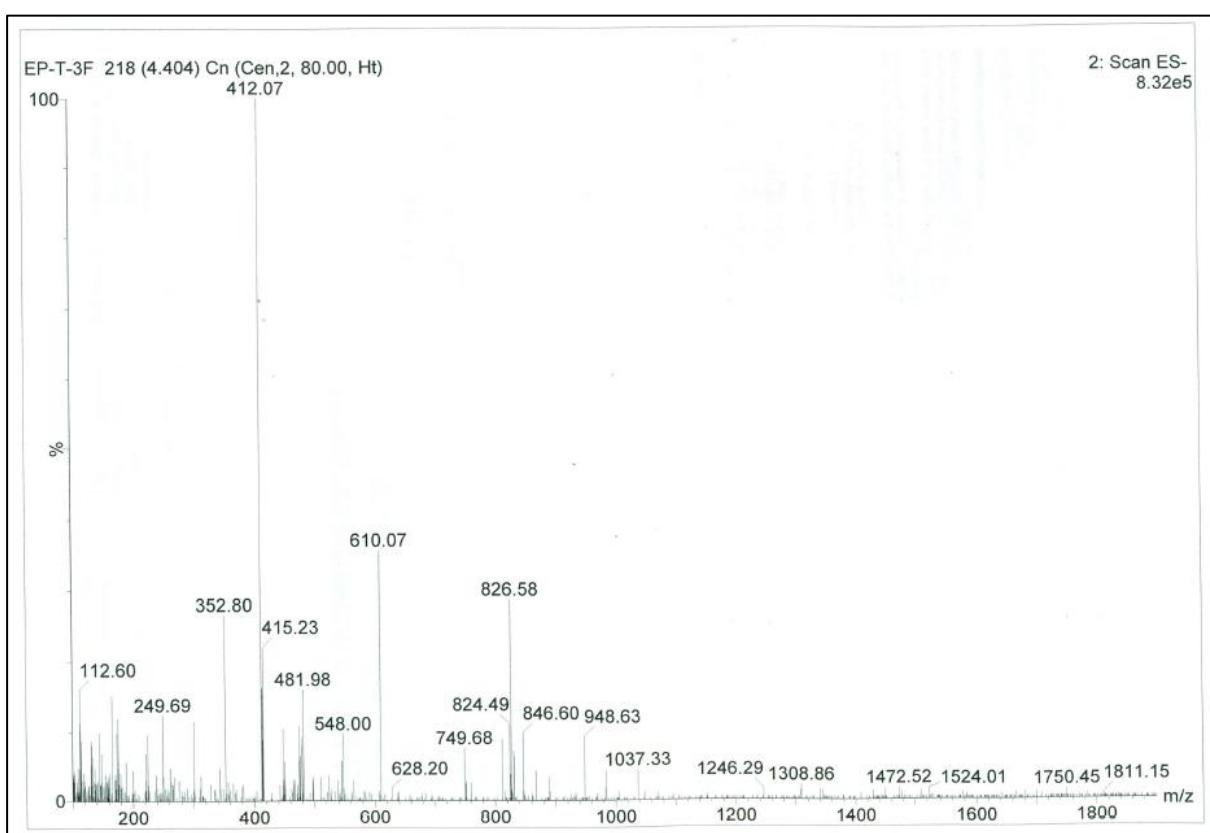
Lab Code: EP-T-3F



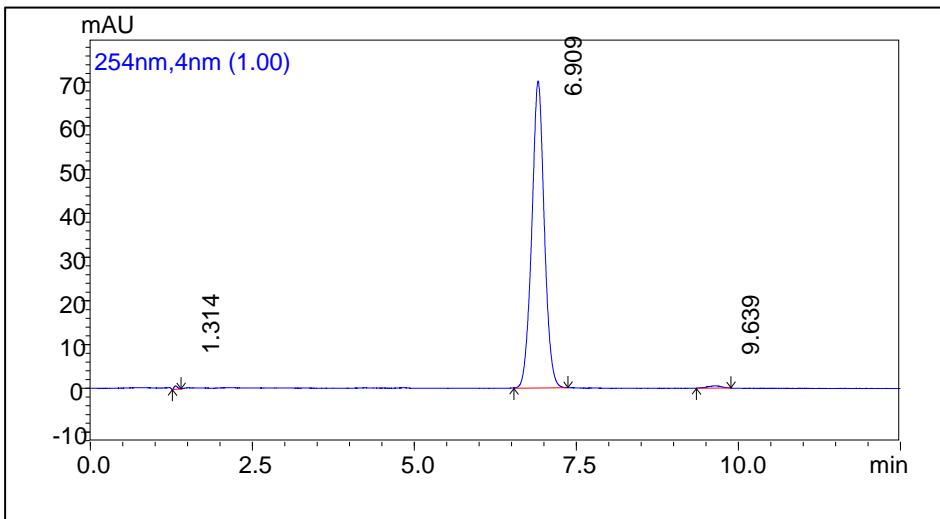
**Figure S57.** Compound **3o** <sup>1</sup>H-NMR spectrum (DMSO-d<sub>6</sub>, 400 MHz).



**Figure S58.** Compound 3o <sup>13</sup>C-NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

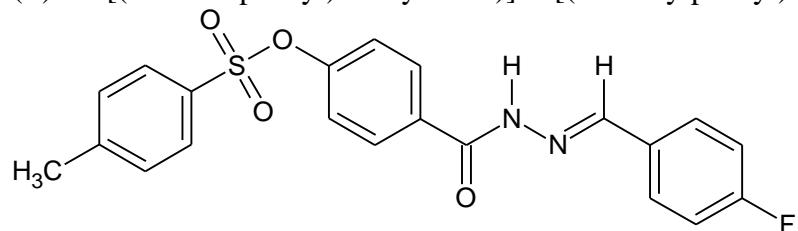


**Figure S59.** Compound 3o ESI MS spectrum.

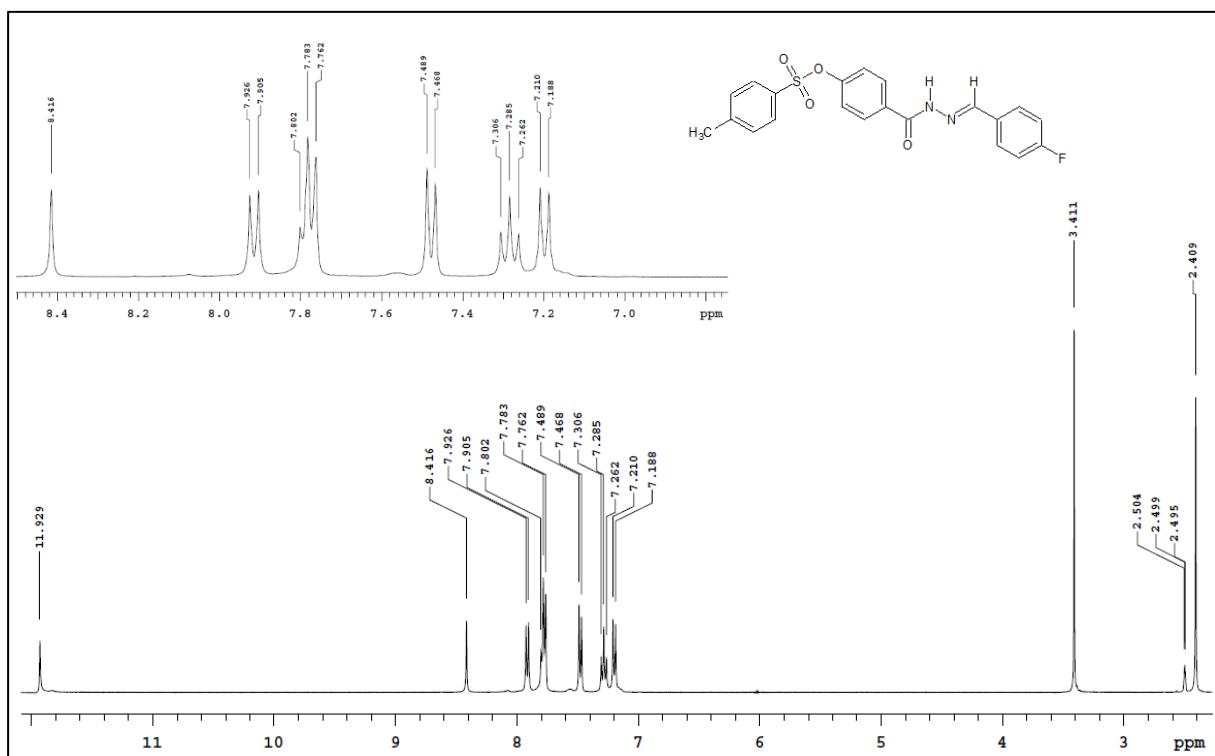


**Figure S60.** Chromatogram of compound **3o** (52 µg/mL) recorded under optimized conditions.

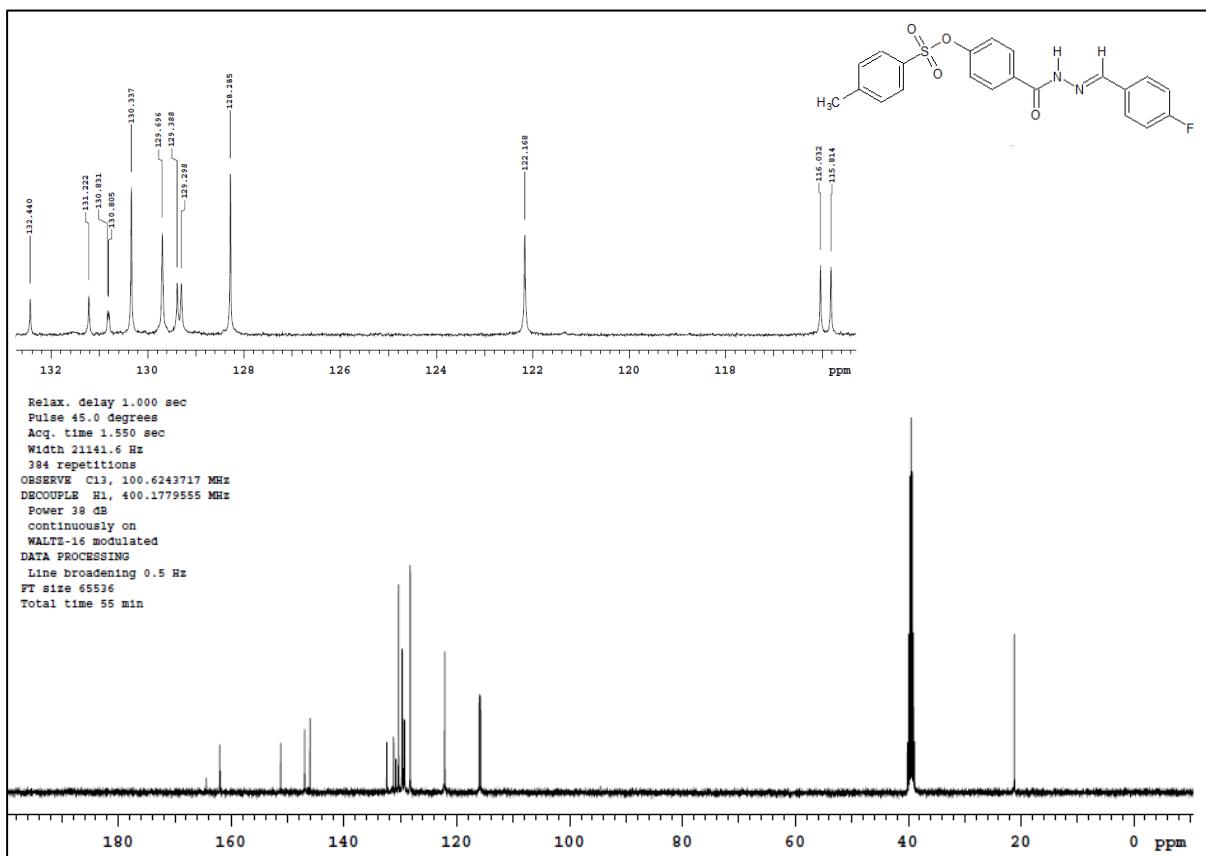
(*E*)-*N'*-[(4-Fluorophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3p**)



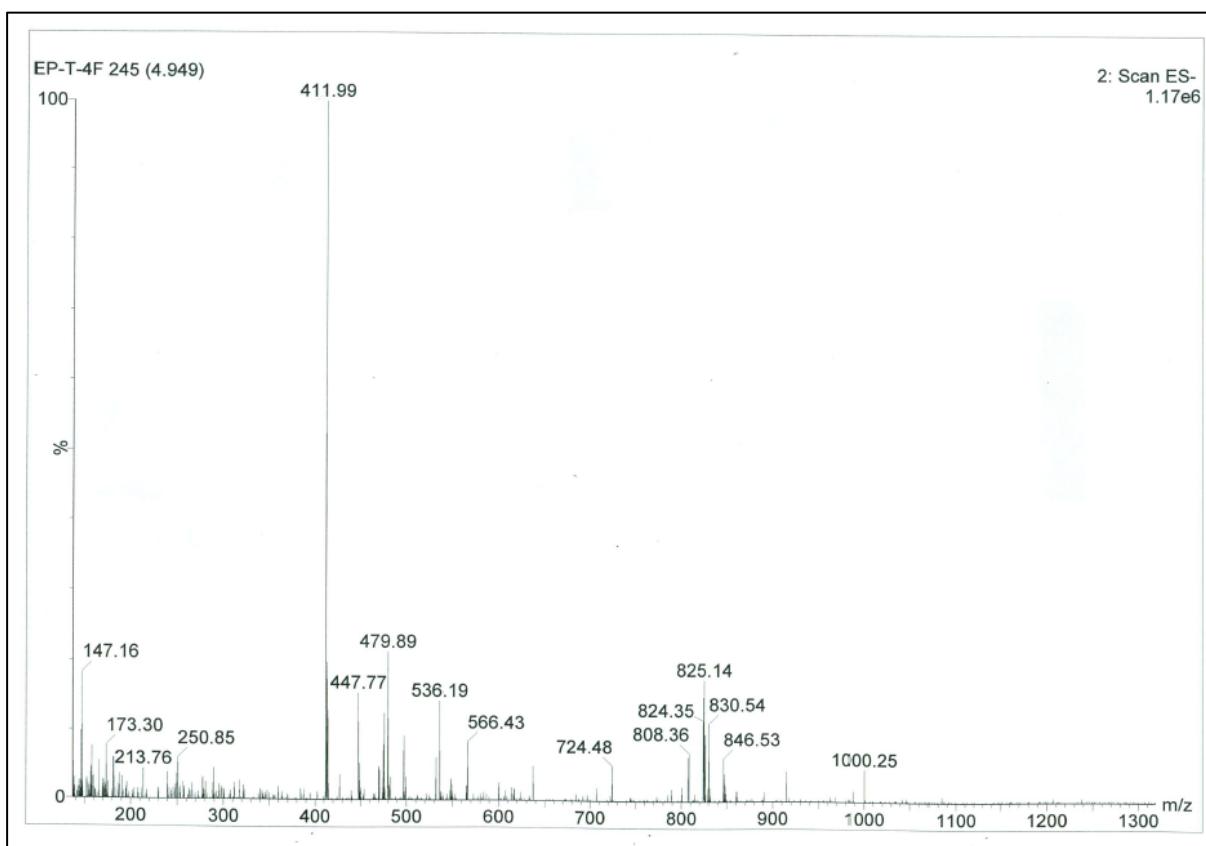
Lab Code: EP-T-4F



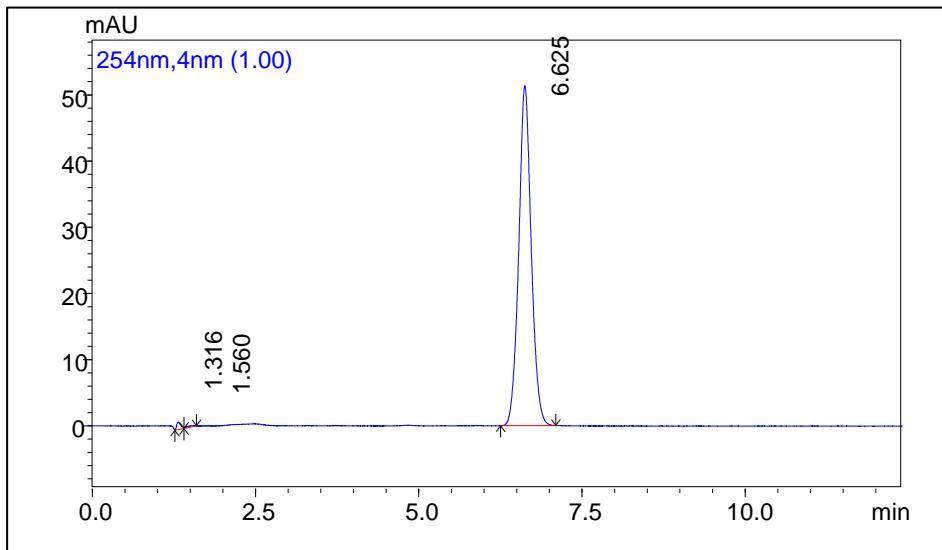
**Figure S61.** Compound **3p**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



**Figure S62.** Compound 3p  $^{13}\text{C}$ -NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

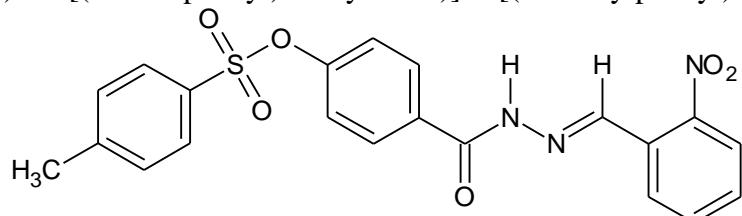


**Figure S63.** Compound 3p ESI MS spectrum.

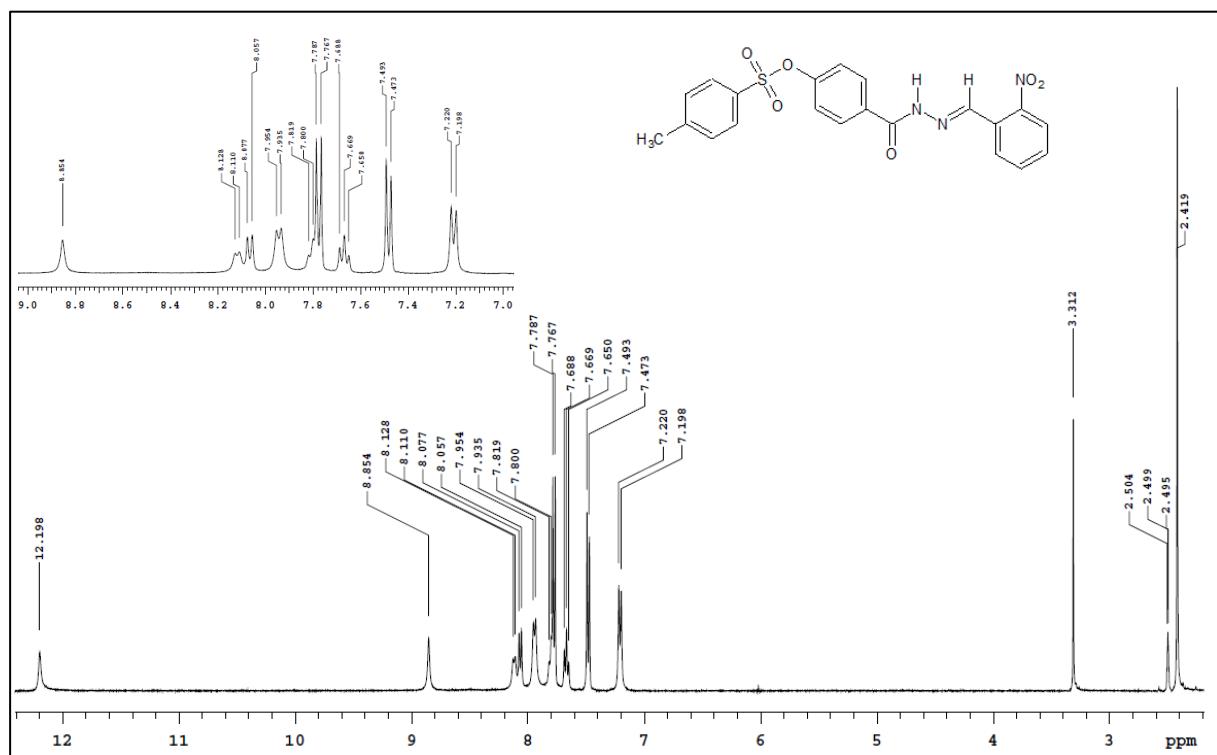


**Figure S64.** Chromatogram of compound **3p** (36 µg/mL) recorded under optimized conditions.

(E)-N'-[(2-Nitrophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3r**)



Lab Code: EP-T-2N



**Figure S65.** Compound 3r  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).

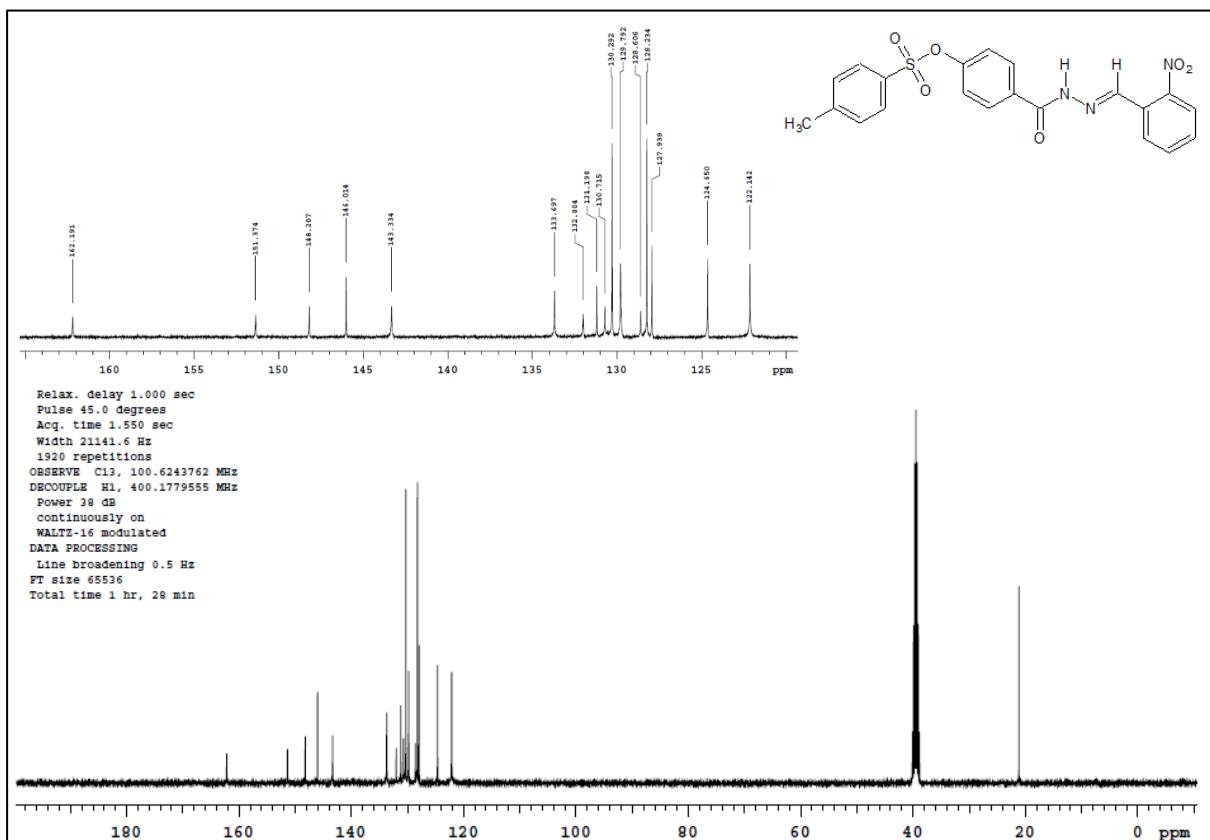


Figure S66. Compound 3r <sup>13</sup>C-NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

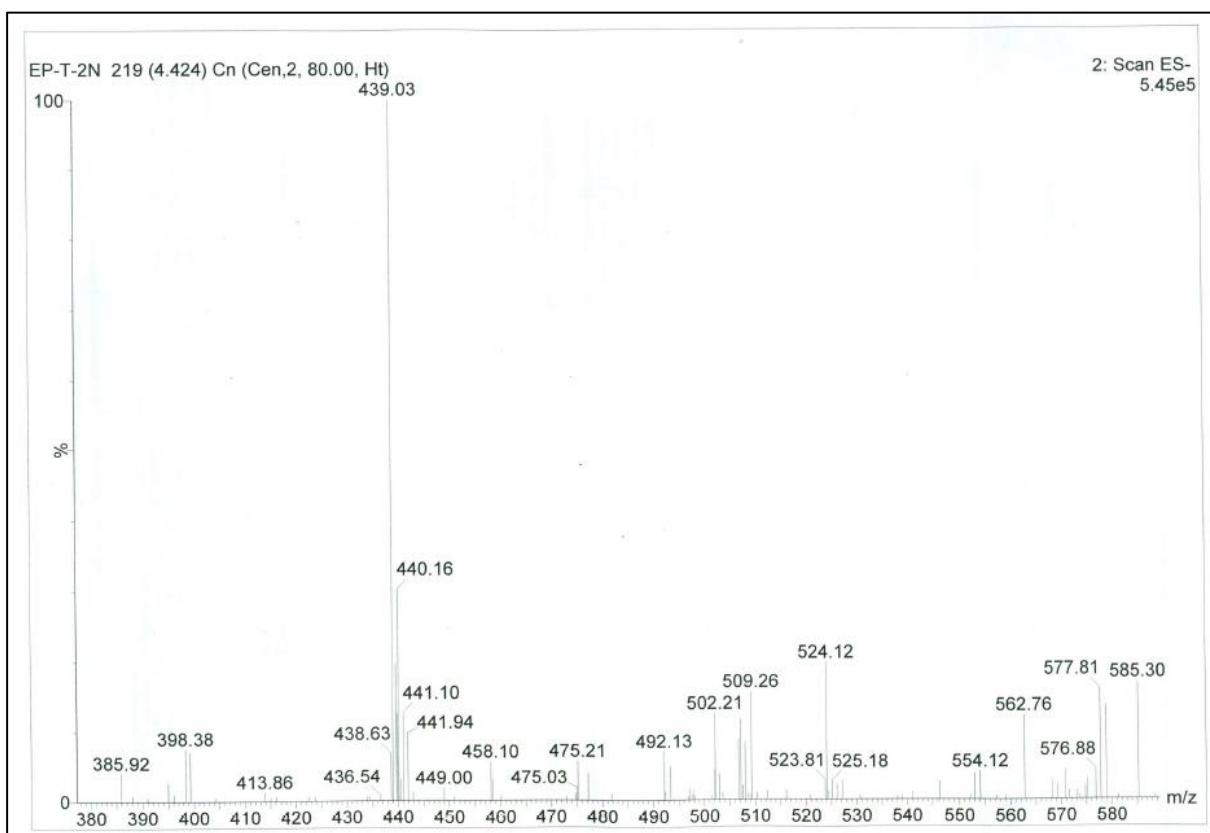
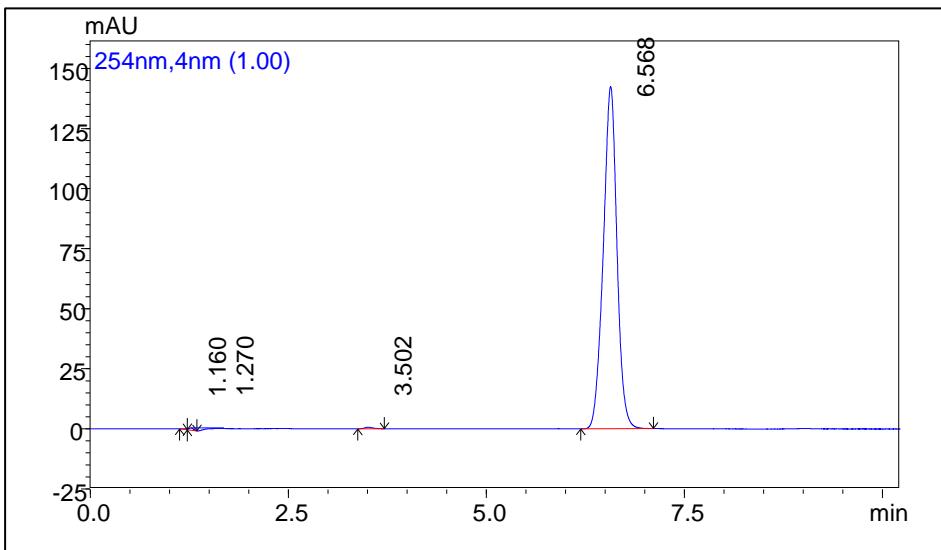
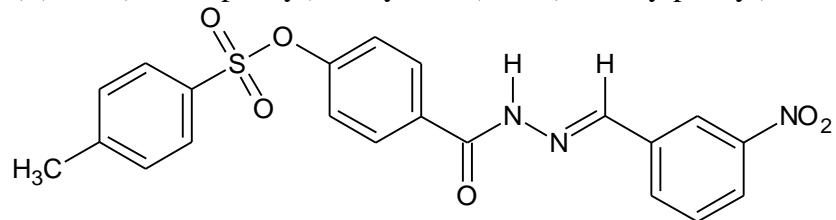


Figure S67. Compound 3r ESI MS spectrum.

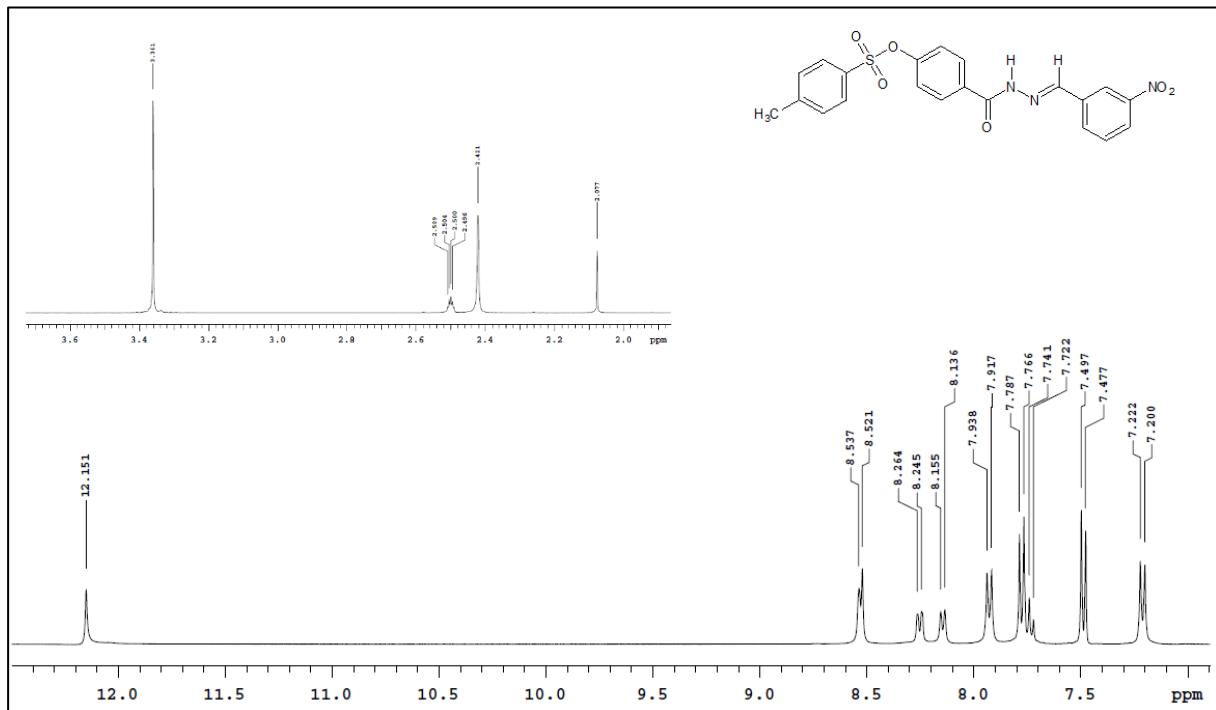


**Figure S68.** Chromatogram of compound **3r** (44 µg/mL) recorded under optimized conditions.

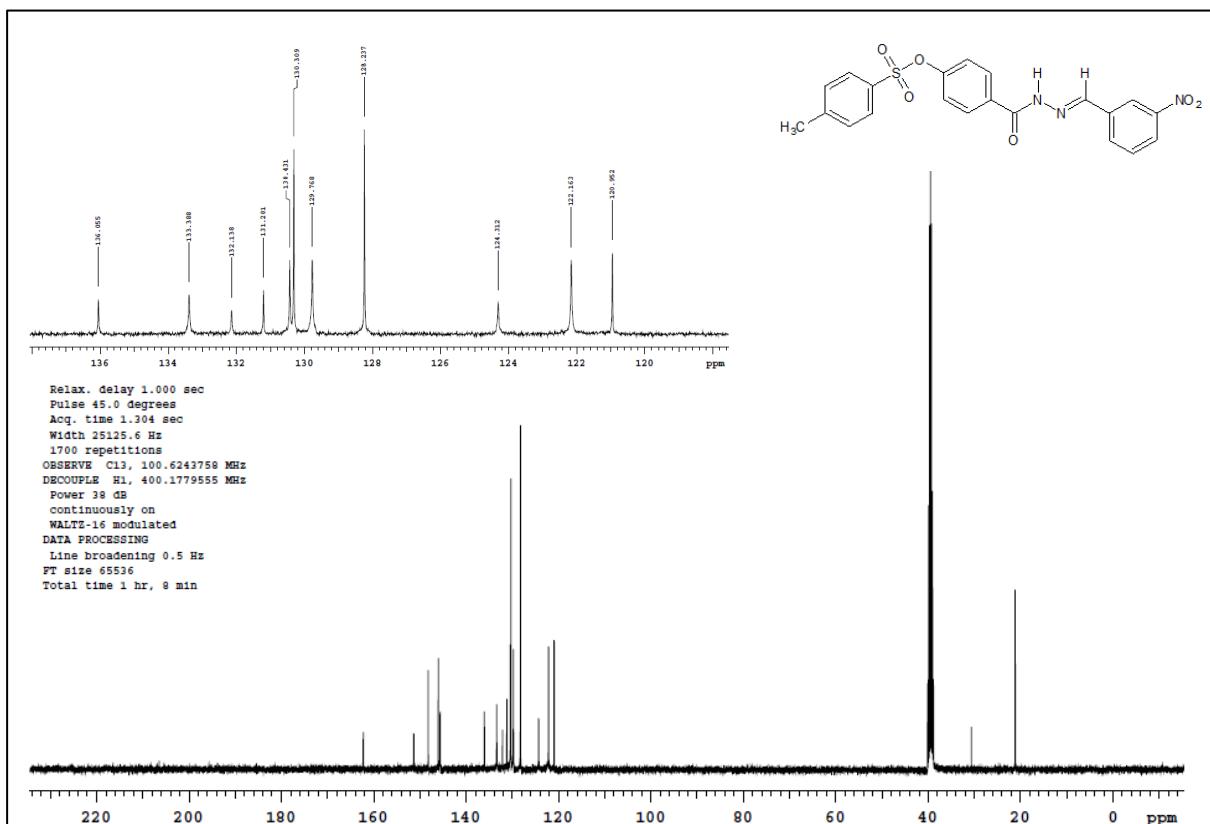
(*E*)-*N'*-[(3-Nitrophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3s**)



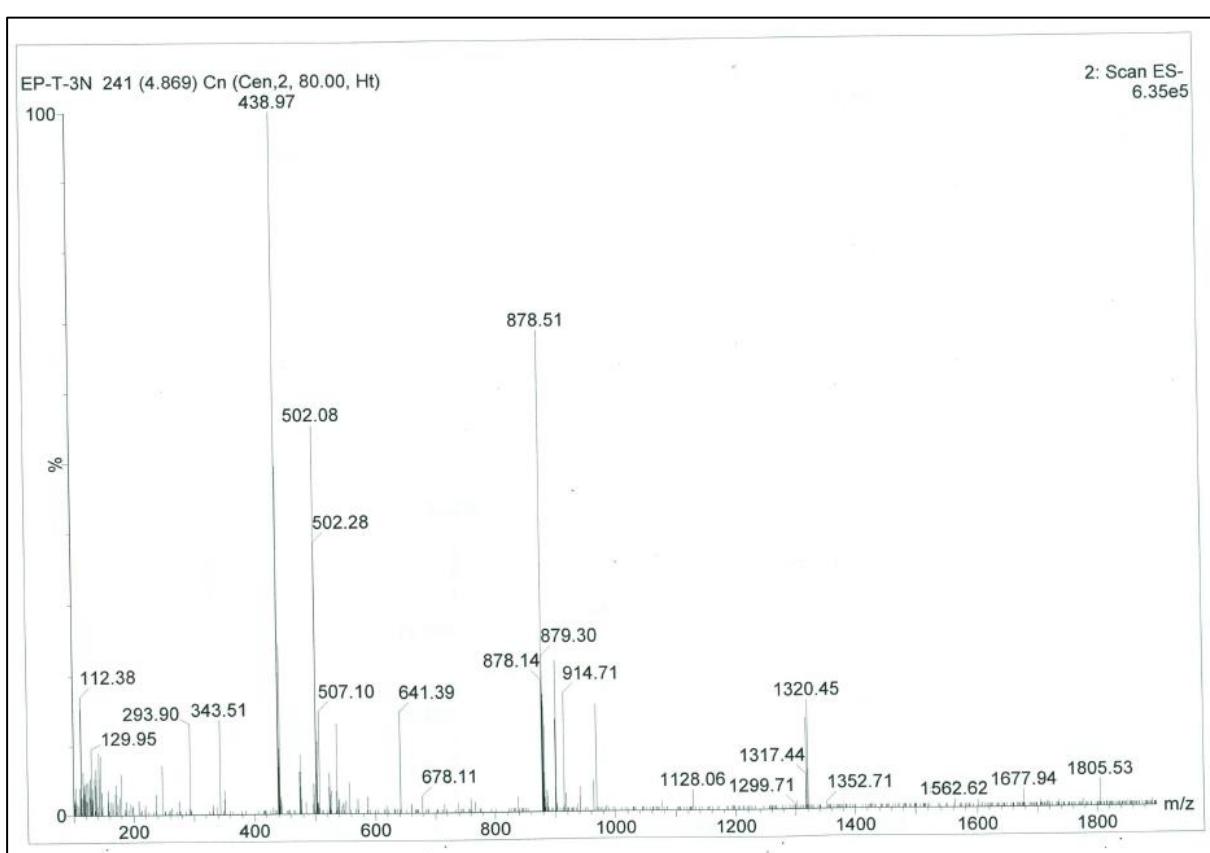
Lab Code: EP-T-3N



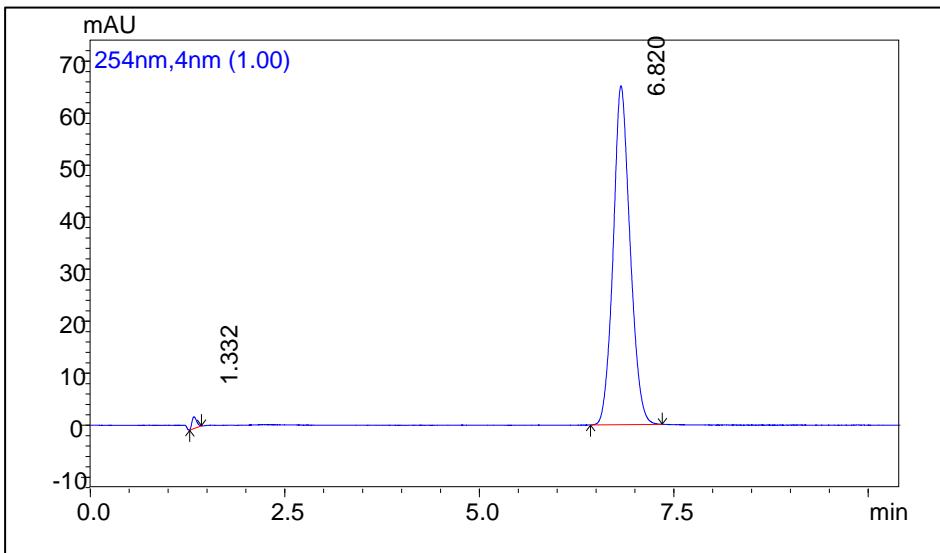
**Figure S69.** Compound **3s**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).



**Figure S70.** Compound 3s  $^{13}\text{C}$ -NMR spectrum (DMSO- $\text{d}_6$ , 100 MHz).

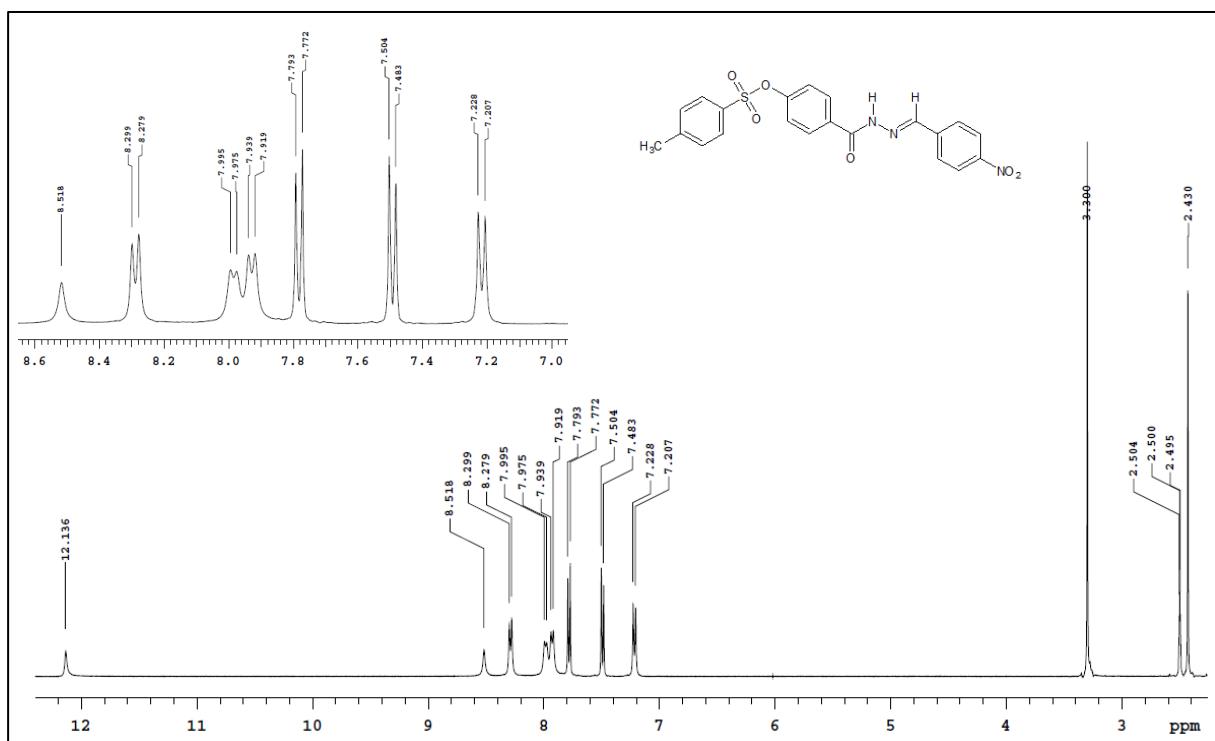
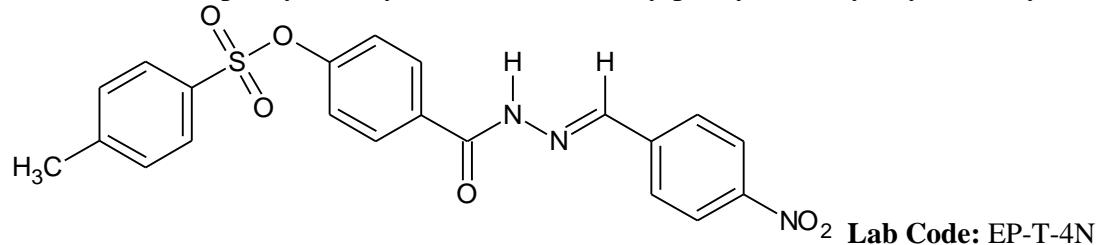


**Figure S71.** Compound 3s ESI MS spectrum.



**Figure S72.** Chromatogram of compound **3s** (32 µg/mL) recorded under optimized conditions.

(*E*)-*N'*-[(4-Nitrophenyl)methylidene]-4-[(4-methylphenyl)sulfonyloxy]benzohydrazide (**3t**)



**Figure S73.** Compound **3t**  $^1\text{H}$ -NMR spectrum (DMSO- $\text{d}_6$ , 400 MHz).

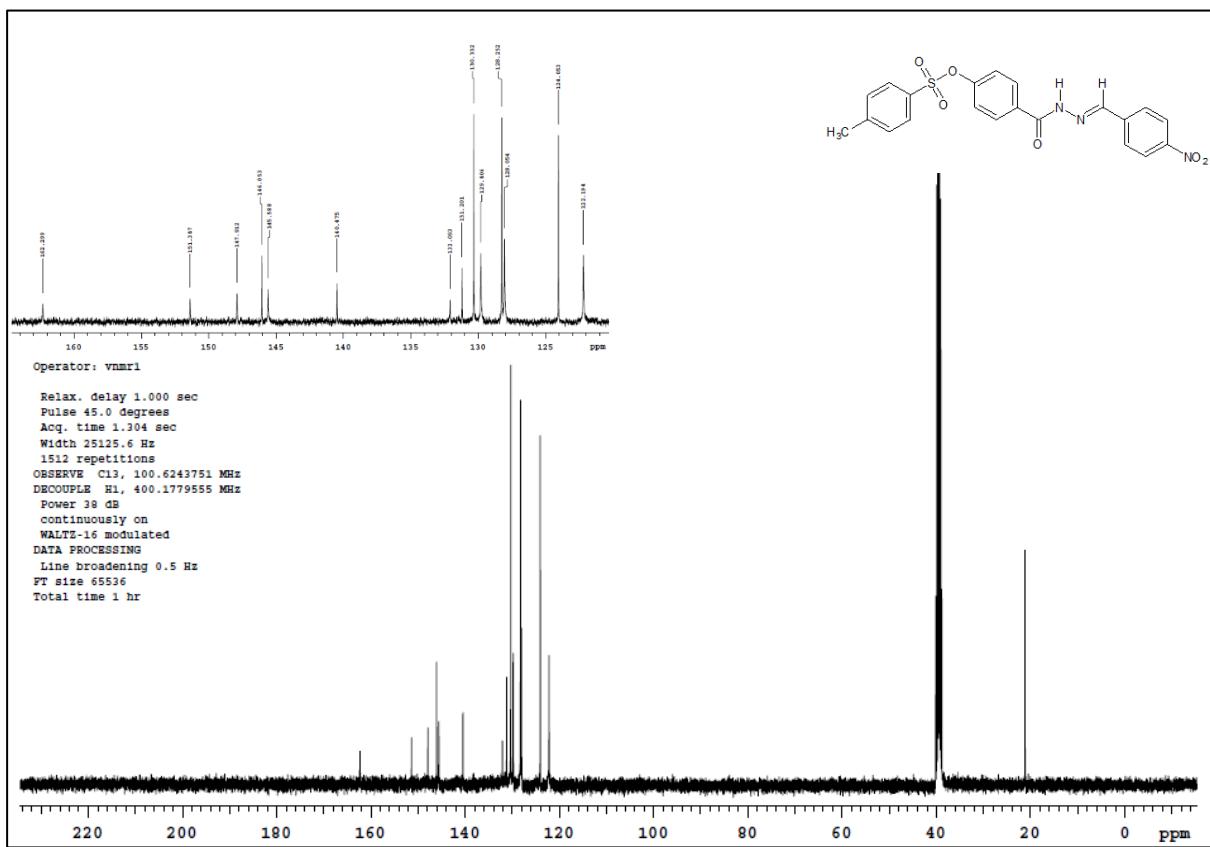


Figure S74. Compound 3t  $^{13}\text{C}$ -NMR spectrum (DMSO-d<sub>6</sub>, 100 MHz).

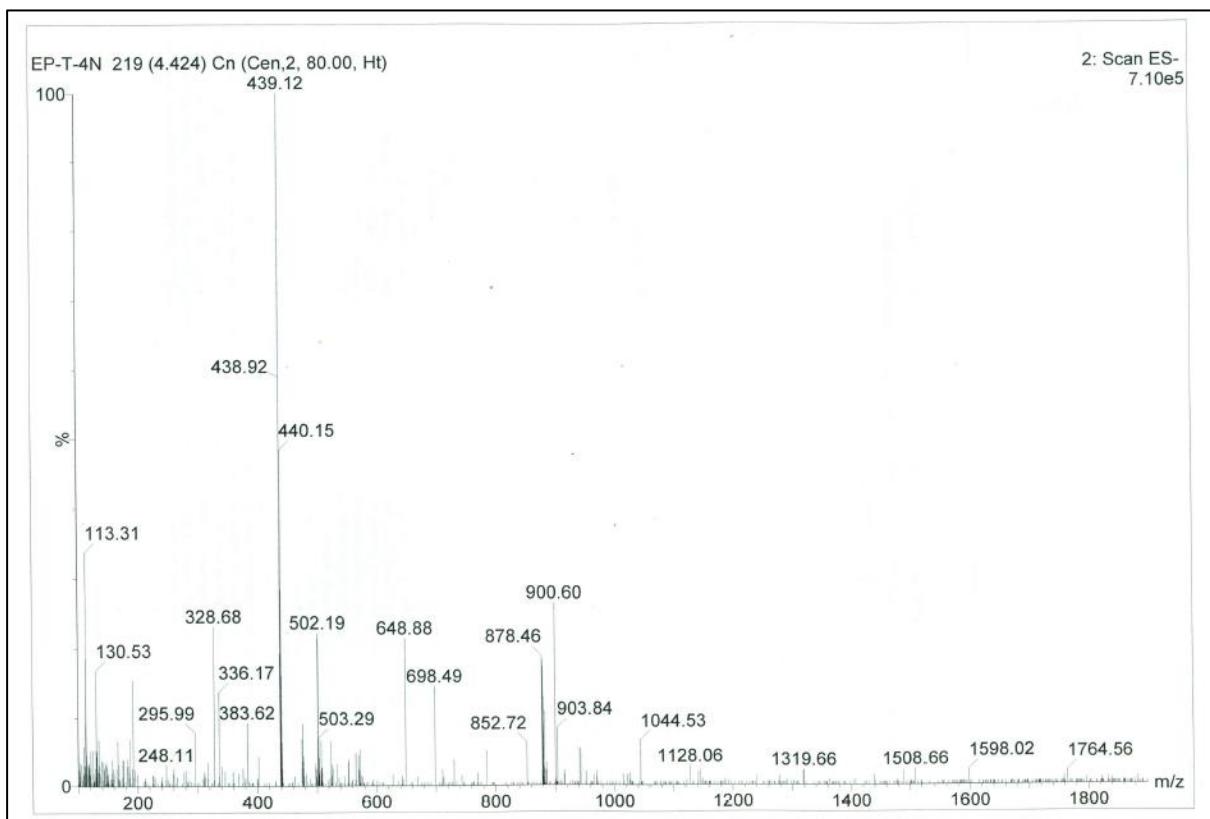
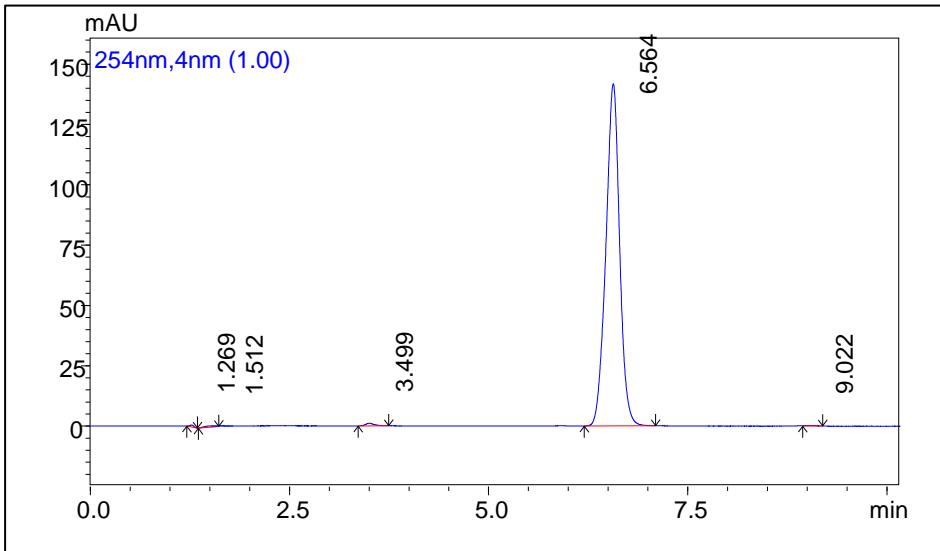


Figure S75. Compound 3t ESI MS spectrum.



**Figure S76.** Chromatogram of compound **3t** (36 µg/mL) recorded under optimized conditions.