

**Supporting Information**  
**Functionalized Guanidinium Chloride Based Colourimetric Sensors for Fluoride and Acetate:  
Single Crystal X-ray Structural Evidence of -NH Deprotonation and Complexation**

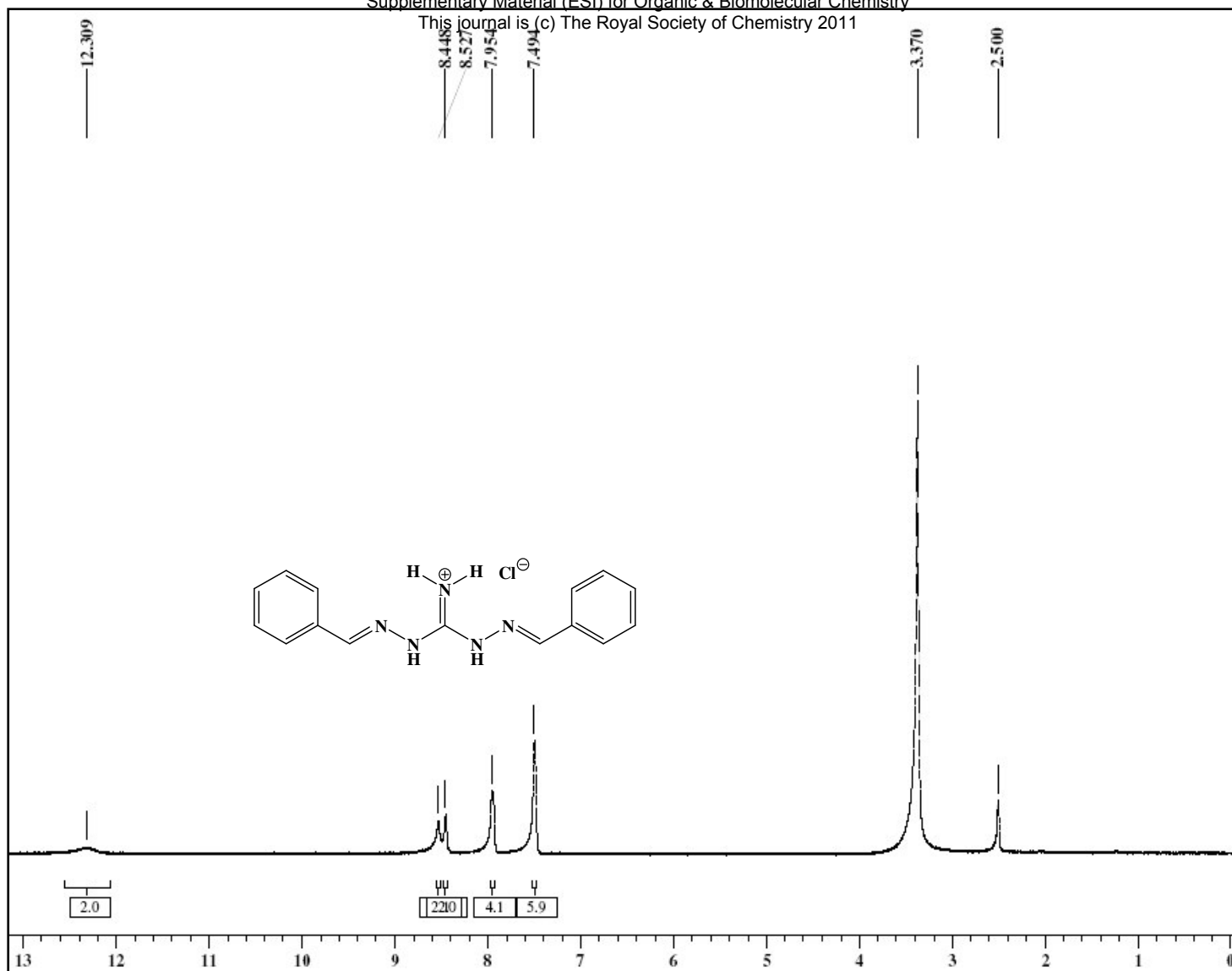
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<b>Contents</b>	<b>Page No.</b>
1. <b>Figure S1.</b> <sup>1</sup> H-NMR spectrum of <b>S1</b> in DMSO-d <sub>6</sub> at 25°C.....	4
2. <b>Figure S2.</b> <sup>13</sup> C-NMR spectrum of <b>S1</b> in DMSO- d <sub>6</sub> at 25°C.....	5
3. <b>Figure S3.</b> HRMS (ESI) Spectrum of <b>S1</b> .....	6
4. <b>Figure S4.</b> <sup>1</sup> H-NMR spectrum of <b>S2</b> in DMSO- d <sub>6</sub> at 25°C.....	7
5. <b>Figure S5.</b> <sup>13</sup> C-NMR spectrum of <b>S2</b> in DMSO- d <sub>6</sub> at 25°C.....	8
6. <b>Figure S6.</b> HRMS (ESI) Spectrum of <b>S2</b> .....	9
7. <b>Figure S7.</b> <sup>1</sup> H-NMR spectrum of <b>S3</b> in DMSO- d <sub>6</sub> at 25°C.....	10
8. <b>Figure S8.</b> <sup>13</sup> C-NMR spectrum of <b>S3</b> in DMSO- d <sub>6</sub> at 25°C.....	11
9. <b>Figure S9.</b> HRMS (ESI) Spectrum of <b>S3</b> .....	12
10. <b>Figure S10.</b> <sup>1</sup> H-NMR spectrum of <b>S4</b> in DMSO- d <sub>6</sub> at 25°C.....	13
11. <b>Figure S11.</b> <sup>13</sup> C-NMR spectrum of <b>S4</b> in DMSO- d <sub>6</sub> at 25°C.....	14
12. <b>Figure S12.</b> HRMS (ESI) Spectrum of <b>S4</b> .....	15
13. <b>Figure S13.</b> <sup>1</sup> H-NMR spectrum of <b>S5</b> in DMSO- d <sub>6</sub> at 25°C.....	16
14. <b>Figure S14.</b> <sup>13</sup> C-NMR spectrum of <b>S5</b> in DMSO- d <sub>6</sub> at 25°C.....	17

15.	<b>Figure S15.</b> HRMS (ESI) Spectrum of <b>S5</b> .....	18
16.	<b>Figure S16.</b> <sup>1</sup> H-NMR spectrum of <b>S6</b> in DMSO- d <sub>6</sub> at 25°C.....	19
17.	<b>Figure S17.</b> <sup>13</sup> C-NMR spectrum of <b>S6</b> in DMSO- d <sub>6</sub> at 25°C .....	20
18.	<b>Figure S18.</b> HRMS (ESI) Spectrum of <b>S6</b> .....	21
19.	<b>Figure S19.</b> <sup>1</sup> H-NMR spectrum of <b>S7</b> in DMSO- d <sub>6</sub> at 25°C .....	22
20.	<b>Figure S20.</b> <sup>13</sup> C-NMR spectrum of <b>S7</b> in DMSO- d <sub>6</sub> at 25°C .....	23
21.	<b>Figure S21.</b> HRMS (ESI) Spectrum of <b>S7</b> .....	24
22.	<b>Figure S22.</b> <sup>1</sup> H-NMR spectrum of <b>S8</b> in DMSO- d <sub>6</sub> at 25°C .....	25
23.	<b>Figure S23.</b> <sup>13</sup> C-NMR spectrum of <b>S8</b> in DMSO- d <sub>6</sub> at 25°C .....	26
24.	<b>Figure S24.</b> HRMS (ESI) Spectrum of <b>S8</b> .....	27
25.	<b>Figure S25.</b> <sup>1</sup> H-NMR spectrum of <b>S9</b> in DMSO- d <sub>6</sub> at 25°C .....	28
26.	<b>Figure S26.</b> <sup>13</sup> C-NMR spectrum of <b>S9</b> in DMSO- d <sub>6</sub> at 25°C .....	29
27.	<b>Figure S27.</b> HRMS (ESI) Spectrum of <b>S9</b> .....	30
28.	<b>Figure S28.</b> <sup>1</sup> H-NMR spectrum of <b>S10</b> in DMSO- d <sub>6</sub> at 25°C.....	31
29.	<b>Figure S29.</b> <sup>13</sup> C-NMR spectrum of <b>S10</b> in DMSO- d <sub>6</sub> at 25°C.....	32
30.	<b>Figure S30.</b> HRMS (ESI) Spectrum of <b>S10</b> .....	33
31.	<b>Figure S31.</b> Optical spectrum of <b>S5-S9</b> in presence of various anions .....	34
32.	<b>Figure S32.</b> Optical spectrum of <b>S10-S12</b> in presence of various anions .....	35
33.	<b>Figure S33.</b> Selectivity study of <b>S9</b> (1x10 <sup>-4</sup> M) in presence of different anions ( 30 equiv.).....	36
34.	<b>Figure S34.</b> UV-Vis titration of <b>S1</b> in presence of F <sup>-</sup> .....	37
35.	<b>Figure S35.</b> UV-Vis titration of <b>S2</b> in presence of F <sup>-</sup> .....	38

36.	<b>Figure S36.</b> UV-Vis titration of <b>S2</b> in presence of $\text{AcO}^-$ .....	39
37.	<b>Figure S37.</b> UV-Vis titration of <b>S2</b> in presence of $\text{H}_2\text{PO}_4^-$ .....	40
38.	<b>Figure S38.</b> UV-Vis titration of <b>S3</b> in presence of $\text{F}^-$ .....	41
39.	<b>Figure S39.</b> UV-Vis titration of <b>S3</b> in presence of $\text{AcO}^-$ .....	42
40.	<b>Figure S40.</b> UV-Vis titration of <b>S3</b> in presence of $\text{H}_2\text{PO}_4^-$ .....	43
41.	<b>Figure S41.</b> UV-Vis titration of <b>S4</b> in presence of $\text{F}^-$ .....	44
42.	<b>Figure S42.</b> UV-Vis titration of <b>S4</b> in presence of $\text{AcO}^-$ .....	45
43.	<b>Figure S43.</b> UV-Vis titration of <b>S6</b> in presence of $\text{F}^-$ .....	46
44.	<b>Figure S44.</b> UV-Vis titration of <b>S6</b> in presence of $\text{AcO}^-$ .....	47
45.	<b>Figure S45.</b> UV-Vis titration of <b>S7</b> in presence of $\text{F}^-$ .....	48
46.	<b>Figure S46.</b> UV-Vis titration of <b>S8</b> in presence of $\text{F}^-$ .....	49
47.	<b>Figure S47.</b> UV-Vis titration of <b>S9</b> in presence of $\text{F}^-$ .....	50
48.	<b>Figure S48.</b> UV-Vis titration of <b>S9</b> in presence of $\text{AcO}^-$ .....	51
49.	<b>Figure S49.</b> UV-Vis titration of <b>S9</b> in presence of $\text{H}_2\text{PO}_4^-$ .....	52
50.	<b>Figure S50.</b> UV-Vis titration of <b>S10</b> in presence of $\text{F}^-$ .....	53
51.	<b>Table S1.</b> Table of Crystallographic parameters.....	54
52.	<b>Table S2.</b> Hydrogen bonding interactions in <b>1</b> .....	55
53.	<b>Table S3.</b> Hydrogen bonding interactions in complex <b>2</b> .....	55
54.	<b>Table S4.</b> Hydrogen bonding interactions in complex <b>3</b> .....	56
55.	<b>Methods and References.</b> .....	57

**Figure S1.**  $^1\text{H}$  NMR spectrum of **S1** in  $\text{DMSO-d}_6$ .

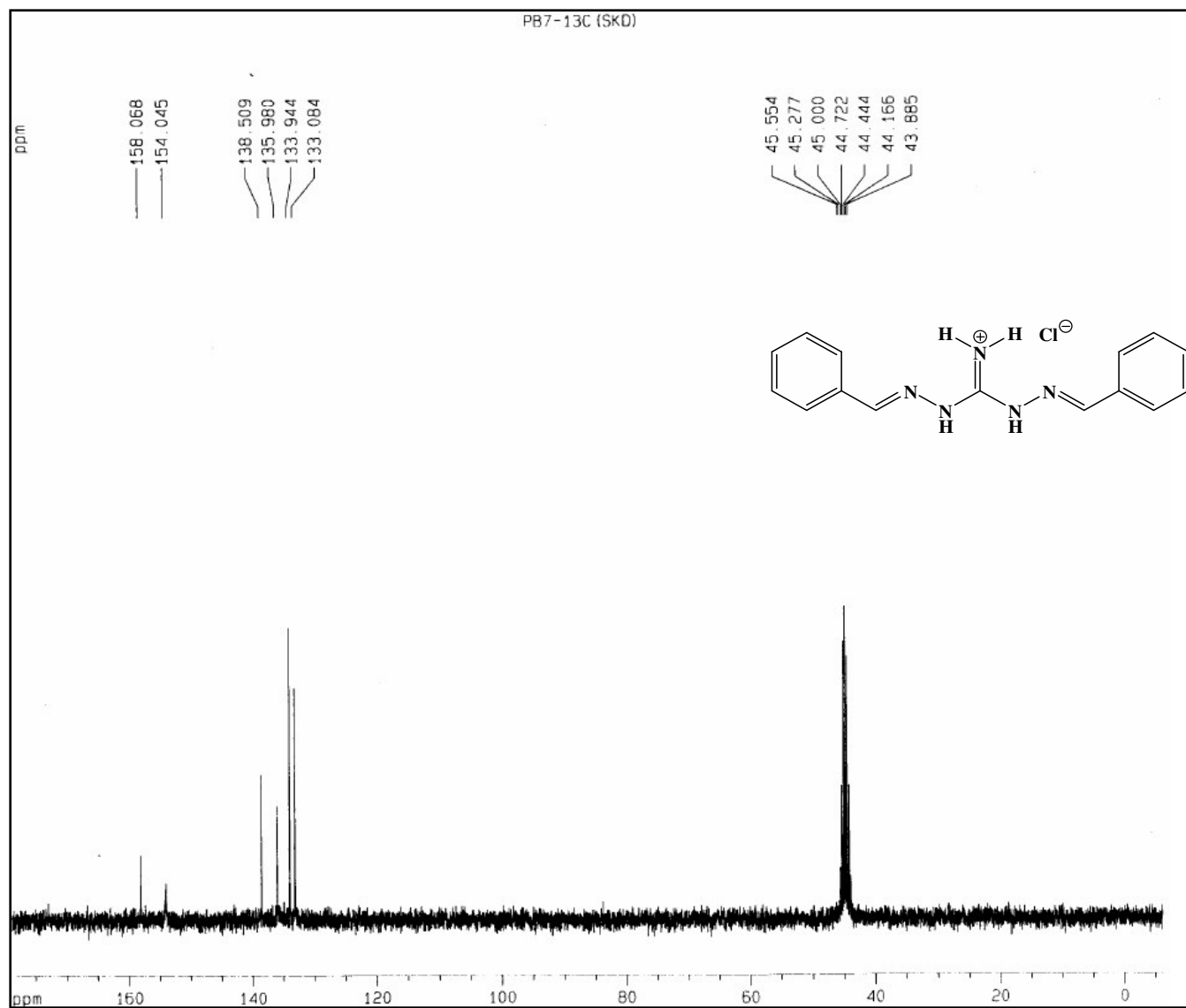


Figure S2.  $^{13}\text{C}$  NMR spectrum of S1 in DMSO- $d_6$ .

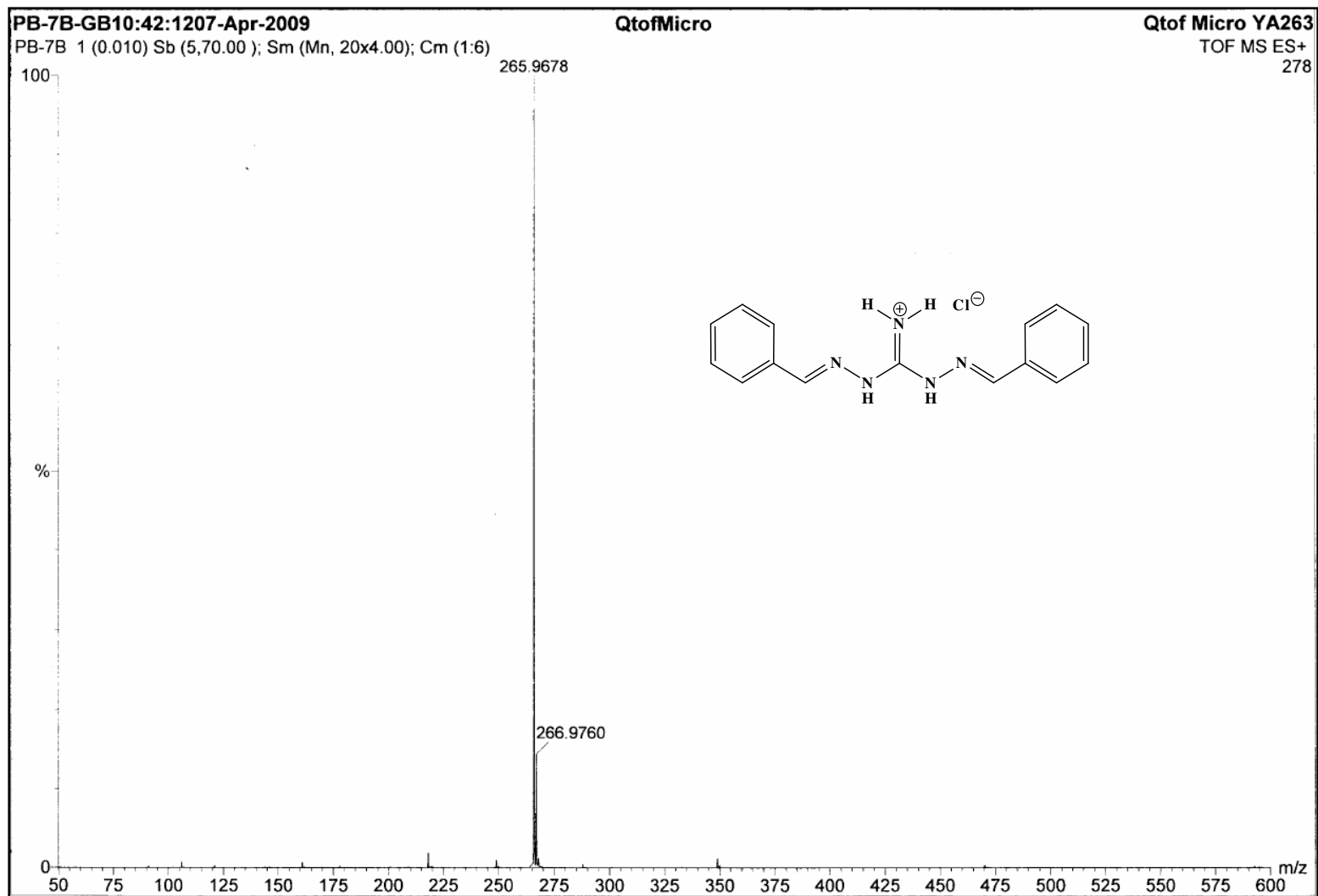


Figure S3. HRMS spectrum of S1.

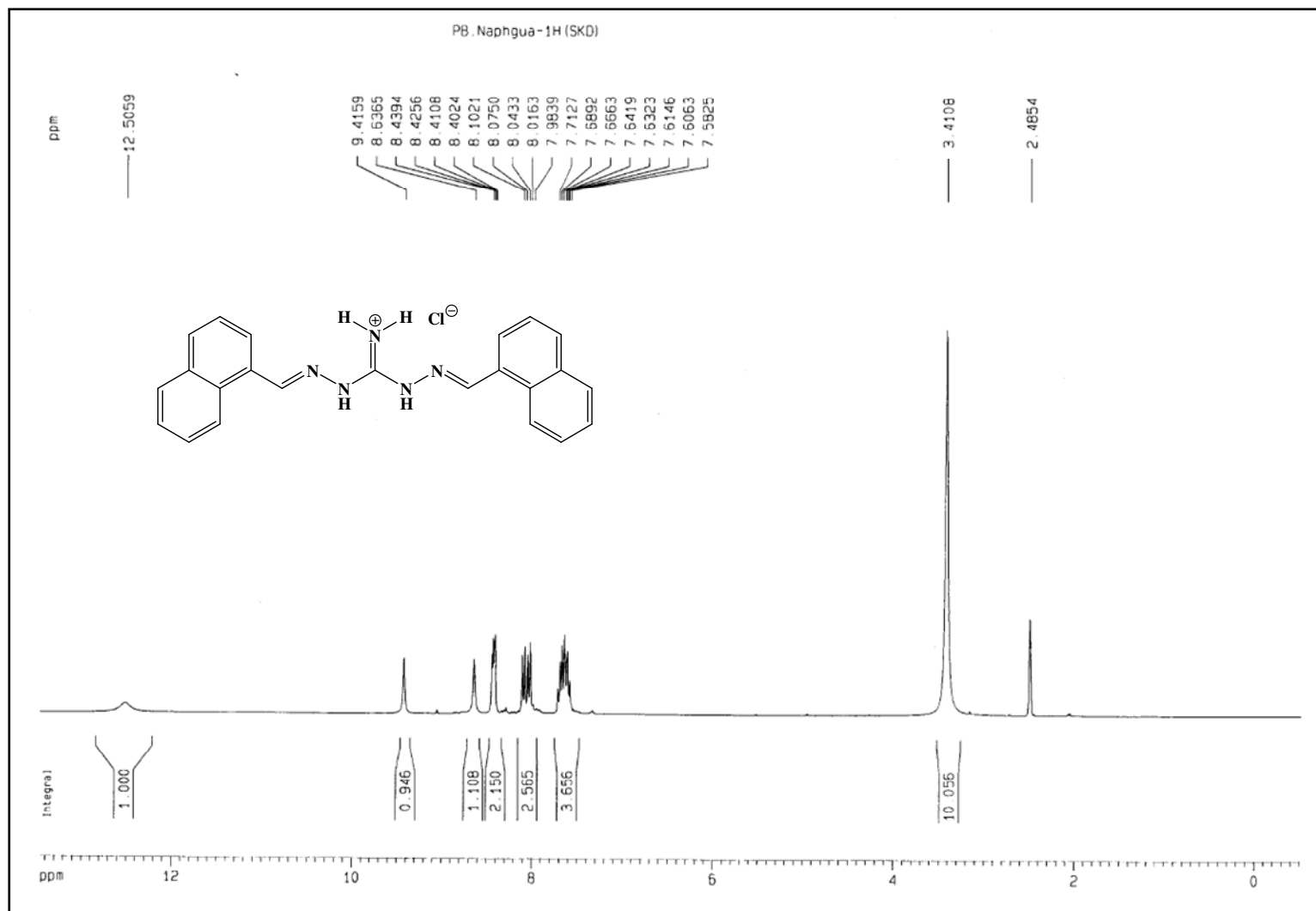


Figure S4. <sup>1</sup>H NMR spectrum of S2 in DMSO-d<sub>6</sub>.

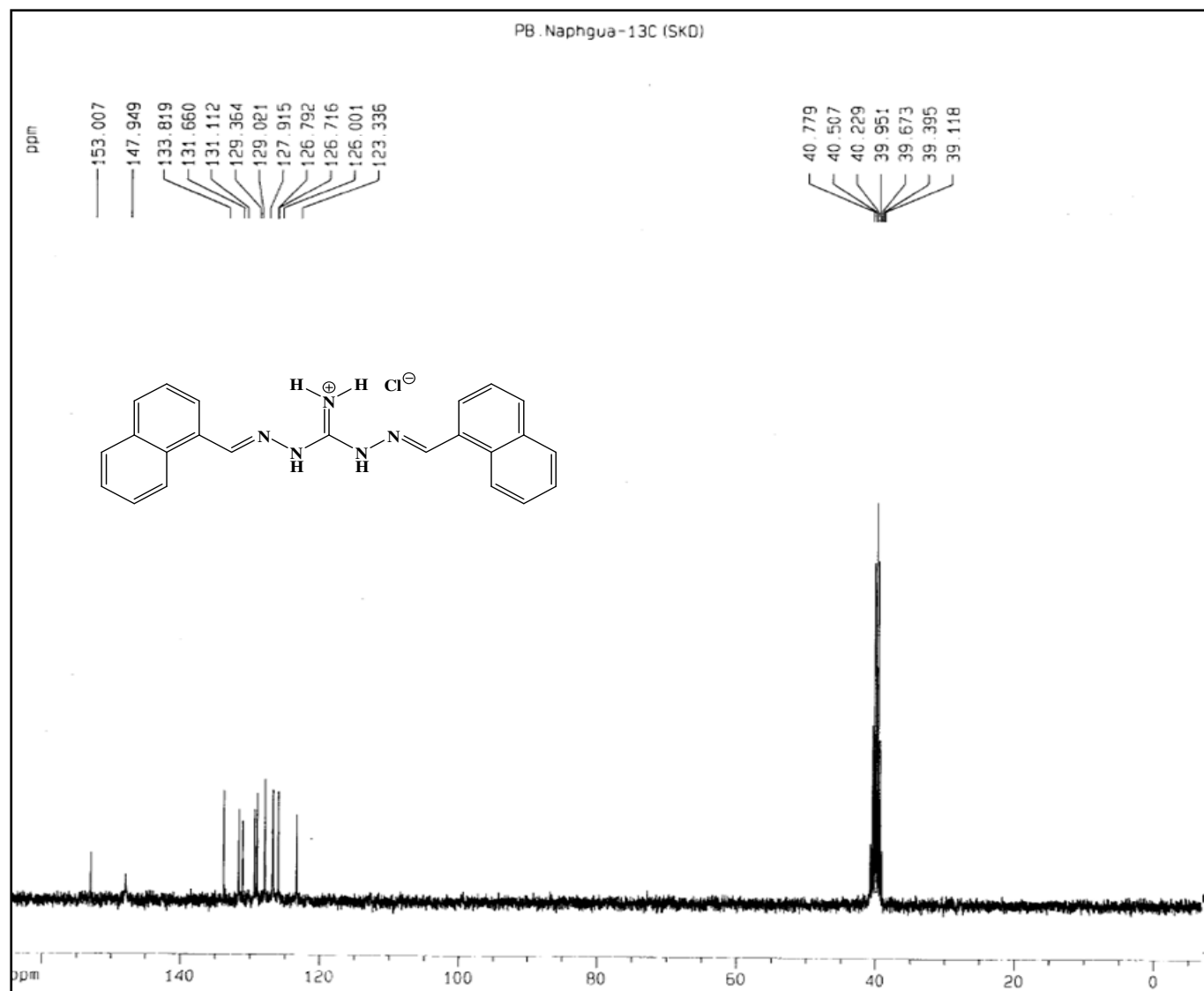


Figure S5.  $^{13}\text{C}$  NMR spectrum of S2 in DMSO- $d_6$ .



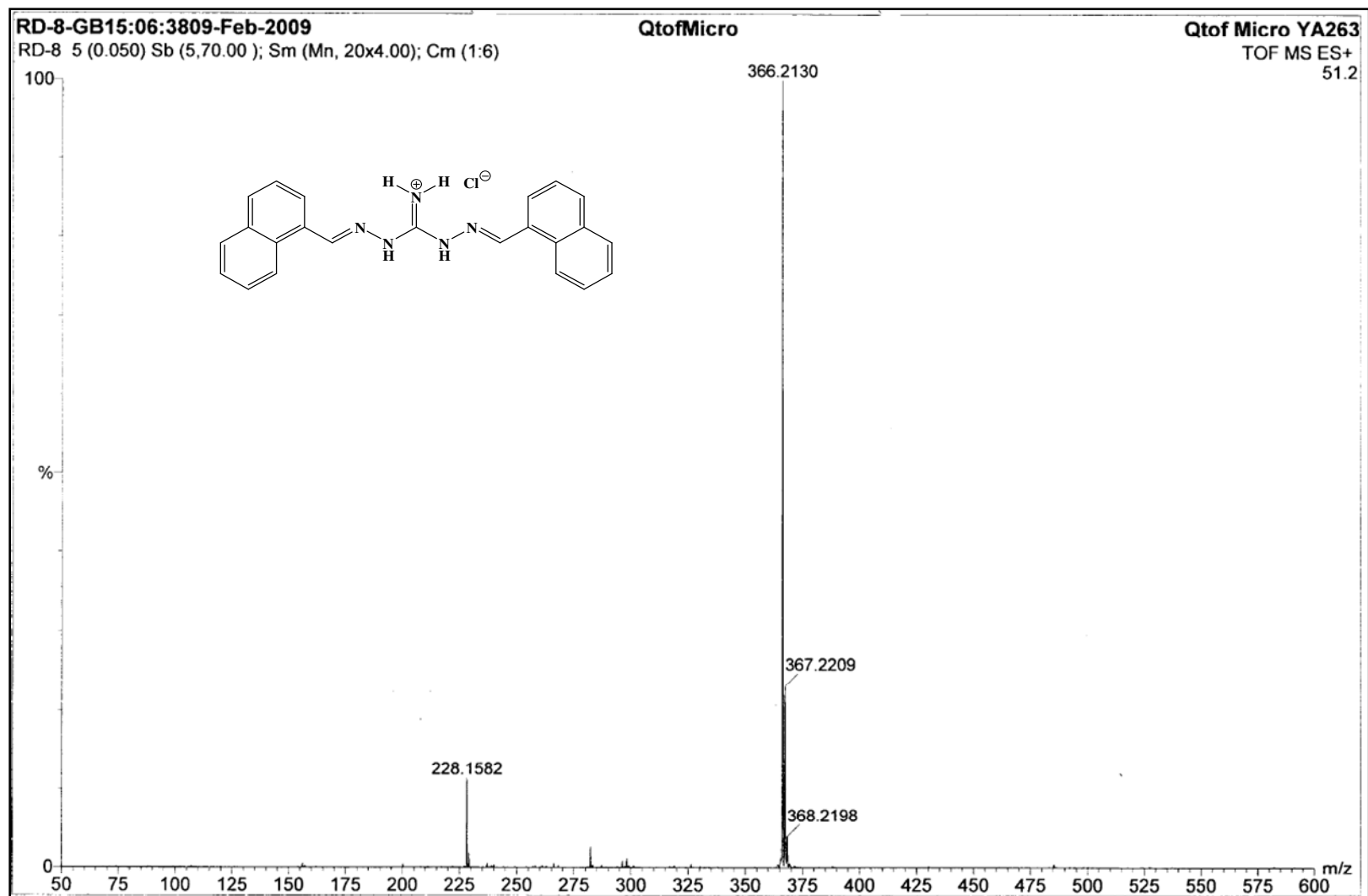
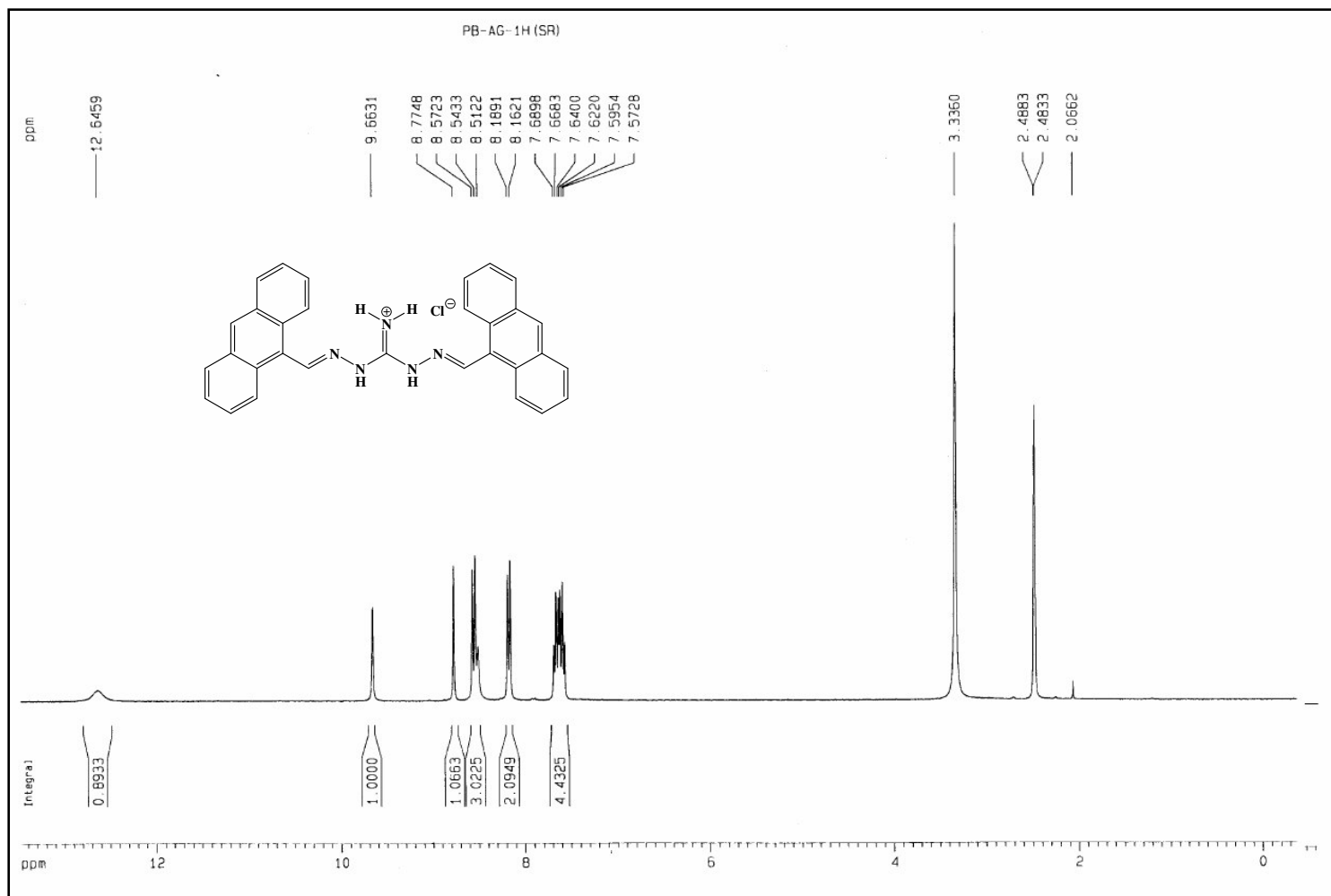


Figure S6. HRMS spectrum of S2.



**Figure S7.** <sup>1</sup>H NMR spectrum of **S3** in DMSO-d<sub>6</sub>.

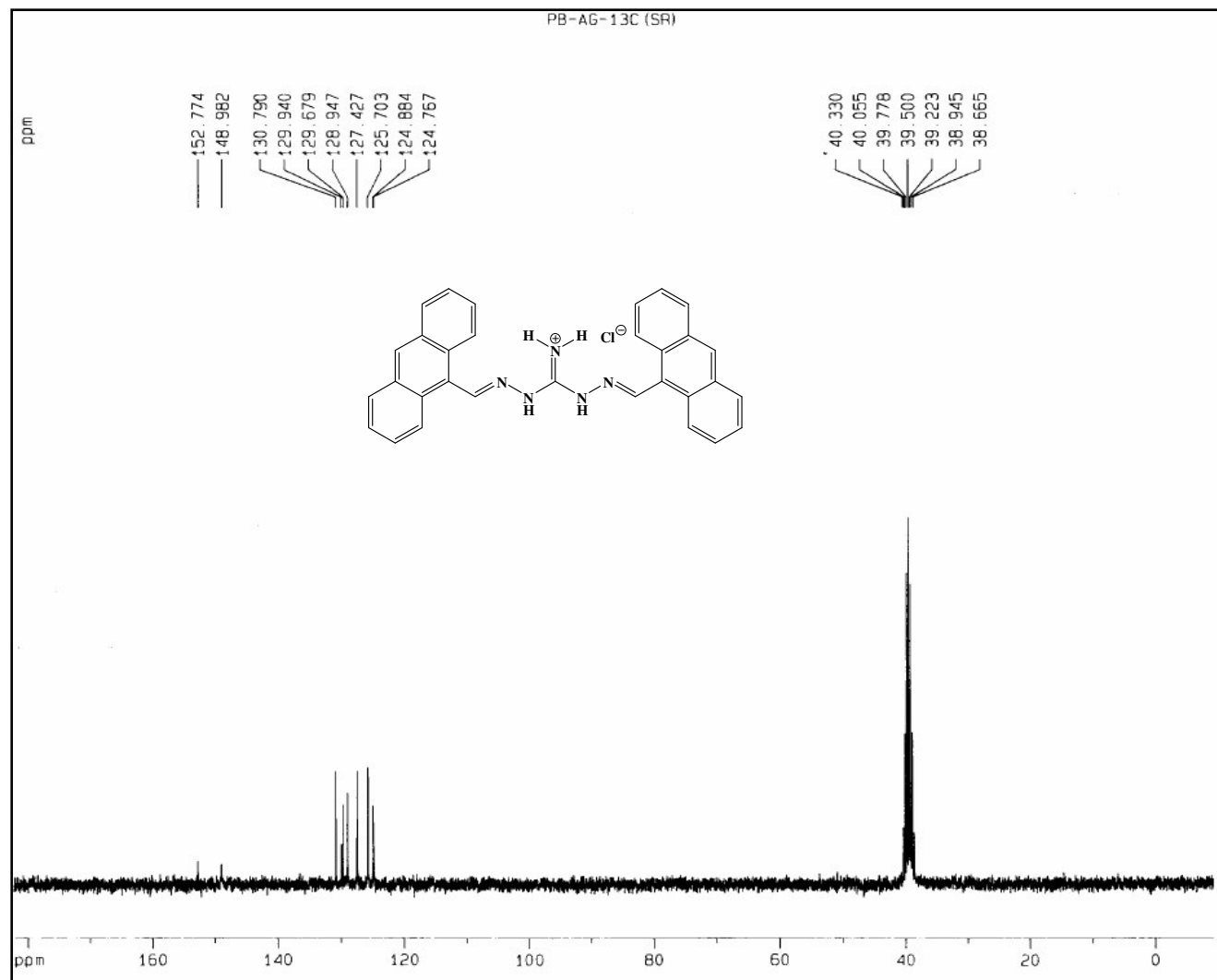
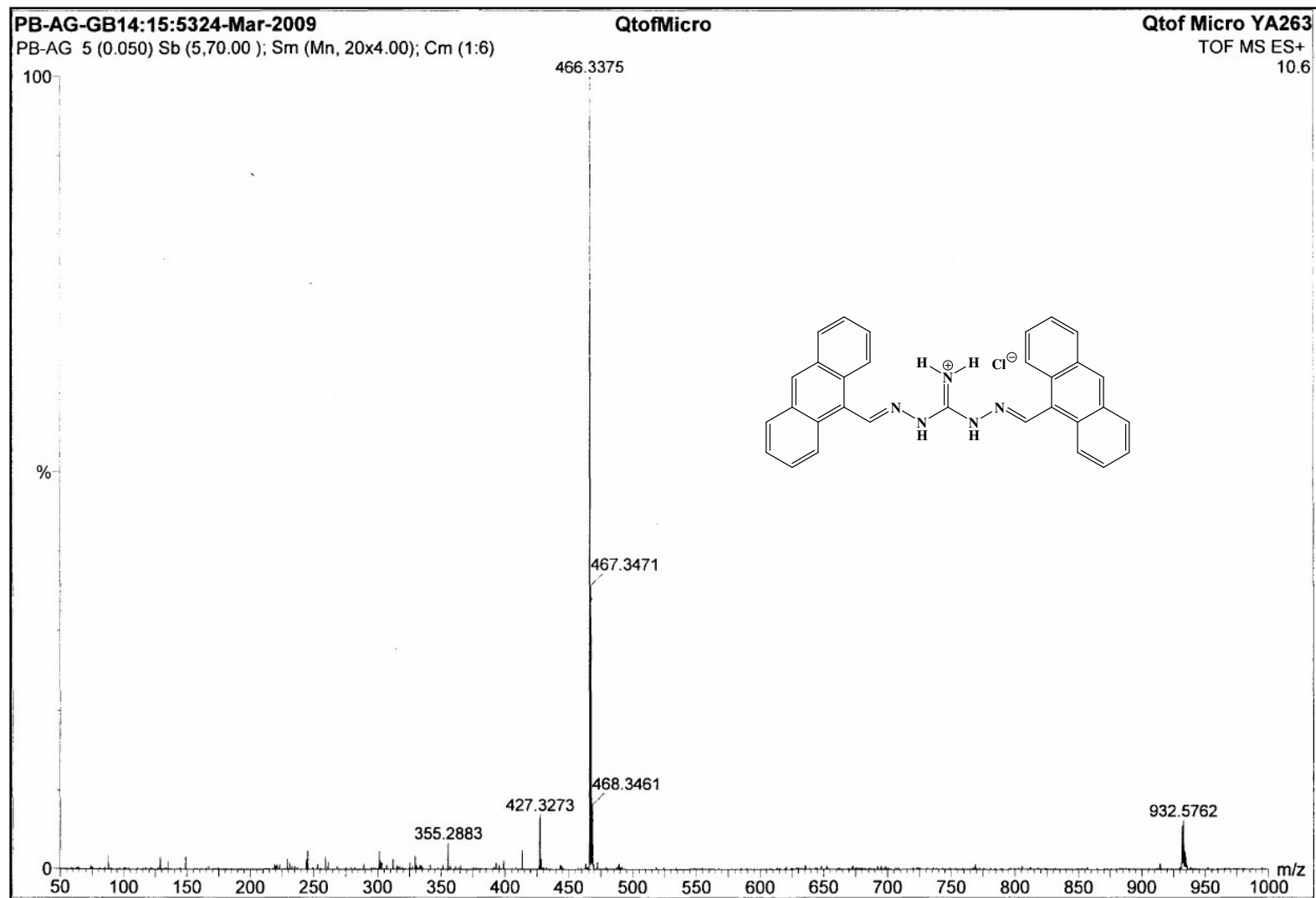


Figure S8.  $^{13}\text{C}$  NMR spectrum of S3 in  $\text{DMSO-d}_6$ .



**Figure S9.** HRMS spectrum of **S3**.

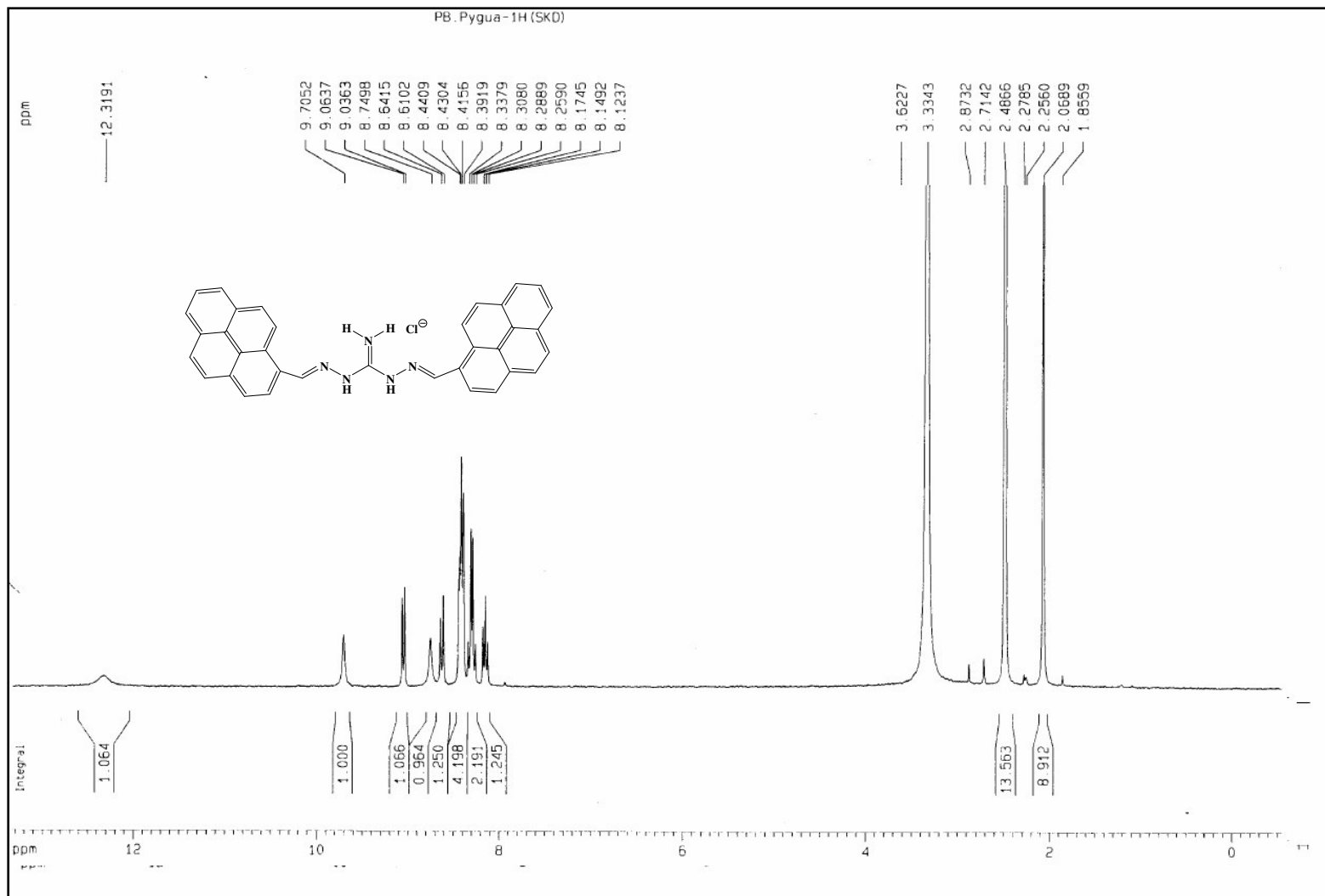
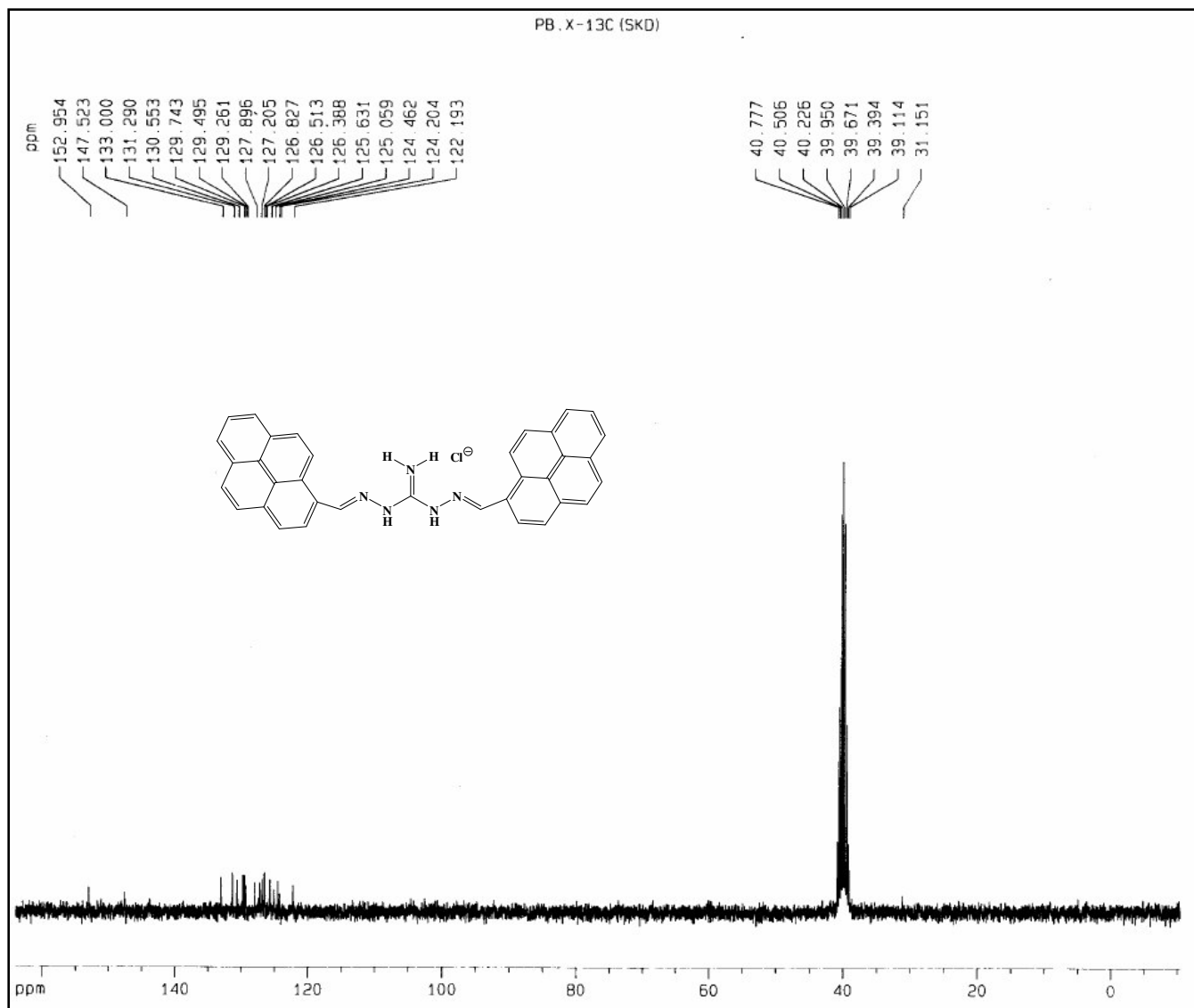


Figure S10. <sup>1</sup>H NMR spectrum of S4 in DMSO-d<sub>6</sub>.



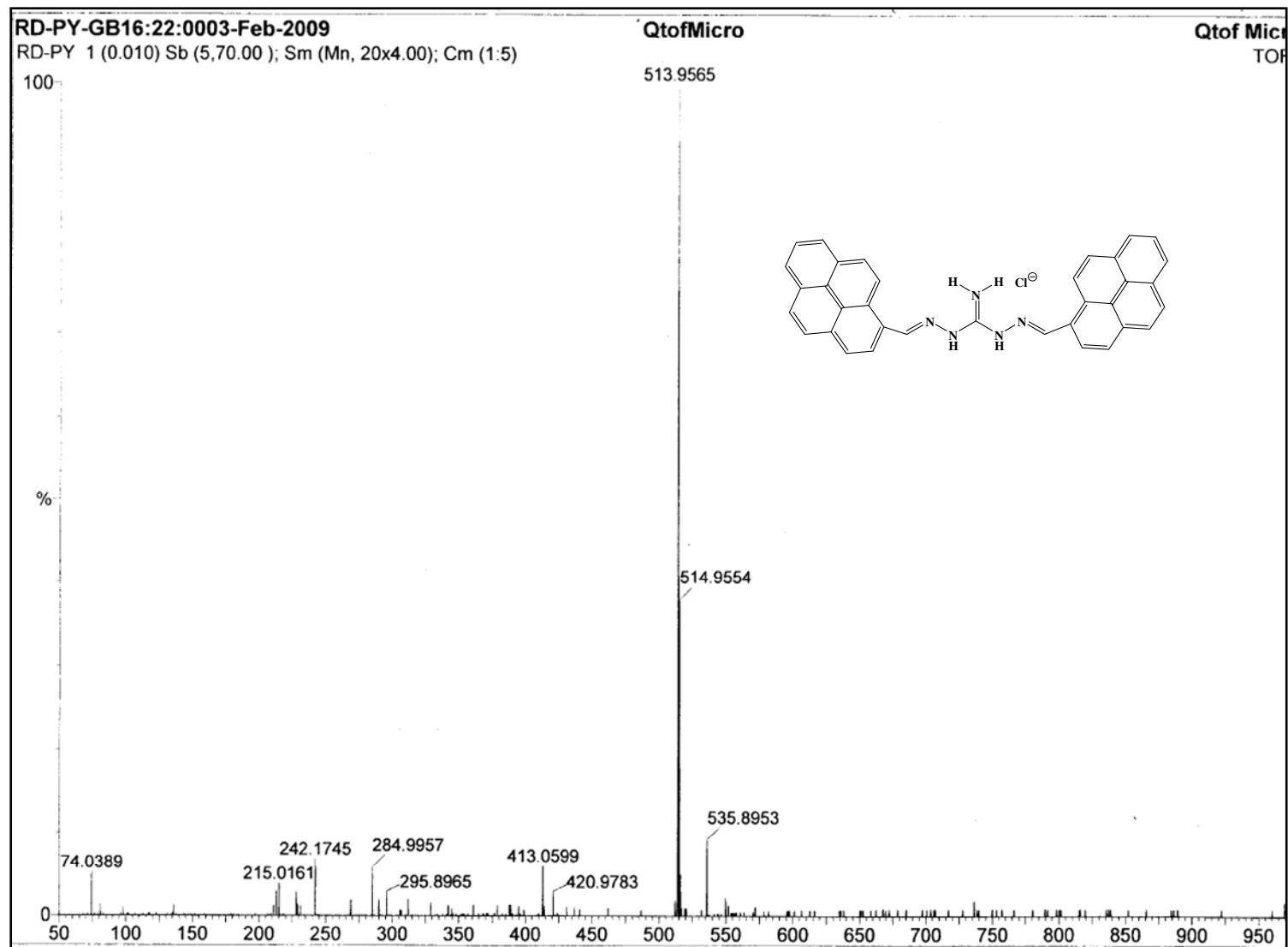


Figure S12. HRMS spectrum of S4.

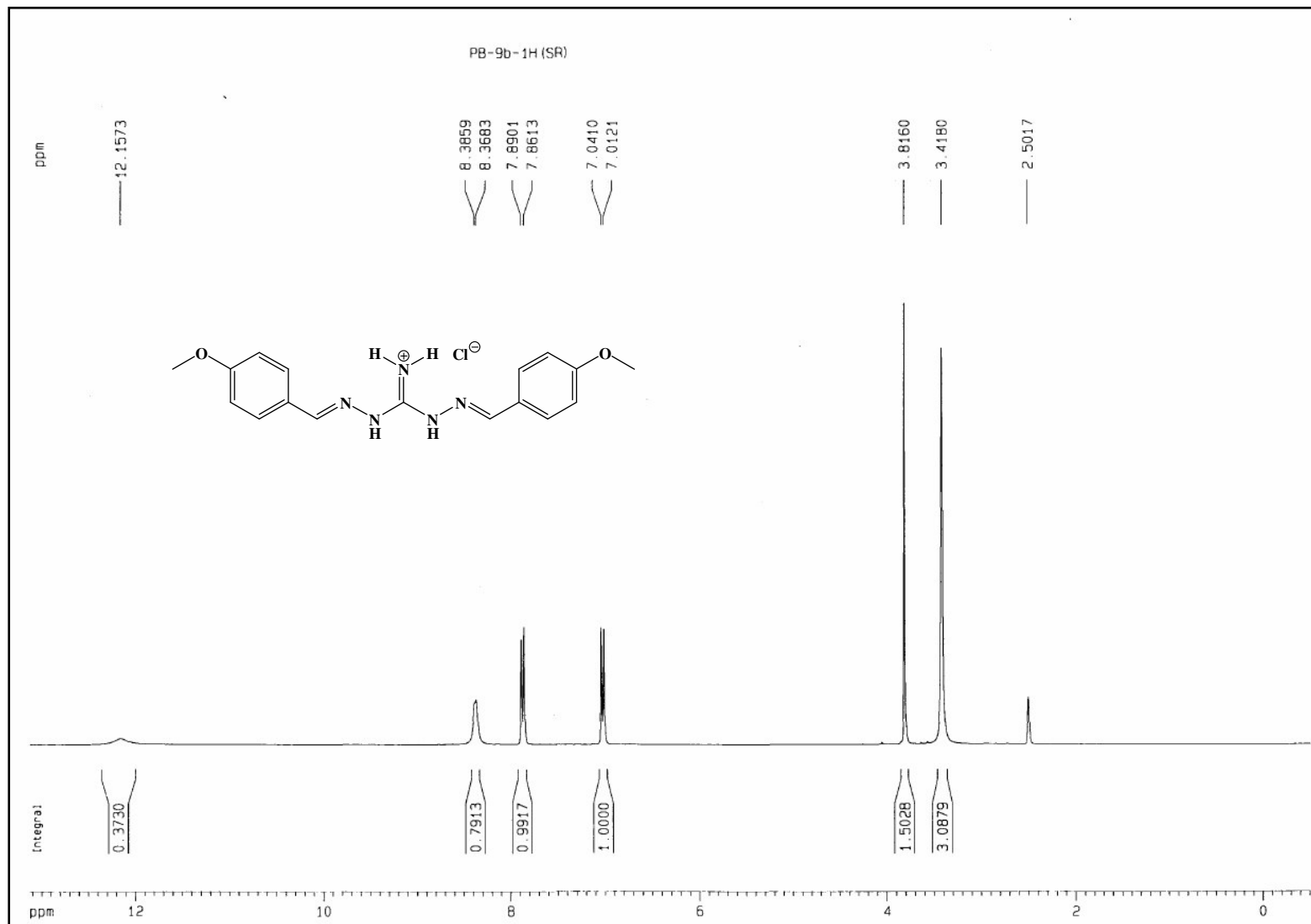


Figure S13.  $^1\text{H}$  NMR spectrum of S5 in  $\text{DMSO-d}_6$ .



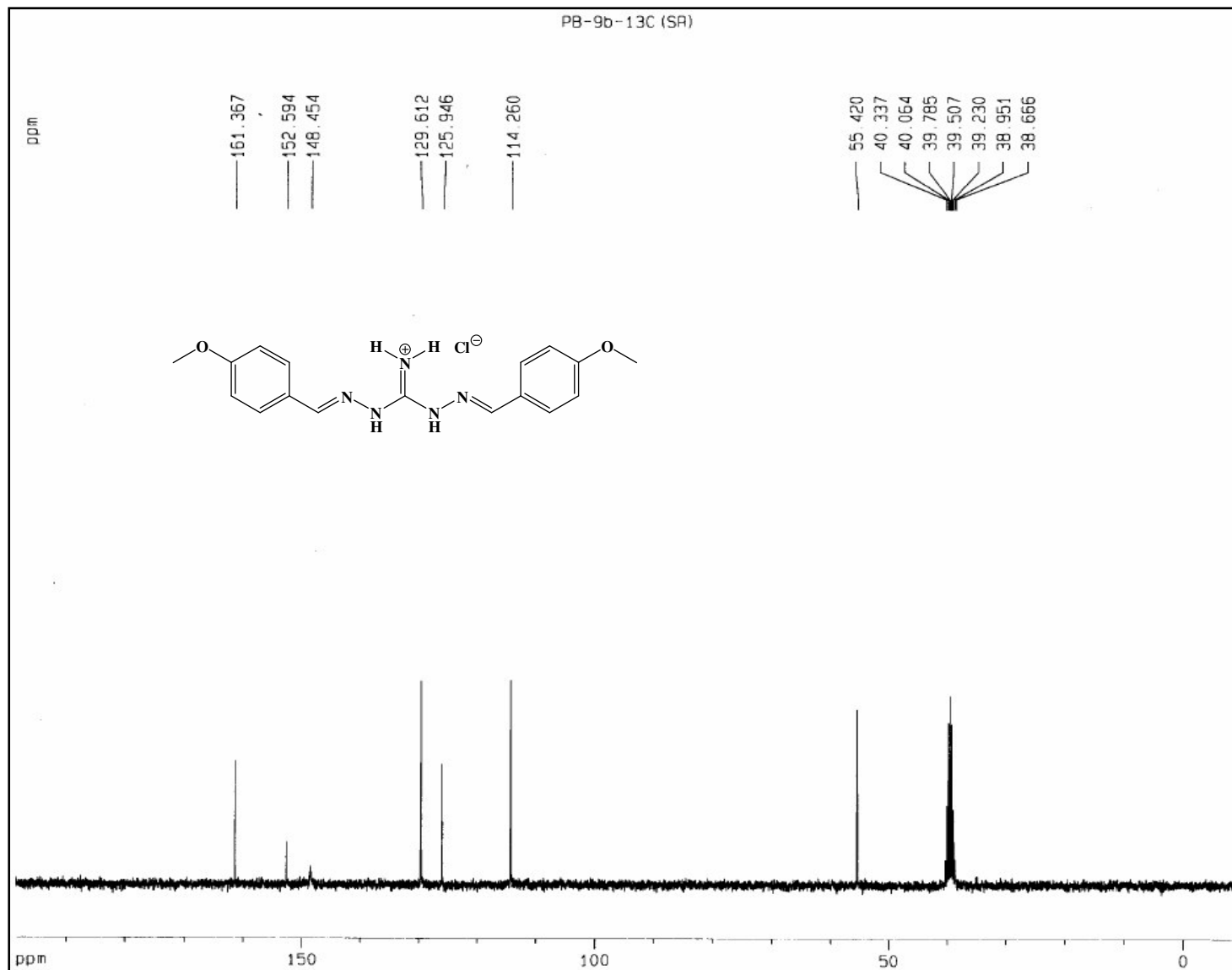


Figure S14.  $^{13}\text{C}$  NMR spectrum of **S5** in  $\text{DMSO-d}_6$ .

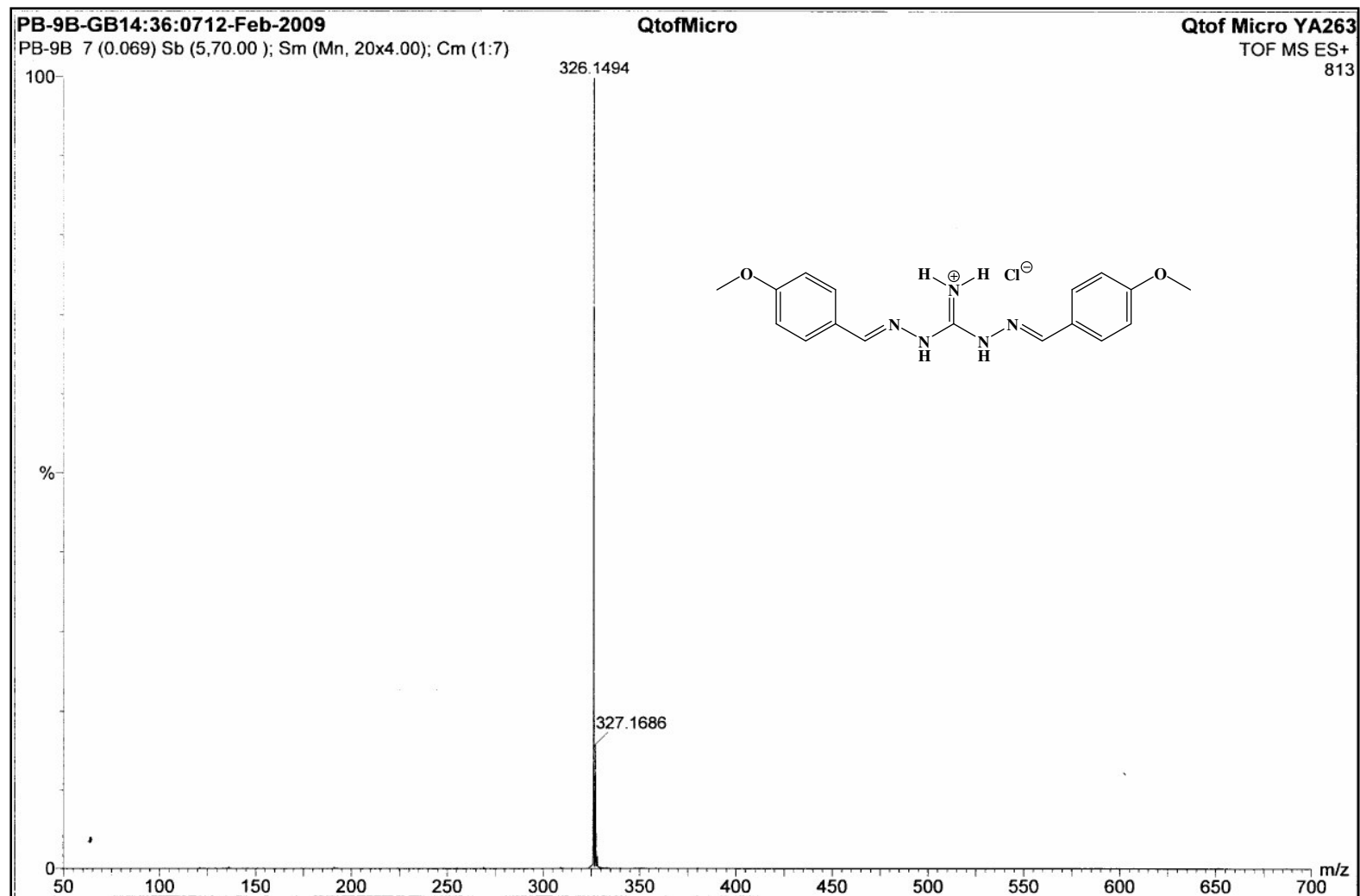


Figure S15. HRMS spectrum of S5.

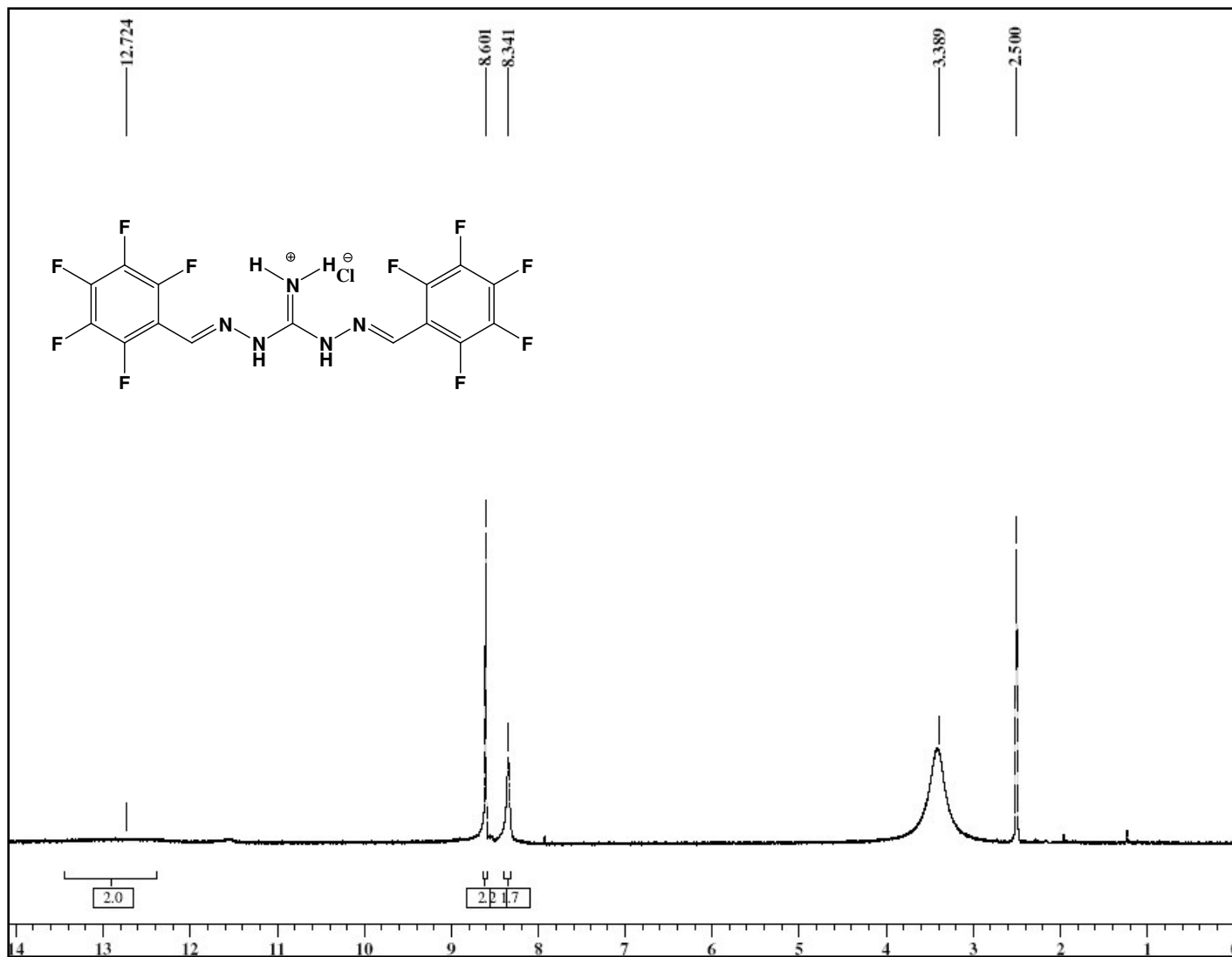


Figure S16.  $^1\text{H}$  NMR spectrum of S6 in  $\text{DMSO-d}_6$ .

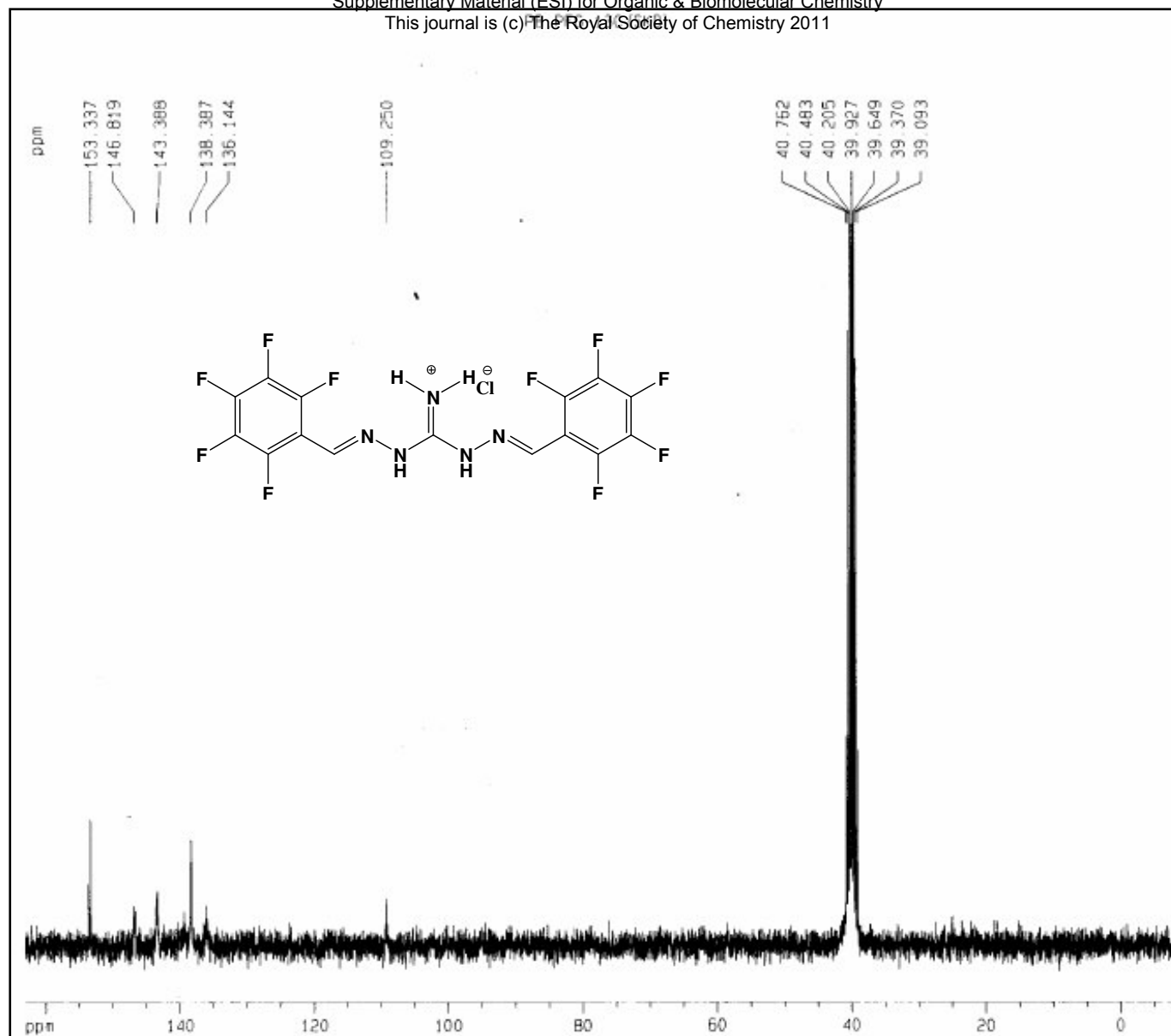


Figure S17.  $^{13}\text{C}$  NMR spectrum of S6 in DMSO- $d_6$ .

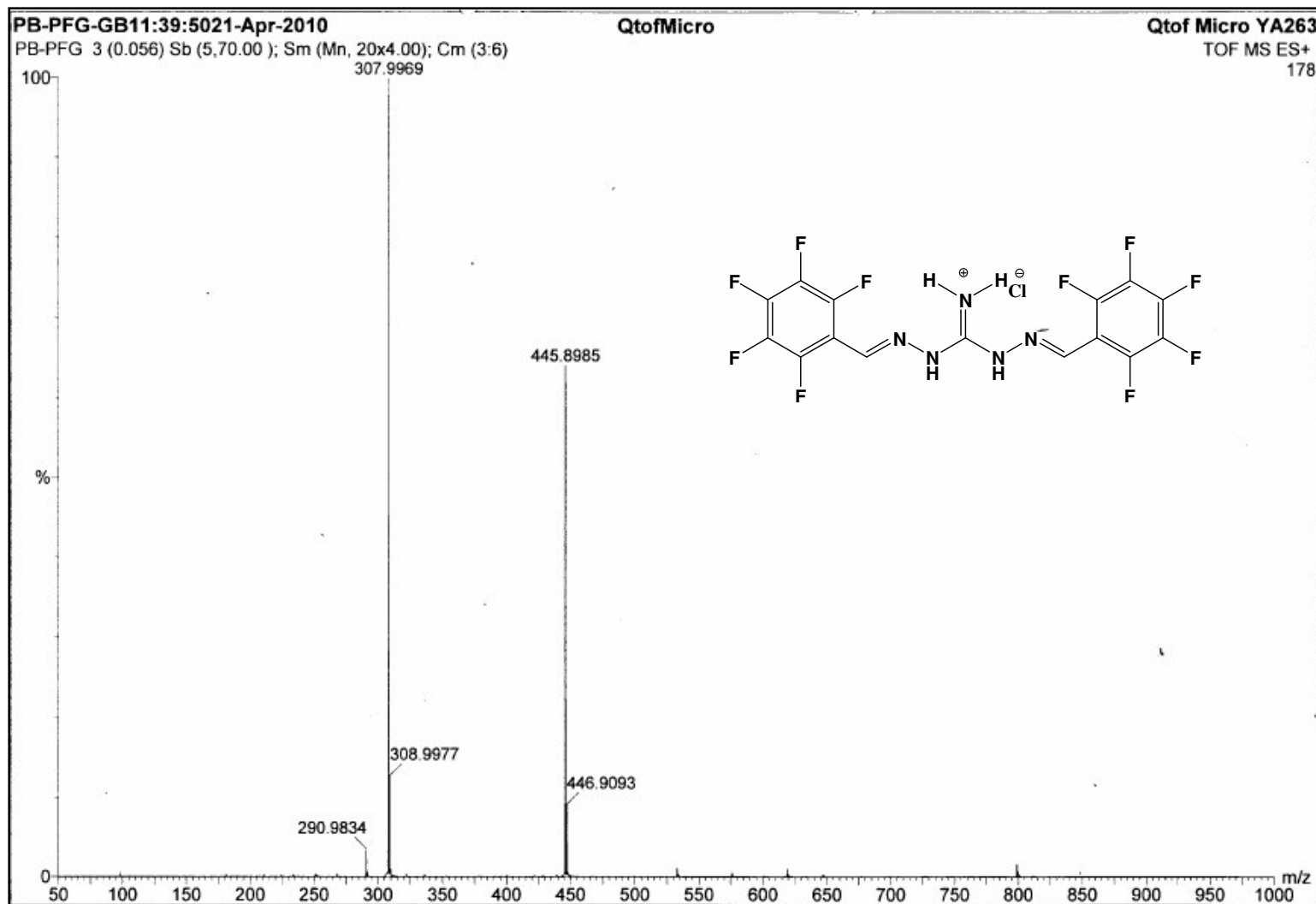


Figure S18. HRMS spectrum of S6.

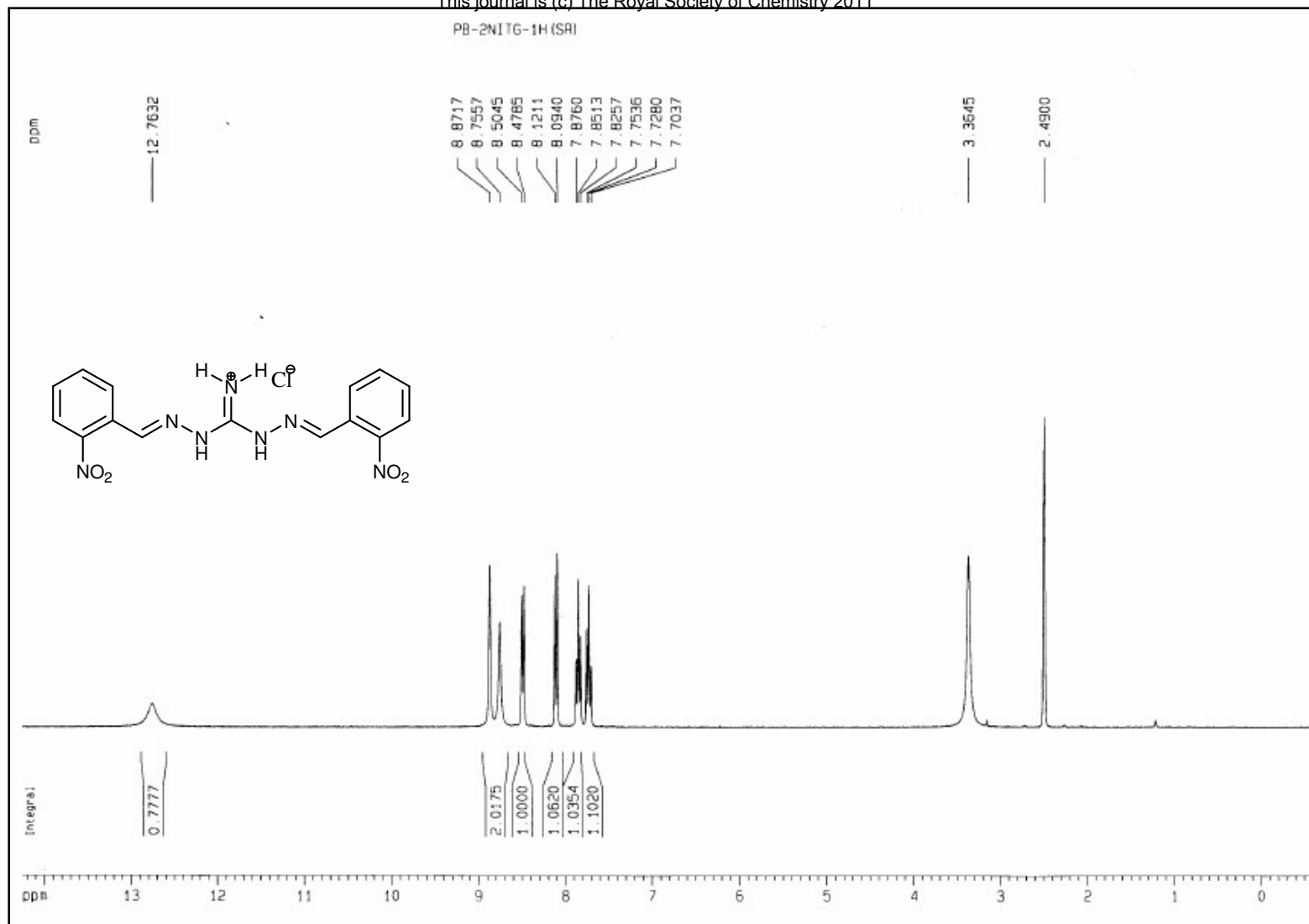
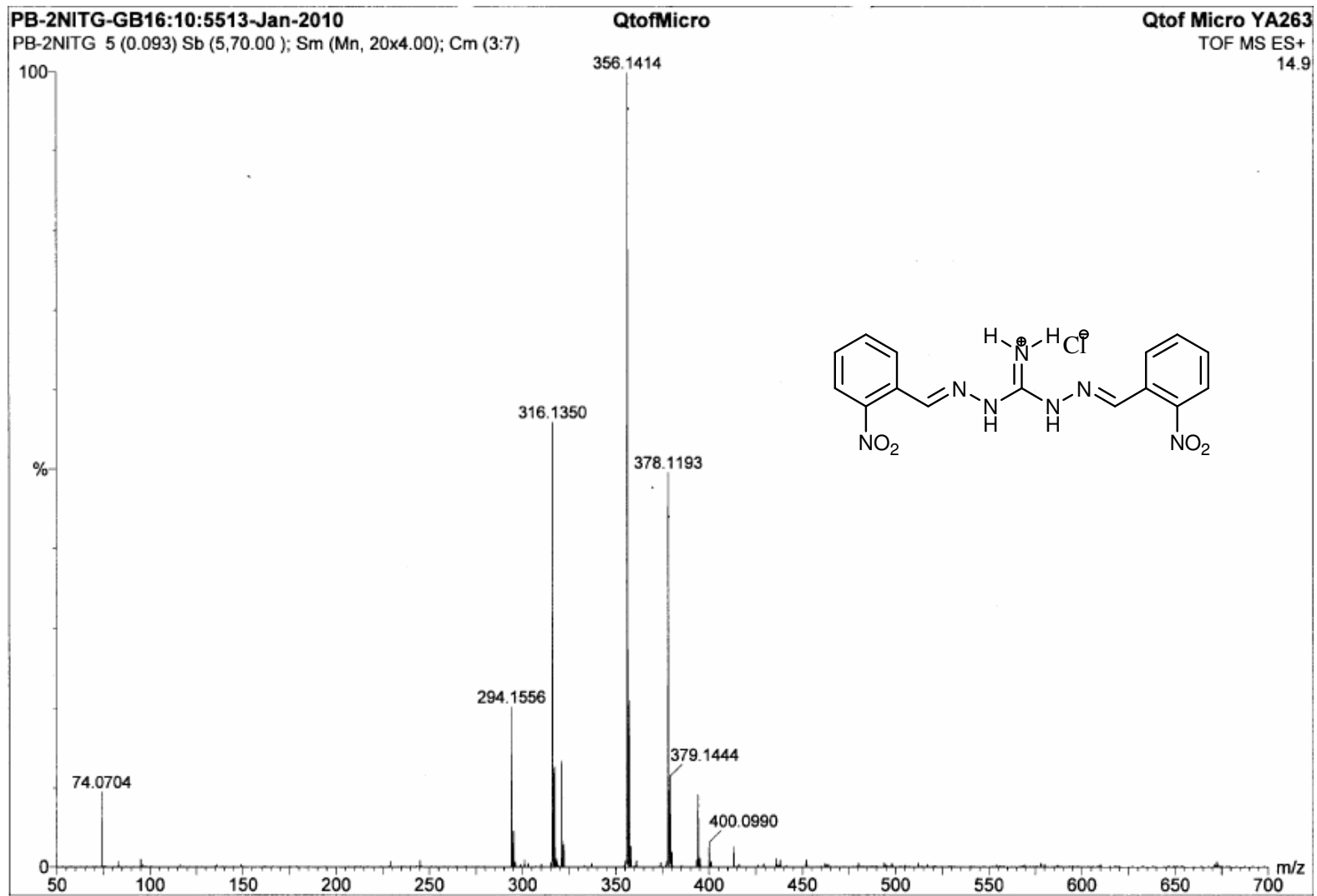


Figure S19.  $^1\text{H}$  NMR spectrum of S7 in DMSO- $d_6$ .





**Figure S21.** HRMS spectrum of S7.





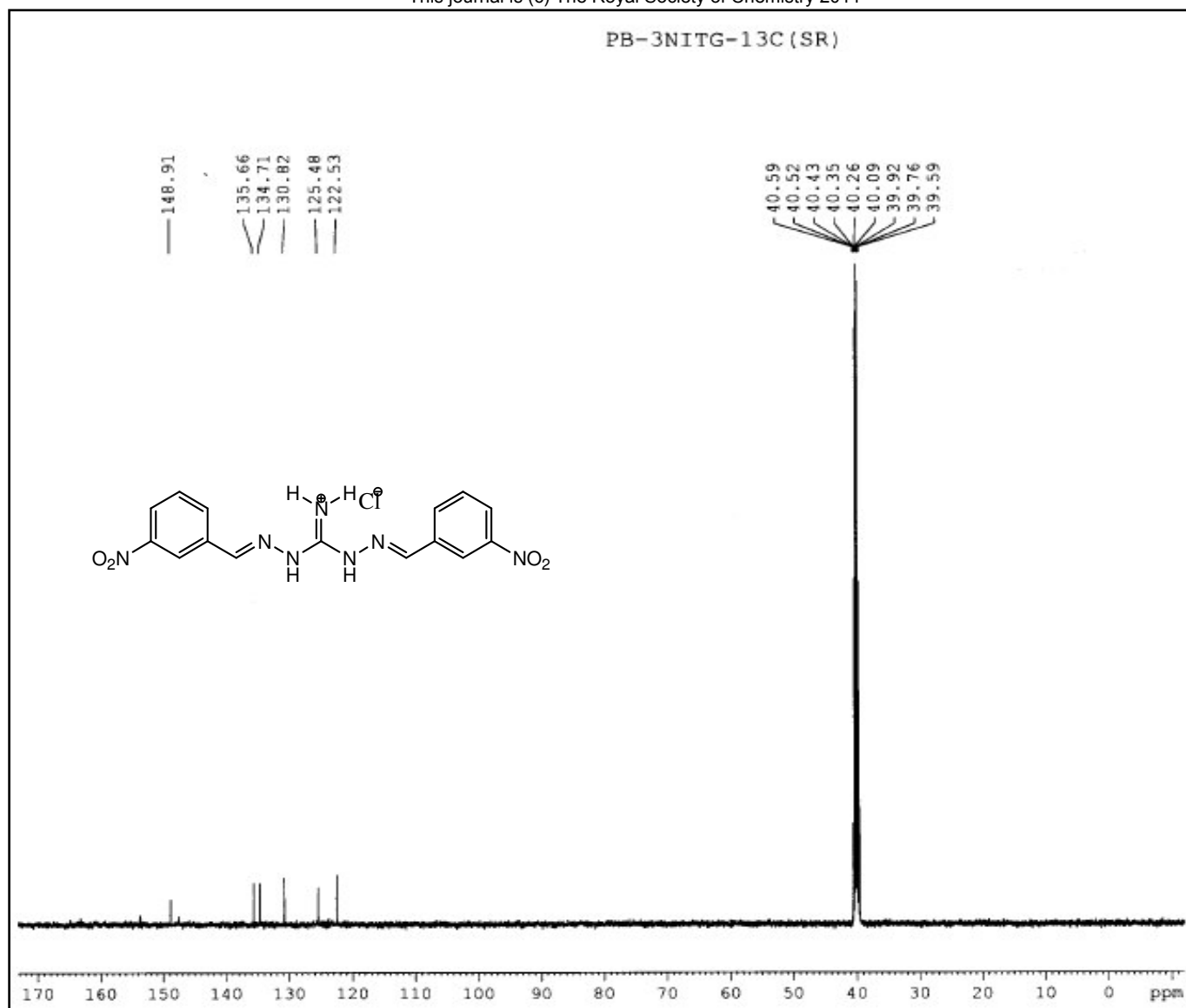


Figure S23.  $^{13}\text{C}$  NMR spectrum of S8 in DMSO- $d_6$ .

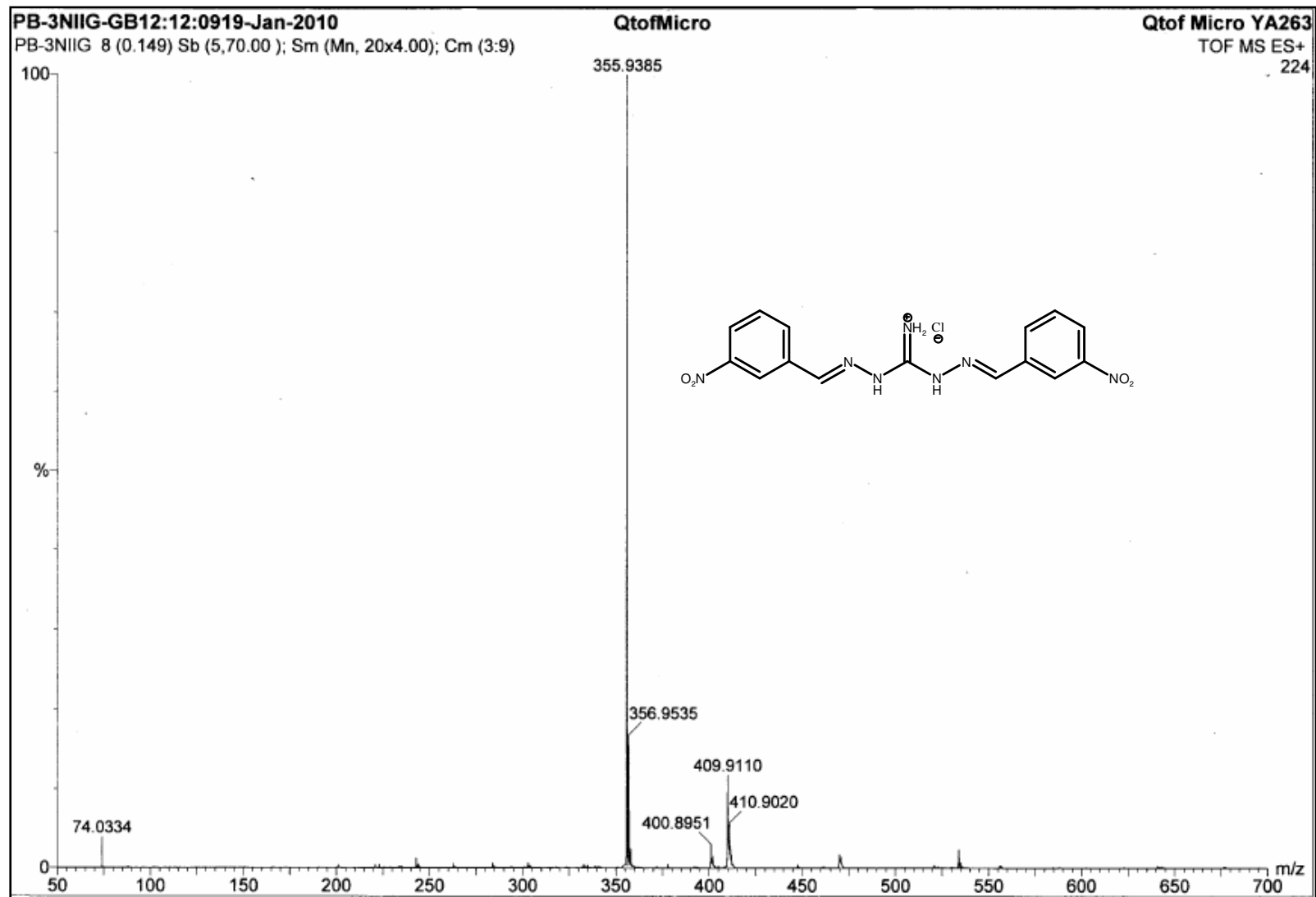


Figure S24. HRMS spectrum of S8.

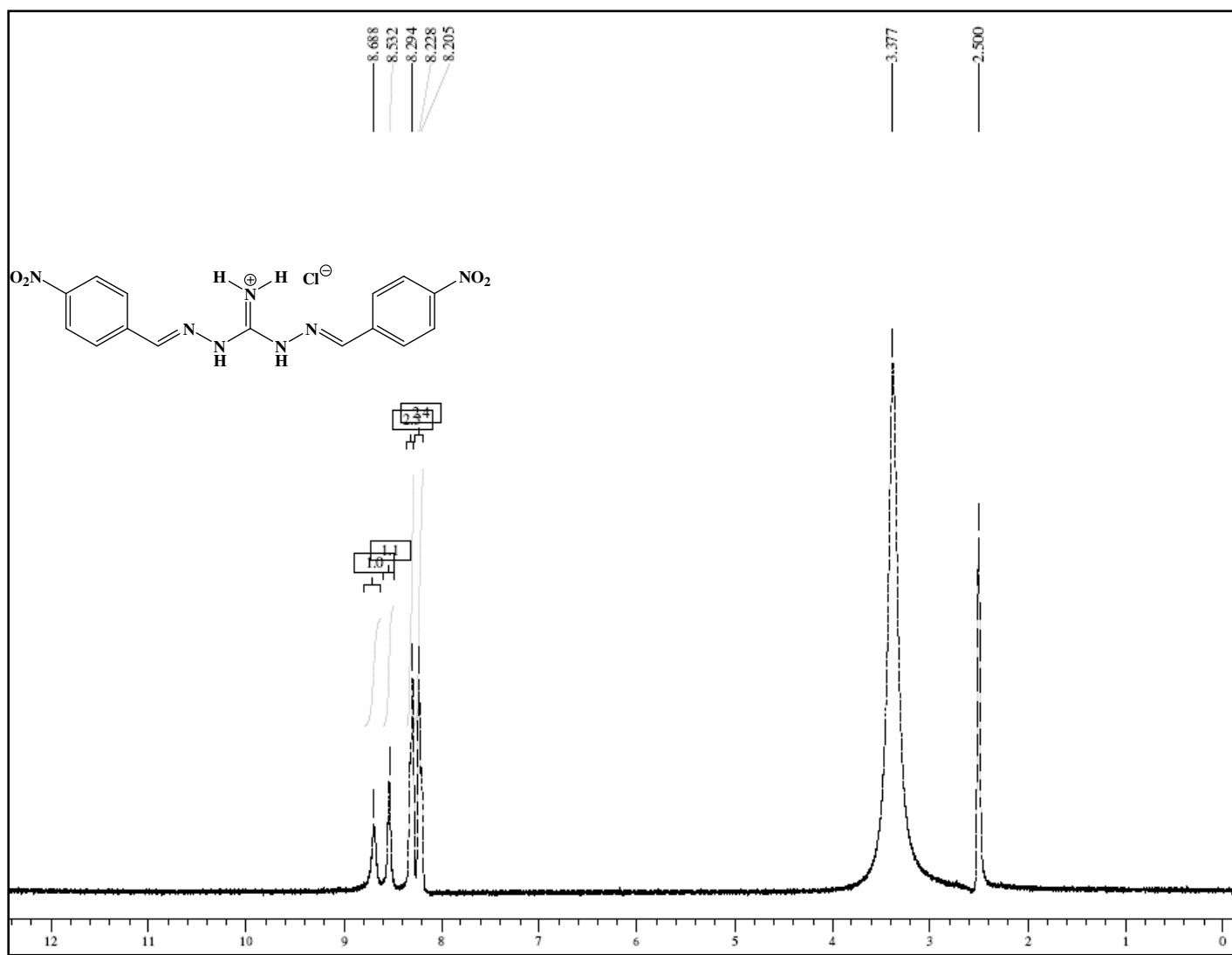


Figure S25.  $^1\text{H}$  NMR spectrum of **S9** in  $\text{DMSO-d}_6$ .

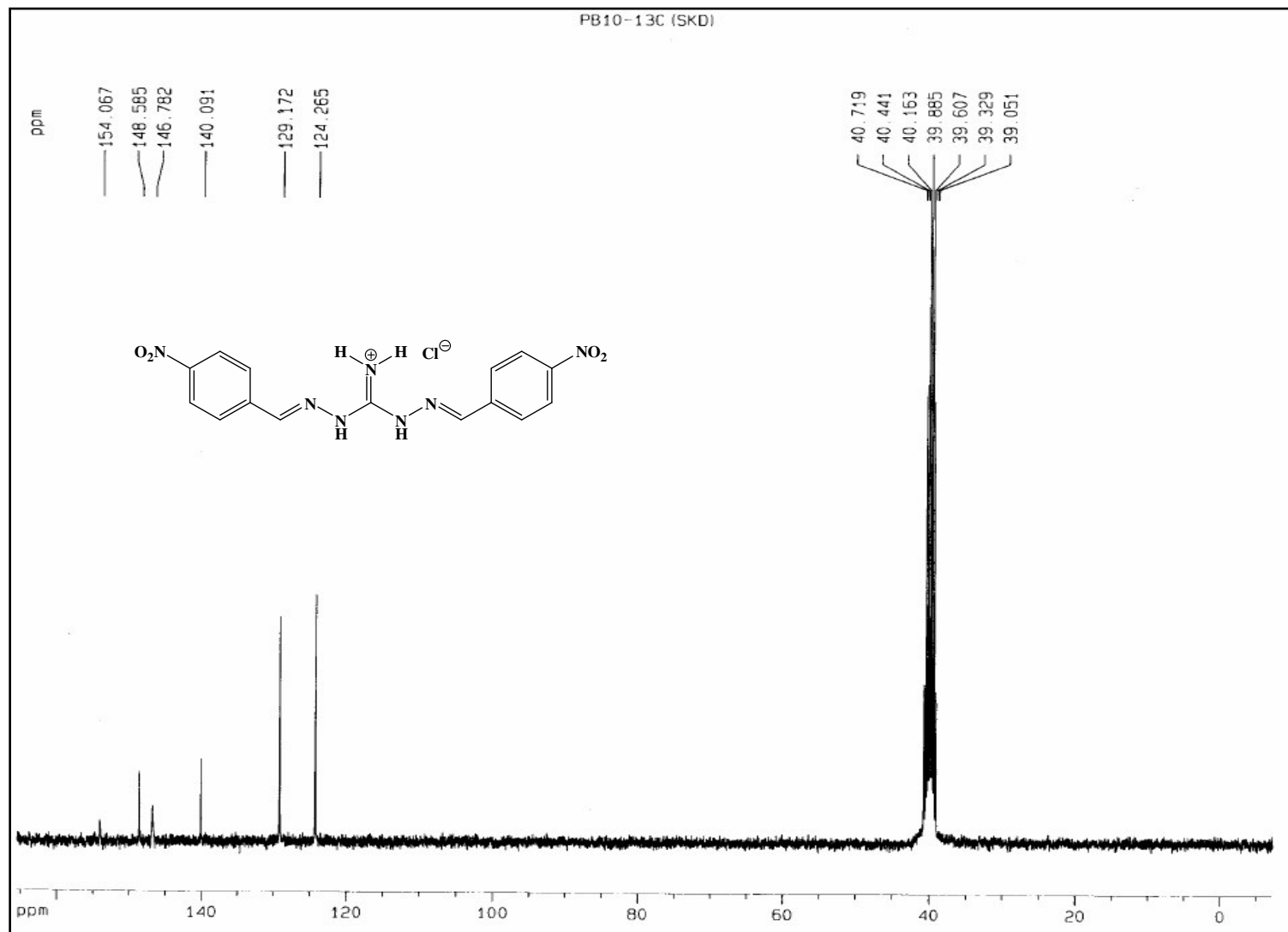


Figure S26.  $^{13}\text{C}$  NMR spectrum of **S9** in  $\text{DMSO-d}_6$ .

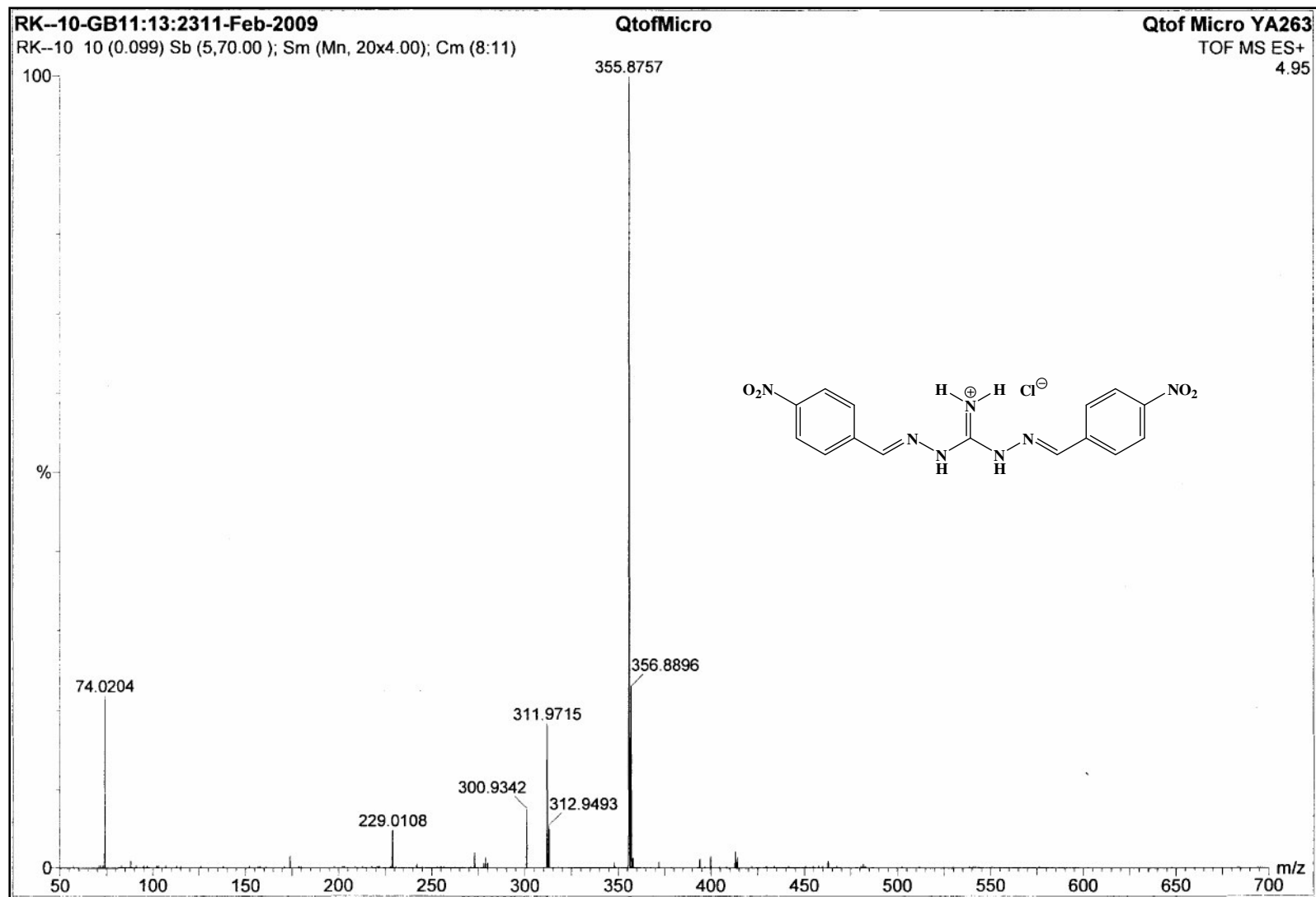


Figure S27. HRMS spectrum of S9.

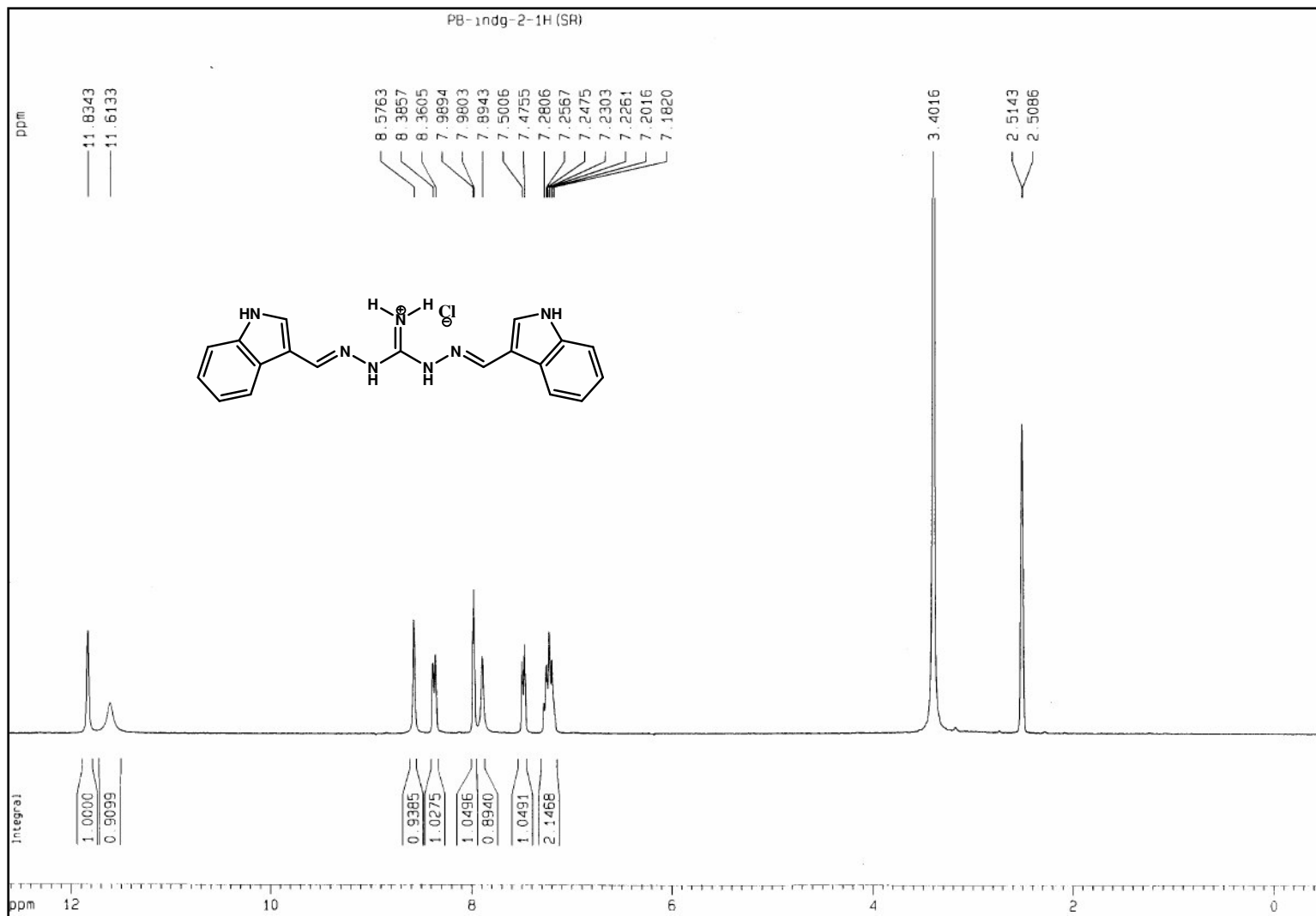


Figure S28.  $^1\text{H}$  NMR spectrum of **S10** in  $\text{DMSO-d}_6$ .

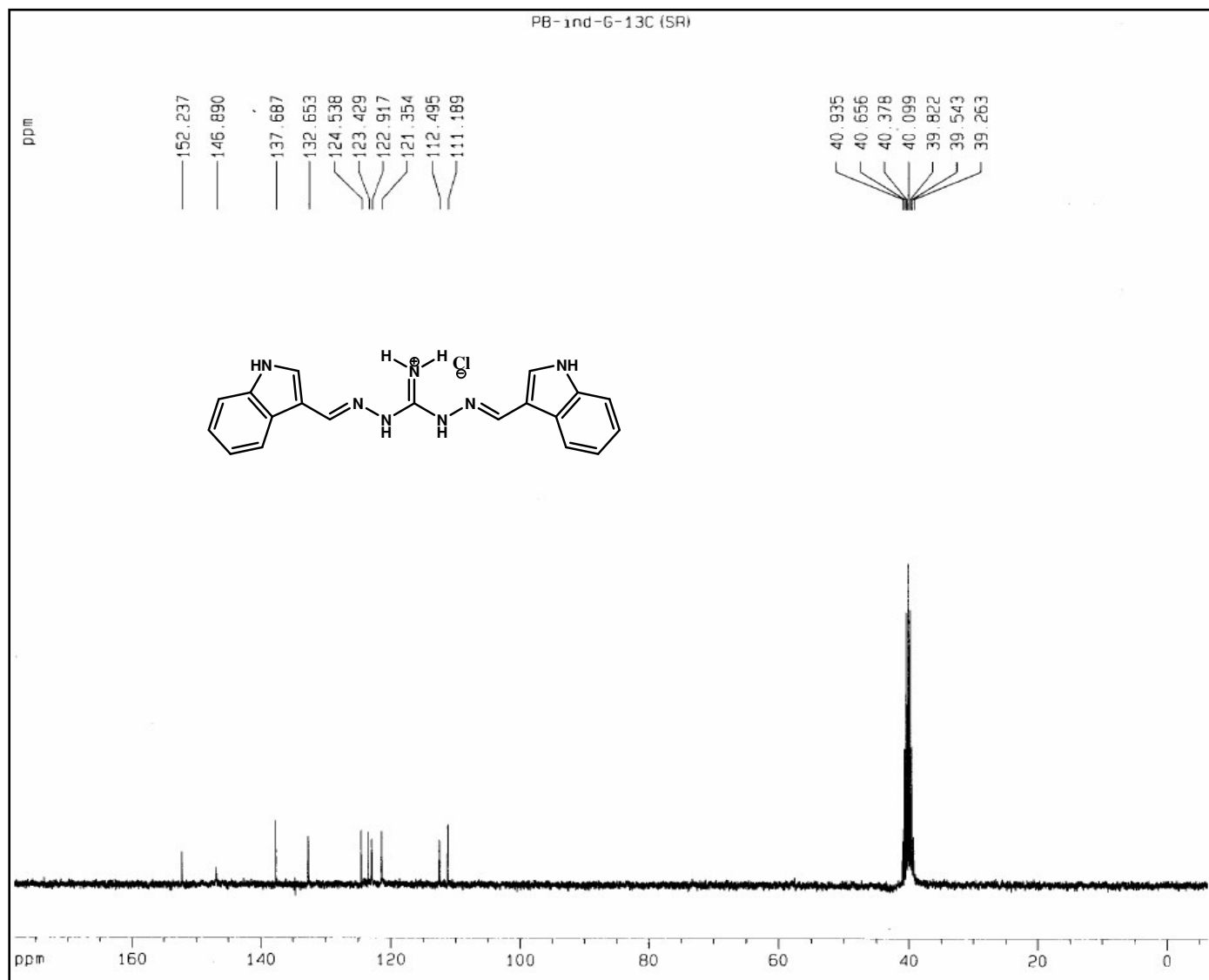


Figure S29.  $^{13}\text{C}$  NMR spectrum of S10 in DMSO- $d_6$ .



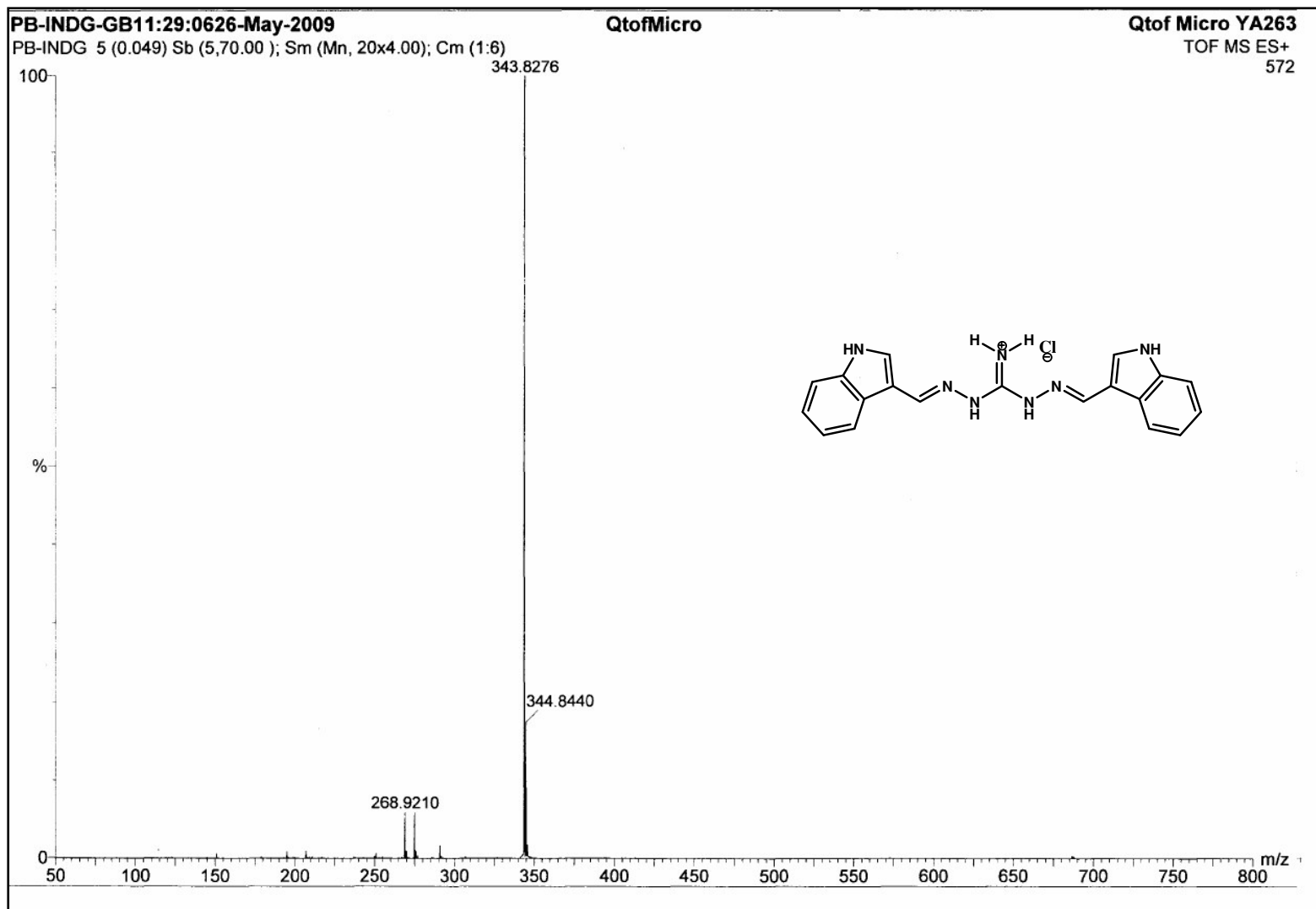
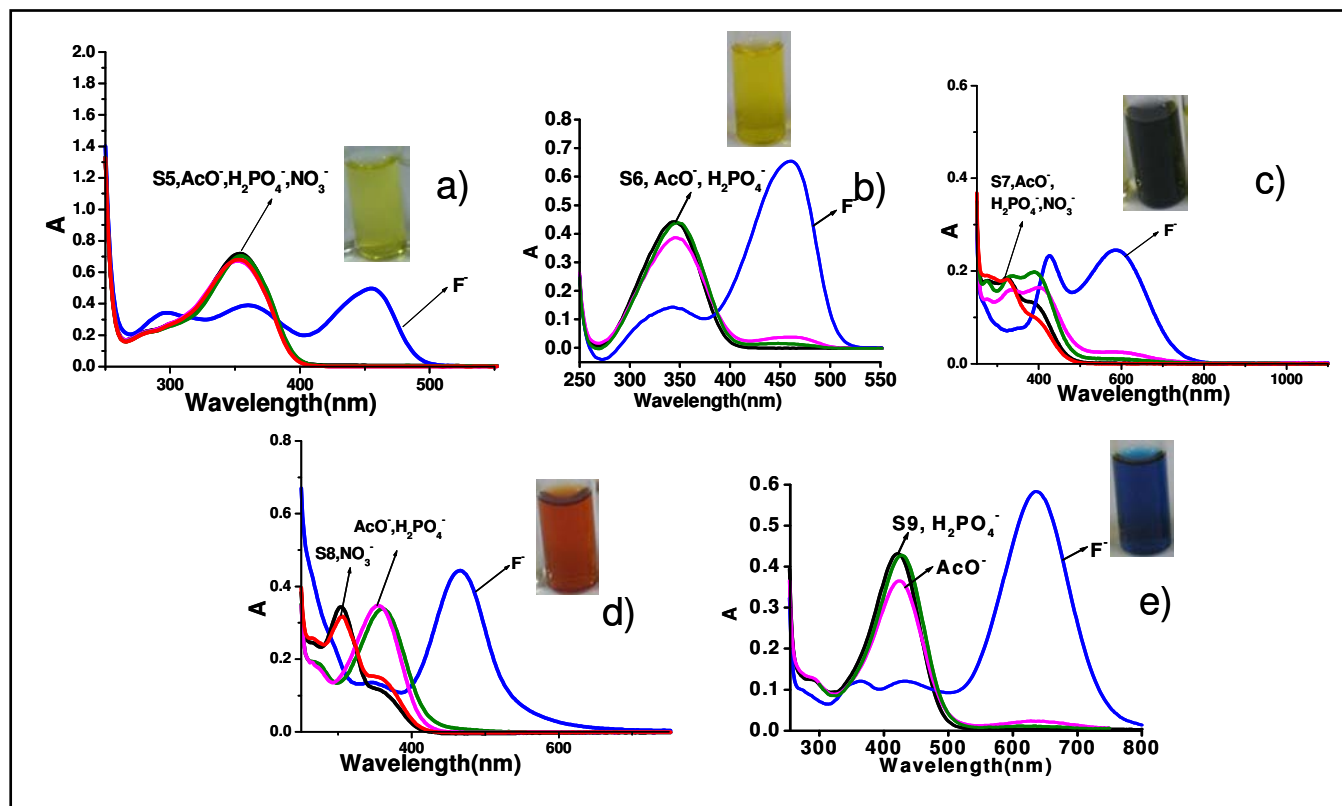
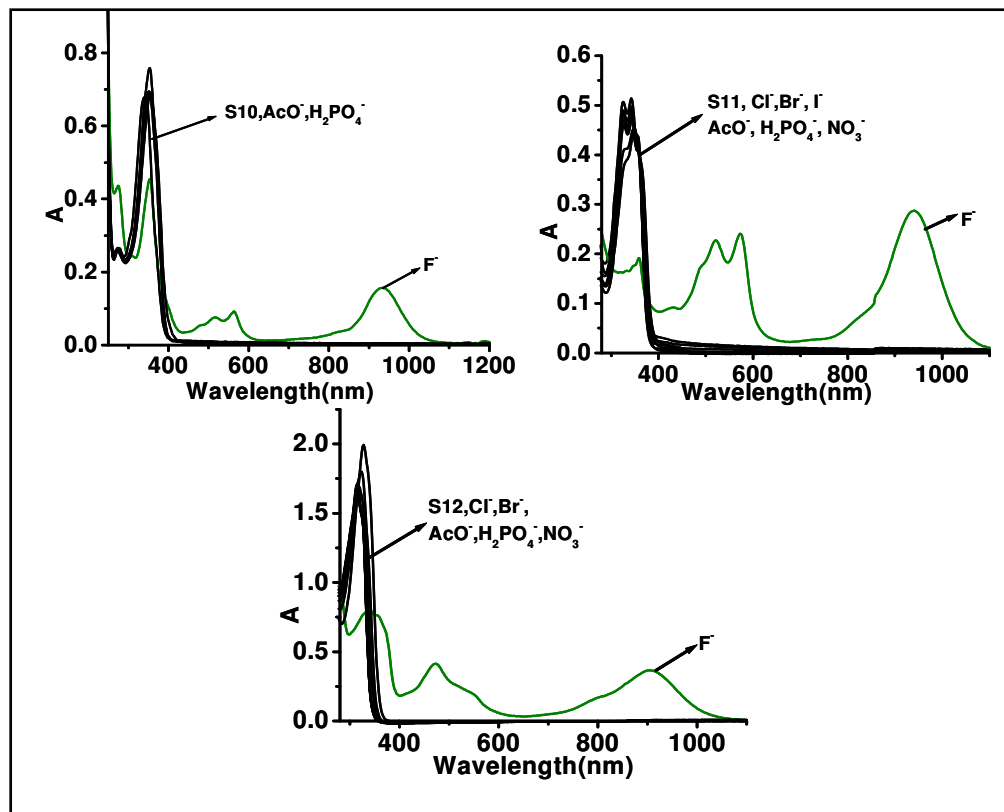


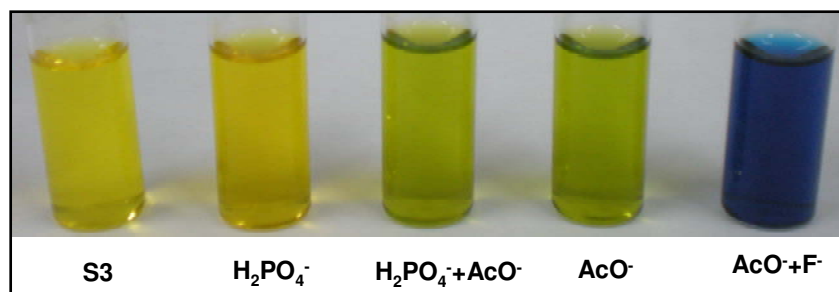
Figure S30. HRMS spectrum of S10.



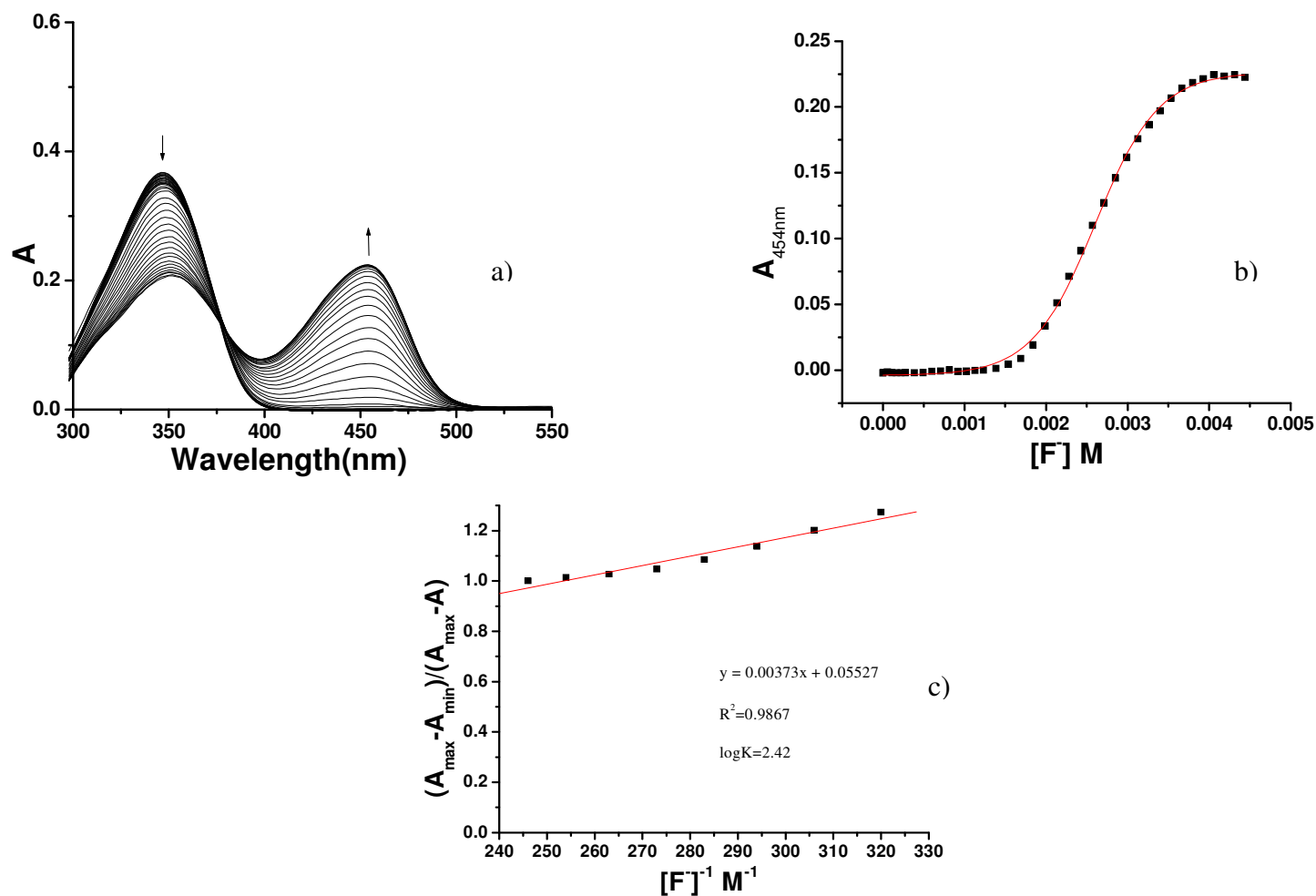
**Figure S31.** Changes in the UV-Vis absorption spectrum a)-e) of **S5-S9** ( $1.0 \times 10^{-4}$  M) in MeCN/DMF (9.6:0.4)(v/v) solution upon addition of 50 equiv of anions.



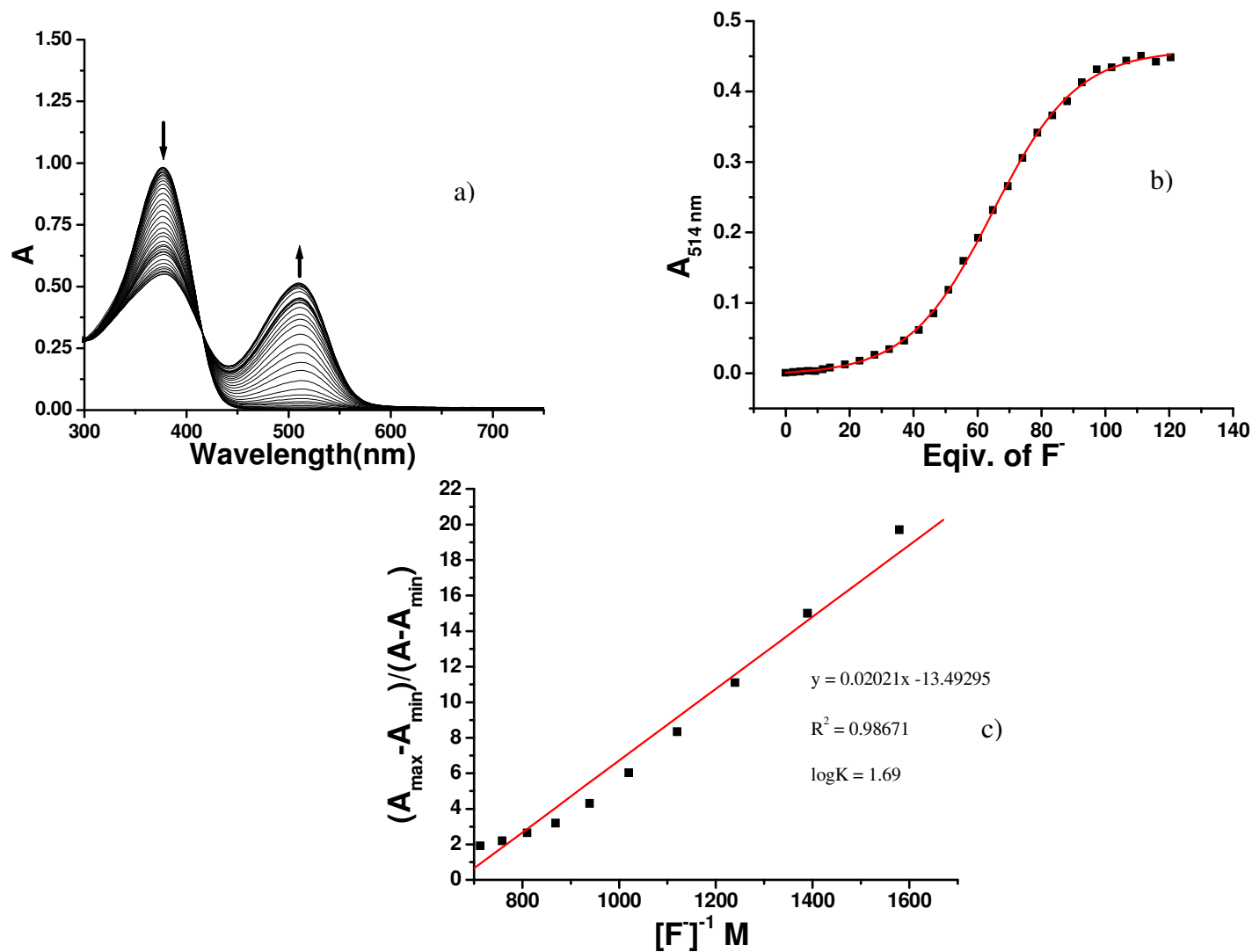
**Figure S32.** Changes in the UV/vis/NIR absorption spectrum of **S10-S12** ( $1.0 \times 10^{-5}$  M) in MeCN/DMF(9.6:0.4)(v/v) solution upon addition of 50 equiv of different anions.



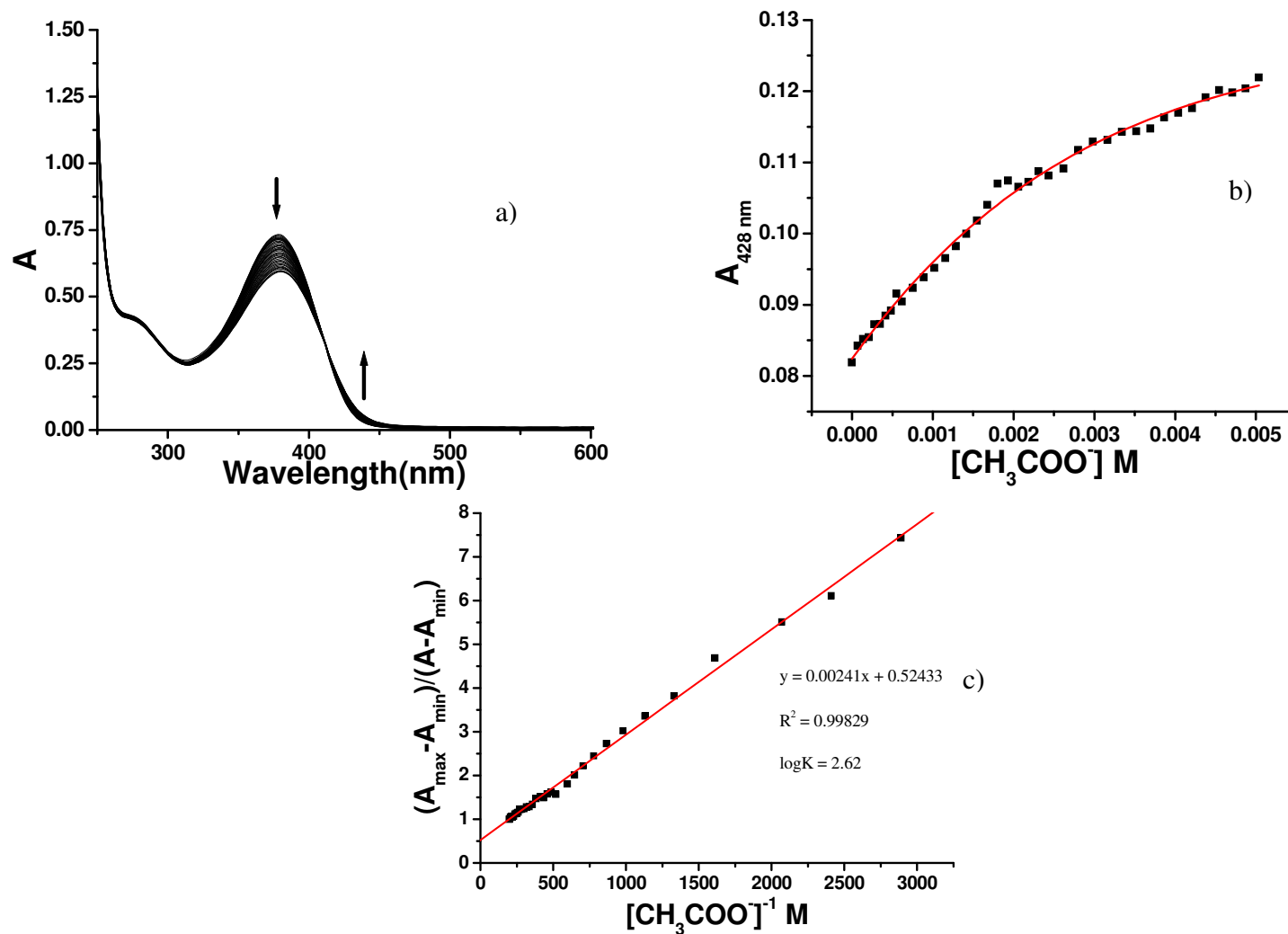
**Figure S33.** Selectivity study of **S9** ( $1 \times 10^{-4}$  M) in presence of different anions (30 equiv.).



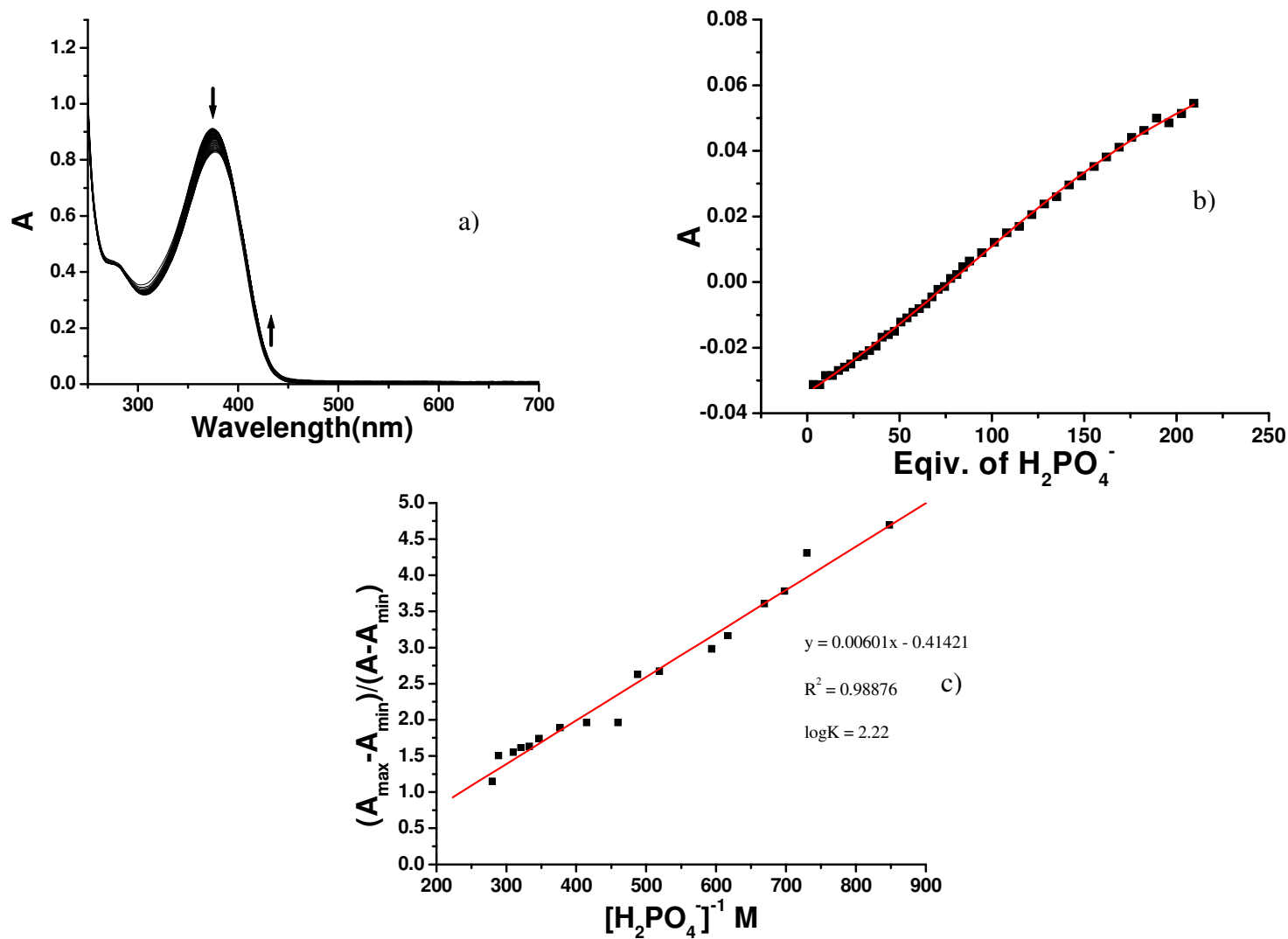
**Figure S34.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S1** in MeCN/DMF (9.6:0.4)(v/v) with a standard solution of 0.01 (M) [Bu<sub>4</sub>N]F in MeCN. b) Absorbance changes for **S1** at 350 nm on addition of various concentration of [Bu<sub>4</sub>N]F. c) Benesi-Hildebrand plot.



**Figure S35.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of S2 in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01(M) [Bu<sub>4</sub>N]F in MeCN. b) Absorbance changes for S2 at 514 nm on addition of various concentration of [Bu<sub>4</sub>N]F. c) Benesi-Hildebrand plot.

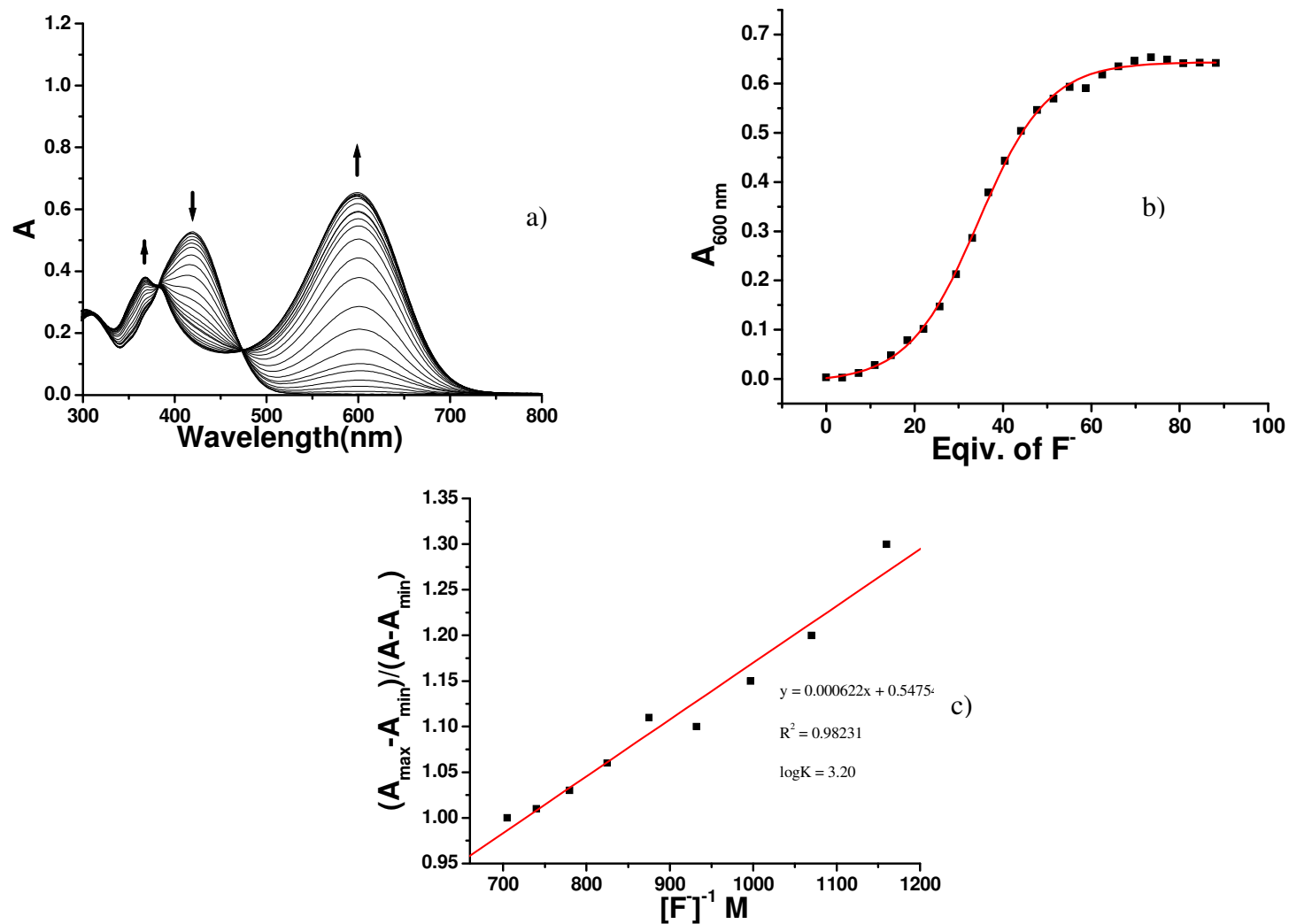


**Figure S36.** a) UV-Vis absorption changes of the titration of a 1.0 × 10<sup>-5</sup> M solution of S2 in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01(M) [Bu<sub>4</sub>N]AcO in MeCN. b) Absorbance changes for S2 at 428 nm on addition of various concentration of [Bu<sub>4</sub>N]AcO. c) Benesi-Hildebrand plot.

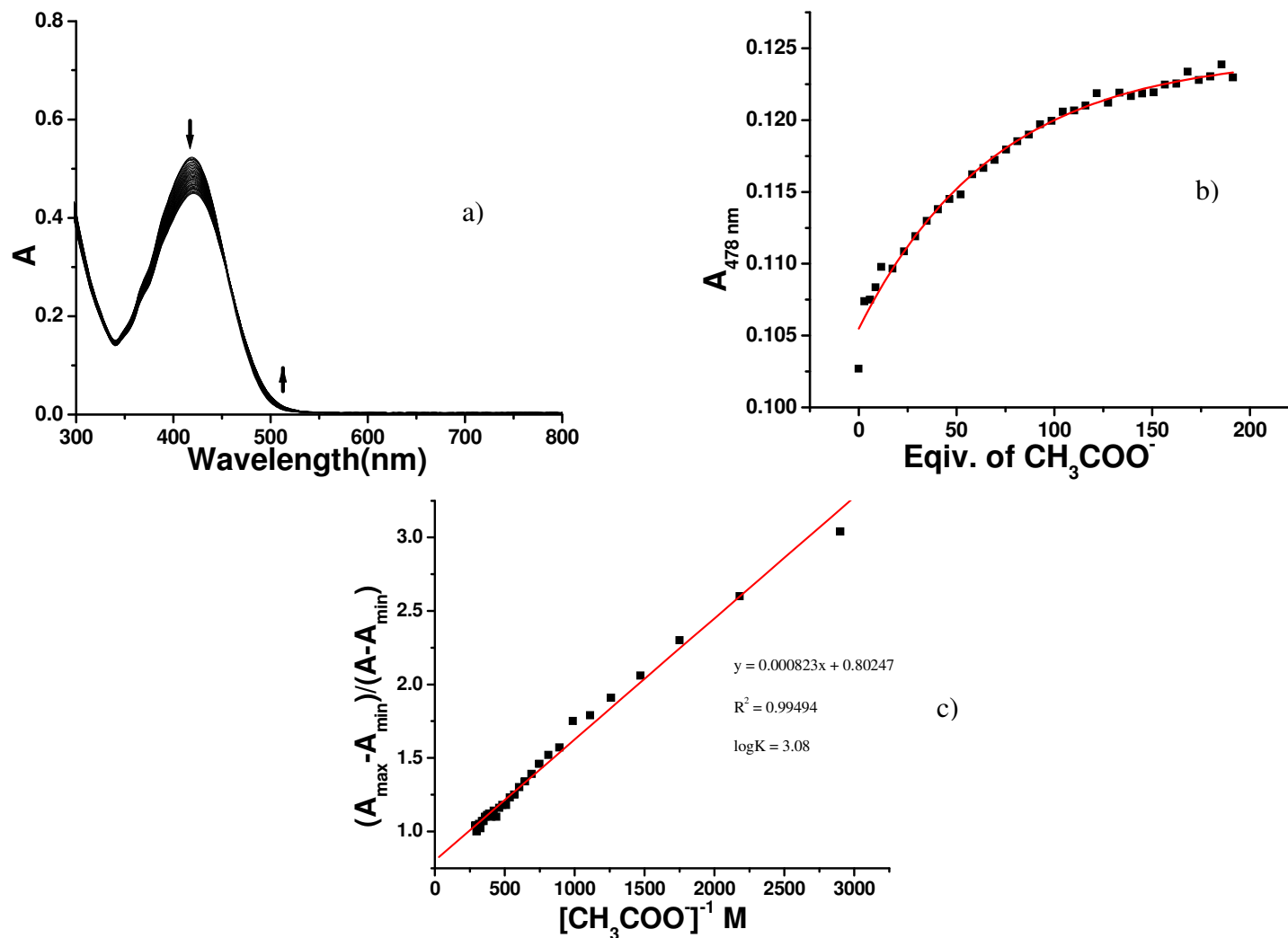


**Figure S37.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S2** in MeCN/DMF (9.6:0.4)(v/v) with a standard solution of 0.01(M) [Bu<sub>4</sub>N]H<sub>2</sub>PO<sub>4</sub> in MeCN. b) Absorbance changes for **S2** at 430 nm on addition of various concentration of [Bu<sub>4</sub>N] H<sub>2</sub>PO<sub>4</sub>. c) Benesi-Hildebrand plot.

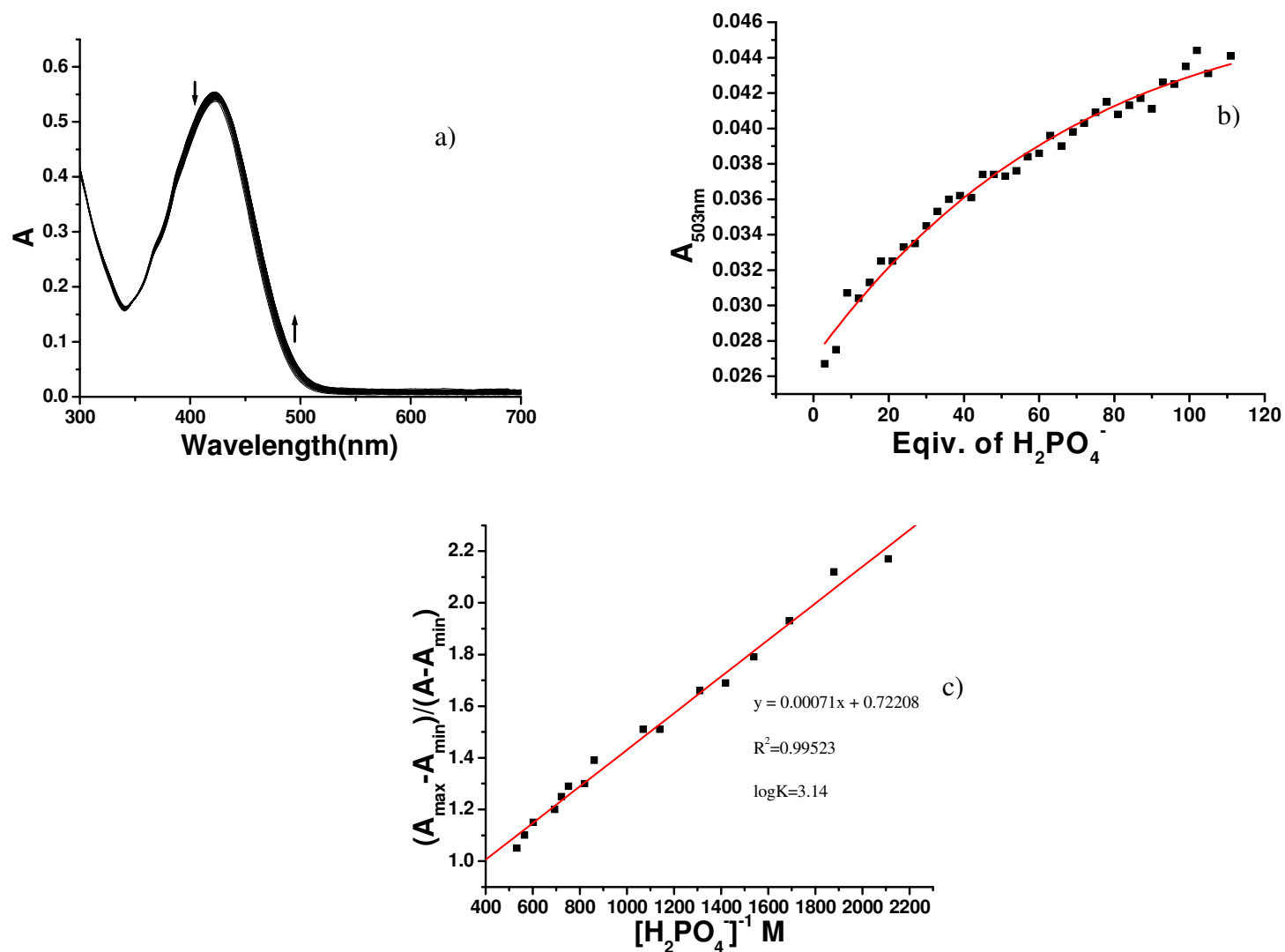




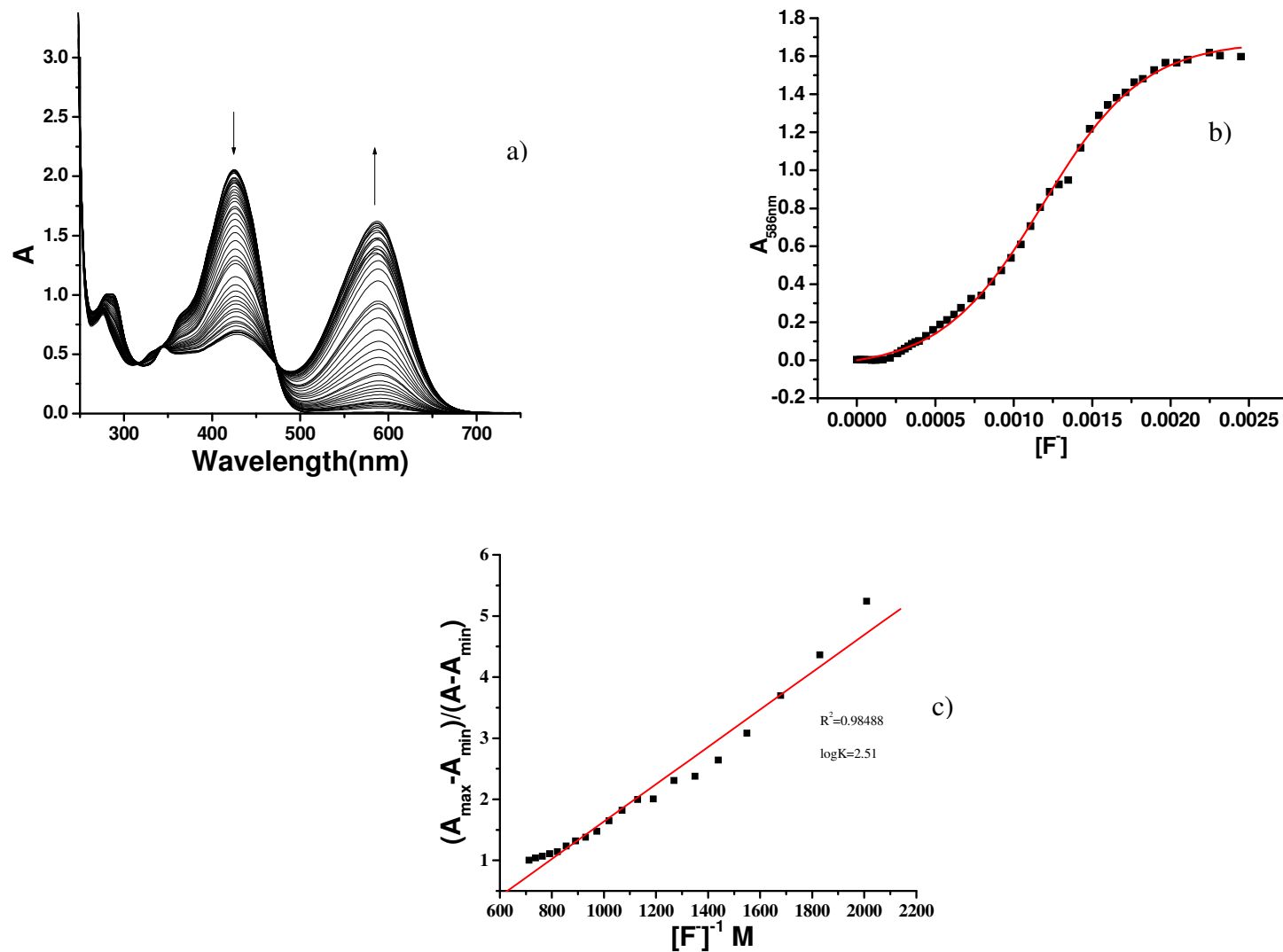
**Figure S38.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5} \text{ M}$  solution of **S3** in in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01(M) [Bu<sub>4</sub>N]F in MeCN. b) Absorbance changes for **S3** at 600 nm on addition of various concentration of [Bu<sub>4</sub>N]F. c) Benesi-Hildebrand plot.



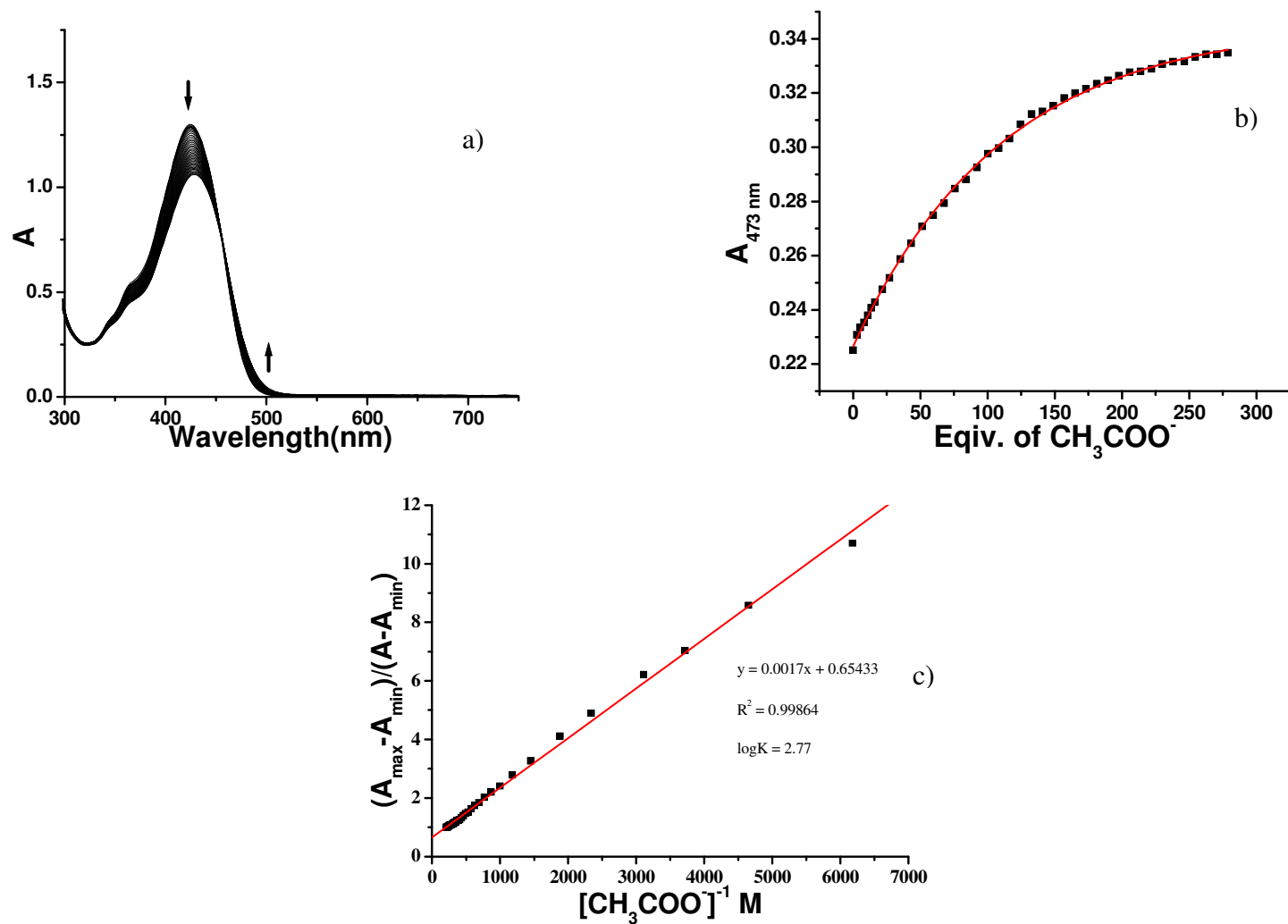
**Figure S39.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S3** in MeCN/DMF (9.6:0.4)(v/v) with a standard solution of 0.01(M) [Bu<sub>4</sub>N]AcO in MeCN. b) Absorbance changes for **S3** at 478 nm on addition of various concentration of [Bu<sub>4</sub>N]AcO. c) Benesi-Hildebrand plot.



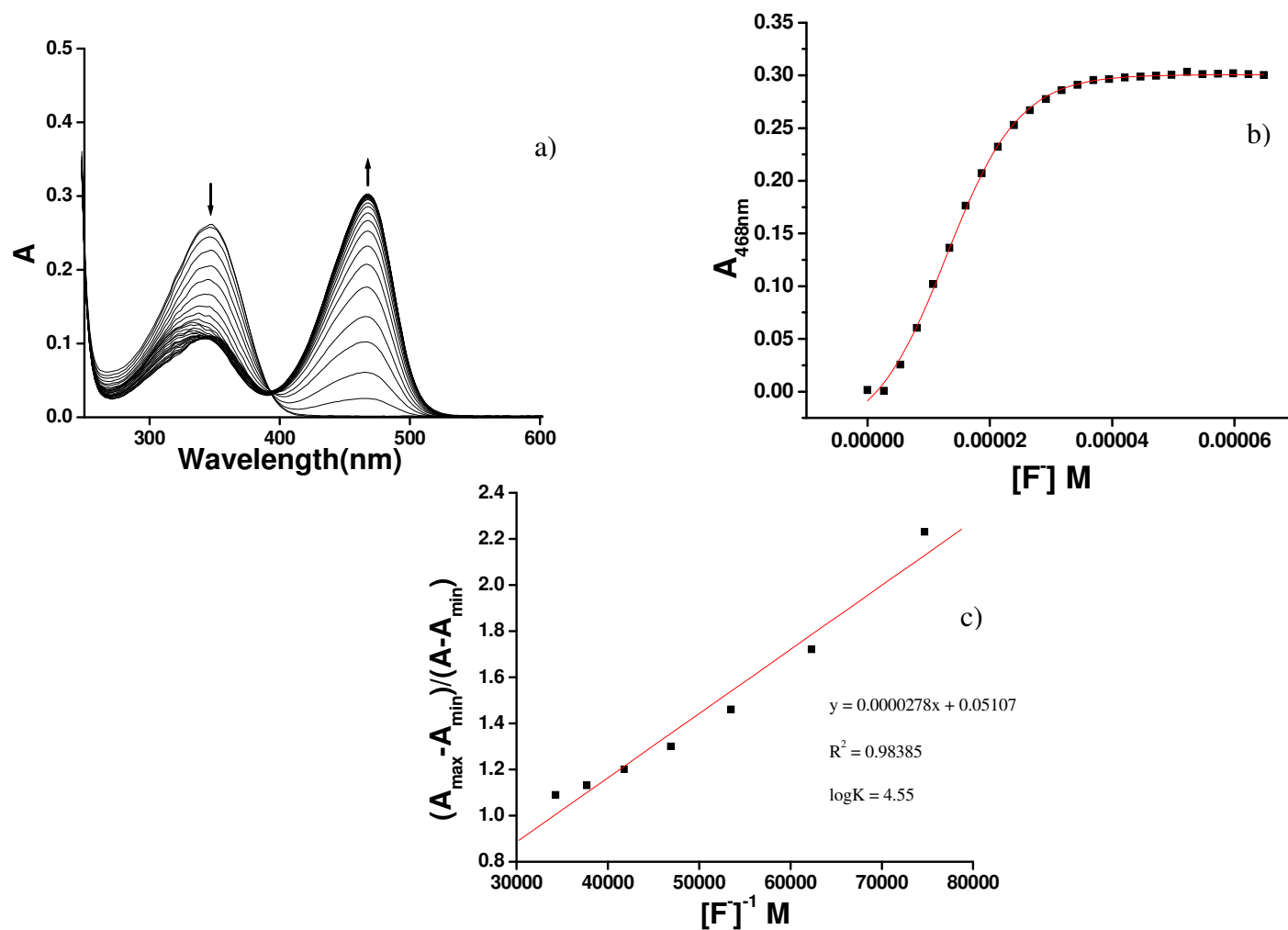
**Figure S40.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S3** in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01(M)  $[\text{Bu}_4\text{N}]\text{H}_2\text{PO}_4$  in MeCN. b) Absorbance changes for **S3** at 503 nm on addition of various concentration of  $[\text{Bu}_4\text{N}]\text{H}_2\text{PO}_4$ . c) Benesi-Hildebrand plot.



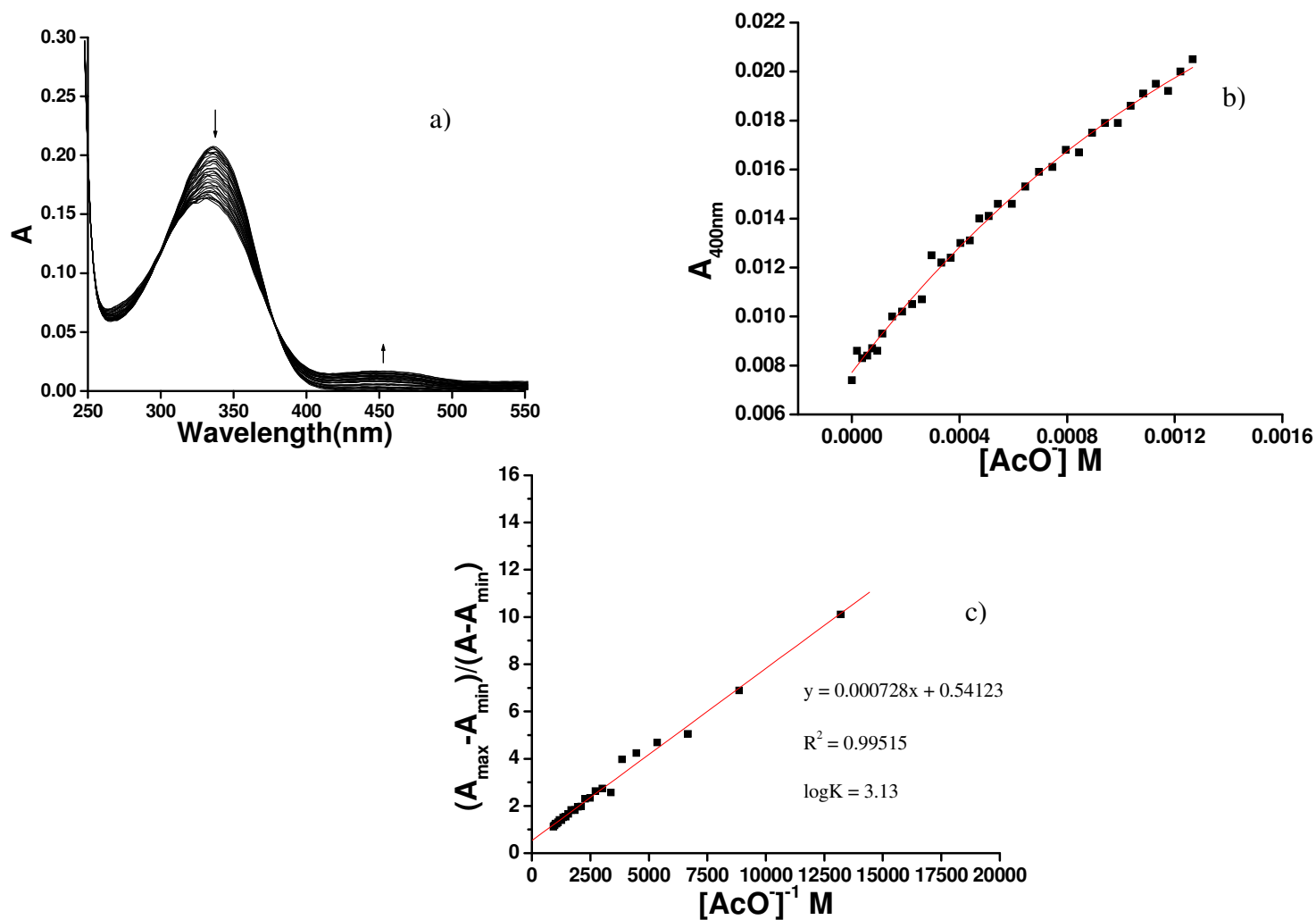
**Figure S41.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of S4 in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01 (M) [Bu<sub>4</sub>N]F in MeCN. b) Absorbance changes for S4 at 586 nm on addition of various concentration of [Bu<sub>4</sub>N]F. c) Benesi-Hildebrand plot.



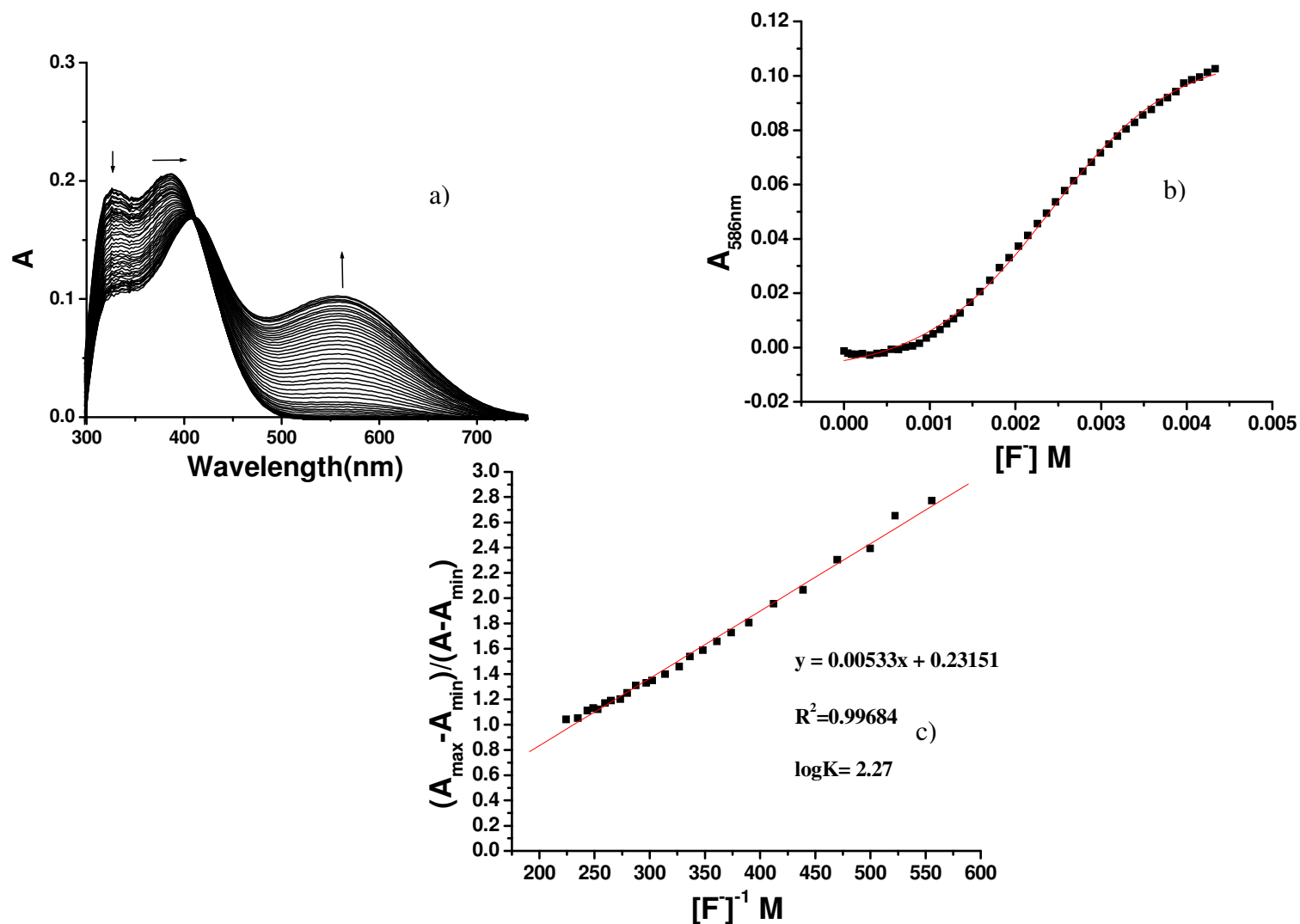
**Figure S42.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of S4 in MeCN/DMF (9.6:0.4)(v/v) with a standard solution of 0.01 (M) [Bu<sub>4</sub>N]AcO in MeCN. b) Absorbance changes for S4 at 473 nm on addition of various concentration of [Bu<sub>4</sub>N]AcO. c) Benesi-Hildebrand plot.



**Figure S43.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S6** in MeCN/DMF (9.6:0.4)(v/v) with a standard solution of 0.01 (M) [Bu<sub>4</sub>N]F in MeCN. b) Absorbance changes for **S6** at 468 nm on addition of various concentration of [Bu<sub>4</sub>N]F. c) Benesi-Hildebrand plot.

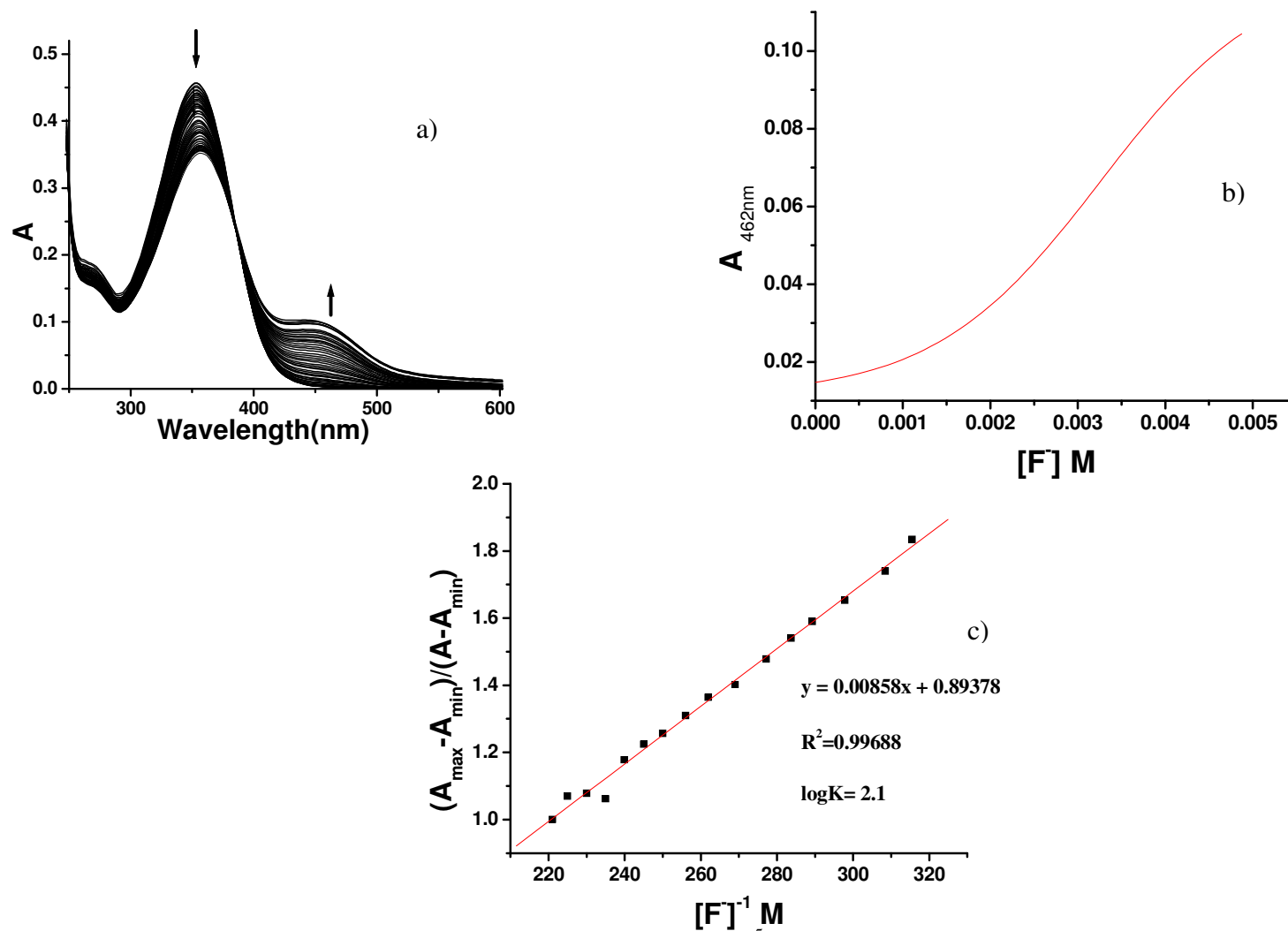


**Figure S44.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of S6 in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01(M) [Bu<sub>4</sub>N]AcO in MeCN. b) Absorbance changes for S6 at 468 nm on addition of various concentration of [Bu<sub>4</sub>N]AcO. c) Benesi-Hildebrand plot.

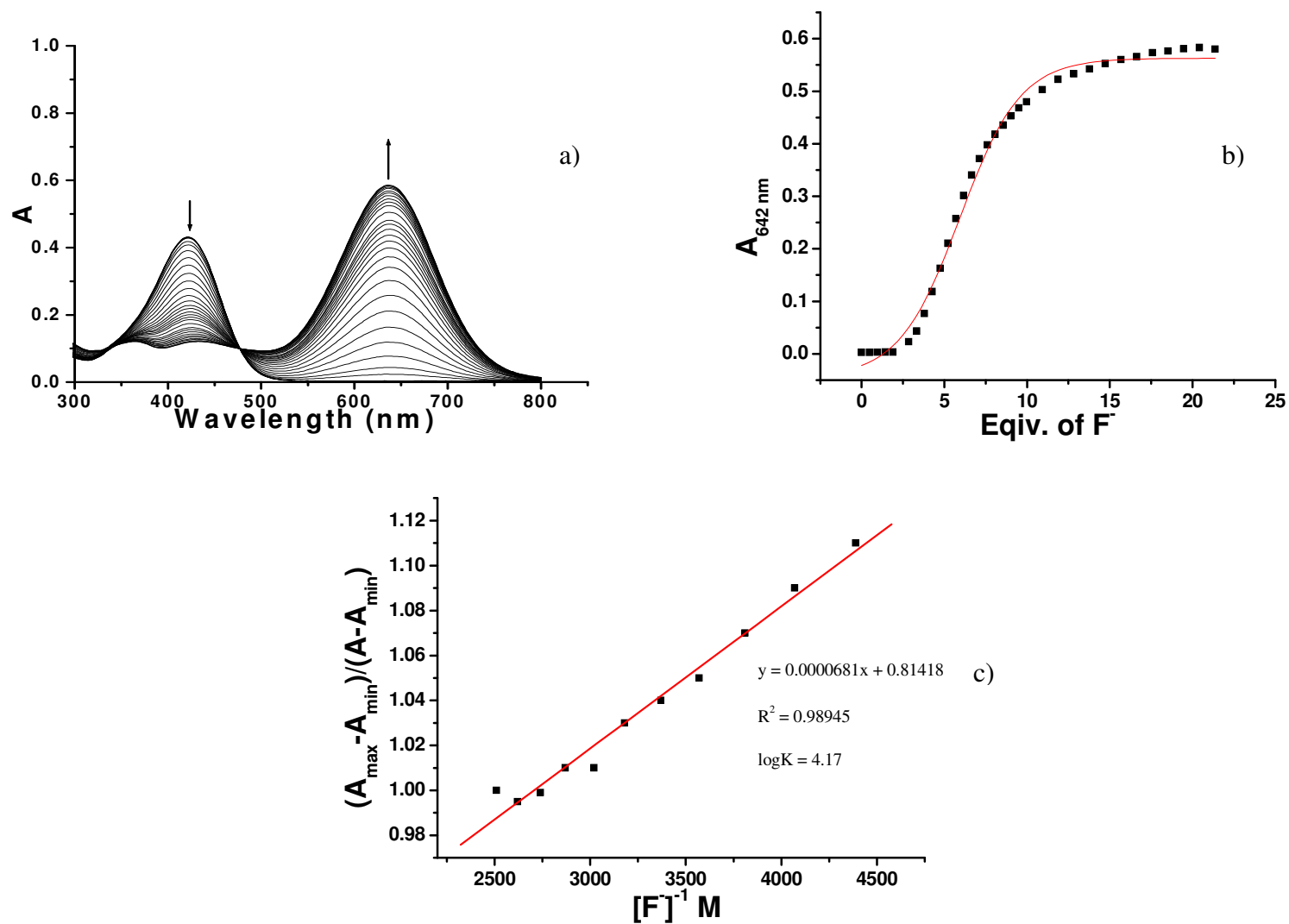


**Figure S45.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of S7 in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01 (M) [Bu<sub>4</sub>N]F in MeCN. b) Absorbance changes for S7 at 586 nm on addition of various concentration of [Bu<sub>4</sub>N]F. c) Benesi-Hildebrand plot.

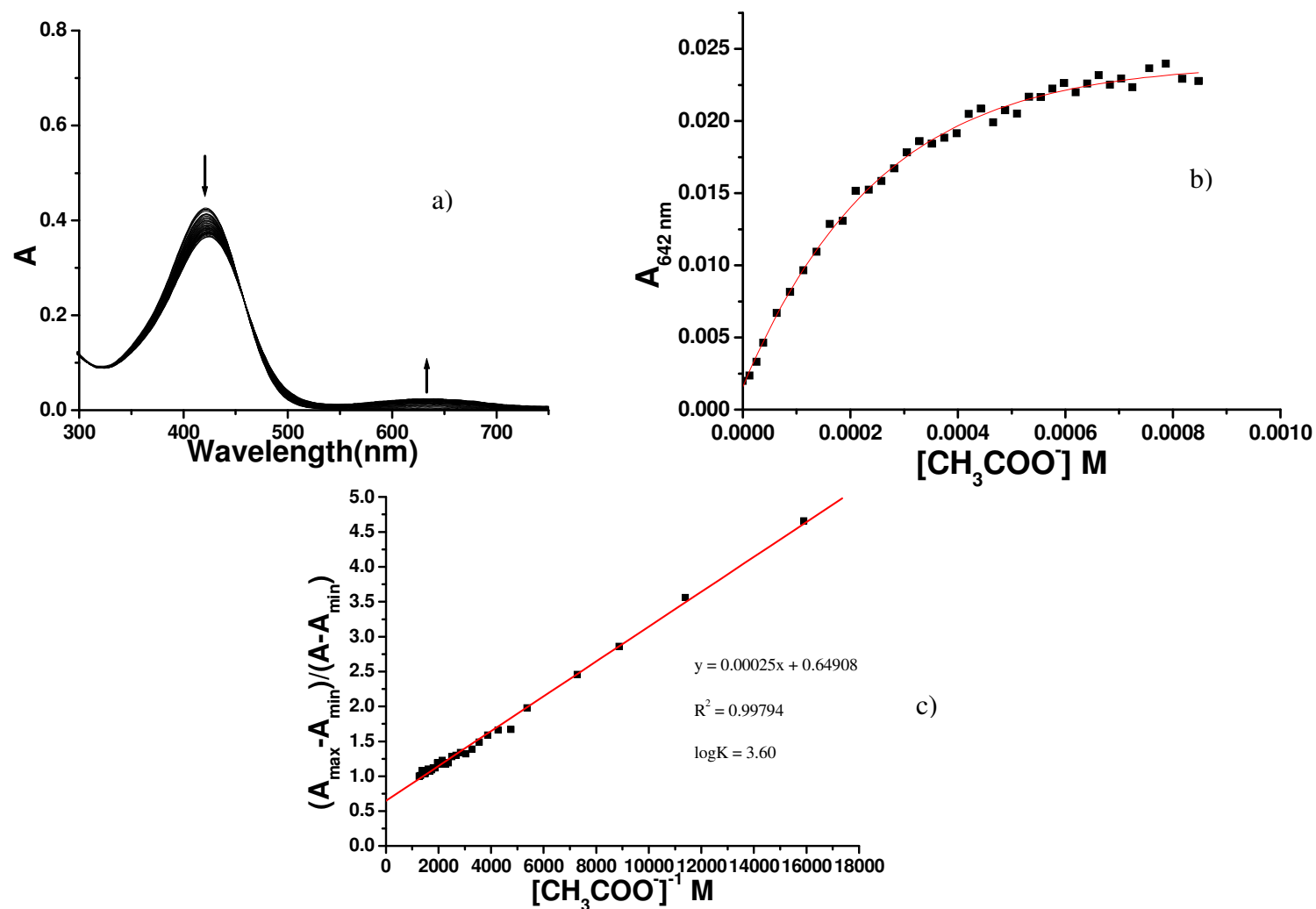




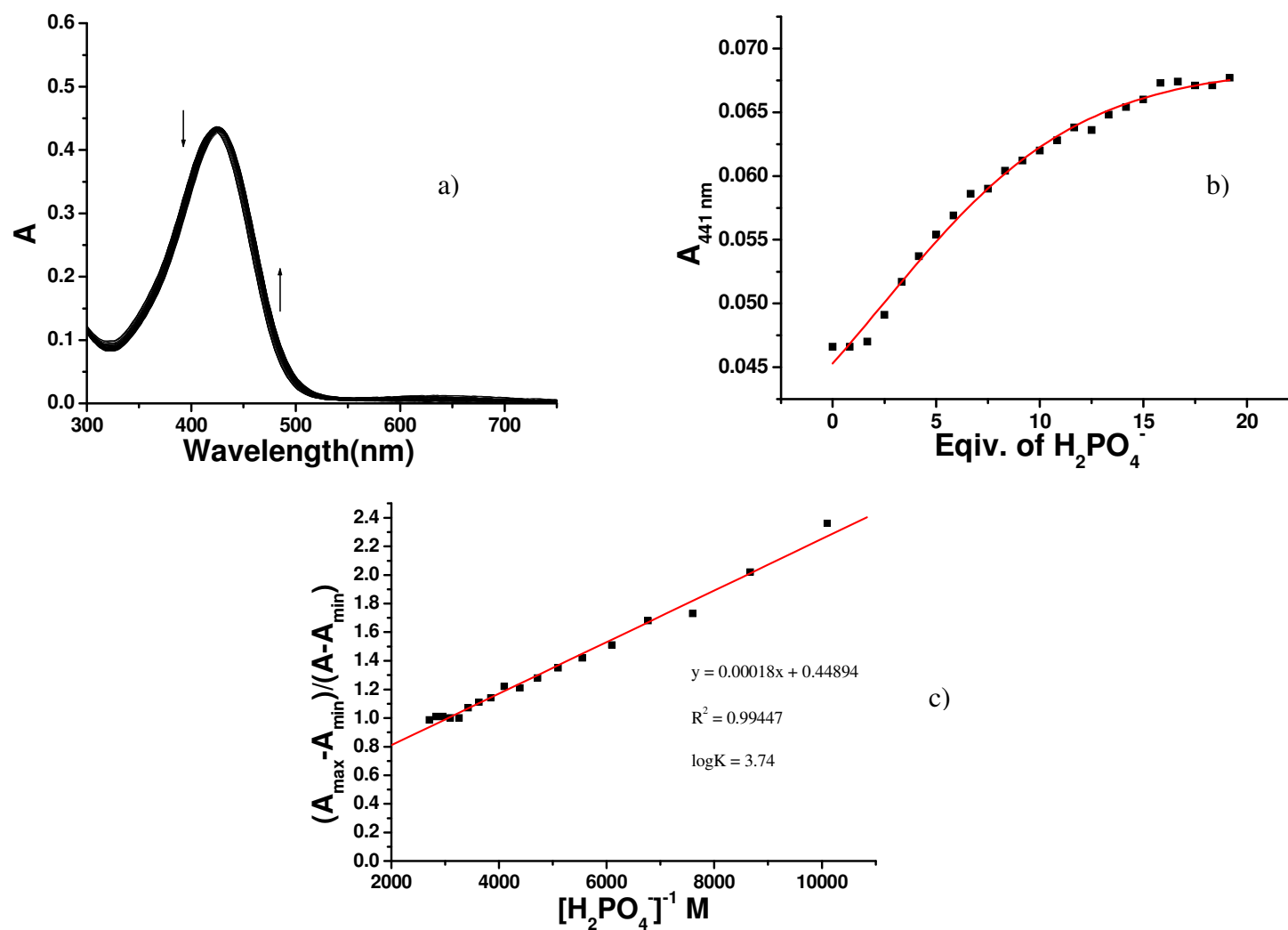
**Figure S46.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S8** in MeCN/DMF (9.6:0.4)(v/v) with a standard solution of 0.01 (M)  $[\text{Bu}_4\text{N}]\text{F}$  in MeCN. b) Absorbance changes for **S8** at 462 nm on addition of various concentration of  $[\text{Bu}_4\text{N}]\text{F}$ . c) Benesi-Hildebrand plot.



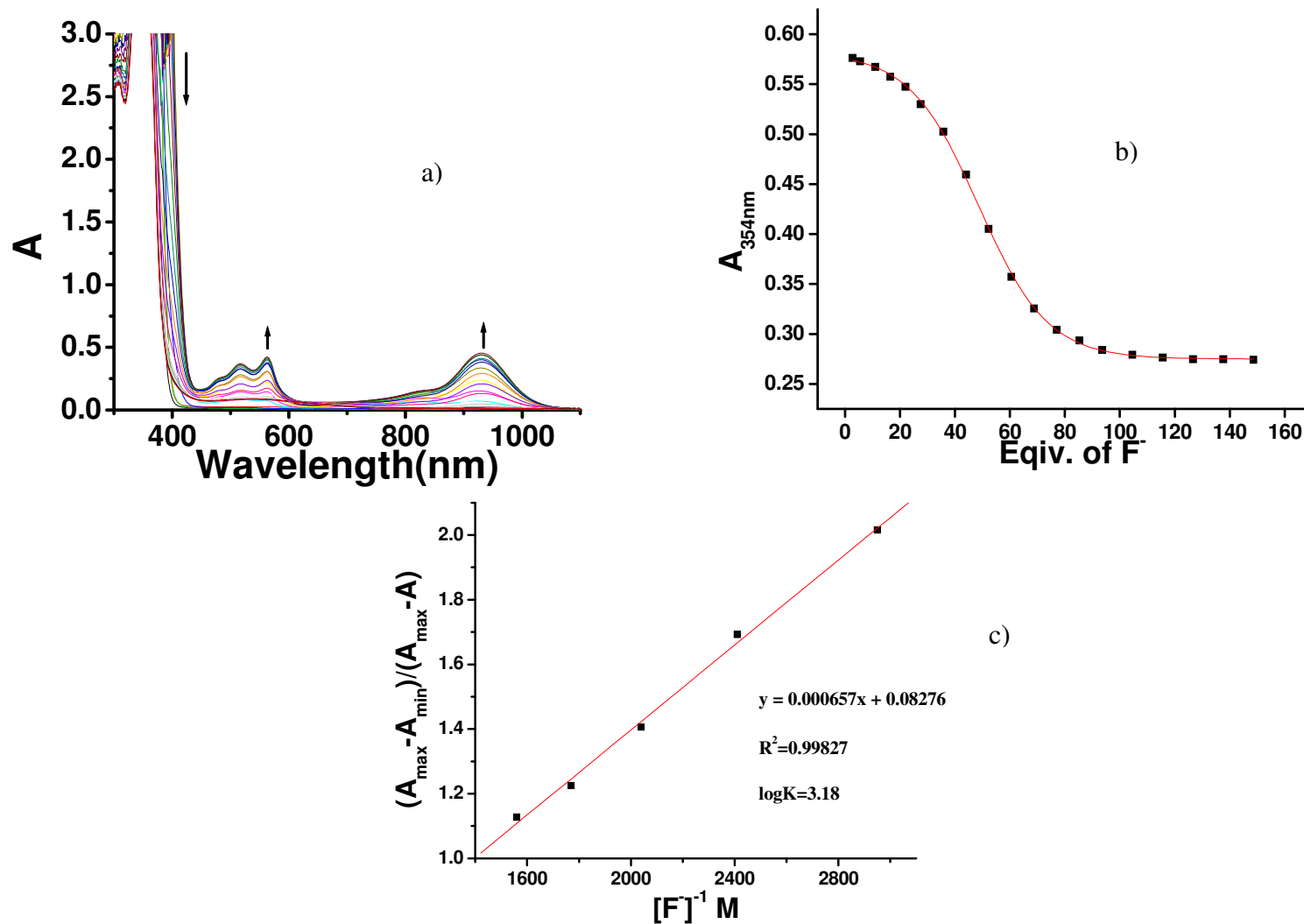
**Figure S47.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S9** in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01 (M) [Bu<sub>4</sub>N]F in MeCN. b) Absorbance changes for **S9** at 642 nm on addition of various concentration of [Bu<sub>4</sub>N]F. c) Benesi-Hildebrand plot.



**Figure S48.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of S9 in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01 (M) [Bu<sub>4</sub>N]AcO in MeCN. b) Absorbance changes for S9 at 642 nm on addition of various concentration of [Bu<sub>4</sub>N]AcO. c) Benesi-Hildebrand plot.



**Figure S49.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5}$  M solution of **S9** in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01 (M)  $[\text{Bu}_4\text{N}]\text{H}_2\text{PO}_4$  in MeCN. b) Absorbance changes for **S9** at 441 nm on addition of various concentration of  $[\text{Bu}_4\text{N}]\text{H}_2\text{PO}_4$ . c) Benesi-Hildebrand plot.



**Figure S50.** a) UV-Vis absorption changes of the titration of a  $1.0 \times 10^{-5} \text{ M}$  solution of **S10** in MeCN/DMF(9.6:0.4)(v/v) with a standard solution of 0.01(M)  $[\text{Bu}_4\text{N}]\text{F}$  in MeCN. b) Absorbance changes for **S10** at 354 nm on addition of various concentration of  $[\text{Bu}_4\text{N}]\text{F}$ . c) Benesi-Hildebrand plot.

**Table S1. Table of Crystallographic parameters**

<b>Parameters</b>	<b>1</b>	<b>Complex 2</b>	<b>Complex 3</b>
<b>Empirical formula</b>	C <sub>16</sub> H <sub>9</sub> F <sub>10</sub> N <sub>5</sub> O	C <sub>36</sub> H <sub>22</sub> F <sub>10</sub> N <sub>5</sub> O <sub>6</sub>	C <sub>37</sub> H <sub>31</sub> N <sub>5</sub> O <sub>4</sub>
<b>Formula weight</b>	477.28	810.59	609.67
<b>crystal system</b>	Monoclinic	Monoclinic	Orthorhombic
<b>Space group</b>	P2(1)/n	P2(1)/m	Pbca
<b>a (Å)</b>	16.012(10)	6.8654(13)	14.5032(10)
<b>b (Å)</b>	11.932(7)	34.567(6)	9.6882(7)
<b>c (Å)</b>	19.682(12)	7.1380(14)	44.522(3)
<b>α (deg)</b>	90.00	90.000	90.000
<b>β (deg)</b>	104.571(8)	98.565(4)	90.000
<b>γ (deg)</b>	90.00	90.000	90.000
<b>V (Å<sup>3</sup>)</b>	3639(4)	1675.1(5)	6255.7 (8)
<b>Z</b>	8	2	8
<b>d<sub>calc</sub> (g/cm<sup>3</sup>)</b>	1.742	1.607	1.295
<b>Crystal size (mm<sup>3</sup>)</b>	0.32 x 0.07 x 0.05	0.15 x 0.09 x 0.08	0.18 x 0.03x 0.02
<b>Diffractometer</b>	Smart CCD	Smart CCD	Smart CCD
<b>F(000)</b>	1904	822	2560
<b>μ MoKα (mm<sup>-1</sup>)</b>	0.184	0.148	0.086
<b>T (K)</b>	120 (2)	100 (2)	100(2)
<b>θ max</b>	24.39	25.00	25.00
<b>ObservedReflections</b>	23147	15838	55819
<b>Parameters refined</b>	633	232	417
<b>R<sub>1</sub>; WR<sub>2</sub></b>	0.0499 ; 0.1123	0.0334 ; 0.0842	0.0879 ; 0.2308
<b>GOF (F2)</b>	1.022	1.078	1.161

**Table S2. Hydrogen bonding interactions in 1.**

<b>D-H...A</b>	<b>D-H (Å)</b>	<b>H...A(Å)</b>	<b>D...A(Å)</b>	<b>∠ D-H...A</b>
N9-H9...O42	0.843	1.944	2.766(5)	165.0
O44-H44...N12	0.800	2.042	2.807(6)	160.0
N29-H29...O44	0.895	1.914	2.790(6)	165.7
O42-H42...N32	0.850	1.982	2.821	169.2

**Table S3. Hydrogen bonding interactions in Complex 2.**

<b>D-H...A</b>	<b>D-H (Å)</b>	<b>H...A(Å)</b>	<b>D...A(Å)</b>	<b>∠ D-H...A (deg)</b>
N11-H11...O25	0.860	2.070	2.8623(18)	152.3
N9-H9...O17	0.860	1.930	2.7916(14)	178.1
O26-H26...O17	0.820	1.810	2.6179(11)	170.6

**Table S4. Hydrogen bonding interactions in Complex 3.**

<b>D-H...A</b>	<b>D-H (Å)</b>	<b>H...A(Å)</b>	<b>D...A(Å)</b>	<b>∠ D-H...A (deg)</b>
O3-H3X...O2	0.820	1.770	2.593(4)	175.40
N2-H2A...O1	0.860	1.930	2.710(4)	149.90
N3-H3A...O1	0.860	2.240	2.970(4)	142.70
N3-H3B...O4	0.860	2.180	2.899(4)	140.80
N4-H4A...O2	0.860	1.920	2.741(4)	158.90



## Methods.

The binding constant values of anions with **S1-S10** have been determined from the absorption data following the modified Benesi–Hildebrand equation.

$$1/\Delta A = 1/\Delta A_{\max} + (1/K[\text{Anion}])(1/\Delta A_{\max}).$$

Here,  $\Delta A = A - A_{\min}$ ,  $\Delta A_{\max} = A_{\max} - A_{\min}$ .

Where,  $A_{\min}$ ,  $A$ ,  $A_{\max}$  are the absorption of **S1-S10** considered in the absence of anions, at an intermediate, and at a concentration of complete concentration.

$K$  is Binding constant,  $[\text{Anion}]$  is concentration of anion.

From the Plot of  $(A_{\max} - A_{\min}) / (A - A_{\min})$  against  $[\text{Anion}]$  for **S1-S10**, the value of  $K$  ( $\pm 10\%$ ) extracted from the slope.

## References

- (1) (a) SAINT and XPREP, 5.1 ed.; Siemens Industrial Automation Inc.: Madison, WI, 1995. Sheldrick, G. M. (b) SADABS, *empirical absorption Correction Program*; University of Göttingen: Göttingen, Germany, 1997.
- (2) Sheldrick, G. M. *SHELXTL Reference Manual: Version 5.1*; Bruker AXS: Madison, WI, 1997.
- (3) Sheldrick, G. M. *SHELXL-97: Program for Crystal Structure Refinement*; University of Göttingen: Göttingen, Germany, 1997.
- (4) Spek, A. L. *PLATON-97*; University of Utrecht: Utrecht, The Netherlands, 1997.
- (5) Mercury 2.2 supplied with Cambridge Structural Database, CCDC, Cambridge, UK.