Novel Thiazolidinedione and Rhodanine Derivatives Regulate Glucose Metabolism, Improve Insulin Sensitivity, and Activate Peroxisome Proliferator Activated Gamma Receptor.

Shaikha S. Al Neyadi[a], Abdu Adem[b], Naheed Amir[b], Mohammad A. Ghattas[c], Ibrahim M. Abdou[a*], and Alaa A. Salem[a*]

[a] Department of Chemistry, College of Science, United Arab Emirates University Al-Ain, United Arab Emirates.

[b] Department of Pharmacology and Therapeutics, College of Medicine and Health Sciences, United Arab Emirates University, Al-Ain, United Arab Emirates.

[c] College of Pharmacy, Al Ain University, Abu Dhabi, United Arab Emirates.

Materials supplied as supporting information.

Figures S1-S16: IR and NMR spectra of synthesized TZDs and RDs. IR spectra (a), ^{1}H-NMR spectra (b), ^{13}C-NMR spectra (c).

Table S1: Docking scores of TZDs and RDs into PPAR-γ crystal structures; PDB:1WM0, PDB:1ZGY and PDB:1I7I.

Captions of figures and tables

Fig S14. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33e

Fig S15. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33f

Fig S16. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33g

Table S1. Table S1. Docking scores of different ligands into PDB:1WM0, PDB:1ZGY and PDB:1I7I PPAR-γ crystal structures.

.

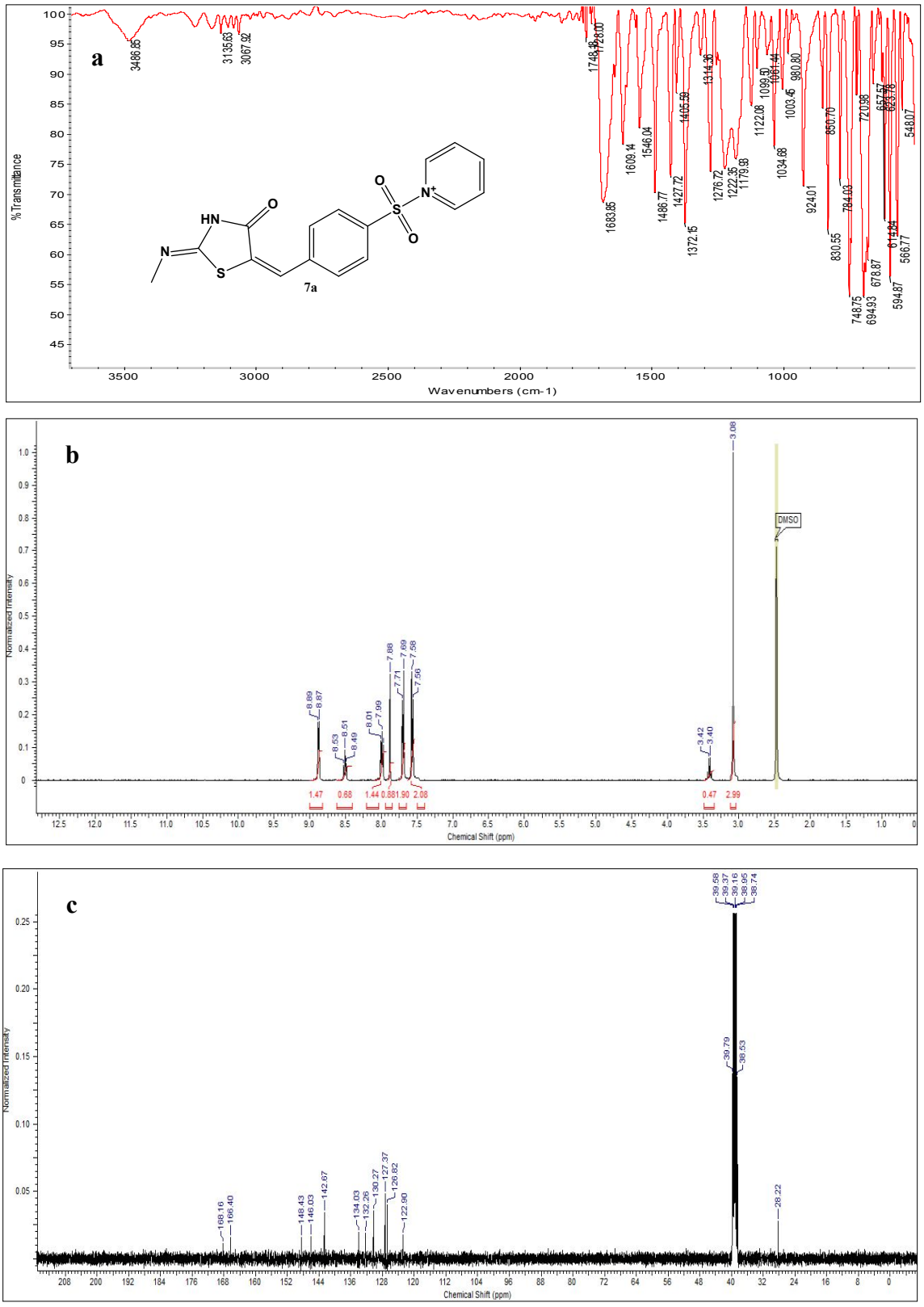


Fig S1. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **7a**

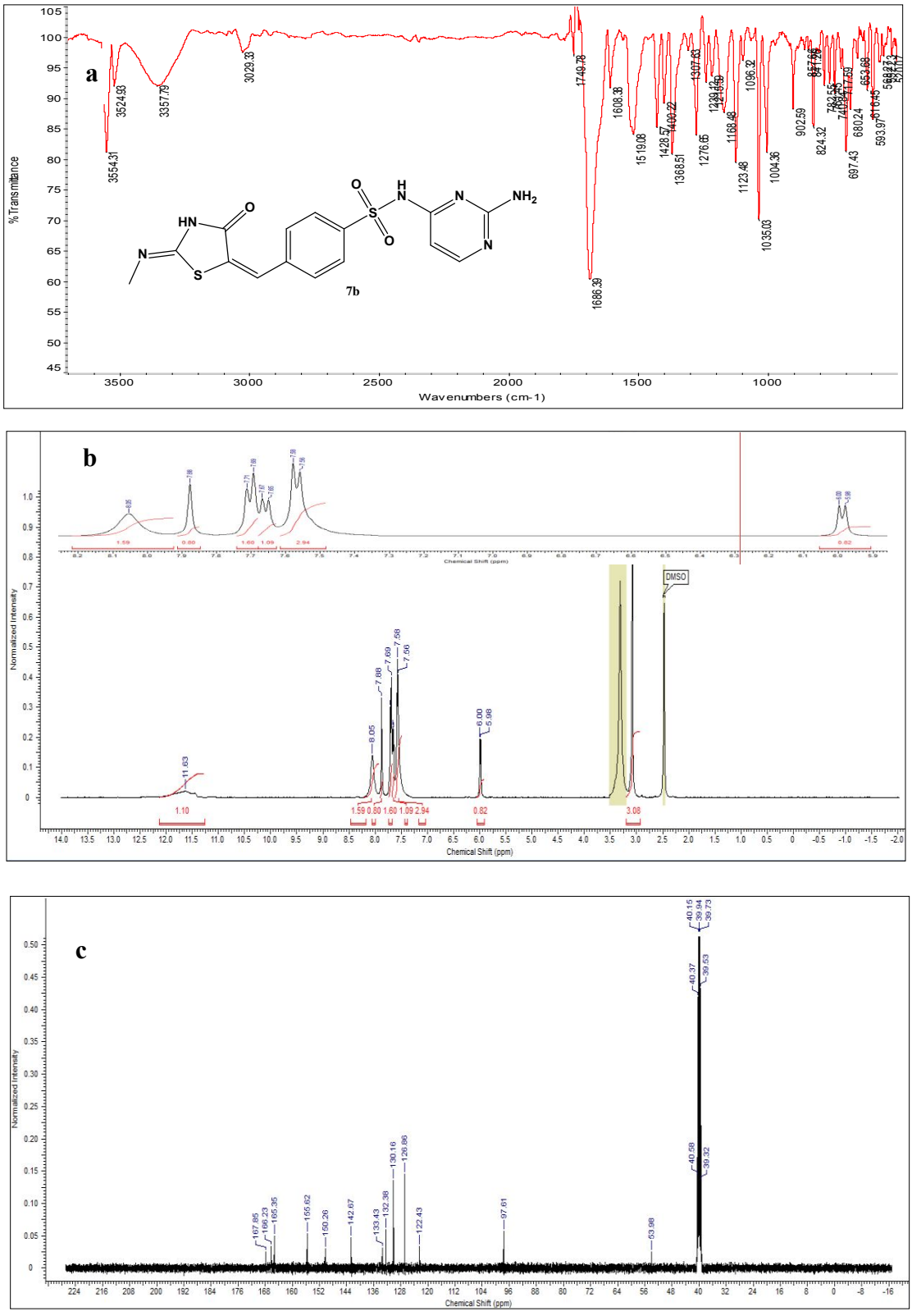


Fig S2. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **7b**

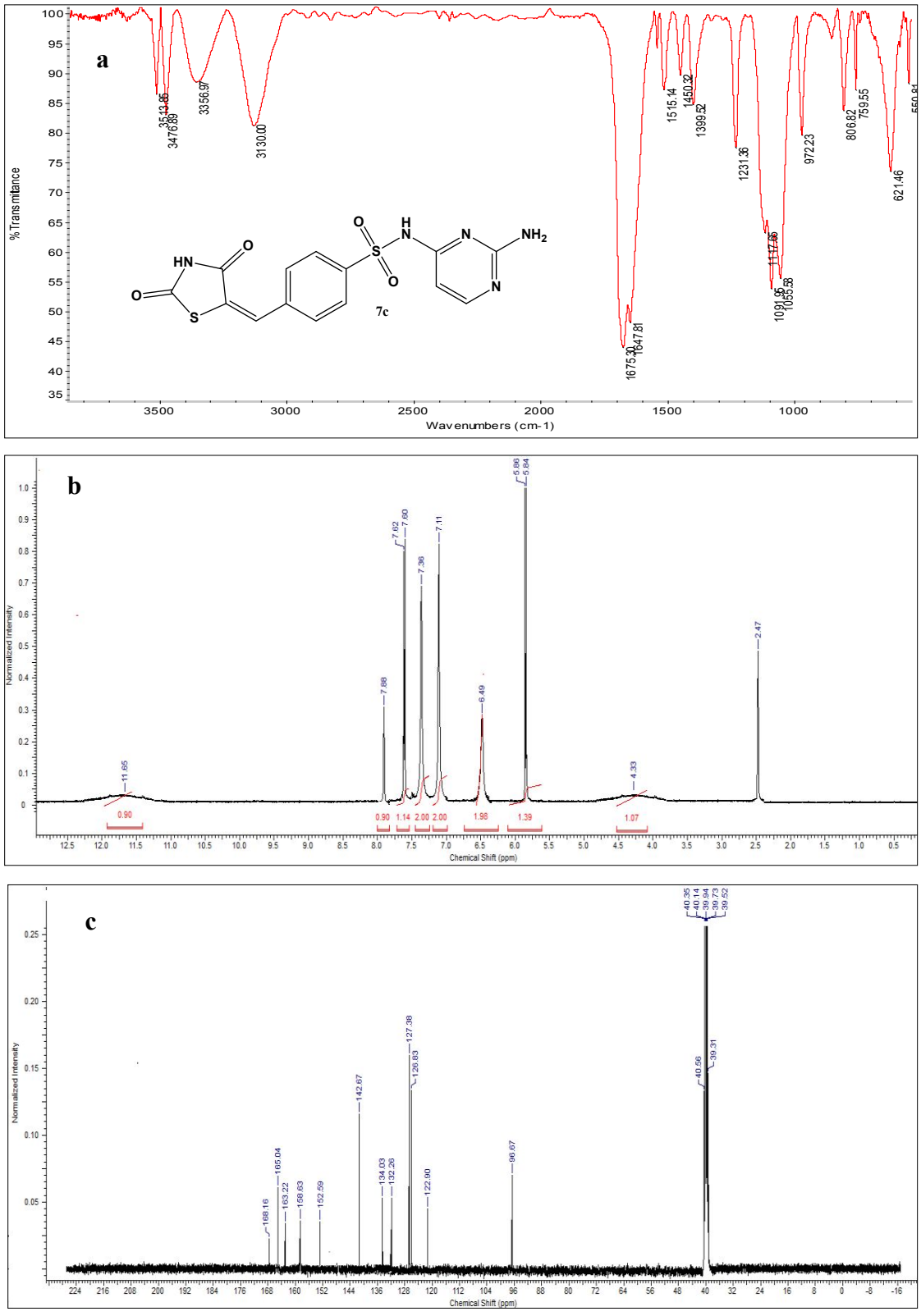


Fig S3. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **7c**

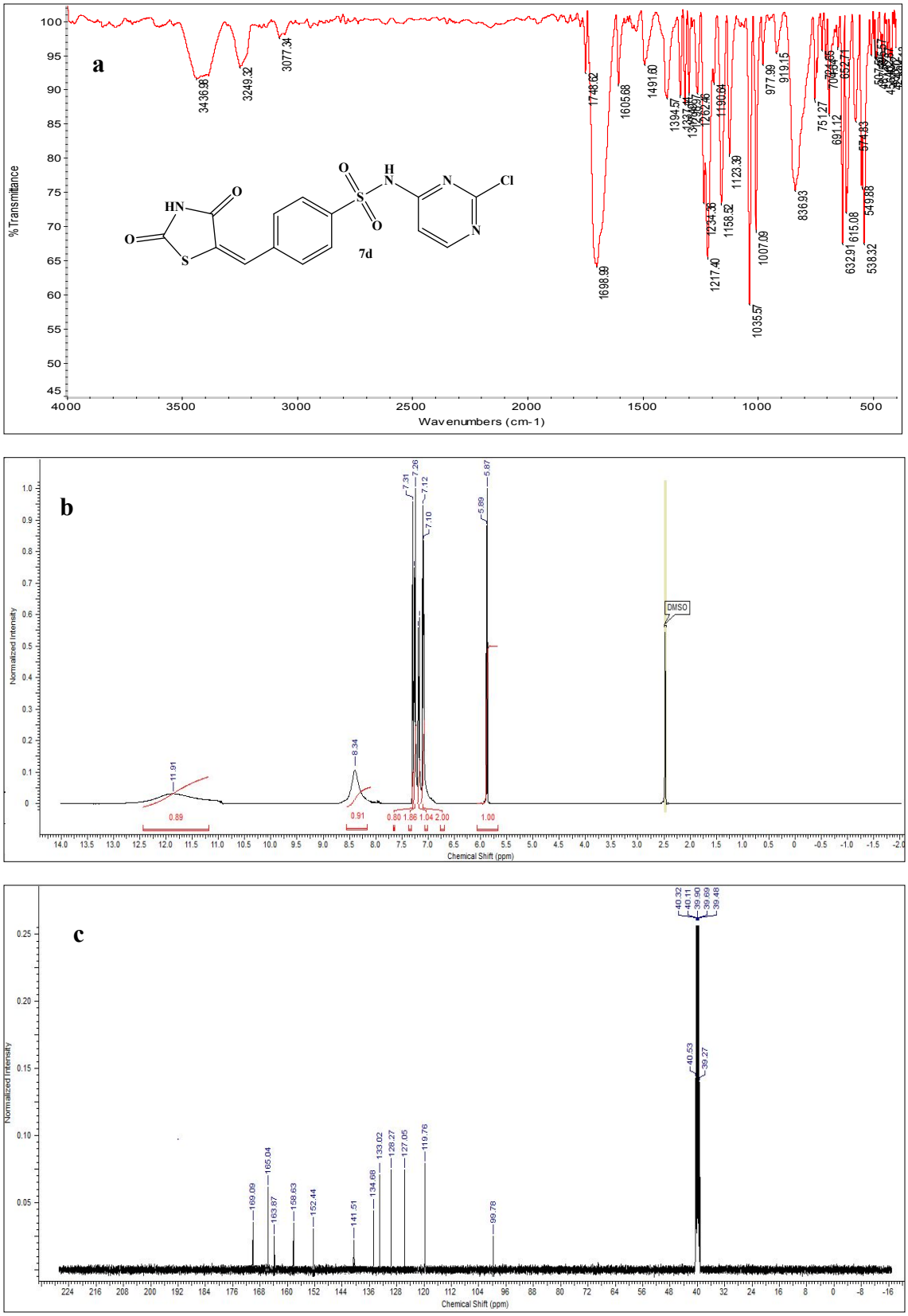


Fig S4. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **7d**

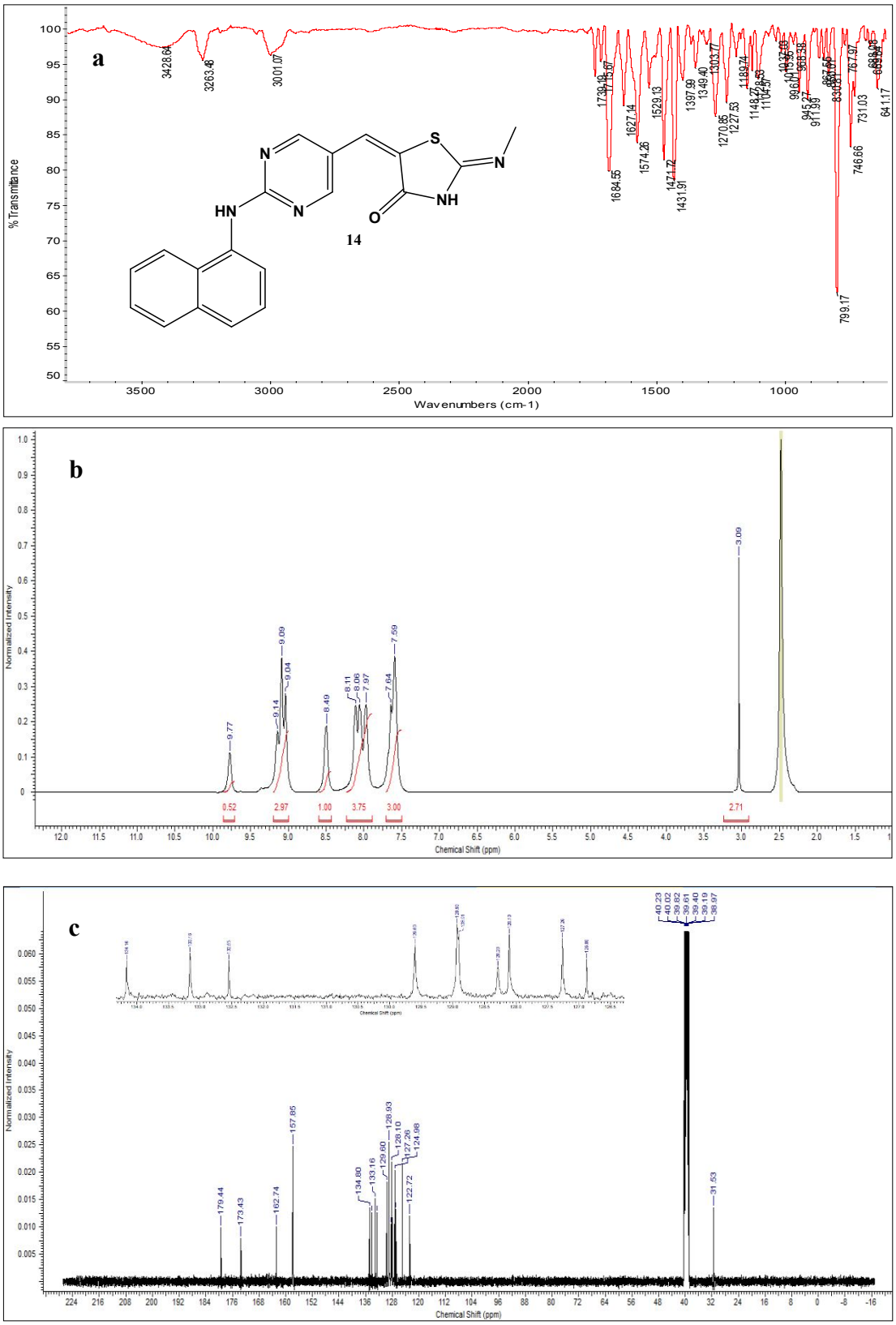


Fig S5. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **14**

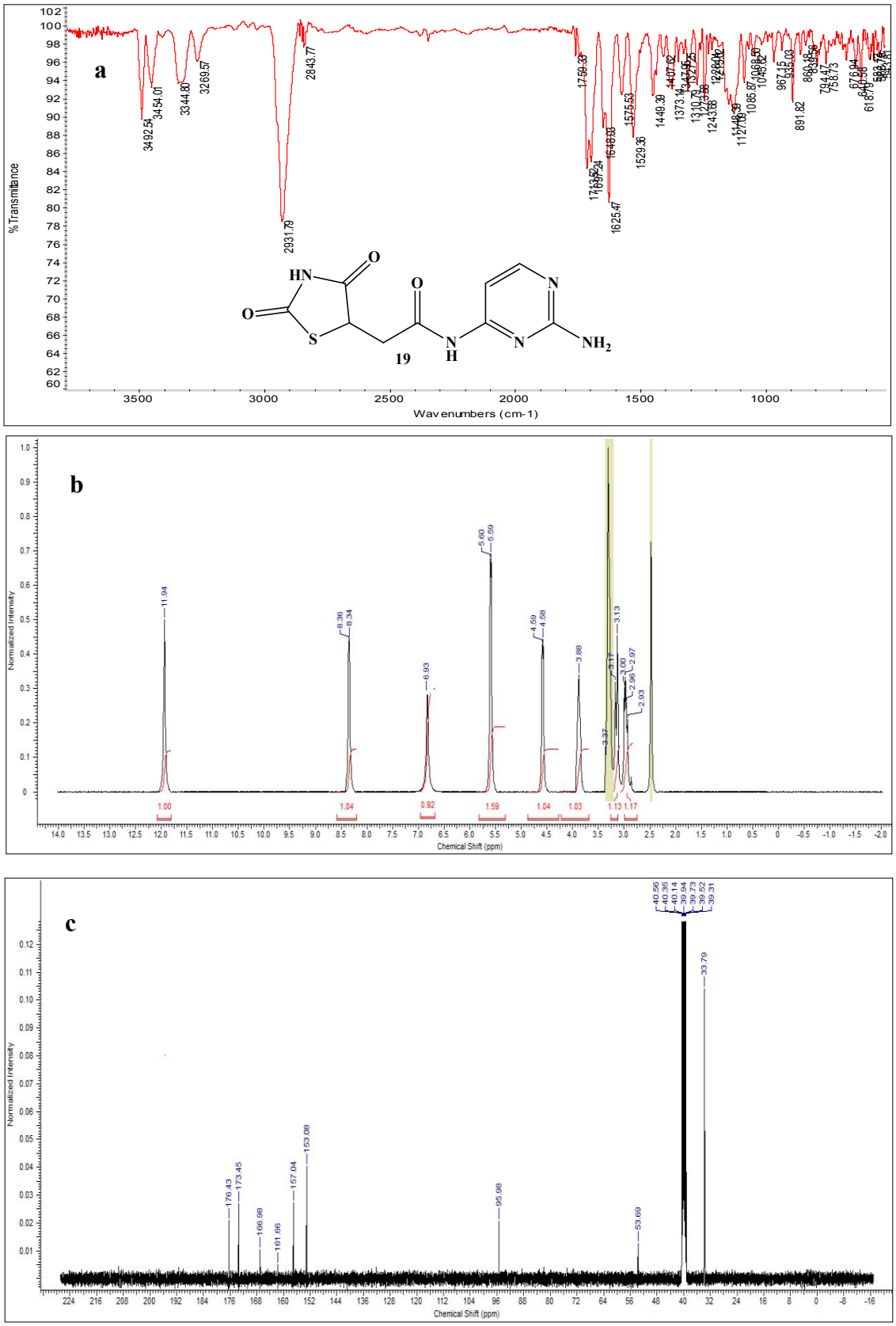


Fig S6. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **19**

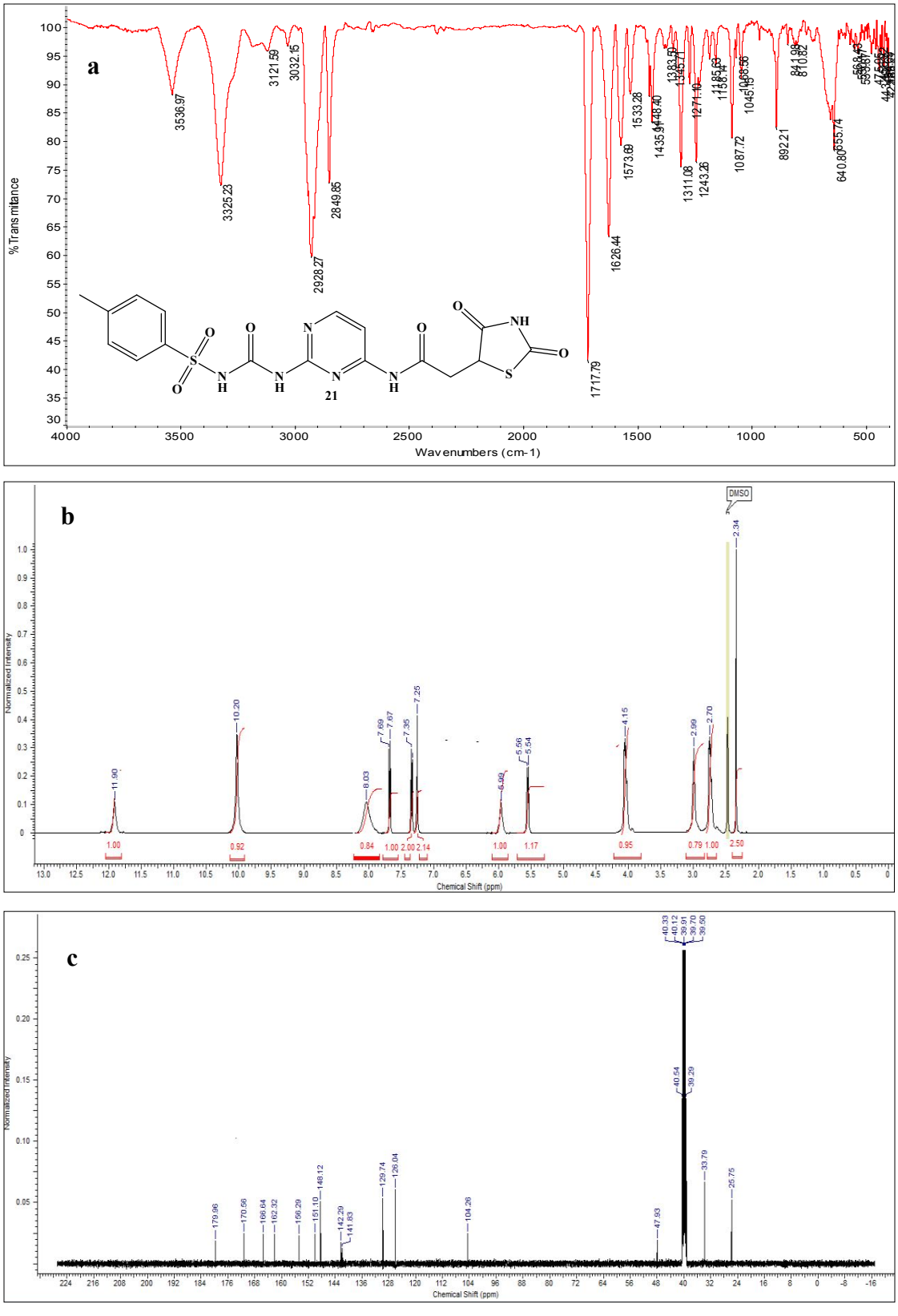


Fig S7. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **21**

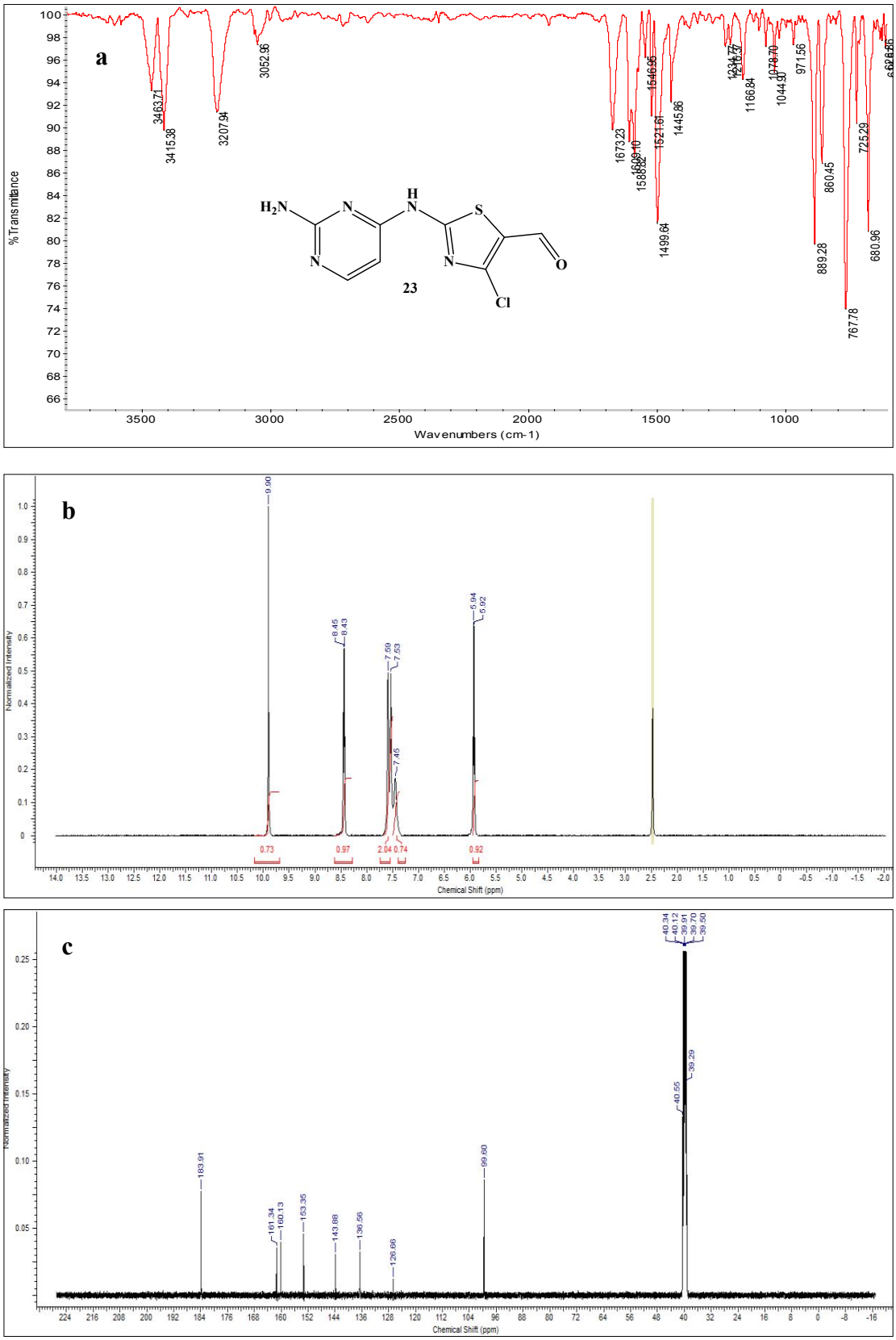
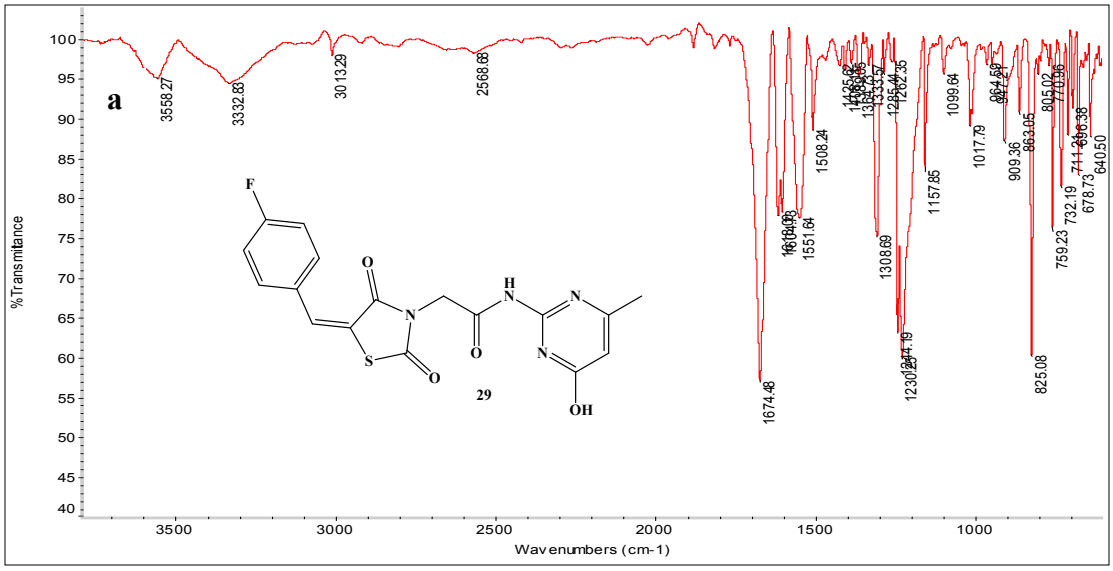
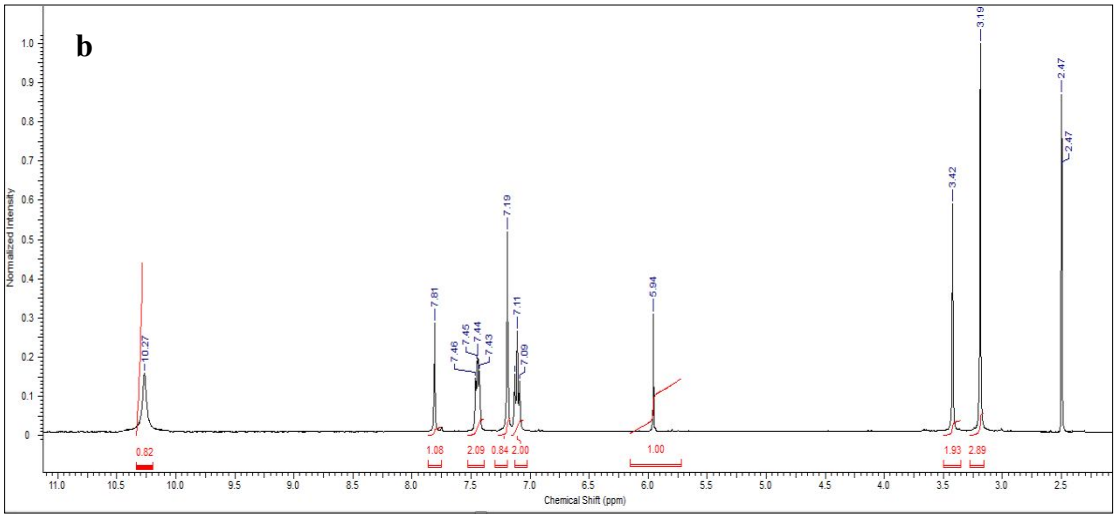


Fig S8. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **23**





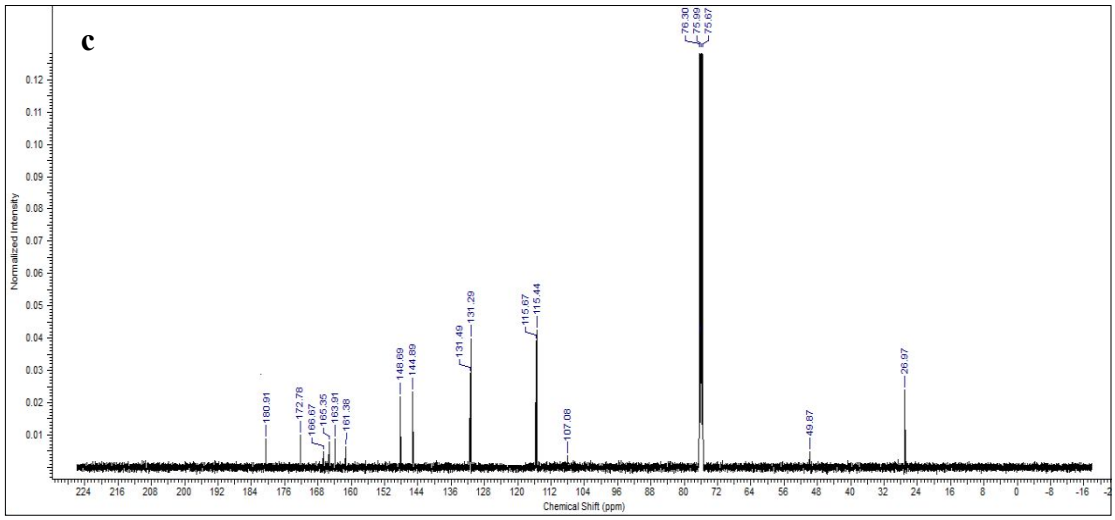


Fig S9. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound **29**

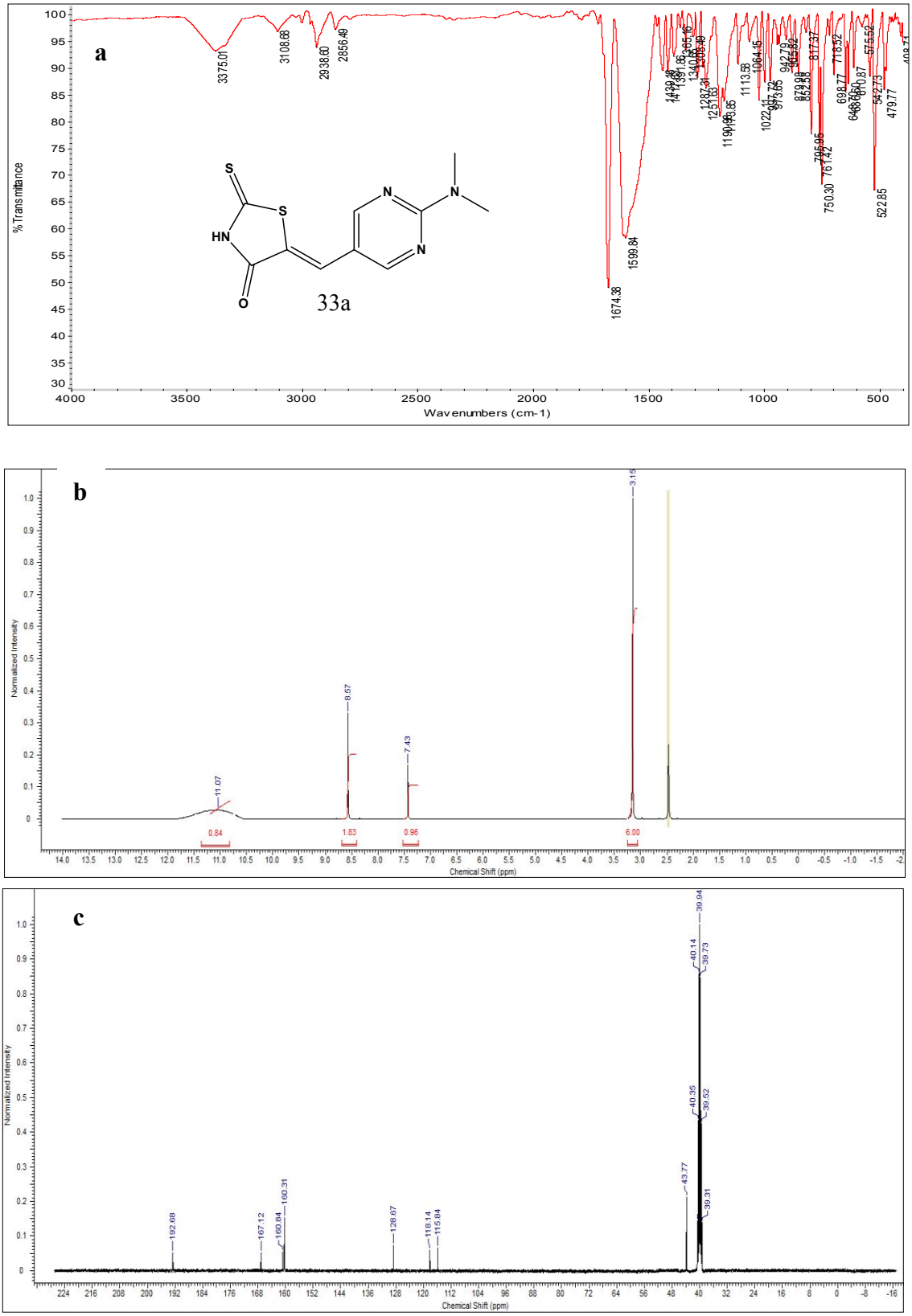


Fig S10. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33a

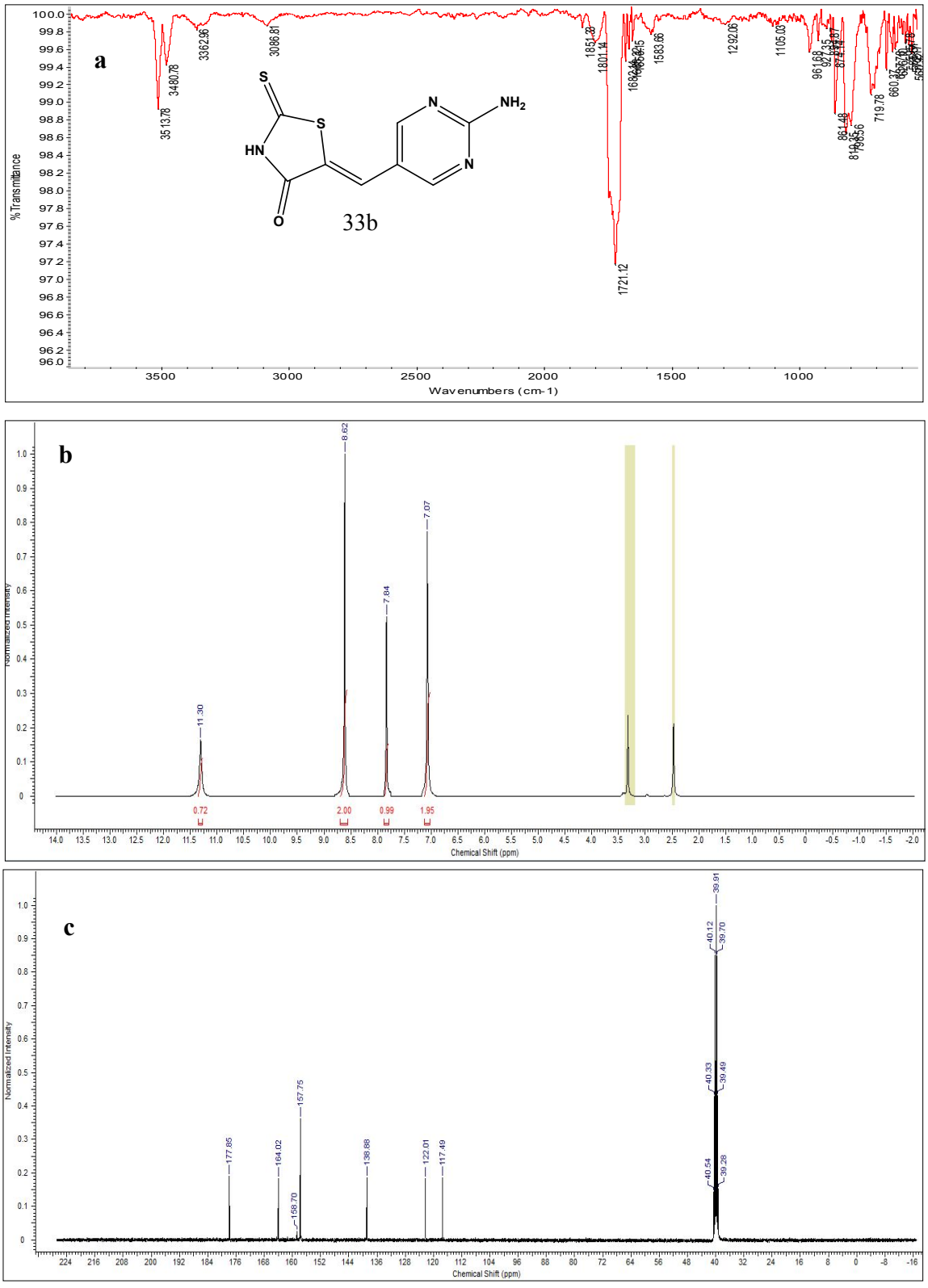


Fig S11. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33b

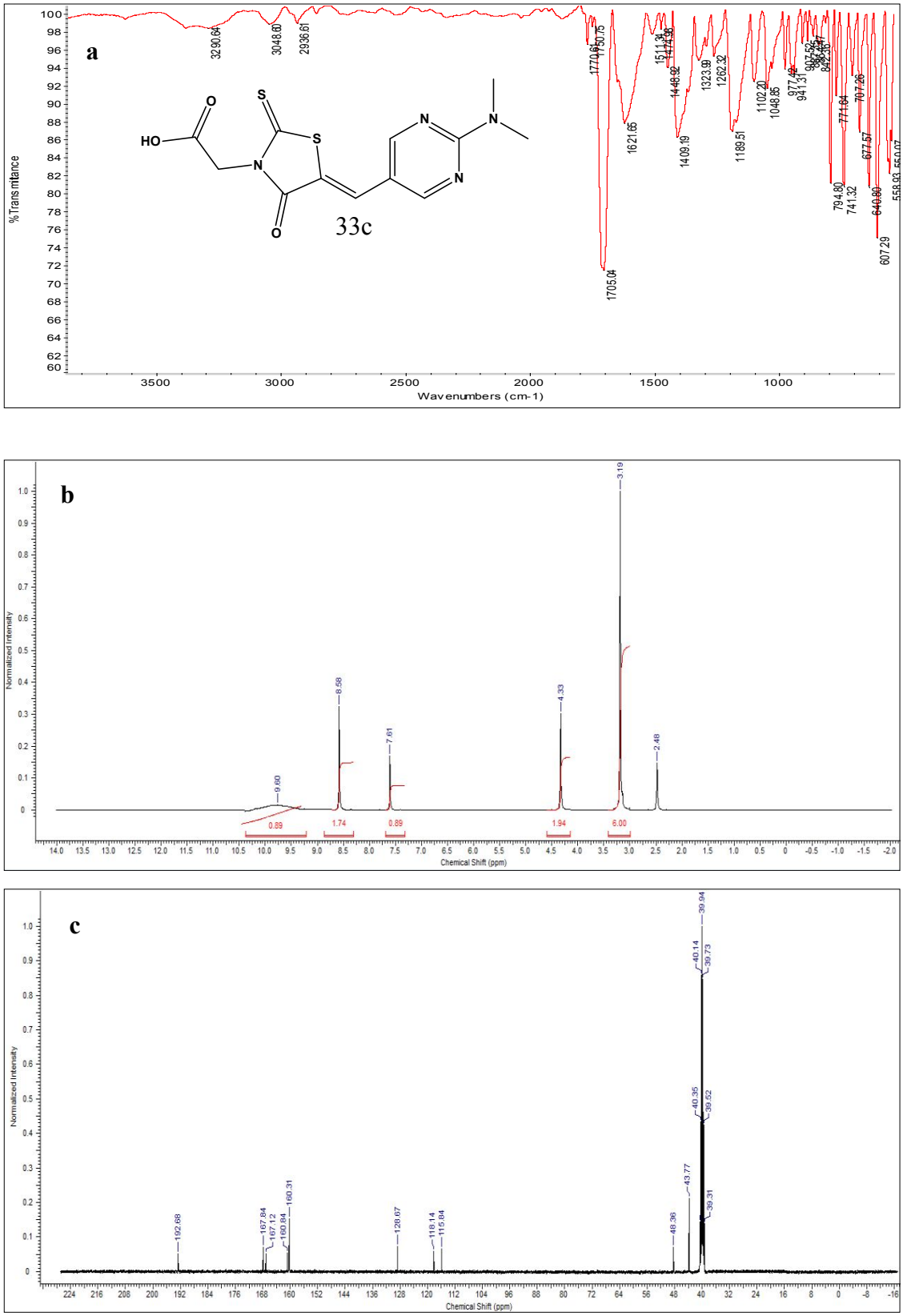


Fig S12. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33c

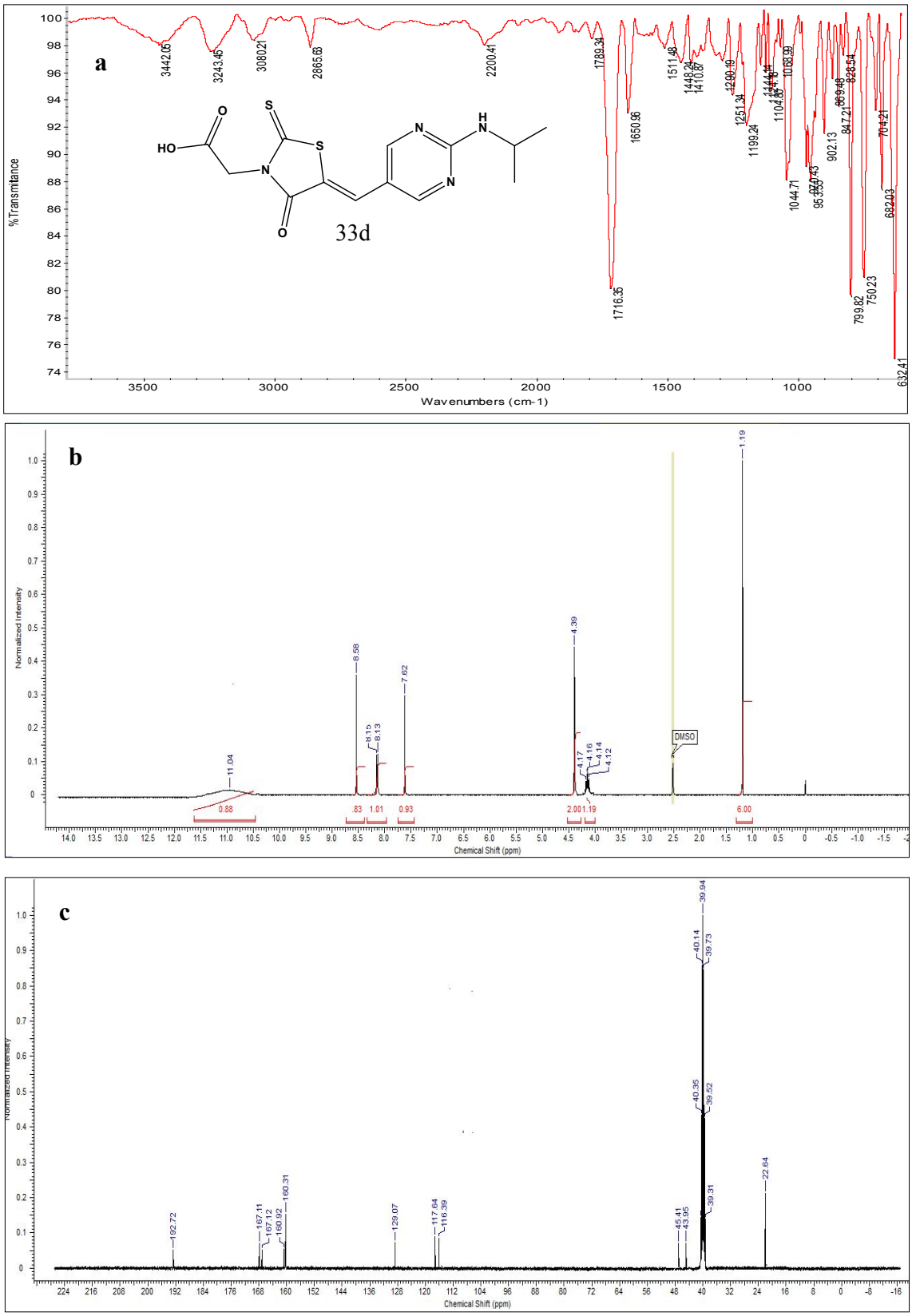


Fig S13. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33d

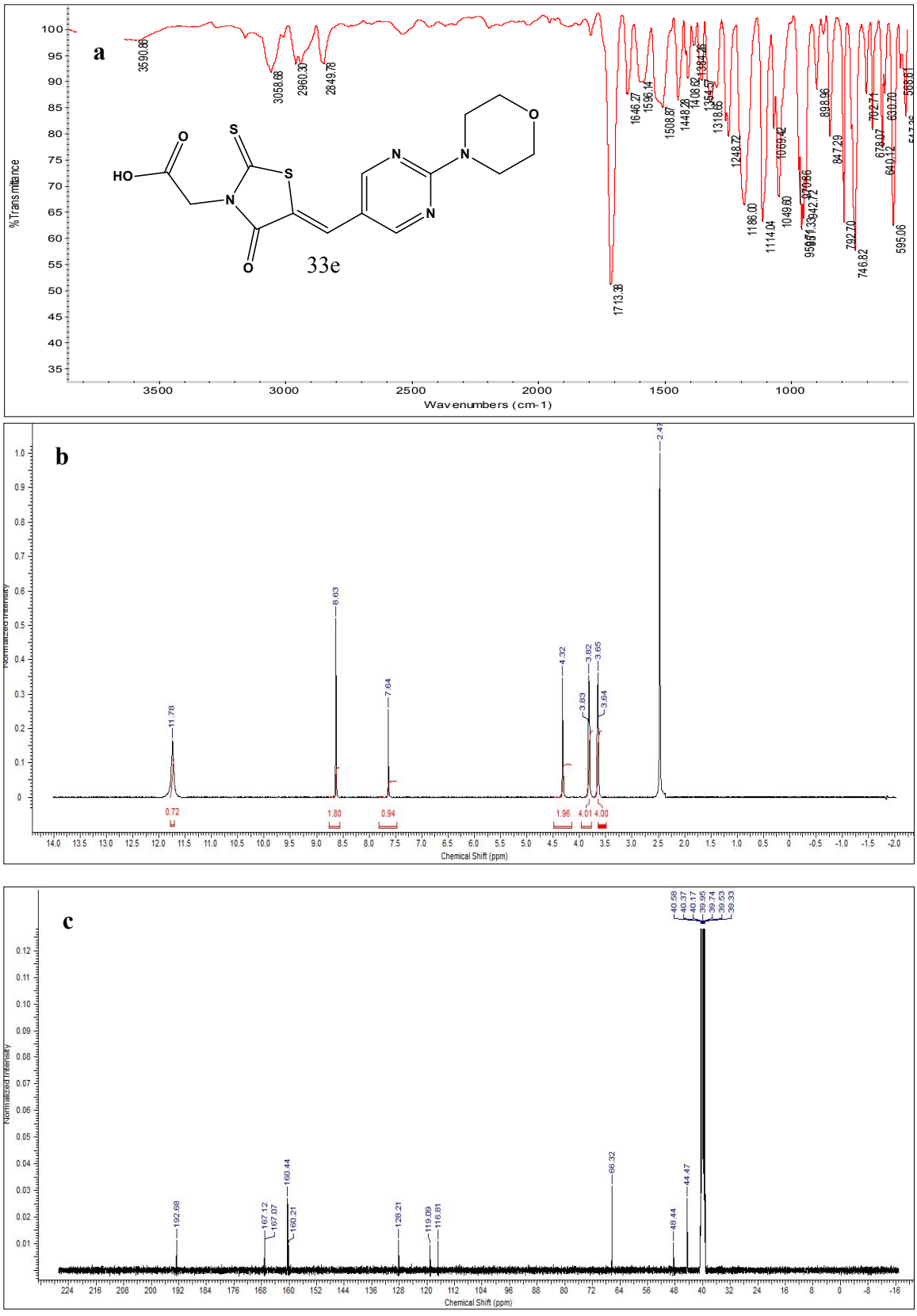


Fig S14. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33e

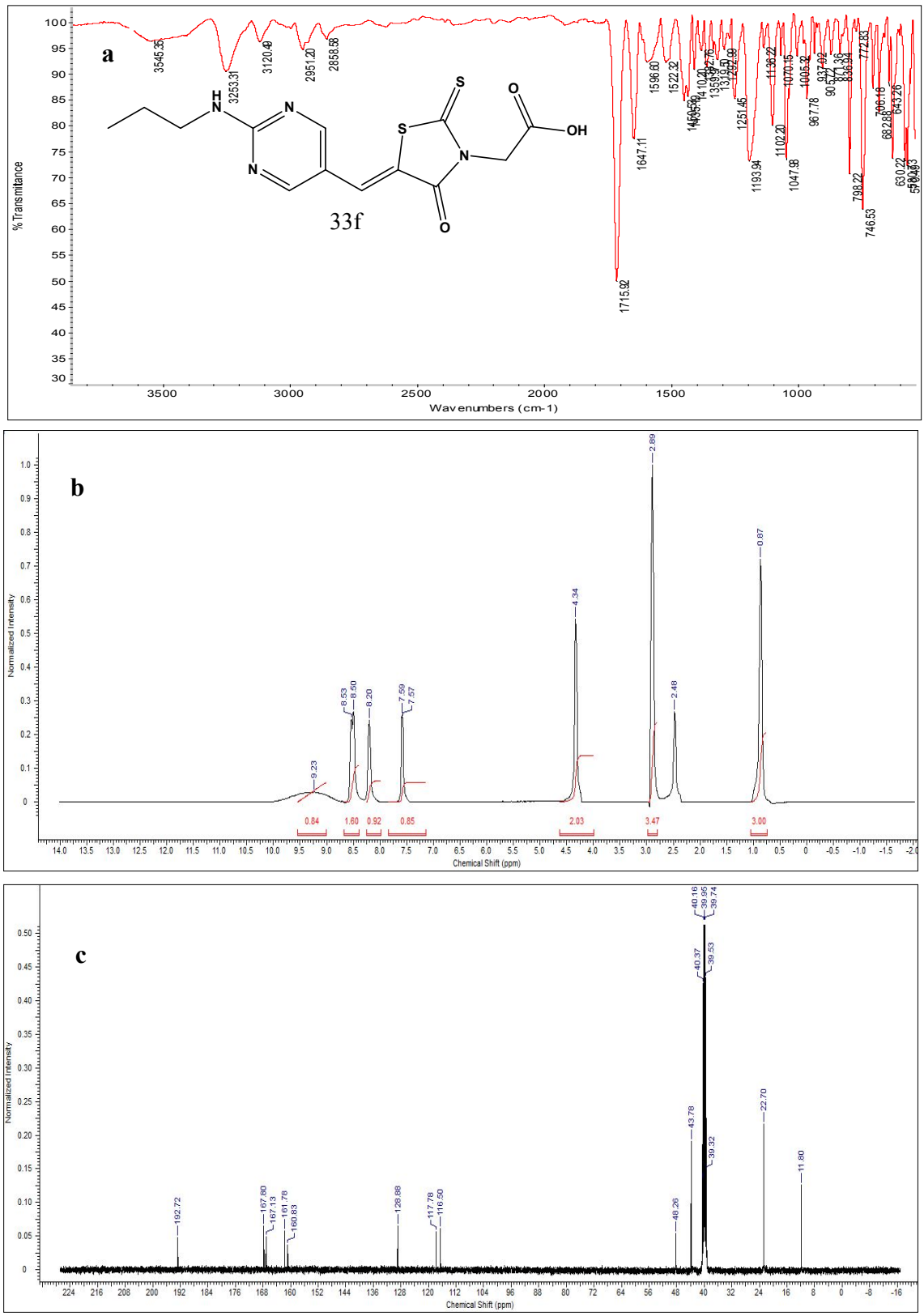


Fig S15. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33f

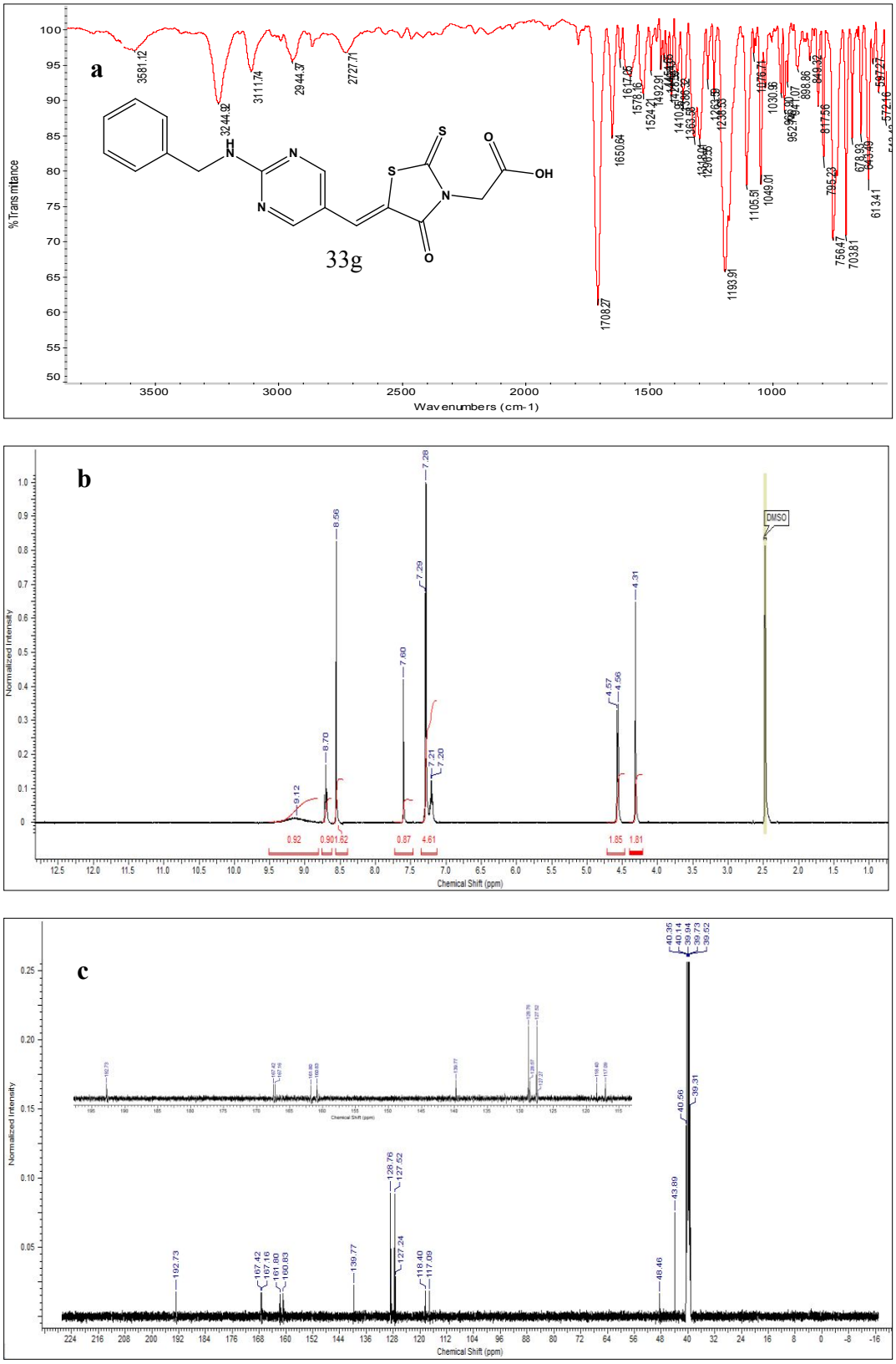
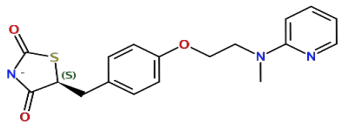
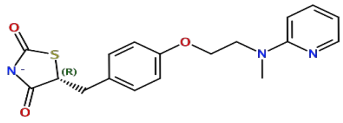
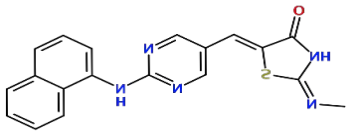
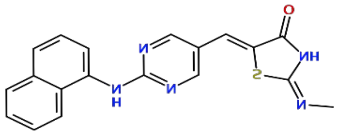
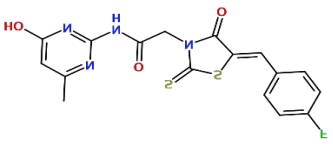
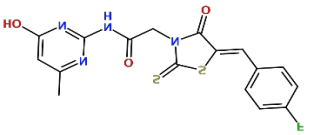
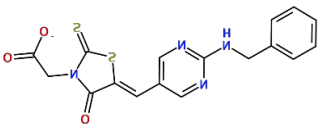
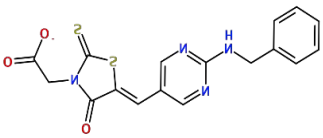
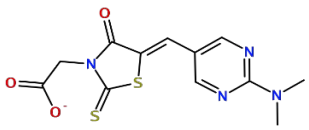
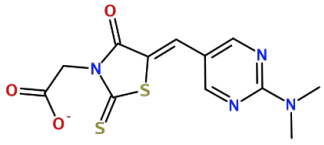
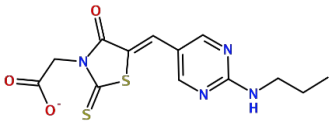
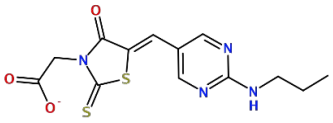
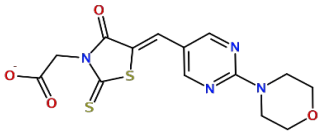
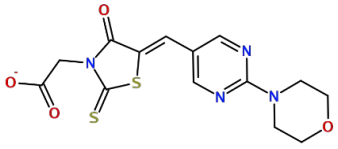
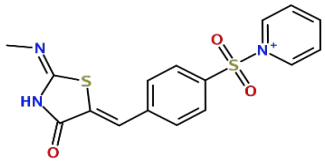
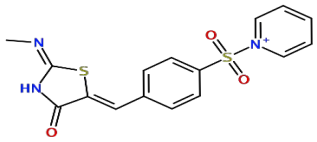
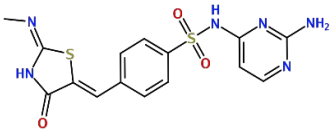
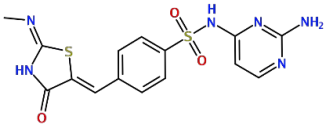
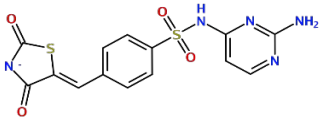
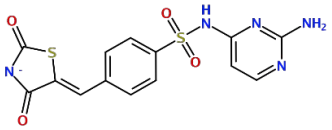
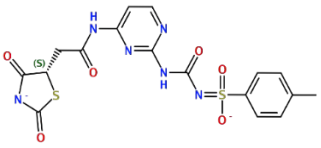
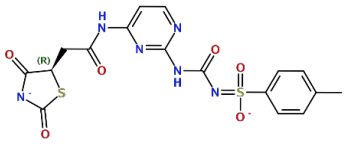
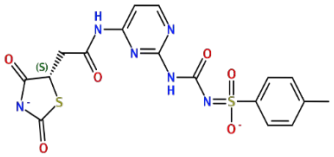
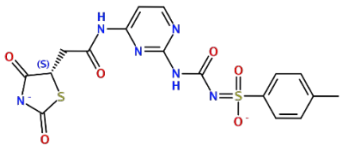
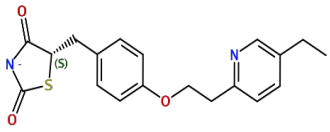
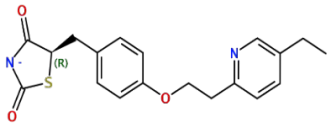
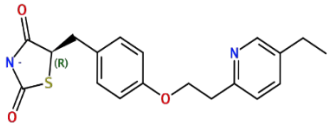
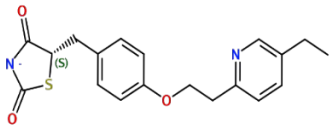


Fig S16. (a) IR spectrum; (b) ^{1}H-NMR spectrum; (c) ^{13}C-NMR spectrum for compound 33g

Table S1. Docking scores of different ligands into PDB:1WM0, PDB:1ZGY and PDB:1I7I PPAR-γ crystal structures.

	Ligand ID	Compond structure	XP docking score (kcal/mol)		
			1WM0	1ZGY	1I7I
1	1ZGY_S		-9.081	-8.628	-8.258
2	1ZGY_R		-2.582	-7.884	-7.999
3	MF1		-8.232	-8.856	-7.219
4	MF1_E		-7.355	-6.572	-8.323
5	MF10		-7.577	-6.181	-9.698
6	MF10_Z		-8.787	-7.708	-7.823
7	MF11		-8.521	-6.068	-7.115
8	MF11_Z		-9.604	-4.94	-6.766
9	MF12		-7.029	-4.729	-5.643
10	MF12_Z		-6.337	-4.285	-5.43

11	MF13		-7.093	-5.186	-6.02
12	MF13_Z		-7.073	-4.461	-5.256
13	MF14		-6.885	-5.041	-6.284
14	MF14_Z		-6.433	-4.794	-6.269
15	MF2		-3.821	-5.284	-4.598
16	MF2_E		-4.742	-4.281	-6.018
17	MF3		-8.008	-6.185	-6.962
18	MF3_E		-7.739	-6.88	-6.954
19	MF4		-7.349	-6.914	-6.559
20	MF4_E		-6.978	-2.001	-7.455
21	MF7_R		-8.816	-6.794	-6.592

22	MF7_R		-6.35	-5.849	-5.325
23	MF7_S		-8.567	-8.296	-6.964
24	MF7_S		-6.767	-5.869	-6.482
25	pioglitazone_R		-10.151	-9.251	-8.927
26	pioglitazone_R		-7.668	-8.304	-8.661
27	pioglitazone_S		-10.12	-9.247	-9.024
28	pioglitazone_S		-10.052	-7.767	-8.978