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Supporting information for article:

Proton tautomerism in 5-dimethylaminomethylidene-4-(*o*-,*m*-,*p*-hydroxyphenyl)-amino-1,3-thiazol-2(5*H*)-ones: synthesis, crystal structure, and spectroscopic studies

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CONTENTS

Figure S16. Calculated spectra for compounds **1** – **3** using DFT/ωB97X-D/6-311G(d,p) method.

Table S1. The reference lengths of double and single Csp^2–N bonds obtained based on structures deposited in Cambridge Structural Database, version 5.42.

	Refcode	**C=N**	**Csp^2–N**
1.	EHITZO	1.282	1.387
2.	FOTQEM	1.269	1.380
3.	HEGMAJ	1.281	1.362
4.	HEGMAJ	1.268	1.372
5.	HEGMEN	1.282	1.381
6.	HEGMIR	1.296	1.363
7.	HEGMOX	1.277	1.369
8.	HEGMOX	1.284	1.371
9.	IKIVIJ	1.291	1.360
10.	JOCKIY	1.280	1.384
11.	JOCKOE	1.288	1.370
12.	JOMCOF	1.271	1.383
13.	JOMKOO	1.271	1.379
14.	LAFJAG	1.297	1.373
15.	NEBHOU	1.283	1.367
16.	NOYYOS	1.277	1.356
17.	OCAGEI	1.272	1.371
18.	POSSOH	1.271	1.382
19.	QAJSEC	1.280	1.368
20.	RALVEI	1.280	1.374
21.	RALVEI	1.266	1.382
22.	ROMXUN	1.278	1.367
23.	SISCAB	1.270	1.373
24.	TIQTIZ	1.285	1.370
25.	TIQTIZ	1.276	1.381
26.	ULACEQ	1.260	1.390
27.	VAMPUW	1.292	1.380
28.	WAGVUY	1.286	1.369

29.	WOGGOQ	1.288	1.380
30.	XOKLAN	1.281	1.368
31.	XOKLER	1.281	1.371
32.	XUBYOK	1.279	1.379
33.	YIKXOI	1.278	1.374
34.	YIKXOI	1.270	1.378
Mean values		**1.279(1)**	**1.374(1)**

Table S2. The reference length of single Csp^2–Csp^2 bond obtained based on structures deposited in Cambridge Structural Database, version 5.42.

	Refcode	**Csp^2–Csp^2**		**Refcode**	**Csp^2–Csp^2**
1.	ADUDIO	1,49	29.	MIZJUC	1,498
2.	AGOMUG	1,495	30.	MUDRIO	1,498
3.	BIVWUZ	1,494	31.	NIPPAF	1,496
4.	CEMHOR	1,492	32.	NIPPAF	1,501
5.	CODYOM	1,493	33.	OHOXIU	1,496
6.	COTPUX	1,482	34.	OHOXIU	1,496
7.	COTPUX	1,489	35.	PUWYEN	1,499
8.	COTPUX	1,498	36.	PUWYIR	1,491
9.	COTPUX	1,509	37.	PUWYOX	1,501
10.	COXWUJ	1,487	38.	QUFKAG	1,497
11.	ECOVEA	1,499	39.	RIMDIC	1,499
12.	FIYPUA	1,497	40.	SEVGOS	1,488
13.	FOYPAL	1,495	41.	SISMUD	1,479
14.	FOYPEP	1,505	42.	SISMUD	1,487
15.	FOYPIT	1,508	43.	SIXFOV	1,489
16.	FUHVUA	1,498	44.	SIXFOV	1,493
17.	GUVVAW	1,493	45.	TOCKED	1,490
18.	HOLHIA	1,492	46.	TUTRAE	1,492
19.	IMMAZO10	1,488	47.	TUTREI	1,497
20.	IMMAZO10	1,493	48.	WABCAH	1,495
21.	INEPAU	1,49	49.	WABCIP	1,494

22.	JARNUO	1,481	50.	WAGGUJ	1,500
23.	JEJFUA	1,506	51.	WAGVUY	1,499
24.	JEJGAH	1,47	52.	WITLUJ	1,501
25.	JOMKAA	1,496	53.	WUYMIO	1,500
26.	KETRIL	1,488	54.	XABNOH	1,494
27.	KISBOE	1,452	55.	XUBYOK	1,503
28.	LIVSOA	1,497	56.	YIXKEX	1,486
			57.	ZANHAA	1,485
			Mean value		**1.493(1)**

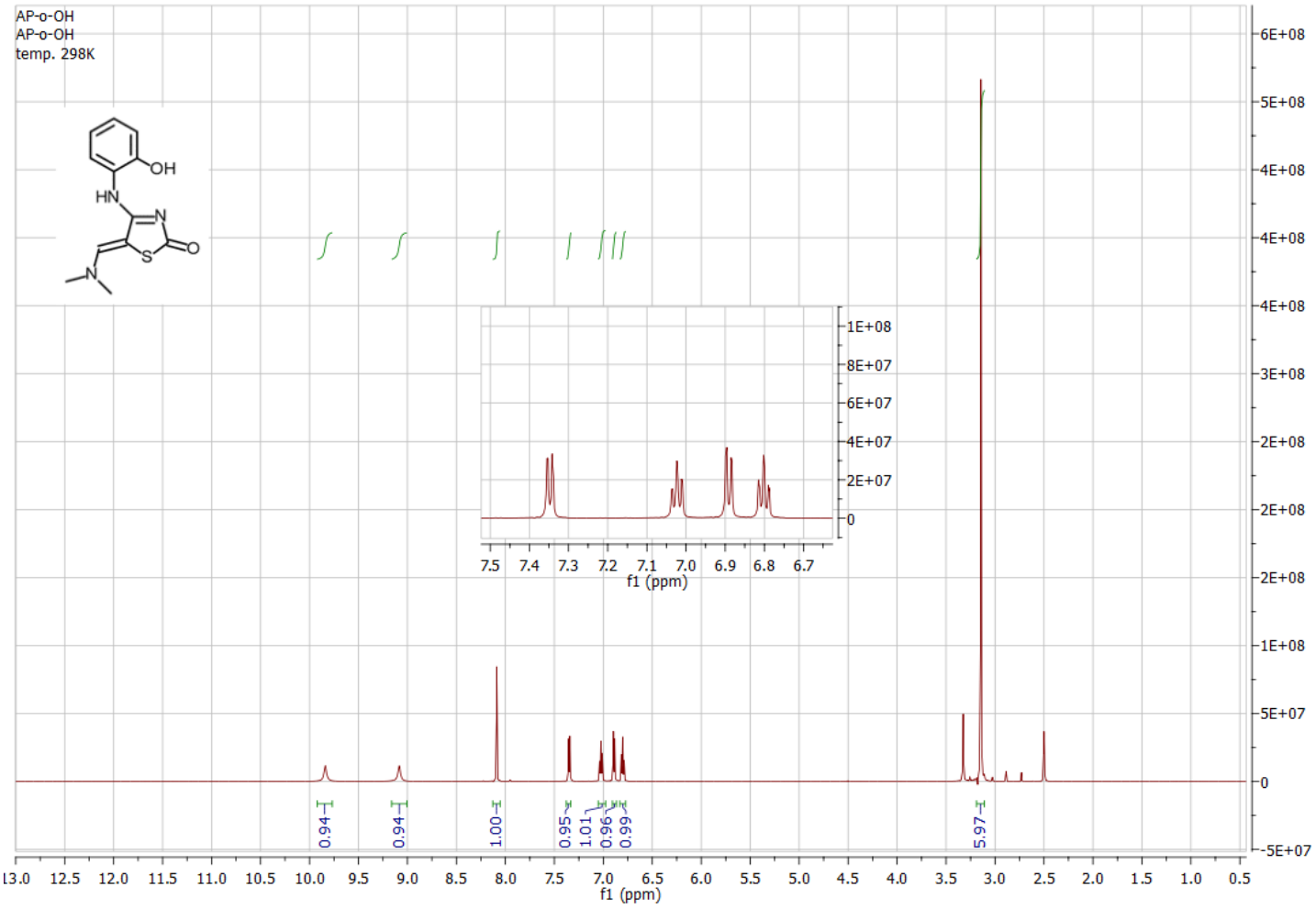

Figure S1. ^{1}H NMR spectra of compound **1**

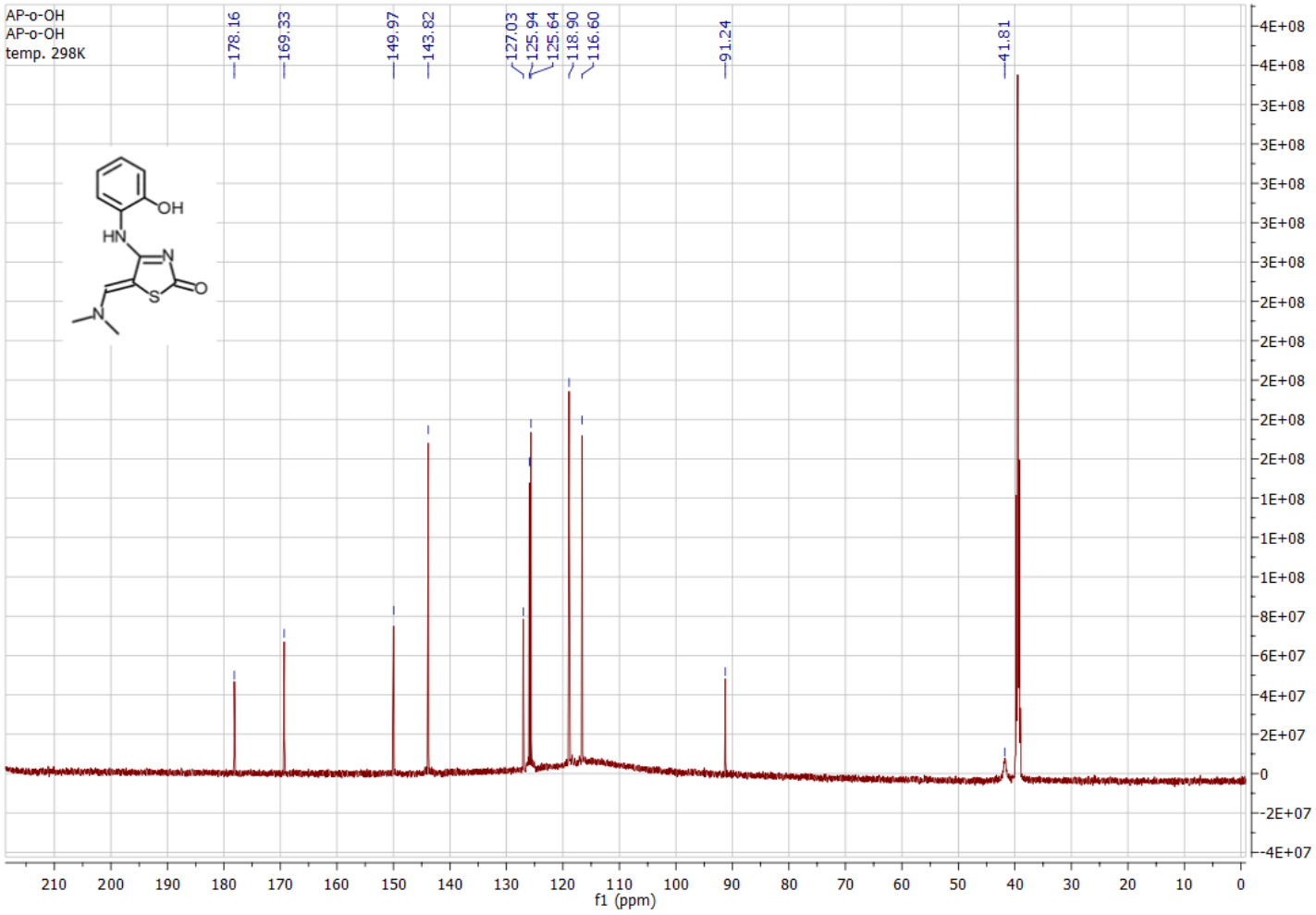

Figure S2. ^{13}C NMR spectra of compound **1**

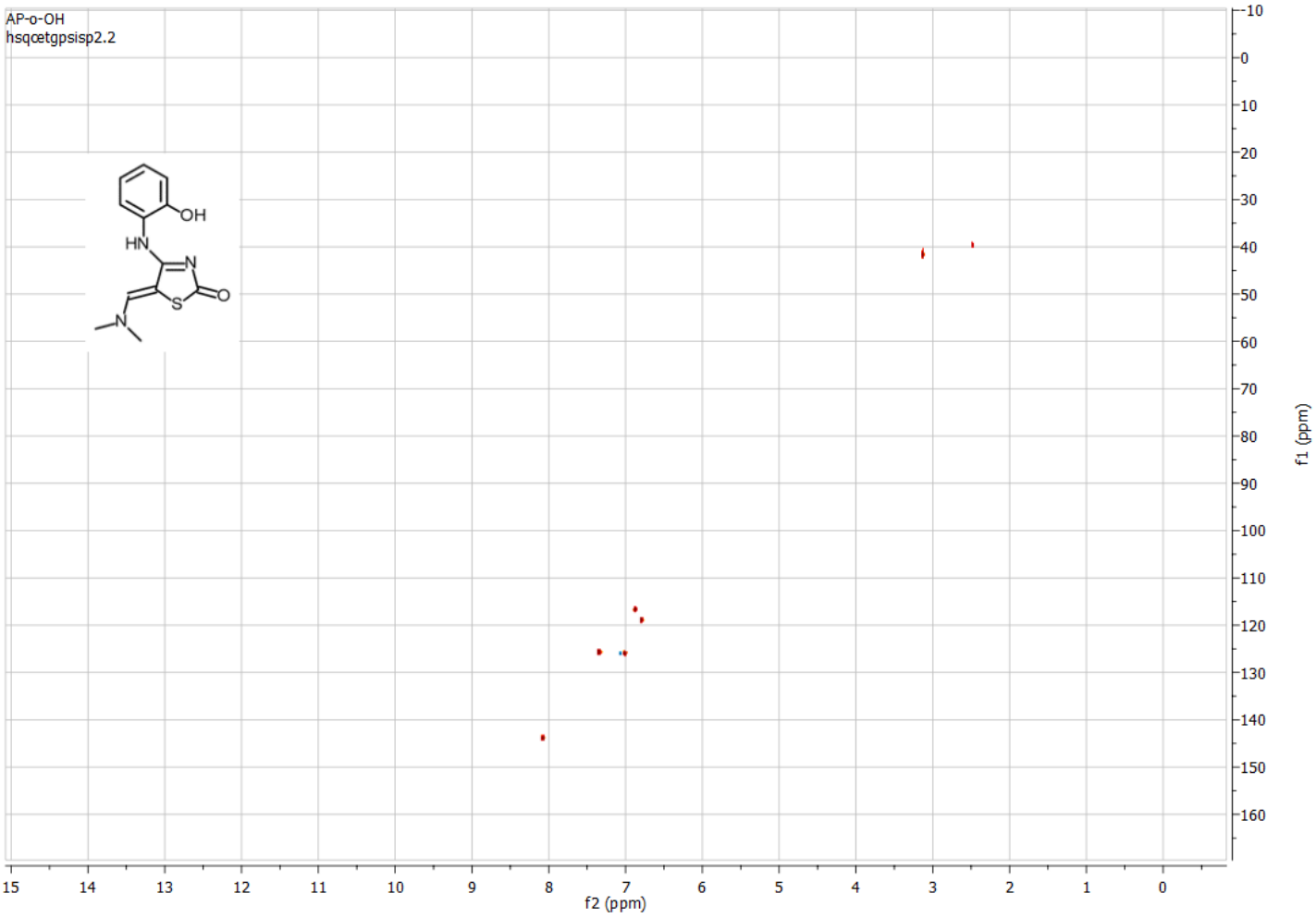

Figure S3. $^{1}H–^{13}C$ HSQC NMR spectra of compound **1**

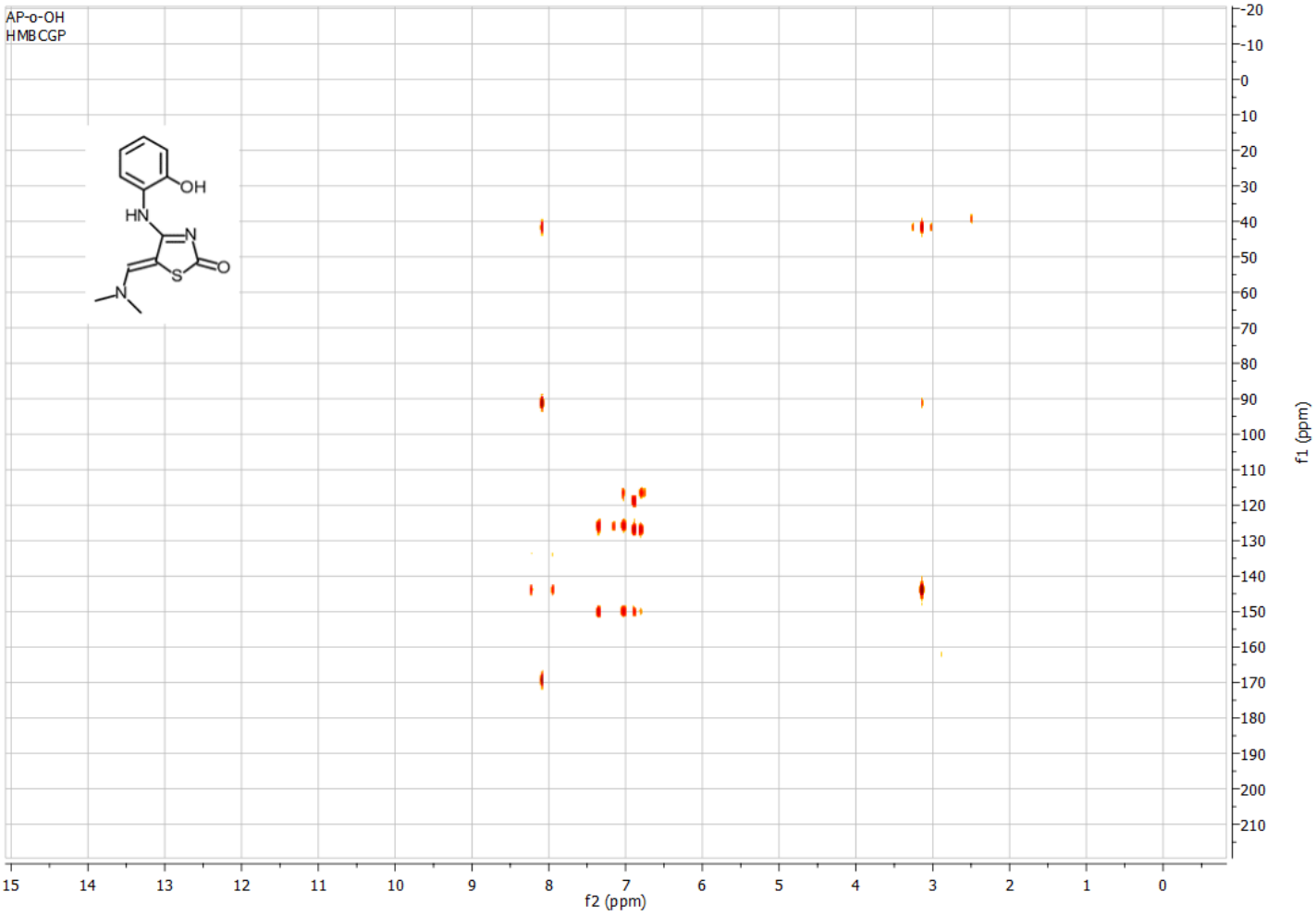

Figure S4. $^{1}H–^{13}C$ HMBC NMR spectra of compound **1**

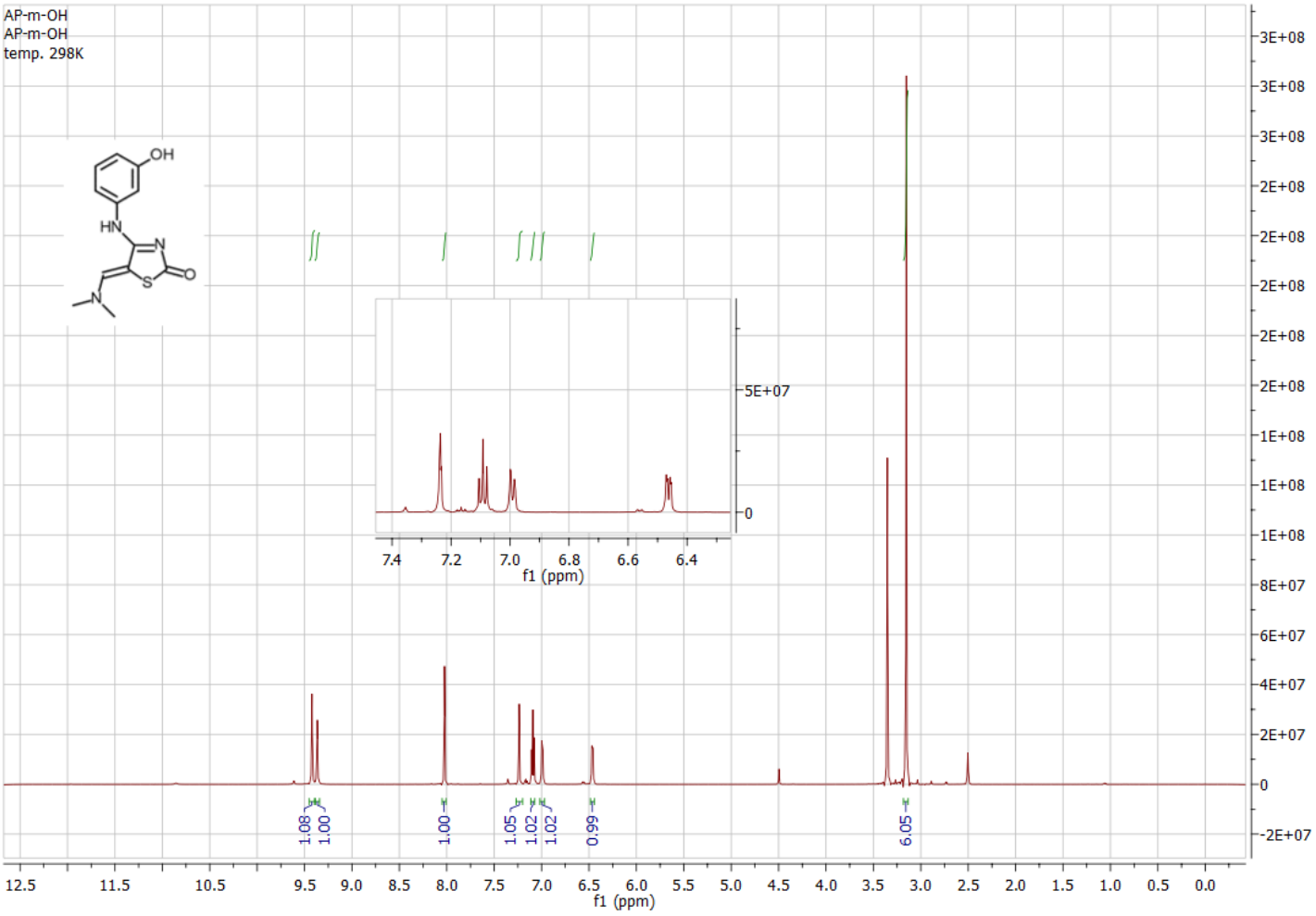

Figure S5. ^{1}H NMR spectra of compound **2·DMF**

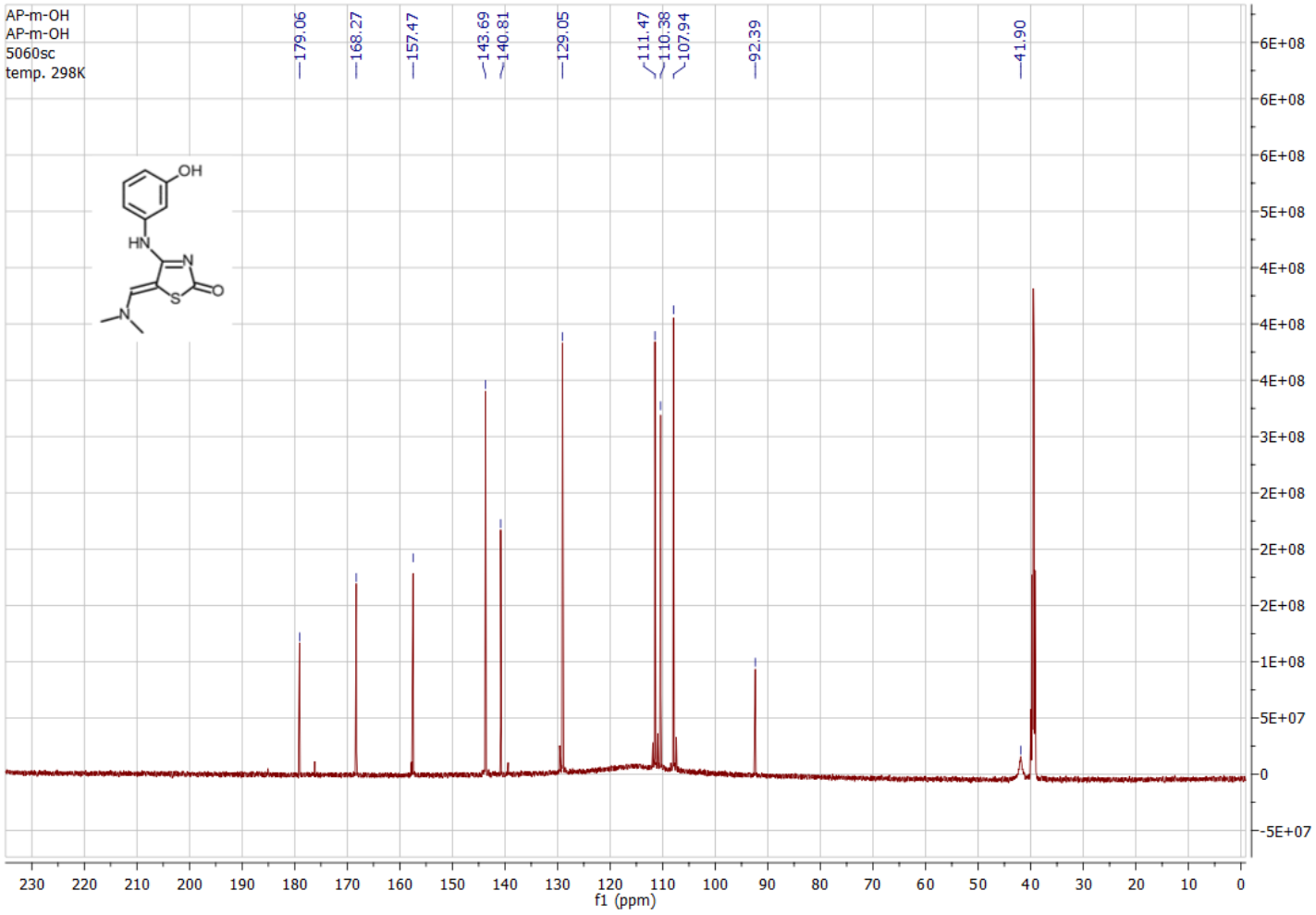

Figure S6. ^{13}C NMR spectra of compound **2·DMF**

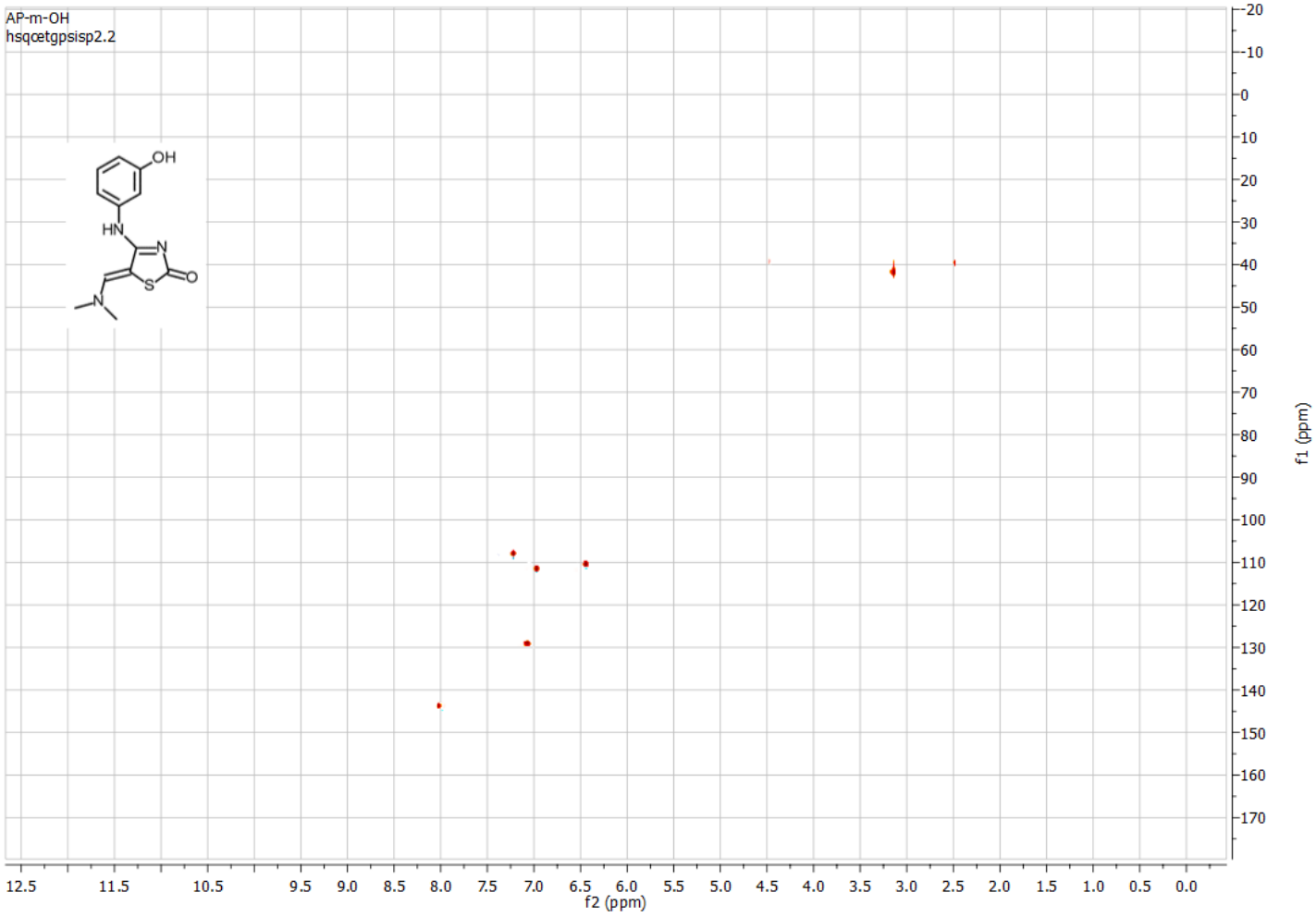

Figure S7. ^{1}H–^{13}C HSQC NMR spectra of compound **2·DMF**

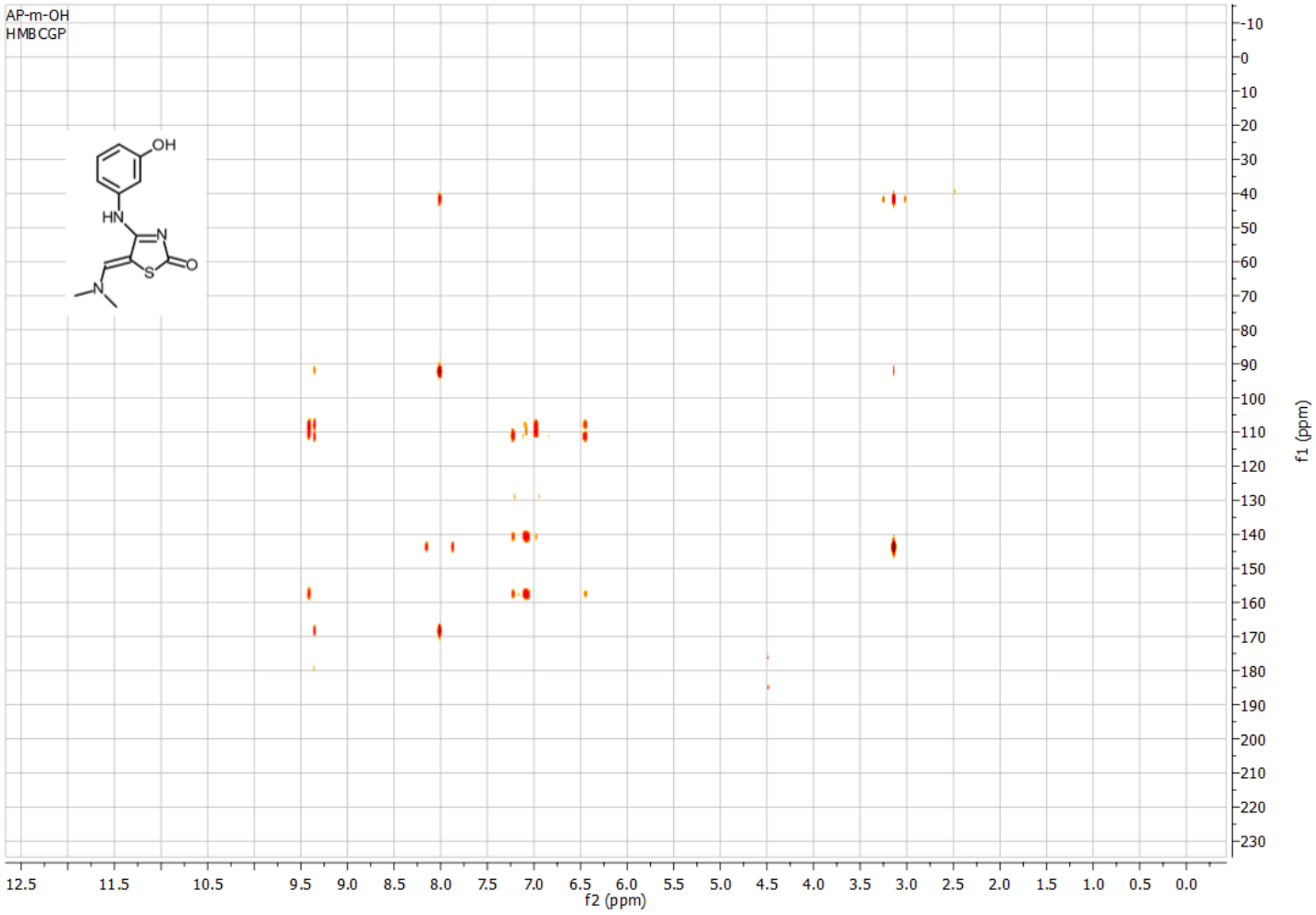

Figure S8. ^{1}H–^{13}C HMBC NMR spectra of compound **2·DMF**

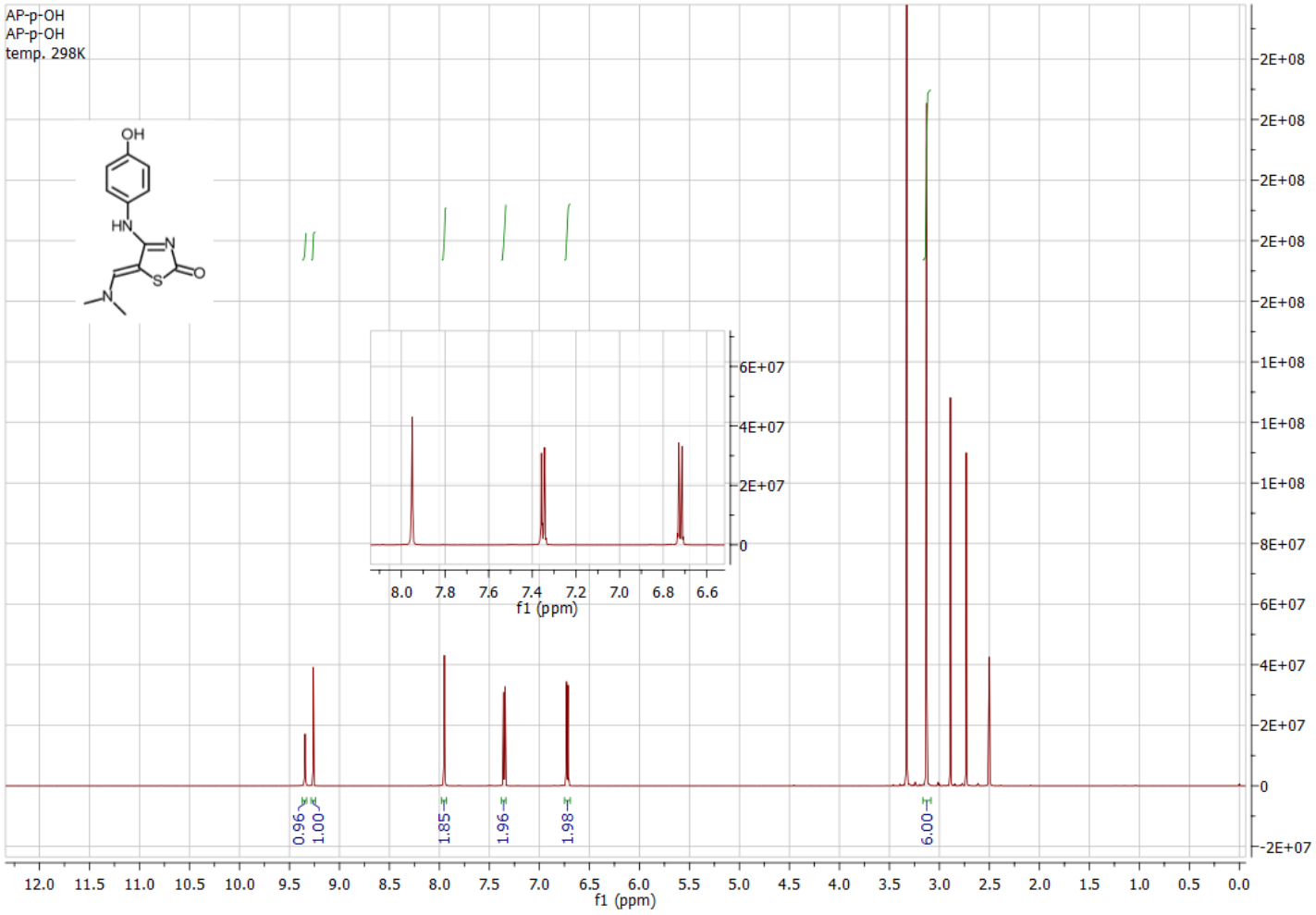

Figure S9. ^{1}H NMR spectra of compound **3·DMF**

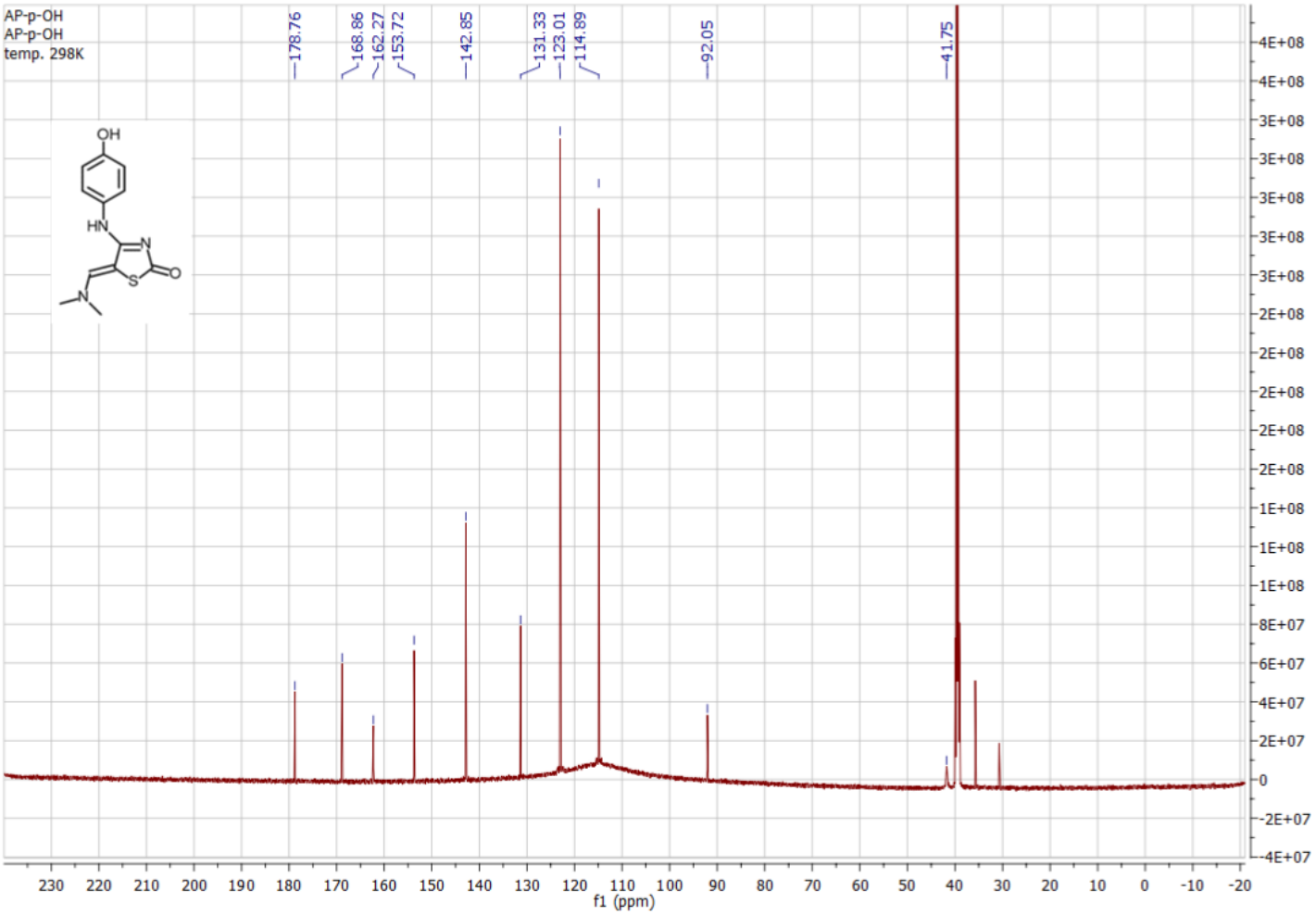

Figure S10. ^{13}C NMR spectra of compound **3·DMF**

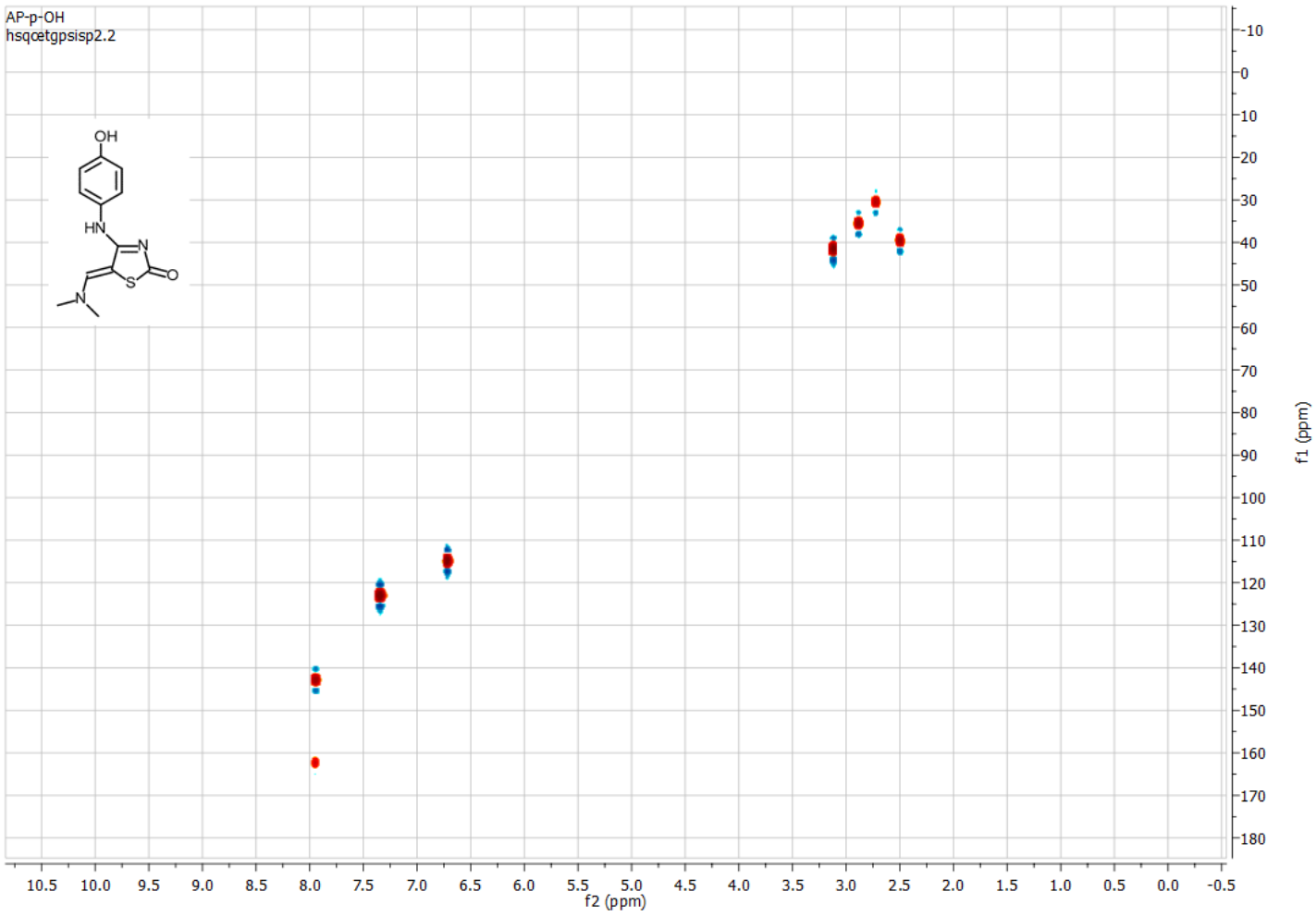

Figure S11. ^{1}H–^{13}C HSQC NMR spectra of compound **3·DMF**

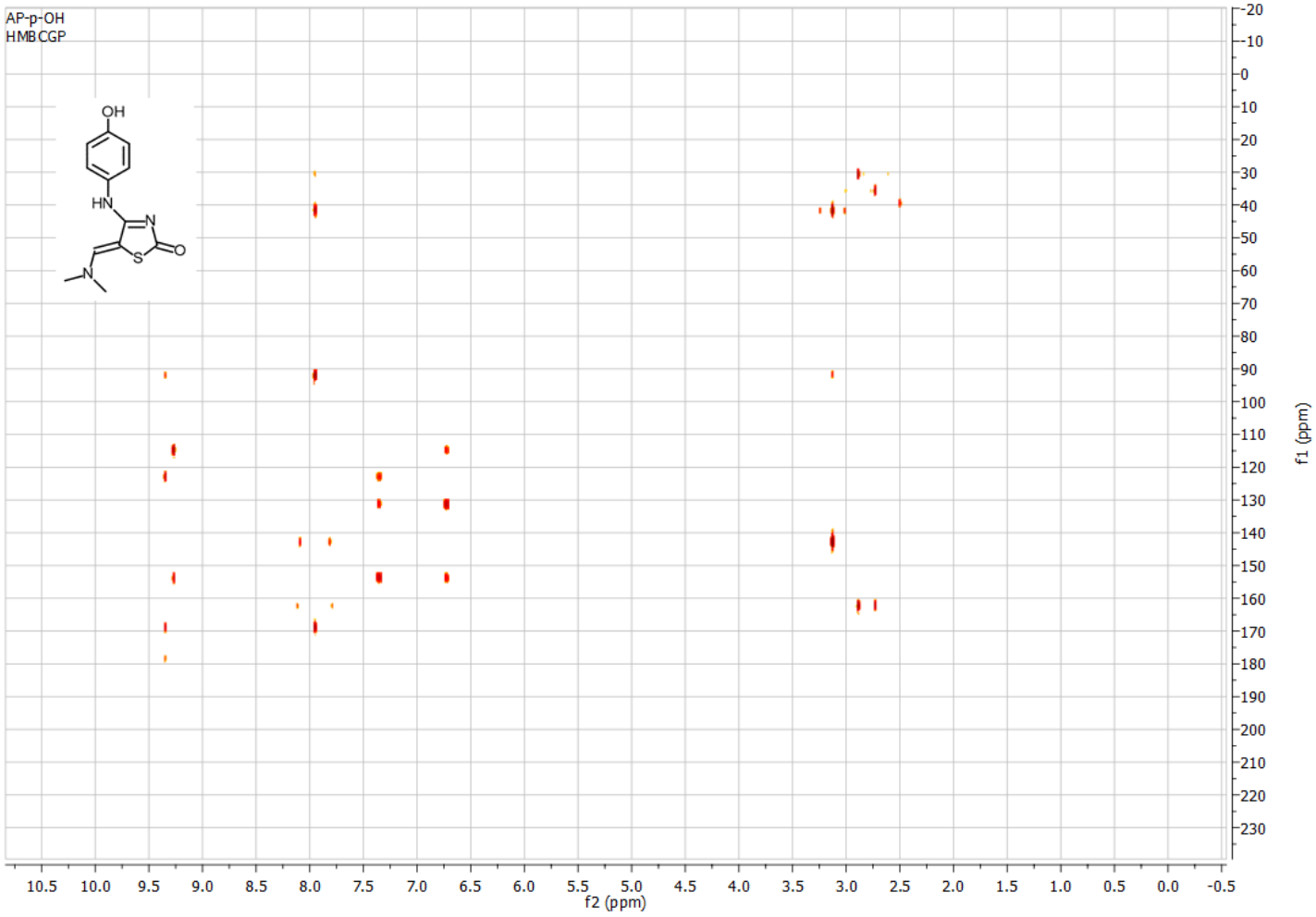

Figure S12. ^{1}H–^{13}C HMBC NMR spectra of compound **3·DMF**

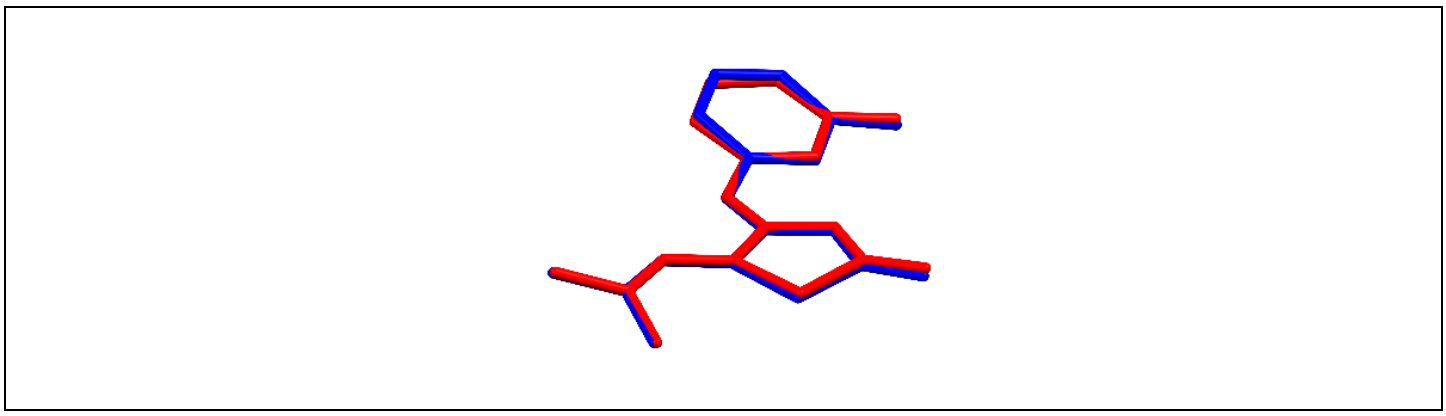

Figure S13. Overlay of two symmetry-independent molecules A (red) and B (blue) by the least-squares fitting of the tiazolin-2-one systems.

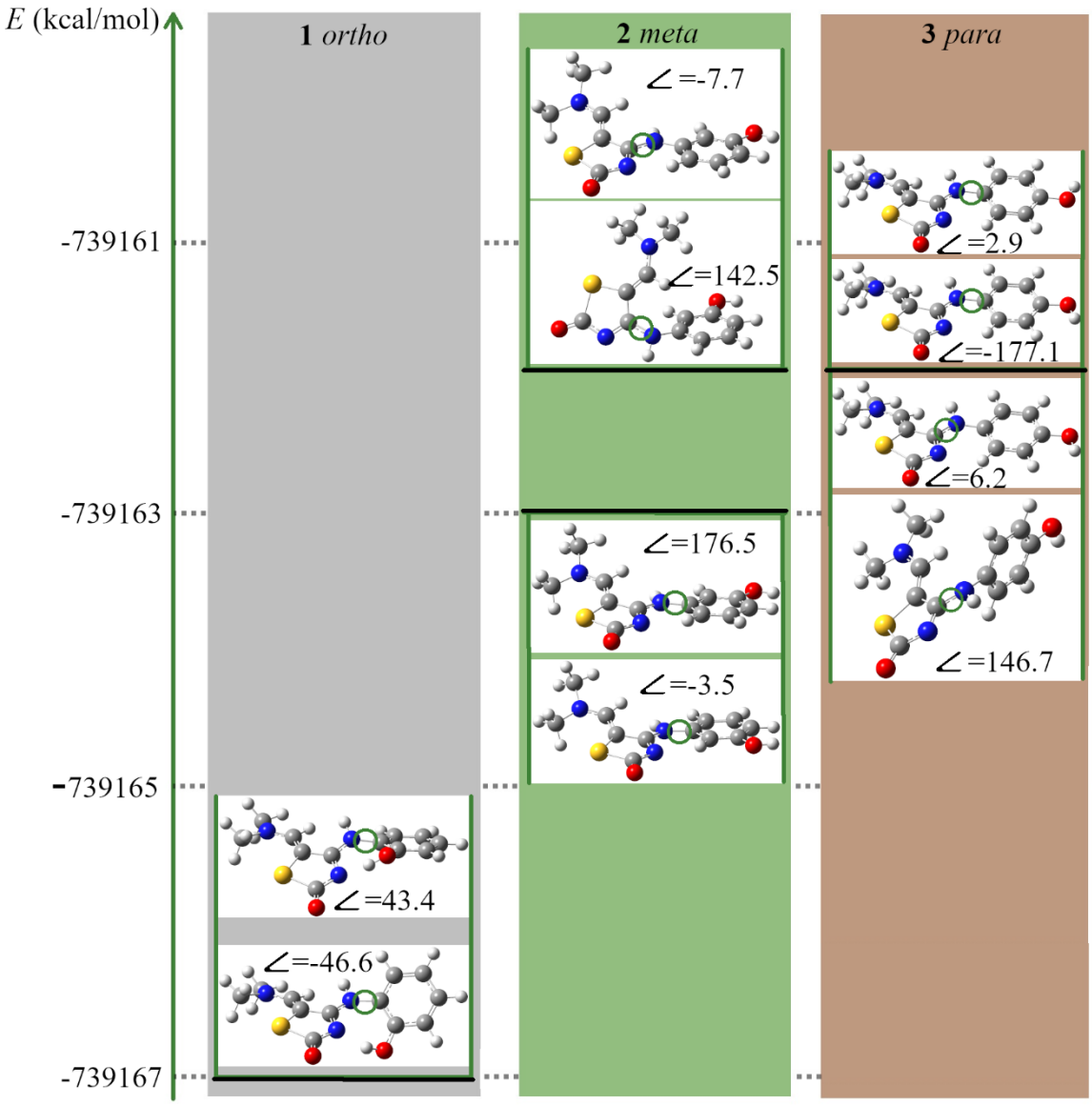

Figure S14. Conformational analysis of substituted molecules in the *ortho* (1), *meta* (2), and *para* (3) positions. The green circle indicates the single bonds around which the molecule fragments were rotated. The values of dihedral angles C9–C8–N7–C4 and N3–C4–N7–C8 are shown.

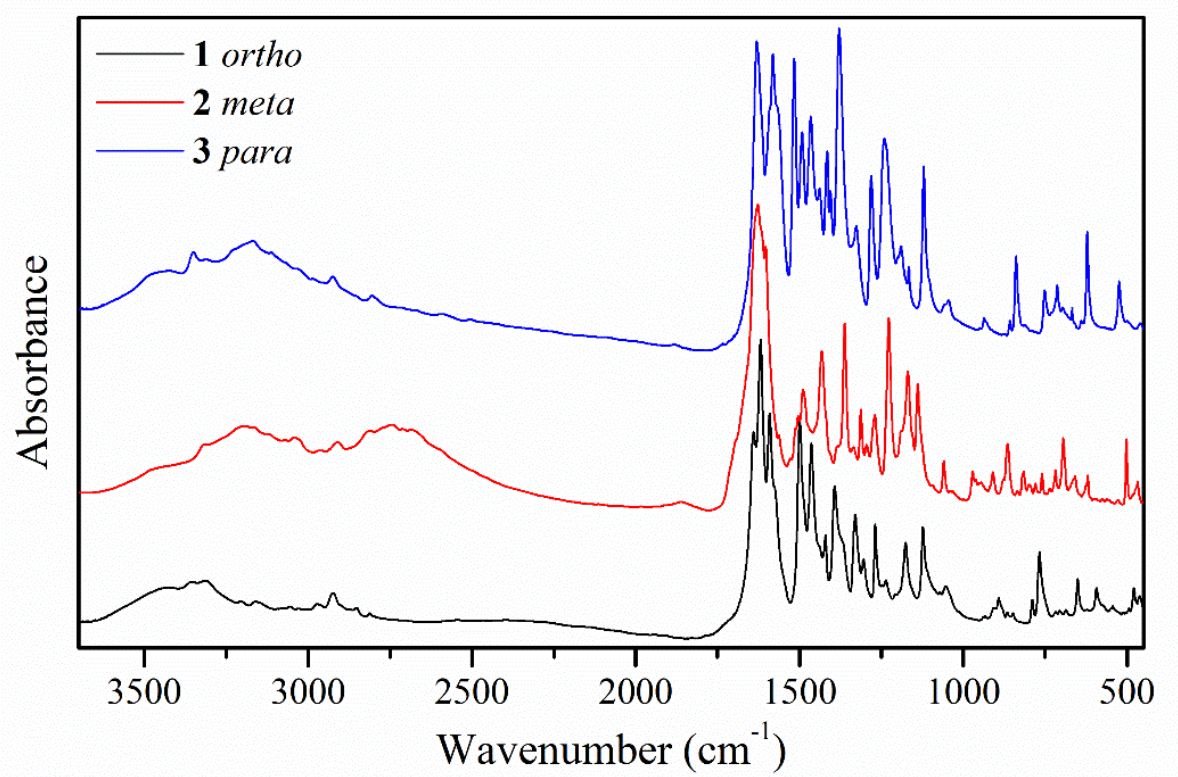

Figure S15. IR spectra of compounds **1** – **3** in the KBr matrix (c=1:1000 for **1** and c=1:500 for **2**, **3**).

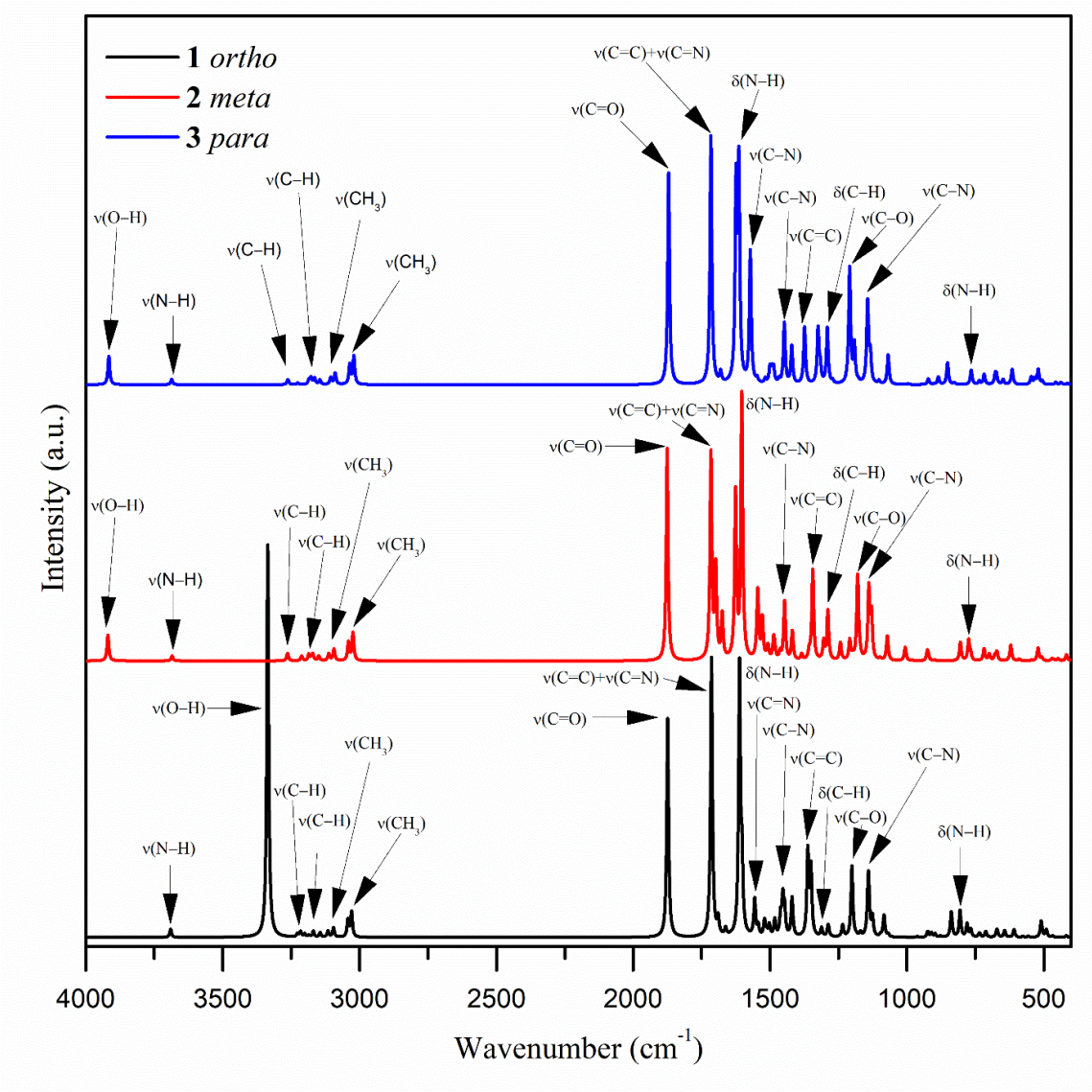

Figure S16. Calculated spectra for compounds **1** – **3** using DFT/ωB97X-D/6-311G(d,p) method.