

Supplementary data contents page

C-8 *N*-ethyl-2-pyrrolidinone substituted flavan-3-ols from the leaves of *Camellia sinensis* var. *pubilimba*

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Figure S1. Purification procedure of compounds **1-40**

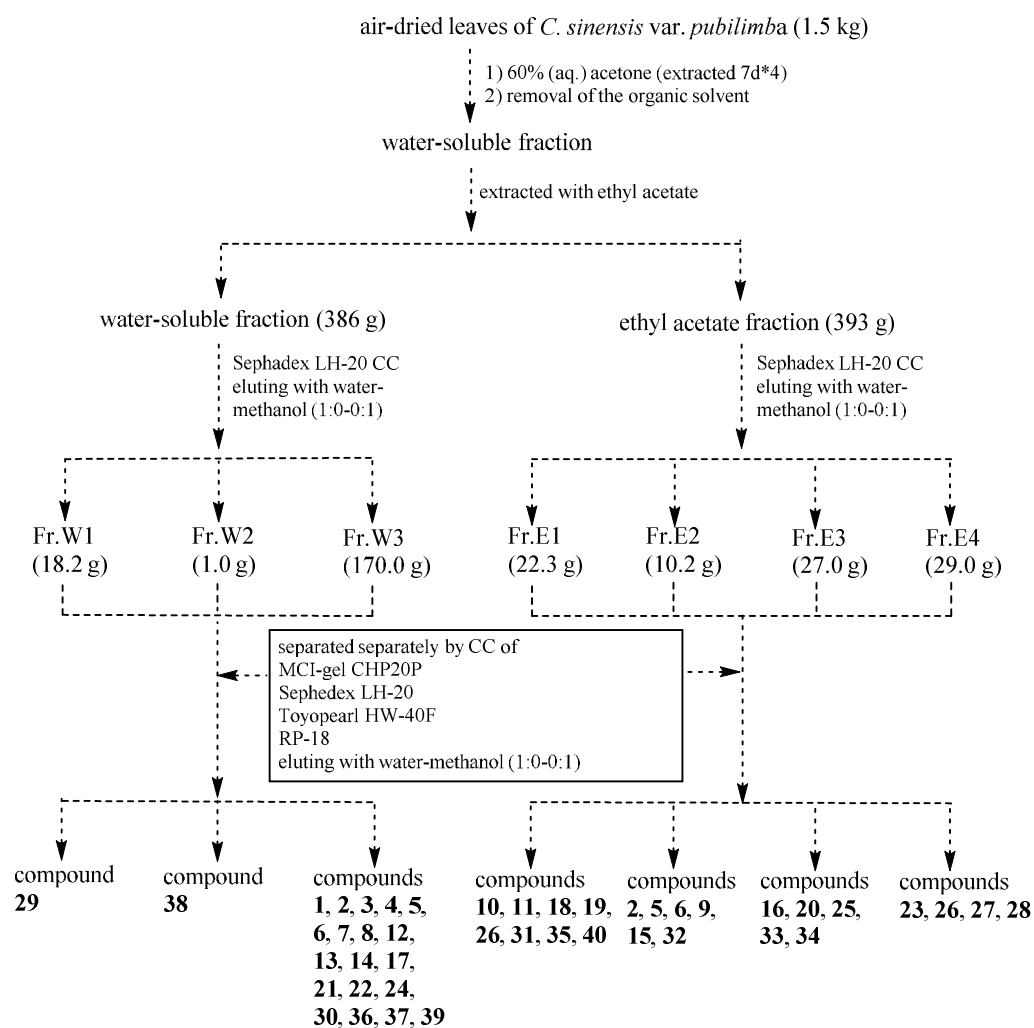


Figure S2. The structures of compounds **15-40** from *C. sinensis* var. *pubilimba*

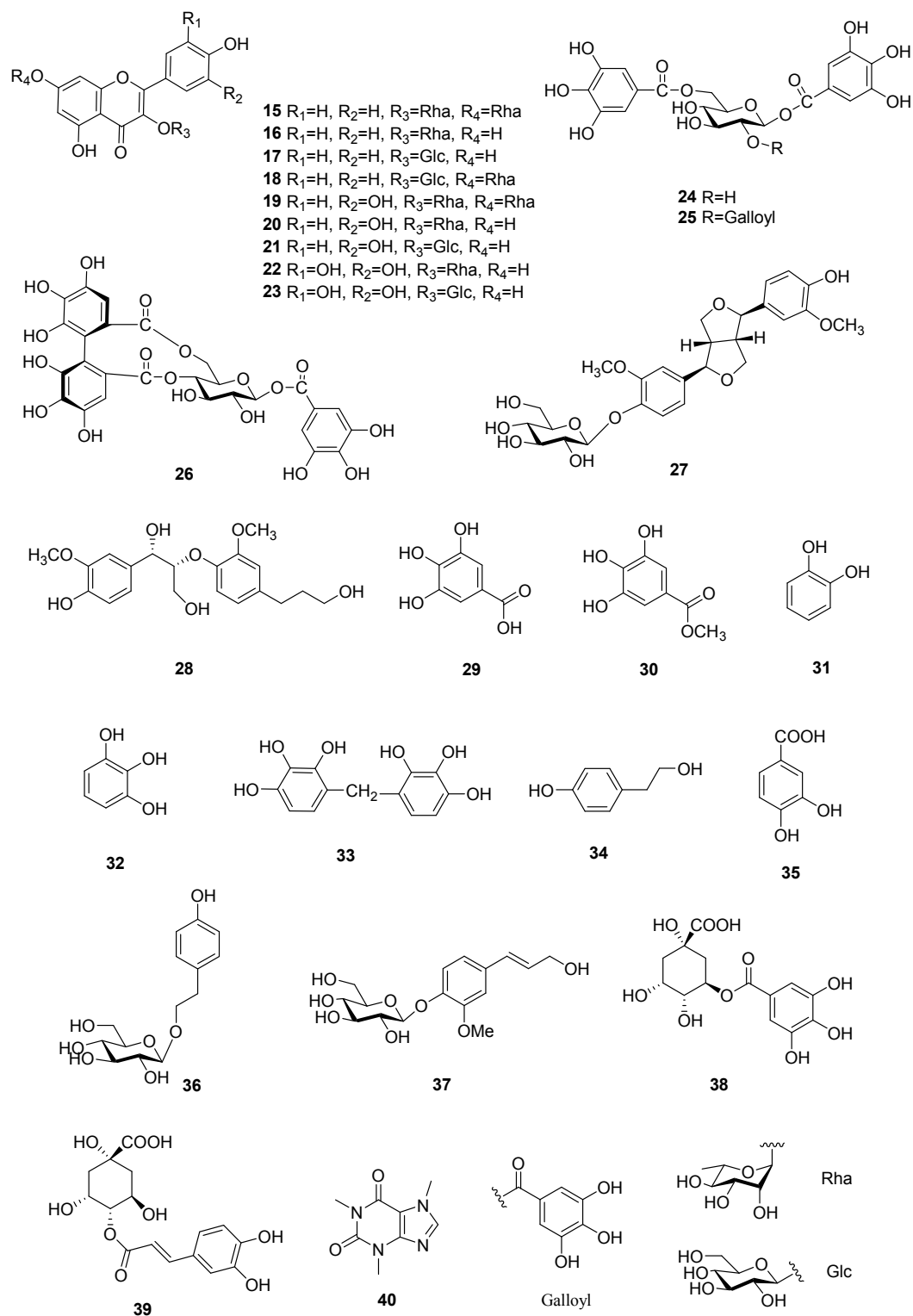


Figure S3. ^1H NMR spectrum of compound **1** in CD_3OD

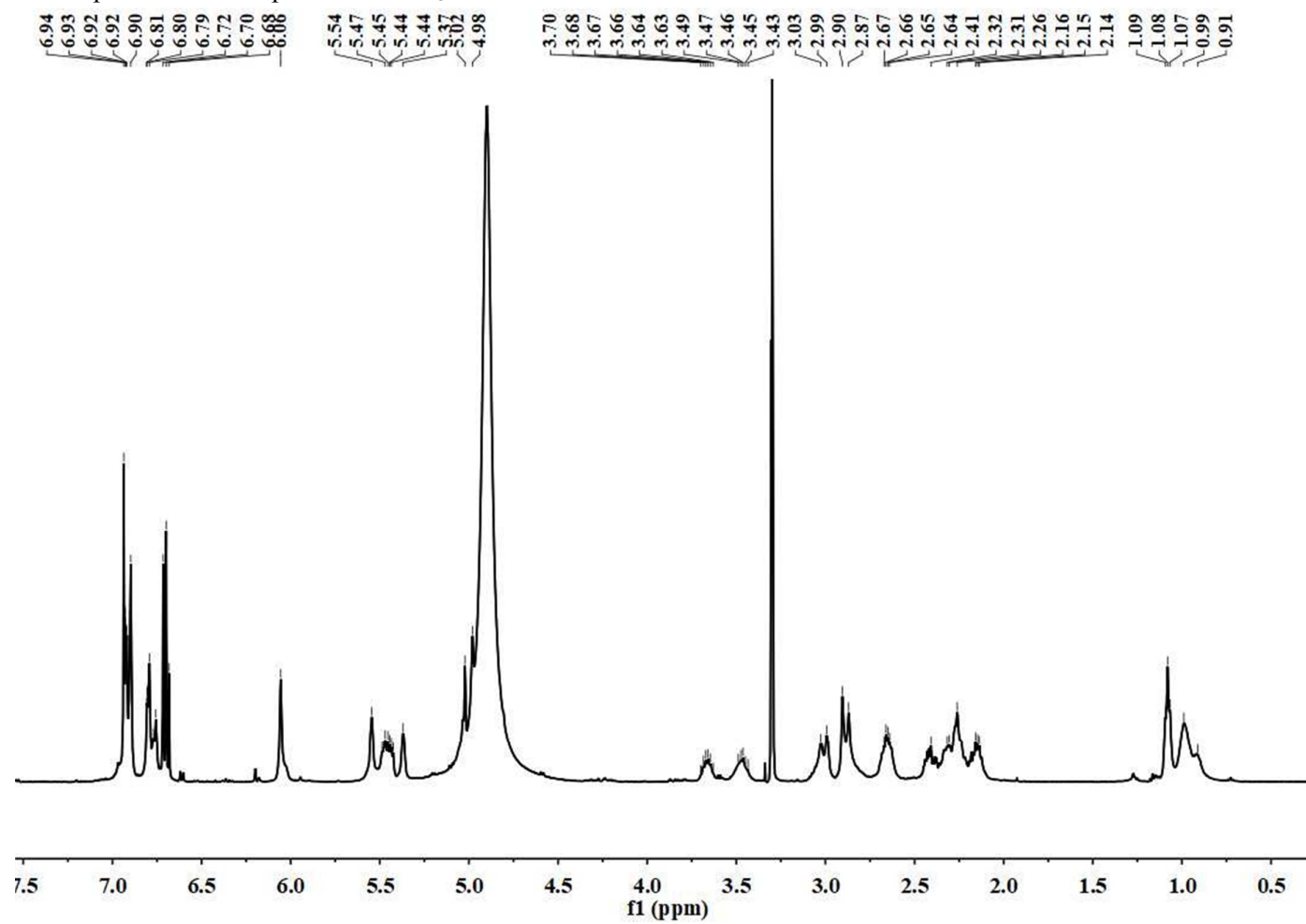


Figure S4. ^{13}C NMR spectrum of compound **1** in CD_3OD

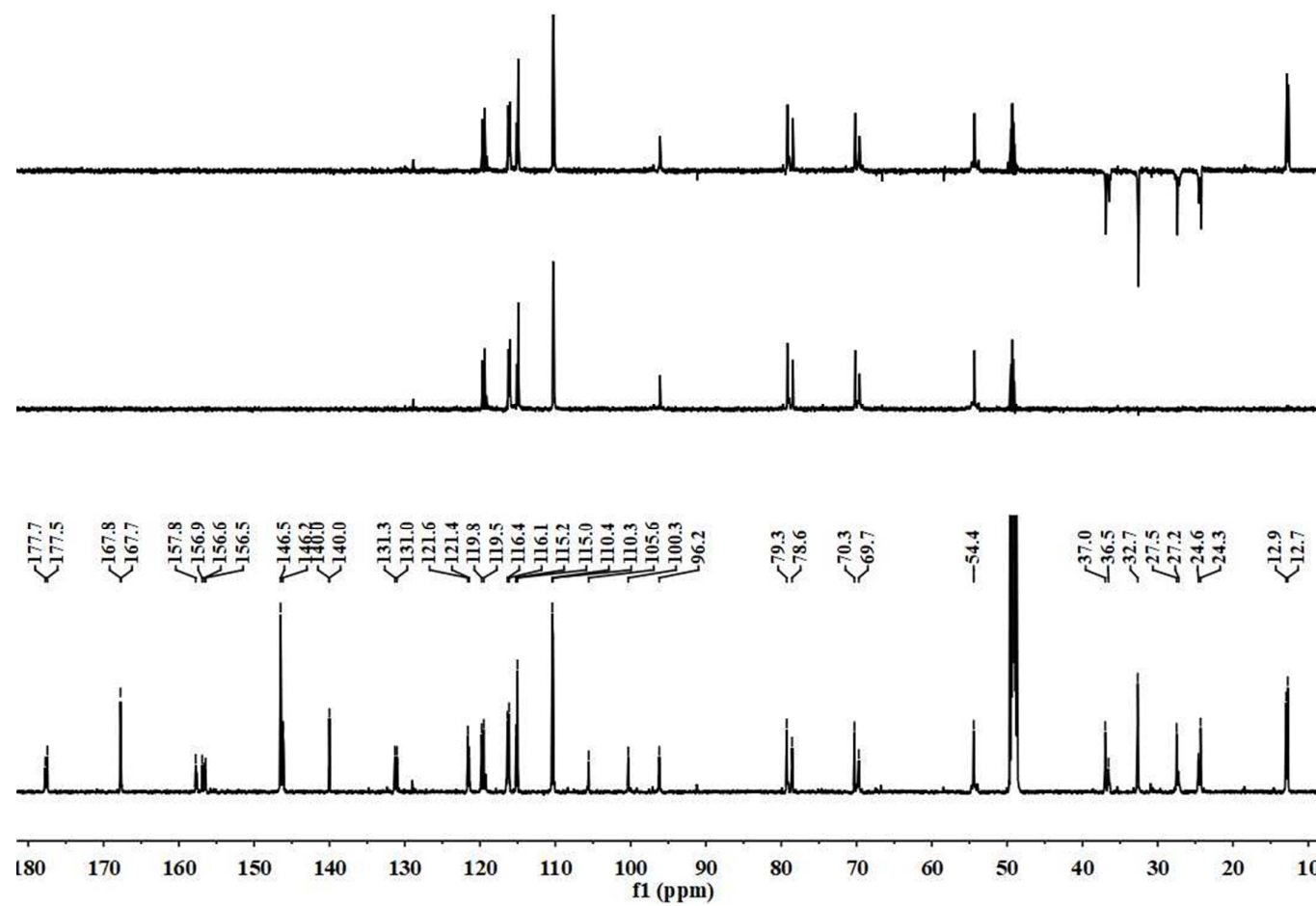


Figure S5. HMQC spectrum of compound **1** in CD₃OD

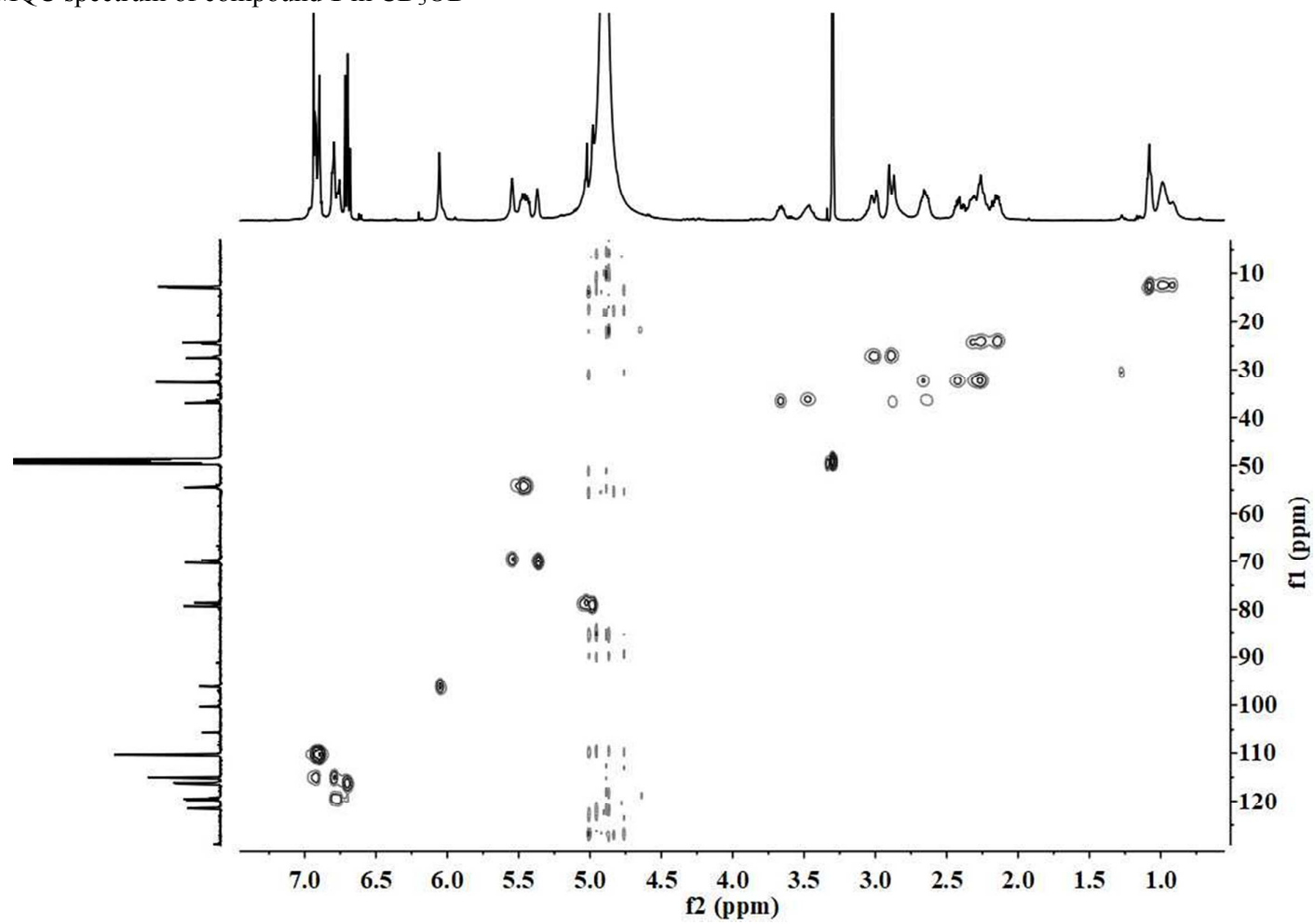


Figure S6. HMBC spectrum of compound **1** in CD₃OD

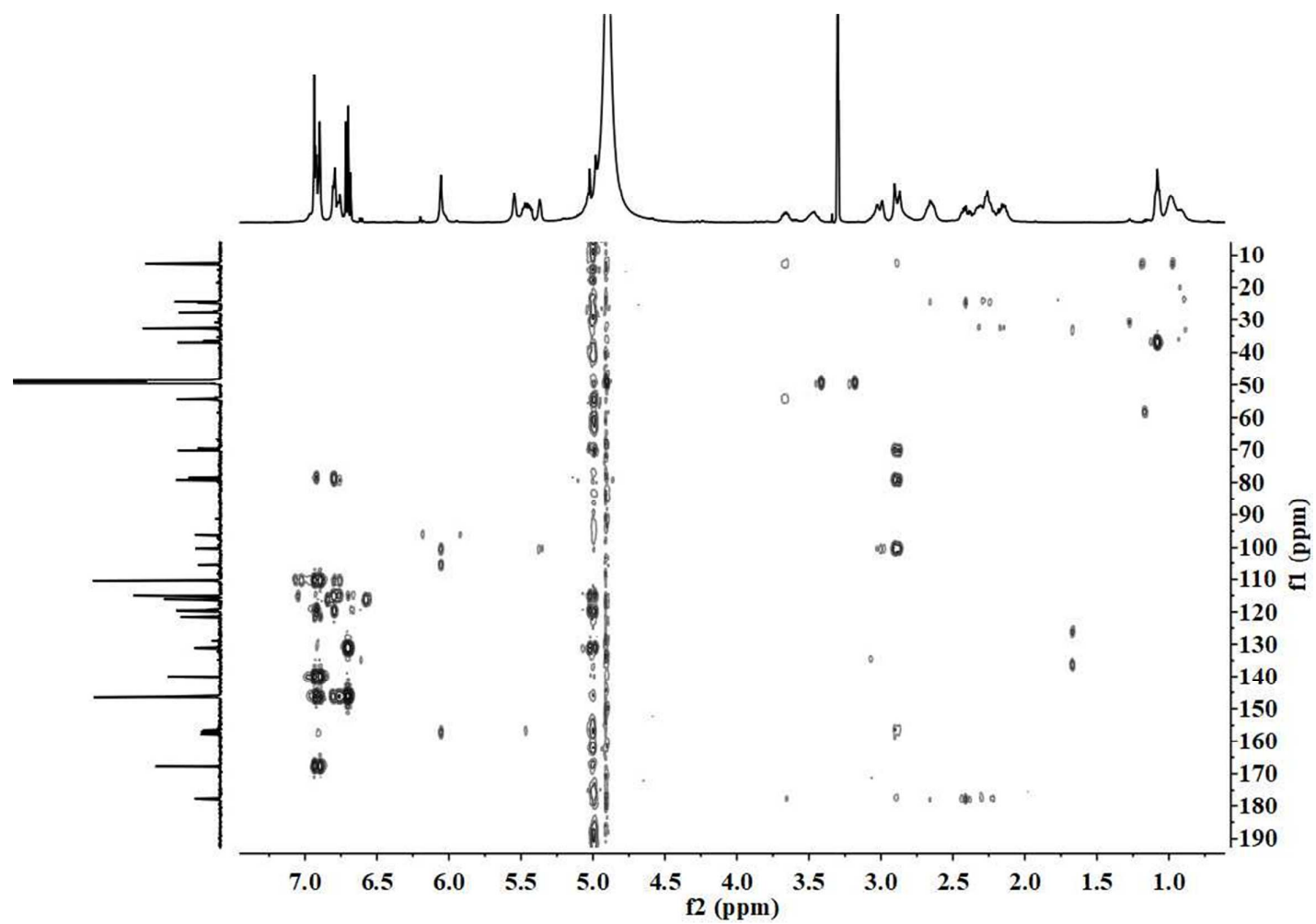


Figure S7. HRESIMS of compound 1

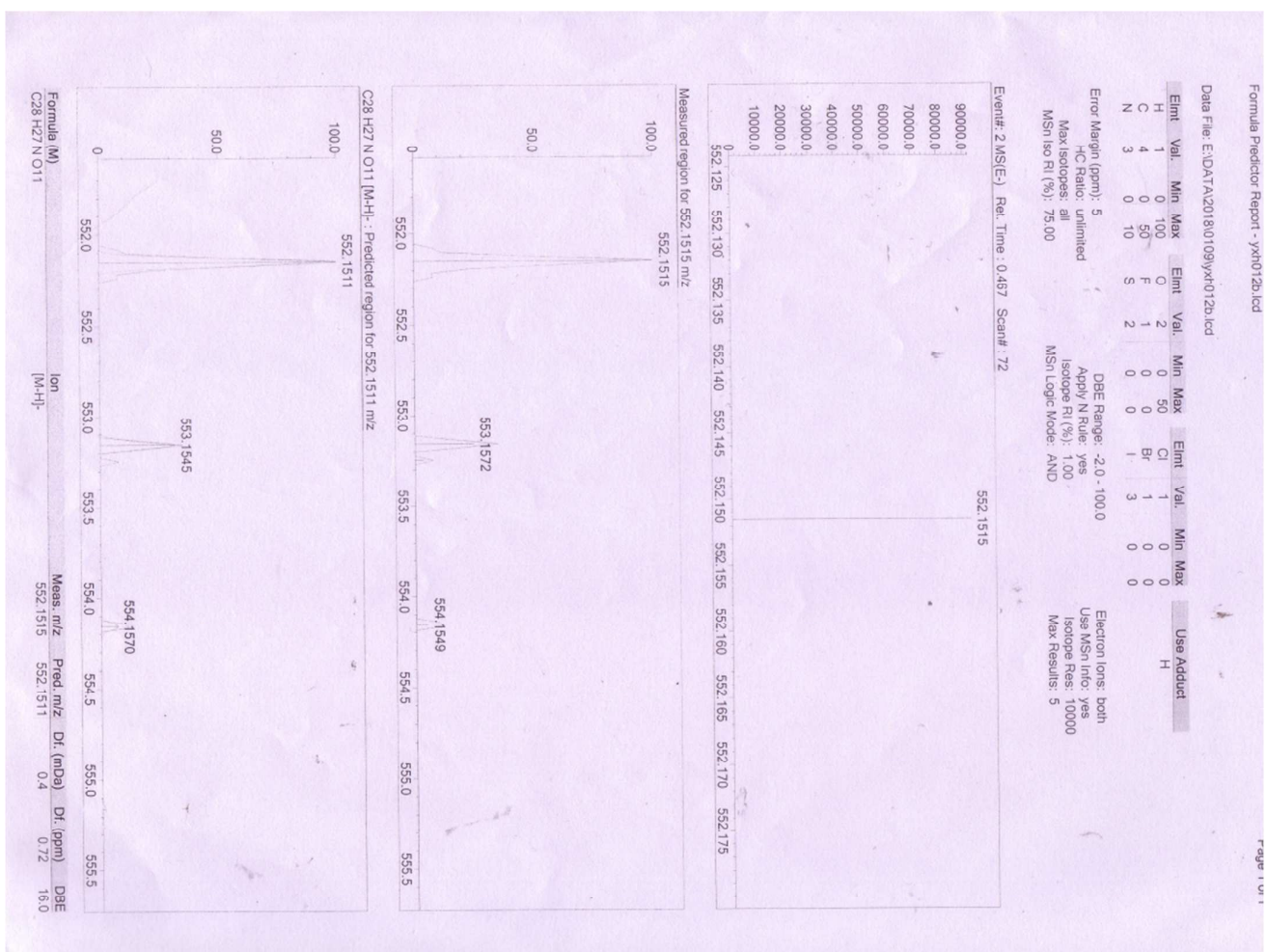


Figure S8. IR spectrum of compound **1**

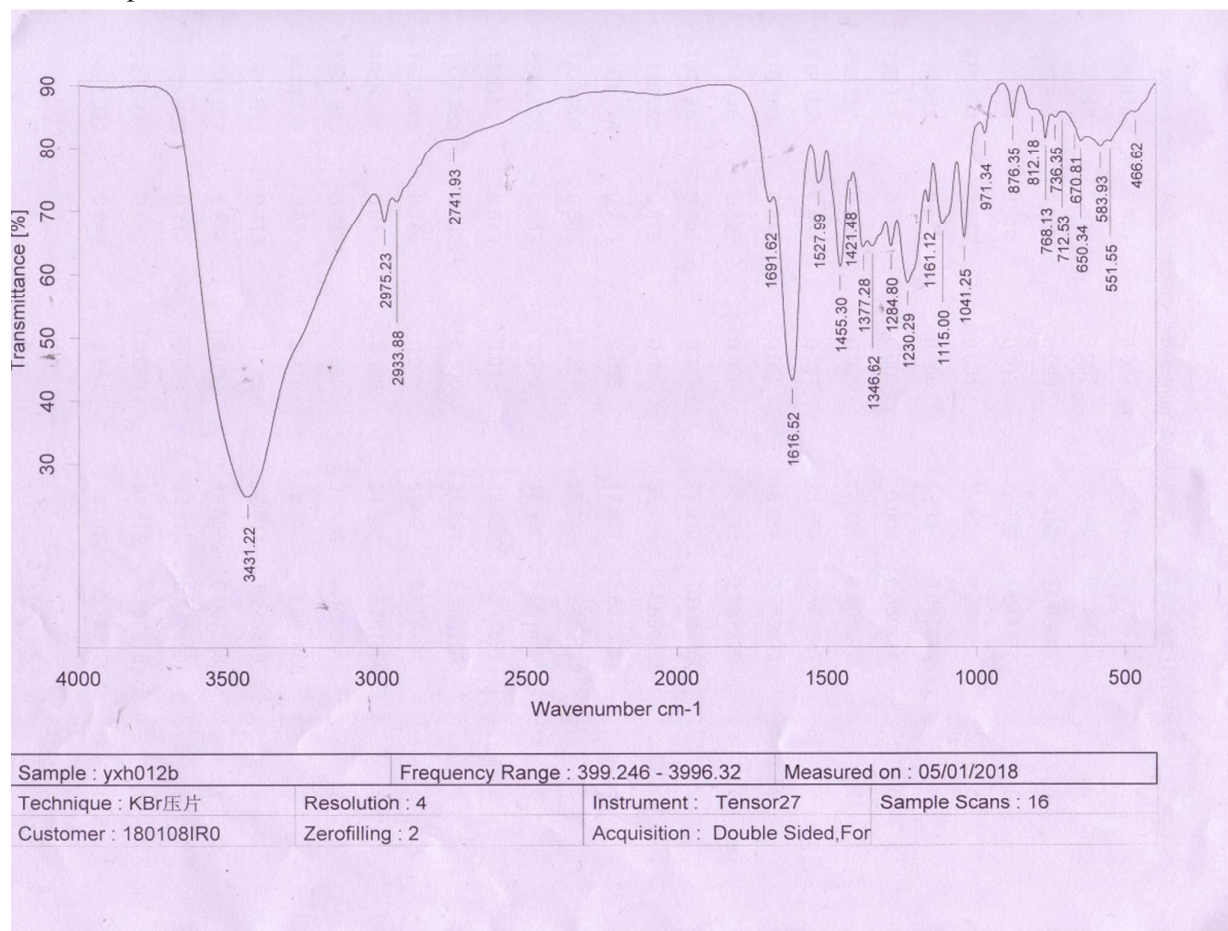
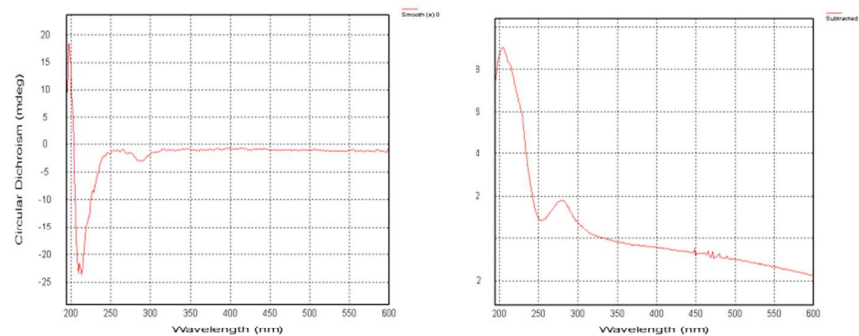


Figure S9. CD and UV spectra of compound **1** in MeOH

YXH012B1



File: CD YXH012B1-1mm(195-600)17031612.dsx

ProBinaryX

Attributes :

- Time Stamp :Thu Mar 16 19:33:53 2017

- File ID : {C3DEECDF-4C01-40a0-817E-FA120119646D}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.0717 mg/mL MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 600nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S10. OR of compound **1** in MeOH

Optical rotation measurement								
Model : P-1020 (A060460638)								
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	34 (1/3)	Sp.Rot	-198.0000	-0.0198 0.0000	17.6 10.00 Cell	Wed Jan 10 18:40:35 2018 0.001000g/mL MeOH YXH012B1	Na 589nm	2 sec 2 sec
No.2	34 (2/3)	Sp.Rot	-196.0000	-0.0196 0.0000	17.6 10.00 Cell	Wed Jan 10 18:40:40 2018 0.001000g/mL MeOH YXH012B1	Na 589nm	2 sec 2 sec
No.3	34 (3/3)	Sp.Rot	-204.0000	-0.0204 0.0000	17.6 10.00 Cell	Wed Jan 10 18:40:46 2018 0.001000g/mL MeOH YXH012B1	Na 589nm	2 sec 2 sec
average -199.3333°								

Figure S11. ^1H NMR spectrum of compound **2** in CD_3OD

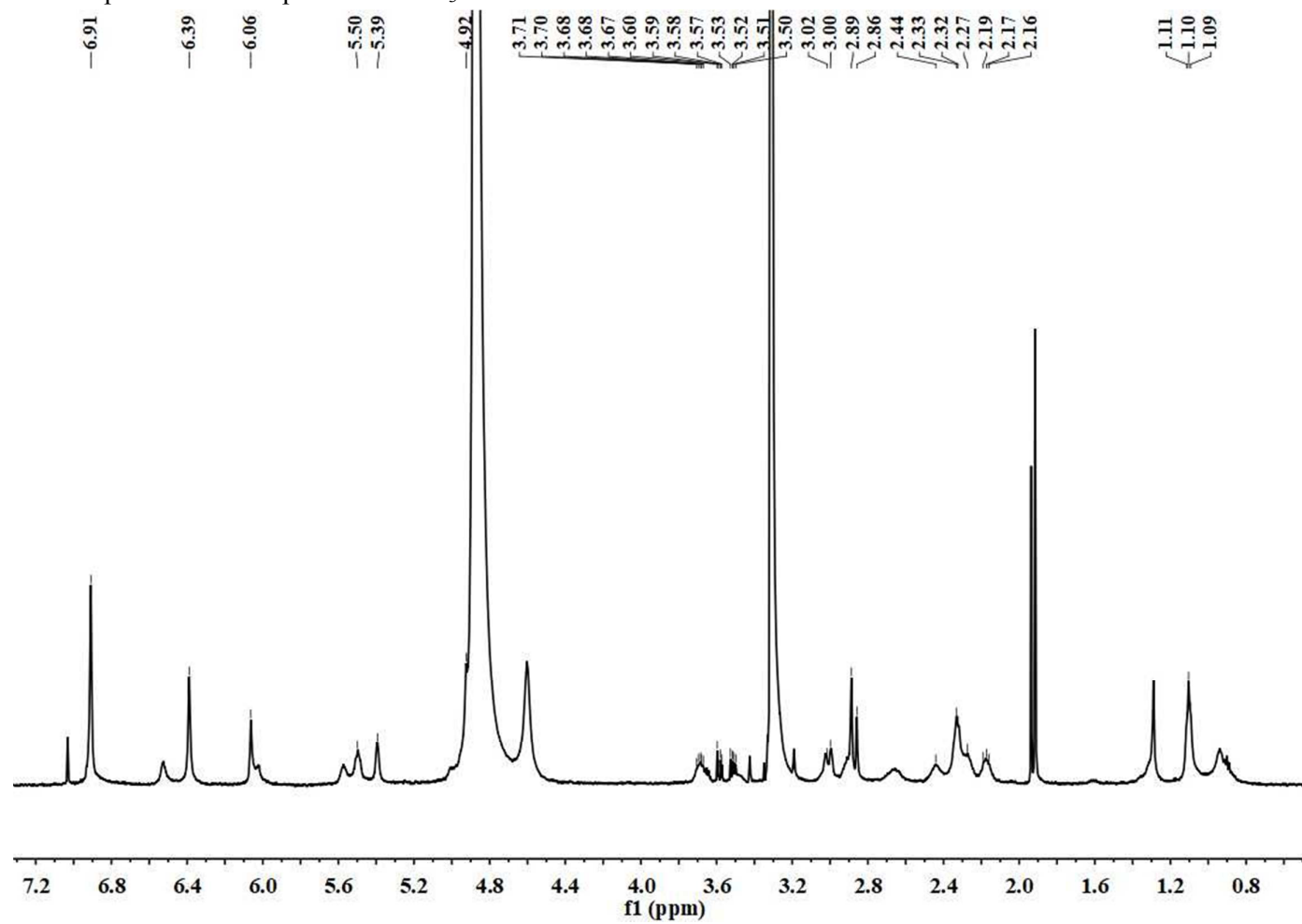


Figure S12. ^{13}C NMR spectrum of compound **2** in CD_3OD

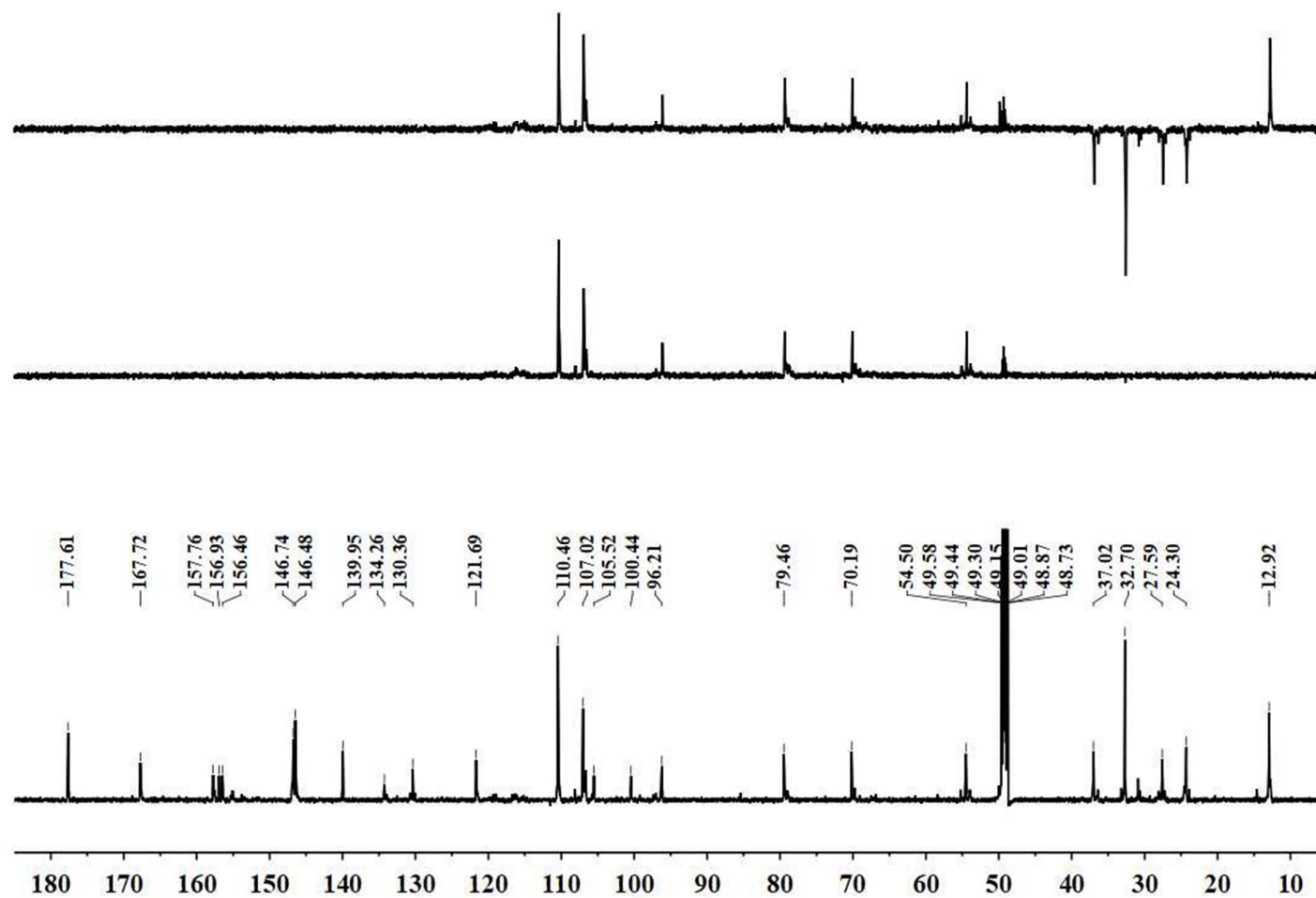


Figure S13. HMQC spectrum of compound **2** in CD₃OD

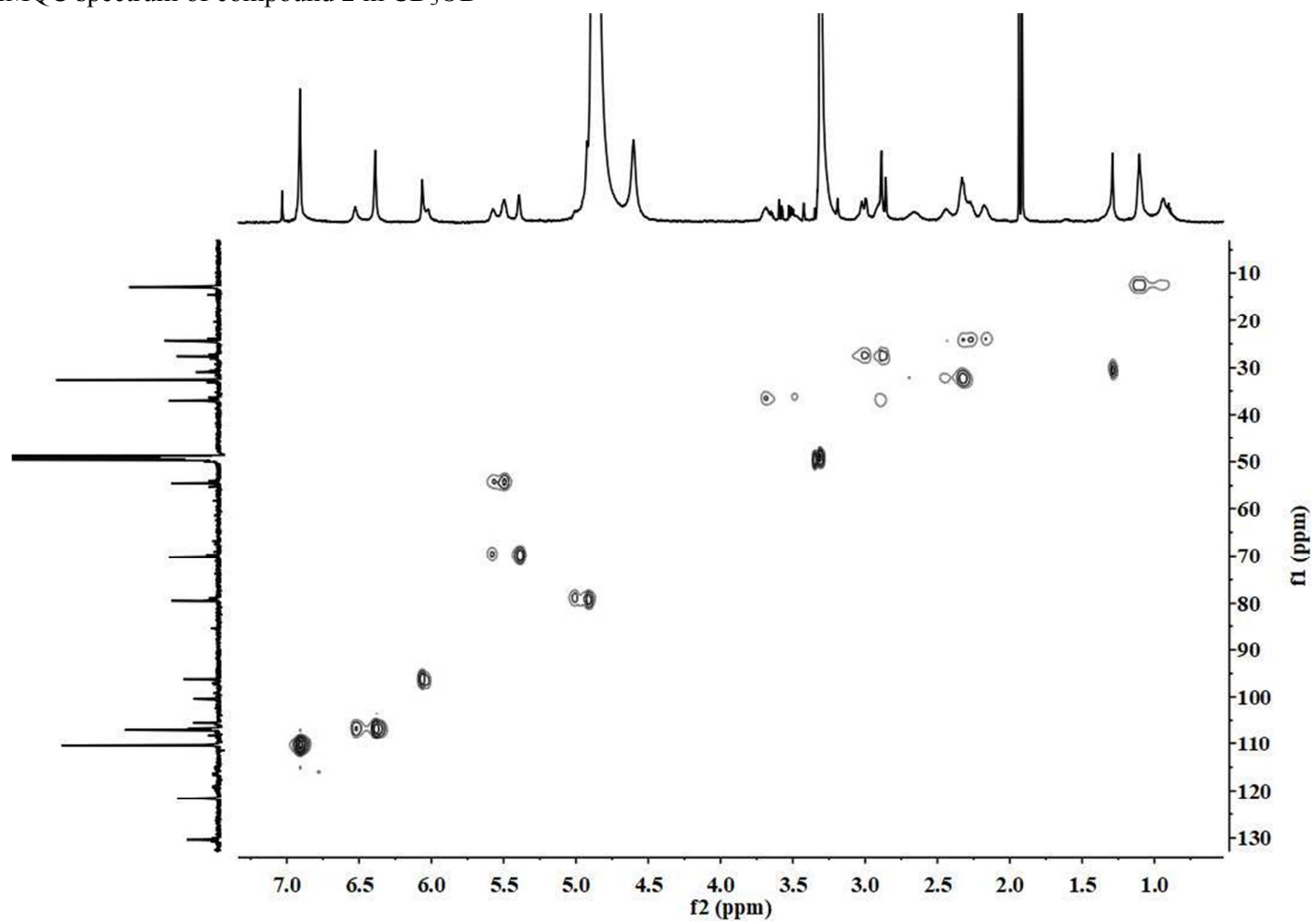


Figure S14. HMBC spectrum of compound **2** in CD₃OD

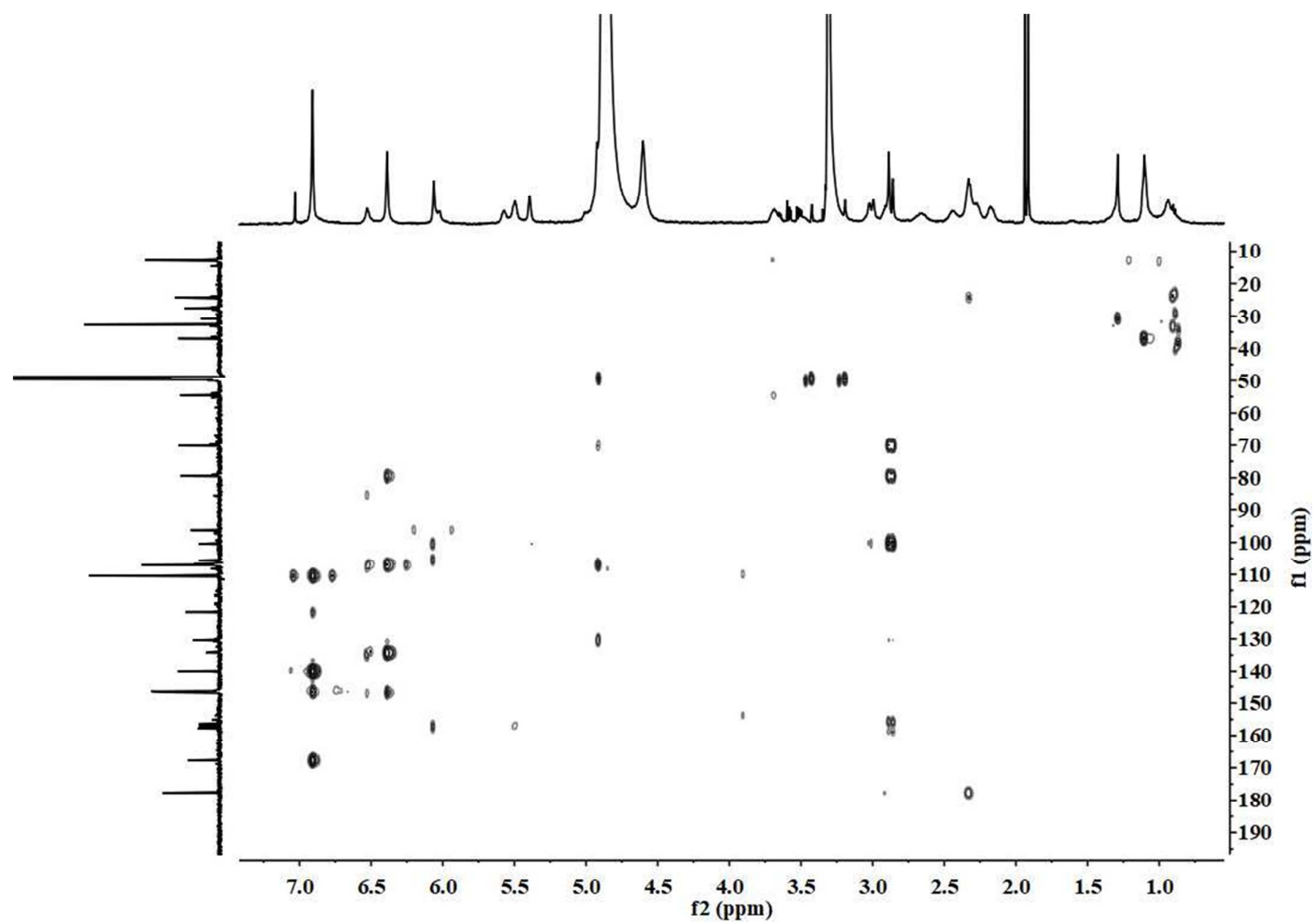
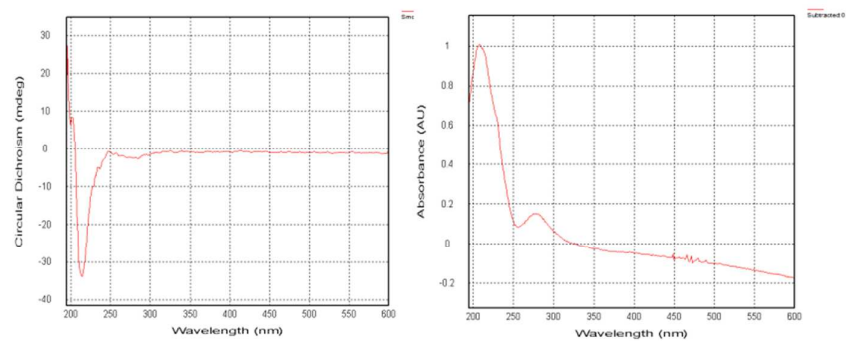


Figure S15. CD and UV spectra of compound **2** in MeOH

YFM048



File: CD YFM048-1mm(195-600)17031613.dsx

ProBinaryX

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- Time Stamp :Thu Mar 16 19:55:09 2017

- File ID : {1E793DD2-6828-49f4-B760-9F7124BBA2FB}

- Is CFR Compliant : false

- Original unaltered data

Remarks:

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.0694 mg/mL MeOH

- Pathlength: 1 mm

Settings:

- Time-per-point: 1s (25us x 40000)

- Wavelength: 195nm - 600nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S16. OR of compound **2** in MeOH

Optical rotation measurement								
Model : P-1020 (A060460638)								
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time
No.1	38 (1/3)	Sp.Rot	-234.0000	-0.0234 0.0000	17.7 10.00 Cell	Wed Jan 10 18:57:31 2018 0.001000g/mL MeOH YFM048	Na 589nm	2 sec 2 sec
No.2	38 (2/3)	Sp.Rot	-236.0000	-0.0236 0.0000	17.6 10.00 Cell	Wed Jan 10 18:57:36 2018 0.001000g/mL MeOH YFM048	Na 589nm	2 sec 2 sec
No.3	38 (3/3)	Sp.Rot	-233.0000	-0.0233 0.0000	17.6 10.00 Cell	Wed Jan 10 18:57:42 2018 0.001000g/mL MeOH YFM048	Na 589nm	2 sec 2 sec
Average -234.3333								

Figure S17. ^1H NMR spectrum of compound **3** in CD_3OD

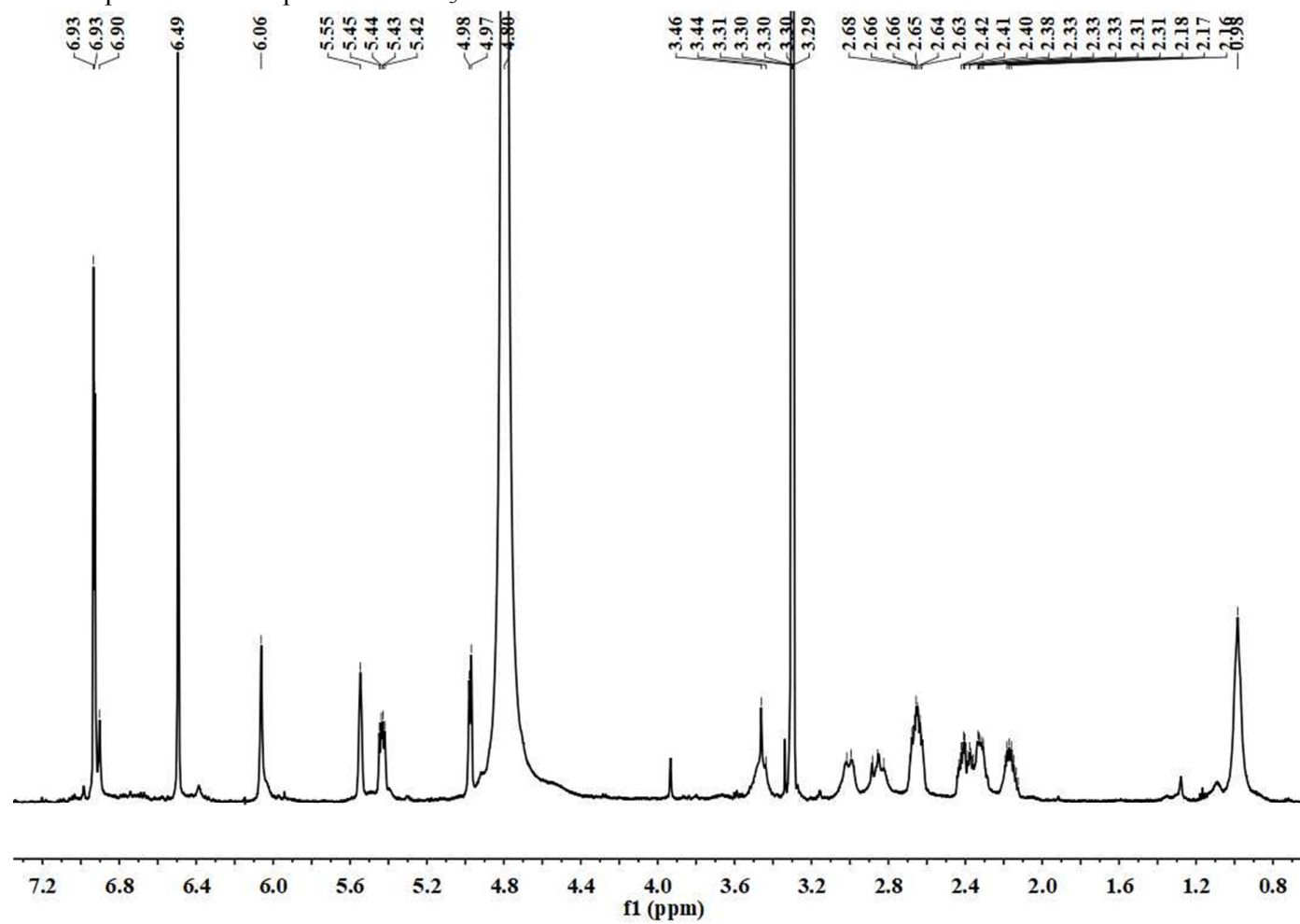


Figure S18. ^{13}C NMR spectrum of compound **3** in CD_3OD

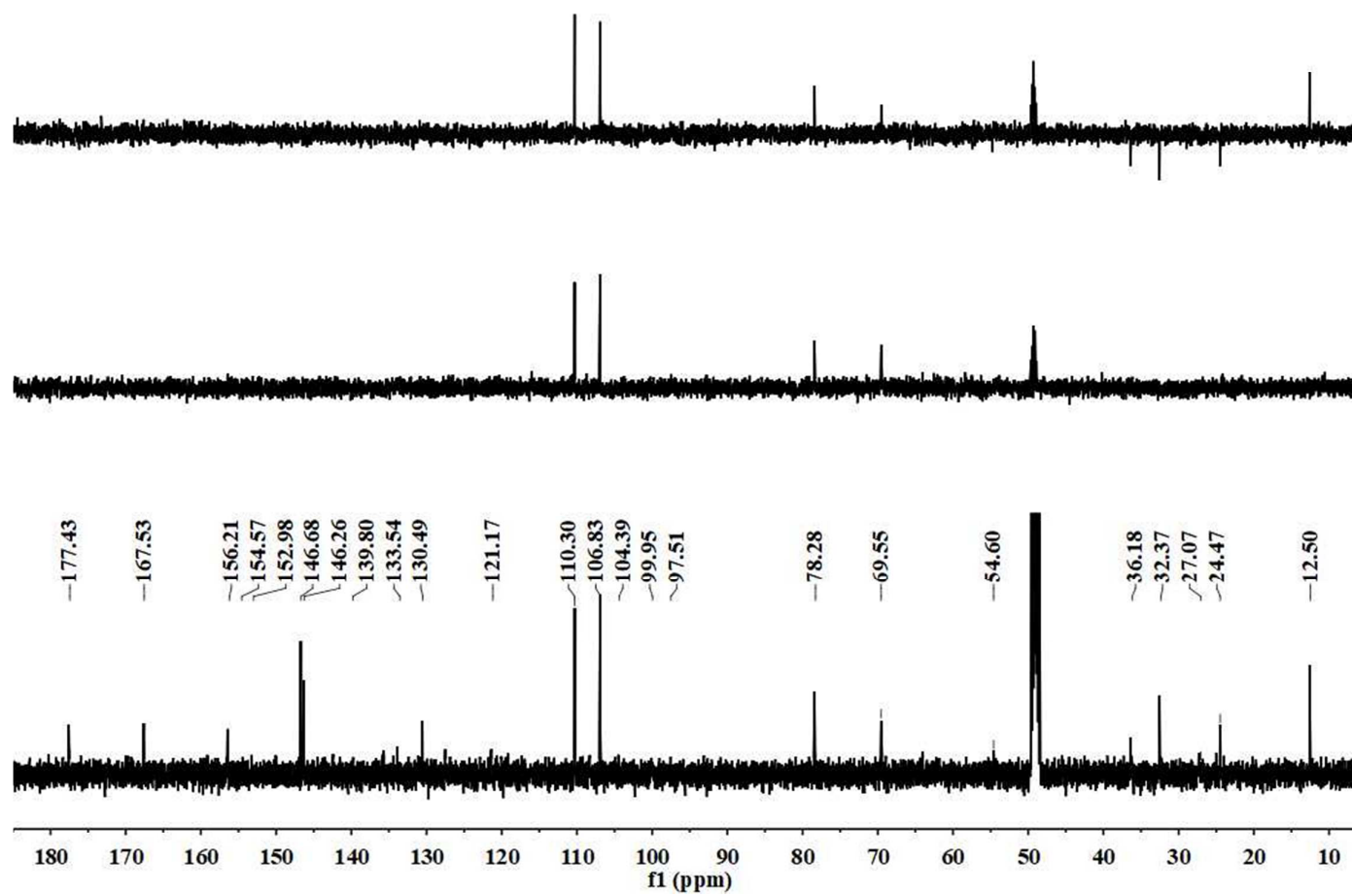


Figure S19. HMQC spectrum of compound **3** in CD₃OD

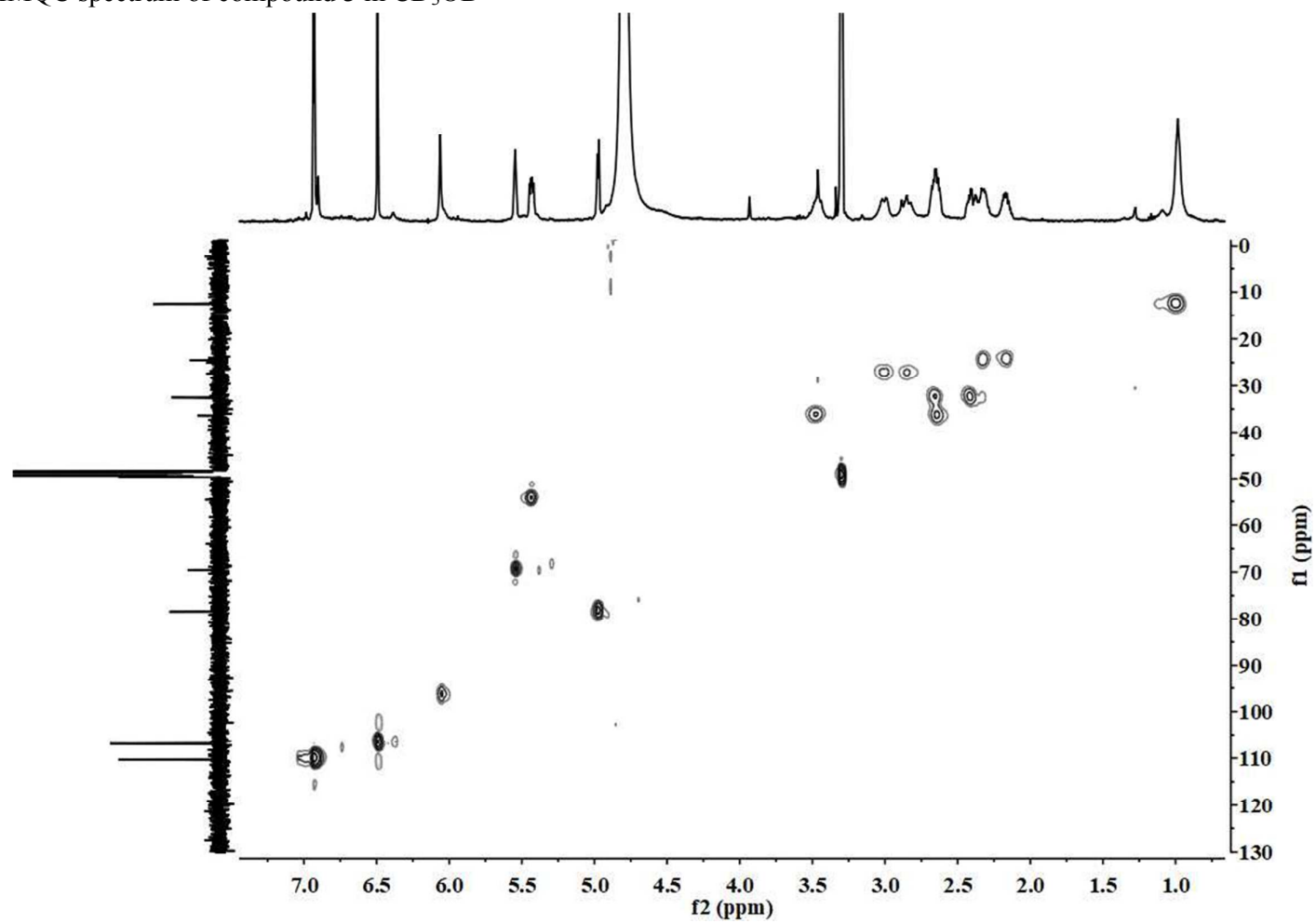


Figure S20. HMBC spectrum of compound **3** in CD₃OD

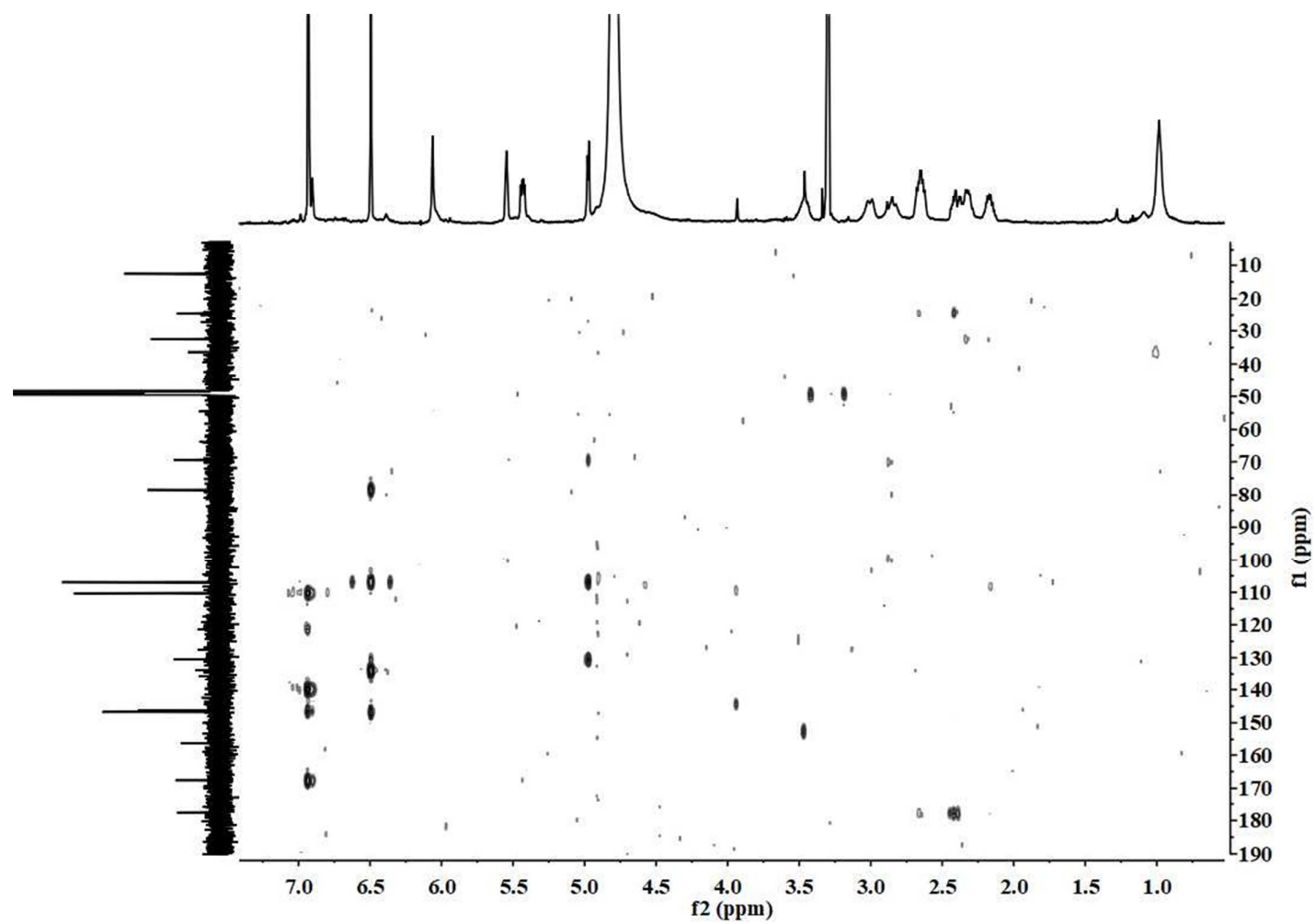
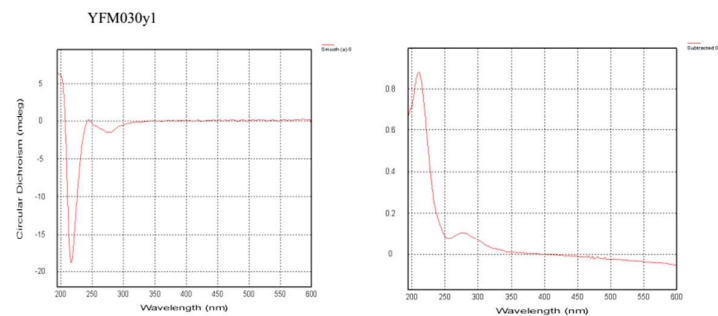


Figure S21. CD and UV spectra of compound **3** in MeOH



File: CD YFM030Y1-1mm(195-600)18050504.dsx

ProBinaryX

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- Time Stamp :Sat May 05 13:47:50 2018

- File ID : {CE74F7EC-45AA-4981-8180-15200C8DA49D}

- Is CFR Compliant : false

- Original data has not been modified.

Remarks:

- User: APLService

- Date: 2018/05/05

- Instrument: 0218

- DetectorType: PMT

- DichOS Calibration Correction Curve: 0218/1

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.0816mg/mL MeOH

- Pathlength: 1 mm

- Temperature: 20°C

Settings:

- Time-per-point: 1s (25us x 40000)

- SE

- Wavelength: 195nm - 600nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S22. OR of compound **3** in MeOH

Optical rotation measurement									
Model : P-1020 (A060460638)									
No.	Sample	Mode	Data	Monitor Blank	Temp. Cell Temp Point	Date Comment Sample Name	Light Filter Operator	Cycle Time Integ Time	
No.1	24 (1/3)	Sp.Rot	28.3330	0.0017 0.0000	19.7 10.00	Wed Jan 17 04:07:44 2018 0.0006g/mL MeOH yfm030y1	Na 589nm	2 sec 2 sec	
No.2	24 (2/3)	Sp.Rot	21.6670	0.0013 0.0000	19.7 10.00	Wed Jan 17 04:07:49 2018 0.0006g/mL MeOH yfm030y1	Na 589nm	2 sec 2 sec	
No.3	24 (3/3)	Sp.Rot	23.3330	0.0014 0.0000	19.7 10.00	Wed Jan 17 04:07:54 2018 0.0006g/mL MeOH yfm030y1	Na 589nm	2 sec 2 sec	
Average +24.4444°									

Figure S23. Circular dichroism (CD) spectra of **1a** and **1b**, **2**, **3**, ECG and EGCG in MeOH

