Supporting information

for

Cuevaenes C–E: Three new triene carboxylic derivatives from *Streptomyces* sp. LZ35Δ*gdmAI*

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[§]These two authors contributed equally to this work.

Spectroscopic data and other relevant information for cuevaenes A–E (1–5)

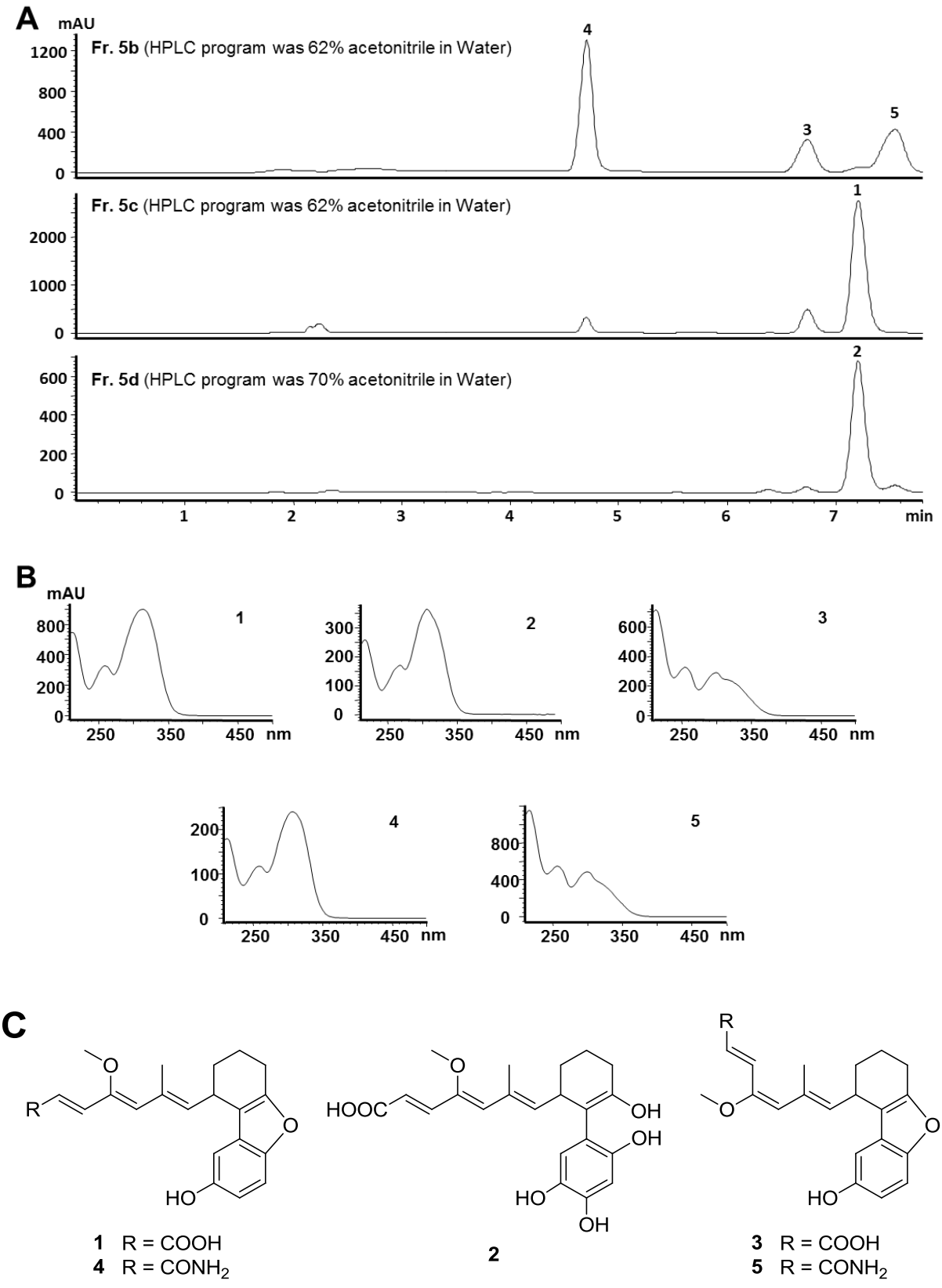

Figure S1: A: HPLC analysis of the constituents of Fr. 5b, Fr.5c and Fr.5d (HPLC were performed on an Agilent 1260 equipped with a YMC-C18 5 μm column (4.6 × 250 mm) and detected at 274 nm on a UV detector. **B**: Ultraviolet absorption curve of compounds **1–5**. **C**: Chemical structure of compounds **1–5**.

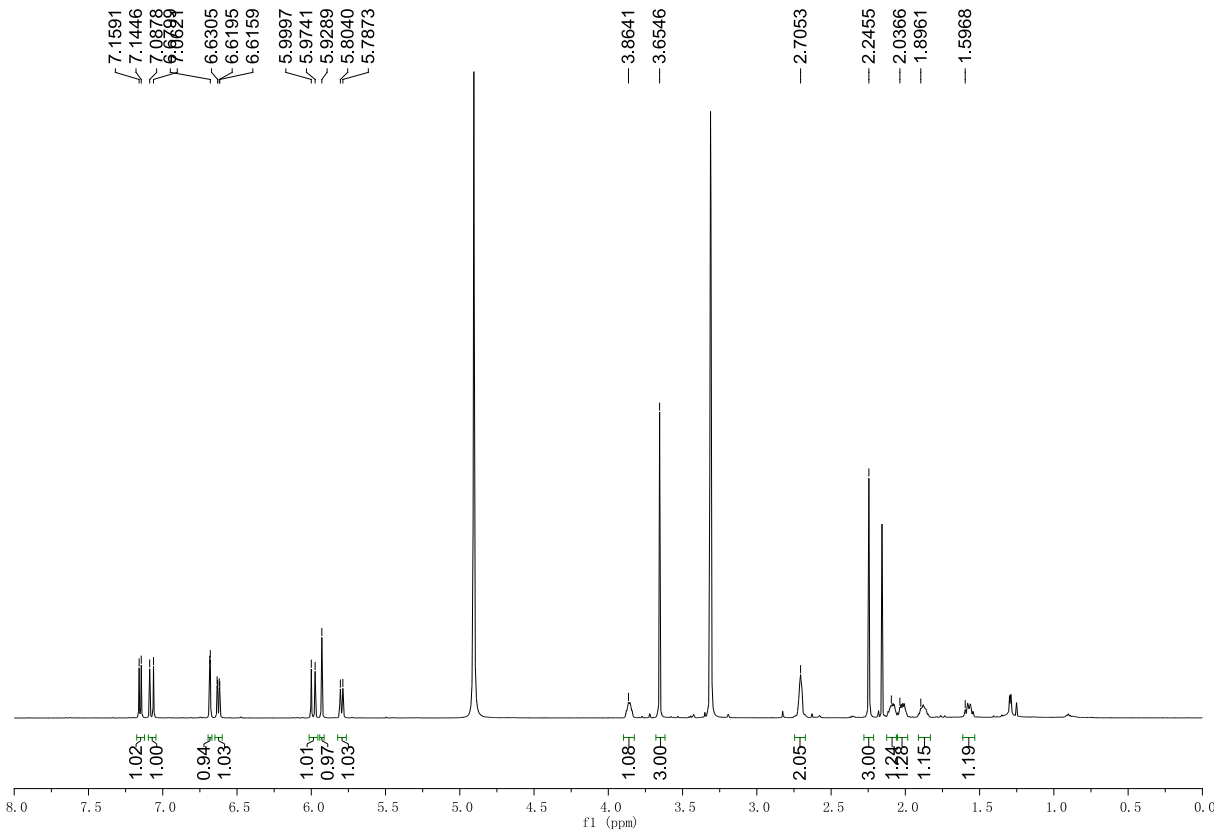

Figure S2: ^{1}H NMR (600 MHz, CD_3OD) spectrum for compound **1**.

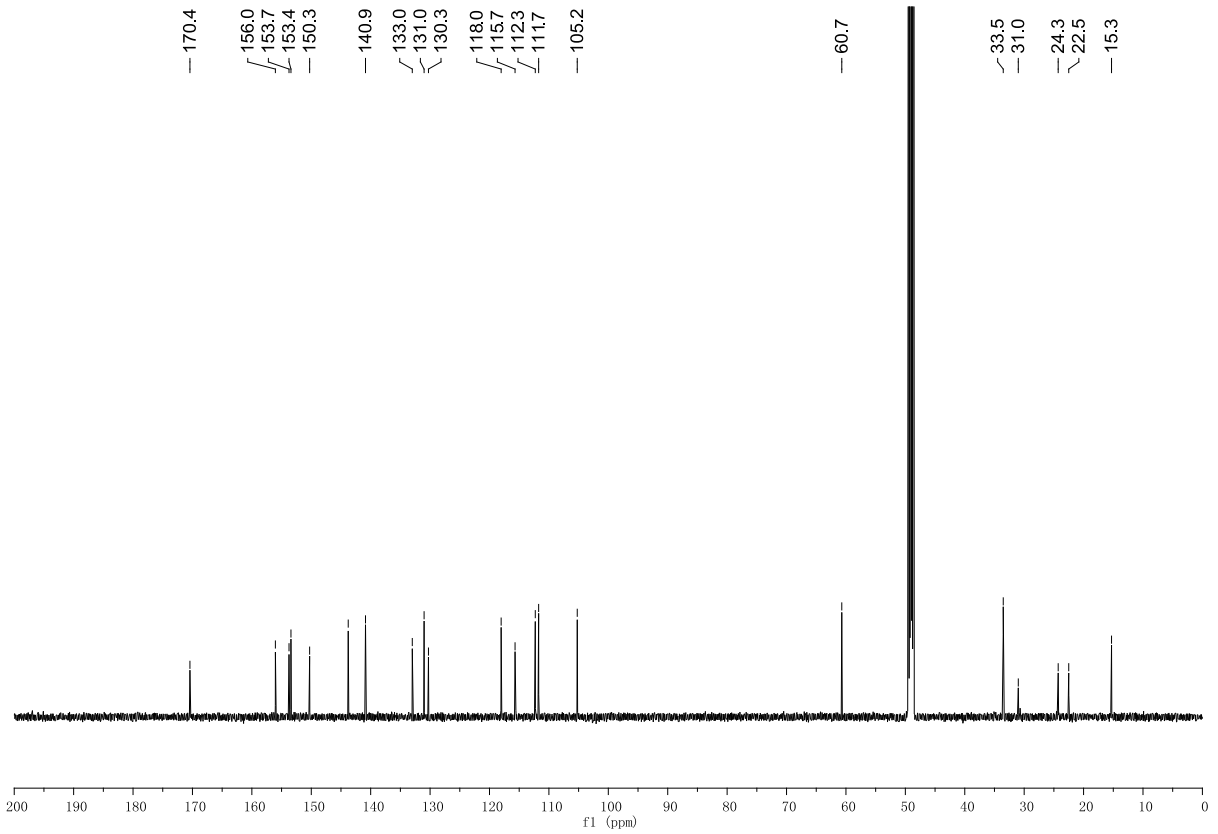

Figure S3: ^{13}C NMR (151 MHz, CD3OD) spectrum for compound **1**.

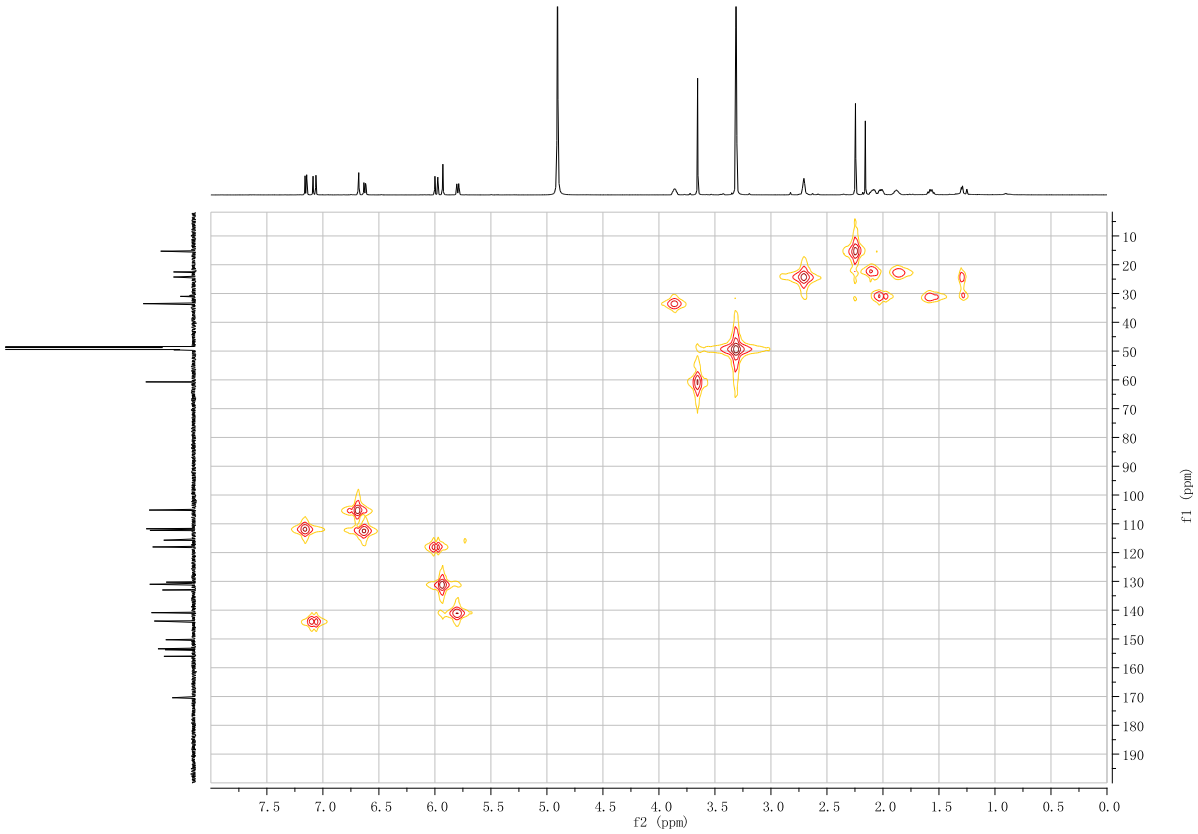

Figure S4: The HSQC spectrum for compound **1**.

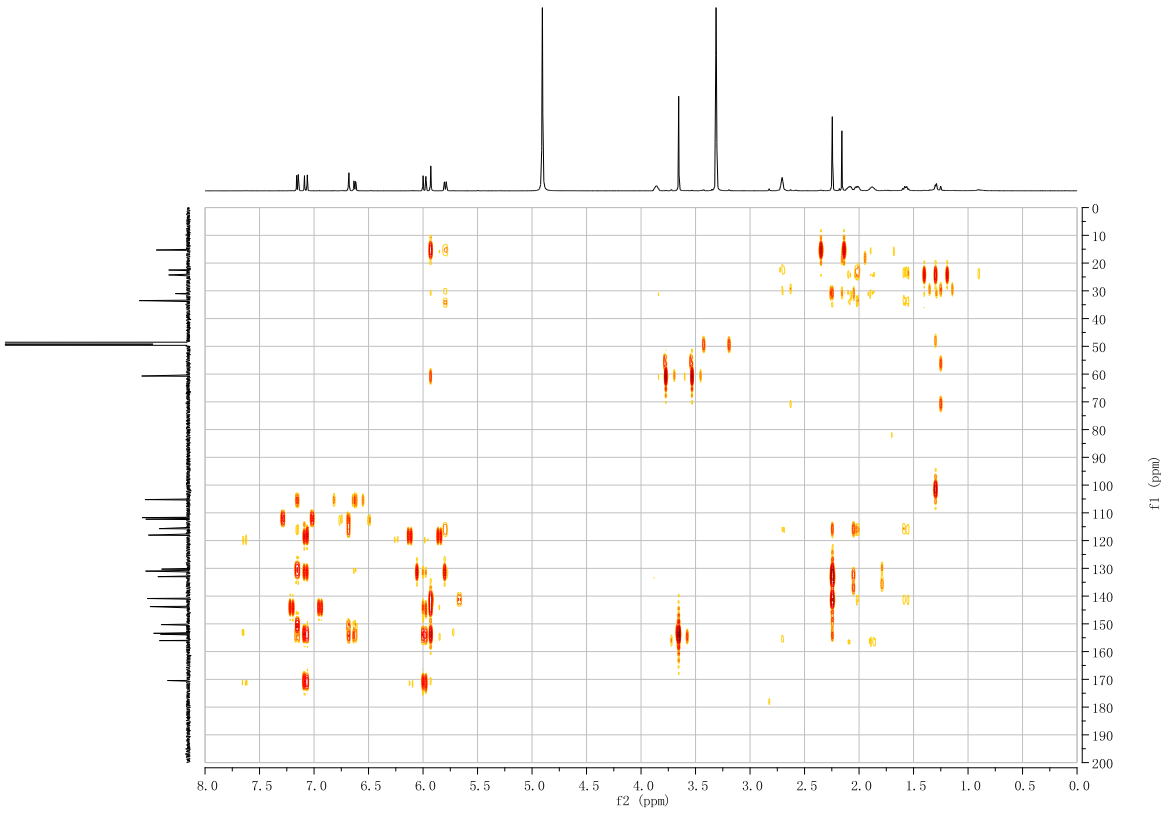

Figure S5: The HMBC spectrum for compound **1**.

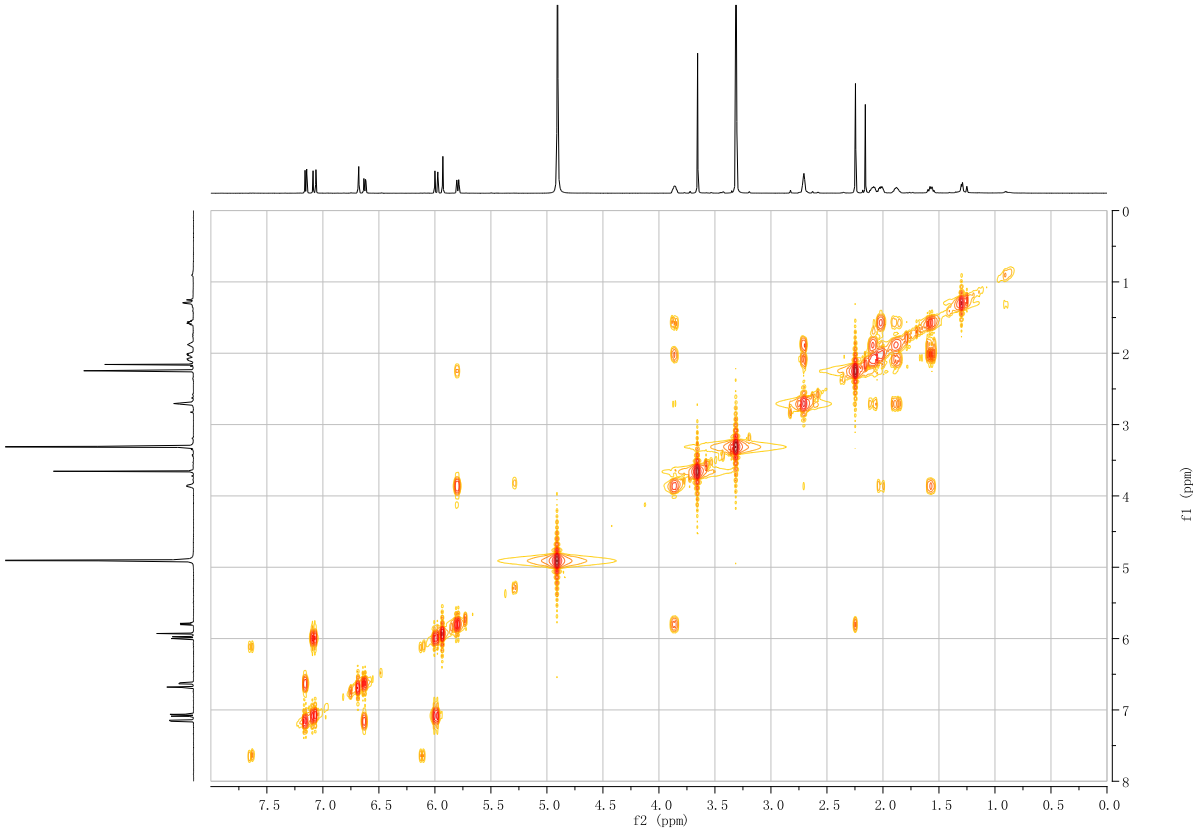

Figure S6: $^{1}H/^{1}H$ COSY spectrum for compound **1**.

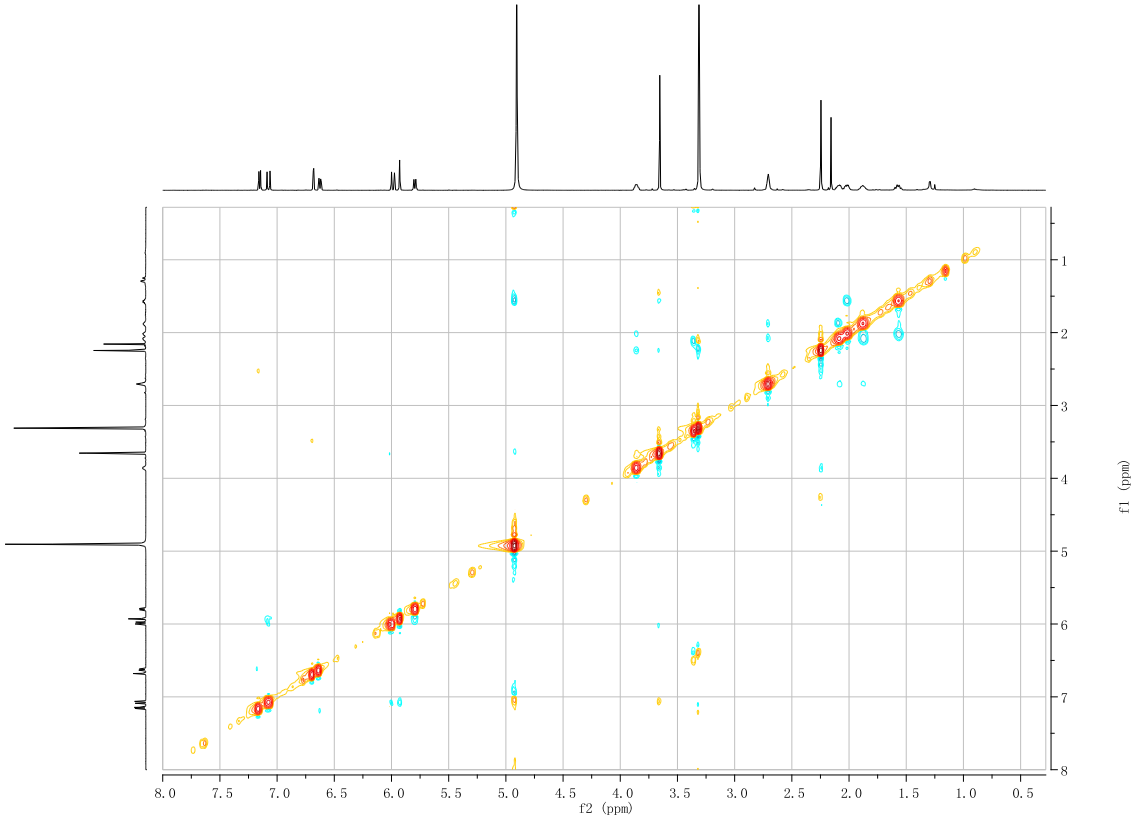

Figure S7: The NOE spectrum for compound **1**.

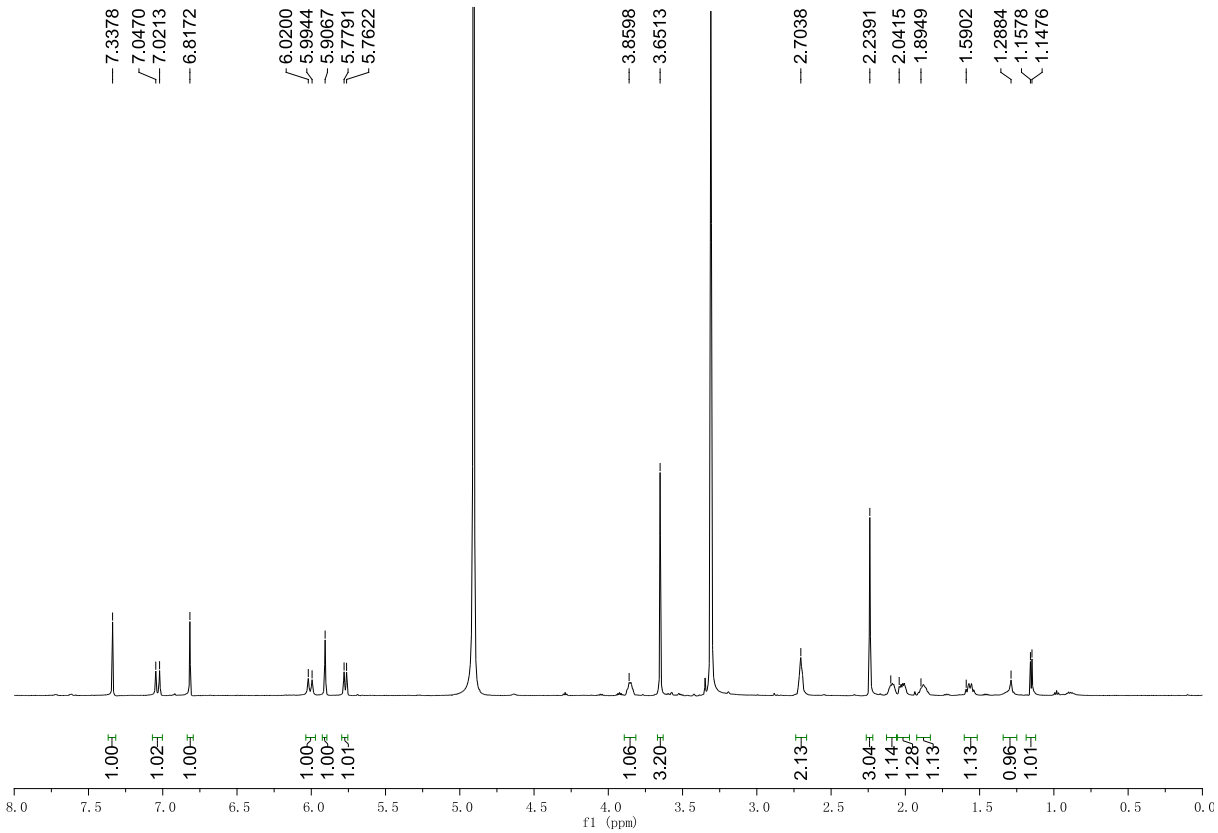

Figure S8: ^{1}H NMR (600 MHz, CD_3OD) spectrum for compound **2**.

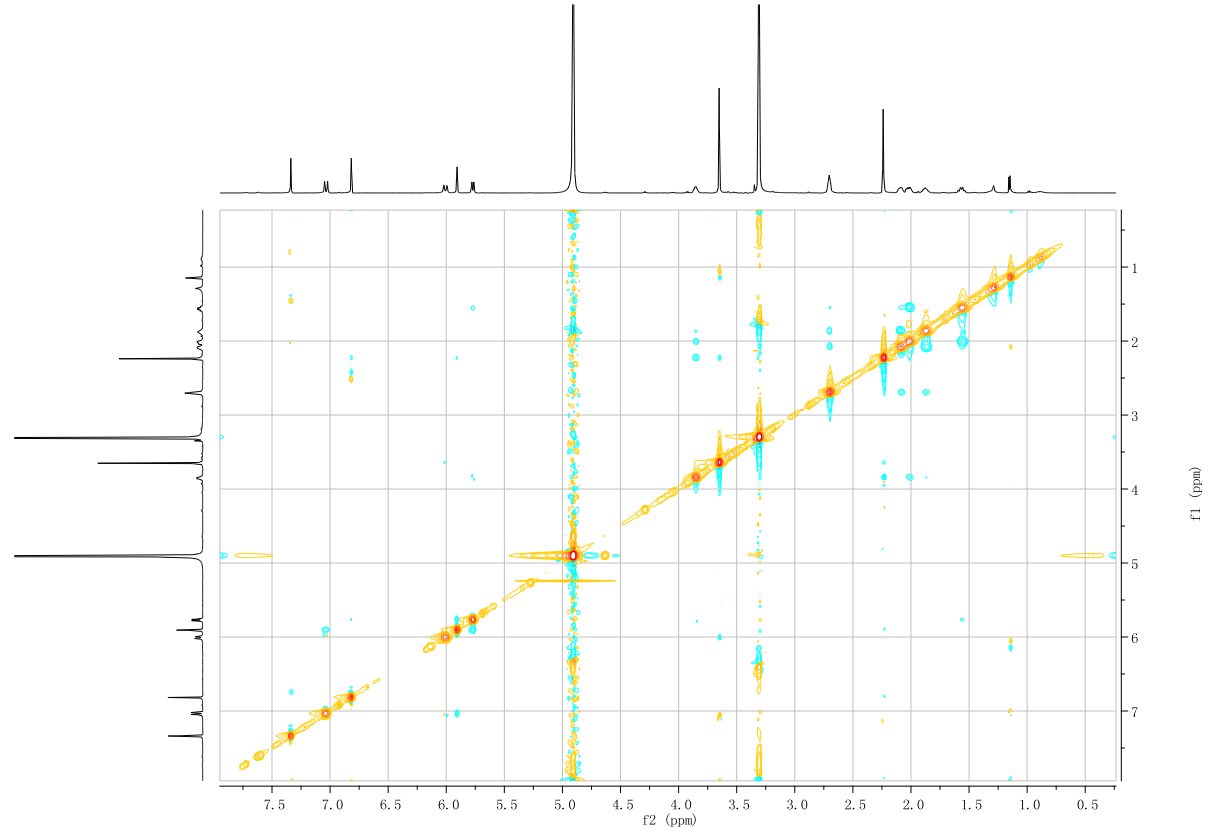

Figure S9: The NOE spectrum for compound **2**.

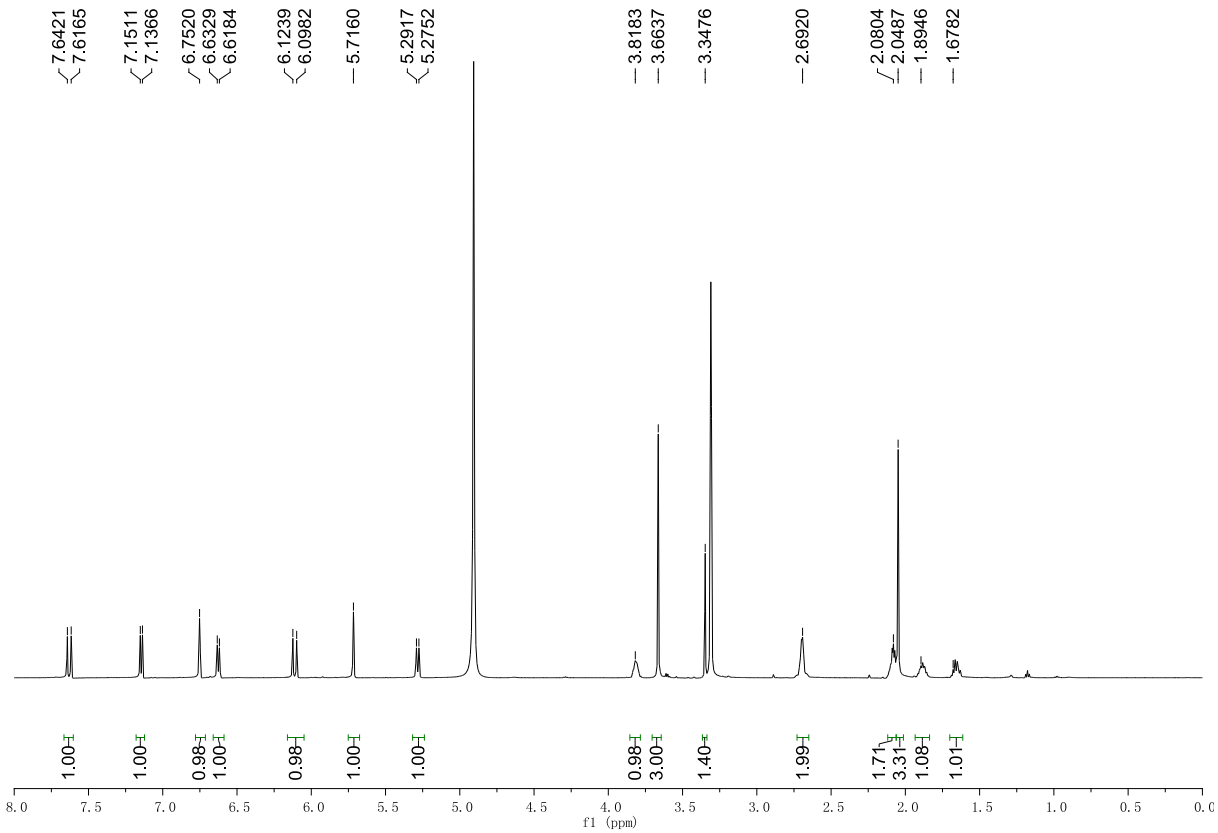

Figure S10: ^{1}H NMR (600 MHz, CD_3OD) spectrum for compound **3**.

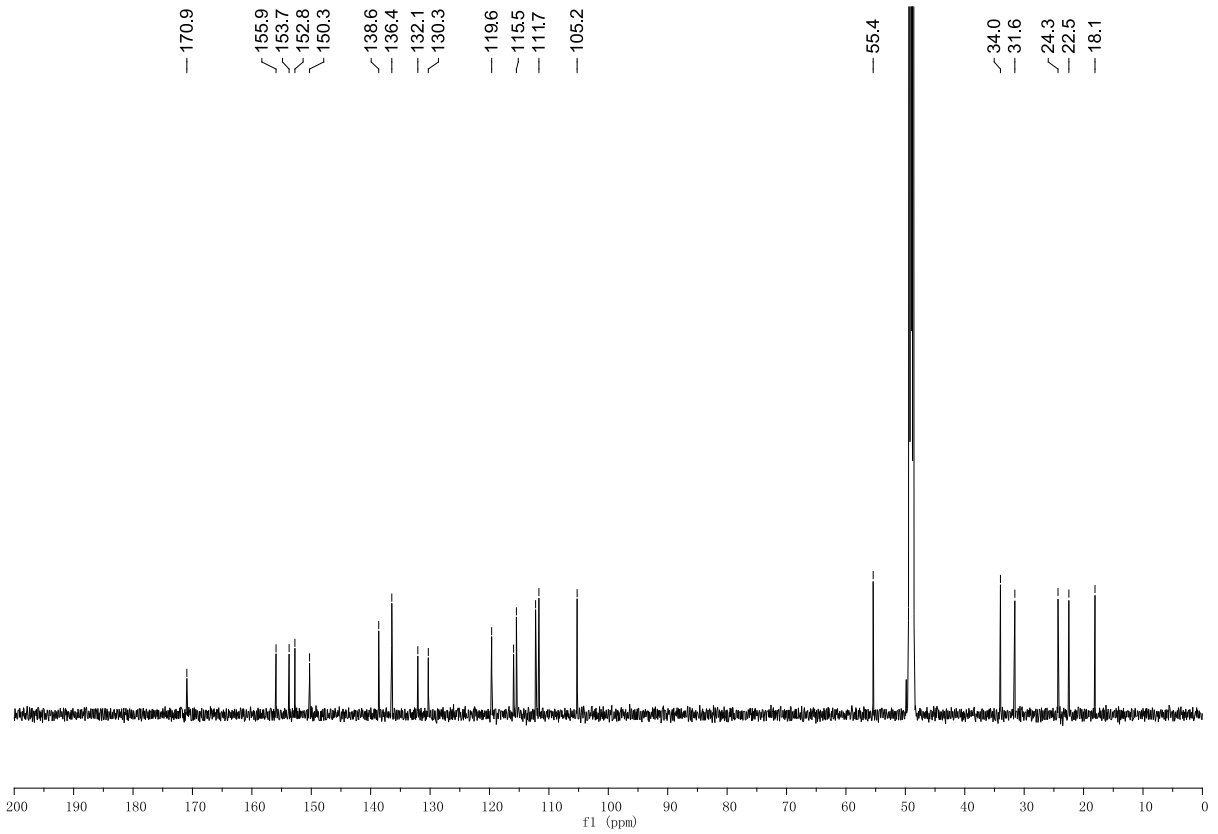

Figure S11. ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **3**.

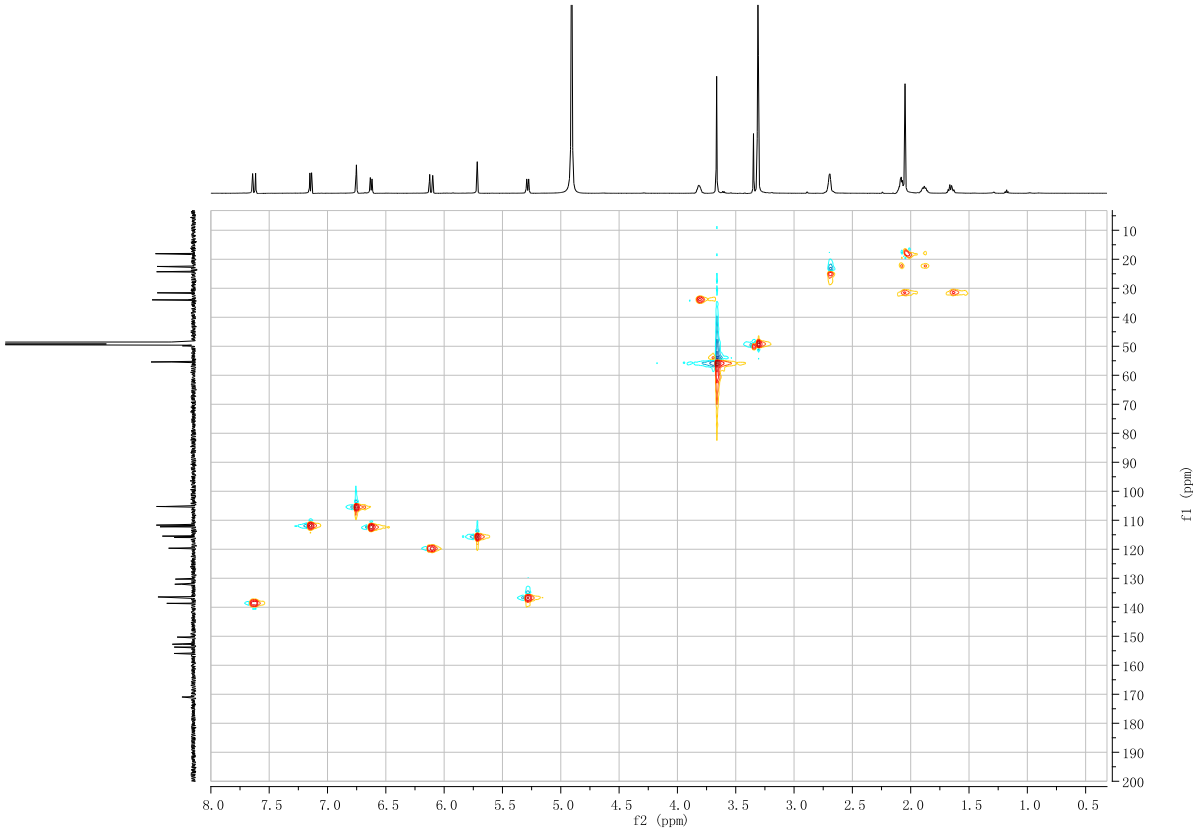

Figure S12: The HSQC spectrum for compound **3**.

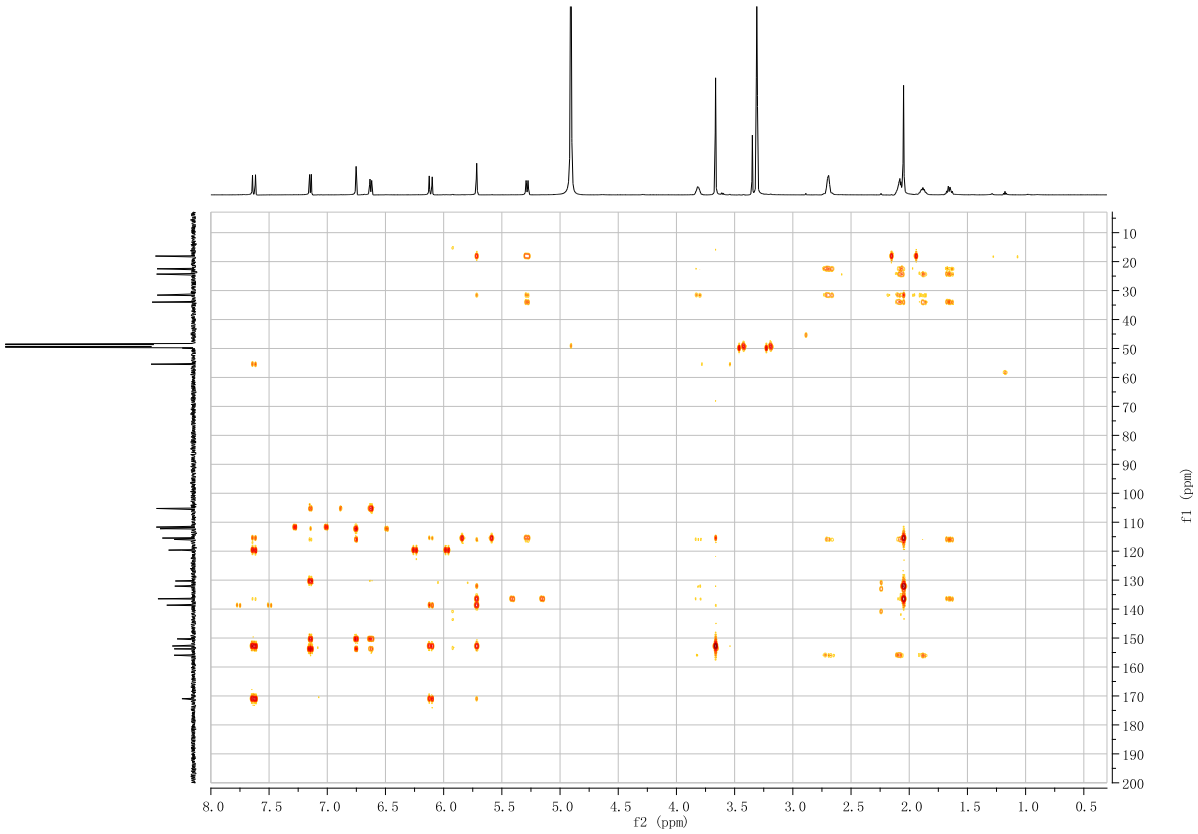

Figure S13: The HMBC spectrum for compound **3**.

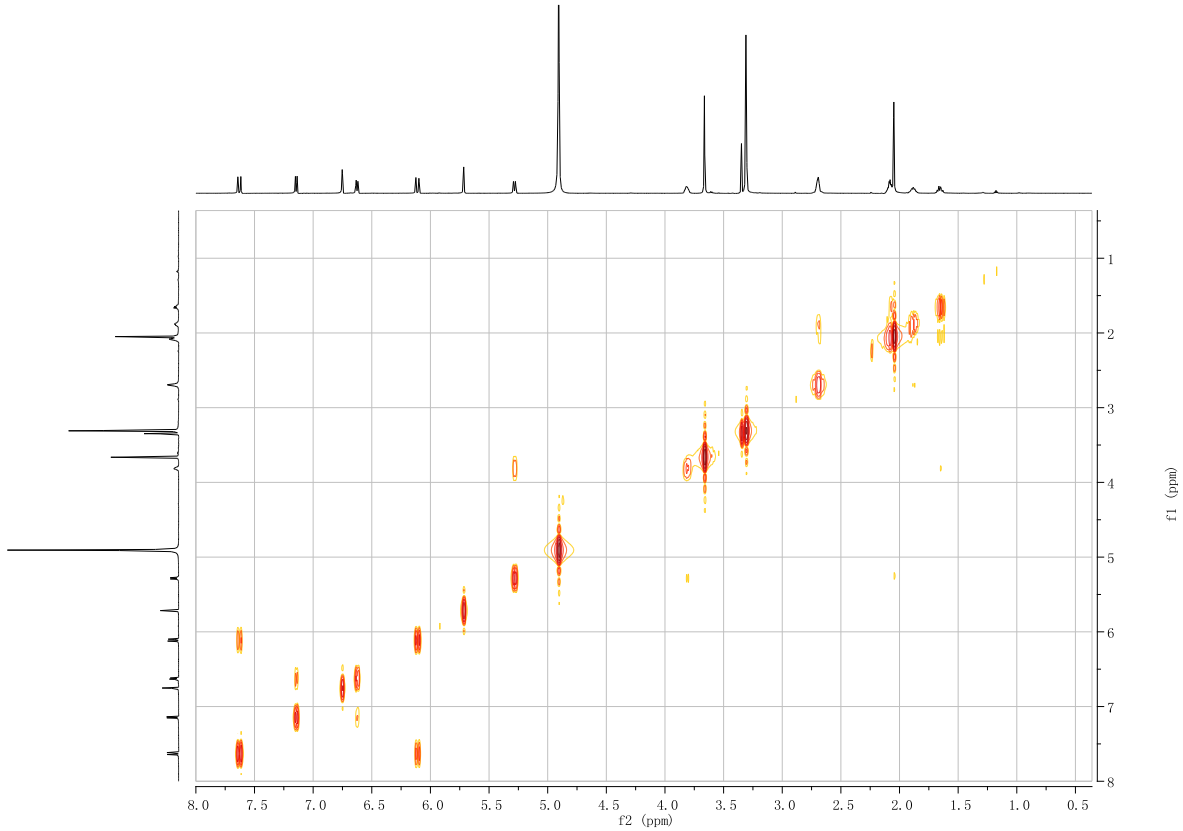

Figure S14: $^{1}H/^{1}H$ COSY spectrum for compound **3**.

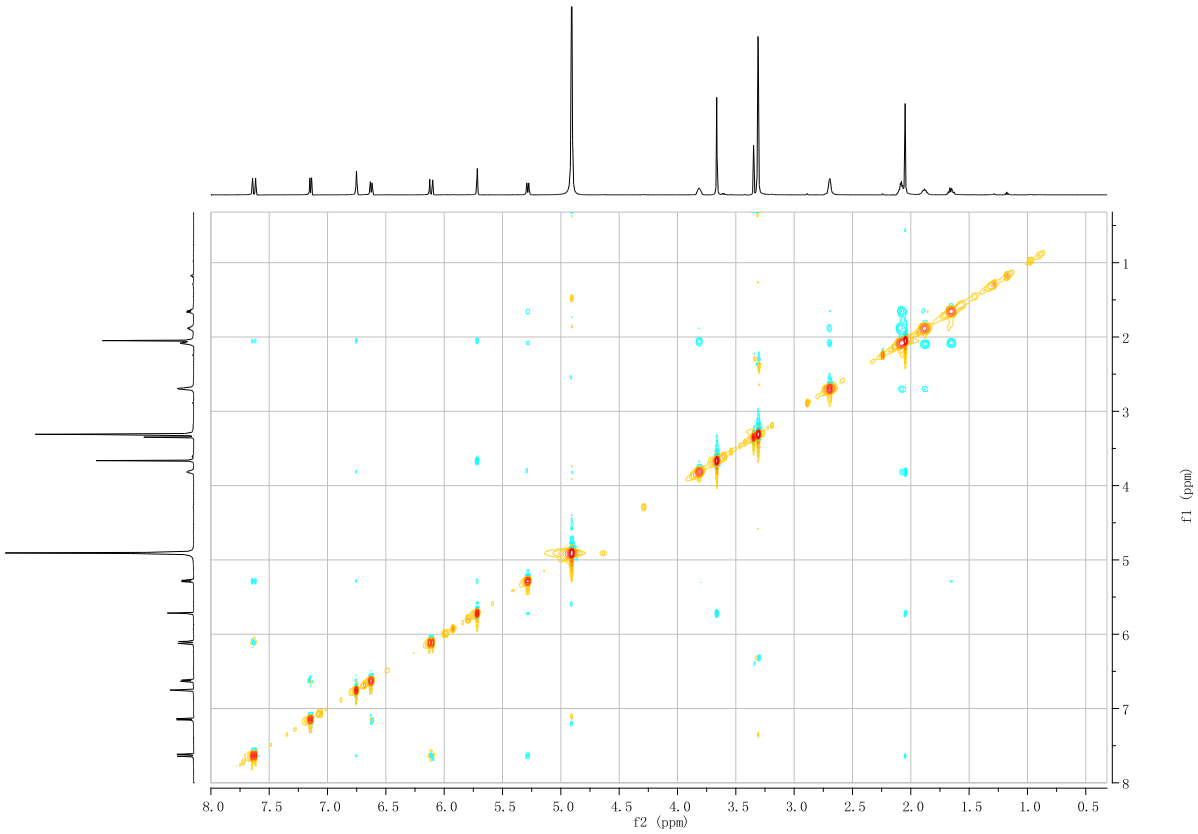

Figure S15: The NOE spectrum for compound **3**.

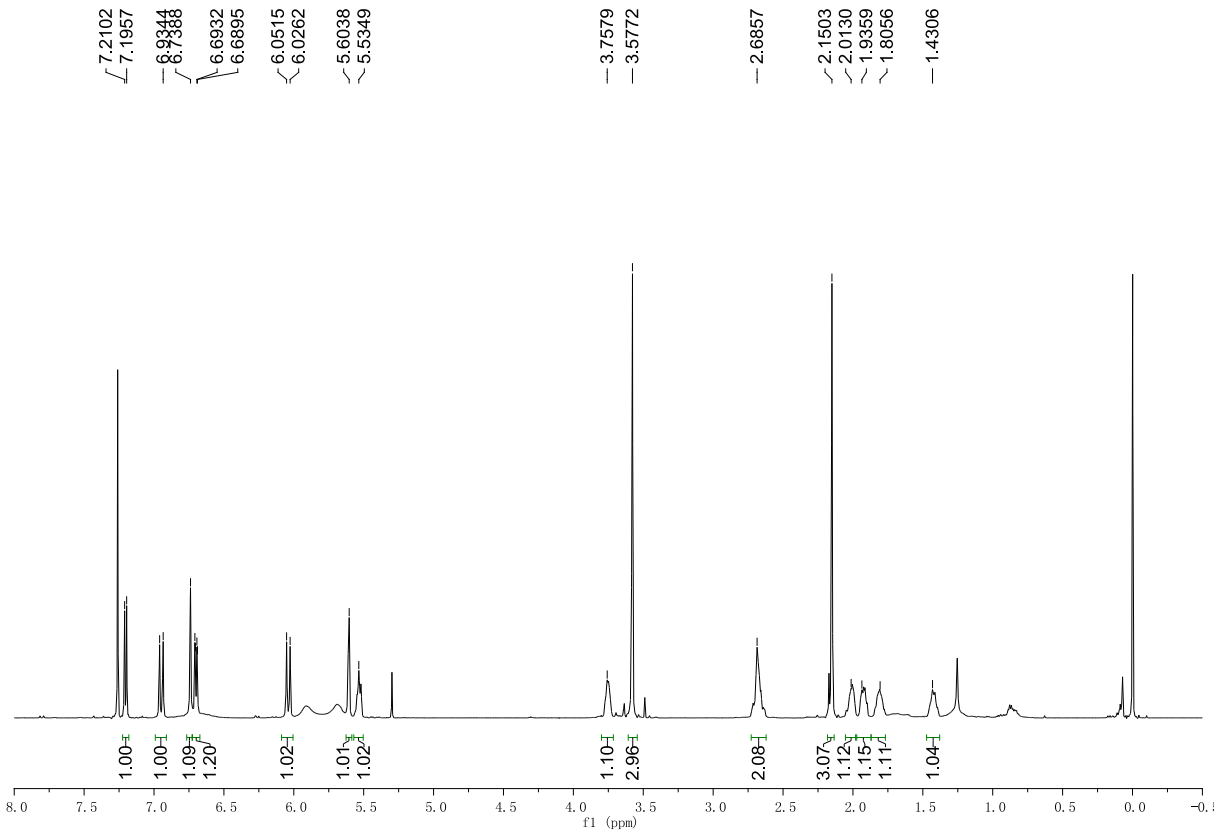

Figure S16: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum for compound **4**.

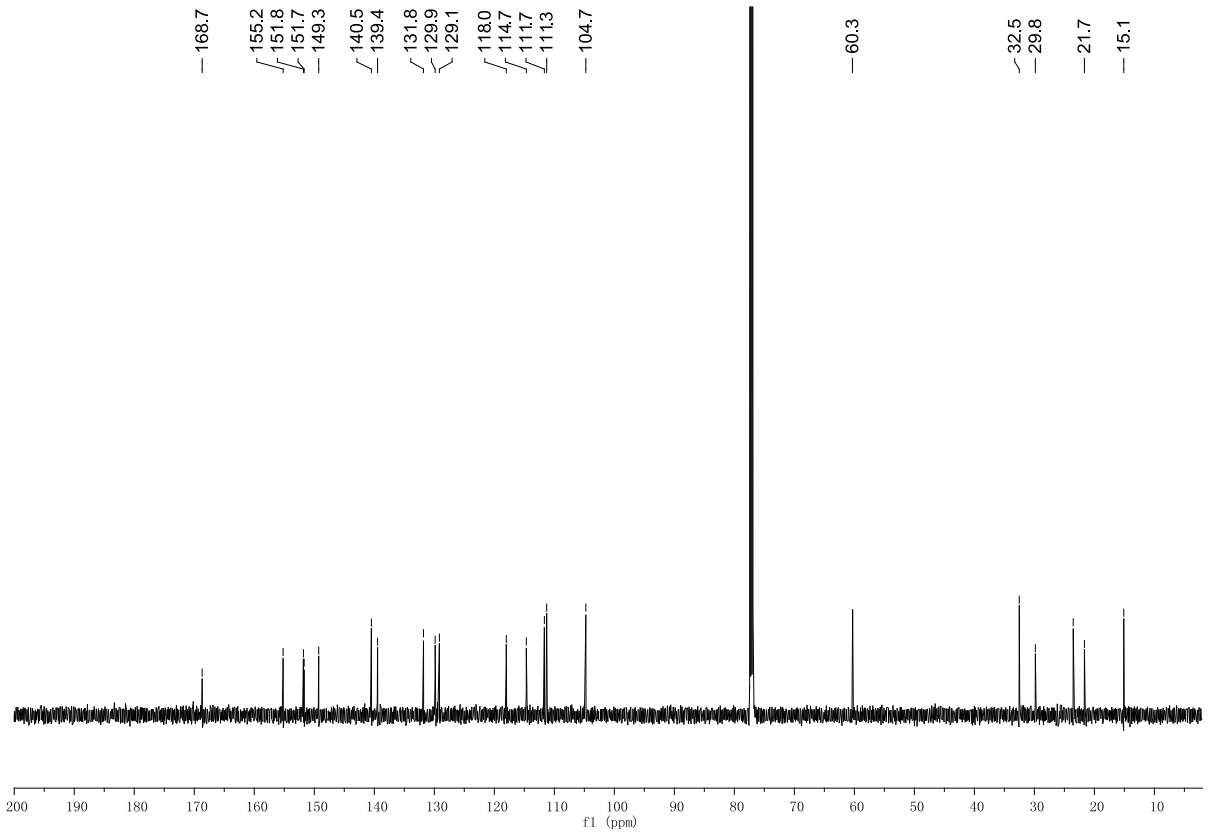

Figure S17: ^{13}C NMR (151 MHz, $CDCl_3$) spectrum for compound **4**.

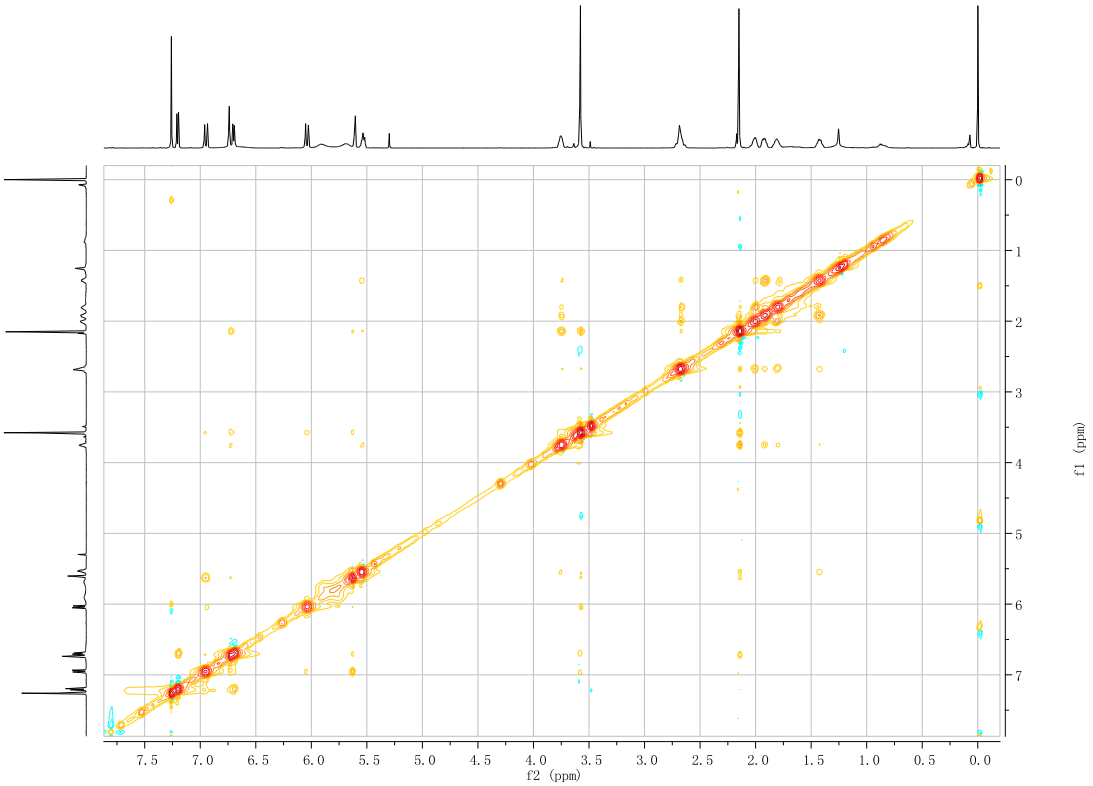

Figure S18: The NOE spectrum for compound **4**.

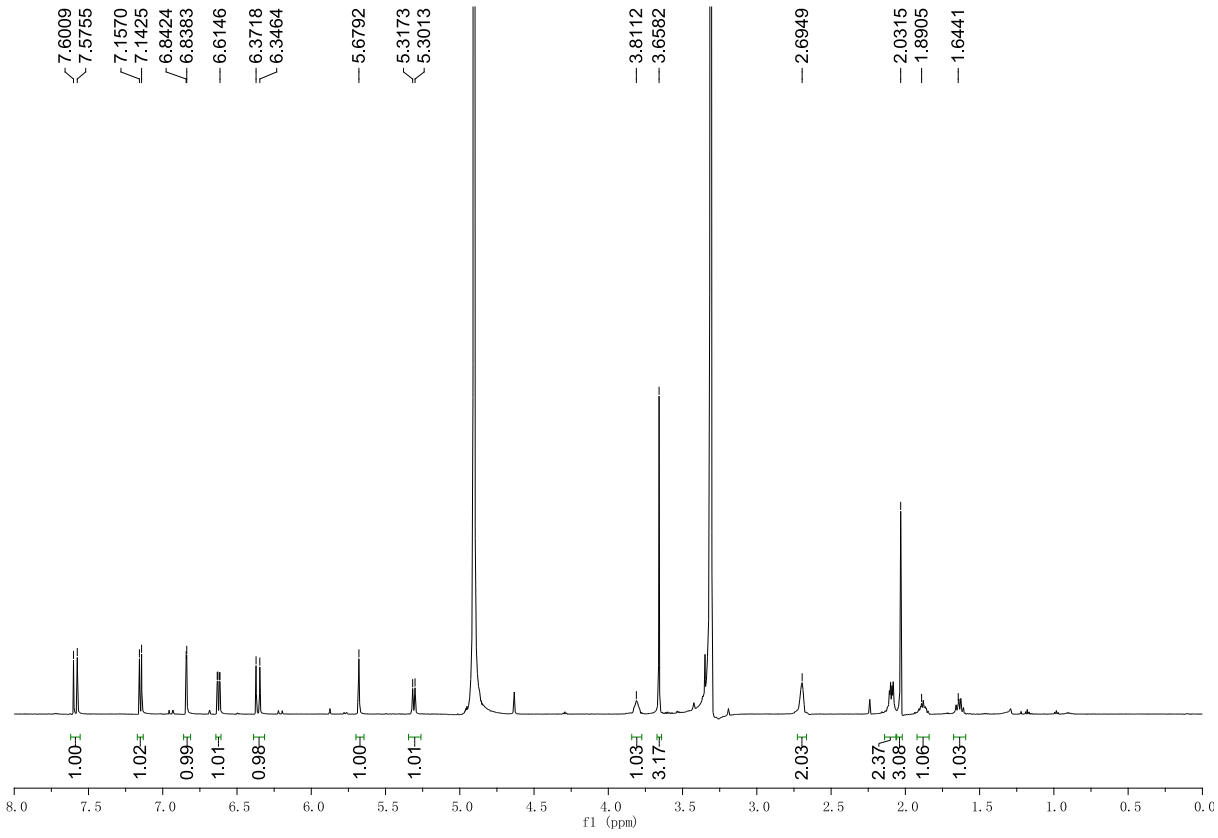

Figure S19: ^{1}H NMR (600 MHz, CD_3OD) spectrum for compound **5**.

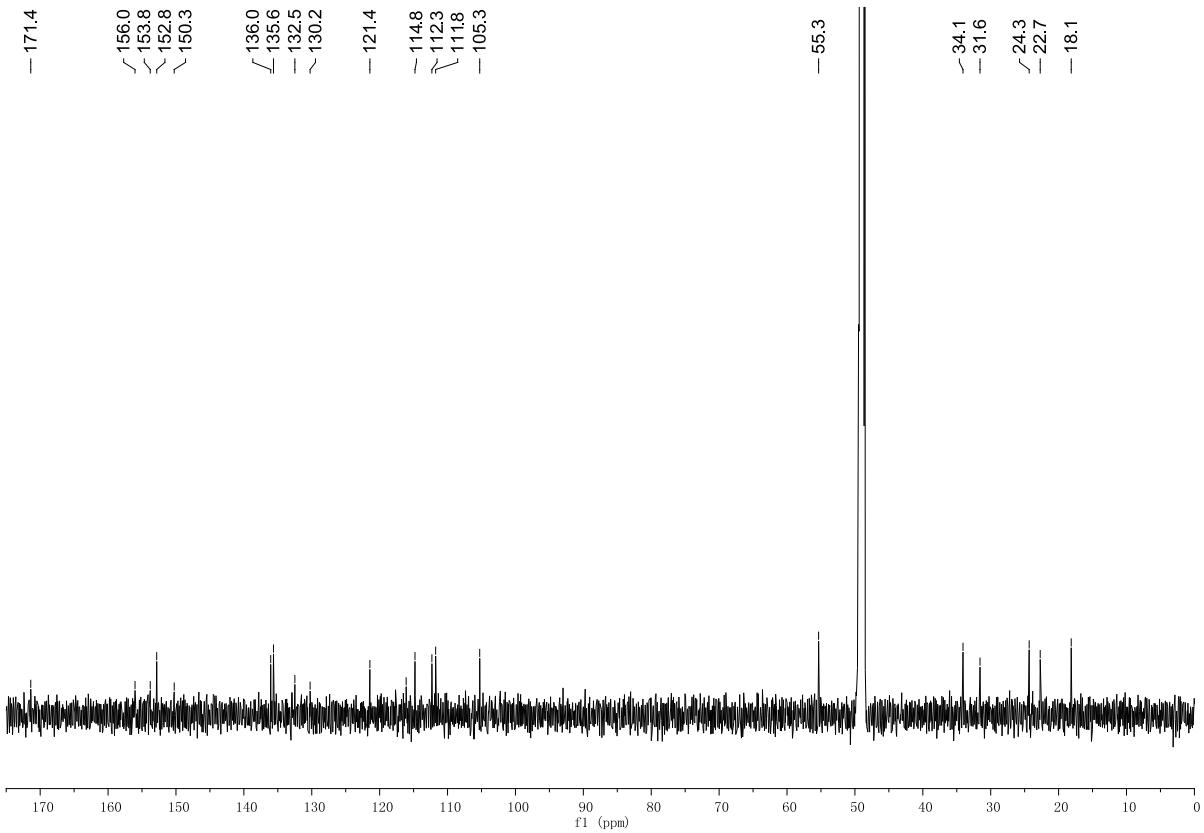

Figure S20: ^{13}C NMR (151 MHz, CD_3OD) spectrum for compound **5**.

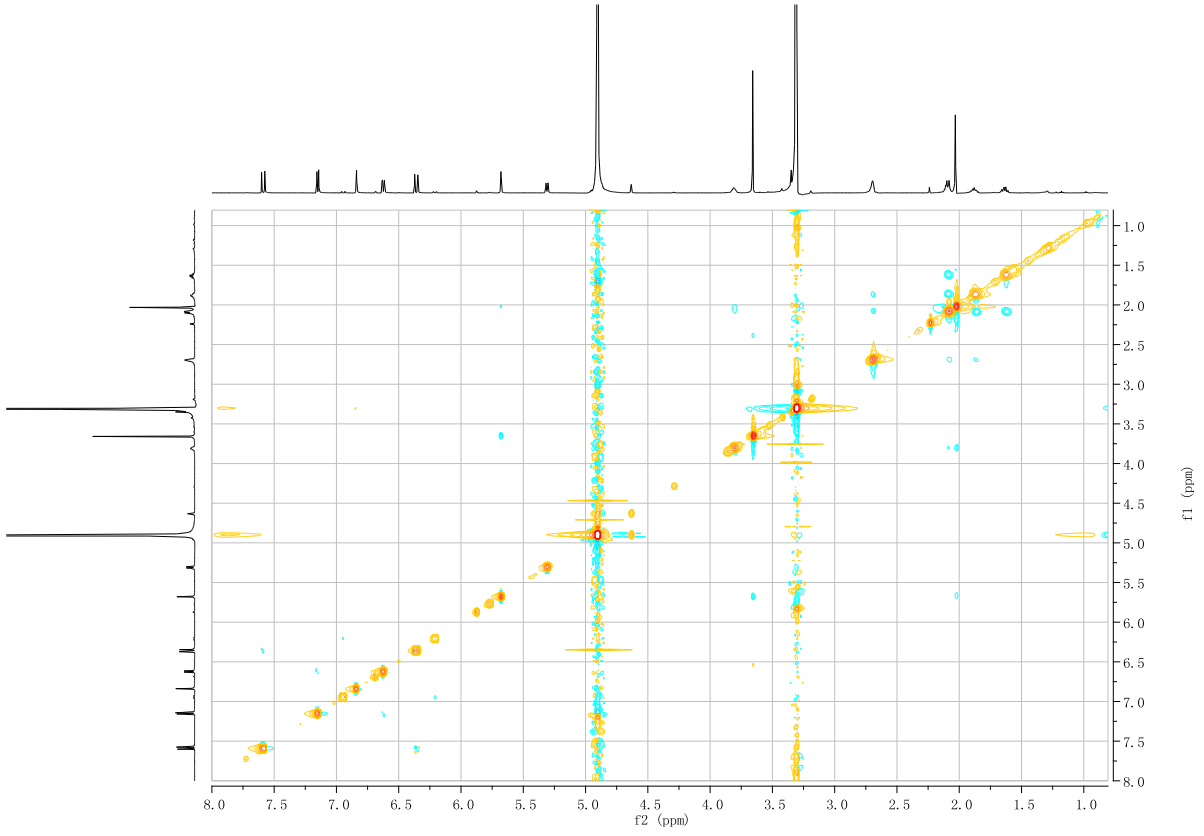

Figure S21: The NOE spectrum for compound **5**.

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CLUSTAL W (1.83) multiple sequence alignment

KR5-ery       RAARTRWSPRGTVLVTGGTGGIGAHVARWLARSG-AEHLVLLGRRGADAPGASELREELT
KR6-ery       GTRESSWEPAGTALVTGGTGALGGHVARHLARCG-VEDLVLVSRRGVDAPGAAELEAELV
KR2-ery       TATSEYAVPGGTILVTGGTAGLGAEVARWLAGRG-AEHLALVSRRGPDTEGVGDLTAELT
KR1-ery       PATDDEWKPTGTVLVTGGTGGVGGQIARWLARRG-APHLLLVSRSGPDADGAGELVAELE
KR1-ave       THQPPTPTPHGTTLITGGTGALATHLTHHLTTHQPTQHLLLTSRTGPHTPHAQHLTTQLQ
KR5-ave       THQPPTPTPHGTTLITGGTGALATHLTHHLTTHQPTQHLLLTSRTGPHTPHAQHLTTQLQ
KR5-cuv       APTEPVAIGEGTVLITGGTGSLGSLVARHLVTEHGVRDLVLVSRQGPDADGATELTNELQ
                     ** *:****.:.  ::: *.    . .* * .* * .:  . .*  :*

KR5-ery       ALGTGVTIAACDVADRARLEAVLAAERAEGRTVSAVMHAAGVSTSTPLDDLTEAEFTEIA
KR6-ery       ALGAKTTITACDVADREQLSKLLEELRGQGRPVRTVVHTAGVPESRPLHEIGELES--VC
KR2-ery       RLGARVSVHACDVSSREPVRELVHGLIEQGDVVRGVVHAAGLPQQVAINDMDEAAFDEVV
KR1-ery       ALGARTTVAACDVTDRESVRELLGGIG-DDVPLSAVFHAAATLDDGTVDTLTGERIERAS
KR1-ave       QKGIHLTITTCDTSNPDQLQQLLNTIPPQH-PLTTVIHTAGILDDATLTNLTPTQLNNVL
KR5-ave       QKGIHLTITTCDTSNPDQLQQLLNTIPPQH-PLTTVIHTAGVNLFAPVSETDAESFSSVT
KR5-cuv       QHGARVRTLSCDLTDRTALAALIDETG----PLTGVVHTAGALADATVDHLDADALATTF
                *      :** :.   :  ::         :  *.*:*.     .:

KR5-ery       DVKVRGTVNLDELC-PDLDA--FVLFSSNAGVWGSPGLASYAAANAFLDGFARRRRSEGA
KR6-ery       AAKVTGARLLDELC-PDAET--FVLFSSGAGVWGSANLGAYSAANAYLDALAHRRRAEGR
KR2-ery       AAKAGGAVHLDELC-SDAEL--FLLFSSGAGVWGSARQGAYAAGNAFLDAFARHRRGRGL
KR1-ery       RAKVLGARNLHELT-RELDLTAFVLFSSFASAFGAPGLGGYAPGNAYLDGLAQQRRSDGL
KR1-ave       RAKAHSAHLLHQLT-QHTPLTAFVLYSSAAATFGAPGQANYAAANAYLDALAHHRHTHHL
KR5-ave       AAKATGAAILHELLLDHETLEHFILFSSGAGAWGSGNQCAYSAANAYLDALATHRQTHGL
KR5-cuv       APKANAAWWLHELT-QDQNLTLFMVFSSLAGVLGSAGQANYAAANSFLDALITHRRSHGL
                *. .:  *.:*   .     *:::** *.. *:     *:..*::**.:  :*:

KR5-ery       PVTSIAWGLWAGQ
KR6-ery       AATSVAWGAWAGE
KR2-ery       PATSVAWGLWAAG
KR1-ery       PATAVAWGTWAGS
KR1-ave       PATSIAWGTWQGN
KR5-ave       PGASIAWGPWAGK
KR5-cuv       PGTSLAWGSWERT
              . :::*** *
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Figure S22: Alignment of modular PKS Ketoreductase (KR) domains. The Asp residue diagnostic of PKS KR specificity is labeled. Those containing the Asp are two known (KR1_ery and KR1_ave) to catalyze reduction with D configuration. Those without the Asp are known to catalyze ketoreduction with L configuration.