

SUPPORTING INFORMATION

Coordination complexes constructed from pyrazole-acetamide and pyrazole-quinoxaline: Effect of hydrogen bonding on the self-assembly process and antibacterial activity

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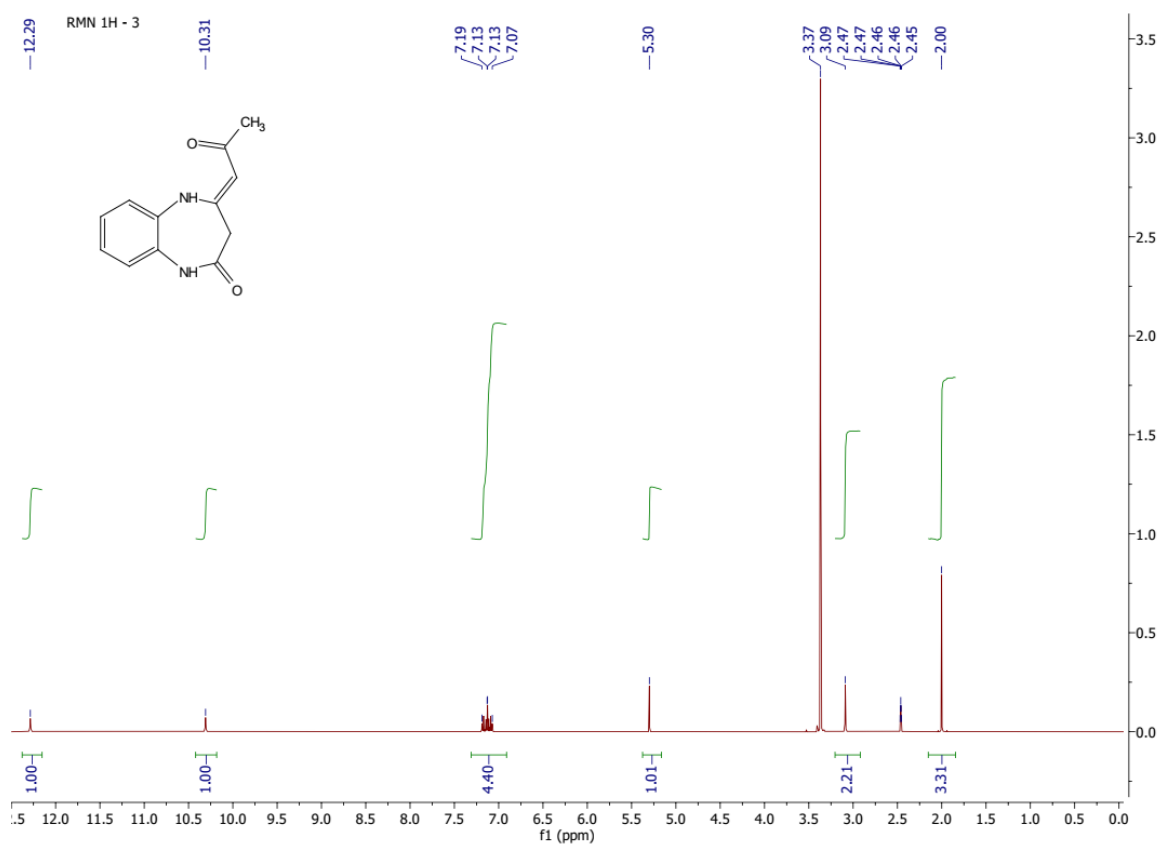


Figure S1. ^1H NMR spectrum of **3**.

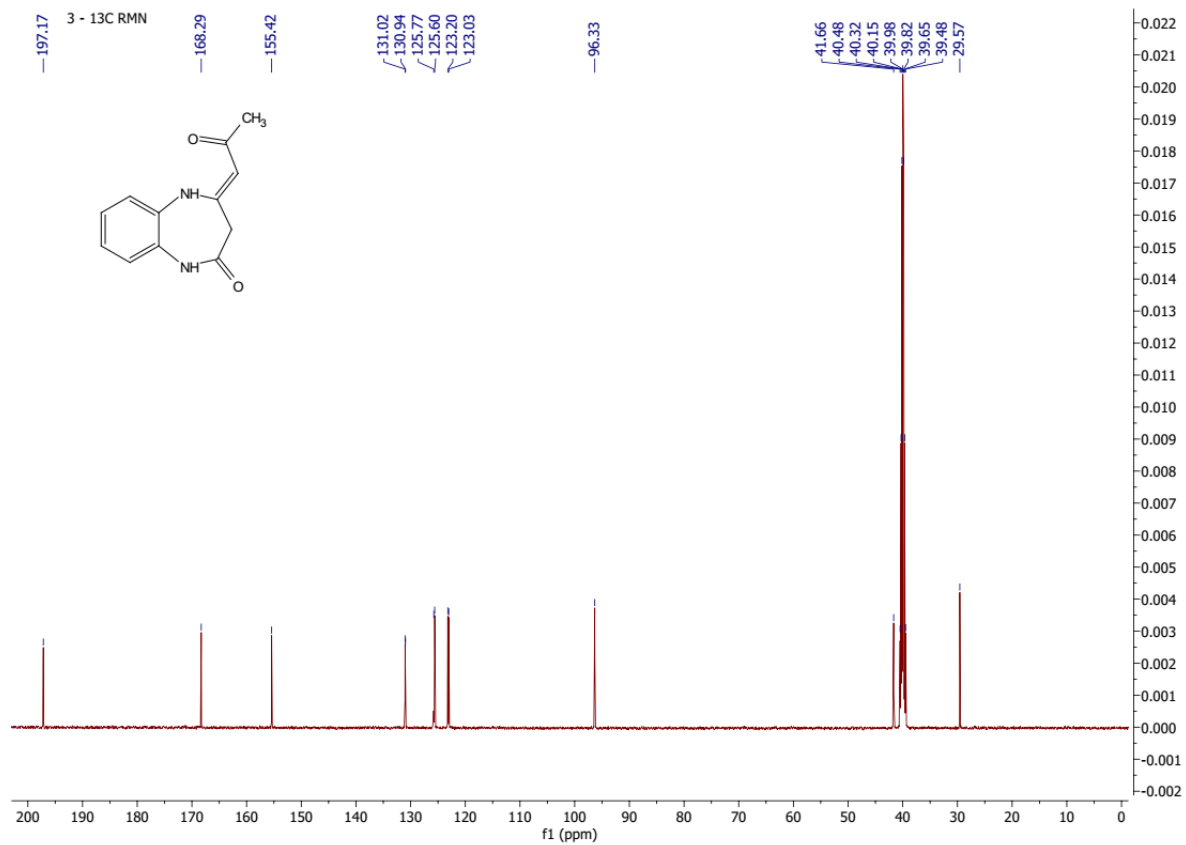


Figure S2. ¹³C NMR spectrum of **3**.

3_210531130729#1 RT: 0.01 AV: 1 NL: 2.63E8
T: FTMS + p ESI Full ms [50.0000-350.0000]

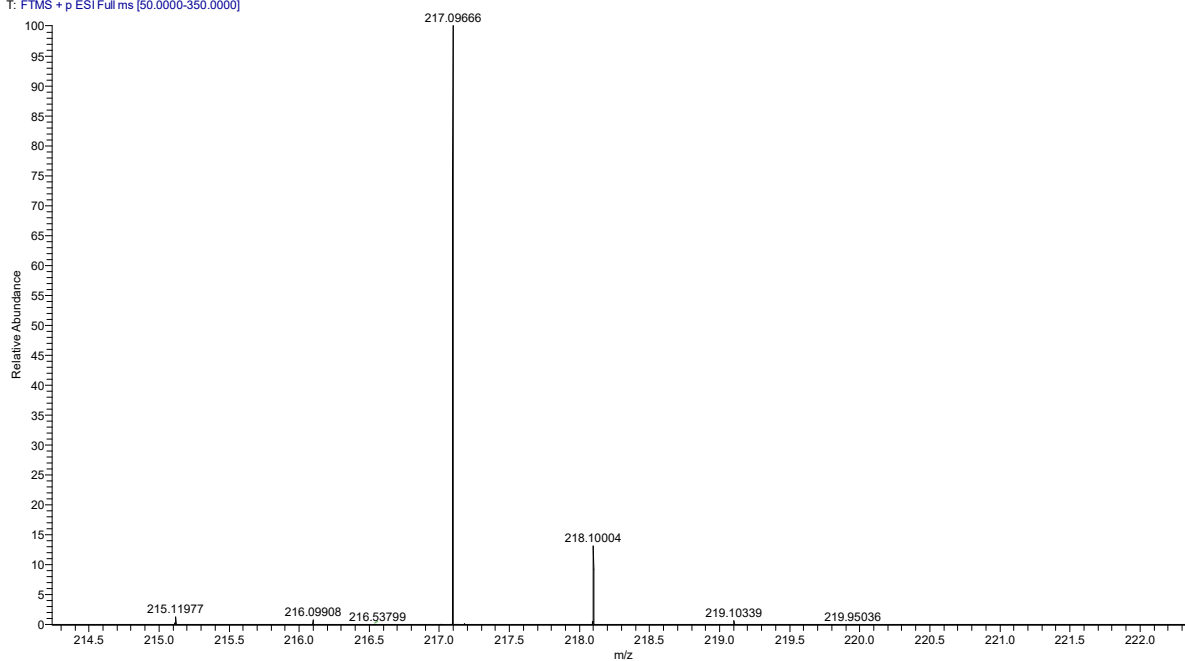


Figure S3. ESI-HRMS spectrum of **3**.

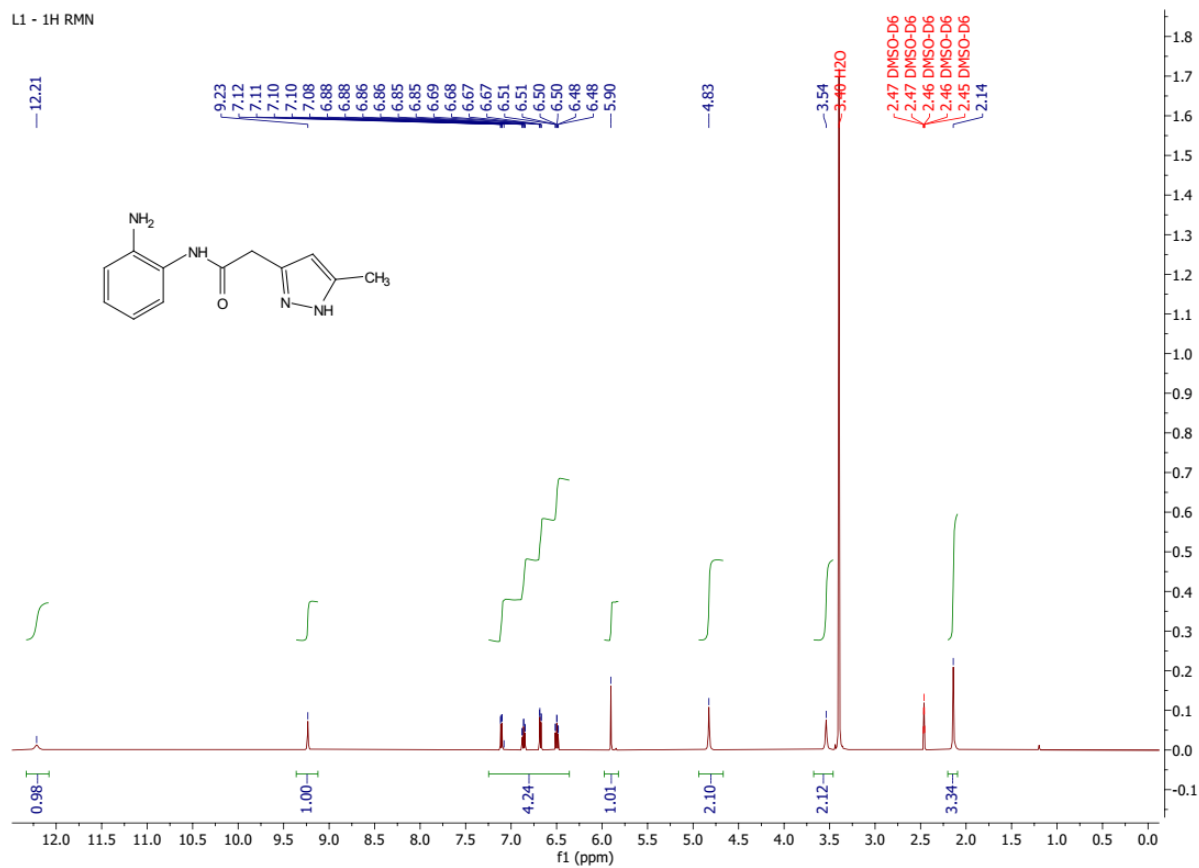


Figure S4. ¹H NMR spectrum of *L1*.

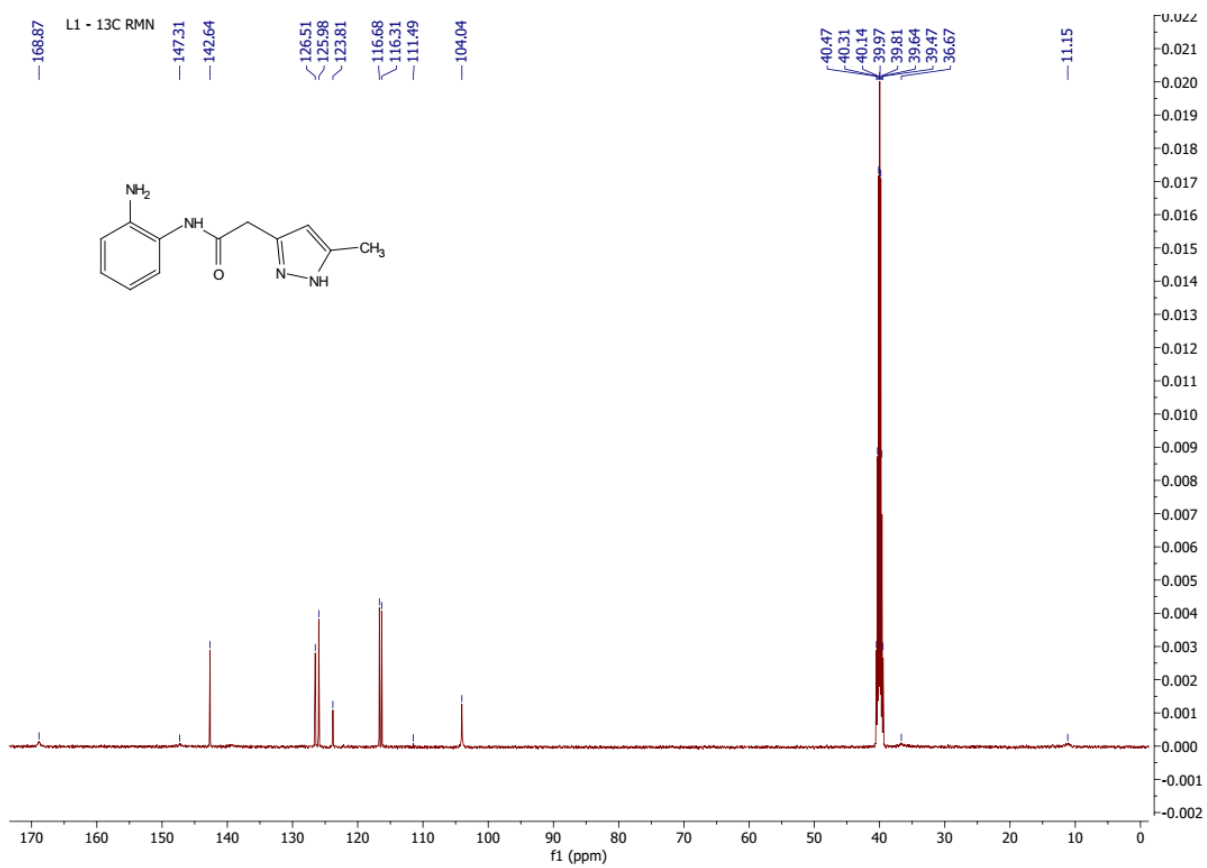


Figure S5. ^{13}C NMR spectrum of *L1*.

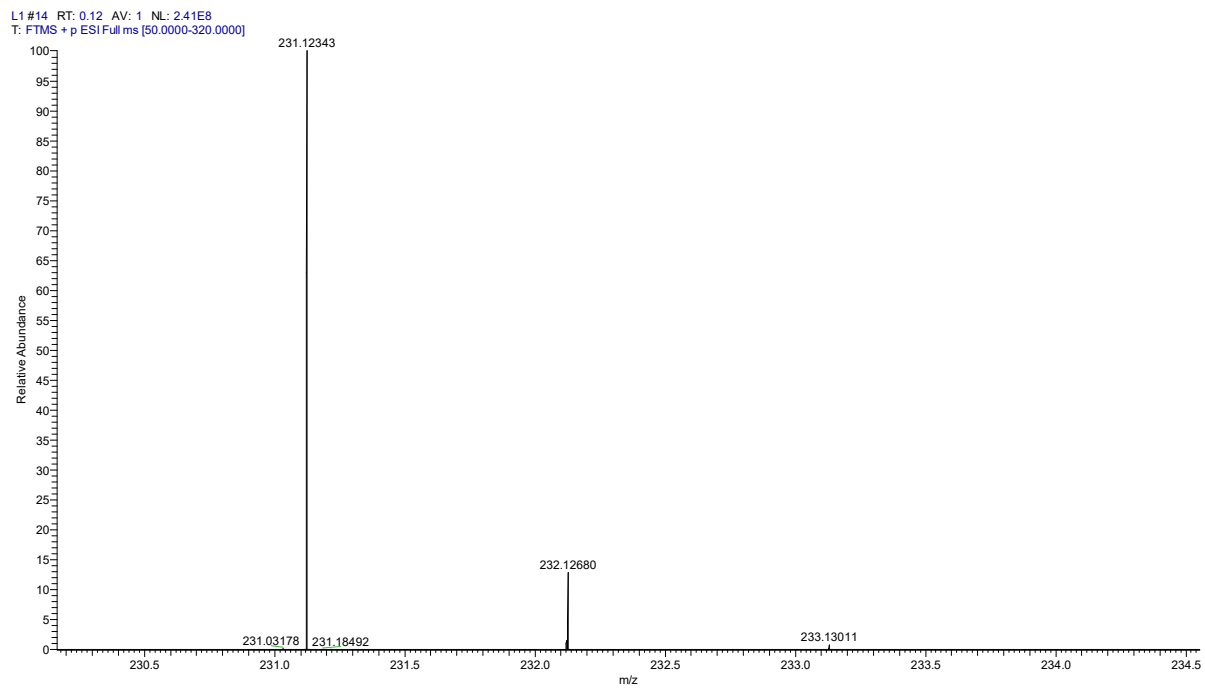


Figure S6. ESI-HRMS spectrum of *L1*.

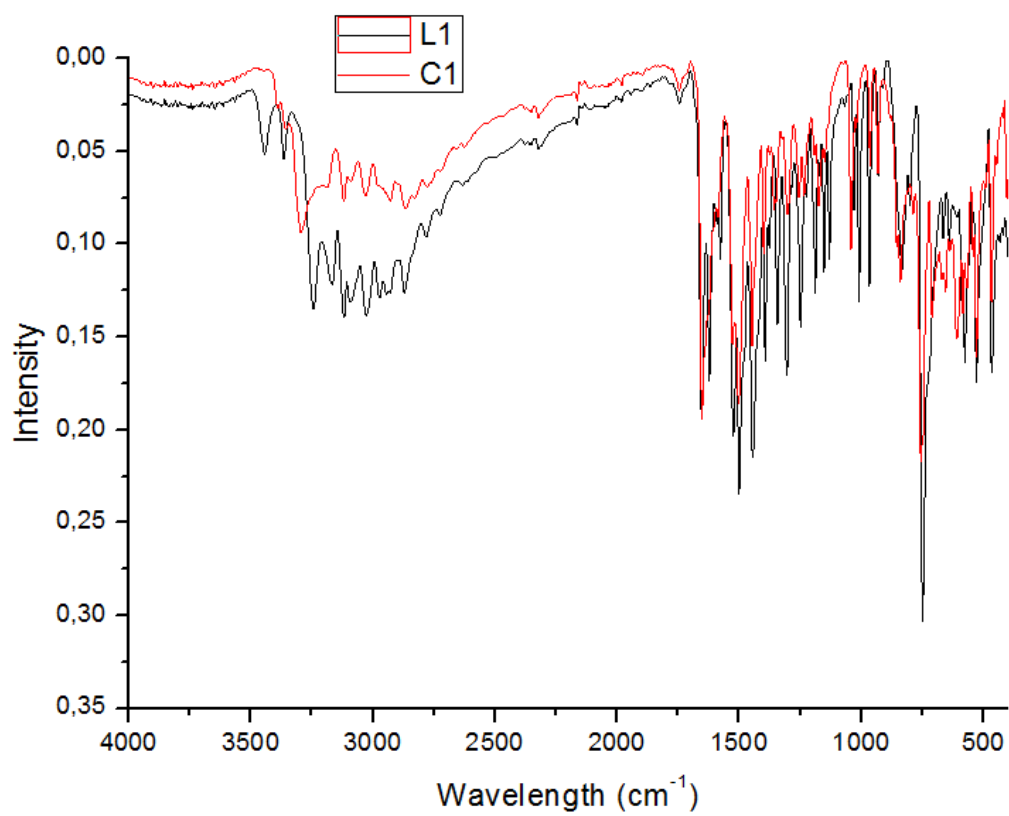


Figure S7. FT-IR comparison plot of C_I and L_I .

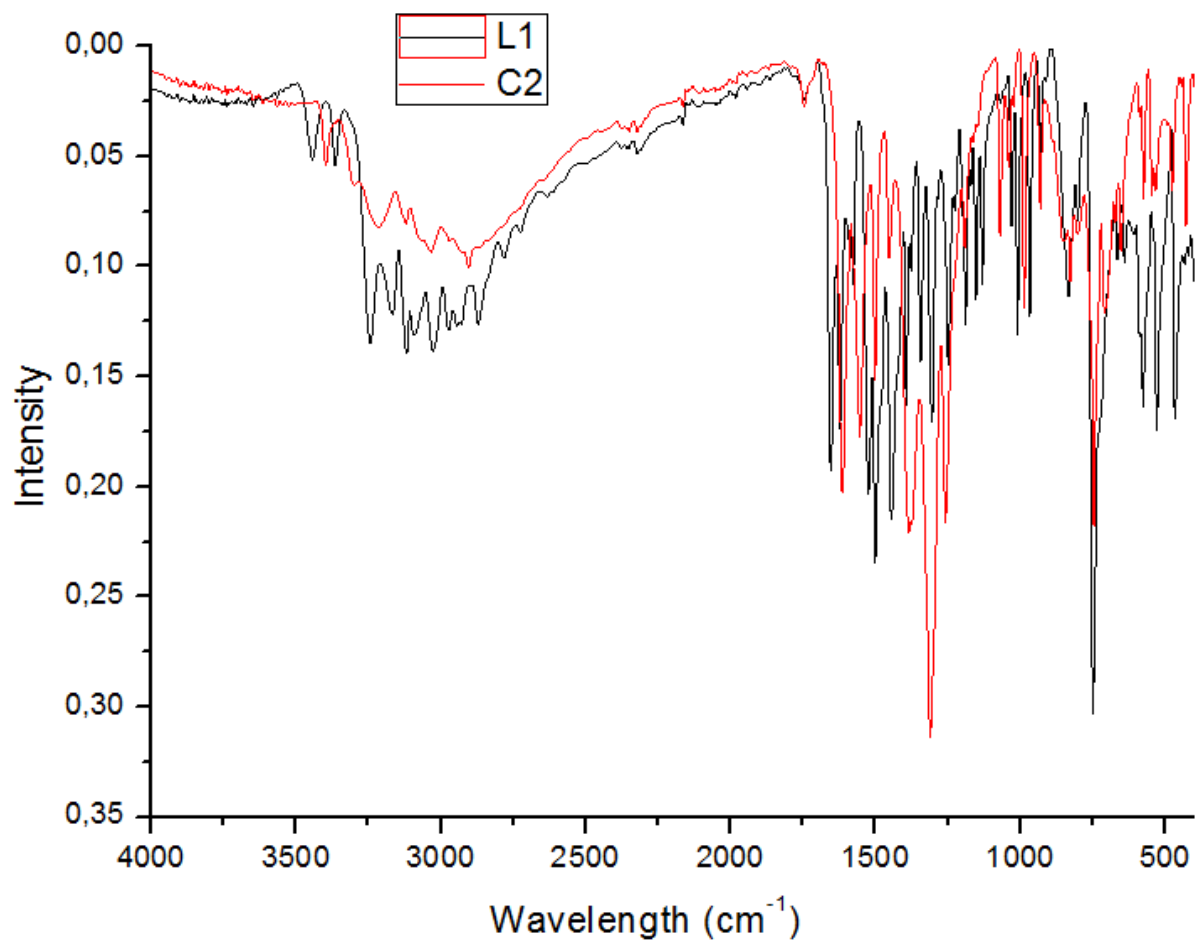


Figure S8. FT-IR comparison plot of C_2 and L_1 .

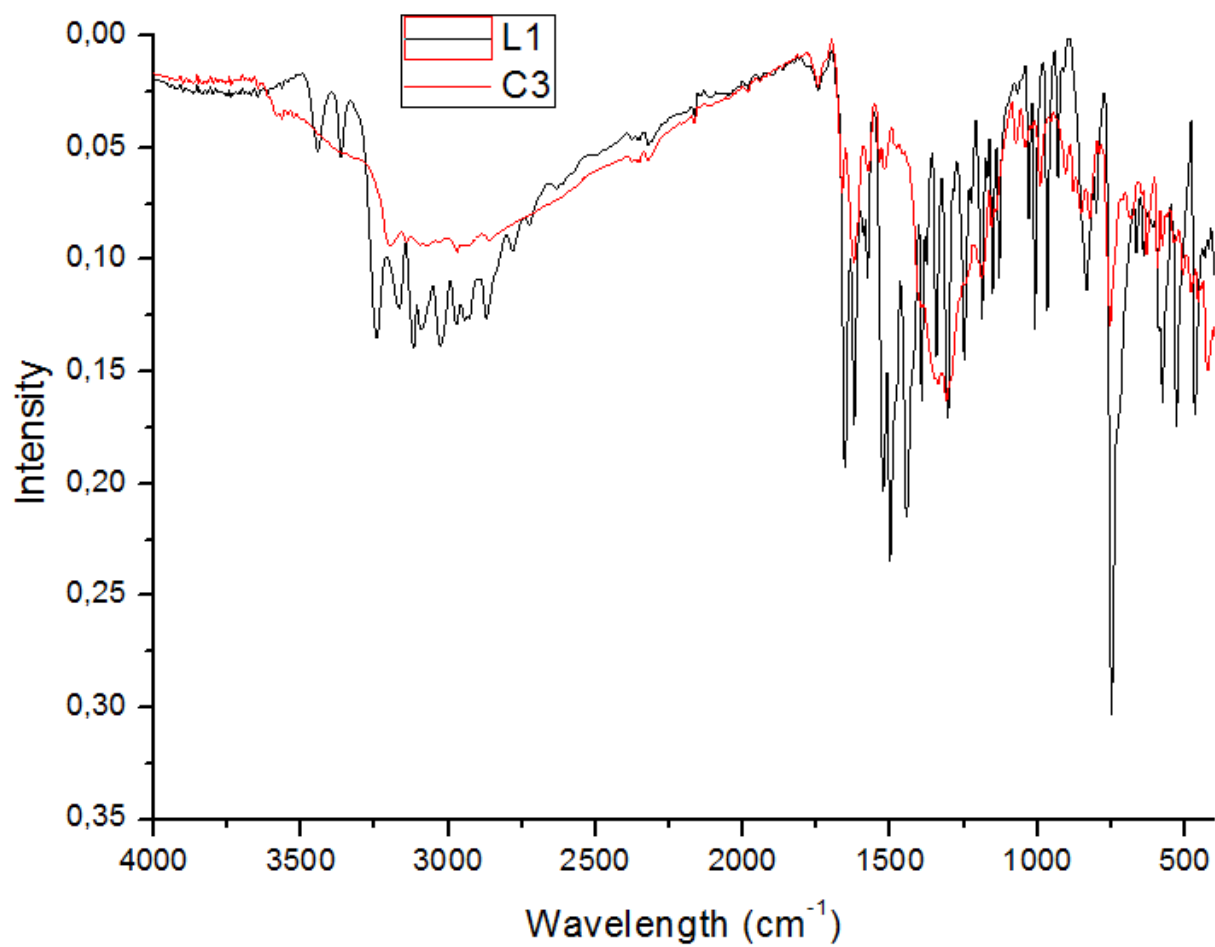


Figure S9. FT-IR comparison plot of C_3 and L_1 .

C1 #1 RT: 0.01 AV: 1 NL: 1.17E9
T: FTMS + p ESI Fullms [450.0000-750.0000]

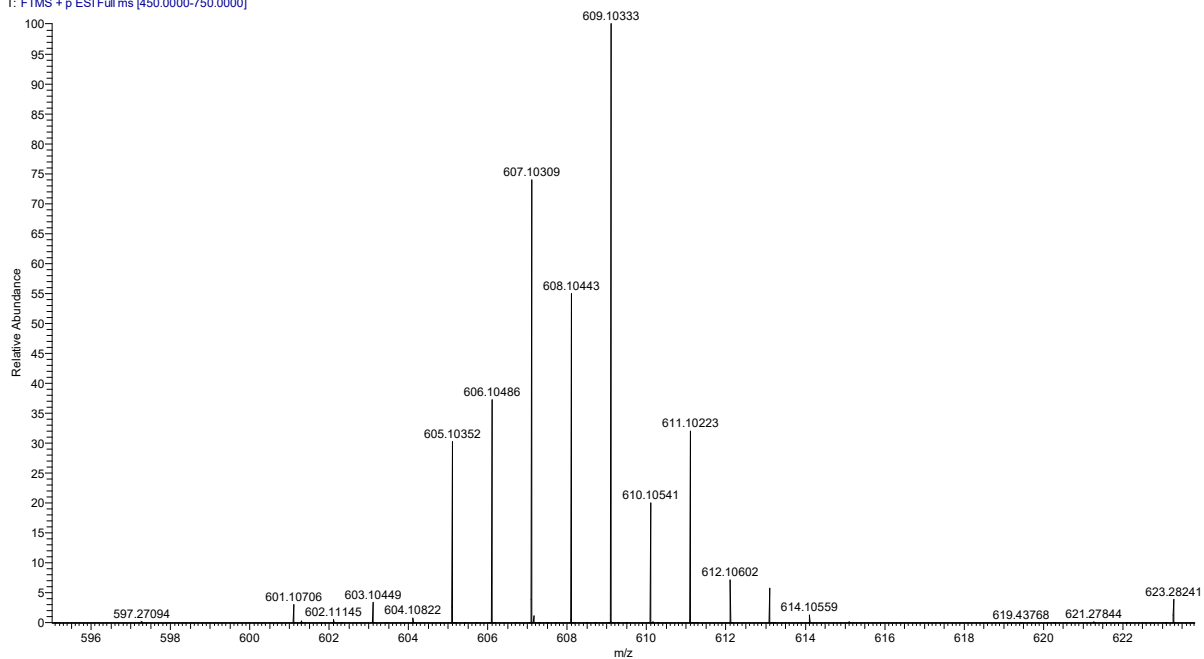


Figure S10. ESI-MS spectrum of C_1 .

C2 #10 RT: 0.09 AV: 1 NL: 3.39E8
T: FTMS + p ESI Full ms [600.0000-800.0000]

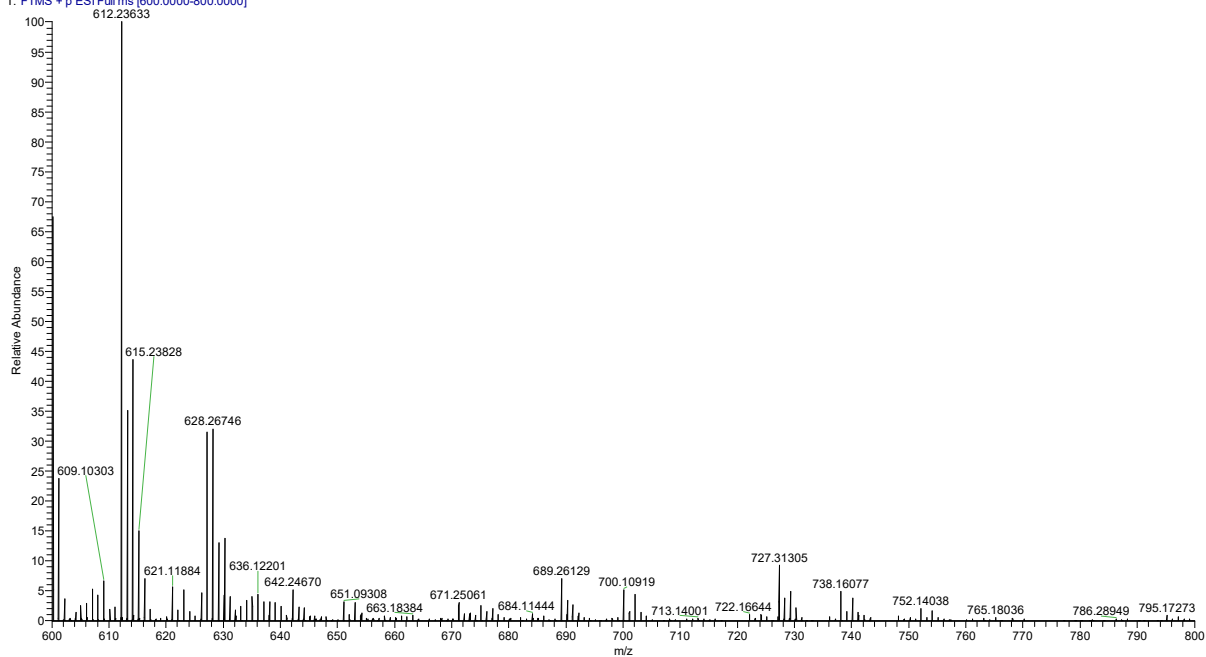


Figure S11. ESI-MS spectrum of C_2 .

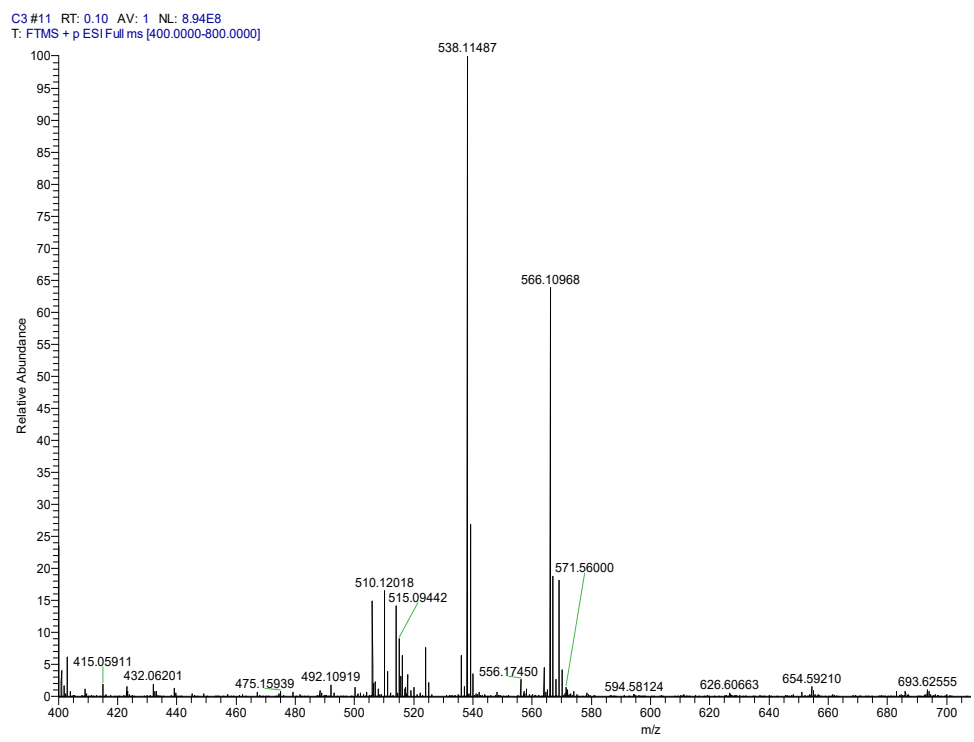


Figure S12. ESI-MS spectrum of C_3 .

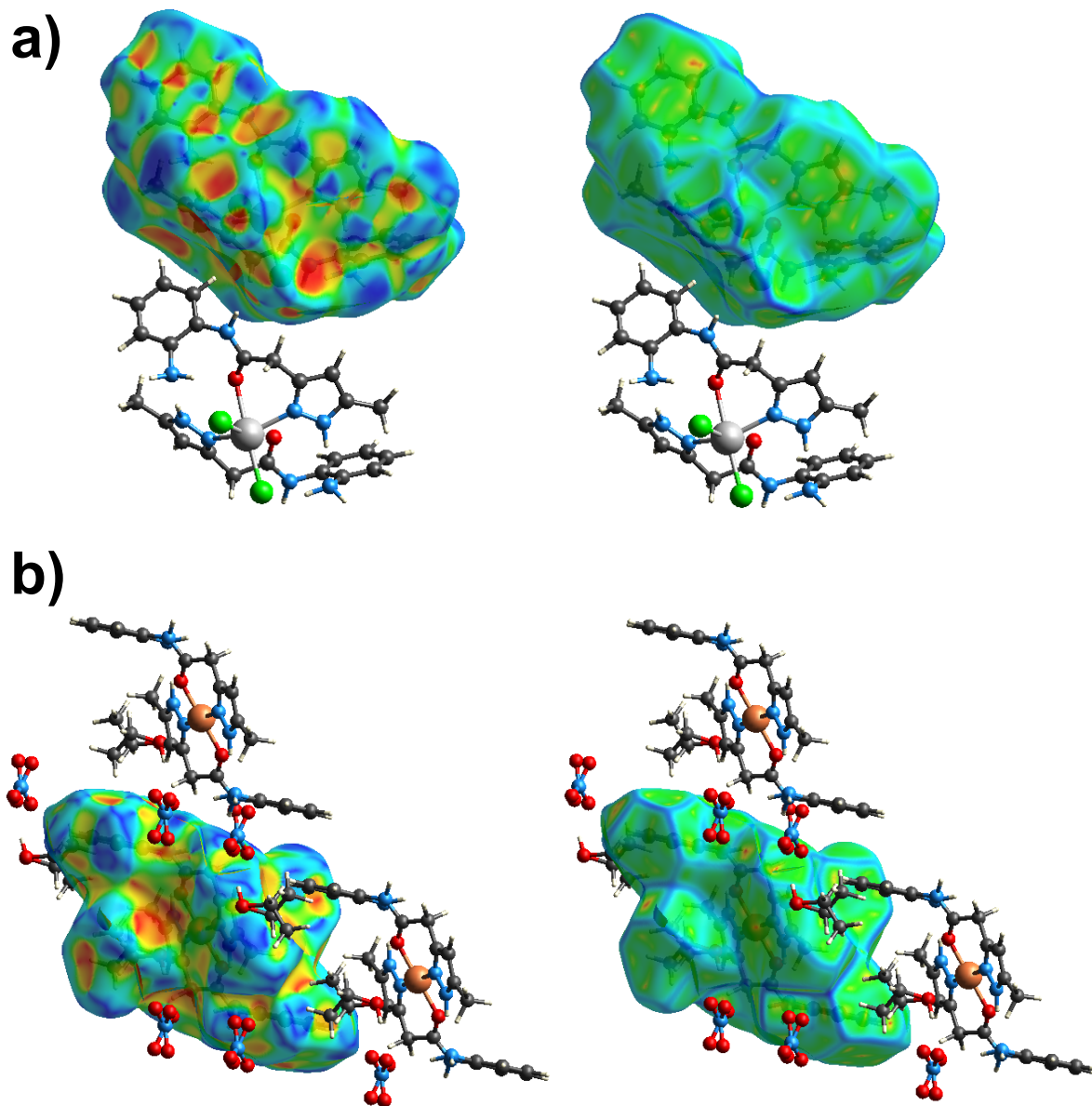


Figure S13. shape index (shown in left side) and curvedness (shown in right side) of C_1 (a) and C_2 (b).

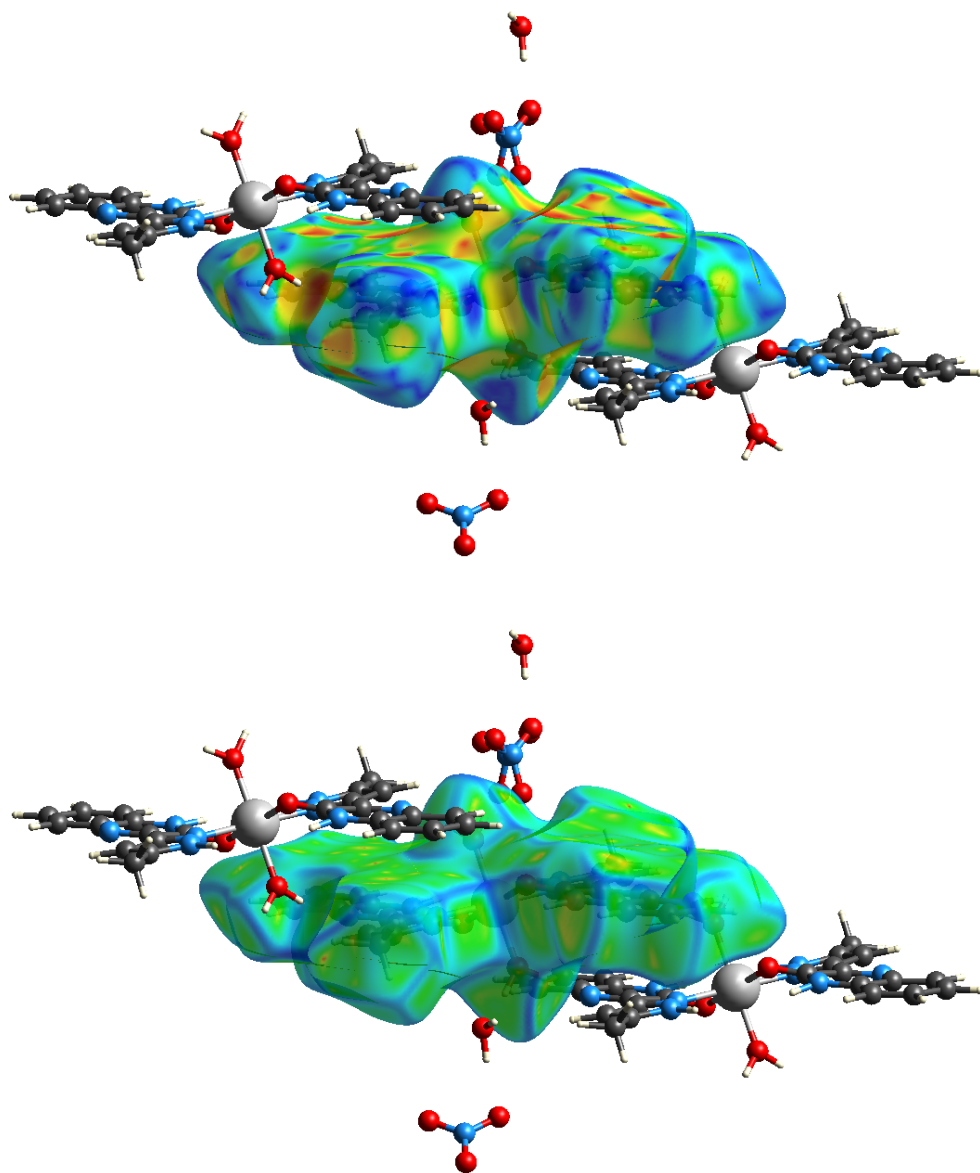


Figure S14. Shape index (*top*) and curvedness (*bottom*) of C₃.

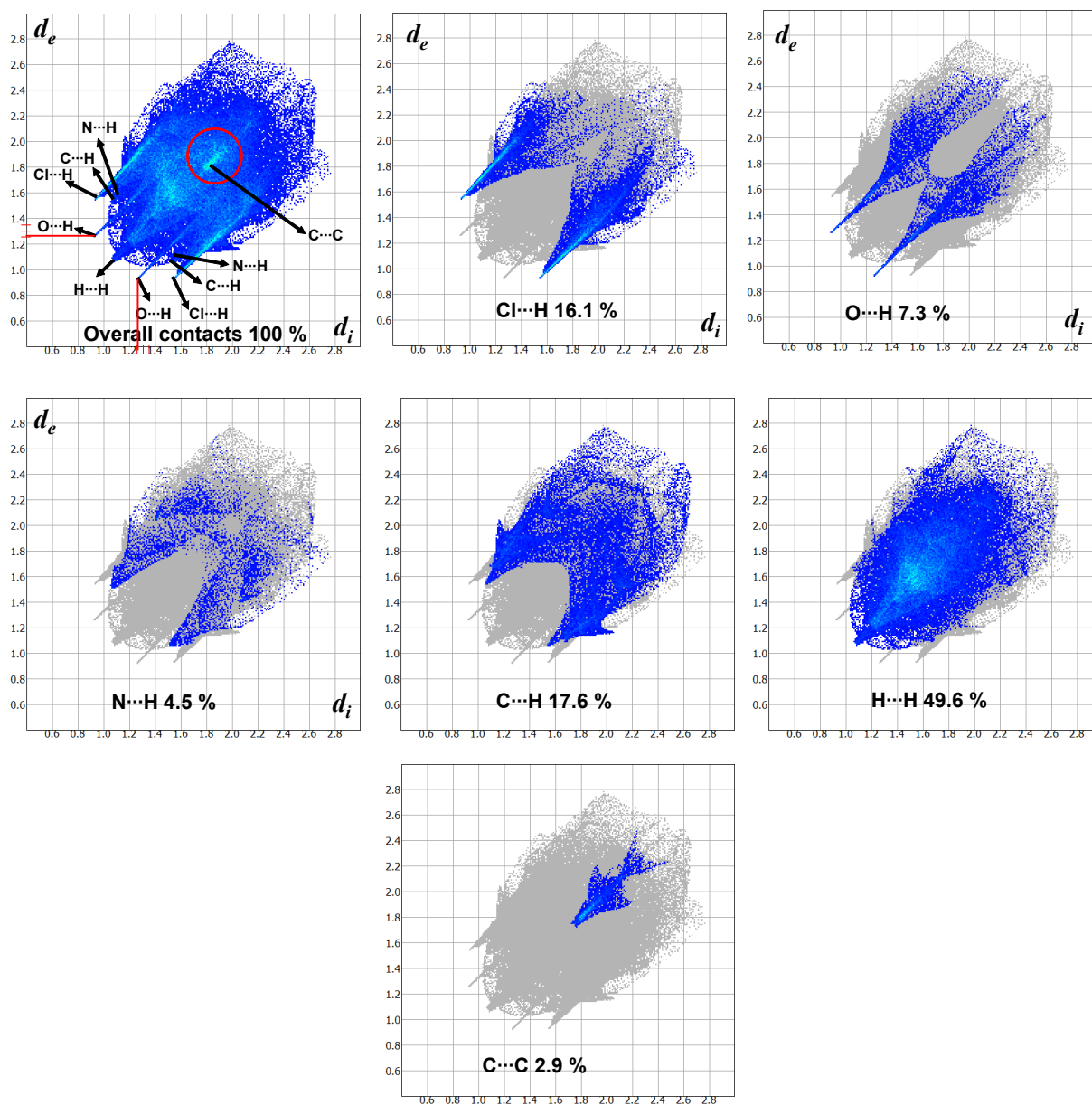


Figure S15. 2D Fingerprint plots derived from Hirshfeld surfaces, displaying various intermolecular interactions for C_1 .

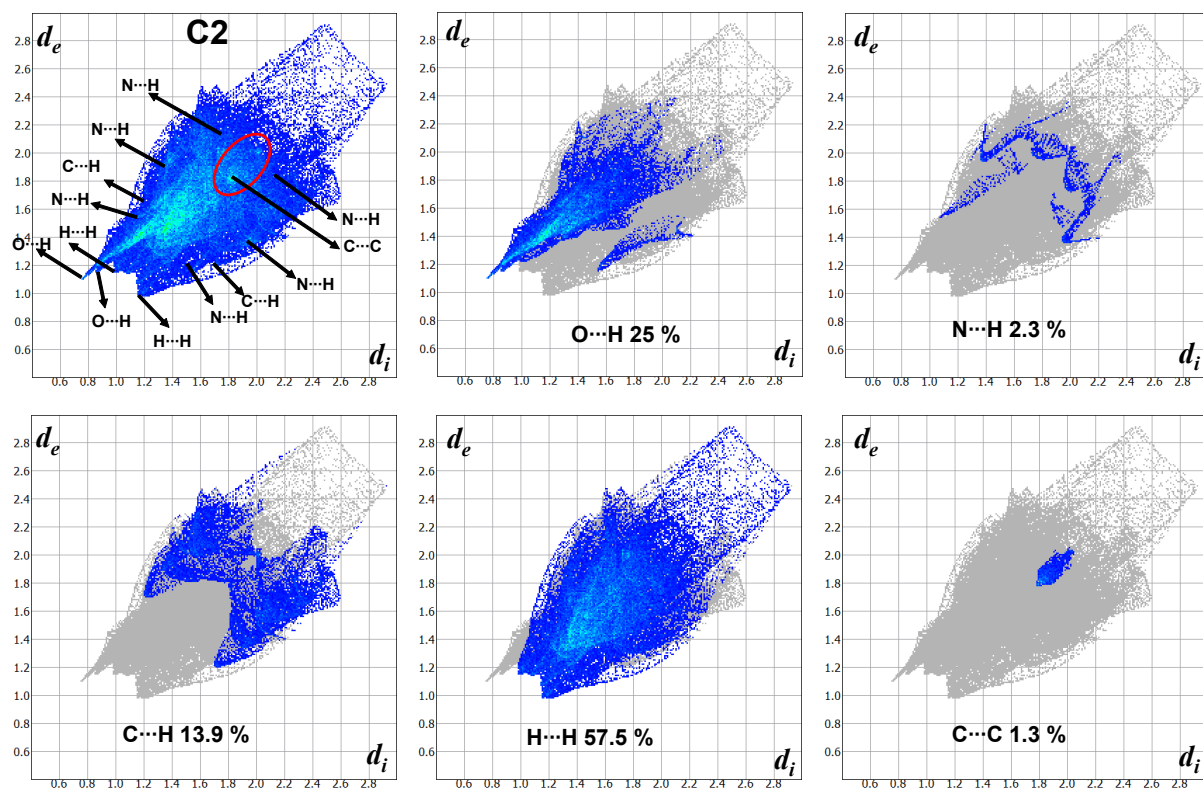


Figure S16. 2D Fingerprint plots derived from Hirshfeld surfaces, displaying various intermolecular interactions for C_2 .

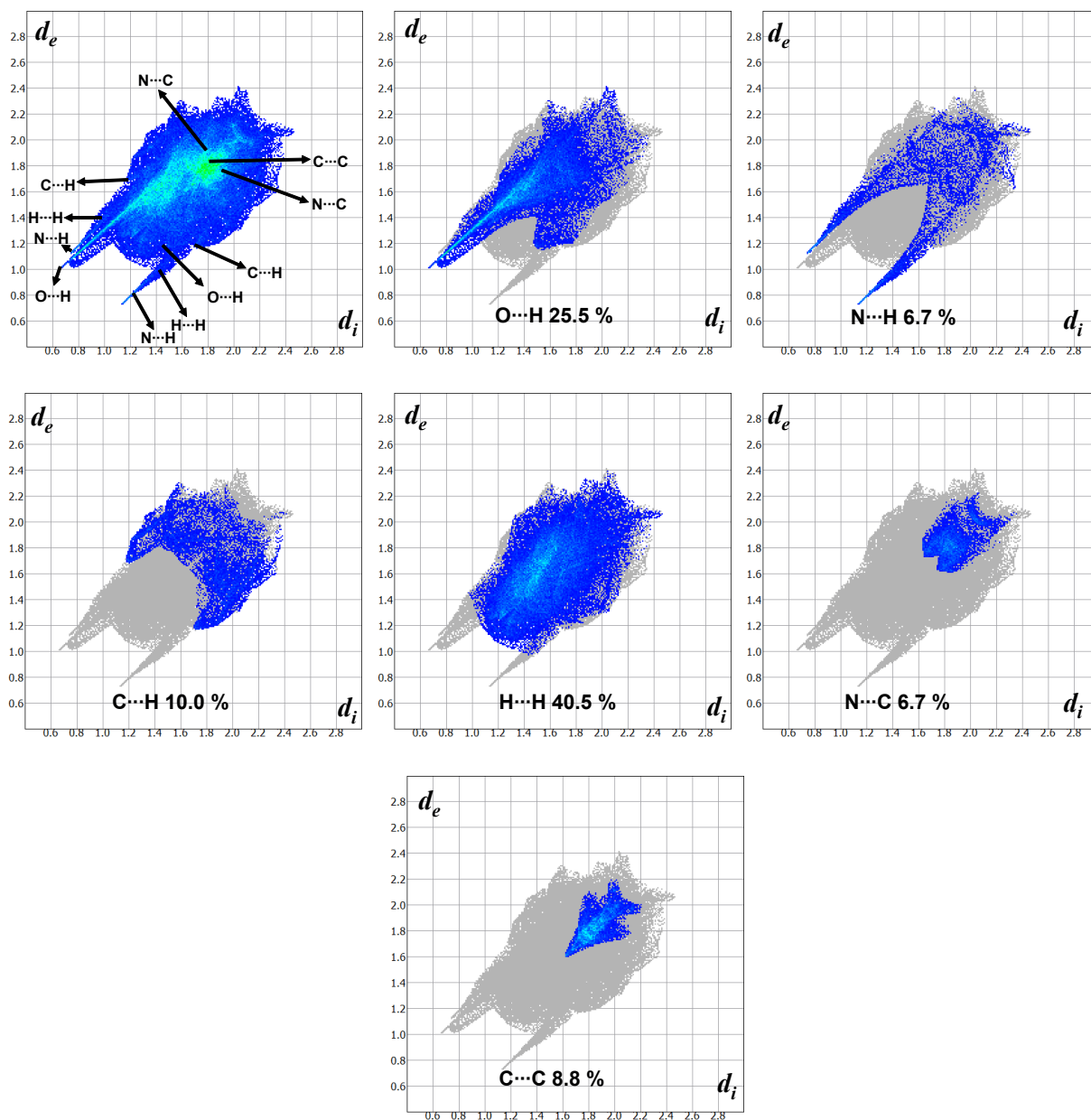


Figure S17. 2D Fingerprint plots derived from Hirshfeld surfaces, displaying various intermolecular interactions for C_3 .