Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

CONTENTS

1. Structural Characterization information

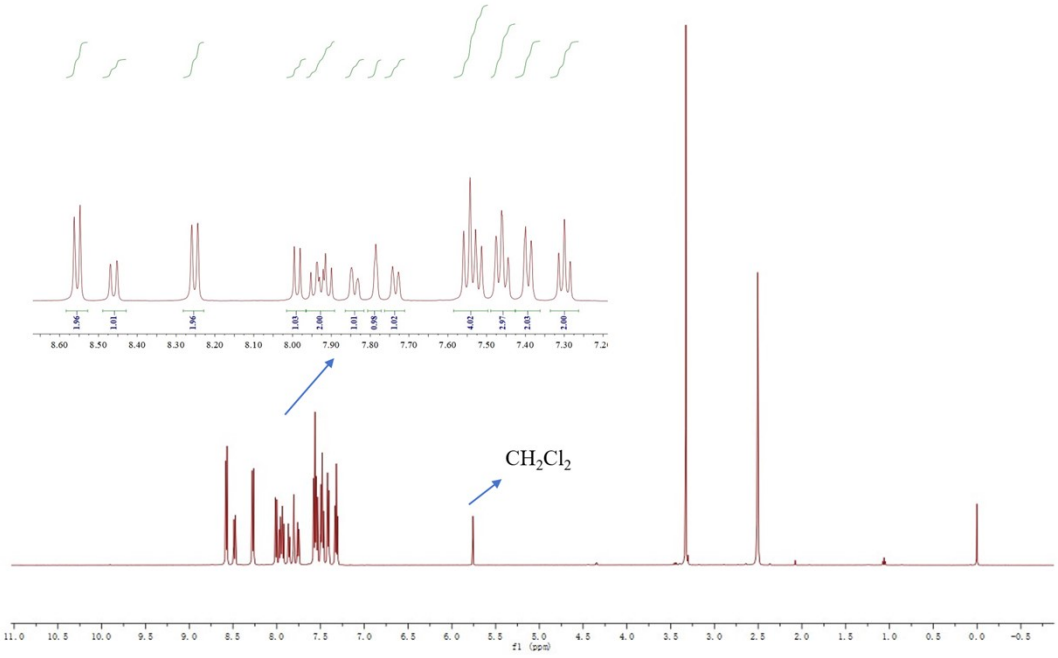

Figure S1 ^{1}H NMR spectrum of compound NI-mPCz

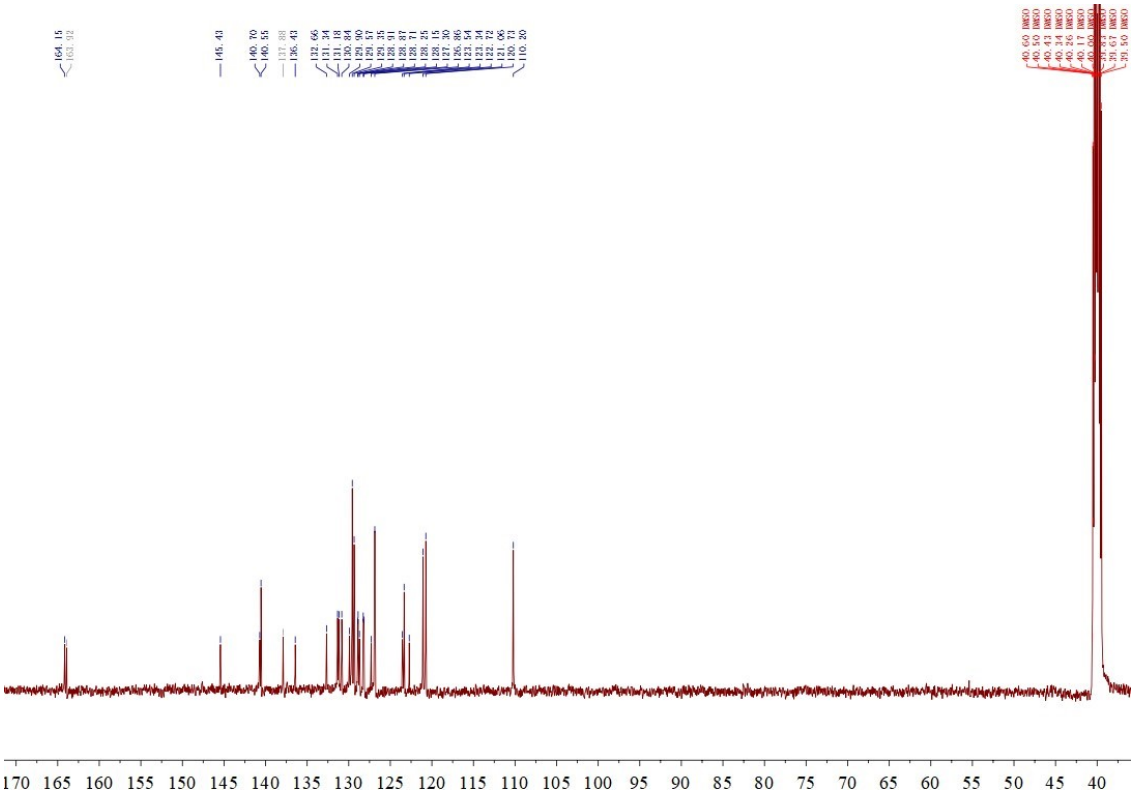

Figure S2 ^{13}C NMR spectrum of compound NI-mPCz

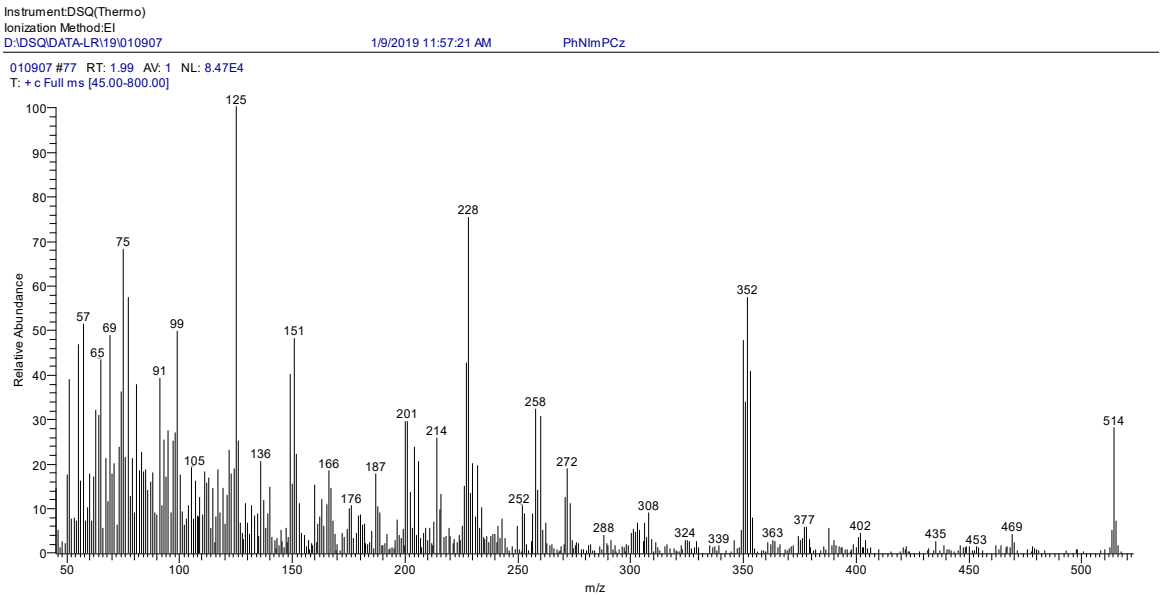

Figure S3 EI-MS spectrum of compound NI-mPCz.

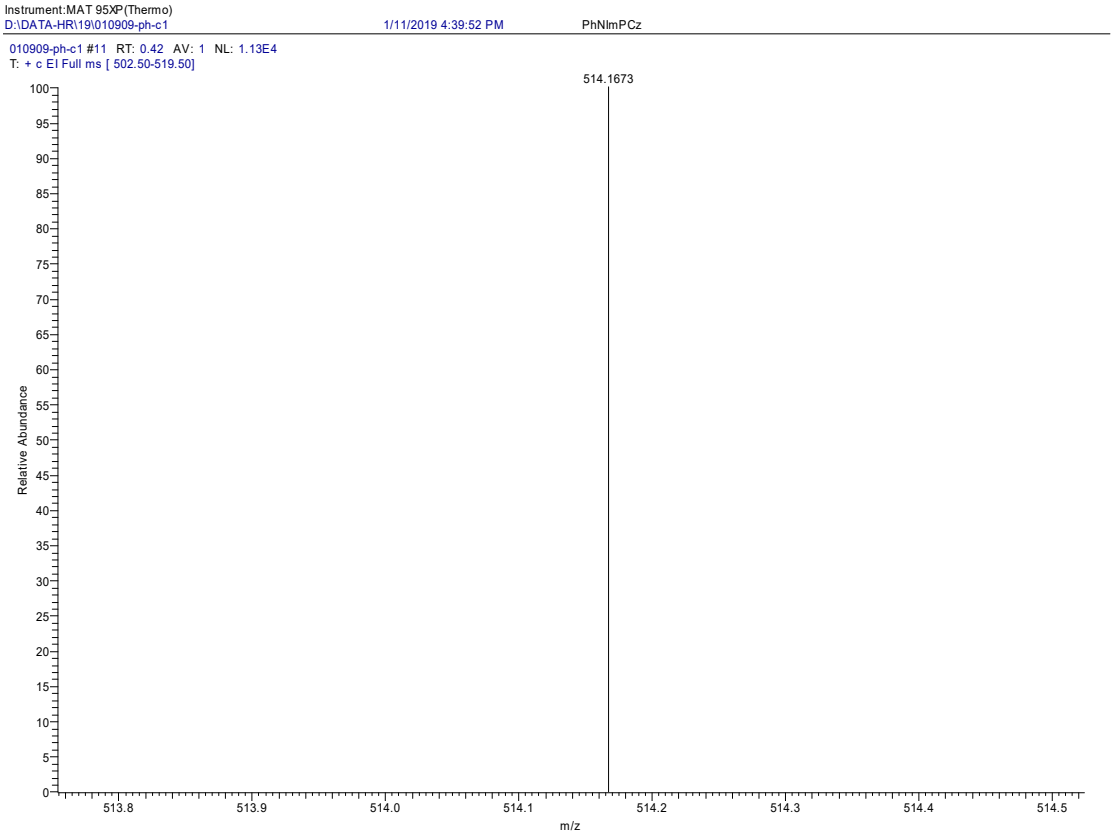

Figure S4 HRMS spectrum of compound NI-mPCz.

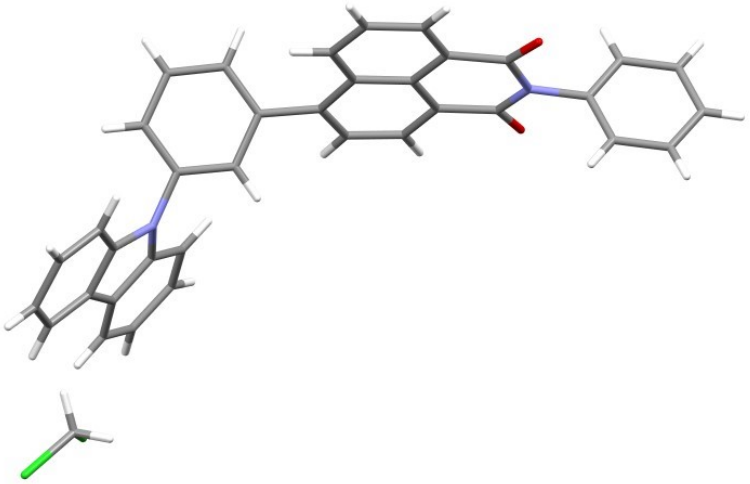

Figure S5 The single-crystal structure of NI-mPCz

2. Supporting Tables

Table 1 Crystal data and structure refinement for NI-mPCz.

Identification code	NI-mPCz
Empirical formula	$C_{37}H_{24}Cl_2N_2O_2$
Formula weight	599.48
Temperature/K	273(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.24880(10)
b/Å	13.19660(10)
c/Å	16.31220(10)
α/°	90
β/°	93.1790(10)
γ/°	90
Volume/Å^3	2847.62(4)

Z	4
ρ_{calc}g/cm^3	1.398
μ/mm^{-1}	2.356
F(000)	1240.0
Crystal size/mm^3	? × ? × ?
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.624 to 148.312
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -20 ≤ l ≤ 20
Reflections collected	20667
Independent reflections	5703 [R_{int} = 0.0208, R_{sigma} = 0.0155]
Data/restraints/parameters	5703/0/161
Goodness-of-fit on F^2	1.078
Final R indexes [I>=2σ (I)]	R_1 = 0.0708, wR_2 = 0.1805
Final R indexes [all data]	R_1 = 0.0740, wR_2 = 0.1831
Largest diff. peak/hole / e Å^{-3}	1.07/-0.58