Electronic Supplementary Information

Heterogeneous single-atom photocatalysts for oxidative Heck reactions†

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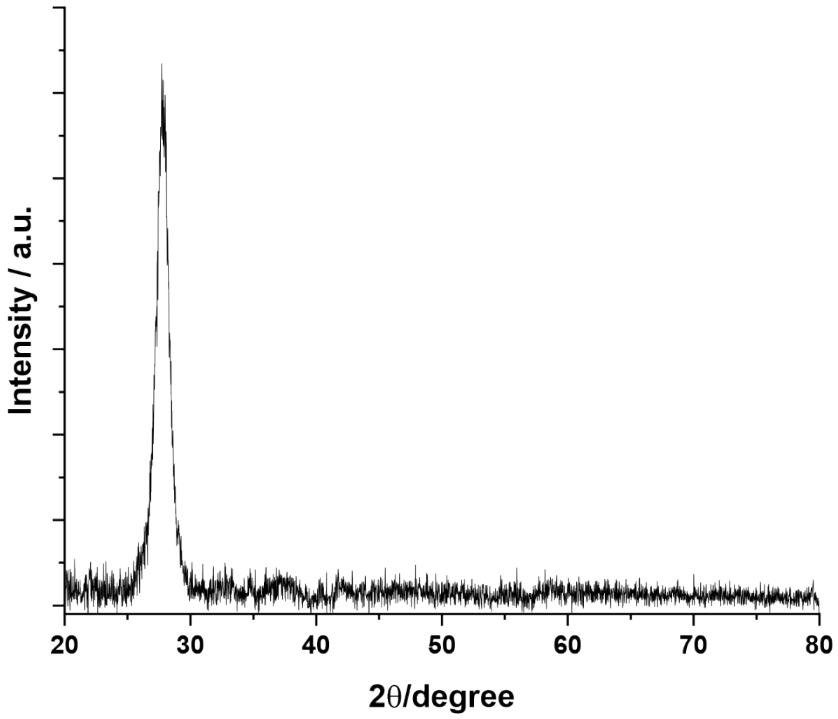


Fig. S1 XRD pattern of $Pd_1/g\text{-}C_3N_4$.

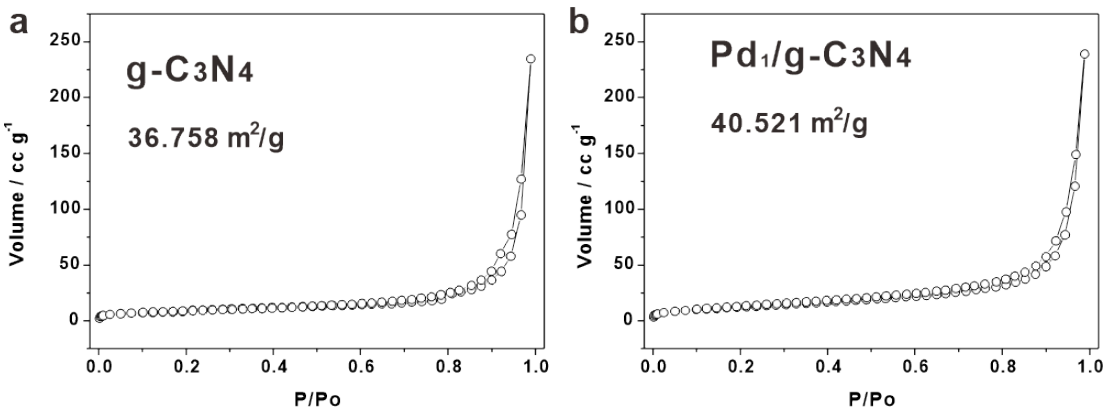


Fig. S2 BET curves of (a) *g*-C_3N_4 and (b) Pd_1/*g*-C_3N_4.

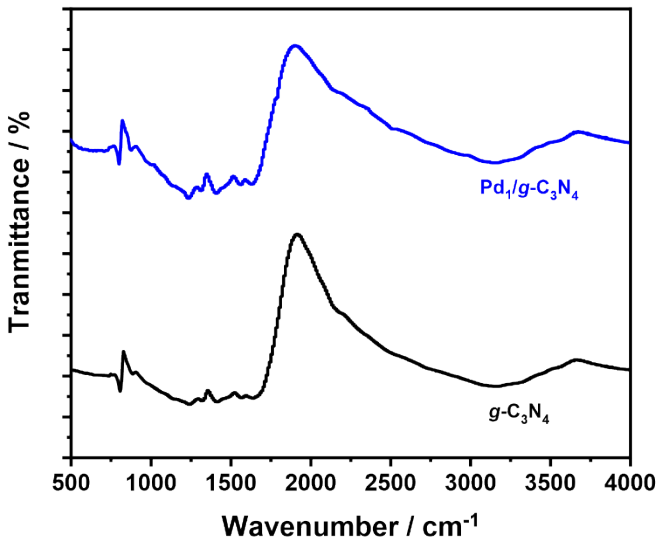


Fig. S3 FTIR spectra of *g*-C_3N_4 and Pd_1/*g*-C_3N_4.

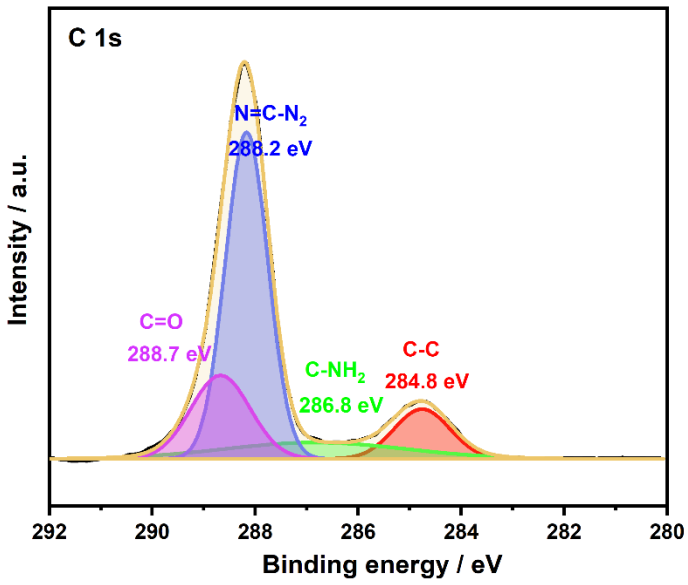


Fig. S4. Core-level XPS of C 1s in pristine *g*-C_3N_4.

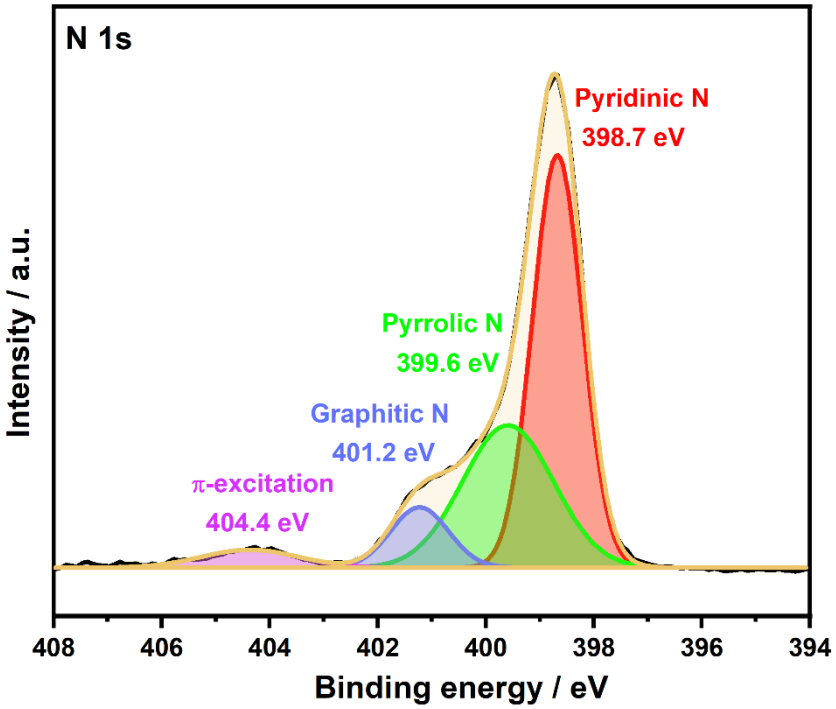


Fig. S5. Core-level XPS of N 1s in pristine *g*-C_3N_4.

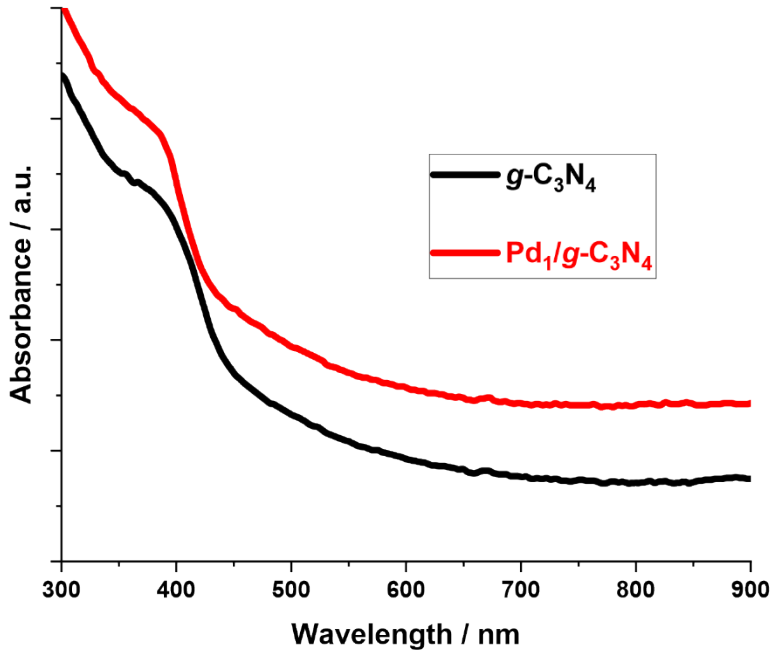


Fig. S6 UV-vis DRS of *g*-C_3N_4 and Pd_1/*g*-C_3N_4.

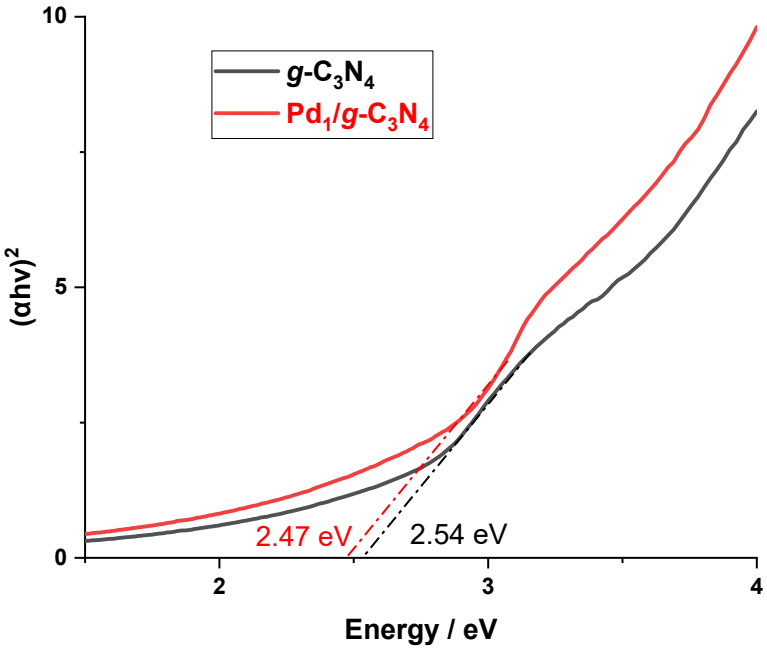


Fig. S7 Tauc plots of g-C_3N_4 and Pd_1/g-C_3N_4 derived from UV-vis spectra

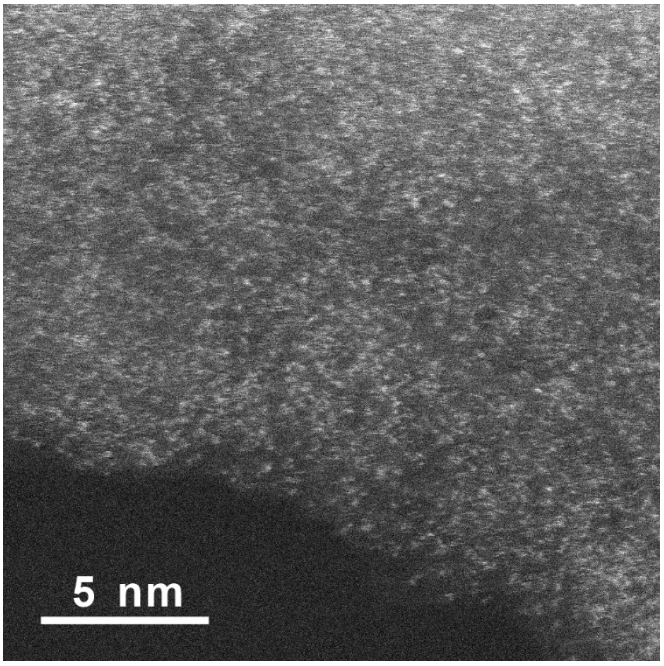


Fig. S8 AC HAADF-STEM image of Pd_1/g-C_3N_4 after 4 h photocatalytic reaction.

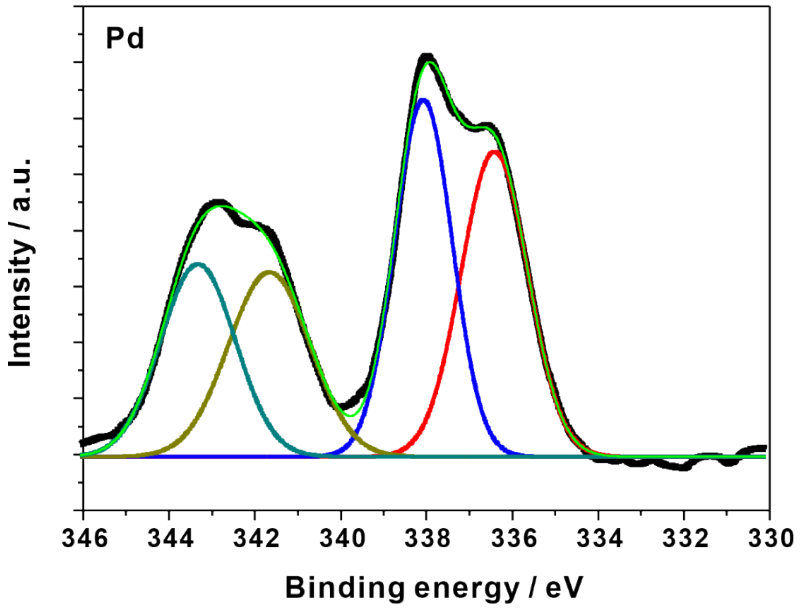


Fig. S9 Core-level XPS of Pd 3d of $Pd_1/g\text{-}C_3N_4$ after 4 h photocatalytic reaction.

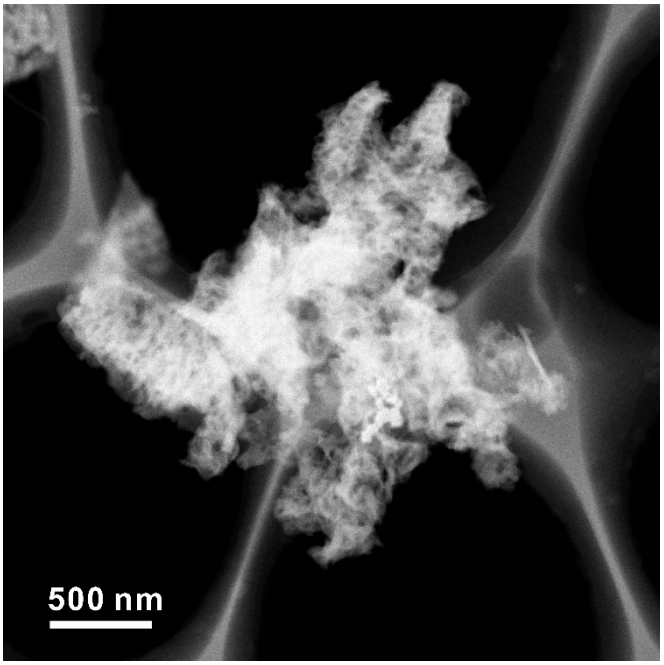


Fig. S10 TEM image of $Pd_1/g\text{-}C_3N_4$ after 6 cycles photocatalytic Heck reaction.

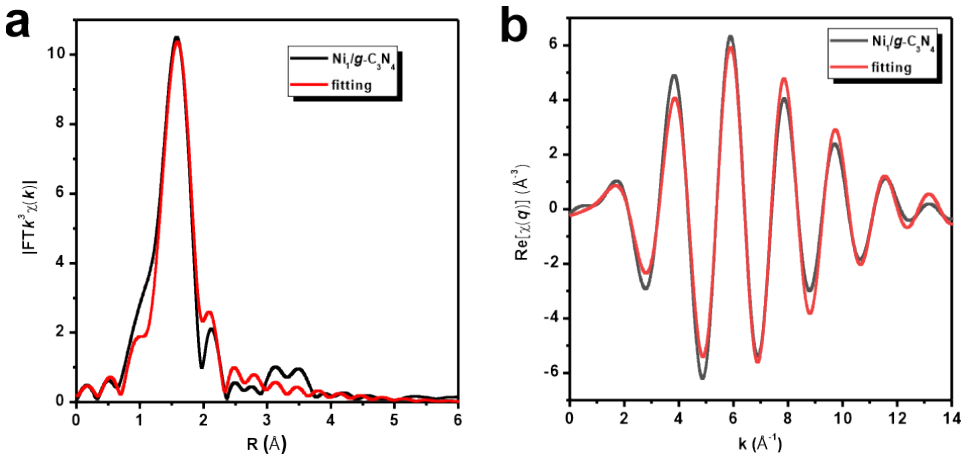


Fig. S11 Fourier-transformed magnitudes of Ni K-edge EXAFS spectra in (c) R space and (d) K space for $Ni_1/g\text{-}C_3N_4$.

Table S1. Structural parameters of $Pd_1/g\text{-}C_3N_4$ at the Pd *K*-edge extracted from quantitative EXAFS curve-fitting using ARTEMIS module of IFEFFIT.

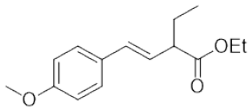
Sample	Path	CN	R(Å)	$\sigma^2(10^{-3}Å^2)$	ΔE_0 (eV)
$Pd_1/g\text{-}C_3N_4$	Pd-N	4.3	2.06	4.1	9.3

CN, coordination number; *R*, bonding distance; σ^2, Debye-Waller factor; ΔE_0, inner potential shift

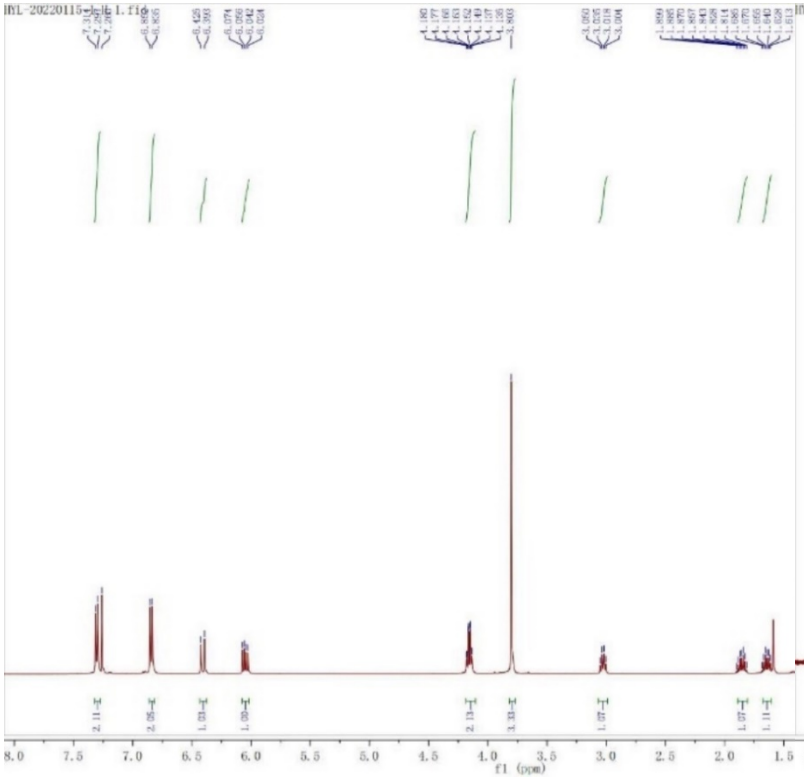
Table S2. Structural parameters of $Ni_1/g\text{-}C_3N_4$ at the Pd *K*-edge extracted from quantitative EXAFS curve-fitting using ARTEMIS module of IFEFFIT.

Sample	Path	CN	R(Å)	$\sigma^2(10^{-3}Å^2)$	ΔE_0 (eV)
$Ni_1/g\text{-}C_3N_4$	Ni-N	7.3	2.03	4.0	-8.4

CN, coordination number; *R*, bonding distance; σ^2, Debye-Waller factor; ΔE_0, inner potential shift



Ethyl(E)-2-ethyl-4-(4-methoxyphenyl)but-3-enoate, PE/EtOAc =40:1, colourless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.5 Hz, 2H), 6.84 (d, *J* = 8.5, 2H), 6.40 (d, *J* = 16.0 Hz, 1H), 6.05 (dd, *J* = 16.0, 9.0 Hz, 1H), 4.18 – 4.13 (m, 2H), 3.80 (s, 3H), 3.02 (dd, *J* = 16.0, 7.5 Hz, 1H), 1.89 – 1.81 (m, 1H), 1.68 – 1.61 (m, 1H), 1.26 (t, *J* = 7.0, 3H), 0.94 (t, *J* = 7.5, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.34, 159.10, 131.50, 129.71, 127.44, 125.47, 113.91, 77.25, 77.00, 76.75, 60.50, 55.28, 51.34, 26.04, 14.24, 11.69.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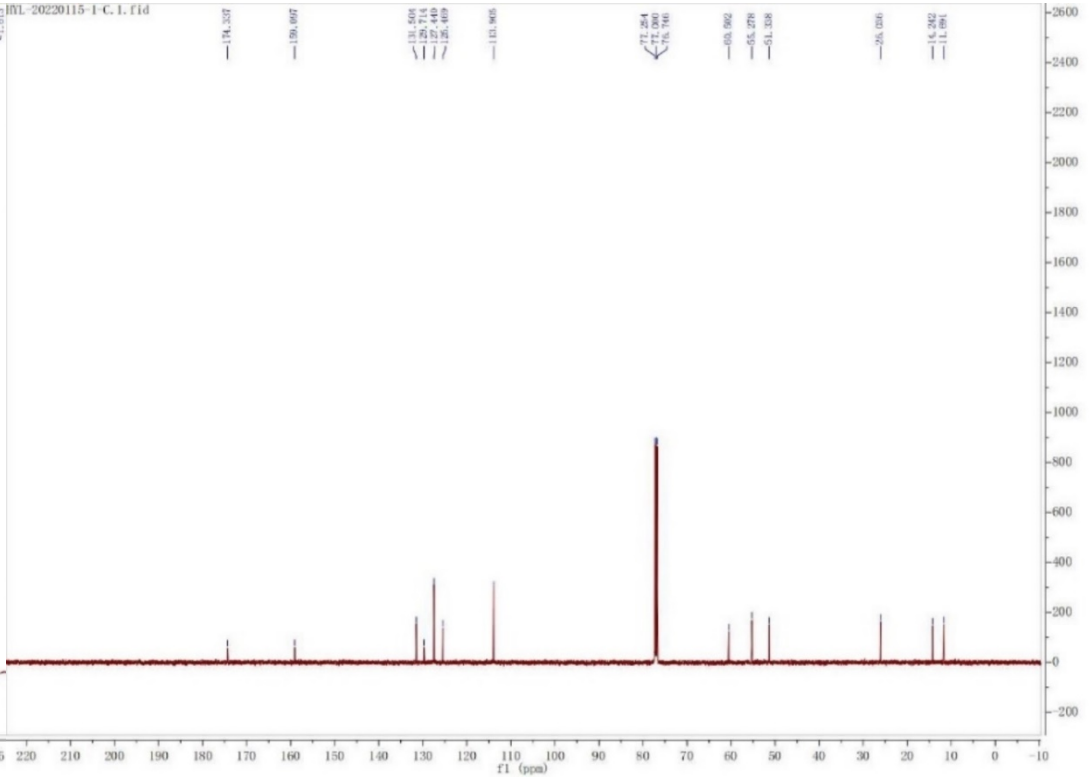
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