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SYNTHESIS, CHARACTERIZATION, HIRSHFELD AND ADMET ESTIMATION STUDIES OF NOVEL 3-(2,4,6-TRIMETHYL-PHENYLAMINO)-BUT-2-ENOATE

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Table S1

Crystallographic data, details of data collection, and structure refinement parameters for compound 3.

Parameters	*Value*
Chemical formula	$C_{15}H_{21}NO_2$
Formula weight (g/mol)	247.33
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P* $2_1/c$
Temperature	100 K
Unit cell dimensions	*a*= 8.5003 (3) Å, *b*= 20.0682 (8) Å, *c*= 8.1720 (4) Å *α*= 90° , *β*= 94.6882°, *γ*=90°
Volume	1389.36(10) $Å^3$
Z	4
Density (calculated)	1.182 g/cm^3
F(000)	536
Radiation type	Mo *Kα*
Theta range for data collection	2.4°–28.3°
Index ranges	−11 ≤ h ≤ 11, − 26 ≤ k ≤ 25, − 10 ≤ l≤ 10
Tmin,Tmax	0.951 ;0.995
Reflections collected	41590
Independent reflections	4960[R(int) = 0.035]
Absorption correction	Multi-scan BRUKER SADABS2016/2
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4960/0/139
Goodness-of-fit on F2	1.068
Δ/σmax	0.002
Refinement	R[F^2>2σ(F^2)], *w*R(F^2), s 0.042, 0.107, 1.03
Final R indices I > 2σ(I)	R1 = 0.035, wR2 = 0.0912
Final R indices all data	R1 = 0.1855, wR2 = 0.1206
Weighting scheme	$w = 1/[\sigma 2(F_o{}^2) + (0.044P)^2 + 0.5544P]$ where $P = (F_o{}^2 + 2F_c{}^2)/3$
Largest diff. peak and hole	0.26 and − 0.23 $eÅ^{-3}$
R.M.S. deviation from mean	0.026 $eÅ^{-3}$

Table S2

Hydrogen-bond geometry in the crystal structure of compound 3.

Hydrogen-bond geometry (Å, °)				
D—*H*···*A*	*D*—*H*	*H*···*A*	*D*···*A*	*D*—*H*···*A*
N1—H1*N*···O2	0.855(17)	2.087(17)	2.7484(14)	133.8(14)
N1—H1*N*···O2^{i}	0.855(17)	2.486(17)	3.1550(14)	135.8(14)
C1—H1C···O2^{ii}	0.98	2.65	3.5084(17)	146

Symmetry codes: (i) −x+1, −y+1, −z+1; (ii) −x+2, −y+1, −z+1

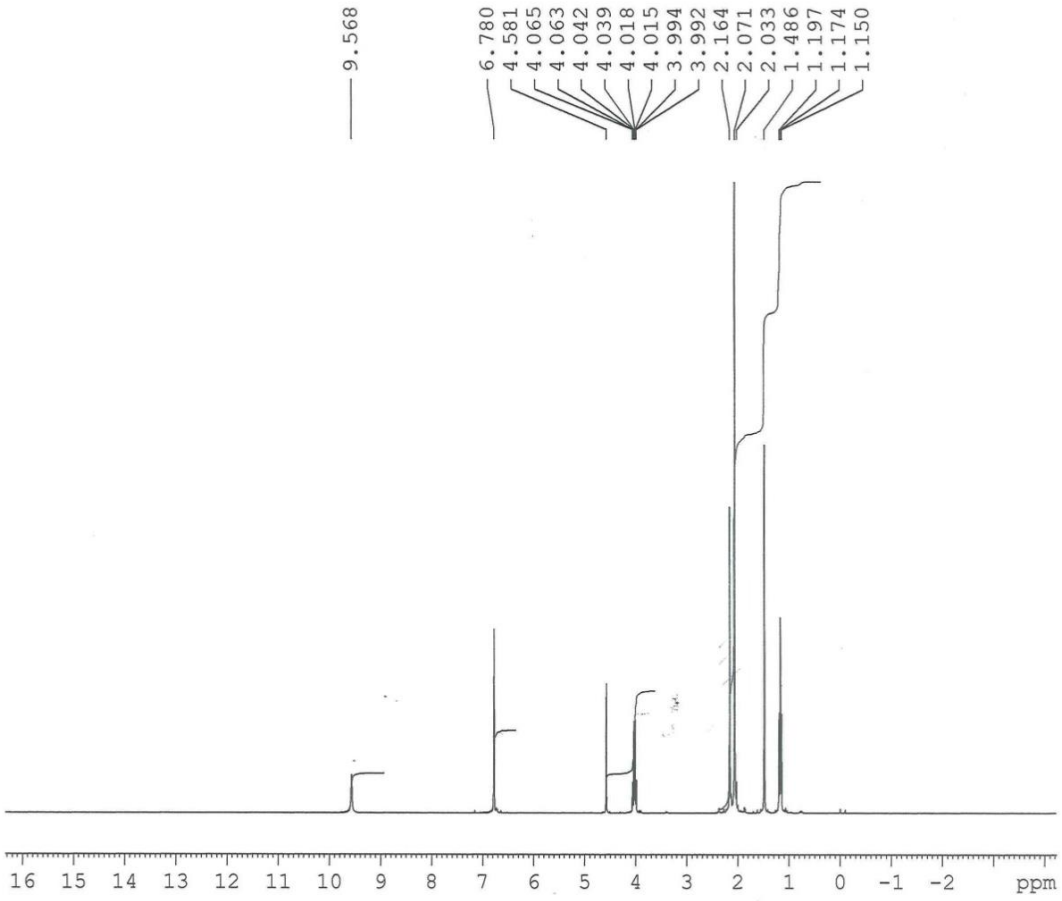

Figure. S1. ^{1}H NMR (300 MHz) spectrum of compound 3.

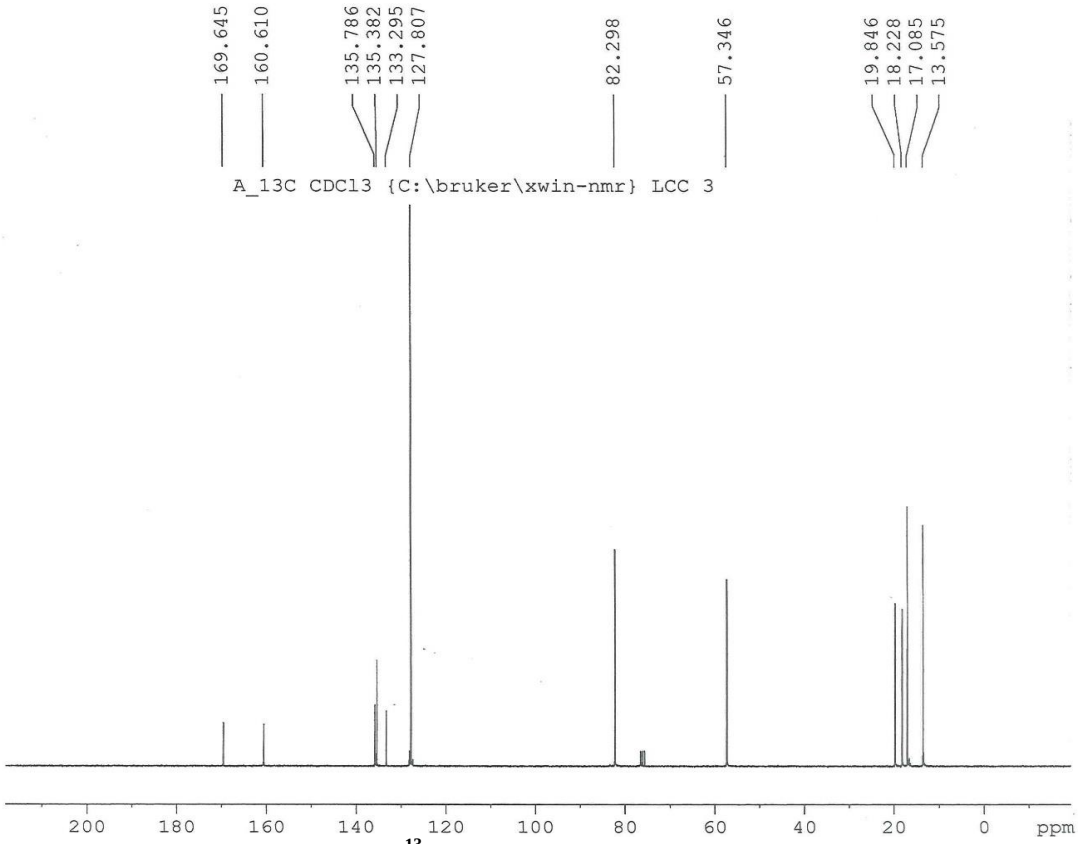

Figure. S2. ^{13}C NMR (75 MHz) spectrum of compound 3.

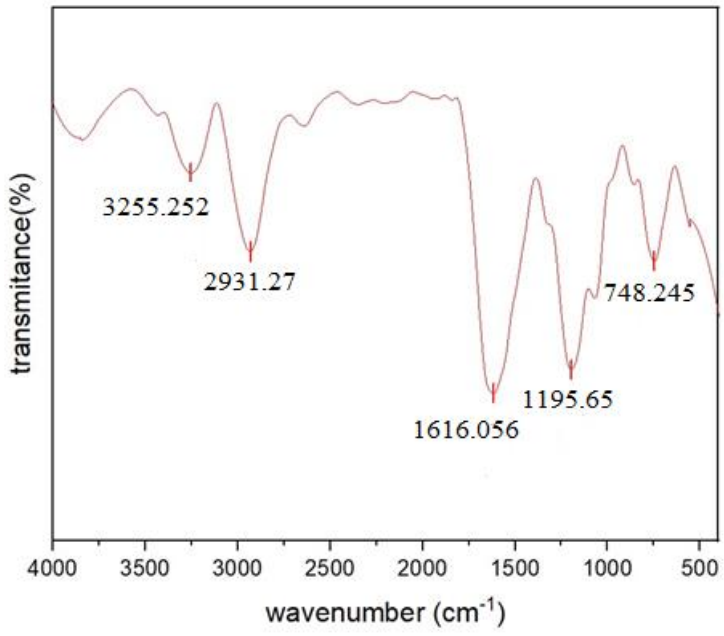

Figure. S3. Experimental infrared spectrum of compound 3.

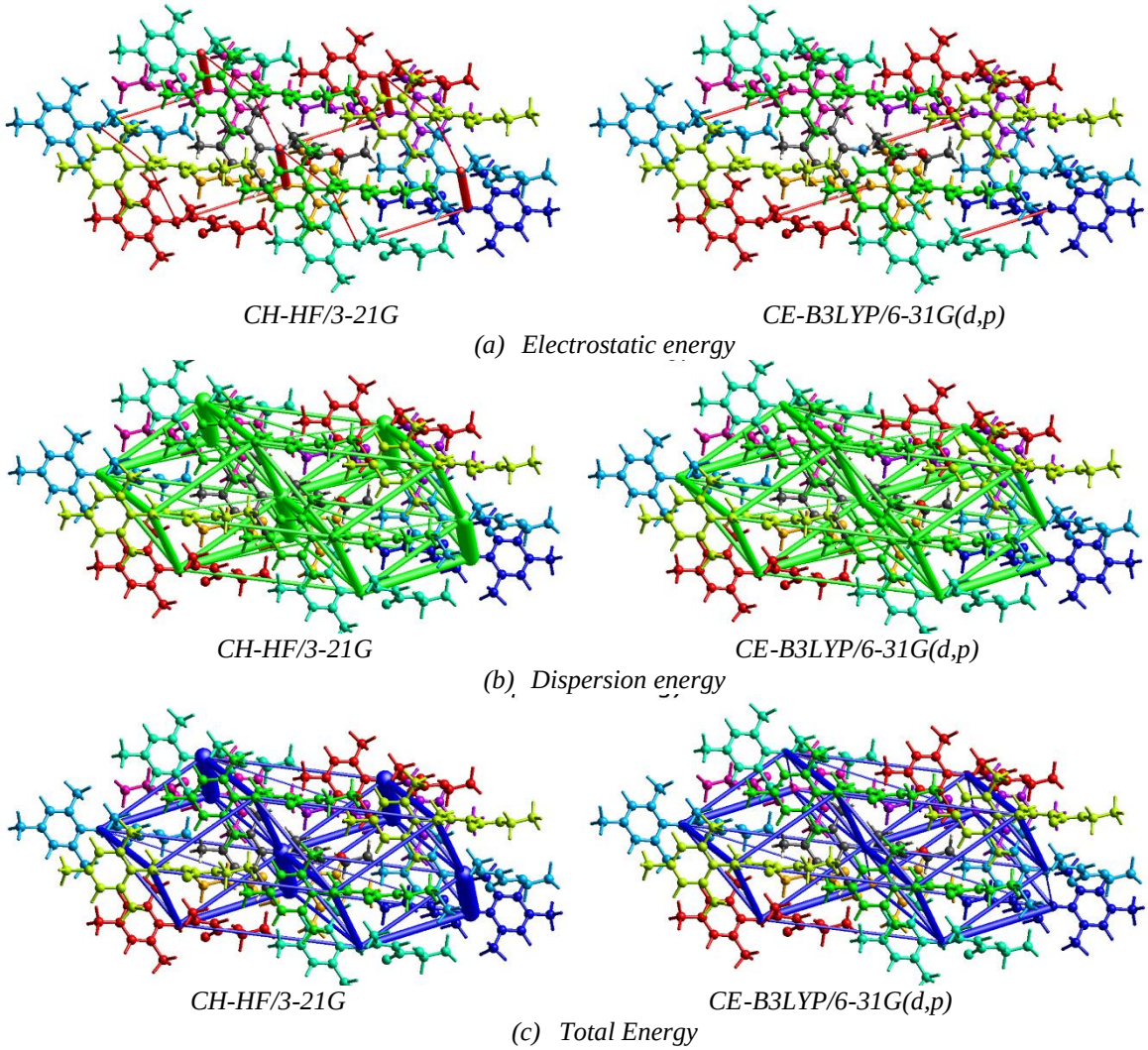

Figure. S4. Energy frameworks corresponding to the different energy components and the total interaction energy. *(a)* Energy framework diagram for separate electrostatic energy, *(b)* dispersion energy and *(c)* the total interaction energy components of the title molecule, results using CE-HF/3-21G (left side) and CE-B3LYP/6–31G(d,p) (right site). The energy factor scale is 100 and the cut-off is5.00kJ/mol.

Table S2

Area percent report of GC.

Peak	*Retention time, min*	*Area, pA·s*	*Height, pA*	*Area, %*
1	4.24139	3.77961	1.23719	0.037229
2	4.70875	7.10704	1.86031	0.070005
3	5.63347	1.67466	0.36761	0.016496
4	6.02592	1285.30859	383.73224	12.66039
5	6.67259	10.70552	2.35478	0.10545
6	6.94303	536.85901	134.27452	5.288104
7	8.37119	2.98387	0.40576	0.029391
8	8.80731	6.41165	0.36927	0.063155
9	9.58086	4.24333	0.67956	0.041797
10	10.84589	8266.28613	466.50247	81.42358
11	18.71644	14.98868	0.49225	0.14764
12	20.27569	11.85334	0.40598	0.116756