ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO: SYNTHESIS, CRYSTAL STRUCTURE, AND DFT STUDY OF N-(2-FLUORO-4-(4,4,5,5-TETRAMETHYL-1,3,2-DIOXIN-2-YL)PHENYL)-3-METHYL-BUTANAMIDE

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Contents:

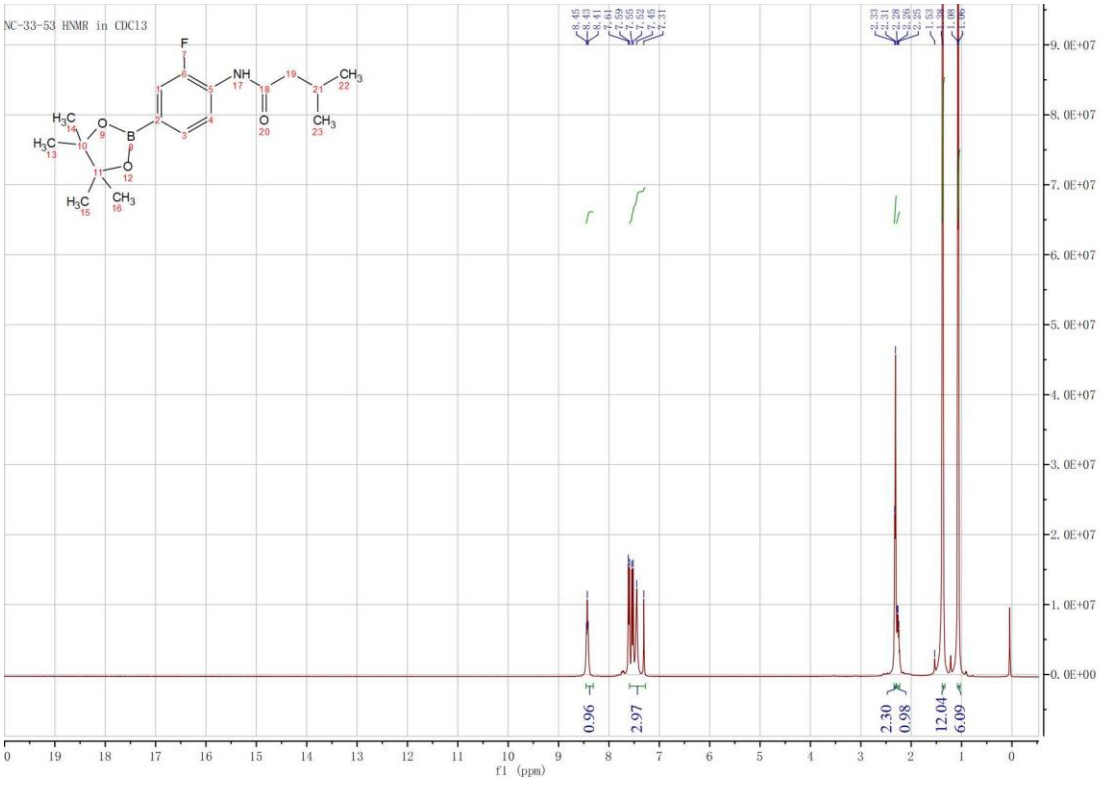

Fig. S1. [1]H-NMR spectrum of **1.**

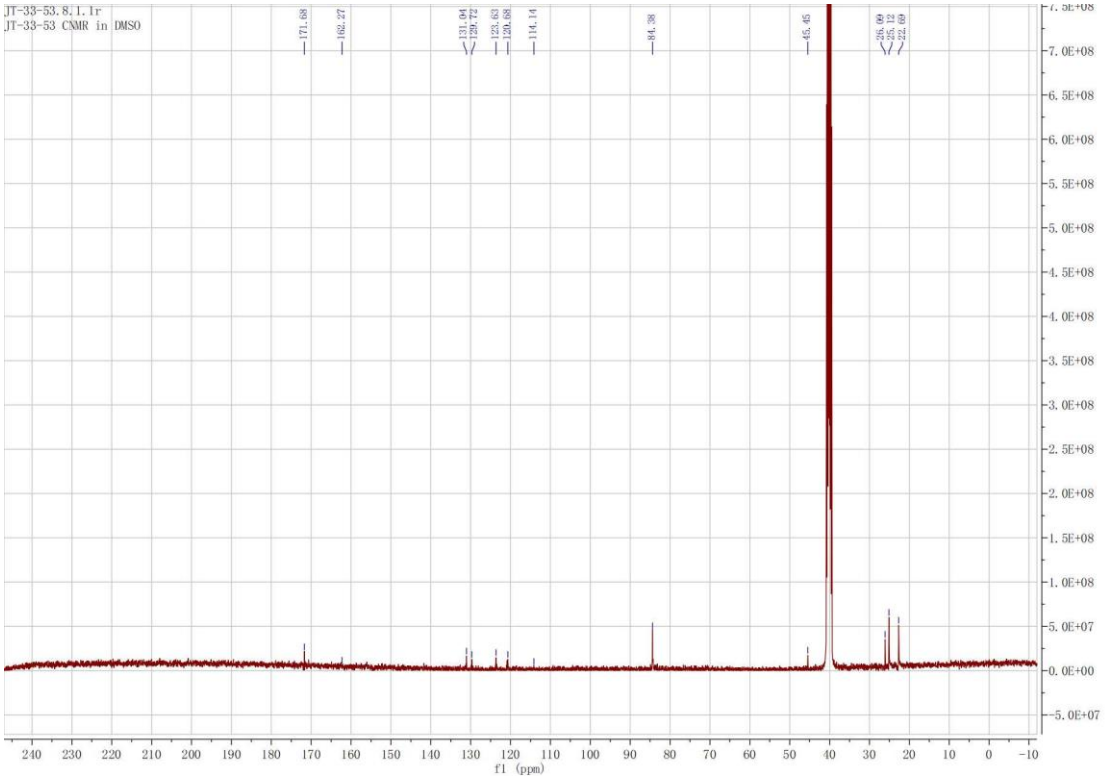

Fig.S2. ^{13}C-NMR spectrum of **1.**

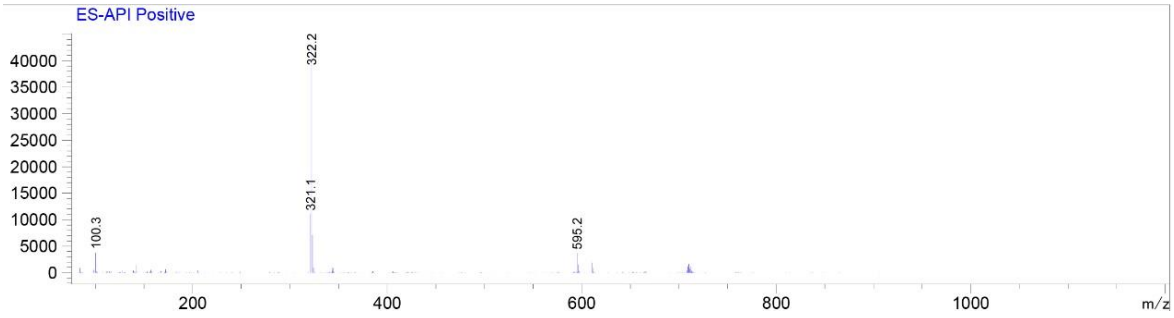

Fig.S3. MS spectrum of **1.**

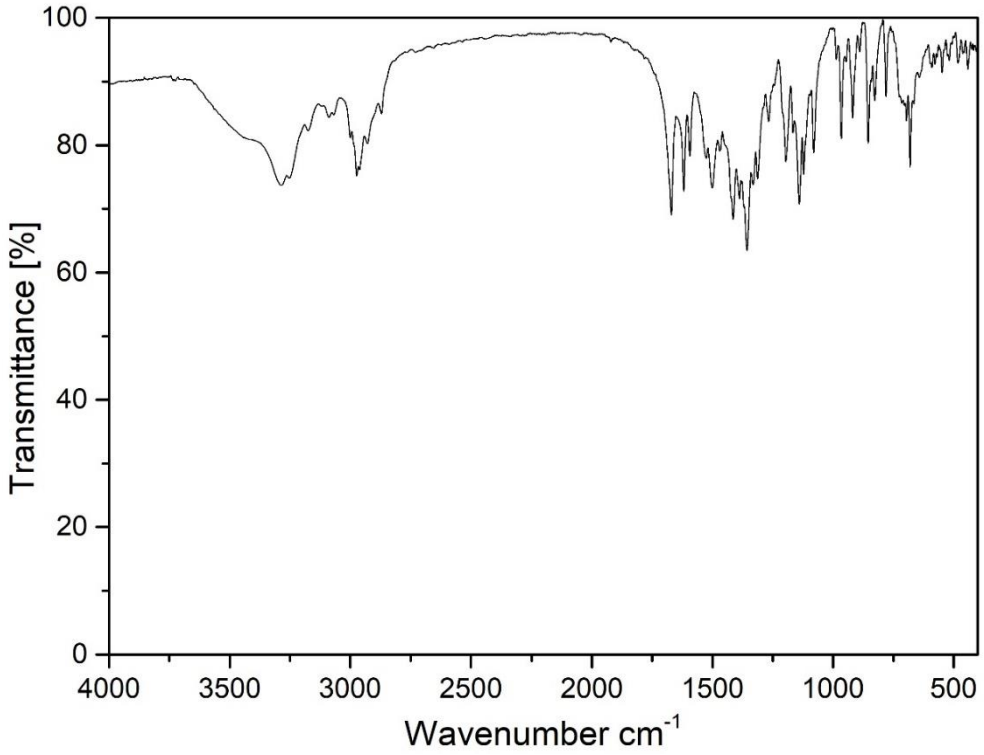

Fig. S4. IR spectrum of **1**

Table.S1. Crystal data and structure refinement for 1

Compound	1
CCDC	2033664
Molecular formula	$C_{17}H_{25}BFNO_3$
Molecular weight	321.19
Crystal system	Monoclinic
Space group	C2
a(Å)	14.6248(17)
b(Å)	12.9570(15)
c(Å)	19.785(3)
α (o)	90
β (o)	108.023(4)
γ (o)	90
V (Å3)	3565.2(7)
T,K	100
Z	8
μ (mm-1)	0.087
Radiation λ (Å)	0.71073
Ranges/indices (h, k, l)	$-18 \leqslant h \leqslant 16$, $-16 \leqslant k \leqslant 15$, $-24 \leqslant l \leqslant 24$
θ limit (o)	5.204 to 52.82
N(hkl)measured,	14986
N(hkl)unique	6057 [$R_{(int)} = 0.0765$]
N(param)refined	428
Diffractometer	Bruker APEX II
Scan mode	φ - ω
Programs	SHELXL-2018/3