Supplementary Information

Synthesis, Crystal Structures, and Molecular Properties of three Nitro-Substituted Chalcones

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Figure S1. ^{1}H NMR (600 MHz, DMSO-d_6) of compound **1a:** (*E*)-1,3-bis(2-nitrophenyl)prop-2-en-1-one.

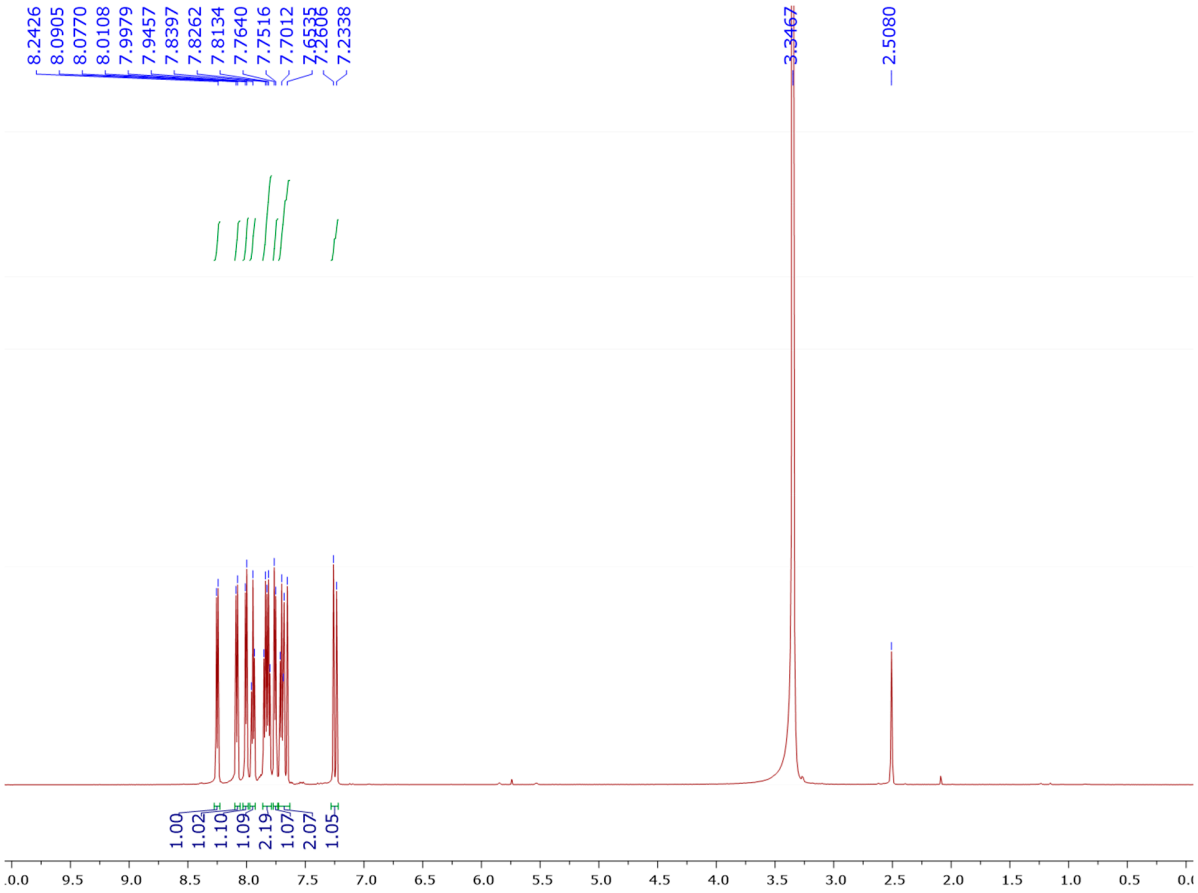

Figure S2. DEPTQ NMR (150 MHz, DMSO-d_6) of compound **1a:** (*E*)-1,3-bis(2-nitrophenyl)prop-2-en-1-one.

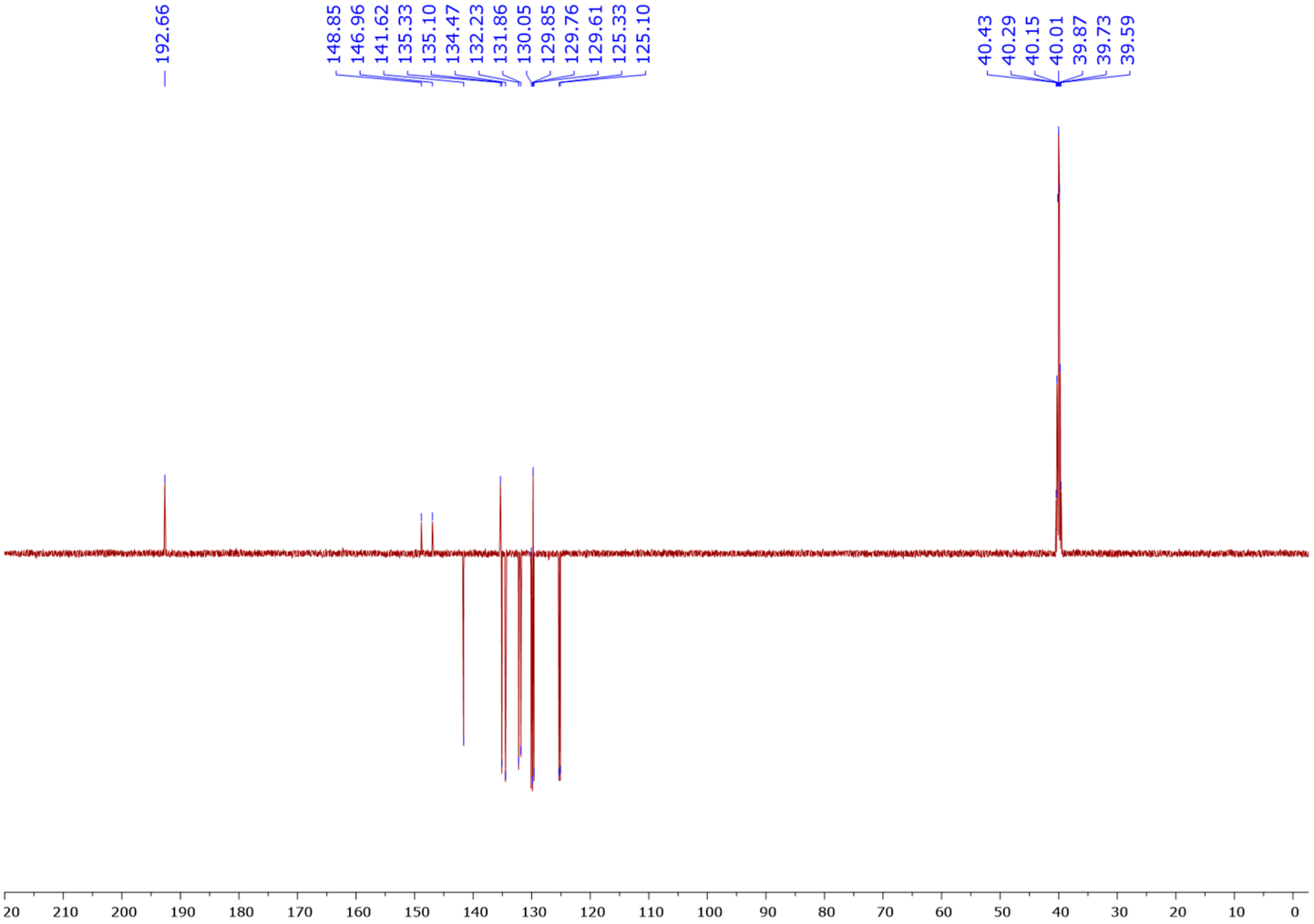

Figure S3. ^{1}H NMR (600 MHz, DMSO-d_6) of compound **1b:** (*E*)-1-(2-nitrophenyl)-3-(3-nitrophenyl)prop-2-en-1-one.

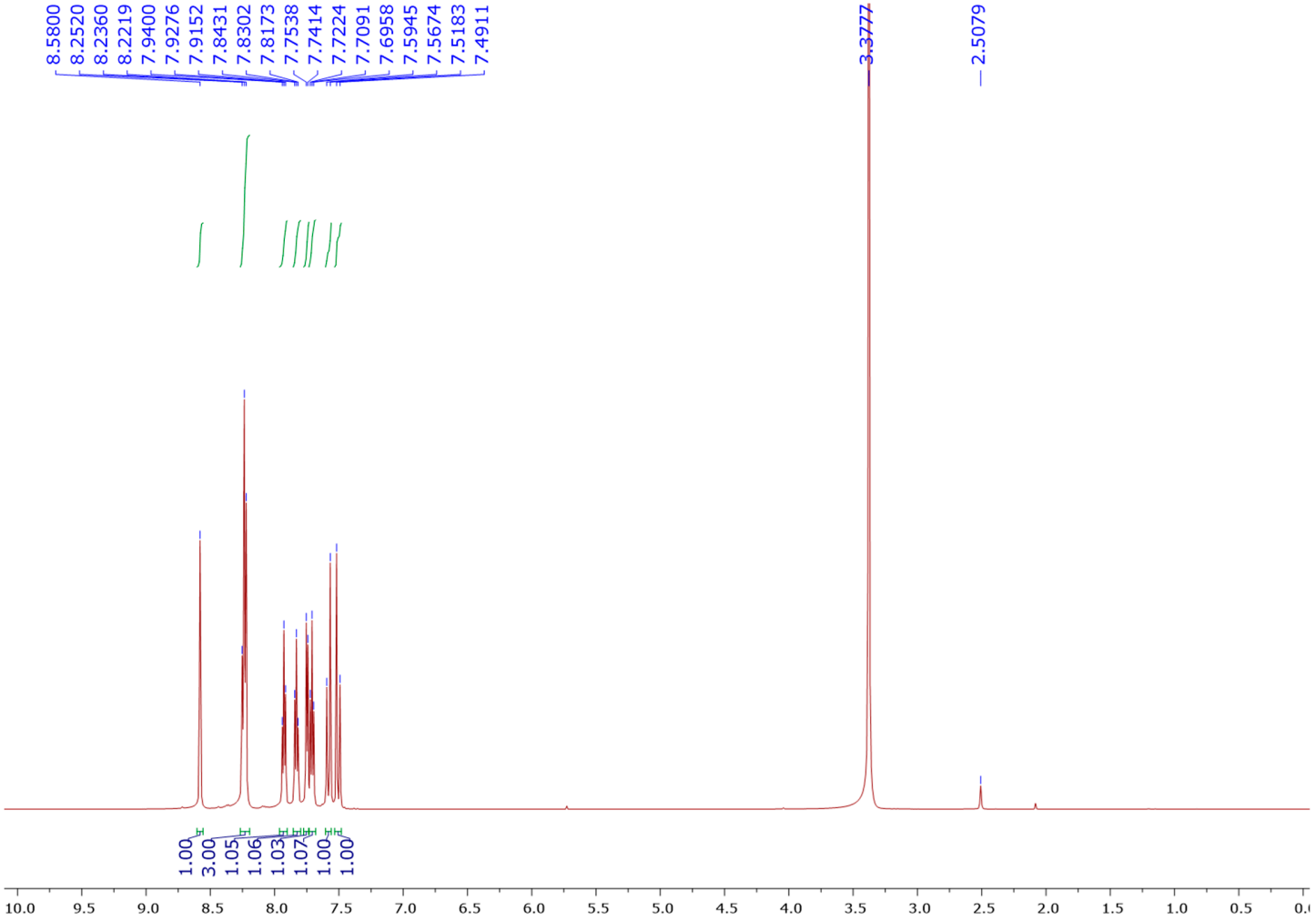

Figure S4. DEPTQ NMR (150 MHz, DMSO-d_6) of compound **1b:** (*E*)-1-(2-nitrophenyl)-3-(3-nitrophenyl)prop-2-en-1-one.

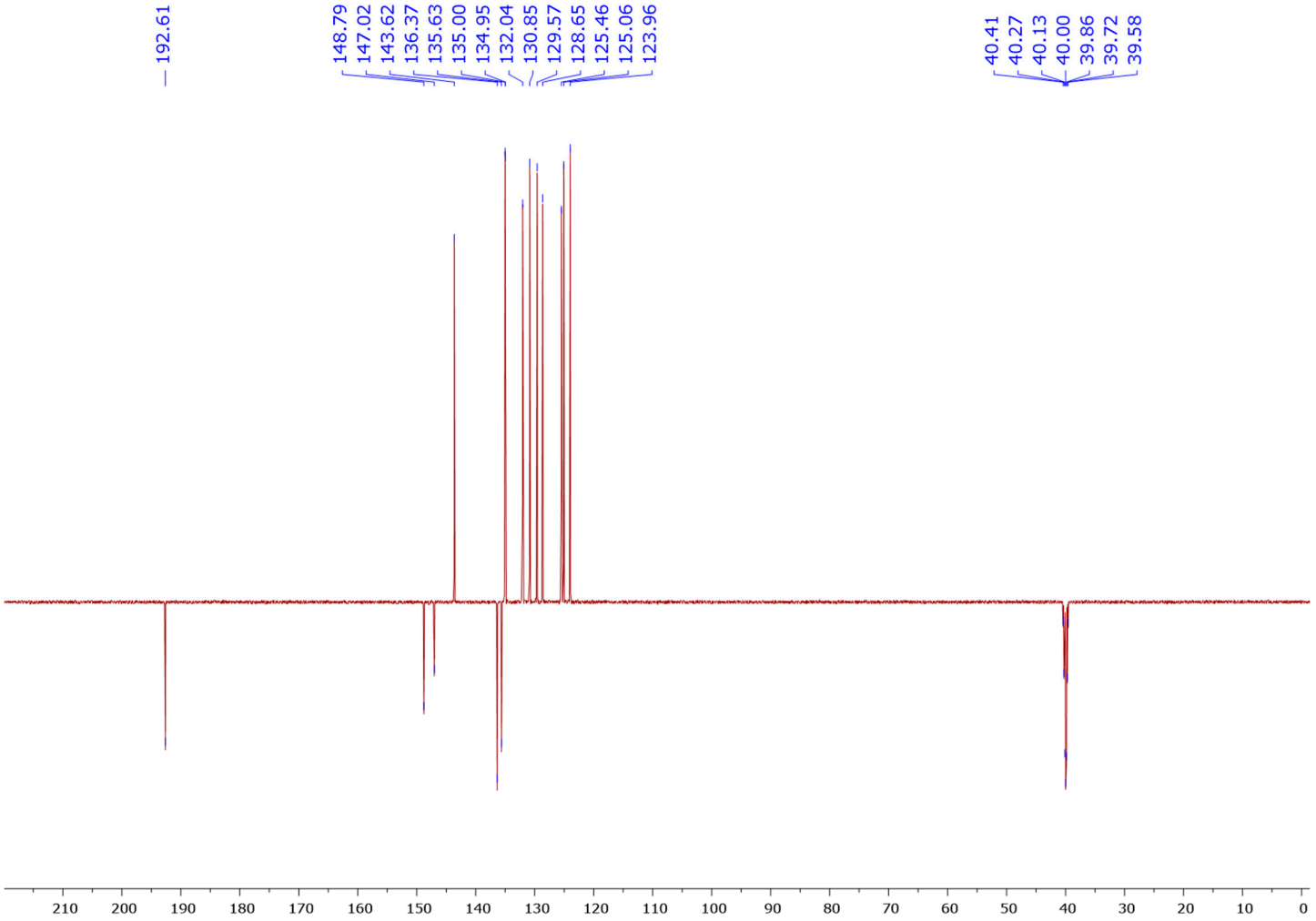

Figure S5. ^{1}H NMR (600 MHz, DMSO-d_6) of compound **1c:** (*E*)-1-(2-nitrophenyl)-3-(4-nitrophenyl)prop-2-en-1-one.

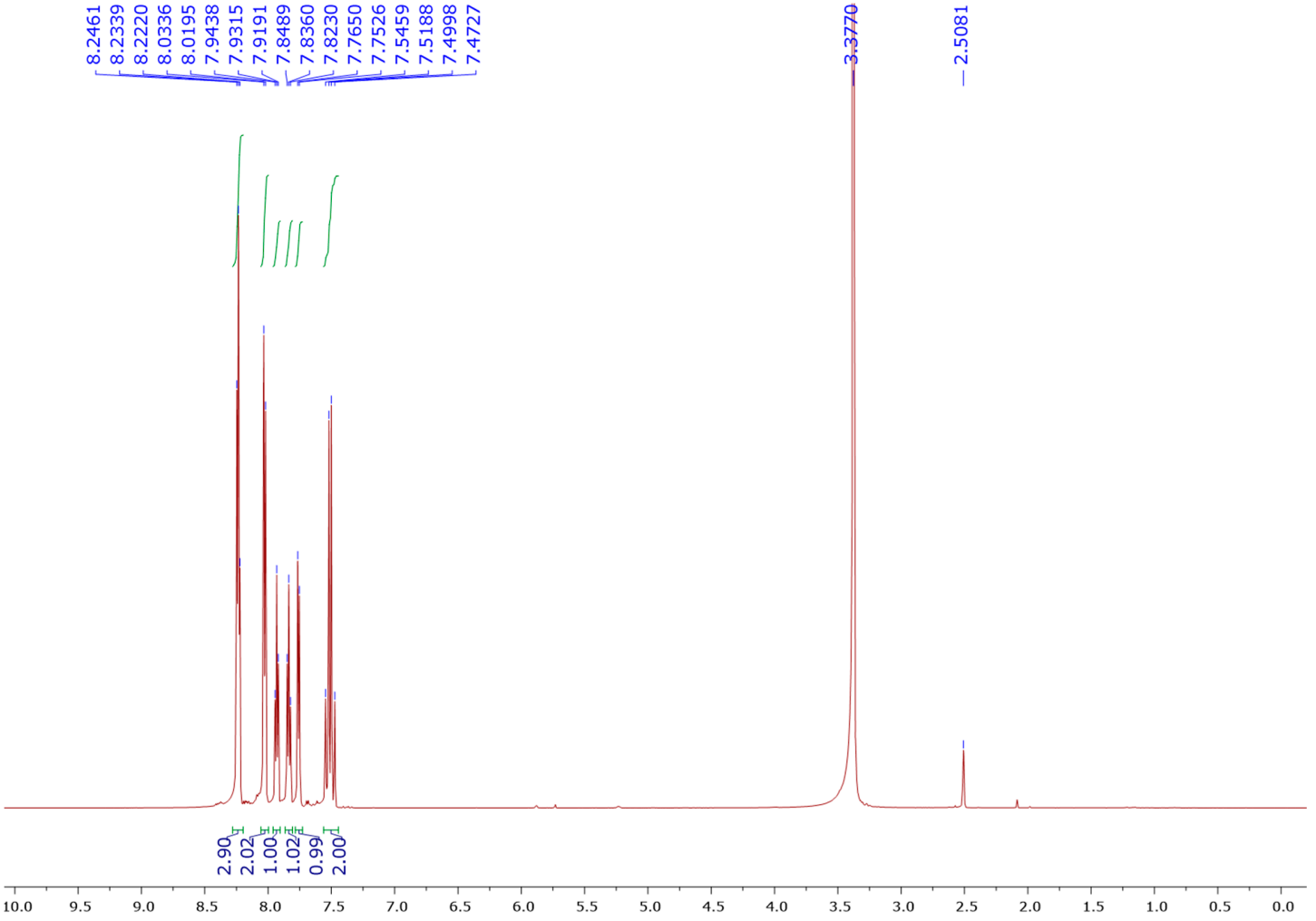

Figure S6. DEPTQ NMR (150 MHz, DMSO-d_6) of compound **1c:** (*E*)-1-(2-nitrophenyl)-3-(4-nitrophenyl)prop-2-en-1-one.

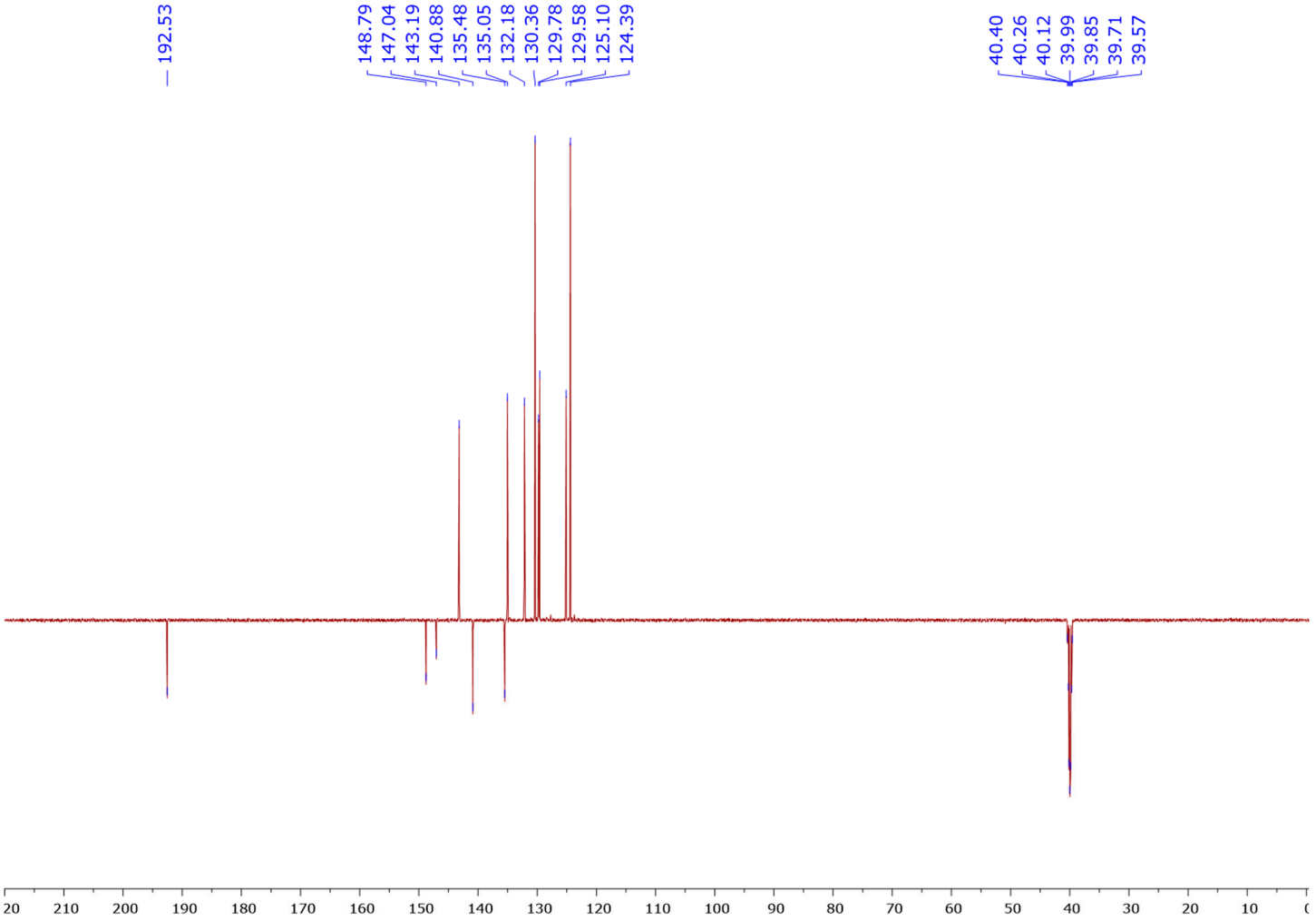

Figure S7. FT-IR Spectrum of **1a-1c.**

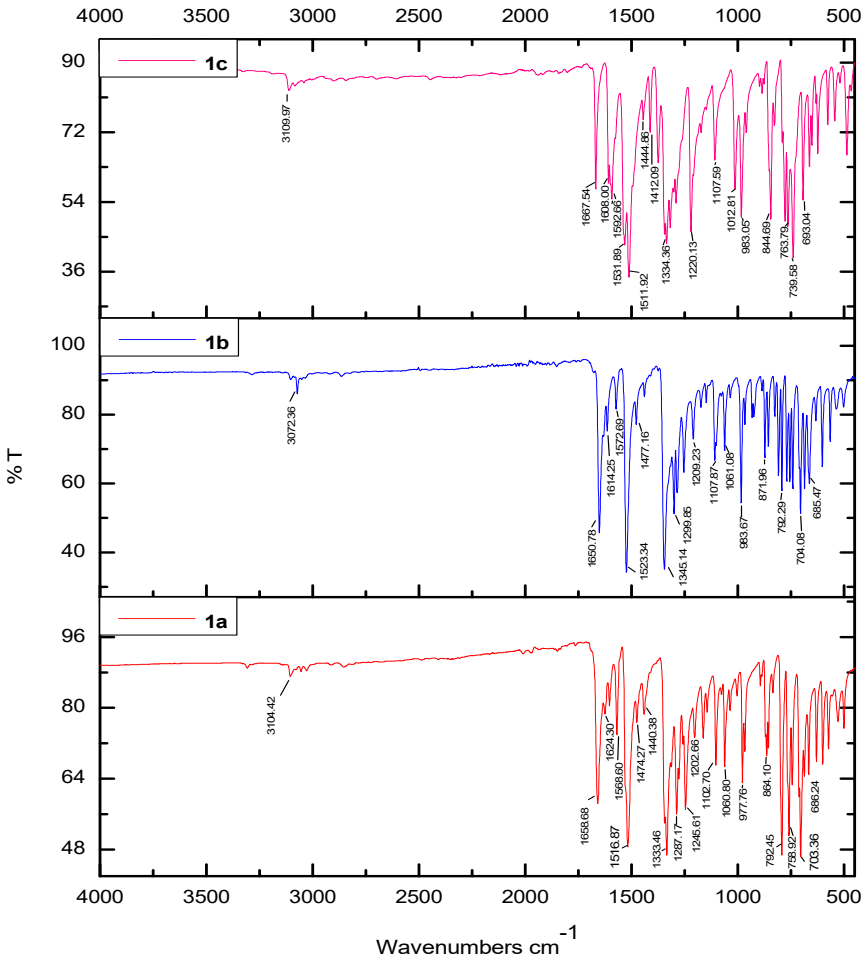

Tabla S1. Assignment of characteristic vibrational frequencies for **1a-1c.**

Assignment	**1a**	**1b**	**1c**
Aromatic C-H stretching vibration	3104	3072	3109
C=O stretching vibration	1658	1650	1667
C = C stretching vibration	1516	1523	1511
N–O asymmetric stretch vibration of NO_2 group	1568	1572	1592
N–O symmetric stretch vibration of NO_2 group	1333	1345	1334
C–H in plane deformation of CH = CH	1202	1209	1220
C = C *trans*	977	983	983

Figure S8. A view of the crystal packing down the *b* axis for compound **1a.**

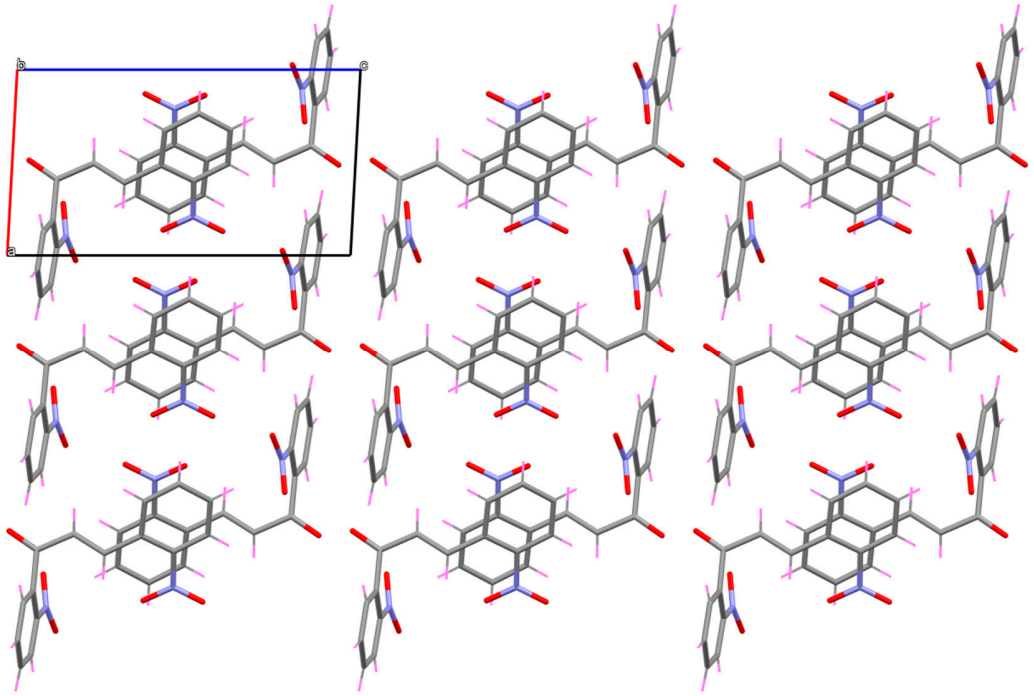

Figure S9. A view of the crystal packing down the *b* axis for compound **1b.**

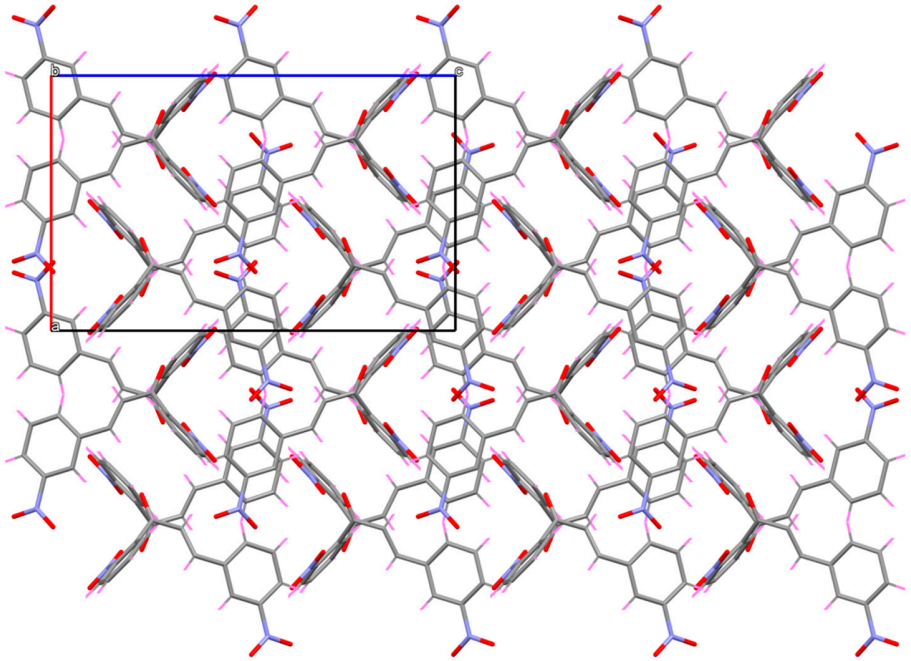

Figure S10. A view of the crystal packing down the *a* axis for compound **1c.**

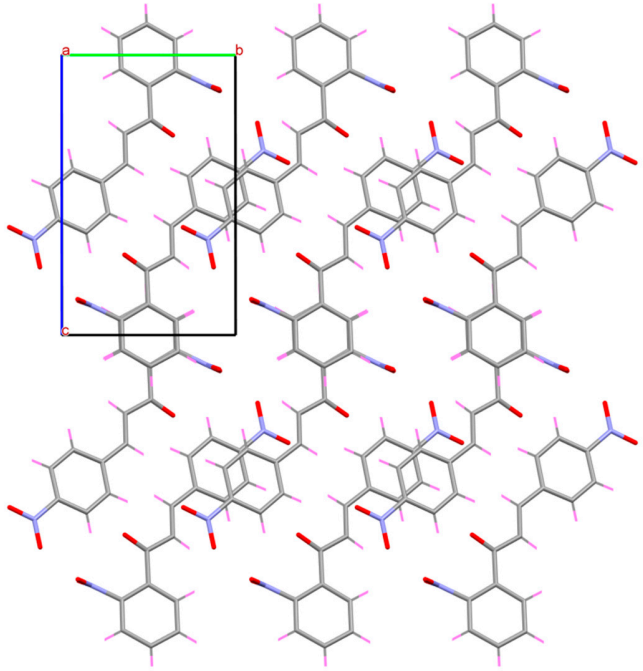

Figure S11. 2D fingerprint plot of **1a**, showing π-π stacking contacts [*de* and *di* represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

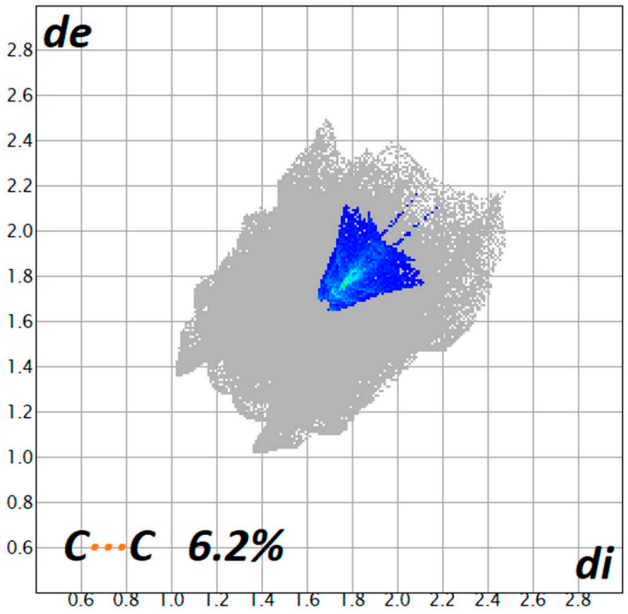

Figure S12. 2D fingerprint plot of **1c**, showing C-H···O contacts [*de* and *di* represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

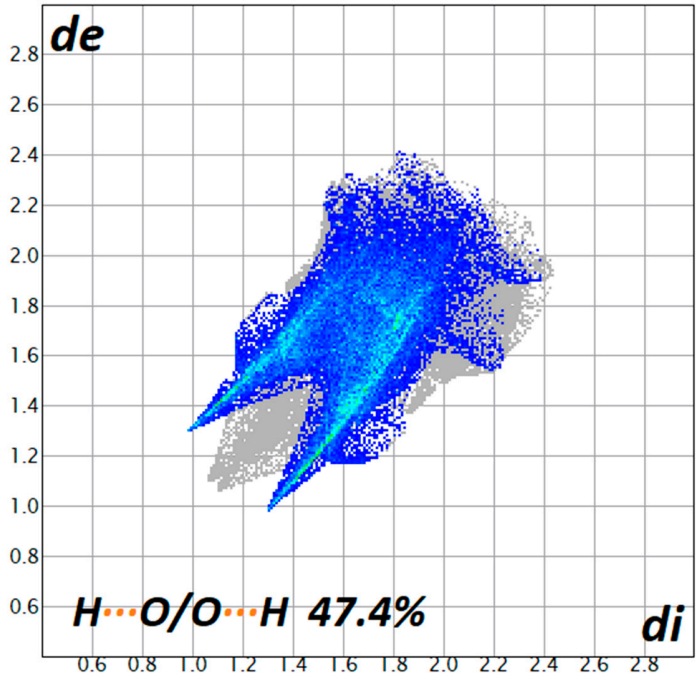

Table S2. Selected Bond lengths [Å] and angles [°] for **1a**

O(1)-N(1)	1.2273(12)
O(2)-N(1)	1.2311(11)
O(3)-N(2)	1.2290(12)
O(4)-N(2)	1.2291(12)
N(1)-C(2')	1.4690(13)
N(2)-C(2)	1.4715(13)
C(1)-C(9)	1.4760(14)
C(2)-C(3)	1.3894(14)
C(3)-C(4)	1.3834(15)
C(4)-C(5)	1.3871(16)
C(5)-C(6)	1.3903(15)
C(7)-O(7)	1.2179(12)
C(7)-C(8)	1.4728(14)
C(7)-C(1')	1.5125(13)
C(8)-C(9)	1.3369(14)
C(1')-C(6')	1.3957(14)
C(1')-C(2')	1.3978(14)
C(2')-C(3')	1.3881(13)
C(3')-C(4')	1.3868(15)
C(5')-C(6')	1.3928(14)
O(1)-N(1)-O(2)	123.38(9)

O(1)-N(1)-C(2')	118.56(9)
O(2)-N(1)-C(2')	118.05(8)
O(3)-N(2)-O(4)	123.18(9)
O(3)-N(2)-C(2)	118.66(9)
O(4)-N(2)-C(2)	118.15(9)
C(6)-C(1)-C(2)	116.05(9)
C(6)-C(1)-C(9)	118.38(9)
C(2)-C(1)-C(9)	125.51(9)
C(3)-C(2)-C(1)	123.00(9)
C(3)-C(2)-N(2)	116.04(9)
C(1)-C(2)-N(2)	120.94(9)
C(4)-C(3)-C(2)	119.13(10)
C(3)-C(4)-C(5)	119.71(10)
C(4)-C(5)-C(6)	120.56(10)
C(5)-C(6)-C(1)	121.53(10)
O(7)-C(7)-C(8)	121.72(9)
O(7)-C(7)-C(1')	119.20(9)
C(8)-C(7)-C(1')	118.90(8)
C(9)-C(8)-C(7)	123.40(9)
C(8)-C(9)-C(1)	122.21(9)
C(6')-C(1')-C(2')	117.44(9)
C(6')-C(1')-C(7)	117.40(9)
C(2')-C(1')-C(7)	125.12(9)
C(3')-C(2')-C(1')	122.62(10)

C(3')-C(2')-N(1)	117.52(9)
C(1')-C(2')-N(1)	119.77(9)
C(4')-C(3')-C(2')	118.72(10)
C(3')-C(4')-C(5')	120.10(9)

Table S3. Selected Bond lengths [Å] and angles [°] for **1b**

O(1)-N(1)	1.2182(19)
O(2)-N(1)	1.2135(19)
O(3)-N(2)	1.219(2)
O(4)-N(2)	1.2216(19)
N(1)-C(2')	1.469(2)
N(2)-C(3)	1.469(2)
C(1)-C(9)	1.465(2)
C(2)-C(3)	1.378(2)
C(1')-C(7)	1.510(2)
C(2')-C(3')	1.380(2)
C(3')-C(4')	1.366(3)
C(7)-O(7)	1.2177(18)
C(7)-C(8)	1.452(2)

C(8)-C(9)	1.324(2)
O(2)-N(1)-O(1)	123.57(16)
O(2)-N(1)-C(2')	118.24(15)
O(1)-N(1)-C(2')	118.19(16)
O(3)-N(2)-O(4)	123.03(17)
O(3)-N(2)-C(3)	118.46(14)
O(4)-N(2)-C(3)	118.50(17)
C(6)-C(1)-C(9)	122.37(14)
C(3)-C(2)-C(1)	119.04(14)
C(4)-C(3)-C(2)	122.77(15)
C(4)-C(3)-N(2)	118.47(15)
C(2)-C(3)-N(2)	118.75(15)
C(3)-C(4)-C(5)	117.92(16)
C(6)-C(5)-C(4)	120.83(16)
C(5)-C(6)-C(1)	120.83(16)
C(2')-C(1')-C(6')	116.89(15)
C(2')-C(1')-C(7)	125.45(15)
C(6')-C(1')-C(7)	117.62(15)
C(3')-C(2')-C(1')	122.82(16)
C(3')-C(2')-N(1)	117.40(15)
C(1')-C(2')-N(1)	119.75(14)
O(7)-C(7)-C(1')	119.33(15)
C(8)-C(7)-C(1')	119.26(13)

Table S4. Selected Bond lengths [Å] and angles [°] for **1c**

O(1)-N(1)	1.199(2)
O(2)-N(1)	1.206(2)
O(3)-N(2)	1.2181(18)
O(4)-N(2)	1.2144(19)
N(1)-C(2')	1.4759(19)
N(2)-C(4)	1.473(2)
C(1)-C(9)	1.466(2)
C(7)-O(7B)	1.214(7)
C(7)-O(7A)	1.251(12)
C(7)-C(8)	1.479(2)
C(7)-C(1')	1.491(2)
C(8)-C(9)	1.321(2)
O(1)-N(1)-O(2)	123.49(16)
O(1)-N(1)-C(2')	118.10(15)
O(2)-N(1)-C(2')	118.30(16)
O(4)-N(2)-O(3)	123.76(16)
O(4)-N(2)-C(4)	118.56(15)
O(3)-N(2)-C(4)	117.68(16)
C(6)-C(1)-C(2)	118.33(14)
C(6)-C(1)-C(9)	118.80(14)
C(2)-C(1)-C(9)	122.83(14)
C(3)-C(2)-C(1)	120.63(15)

C(4)-C(3)-C(2)	119.21(13)
C(3)-C(4)-C(5)	122.21(14)
C(3)-C(4)-N(2)	119.74(14)
C(5)-C(4)-N(2)	118.03(15)
C(4)-C(5)-C(6)	118.04(15)
C(5)-C(6)-C(1)	121.57(14)
O(7B)-C(7)-C(8)	121.7(4)
O(7A)-C(7)-C(8)	118.1(9)
O(7B)-C(7)-C(1')	117.4(5)
O(7A)-C(7)-C(1')	120.0(7)
C(8)-C(7)-C(1')	119.85(13)
C(9)-C(8)-C(7)	120.50(15)
C(8)-C(9)-C(1)	128.26(15)
C(6')-C(1')-C(2')	116.22(14)
C(6')-C(1')-C(7)	122.56(13)
C(2')-C(1')-C(7)	121.03(13)
C(3')-C(2')-C(1')	123.05(14)
C(3')-C(2')-N(1)	116.07(13)
C(4')-C(5')-C(6')	120.14(15)
C(5')-C(6')-C(1')	121.58(14)

Table S5. Hydrogen-bond geometry for **1a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C9-H9...O3	0.95	2.33	2.672 (13)	100.3

Table S6. Hydrogen-bond geometry for **1b** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C8-H8...O1	0.93	2.56	3.37(2)	146.4
C2-H2...O7	0.93	2.56	3.37(2)	145.3

Table S7. Hydrogen-bond geometry for **1c** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)-H(3)...O(7A)	0.93	2.40	3.103(4)	102.7
C9-H9...O7B	0.93	2.46	2.798(9)	101.7