Synthesis

Reviews and Full Papers in Chemical Synthesis

Supporting Information

for DOI: 10.1055/s-0034-1380185

Thieme

Novel One-Pot, Multicomponent Synthetic Strategy for the Synthesis of Pyrrolo[1,2-*a*]benzimidazole and Pyrrolo[1,2-*a*]quinoxaline Derivatives

Emilian Georgescu,[a] Alina Nicolescu,[b,c] Florentina Georgescu,[d] Sergiu Shova,[c,e] Florina Teodorescu,[b] Ana-Maria Macsim,[c] Calin Deleanu.[b,c]*

[a] Research Center Oltchim, St. Uzinei 1, RO-240050 Ramnicu Valcea, Romania.
[b] "C. D. Nenitescu" Centre of Organic Chemistry, Roumanian Academy, Spl. Independentei 202-B, RO-060023 Bucharest, Romania.
[c] "Petru Poni" Institute of Macromolecular Chemistry, Roumanian Academy, Aleea Grigore Ghica Voda 41-A, RO-700487 Iasi, Romania.
[d] Research Dept., Teso Spec S. R. L., Str. Muncii 53, RO-915200 Fundulea, Calarasi, Romania.
[e] Institute of Chemistry, Academy of Sciences, Str. Academiei 3, MD-2028, Chisinau, Republic of Moldova.
E-mail: calin.deleanu@yahoo.com
Received: The date will be inserted once the manuscript is accepted.

Supporting Information

Materials and Methods.

X-Ray crystallographic measurements were carried out with an Oxford-Diffraction XCALIBUR E CCD diffractometer equipped with graphite-monochromated Mo-Kα radiation. Single crystals were positioned at 40 mm from the detector and 346, 298 and 424 frames were measured each for 150, 200 and 150 s over 1° scan width for **4a**, **5c** and **8c**, respectively. The unit cell determination and data integration were carried out using the CrysAlis package of Oxford Diffraction.[1] The structures were solved by direct methods using Olex2[2] and refined by full-matrix least-squares on F^2 with SHELXL-97.[3] Atomic displacements for non-hydrogen, atoms were refined using an anisotropic model. All H atoms were introduced in idealized positions (dCH = 0.96 Å) using the riding model with their isotropic displacement parameters fixed at 120% of their riding atom. In the absence of significant anomalous scattering, the absolute configuration for 4a and 5c structures could not be reliably determined. Friedel pairs were merged and any references to the Flack parameter were removed. The **8c** sample gave a weak diffraction and the resolution of the collected X-ray data has been estimated to be 1.0 Å. Nevertheless the structure could be solved and electron density of the molecule was well defined allowing to determine the atomic connectivity and to refine the model with anisotropic temperature factors. Trifluoracetic acid and water solvate molecules were found to be severely disordered and their positional parameters were refined in combination with PART and SADI restraints using isotropic model for non-H atoms. Taking into account these areas of possible solvent inclusion, the "*Use solvent mask routine*" subroutine of the Olex2 was used to account for the scattering from a disordered solvent molecule. As the result, the value of R_{1obs} has been reduced from 0.1551 to 0.0995. The molecular plots were obtained using the Olex2 program.

X-ray crystallography

These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK).

4a: $C_{27}H_{20}N_2O_3$, Mr = 420.45 g mol^{-1}, size 0.40×0.02×0.02 mm^3, monoclinic, space group $P2_1$, a = 4.5150(7) Å, b = 9.9297(13) Å, c = 22.904(4) Å, β = 91.867(14)°, V = 1026.3(3) Å^3, Z = 2, ρ_{calcd} = 1.361 g cm^{-3}, μ(Mo$K\alpha$) = 0.090 mm^{-1}, F(000) = 440, 7599 reflections in h(-4/5), k(-12/12), l(-28/28), measured in the range 3.56 ≤ Θ ≤ 51.98, T = 173 K, completeness Θ_{max}=99.91%, 2156 independent reflections, R_{int} = 0.1328, 290 parameters, 1 restraints, R_{1obs}=0.0967, wR_{2obs} = 0.1749, R_{1all} = 0.1664, wR_{2all} = 0.2003, GoF = 1.036, largest difference peak and hole: 0.34/-0.31 e A^{-3}. CCDC – 980024.

5c: $C_{28}H_{22}F_2N_2O_3$, Mr = 472.48 g mol^{-1}, size 1.00×0.70×0.03 mm^3, triclinic, space group P-1, a = 7.1282(14) Å, b = 8.8913(18) Å, c = 19.611(3) Å, α = 102.928(15)°, β = 91.713(14)°, γ = 106.364(17)°, V = 1156.6(4) Å^3, Z = 2, ρ_{calcd} = 1.357 g cm^{-3}, μ(Mo$K\alpha$) = 0.100 mm^{-1}, F(000) = 492, 7429 reflections in h(-8/7), k(-10/10), l(-14/24), measured in the range 4.92 ≤ Θ ≤ 52.00, T = 173 K, completeness Θ_{max}=98.90%, 4479 independent reflections, R_{int} = 0.0722, 317 parameters, 0 restraints, R_{1obs}=0.0694, wR_{2obs} = 0.12038, R_{1all} = 0.1547, wR_{2all} = 0.1502, GoF = 0.939, largest difference peak and hole: 0.29/-0.32 e A^{-3}. CCDC – 980025.

8c: $C_{21.7}H_{18.55}F_{3.55}N_2O_{5.05}$, Mr = 455.59 g mol^{-1}, size 0.50×0.05×0.05 mm^3, triclinic, space group P-1, a = 3.8246(5) Å, b = 13.713(2) Å, c = 20.895(3) Å, α = 104.754(14)°, β = 93.402(13)°, γ = 90.436(12)°, V = 1057.6(3) Å^3, Z = 2, ρ_{calcd} = 1.431 g cm^{-3}, μ(Mo$K\alpha$) = 0.122 mm^{-1}, F(000) = 470, 6743 reflections in h(-8/7), k(-12/15), l(-23/17), measured in the range 3.08 ≤ Θ ≤ 46.52, T = 160 K, completeness Θ_{max}=99.40%, 3031 independent reflections, R_{int} = 0.1099, 293 parameters, 14 restraints, R_{1obs}=0.0995, wR_{2obs} = 0.2308, R_{1all} = 0.1667, wR_{2all} = 0.2636, GoF = 0.959, largest difference peak and hole: 0.31/-0.27 e A^{-3}. CCDC – 1036766.

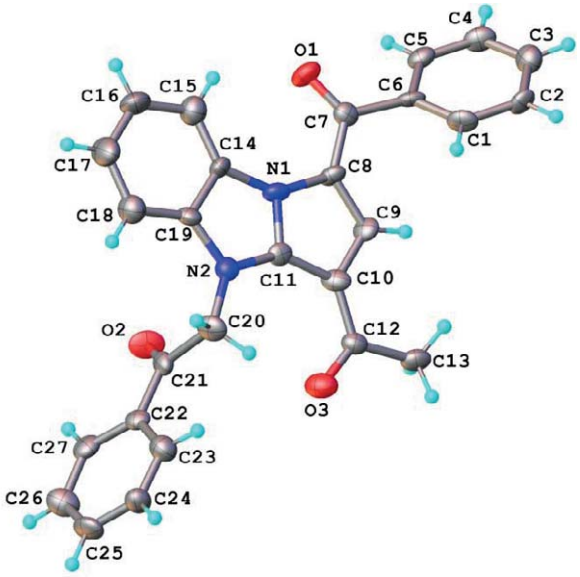


Figure 1S. X-ray molecular structure of compound **4a**. Thermal ellipsoids are drawn at 50% probability level.

Table 1S. Bond lengths (Å) for compound **4a**.

O1-C7	**1.223(9)**	**C9-C10**	**1.40(1)**
O2-C21	1.22(1)	C10-C11	1.42(1)
O3-C12	1.246(9)	C10-C12	1.42(1)
N1-C8	1.43(1)	C12-C13	1.50(1)
N1-C11	1.381(9)	C14-C15	1.36(1)
N1-C14	1.42(1)	C14-C19	1.41(1)
N2-C11	1.37(1)	C15-C16	1.39(1)
N2-C19	1.41(1)	C16-C17	1.39(1)
N2-C20	1.47(1)	C17-C18	1.37(1)
C1-C2	1.39(1)	C18-C19	1.38(1)
C1-C6	1.40(1)	C20-C21	1.53(1)
C2-C3	1.40(1)	C21-C22	1.46(1)
C3-C4	1.34(1)	C22-C23	1.44(1)
C4-C5	1.36(1)	C22-C27	1.39(1)
C5-C6	1.38(1)	C23-C24	1.35(1)
C6-C7	1.49(1)	C24-C25	1.36(1)
C7-C8	1.43(1)	C25-C26	1.38(1)
C8-C9	1.37(1)	C26-C27	1.41(1)

Table 2S. Bond angles (º) for compound **4a**.

C11N1C8	108.2(6)	N2C11C10	141.7(8)
C11N1C14	109.6(6)	O3C12C10	122.8(8)
C14N1C8	142.2(7)	O3C12C13	118.7(7)
C11N2C19	109.2(6)	C10C12C13	118.5(8)
C11N2C20	127.5(7)	C15C14N1	133.2(9)
C19N2C20	123.2(7)	C15C14C19	120.8(8)
C2C1C6	121.5(7)	C19C14N1	105.9(7)
C1C2C3	117.7(8)	C14C15C16	117.1(9)
C4C3C2	120.6(8)	C17C16C15	121.6(9)
C3C4C5	121.3(8)	C18C17C16	122.2(9)
C4C5C6	121.0(8)	C17C18C19	115.8(9)
C1C6C7	122.9(7)	N2C19C14	107.6(7)
C5C6C1	117.7(8)	C18C19N2	130.0(7)
C5C6C7	119.2(7)	C18C19C14	122.4(8)
O1C7C6	119.3(7)	N2C20C21	111.3(7)
O1C7C8	122.1(8)	O2C21C20	120.4(7)
C8C7C6	118.6(7)	O2C21C22	121.9(8)
N1C8C7	123.9(7)	C22C21C20	117.7(8)
C9C8N1	104.6(7)	C23C22C21	123.0(7)
C9C8C7	131.5(8)	C27C22C21	119.0(8)
C8C9C10	113.9(8)	C27C22C23	118.0(8)
C9C10C11	102.6(8)	C24C23C22	120.6(9)
C9C10C12	128.7(8)	C23C24C25	121.7(9)

C12C10C11	128.5(8)	C24C25C26	119.5(8)
N1C11C10	110.7(7)	C25C26C27	120.8(9)
N2C11N1	107.7(7)	C22C27C26	119.3(9)

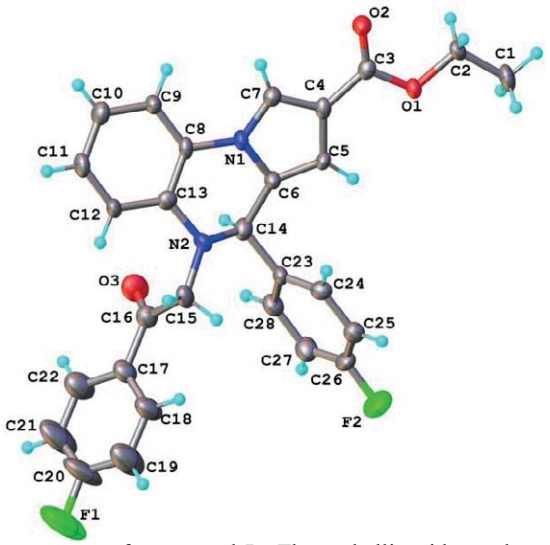


Figure 2S. X-ray molecular structure of compound **5c**. Thermal ellipsoids are drawn at 50% probability level.

Table 3S. Bond lengths (Å) for compound **5c**.

F1-C20	1.374(5)	C9-C10	1.383(4)
F2-C26	1.363(4)	C10-C11	1.371(5)
O1-C2	1.455(3)	C11-C12	1.376(5)
O1-C3	1.346(4)	C12-C13	1.396(4)
O2-C3	1.200(4)	C14-C23	1.506(5)
O3-C16	1.219(4)	C15-C16	1.518(4)
N1-C6	1.393(4)	C16-C17	1.482(5)
N1-C7	1.360(4)	C17-C18	1.387(5)
N1-C8	1.412(3)	C17-C22	1.380(4)
N2-C13	1.402(4)	C18-C19	1.381(6)
N2-C14	1.479(3)	C19-C20	1.355(5)
N2-C15	1.438(4)	C20-C21	1.341(6)
C1-C2	1.497(4)	C21-C22	1.396(6)
C3-C4	1.468(4)	C23-C24	1.382(4)
C4-C5	1.421(5)	C23-C28	1.388(4)
C4-C7	1.363(4)	C24-C25	1.356(5)
C5-C6	1.356(4)	C25-C26	1.365(5)
C6-C14	1.495(5)	C26-C27	1.366(4)
C8-C9	1.390(5)	C27-C28	1.403(5)
C8-C13	1.382(5)		

Table 4S. Bond angles (º) for compound **5c**.

C3O1C2	113.9(3)	C12C13N2	123.5(3)
C6N1C8	121.7(3)	N2C14C6	107.1(3)
C7N1C6	109.6(2)	N2C14C23	112.2(3)
C7N1C8	128.7(3)	C6C14C23	112.8(3)
C13N2C14	114.7(3)	N2C15C16	115.8(3)
C13N2C15	119.5(3)	O3C16C15	120.3(3)
C15N2C14	118.8(3)	O3C16C17	123.1(3)
O1C2C1	107.8(3)	C17C16C15	116.6(3)
O1C3C4	111.9(3)	C18C17C16	122.3(3)
O2C3O1	123.7(3)	C22C17C16	118.9(4)
O2C3C4	124.4(3)	C22C17C18	118.8(4)
C5C4C3	130.4(3)	C19C18C17	121.8(4)
C7C4C3	121.6(4)	C20C19C18	117.0(5)
C7C4C5	107.9(3)	C19C20F1	115.8(5)
C6C5C4	107.6(3)	C21C20F1	120.2(5)
N1C6C14	116.2(3)	C21C20C19	124.0(5)
C5C6N1	107.3(3)	C20C21C22	119.1(4)
C5C6C14	136.3(3)	C17C22C21	119.4(4)

N1C7C4	107.7(3)	C24C23C14	122.9(3)
C9C8N1	120.3(3)	C24C23C28	118.5(3)
C13C8N1	117.6(3)	C28C23C14	118.6(3)
C13C8C9	122.0(3)	C25C24C23	121.8(3)
C10C9C8	119.5(3)	C24C25C26	118.6(3)
C11C10C9	118.8(4)	F2C26C25	119.1(3)
C10C11C12	121.8(3)	F2C26C27	117.7(4)
C11C12C13	120.4(3)	C25C26C27	123.2(4)
C8C13N2	119.0(3)	C26C27C28	117.3(4)
C8C13C12	117.4(3)	C23C28C27	120.6(3)

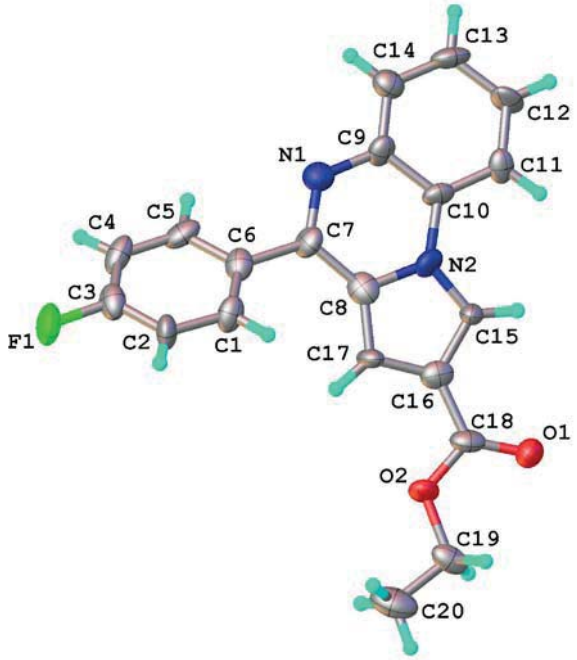


Figure 3S. X-ray molecular structure of compound **8c**. Thermal ellipsoids are drawn at 50% probability level.

Table 5S. Bond lengths (Å) for compound **8c**

F1-C3	1.38(1)	C12-C11	1.34(1)
O2-C18	1.34(1)	C16-C15	1.41(1)
O2-C19	1.44(1)	C6-C1	1.40(1)
N2-C10	1.39(1)	C6-C5	1.42(2)
N2-C8	1.43(1)	C1-C2	1.37(1)
N2-C15	1.32(1)	C3-C4	1.36(2)
O1-C18	1.26(1)	C3-C2	1.38(2)
N1-C9	1.39(1)	C4-C5	1.36(2)
N1-C7	1.33(1)	F7-C23	1.35(1)
C10-C9	1.42(1)	F6-C23	1.35(1)
C10-C11	1.39(1)	F5-C23	1.34(1)
C14-C9	1.35(2)	C24-O6	1.21(1)
C14-C13	1.37(2)	C24-O5	1.276(9)
C18-C16	1.44(2)	C24-C23	1.55(1)
C19-C20	1.45(2)	F2-C22	1.37(1)
C8-C7	1.42(2)	F4-C22	1.37(1)
C8-C17	1.39(2)	F3-C22	1.37(1)
C7-C6	1.50(2)	C22-C21	1.51(1)
C17-C16	1.38(1)	O3-C21	1.33(2)
C13-C12	1.39(2)	O4-C21	1.33(2)

Table 6S. Bond angles (º) for compound **8c**

C18-O2-C19	118.1(9)	C1-C6-C7	121.0(11)
C10-N2-C8	120.7(10)	C1-C6-C5	120.4(11)
C15-N2-C10	130.0(10)	C5-C6-C7	118.6(11)
C15-N2-C8	109.1(9)	C2-C1-C6	119.6(11)

C7-N1-C9	122.7(10)	C4-C3-F1	118.7(11)
N2-C10-C9	118.5(10)	C4-C3-C2	124.2(11)
N2-C10-C11	123.6(10)	C2-C3-F1	117.0(11)
C11-C10-C9	117.8(10)	N2-C15-C16	109.0(10)
C9-C14-C13	120.9(12)	C5-C4-C3	118.8(11)
O2-C18-C16	113.6(11)	C1-C2-C3	118.1(11)
O1-C18-O2	121.3(11)	C4-C5-C6	118.8(11)
O1-C18-C16	125.0(11)	O6-C24-O5	123(2)
O2-C19-C20	107.6(10)	O6-C24-C23	109.2(17)
N1-C9-C10	119.4(10)	O5-C24-C23	127.6(19)
C14-C9-N1	120.3(11)	F7-C23-F6	97.0(16)
C14-C9-C10	120.2(11)	F7-C23-C24	103.7(17)
C7-C8-N2	118.3(10)	F6-C23-C24	121.9(18)
C17-C8-N2	106.1(10)	F5-C23-F7	101.7(17)
C17-C8-C7	135.6(11)	F5-C23-F6	126(2)
N1-C7-C8	120.3(10)	F5-C23-C24	102.6(15)
N1-C7-C6	118.6(10)	F2-C22-F4	106.0(16)
C8-C7-C6	121.1(11)	F2-C22-F3	110.2(16)
C16-C17-C8	108.2(10)	F2-C22-C21	113.6(10)
C14-C13-C12	119.3(11)	F4-C22-F3	100.4(17)
C11-C12-C13	120.7(11)	F4-C22-C21	112.6(10)
C17-C16-C18	127.5(11)	F3-C22-C21	113.0(9)
C17-C16-C15	107.6(10)	O3-C21-C22	119.9(14)
C15-C16-C18	124.9(11)	O3-C21-O4	123(2)
C12-C11-C10	121.0(11)	O4-C21-C22	103.7(15)

References

[1] CrysAlis RED, Oxford Diffraction Ltd.,Version 1.171.34.76, 2003.

[2] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, “OLEX2: a complete structure solution, renement and analysis program”, *J. Appl. Cryst*., **2009**, *42*, 339-341.

[3] G. M. Sheldrick, SHELXS, *Acta Cryst*., **2008**, *A64*, 112-122

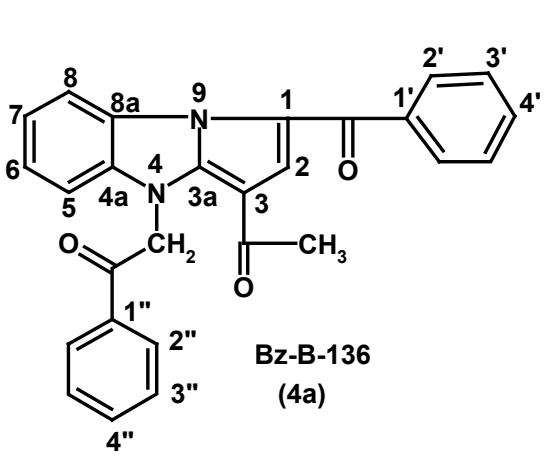
Novel One-Pot, Multicomponent Synthetic Strategy for the Synthesis of Pyrrolo[1,2-*a*]benzimidazole and Pyrrolo[1,2-*a*]quinoxaline Derivatives

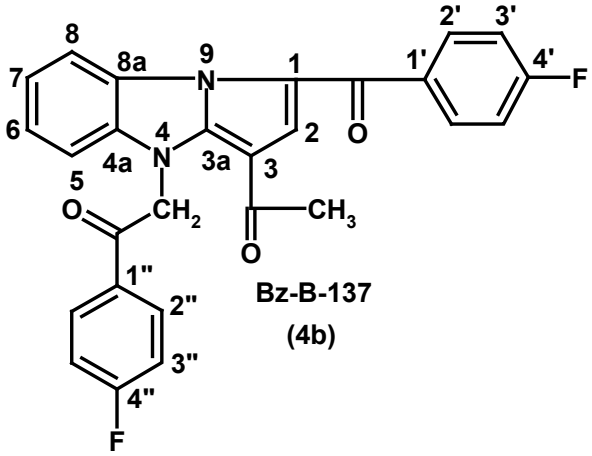
Emilian Georgescu,[a] Alina Nicolescu,[b,c] Florentina Georgescu,[d] Sergiu Shova,[c,e] Florina Teodorescu,[b] Ana-Maria Macsim,[c] Calin Deleanu.[b,c]*

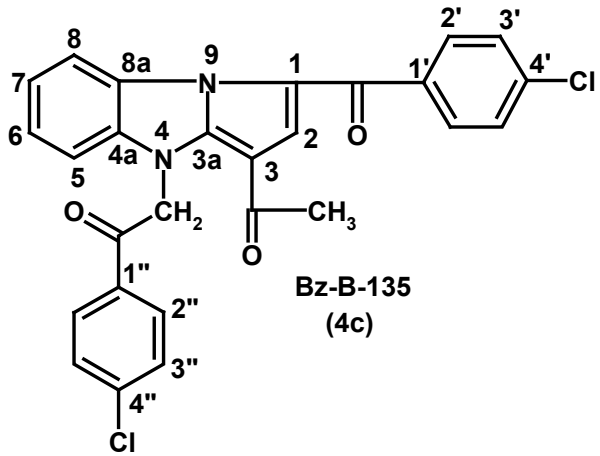
[a] Research Center Oltchim, St. Uzinei 1, RO-240050 Ramnicu Valcea, Romania.
[b] "C. D. Nenitescu" Centre of Organic Chemistry, Roumanian Academy, Spl. Independentei 202-B, RO-060023 Bucharest, Romania.
[c] "Petru Poni" Institute of Macromolecular Chemistry, Roumanian Academy, Aleea Grigore Ghica Voda 41-A, RO-700487 Iasi, Romania.
[d] Research Dept., Teso Spec S. R. L., Str. Muncii 53, RO-915200 Fundulea, Calarasi, Romania.
[e] Institute of Chemistry, Academy of Sciences, Str. Academiei 3, MD-2028, Chisinau, Republic of Moldova.
E-mail: calin.deleanu@yahoo.com

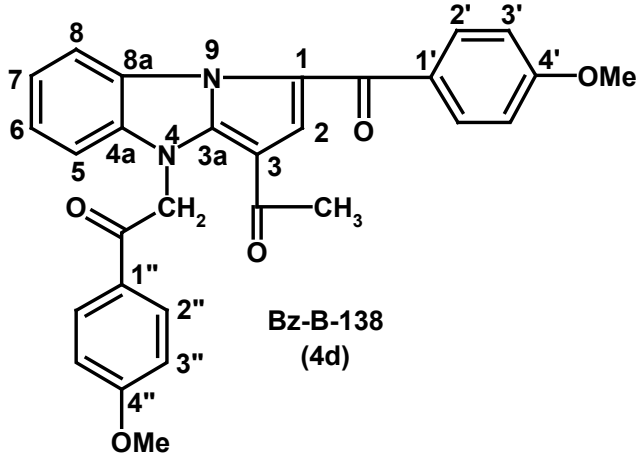
Information for NMR Spectra

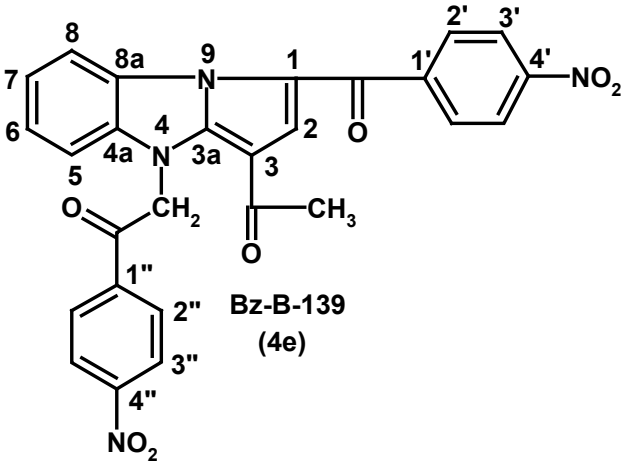
^{1}H- and ^{13}C-NMR spectra are provided below as pdf files for the following compounds:



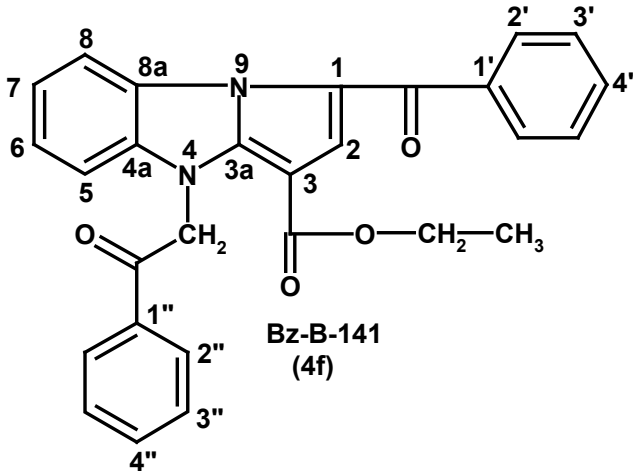




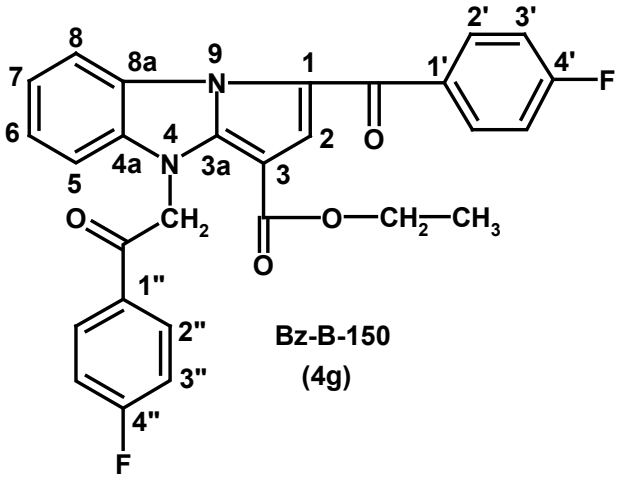




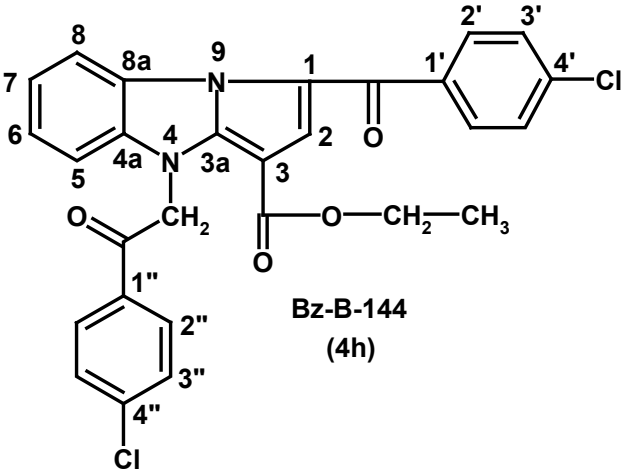
Bz-B-139
(4e)



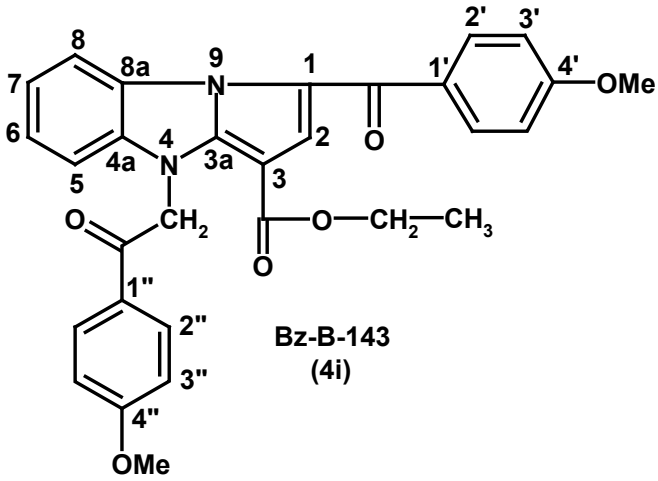
Bz-B-141
(4f)



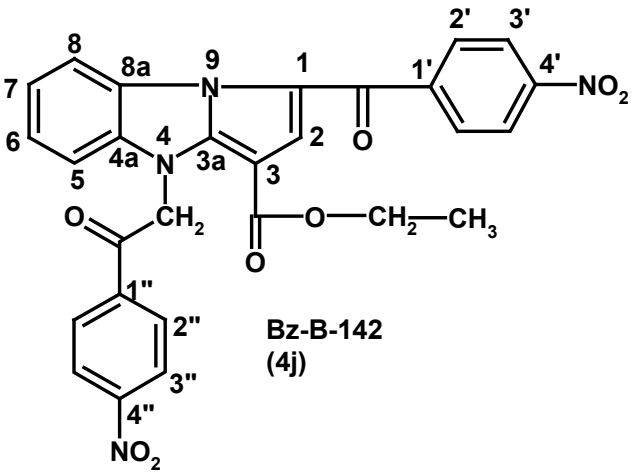
Bz-B-150
(4g)



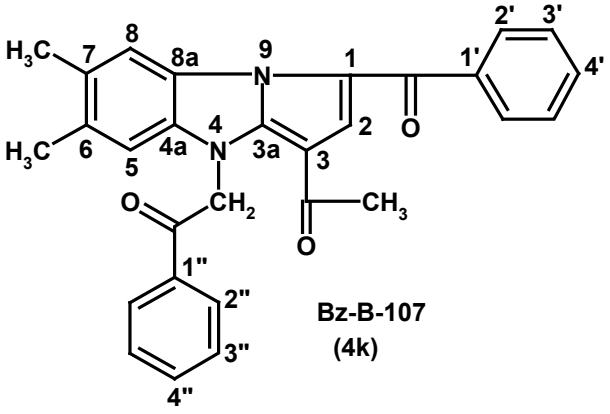
Bz-B-144
(4h)



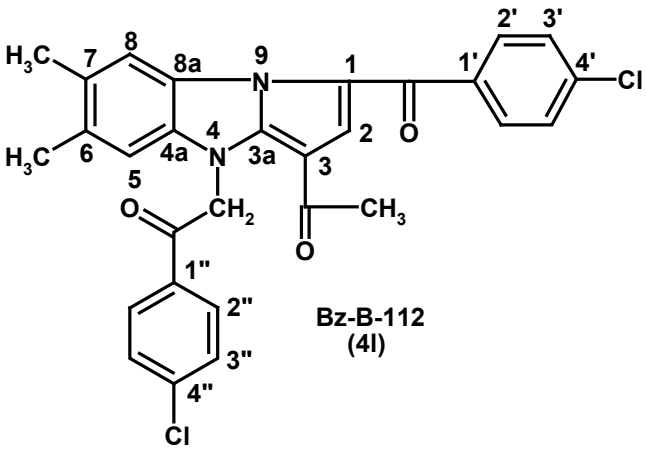
Bz-B-143
(4i)



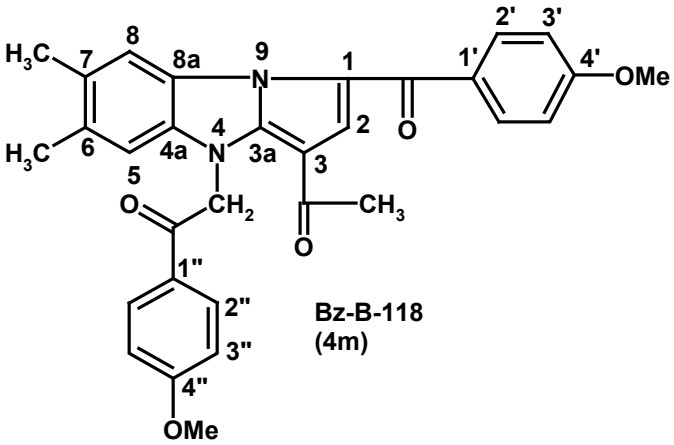
Bz-B-142
(4j)



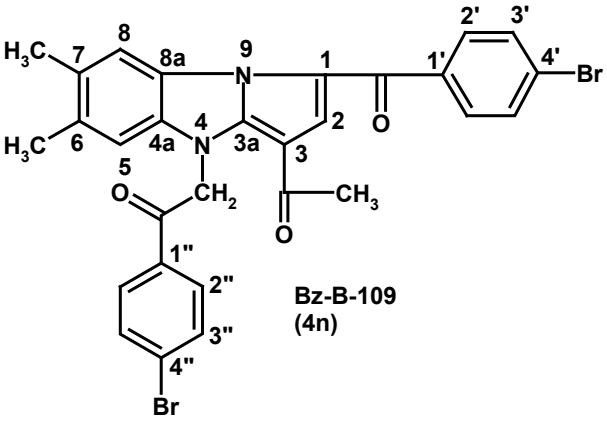
Bz-B-107
(4k)



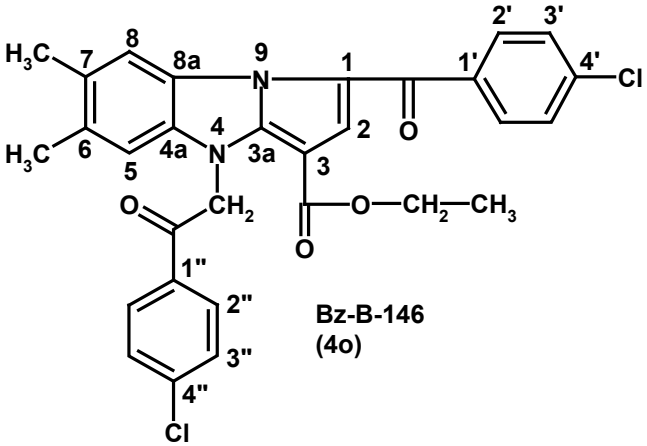
Bz-B-112
(4l)



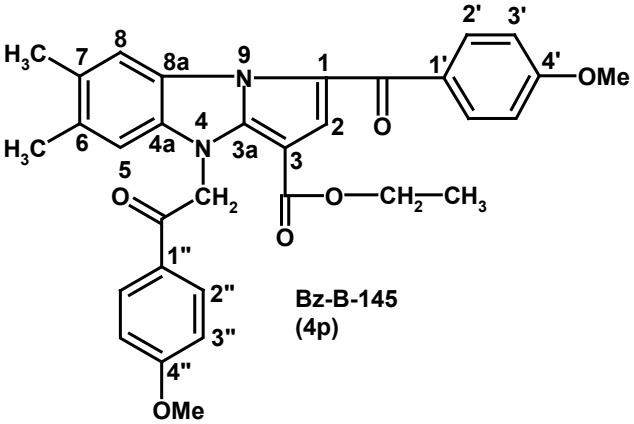
Bz-B-118
(4m)



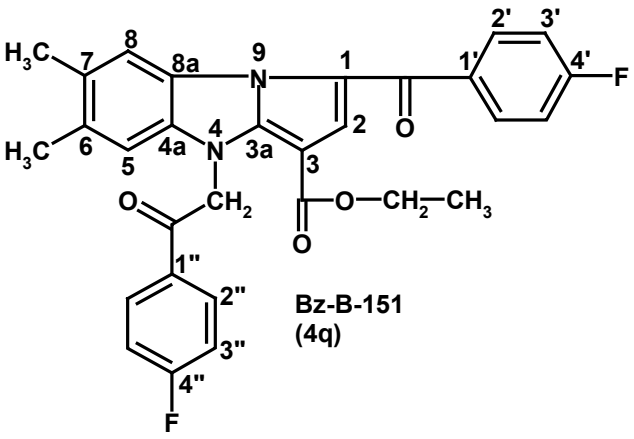
Bz-B-109
(4n)



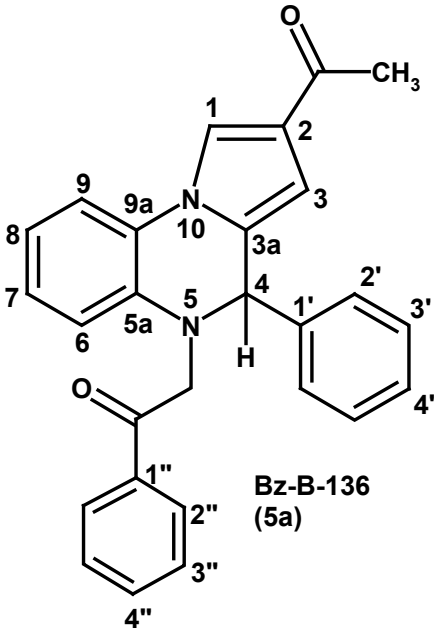
Bz-B-146
(4o)



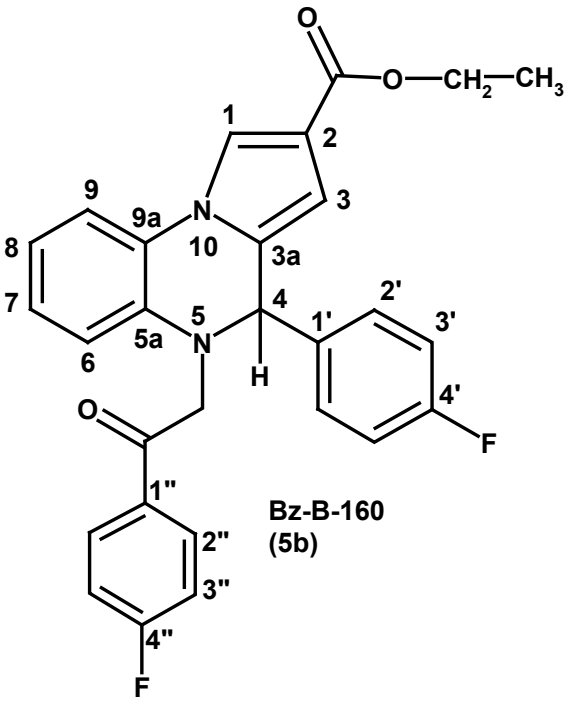
Bz-B-145
(4p)



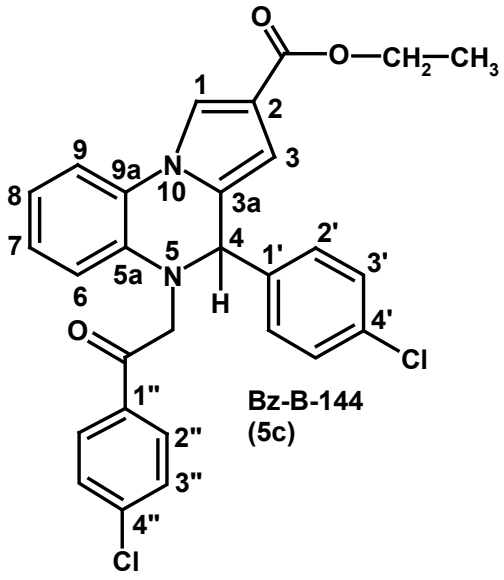
Bz-B-151
(4q)



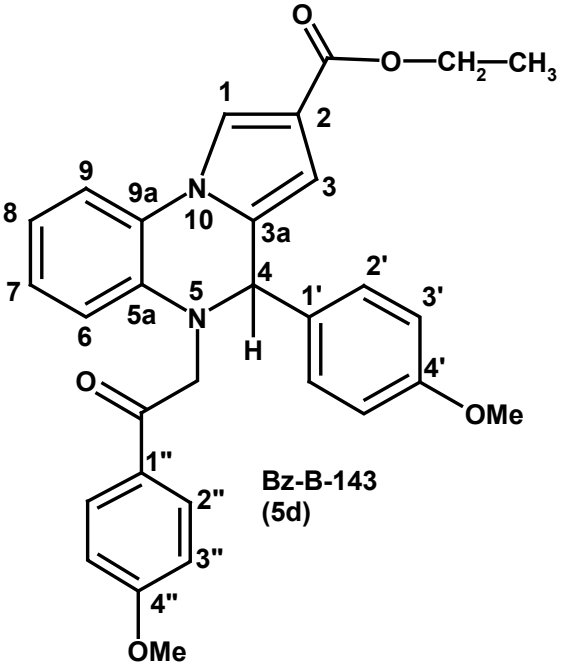
Bz-B-136
(5a)



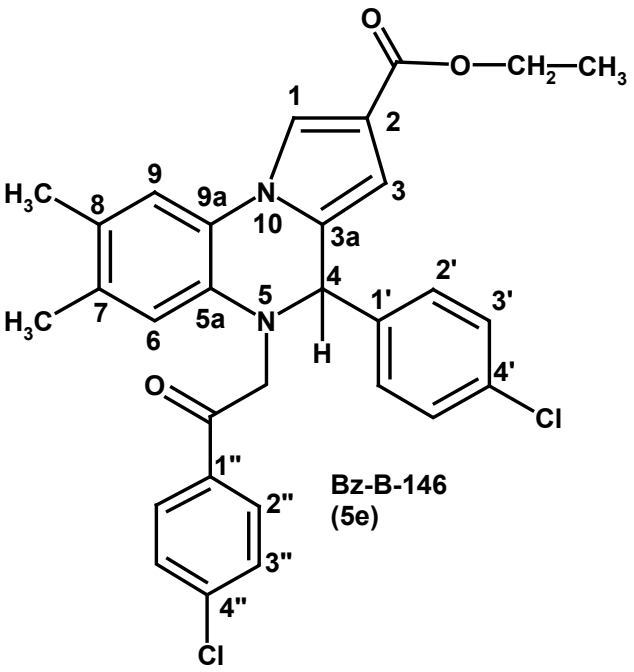
Bz-B-160
(5b)



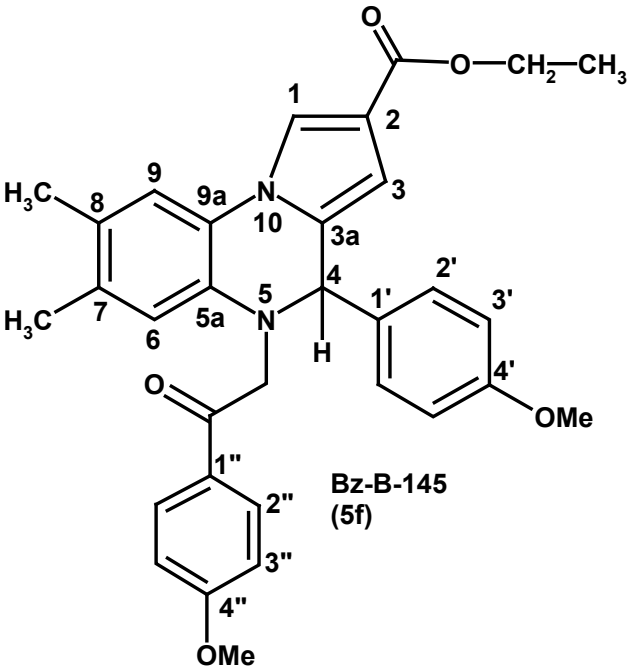
Bz-B-144
(5c)



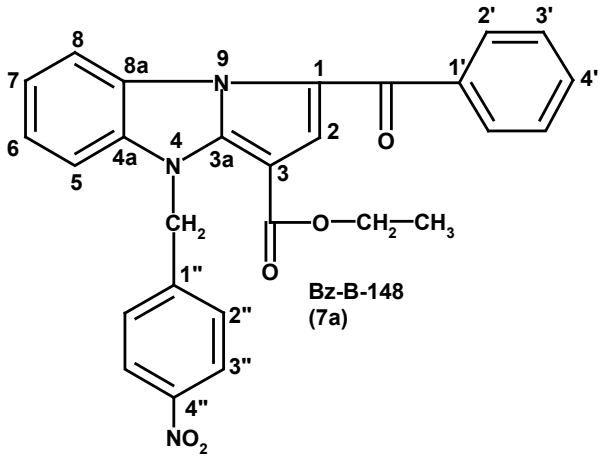
Bz-B-143
(5d)



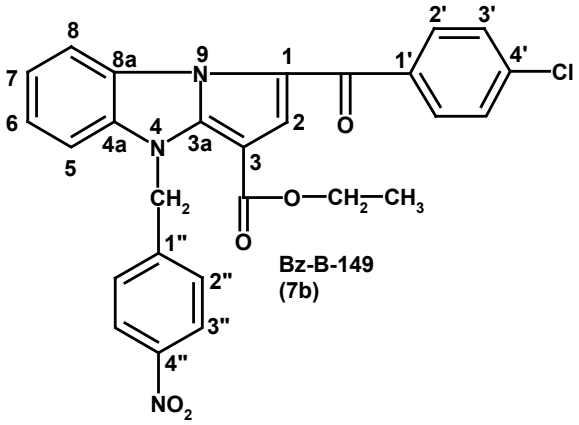
Bz-B-146
(5e)



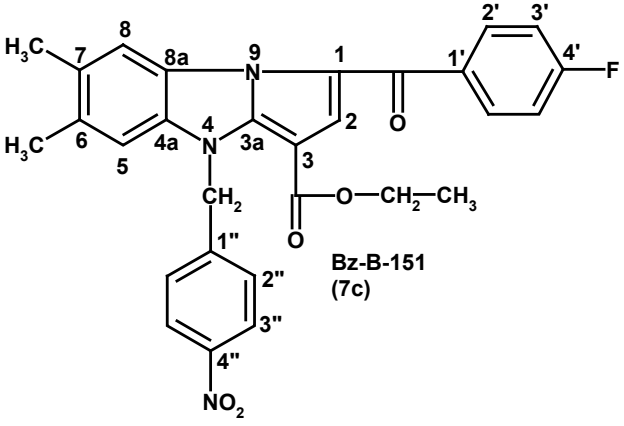
Bz-B-145
(5f)



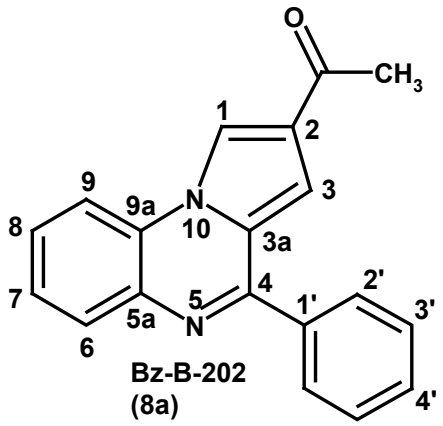
Bz-B-148
(7a)



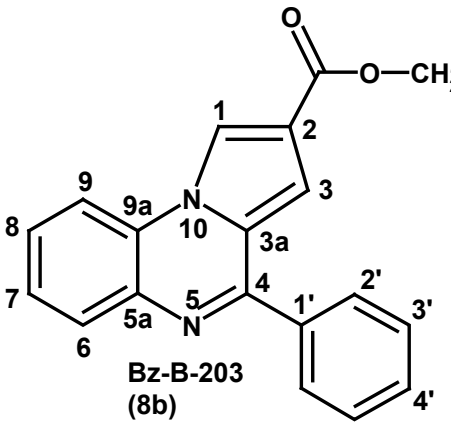
Bz-B-149
(7b)



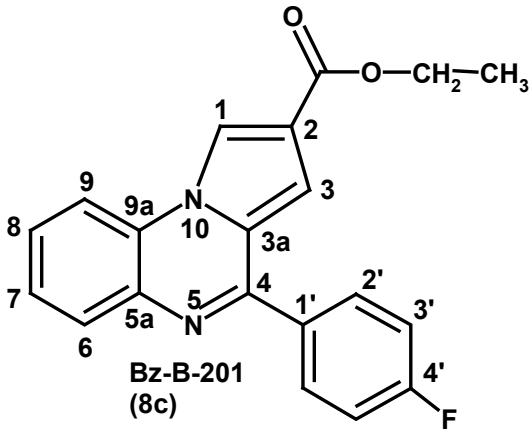
Bz-B-151
(7c)



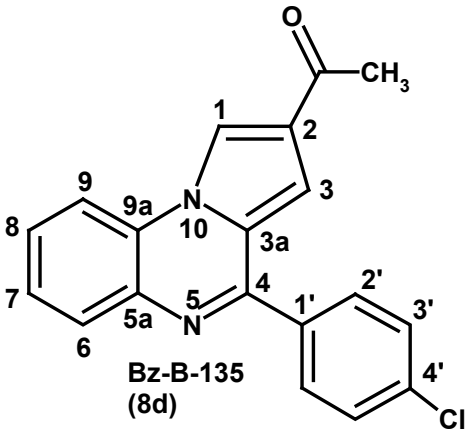
Bz-B-202
(8a)



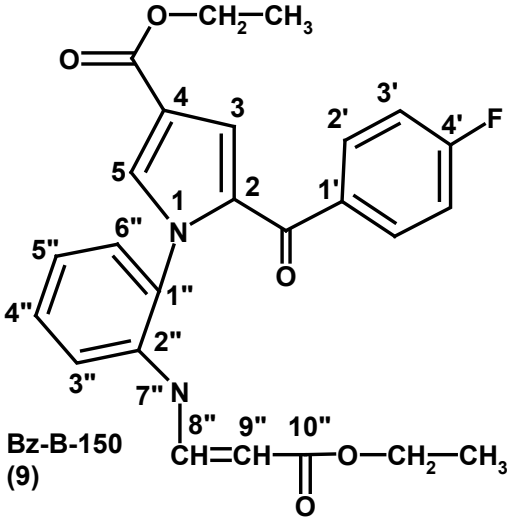
Bz-B-203
(8b)



Bz-B-201
(8c)



Bz-B-135
(8d)

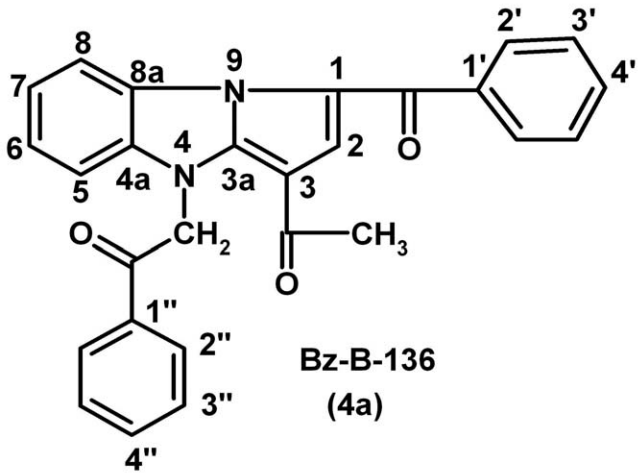


Bz-B-150
(9)

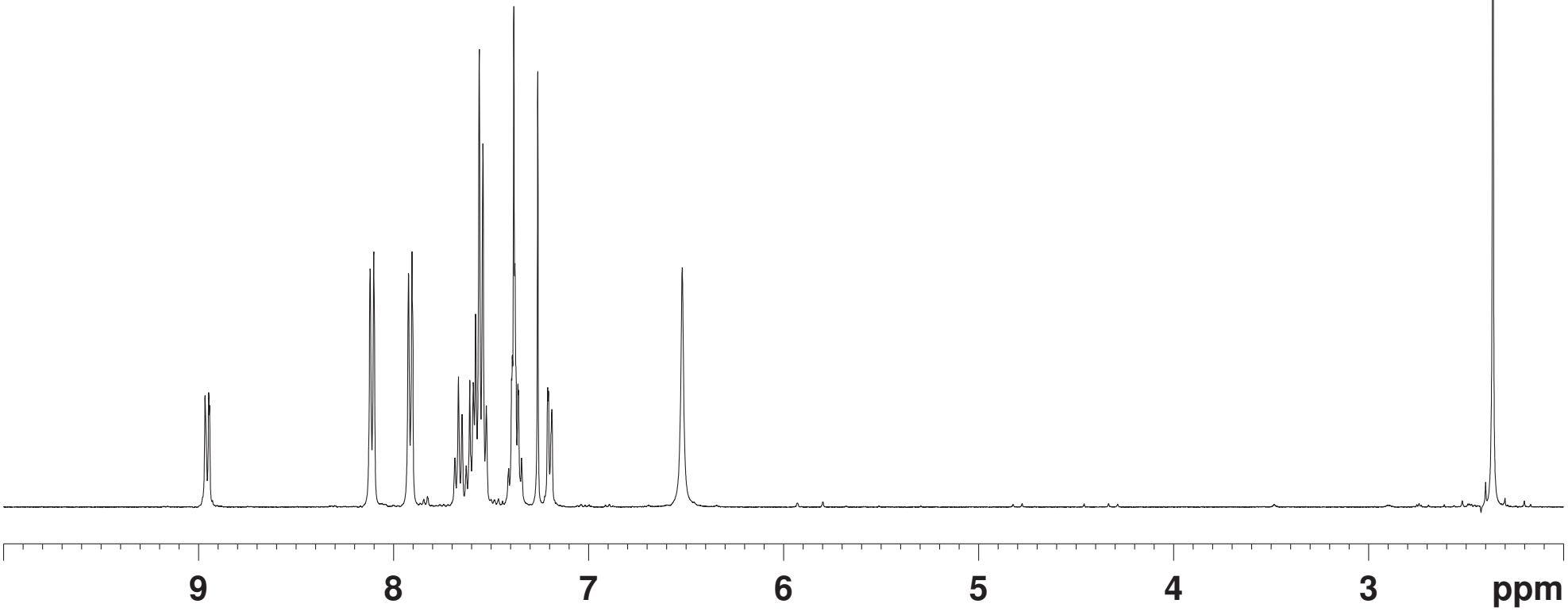
Parameter Set:!H1-BBFOa-44 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24600

Sample name and description:Bz-B-136 (4a)

p.t. 248-250 °C



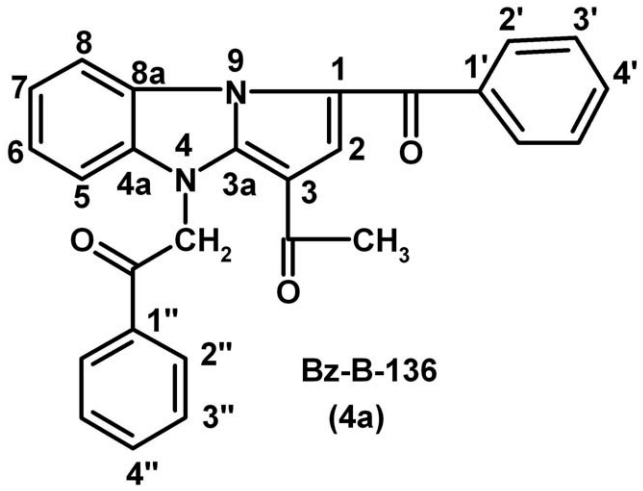
Bz-B-136
(4a)



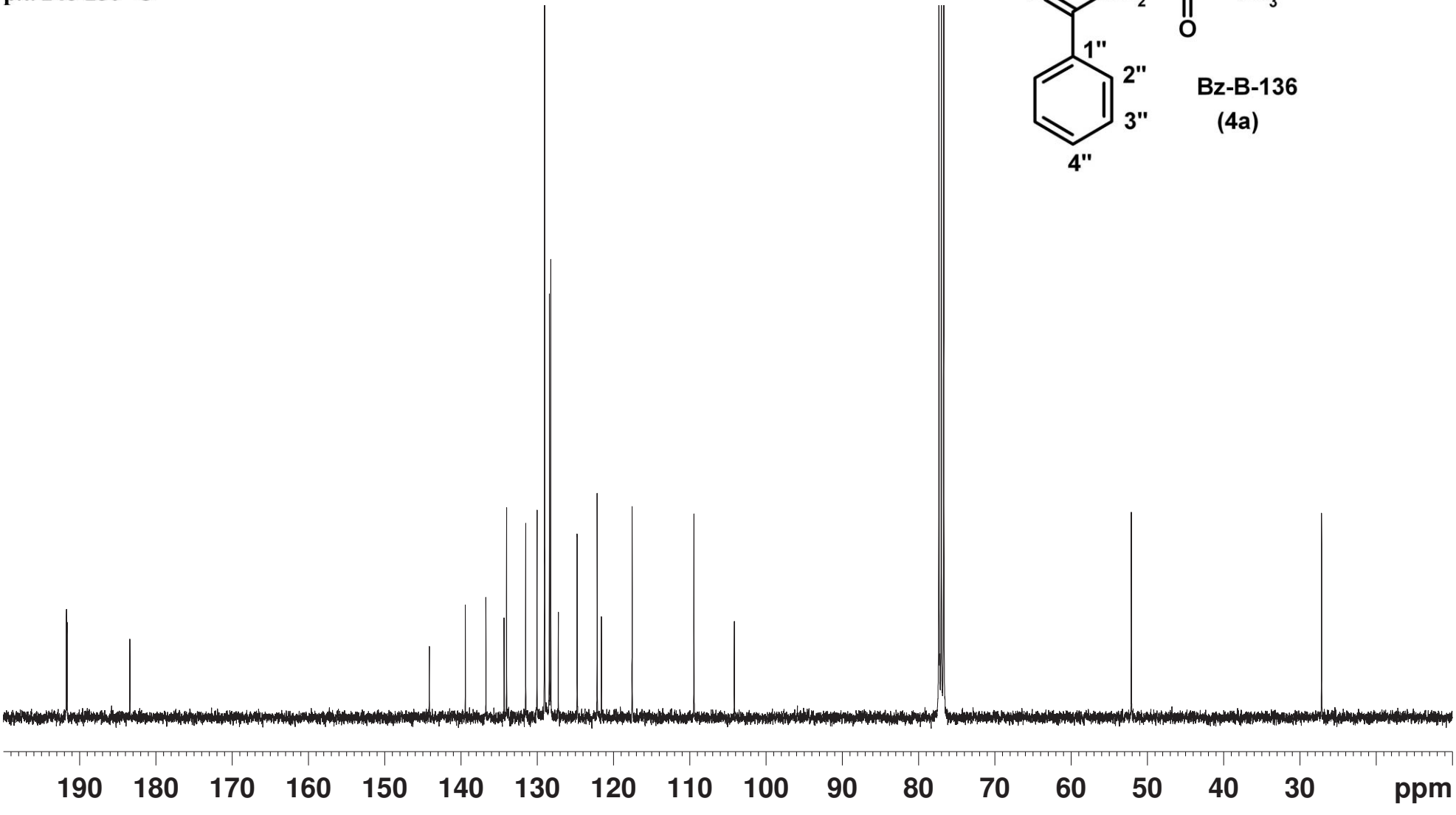
Parameter Set:!C13-CPD-BBFOa-44 TS1.3PL8.NMR
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24471

Sample name and description:Bz-B-136 (4a)

p.t. 248-250 °C



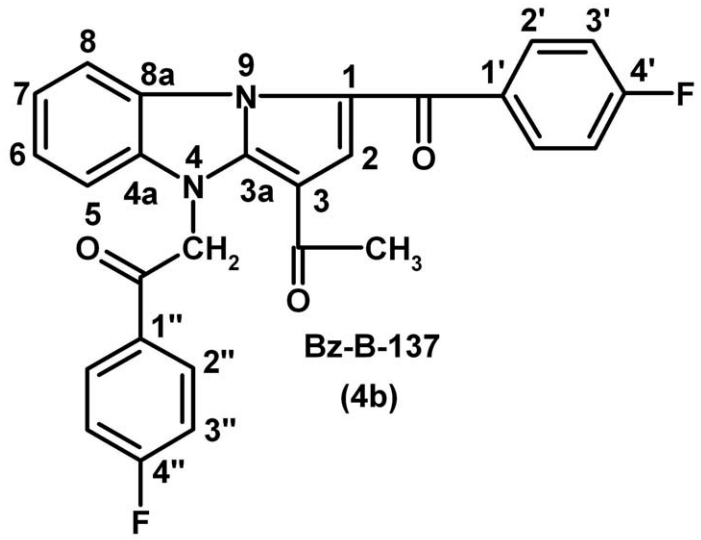
Bz-B-136
(4a)



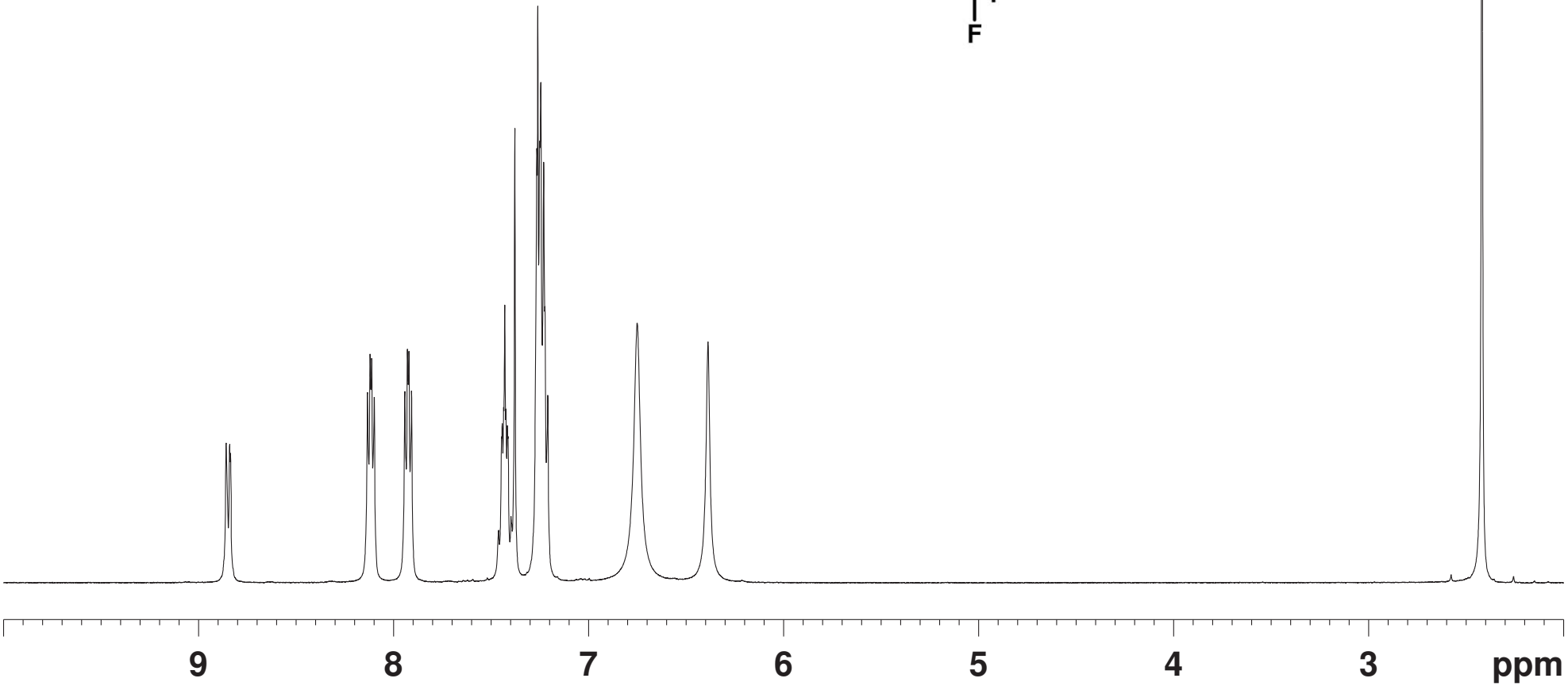
Parameter Set:!H1-BBFOa-44 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24489

Sample name and description:Bz-B-137 (4b)

p.t. 246-247 °C
in CDCl3 with TFA



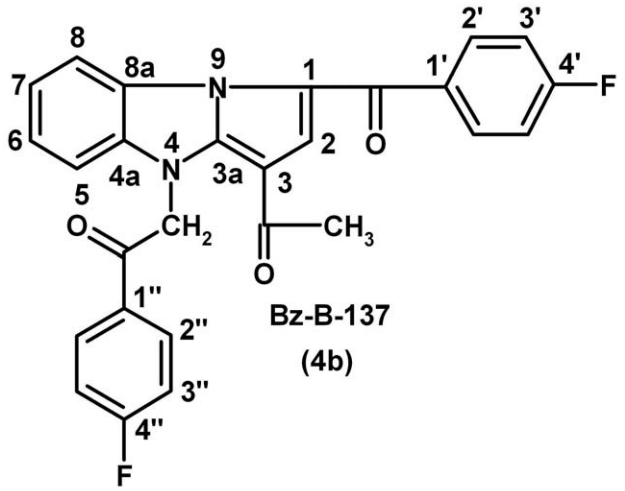
Bz-B-137
(4b)



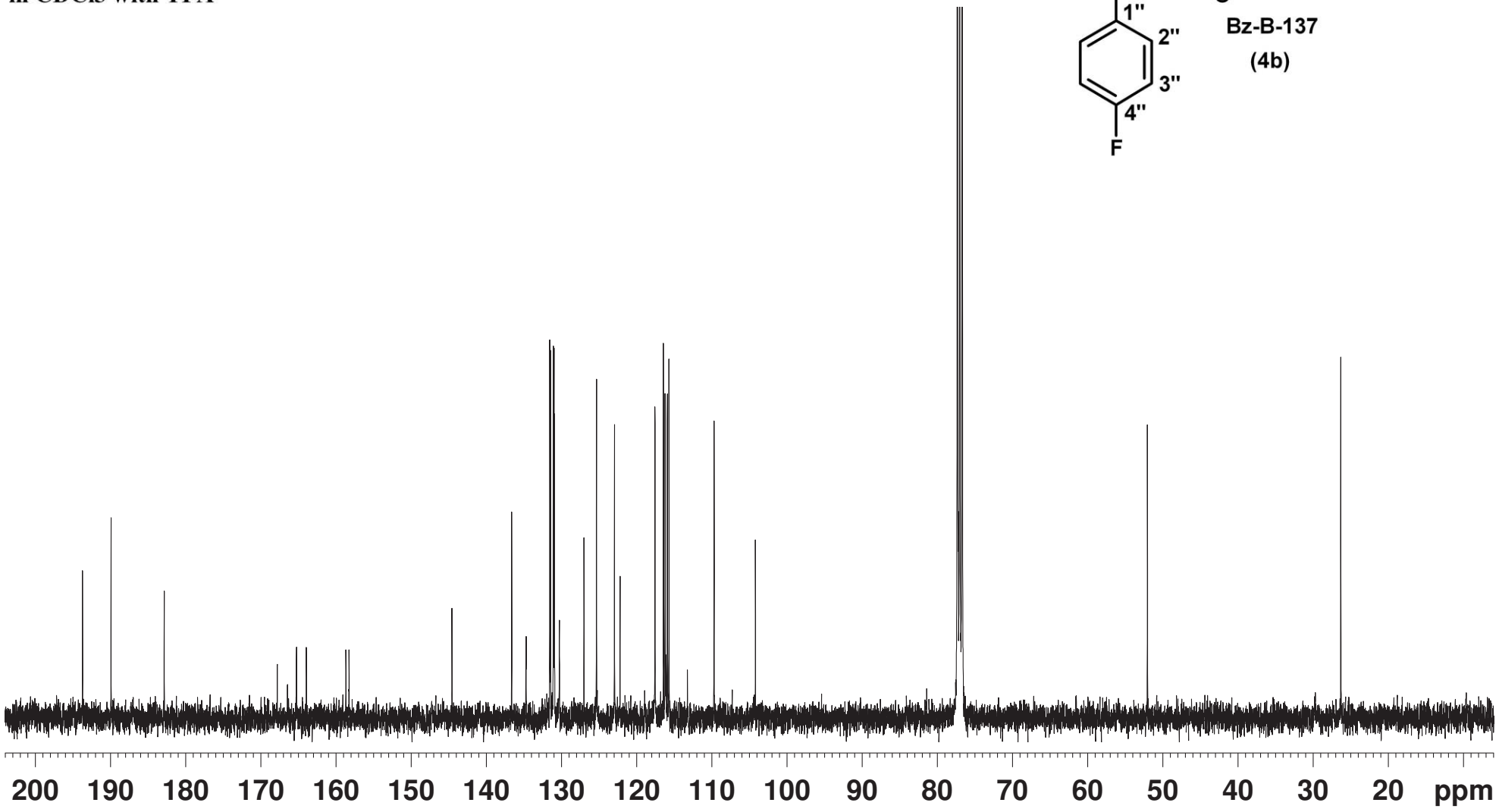
Parameter Set:!C13-CPD-BBFOa-44 TS1.3PL8.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24489

Sample name and description:Bz-B-137 (4b)

p.t. 246-247 °C
in CDCl3 with TFA



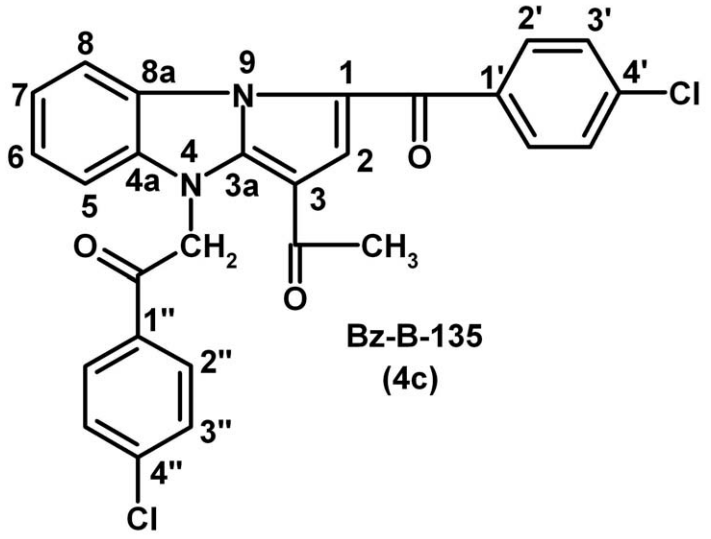
Bz-B-137
(4b)

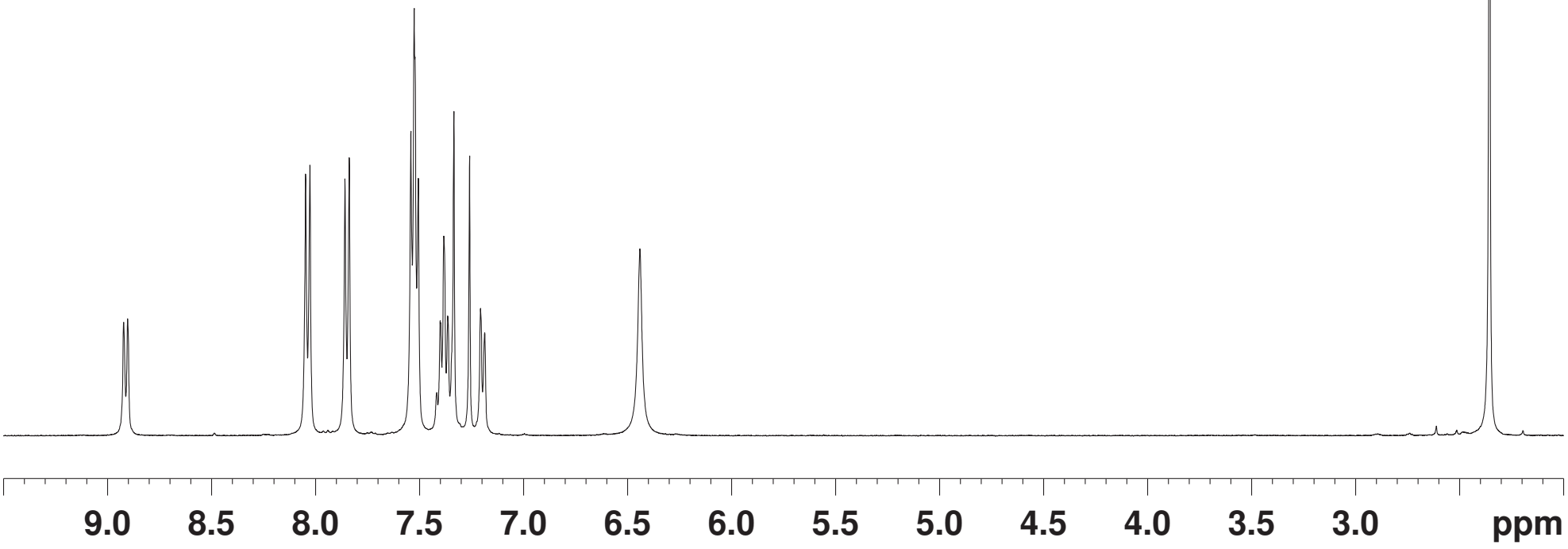


Parameter Set:!H1-BBFOa-44 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24462

Sample name and description:Bz-B-135 (4c)

p.t. 268-270 °C

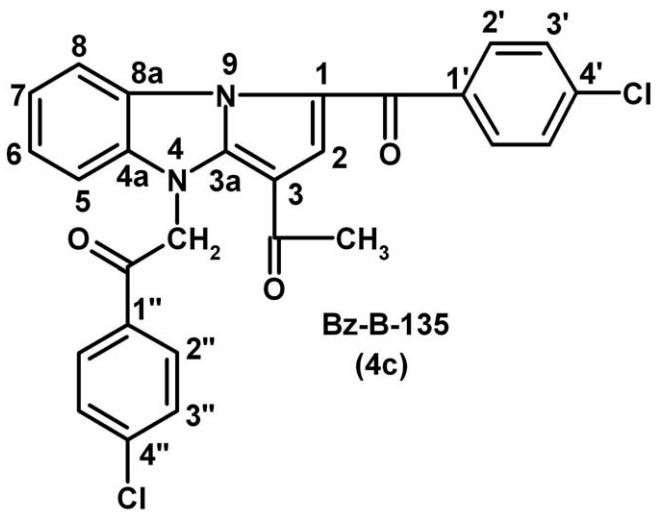




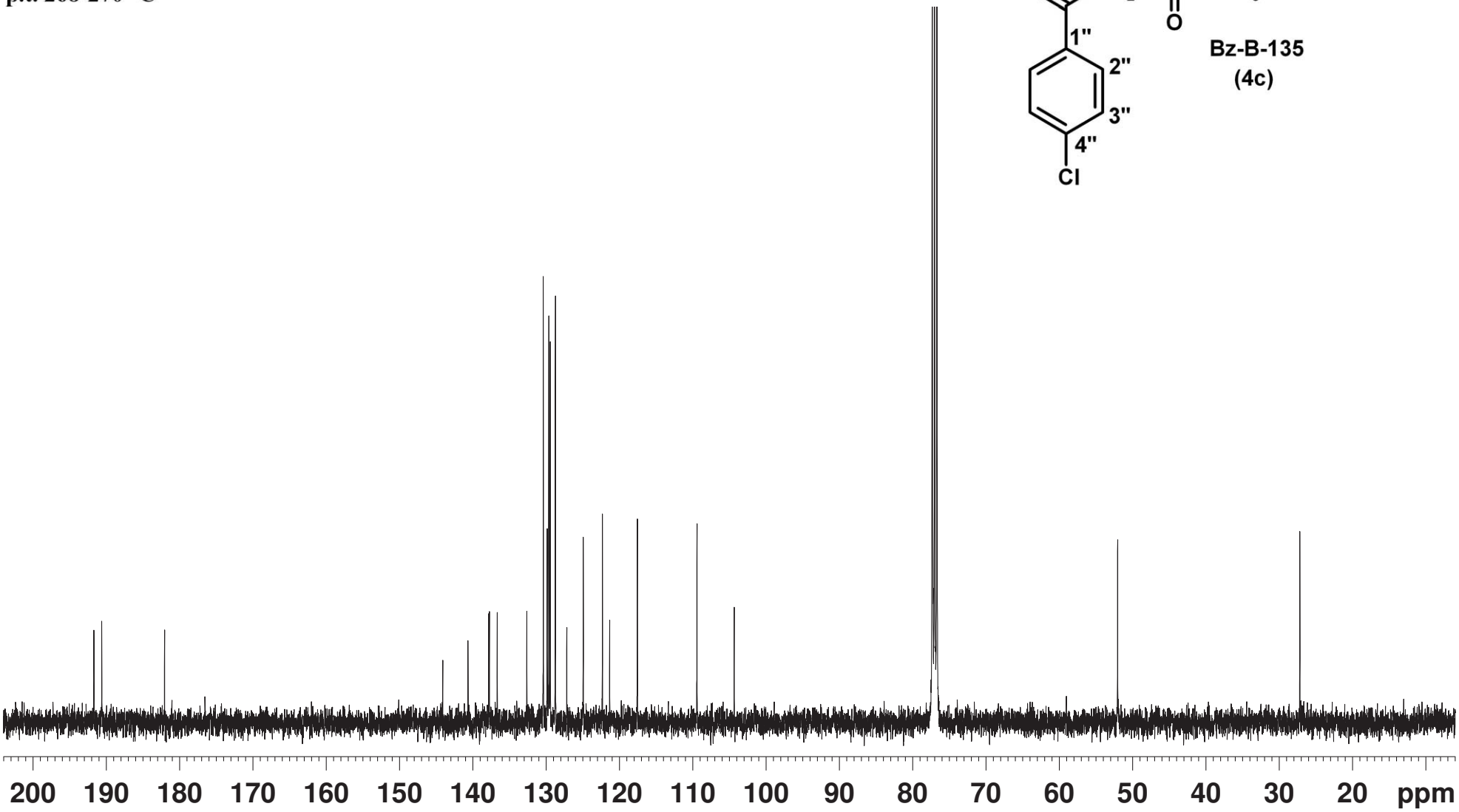
Parameter Set:!C13-CPD-BBFOa-44 TS1.3PL8.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24462

Sample name and description:Bz-B-135 (4c)

p.t. 268-270 °C



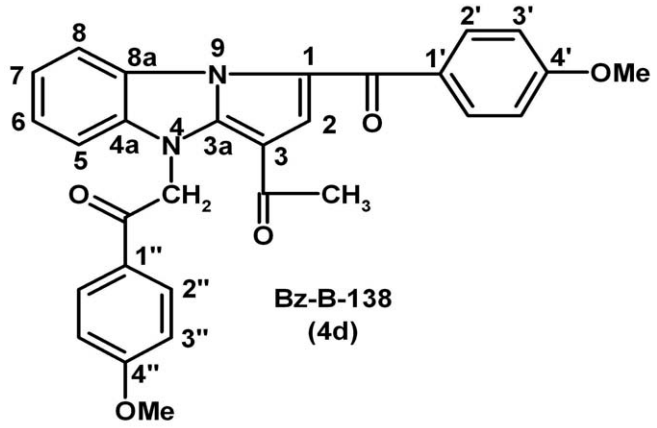
Bz-B-135
(4c)



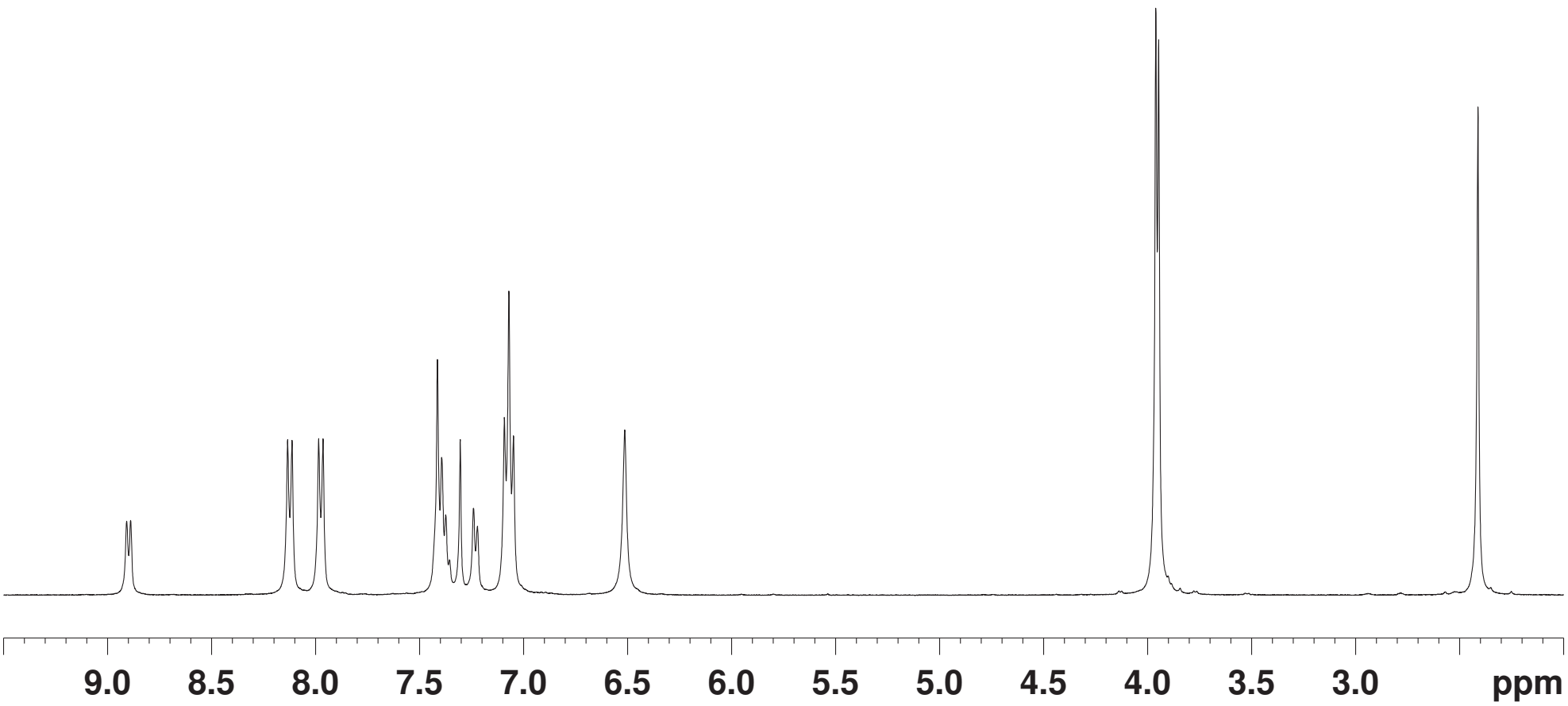
Parameter Set:!H1-BBFOa-44 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24567

Sample name and description:Bz-B-138 (4d)

p.t. 231-233 °C



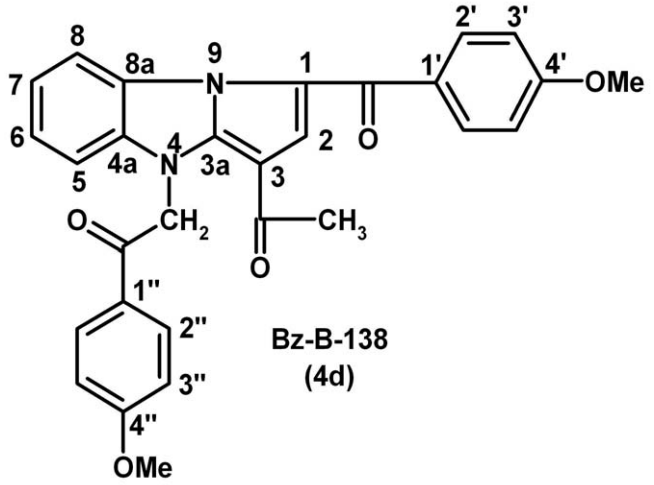
Bz-B-138
(4d)



Parameter Set:!C13-CPD-BBFOa-44 TS1.3PL8.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24567

Sample name and description:Bz-B-138 (4d)

p.t. 231-233 °C



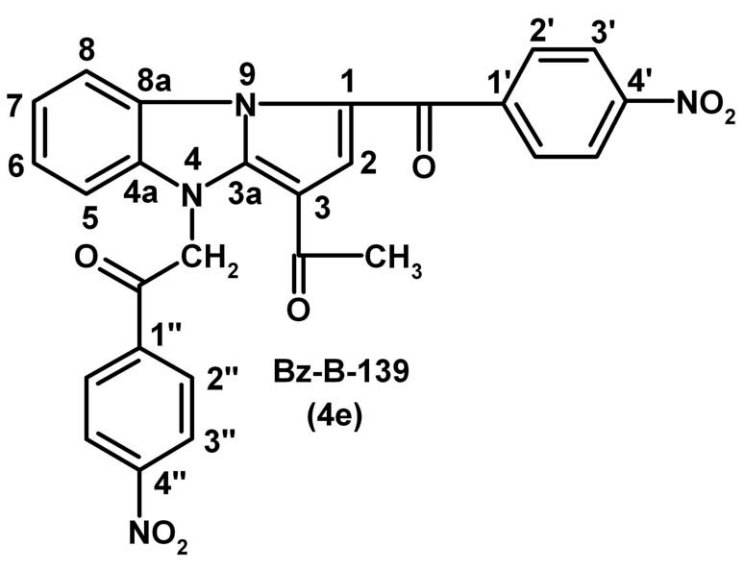
Bz-B-138
(4d)

Parameter Set:!H1-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24584

Sample name and description: Bz-B-139 (4e)

p.t. 273-275 °C

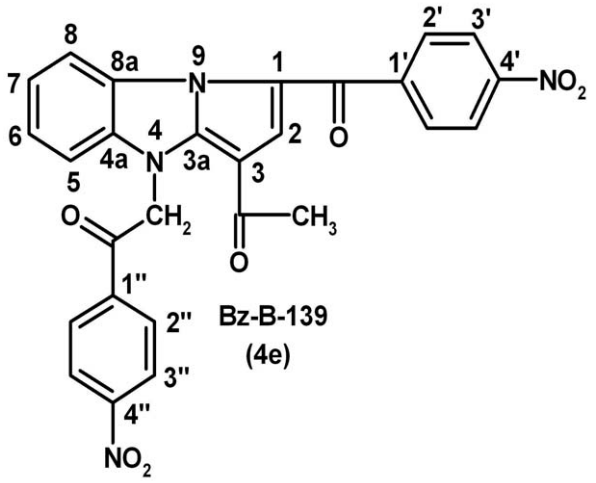


Bz-B-139
(4e)

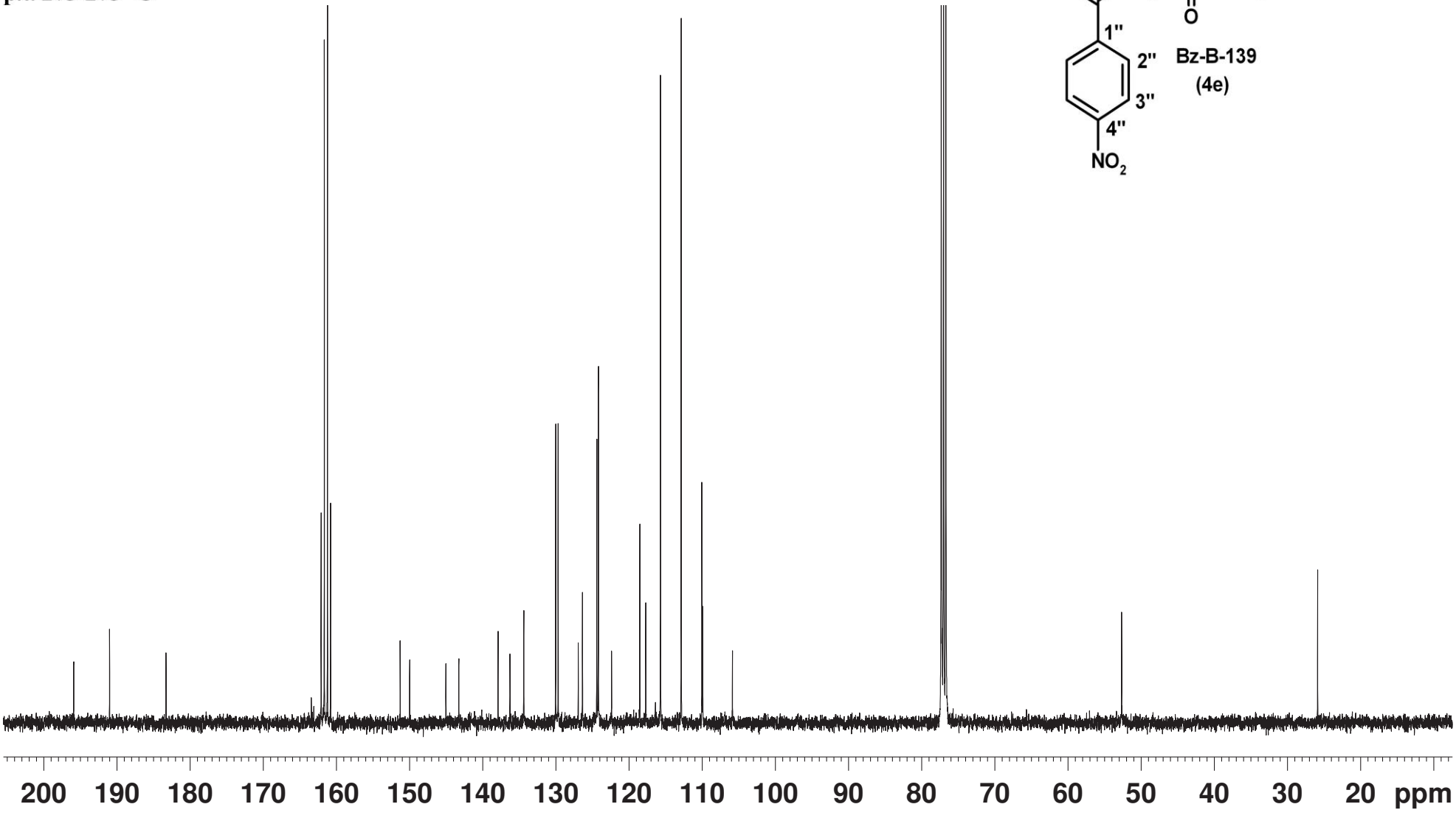
Parameter Set:!C13-CPD-BBFOa-44 TS1.3PL8.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24584

Sample name and description:Bz-B-139 (4e)

p.t. 273-275 °C



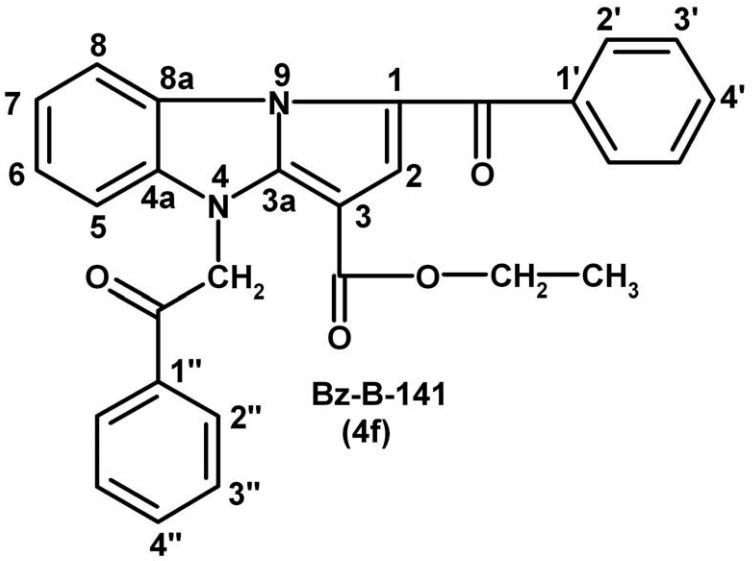
Bz-B-139
(4e)



Parameter Set:!H1-BBFOa-44 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24570

Sample name and description:Bz-B-141 (4f)

p.t. 232-234 °C

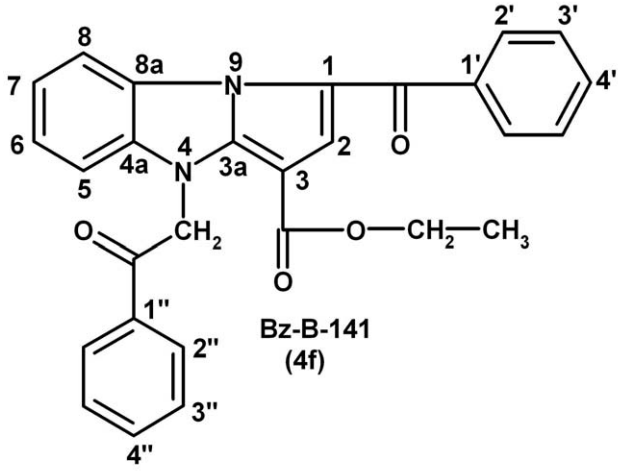


Bz-B-141
(4f)

Parameter Set:!C13-CPD-BBFOa-44 TS1.3PL8.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24570

Sample name and description:Bz-B-141 (4f)

p.t. 232-234 °C

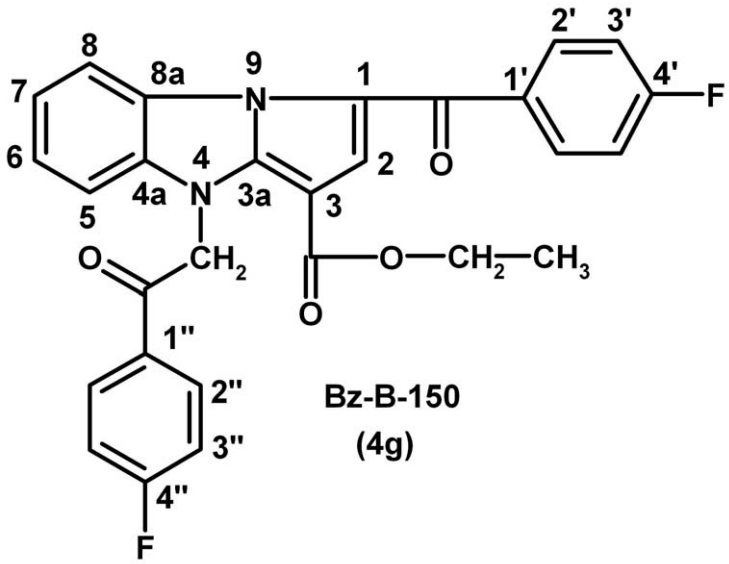


Bz-B-141
(4f)

Parameter Set #H1-QNP-34 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24901

Sample name and description:Bz-B-150 (4g)

p.t. 215-217 °C

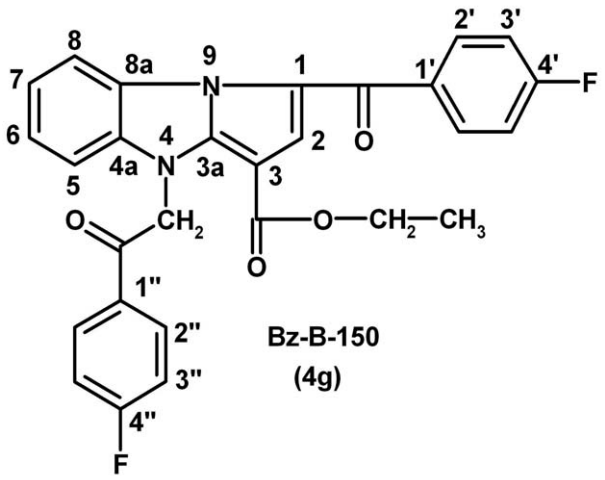


Bz-B-150
(4g)

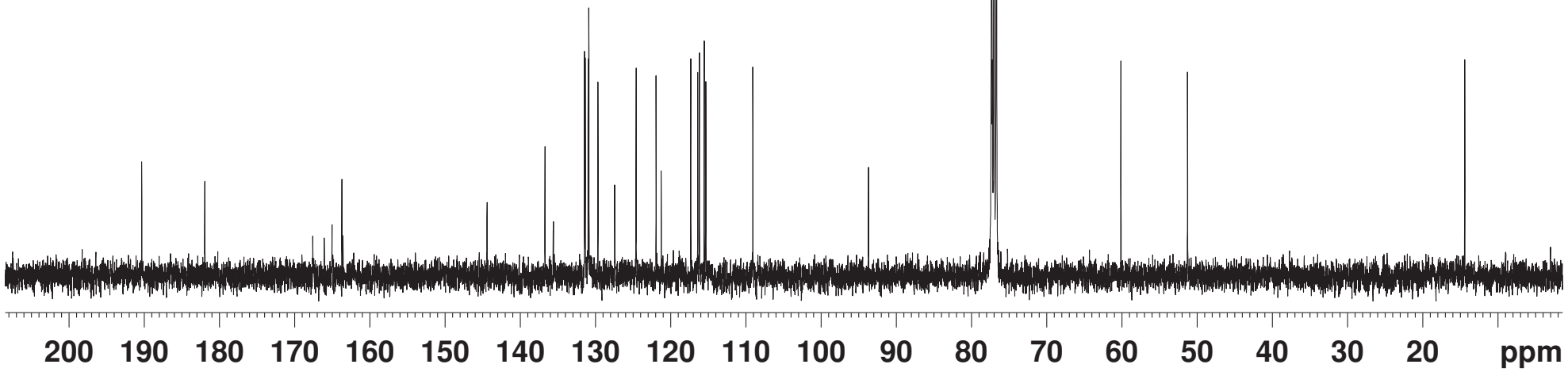
Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24901

Sample name and description:Bz-B-150 (4g)

p.t. 215-217 °C



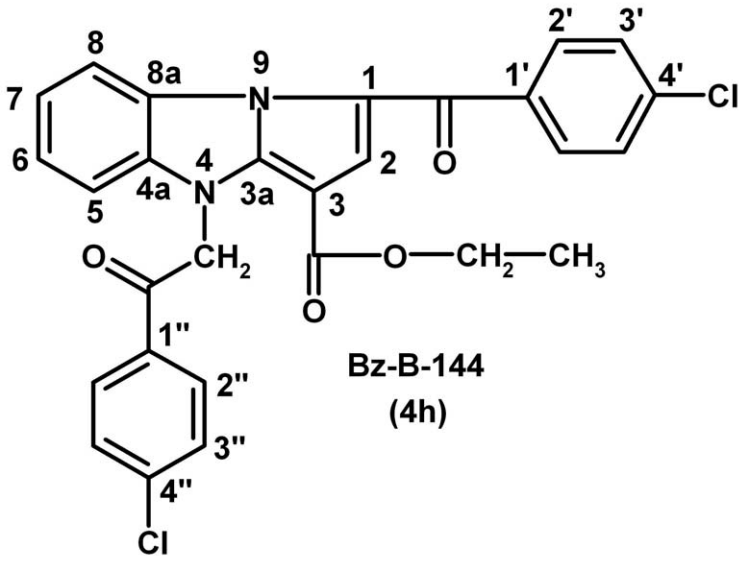
Bz-B-150
(4g)



Parameter !H1-BBFOa-44 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24575

Sample name and description:Bz-B-144 (4h)

p.t. 238-240 °C

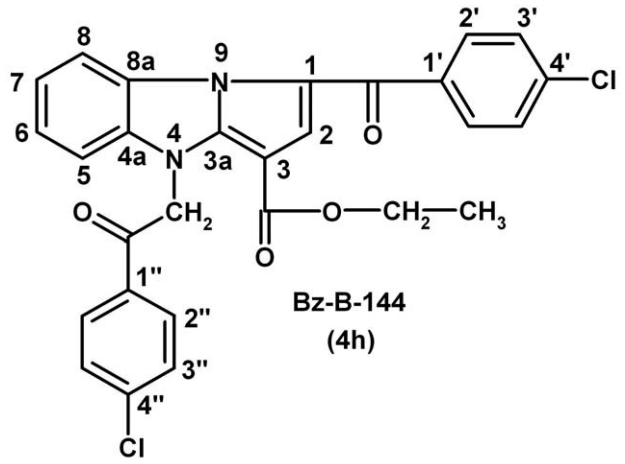


Bz-B-144
(4h)

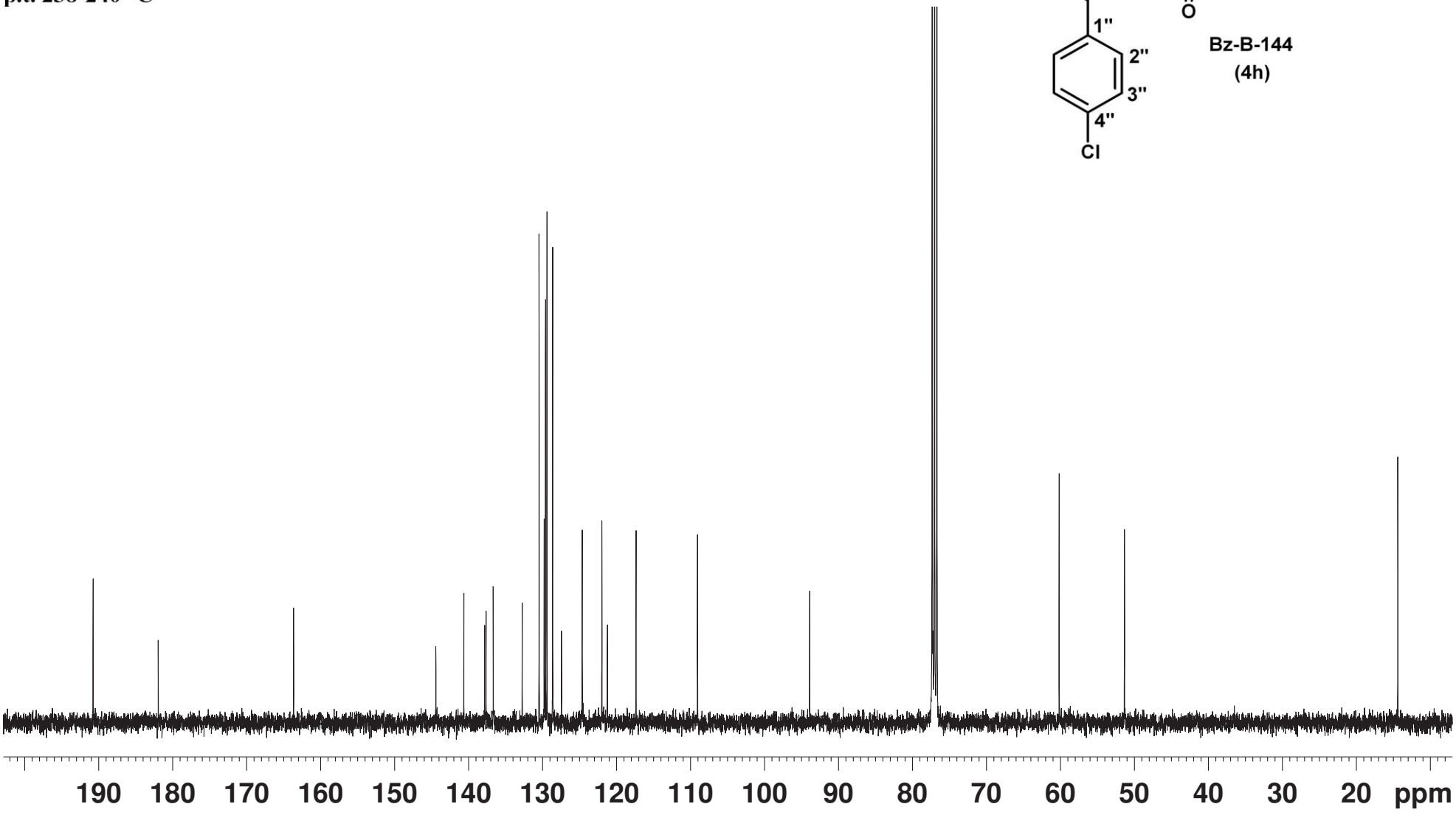
Parameter Set !C13-CPD-BBFOa-44 TS1.3PL8.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24575

Sample name and description:Bz-B-144 (4h)

p.t. 238-240 °C



Bz-B-144
(4h)

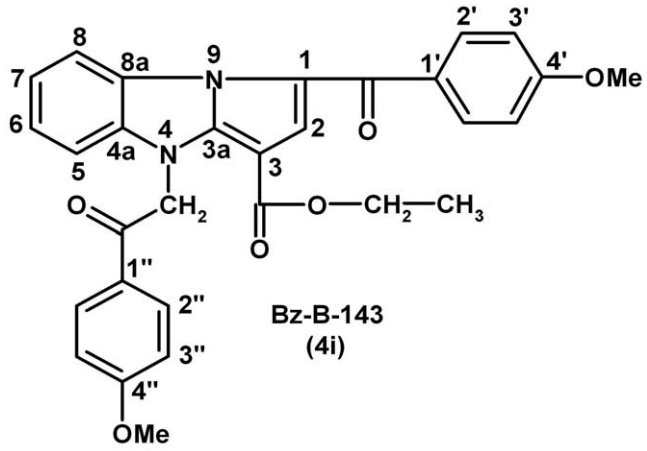


Parameter Set: %H1-BBIa-42. TS 2.1PL6.
Instrument: Bruker Avance III 400 (ICMPP)

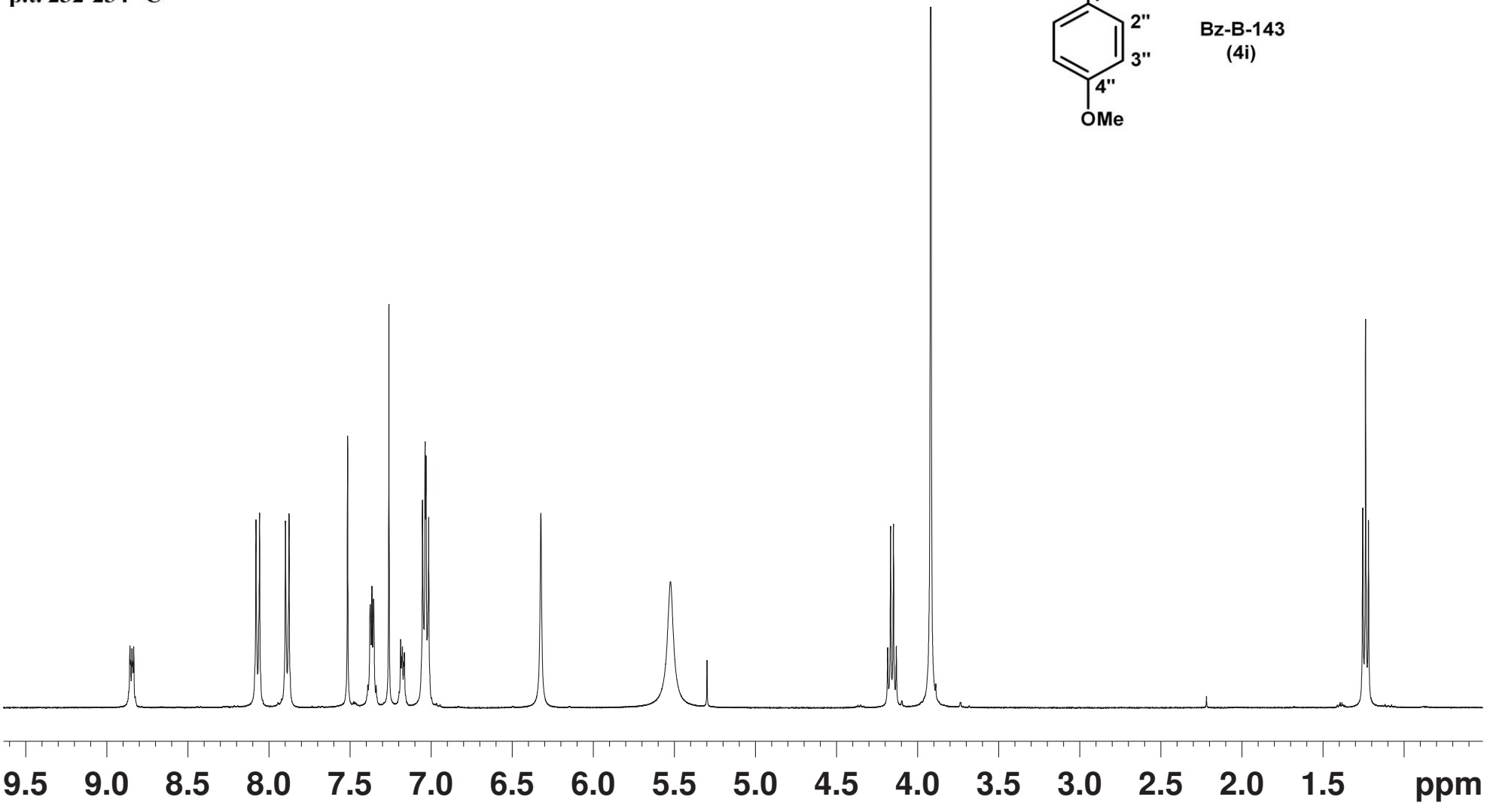
Registry No.:7615

Sample name and description:Bz-B-143 (4i)

p.t. 232-234 °C



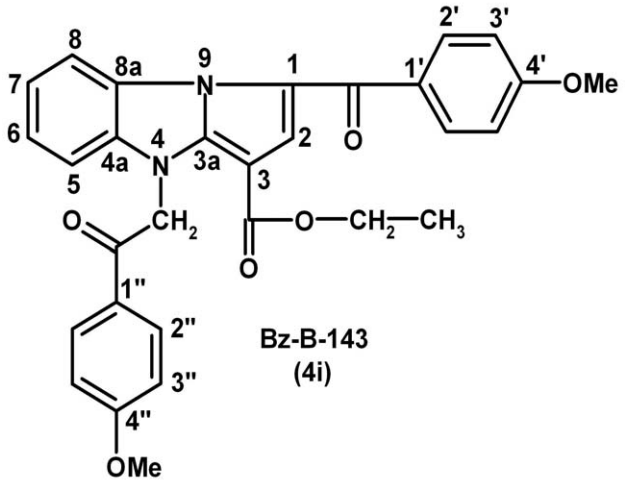
Bz-B-143
(4i)



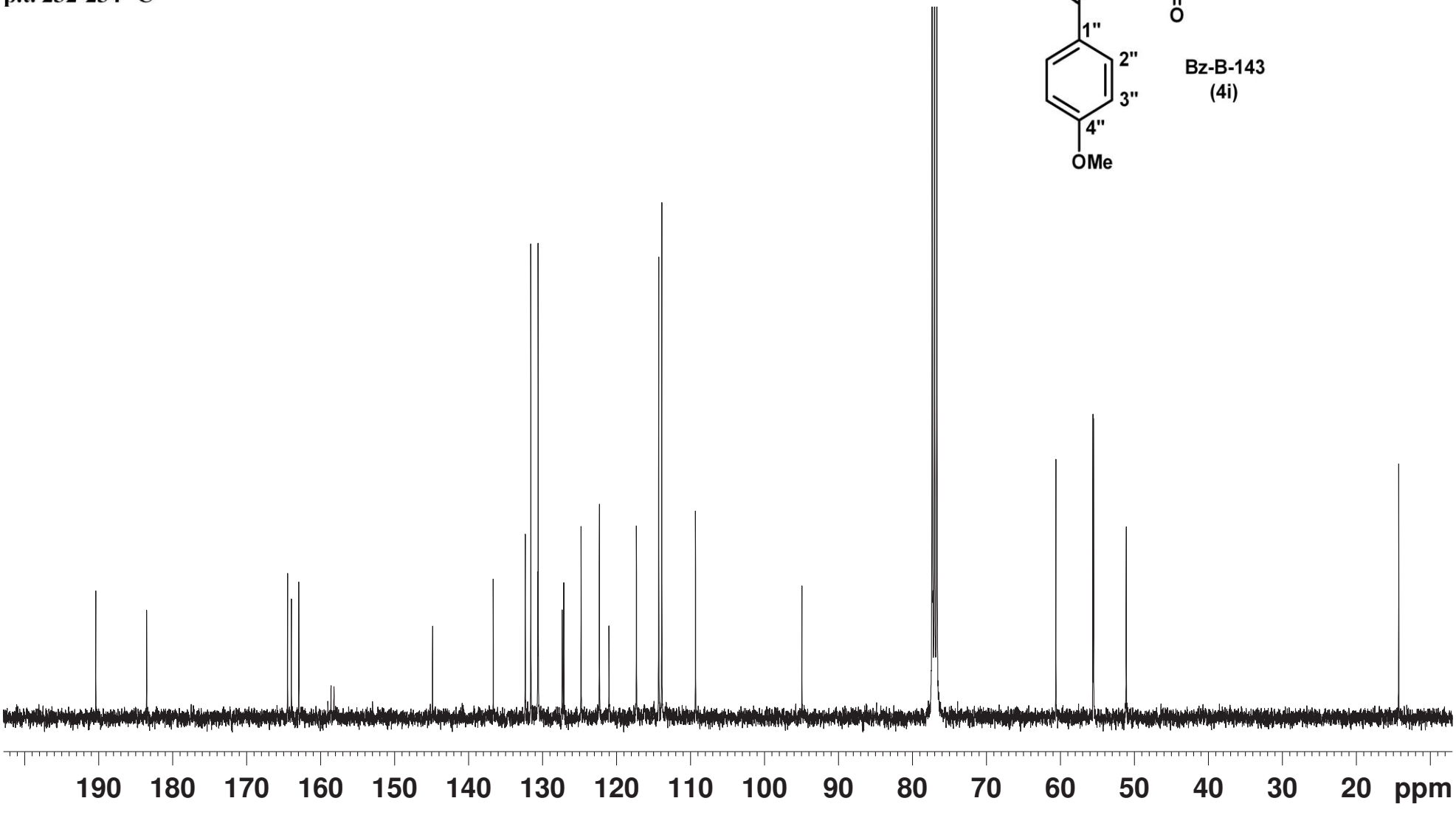
Parameter Set !C13-CPD-BBFOa-44 TS1.3PL10.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:24572

Sample name and description:Bz-B-143 (4i)

p.t. 232-234 °C



Bz-B-143
(4i)

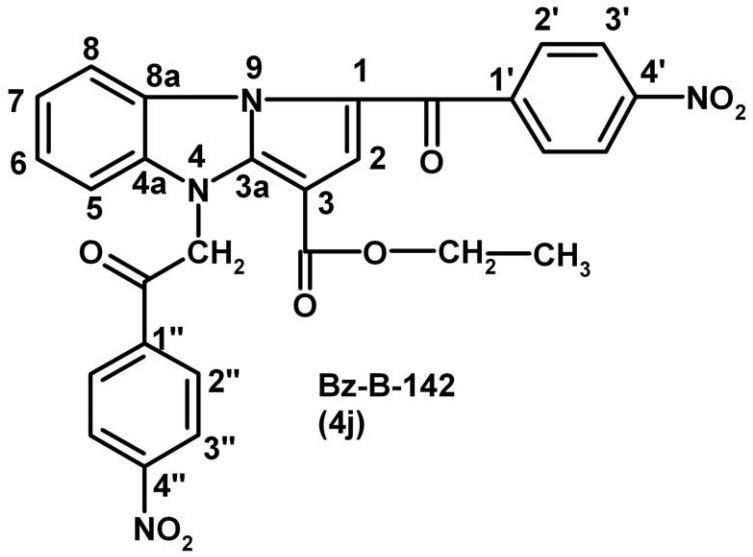


Parameter Set: %H1-BBIa-42 TS2.1PL6.
Instrument: Bruker Avance III 400 (ICMPP)

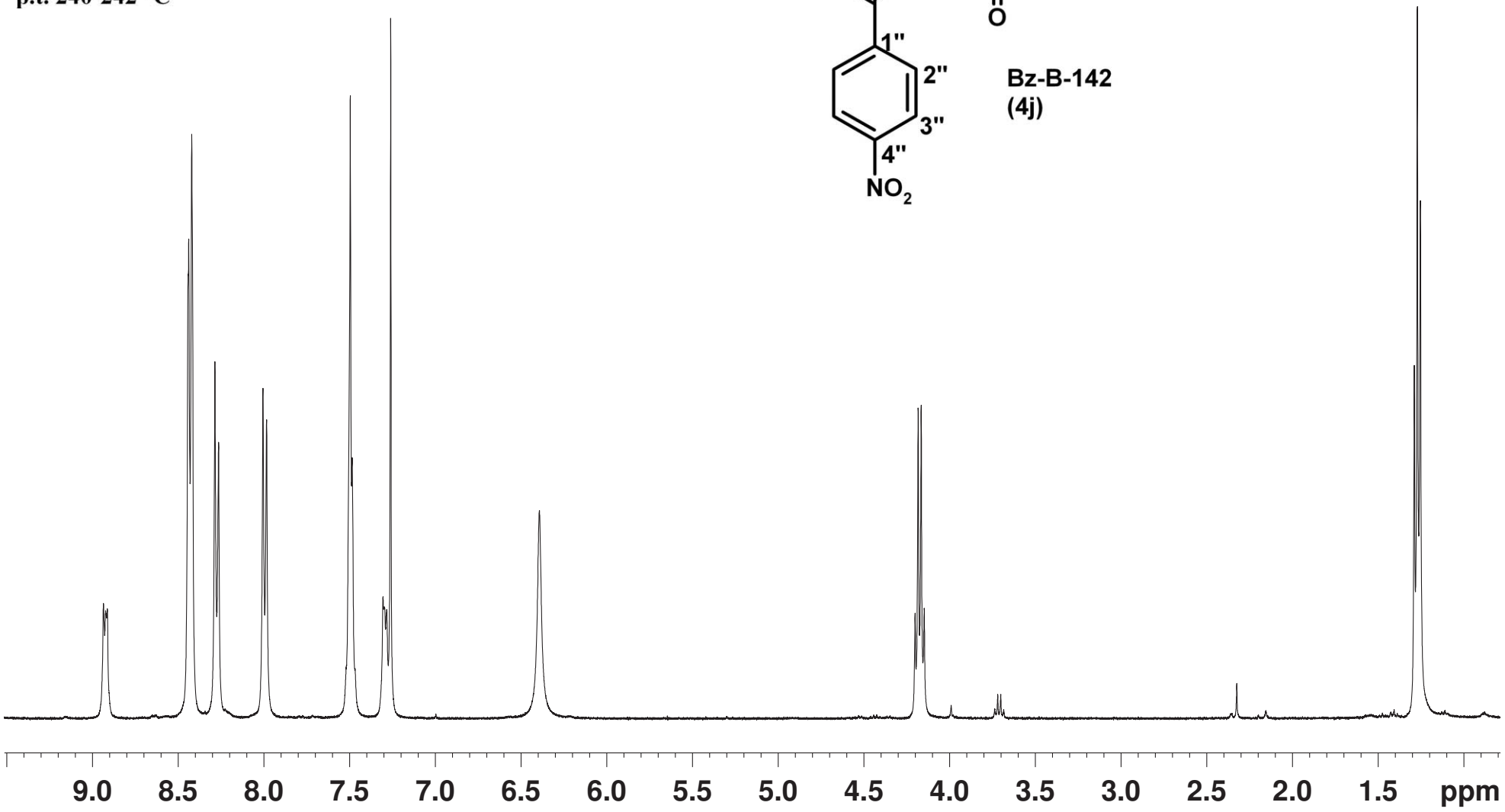
Registry No.:7602

Sample name and description: Bz-B-142 (4j)

p.t. 240-242 °C



Bz-B-142
(4j)

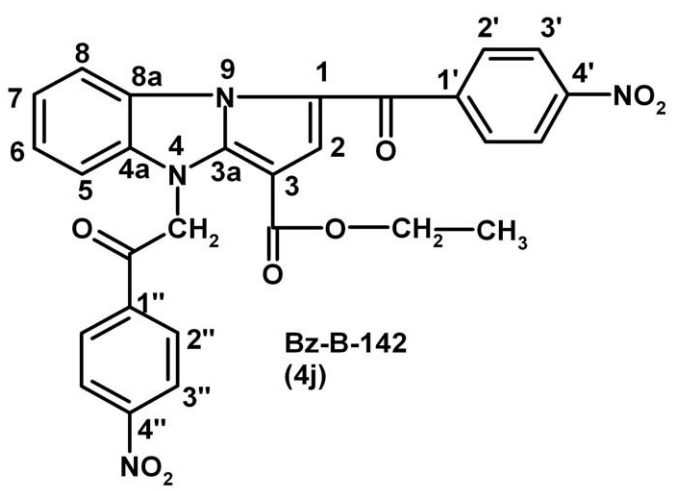


Parameter Set : !C13-CPD-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24577

Sample name and description: Bz-B-142 (4j)

p.t. 240-242 °C

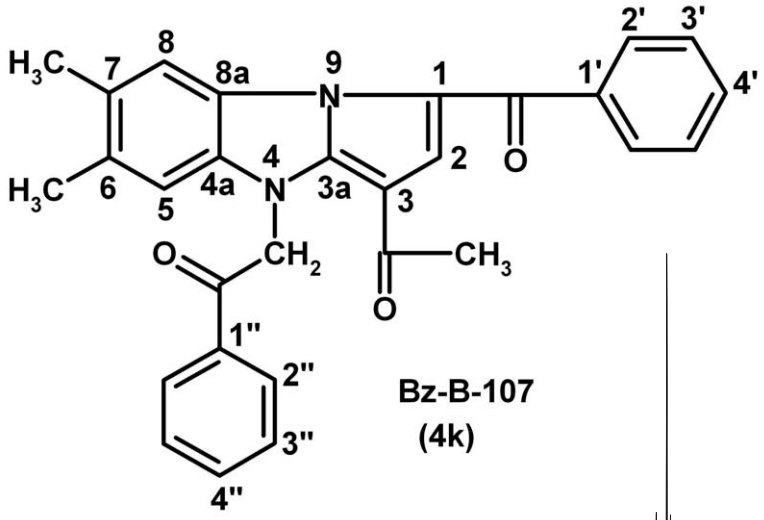


Parameter Set: %H1-BBIa-42. TS 2.1PL6.
Instrument: Bruker Avance III 400 (ICMPP)

Registry No.:6942

Sample name and description: Bz-B-107 (4k)

p.t. 305-307 °C

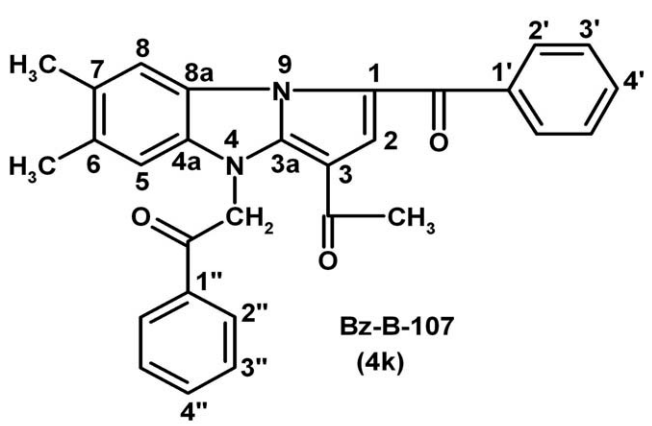


Bz-B-107
(4k)

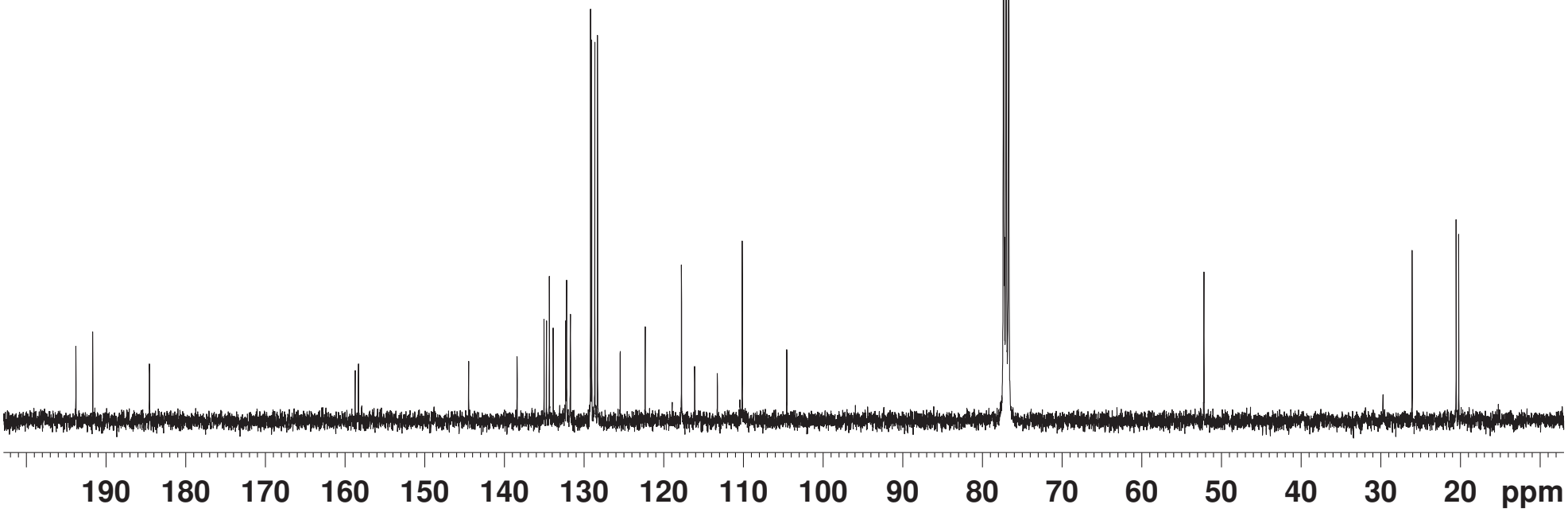
Parameter Set !C13-CPD-BBFOa-44 TS1.3PL10.
System: Bruker Avance DRX 400 (ICMPP)
Registry No.:22685

Sample name and description:Bz-B-107 (4k)

p.t. 305-307 °C



Bz-B-107
(4k)

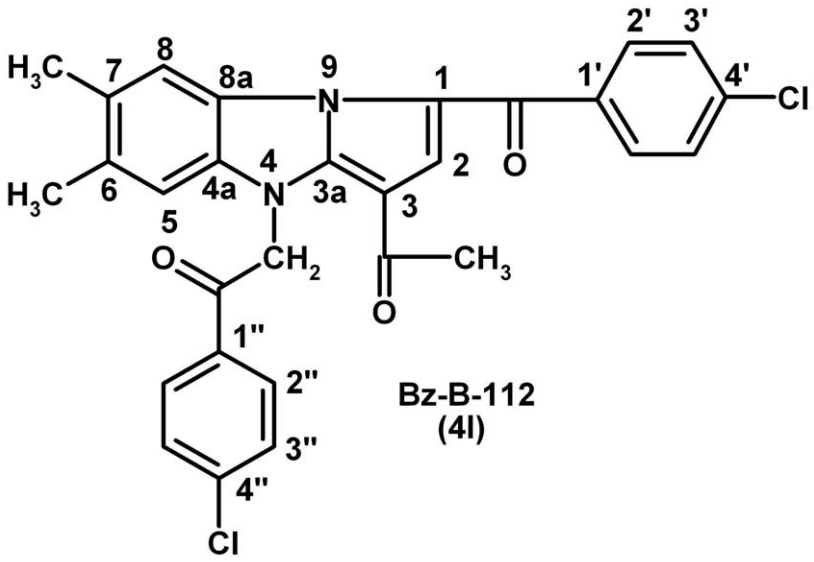


Parameter Set:#H1-QNP-34 TS1.3PL8.
NMR System: Bruker Avance DRX 400 (ICMPP)

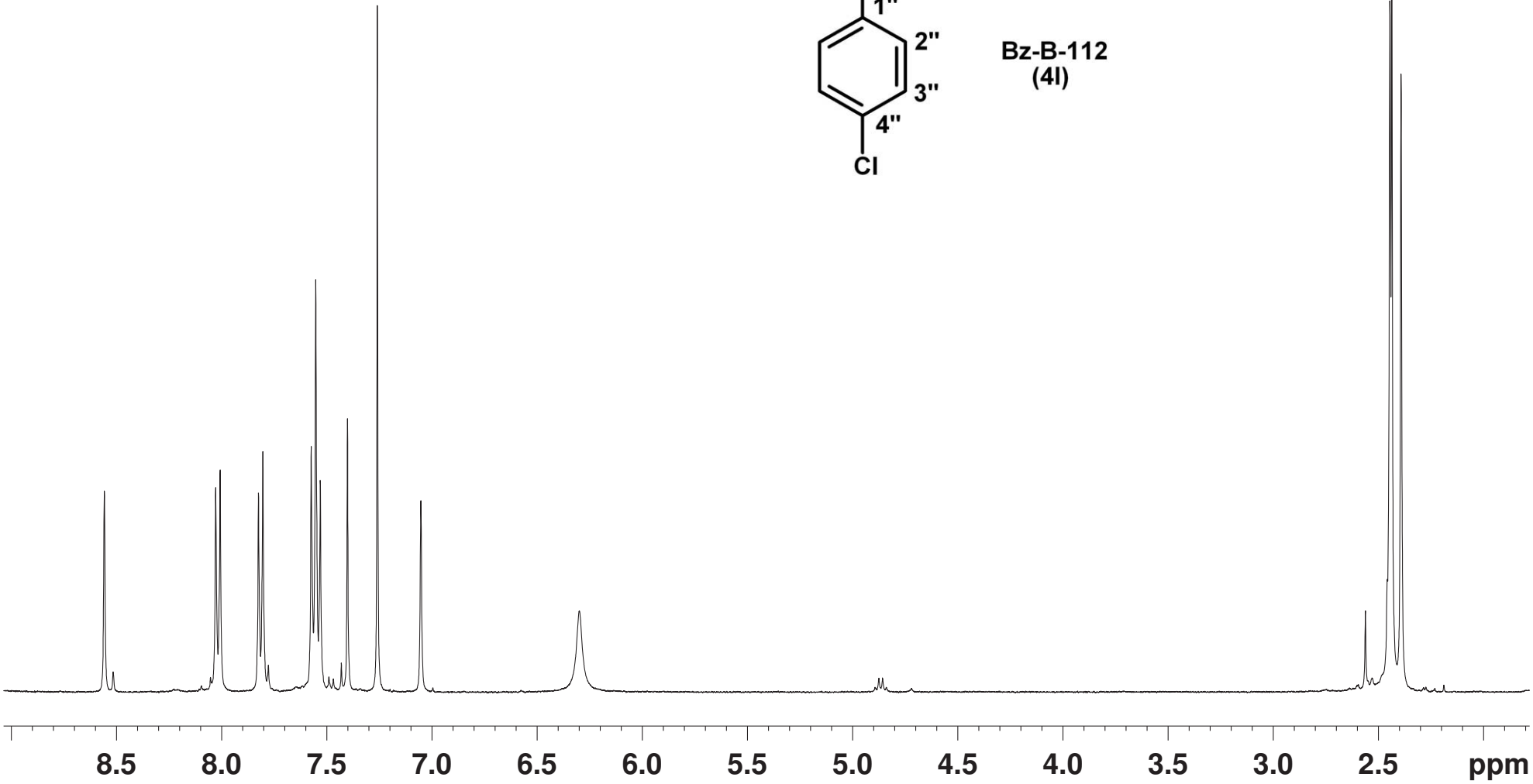
Registry No.:25176

Sample name and description: Bz-B-112 (4l)

p.t. 292-294 °C



Bz-B-112
(4l)

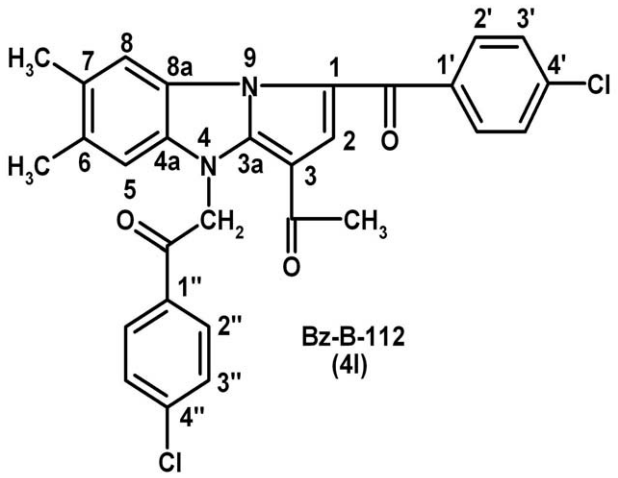


Parameter Set:#C13-CPD-QNP-34 TS1.3PL8
System: Bruker Avance DRX 400 (ICMPP)

Registry No.:25176

Sample name and description: Bz-B-112 (4l)

p.t. 292-294 °C



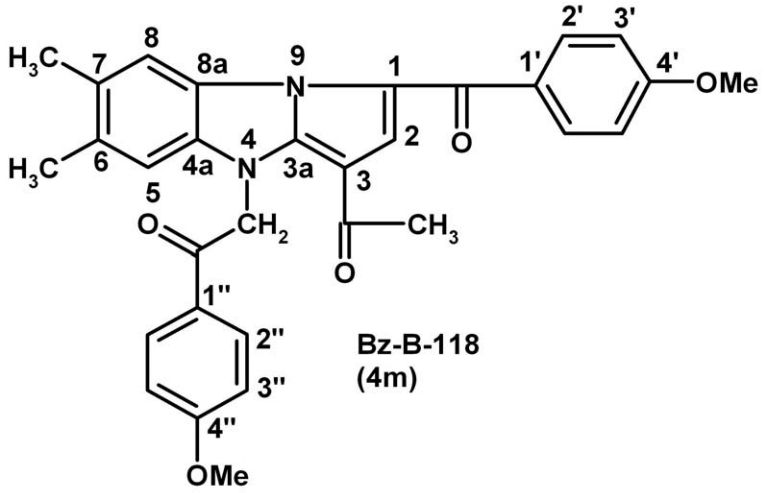
Bz-B-112
(4l)

Parameter Set: %H1-BBIa-42. TS 2.1PL6.
Instrument: Bruker Avance III 400 (ICMPP).

Registry No.:7094

Sample name and description: Bz-B-118 (4m)

p.t. 272-274 °C



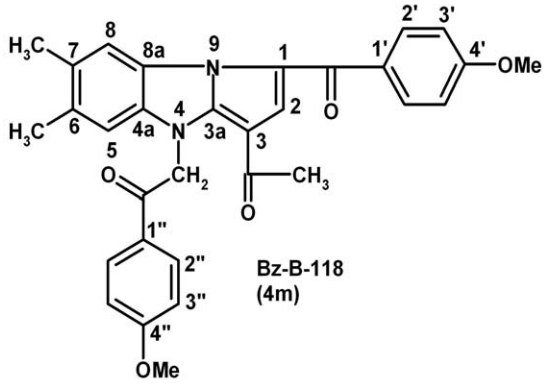
Bz-B-118
(4m)

Parameter Set : !C13-CPD-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:23225

Sample name and description: Bz-B-118 (4m)

p.t. 272-274 °C

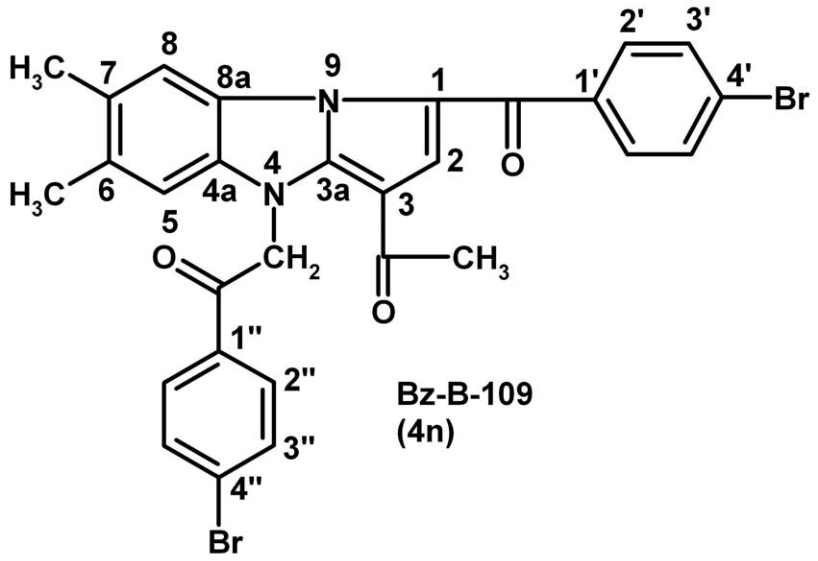


Bz-B-118
(4m)

Parameter Set:!H1-BBFOa-44. TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)
Registry No.:22689

Sample name and description: Bz-B-109 (4n)

p.t. 290-292 °C



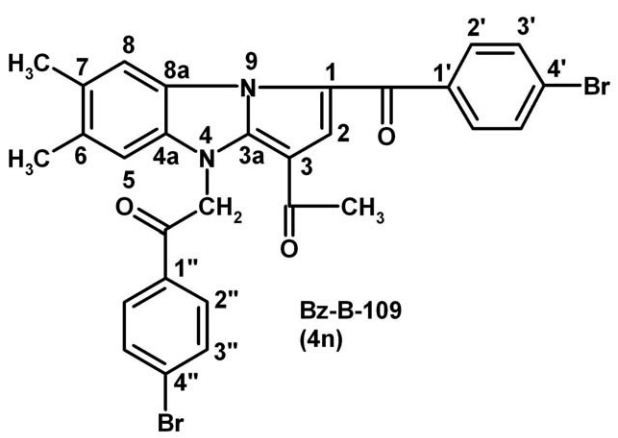
Bz-B-109
(4n)

Parameter Set : !C13-CPD-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

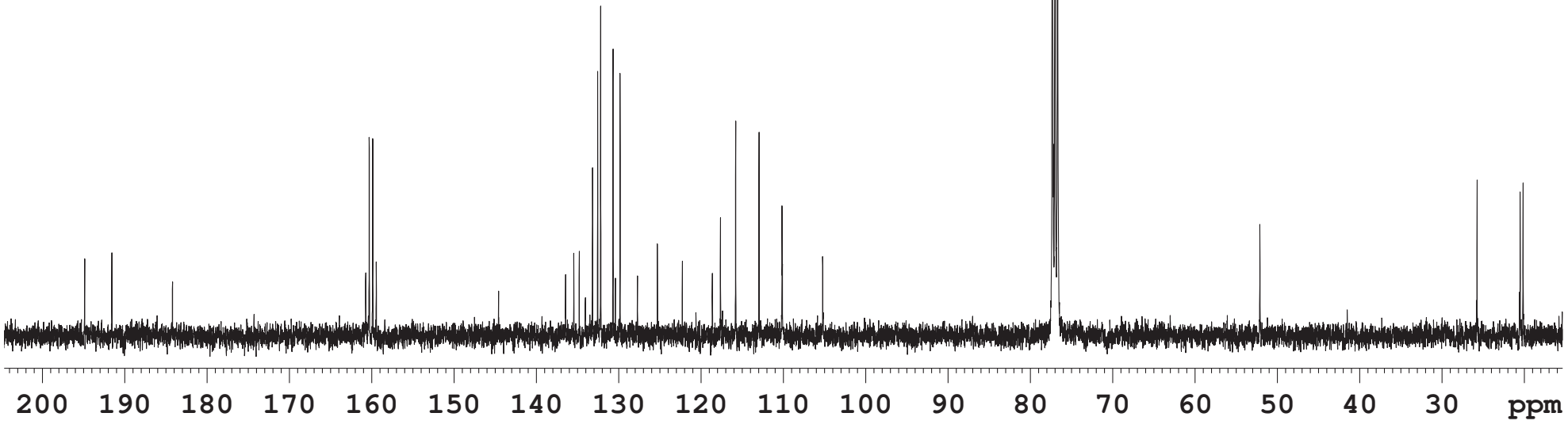
Registry No.:22689

Sample name and description: Bz-B-109 (4n)

p.t. 290-292 °C



Bz-B-109
(4n)

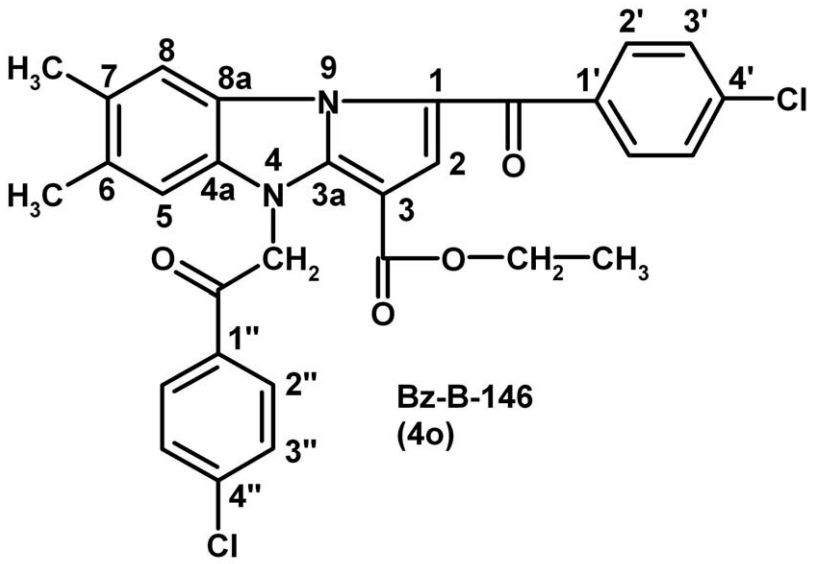


Parameter Set:!H1-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

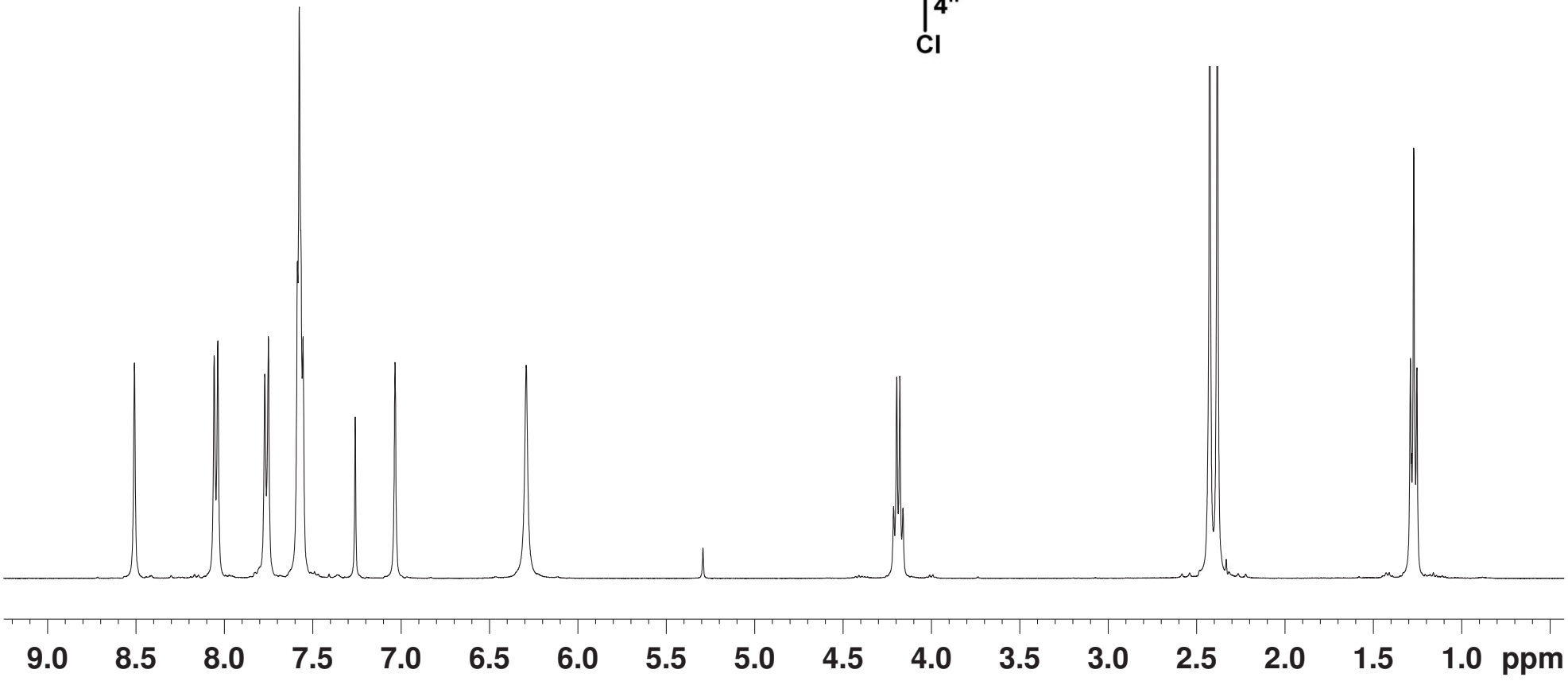
Registry No.:24588

Sample name and description: Bz-B-146 (4o)

p.t. 285-287 °C



Bz-B-146
(4o)

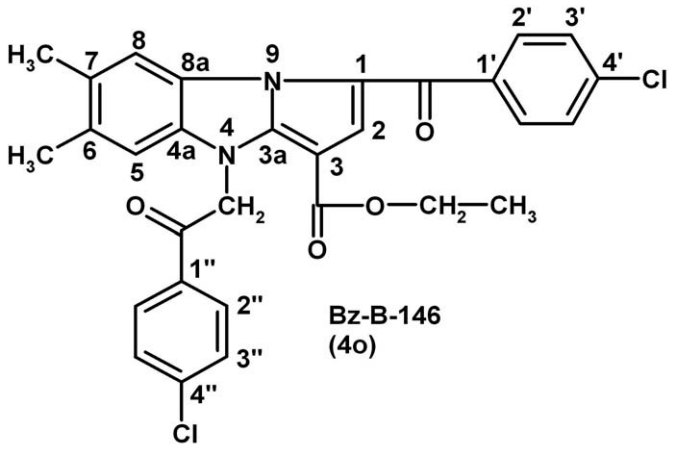


Parameter Set : !C13-CPD-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

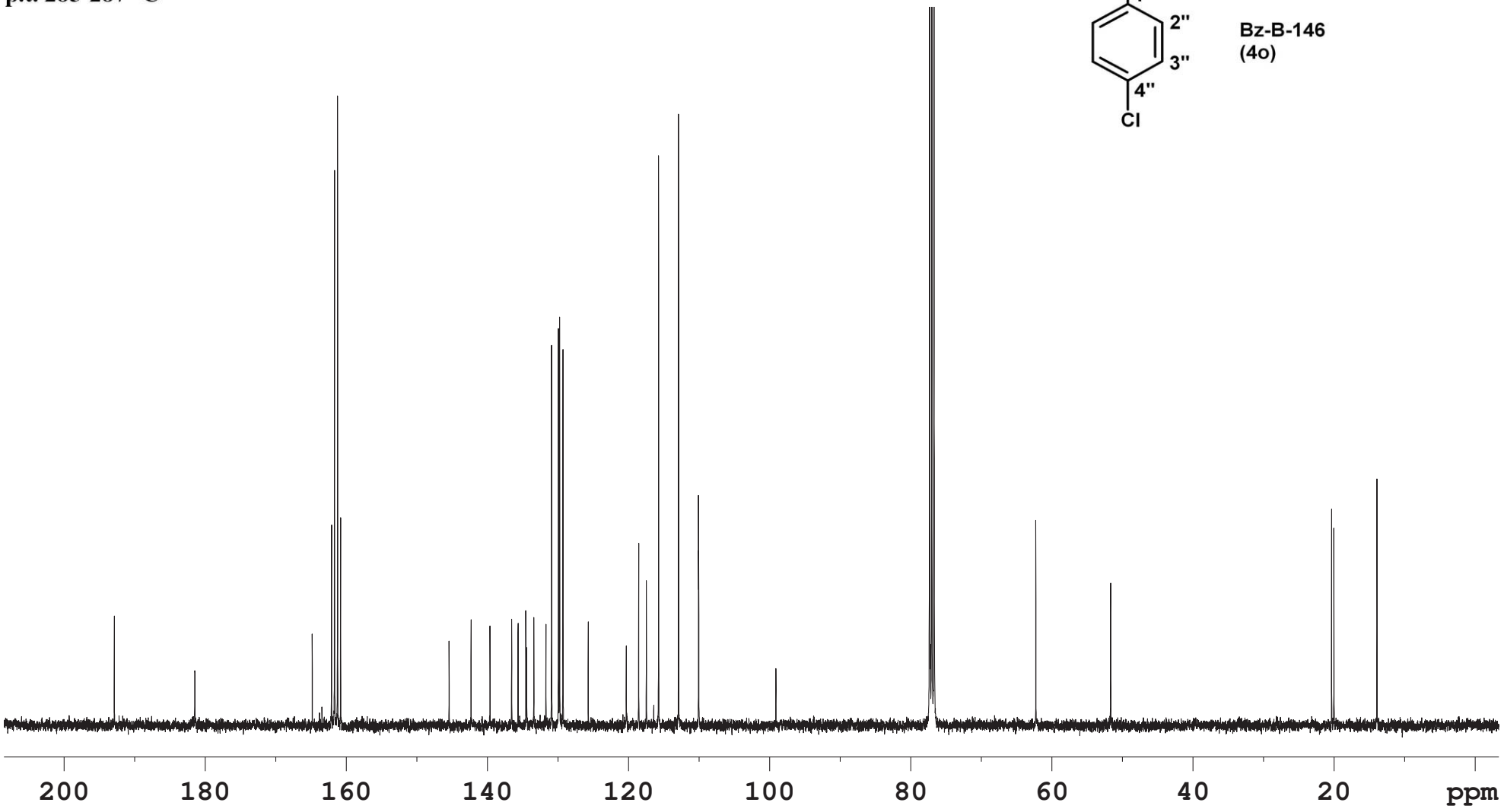
Registry No.:24588

Sample name and description: Bz-B-146 (4o)

p.t. 285-287 °C



Bz-B-146
(4o)

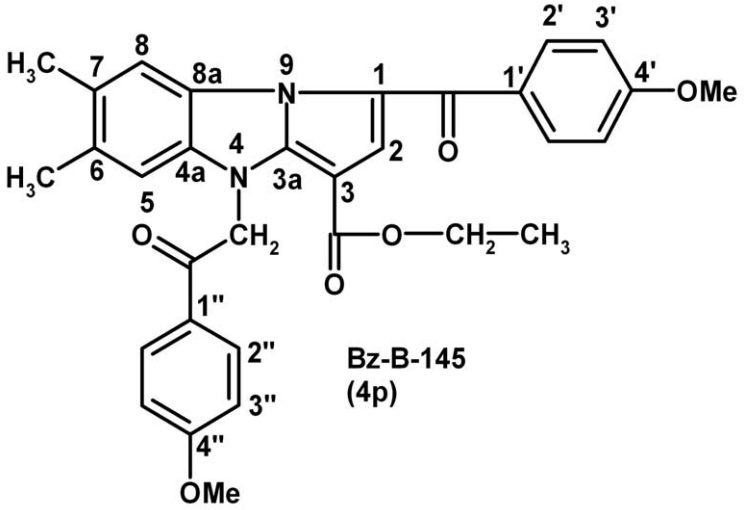


Parameter Set:!H1-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24615

Sample name and description: Bz-B-145 (4p)

p.t. 274-276 °C

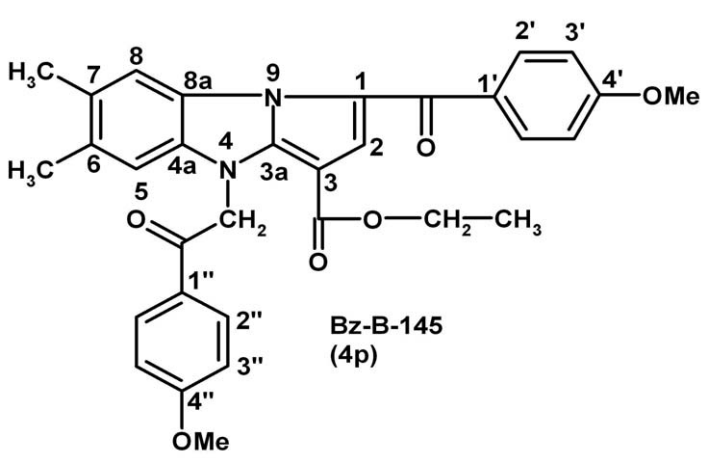


Parameter Set : !C13-CPD-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

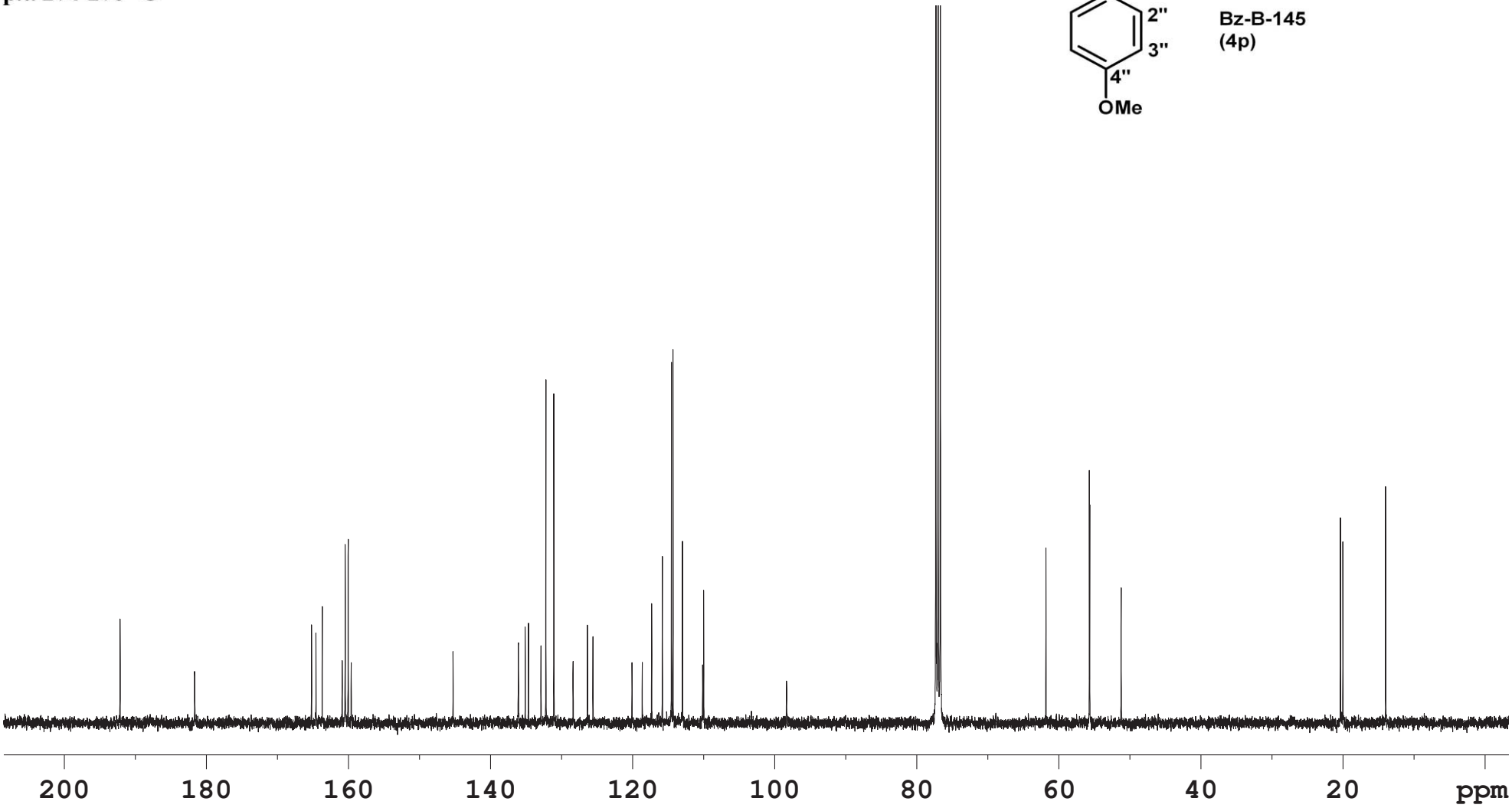
Registry No.:24615

Sample name and description: Bz-B-145 (4p)

p.t. 274-276 °C



Bz-B-145
(4p)

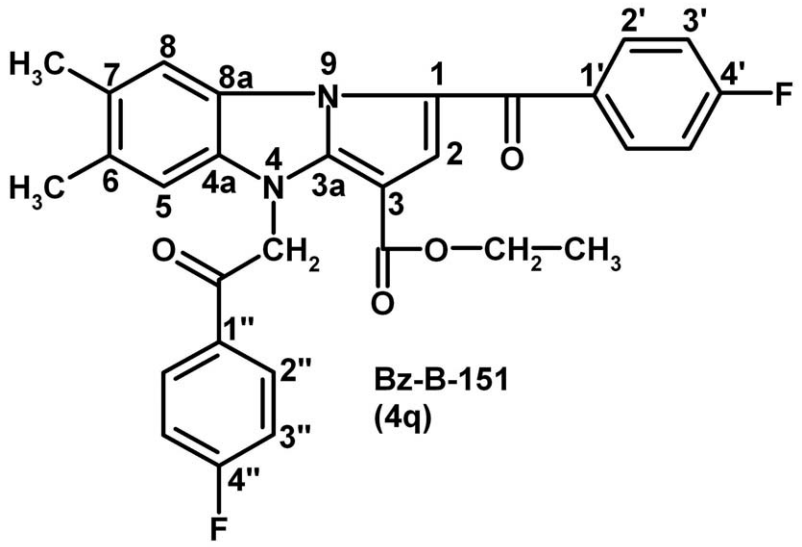


Parameter Set: #H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

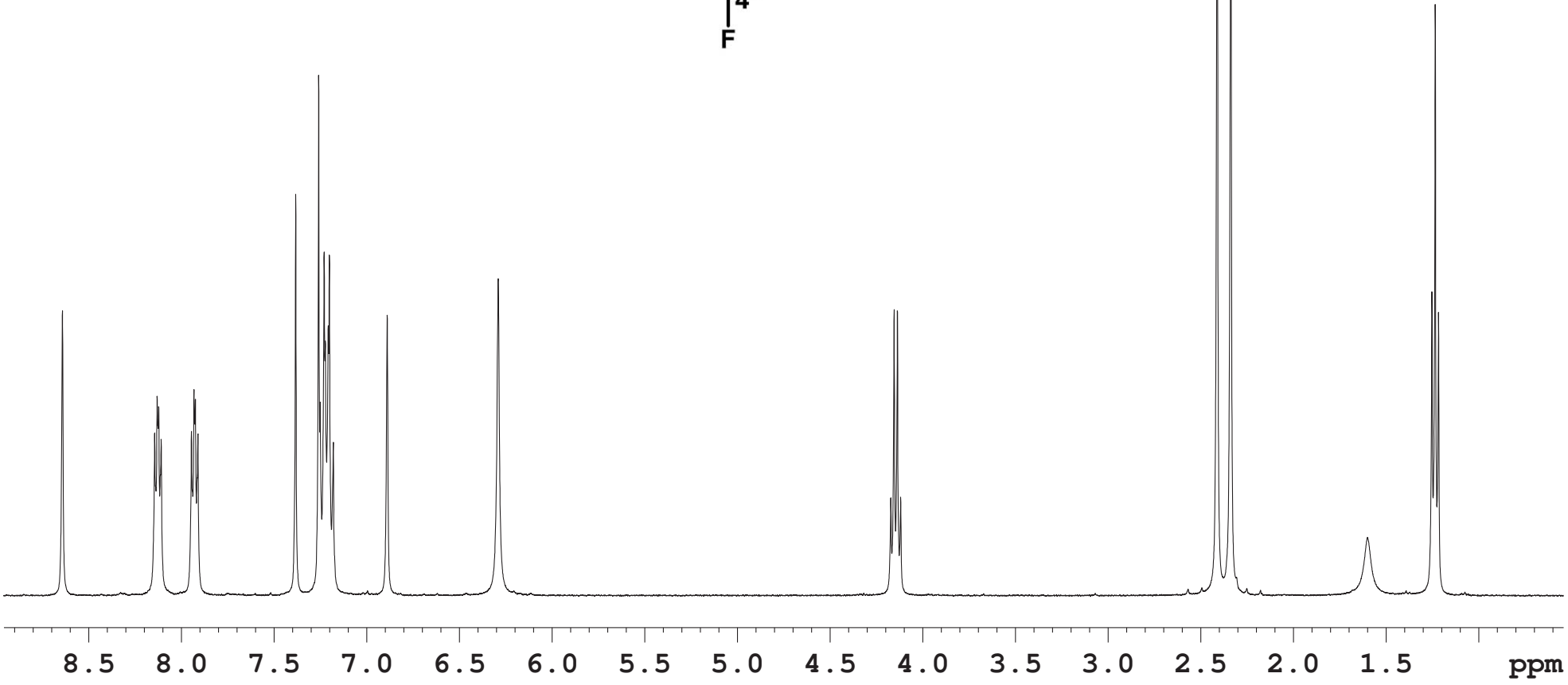
Registry No.:24902

Sample name and description: Bz-B-151 (4q)

p.t. 248-250 °C



Bz-B-151
(4q)

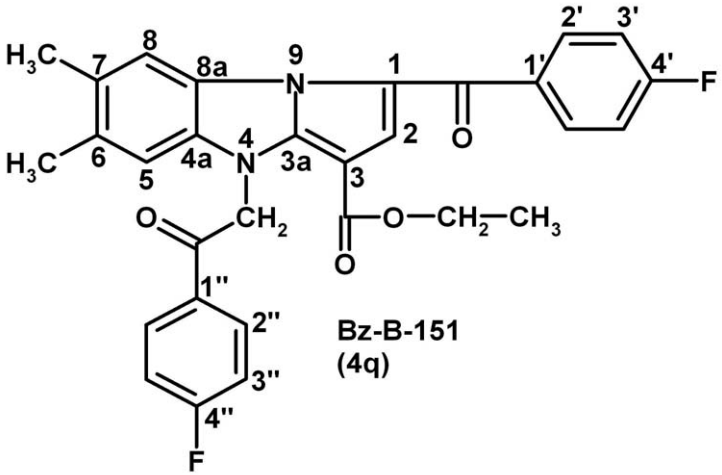


Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24902

Sample name and description: Bz-B-151 (4q)

p.t. 248-250 °C

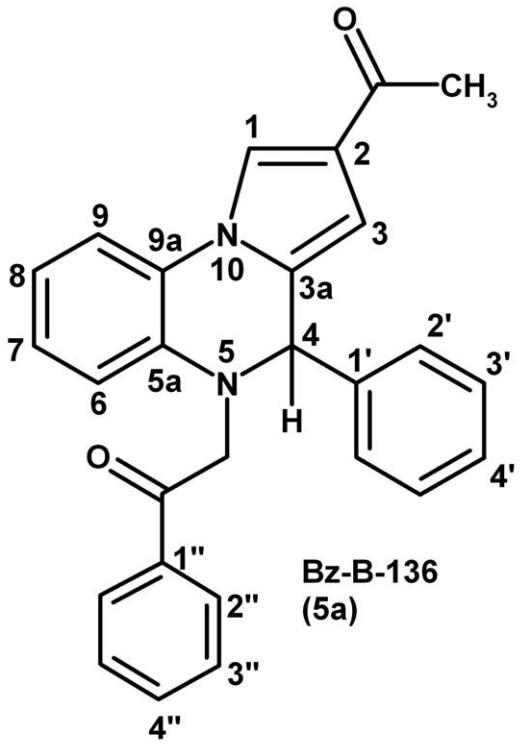


Parameter Set:!H1-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24601

Sample name and description: Bz-B-136 (5a)

p.t. 192-194 °C



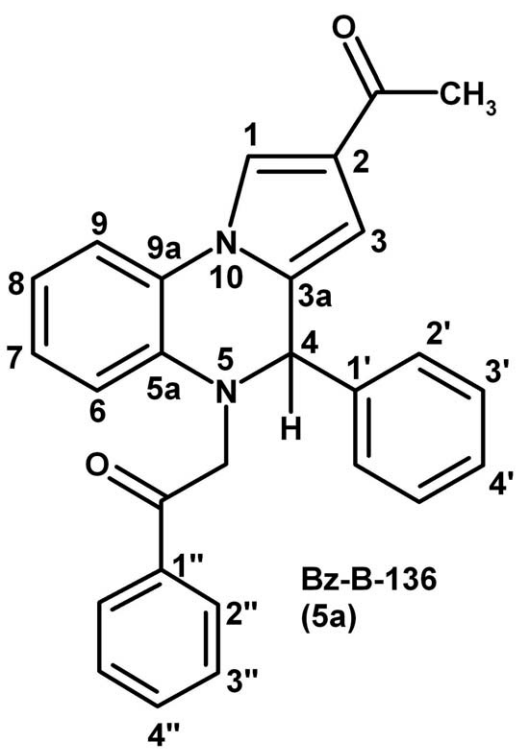
Bz-B-136
(5a)

Parameter Set : !C13-CPD-BBFOa-44 TS1.3PL8
Instrument: Bruker Avance DRX 400 (ICMPP)

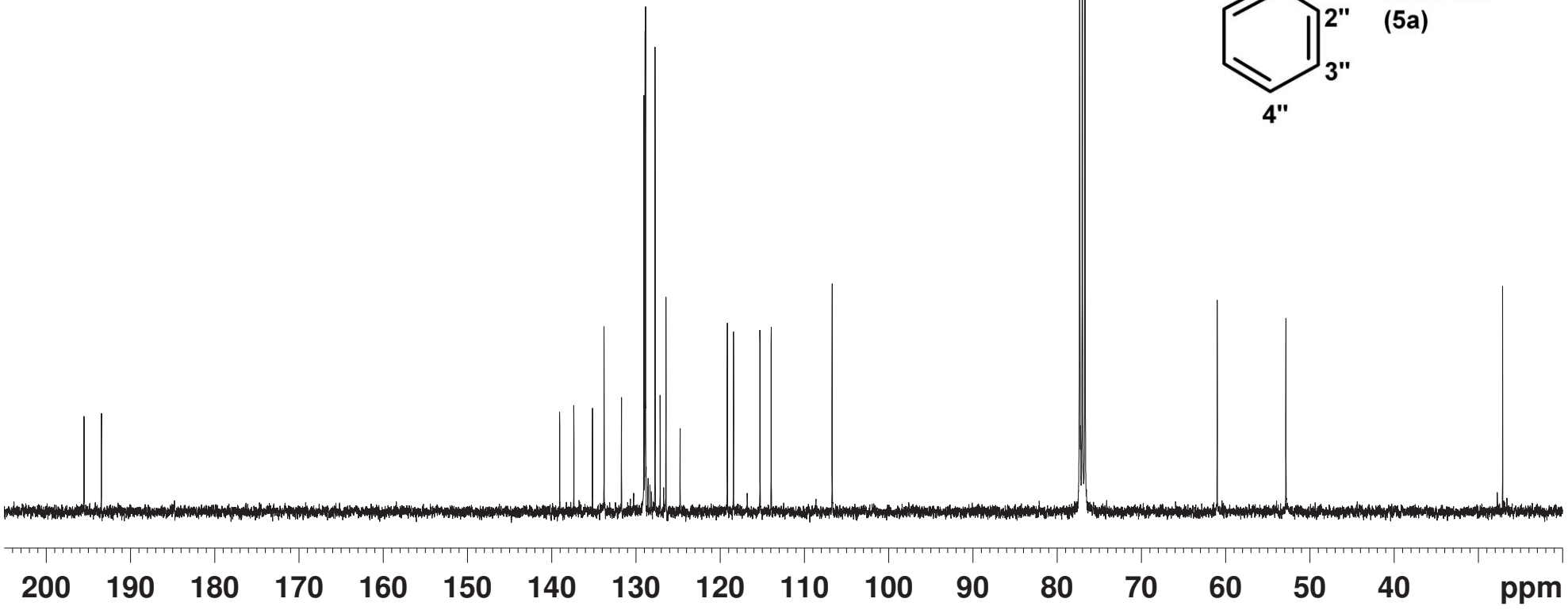
Registry No.:24601

Sample name and description: Bz-B-136 (5a)

p.t. 192-194 °C



Bz-B-136
(5a)

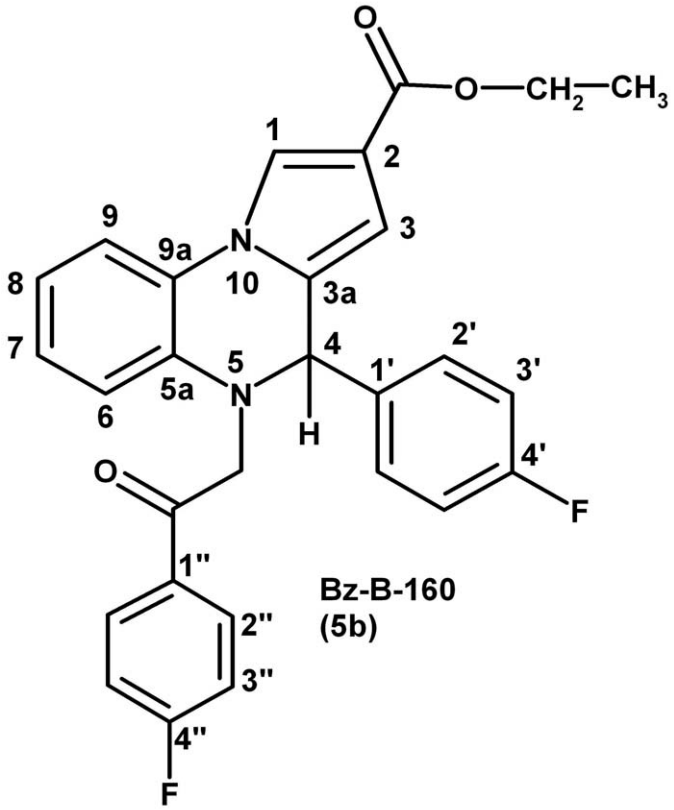


Parameter Set:#H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:25849

Sample name and description: Bz-B-160 (5b)

p.t. 155-157 °C



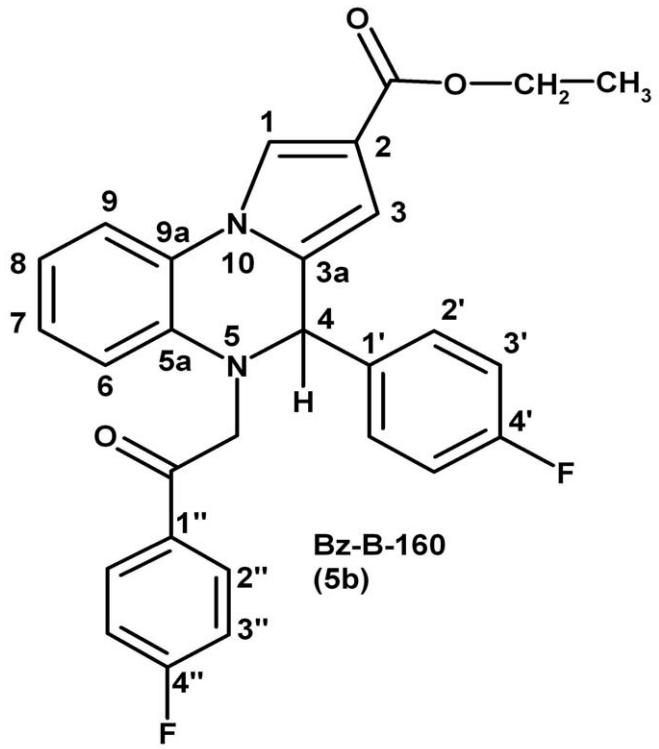
Bz-B-160
(5b)

Parameter Set:#C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:25500

Sample name and description: Bz-B-160 (5b)

p.t. 155-157 °C



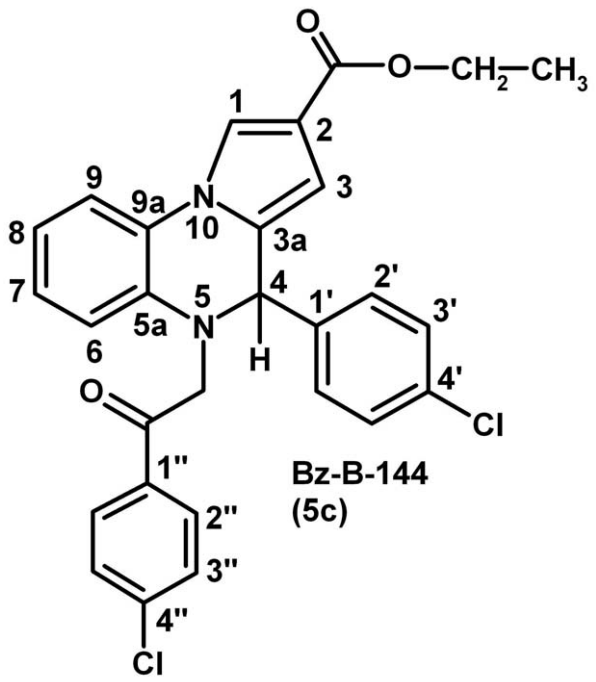
Bz-B-160
(5b)

Parameter Set: !H1-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24574

Sample name and description: Bz-B-144 (5c)

p.t. 172-174 °C



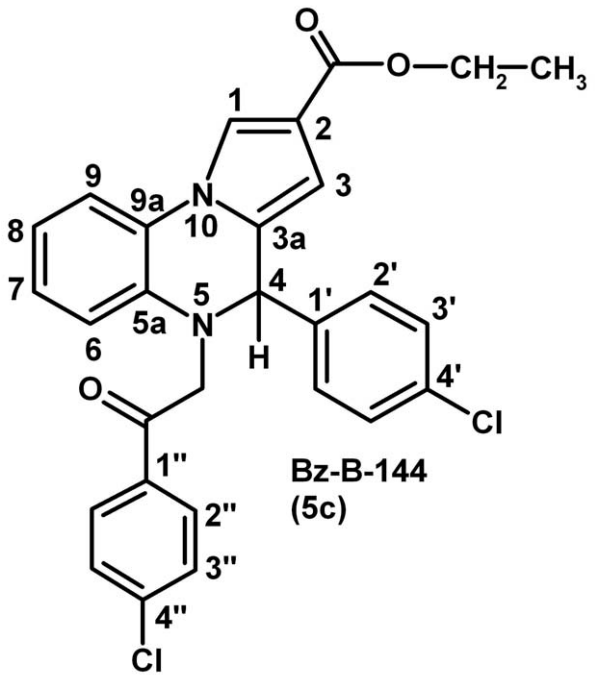
Bz-B-144
(5c)

Parameter Set: !C13-CPD-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24574

Sample name and description: Bz-B-144 (5c)

p.t. 172-174 °C



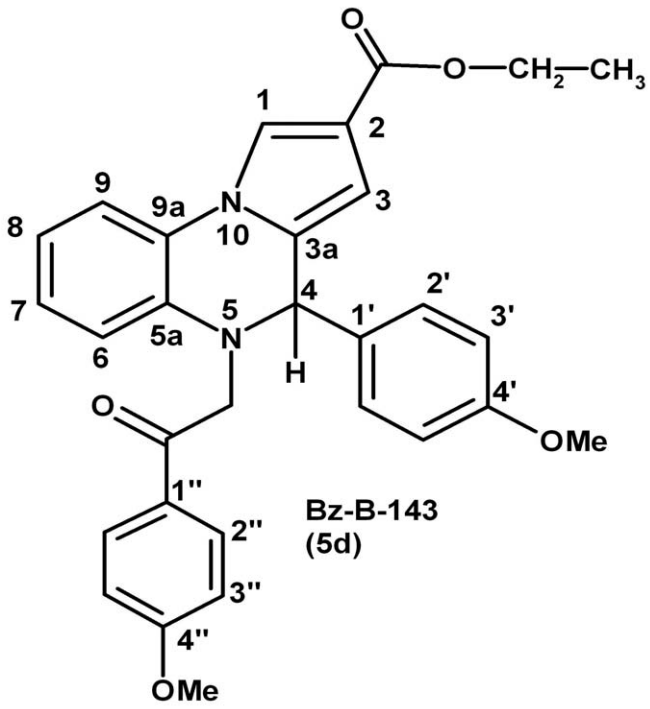
Bz-B-144
(5c)

Parameter Set: #H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

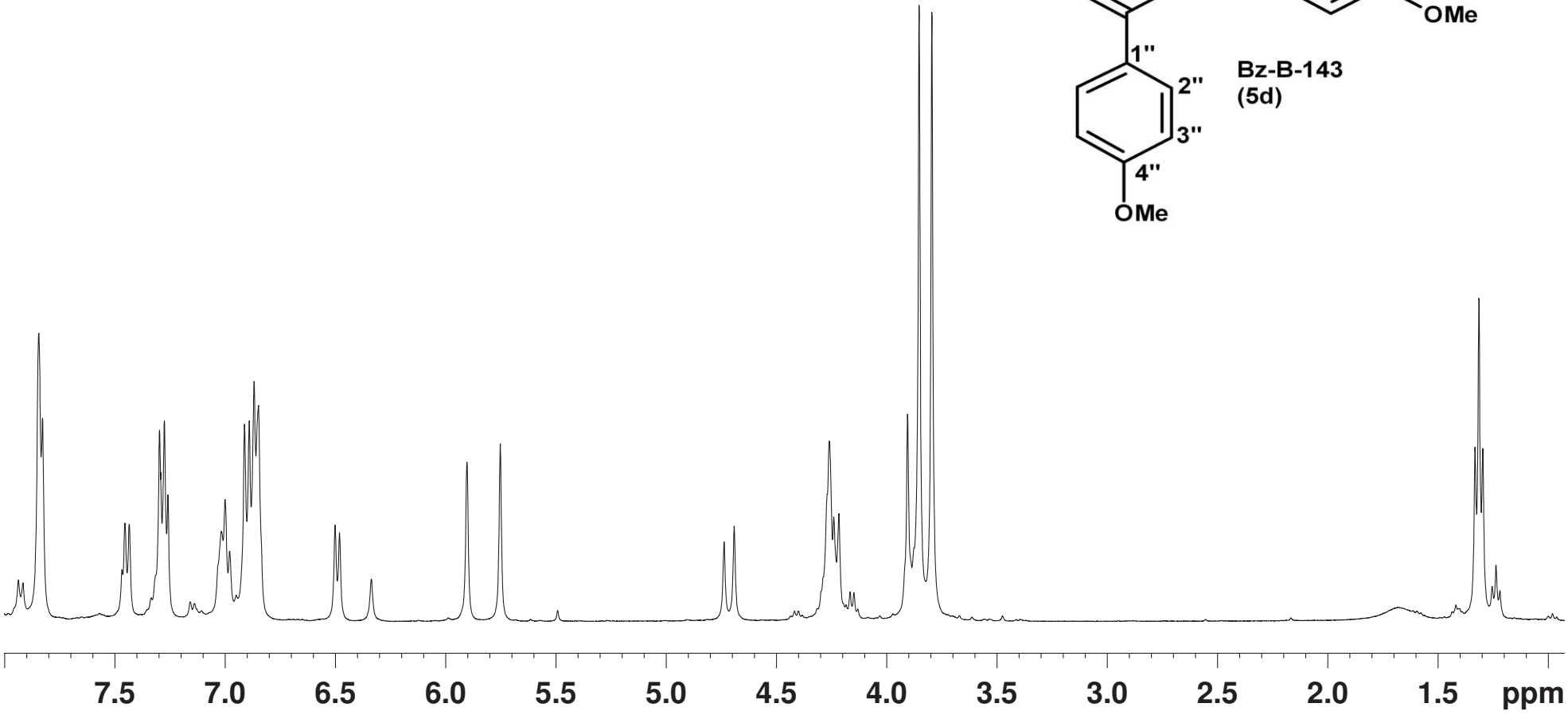
Registry No.:25518

Sample name and description: Bz-B-143 (5d)

p.t. 174-176 °C



Bz-B-143
(5d)

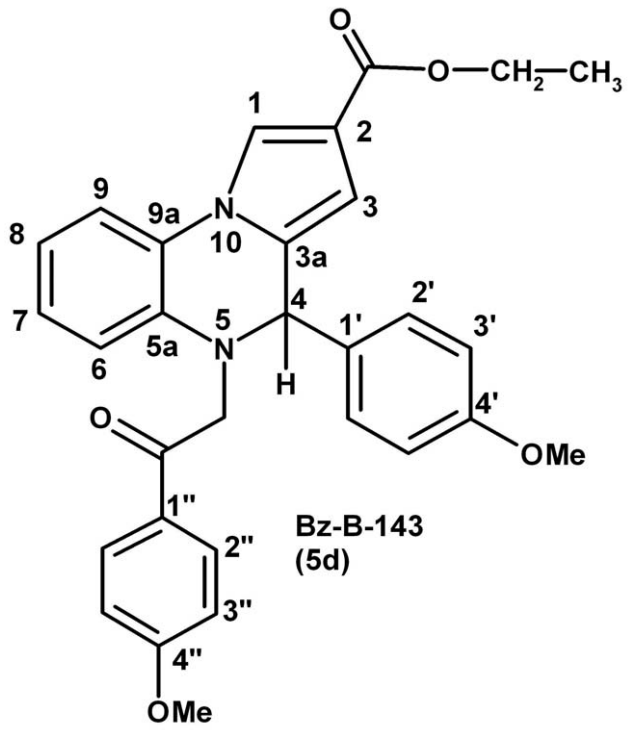


Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:25518

Sample name and description: Bz-B-143 (5d)

p.t. 174-176 °C



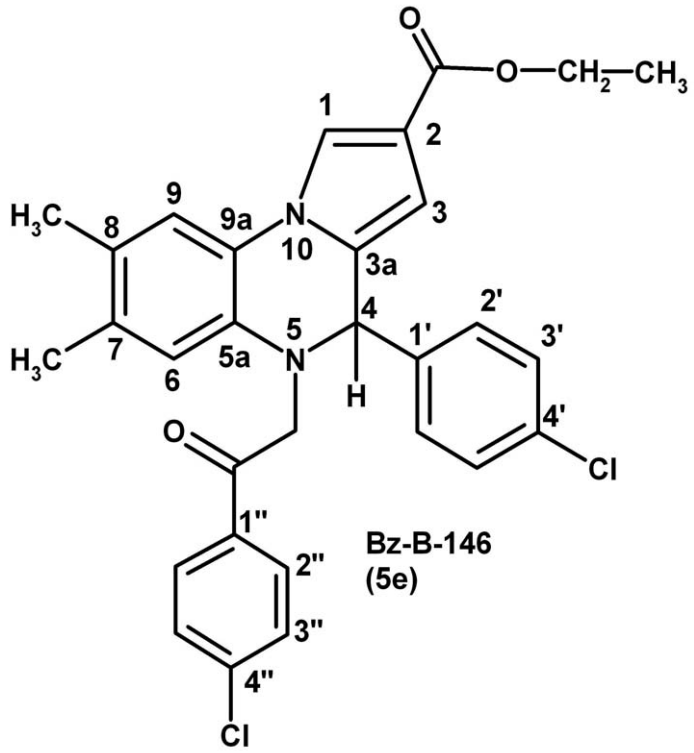
Bz-B-143
(5d)

Parameter Set: !H1-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

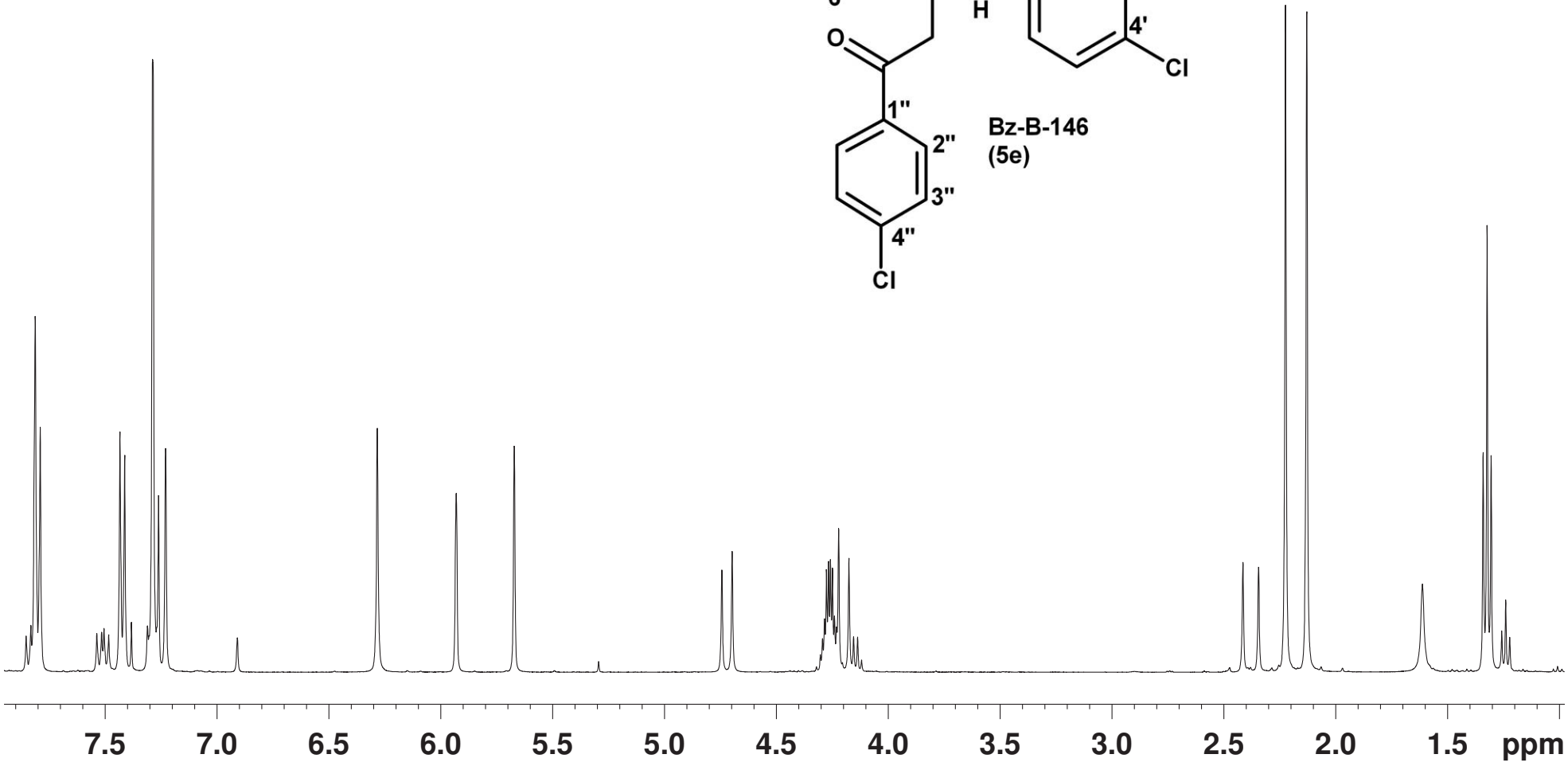
Registry No.:24576

Sample name and description: Bz-B-146 (5e)

p.t. 176-178 °C



Bz-B-146
(5e)

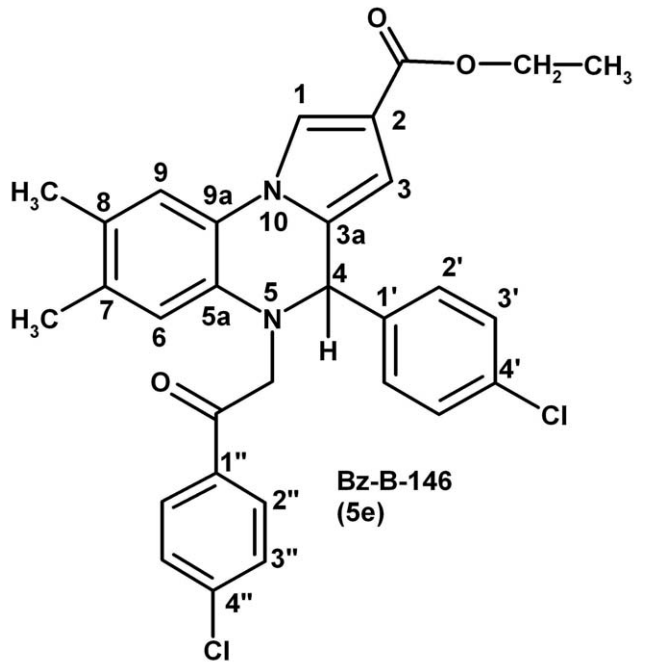


Parameter Set: !C13-CPD-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

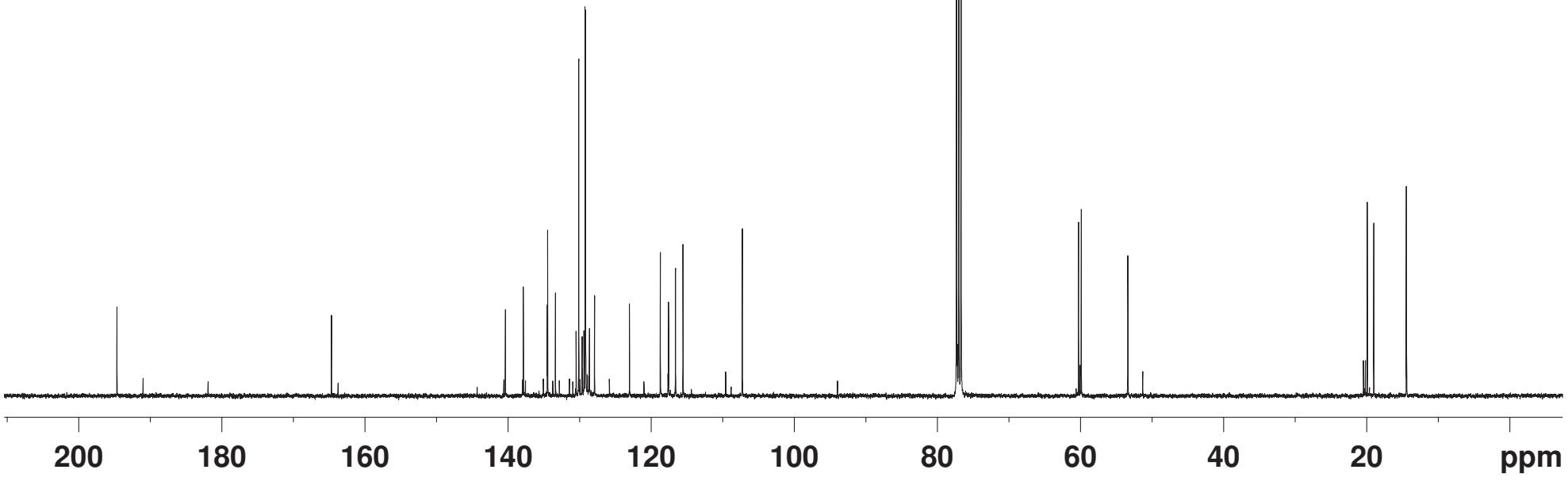
Registry No.:24576

Sample name and description: Bz-B-146 (5e)

p.t. 176-178 °C



Bz-B-146
(5e)

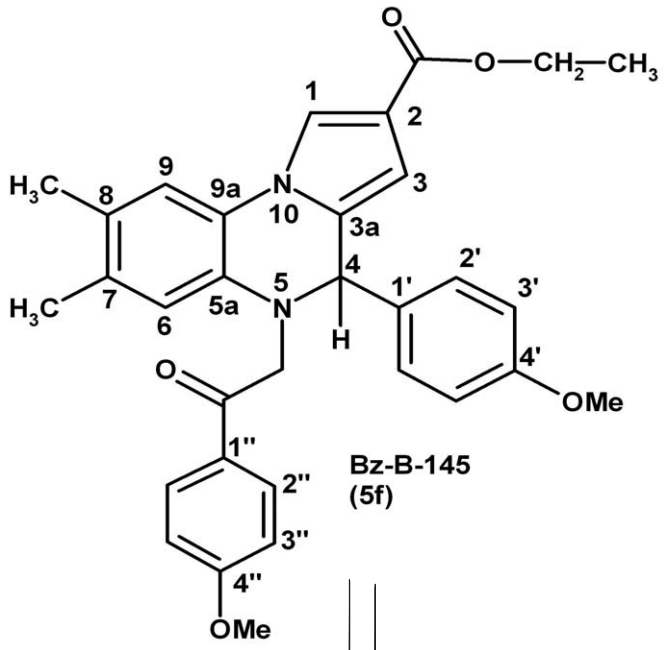


Parameter Set: !H1-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24621

Sample name and description: Bz-B-145 (5f)

p.t. 181-183 °C



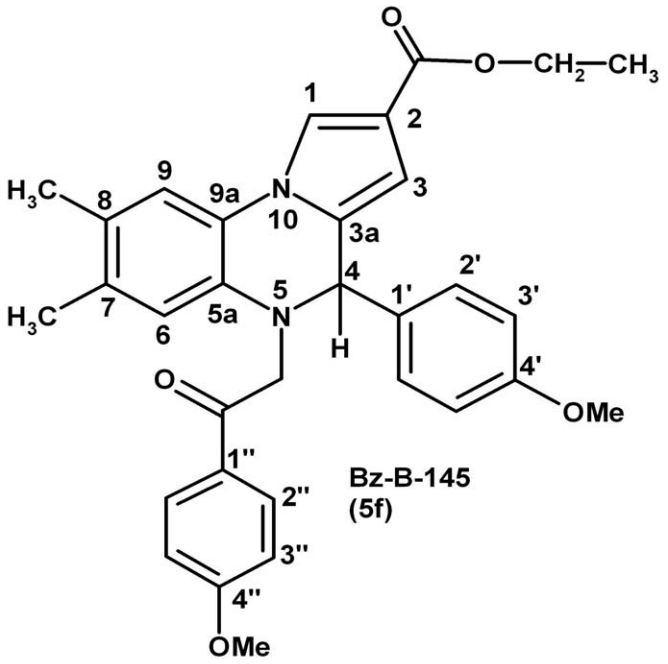
Bz-B-145
(5f)

Parameter Set: !C13-CPD-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

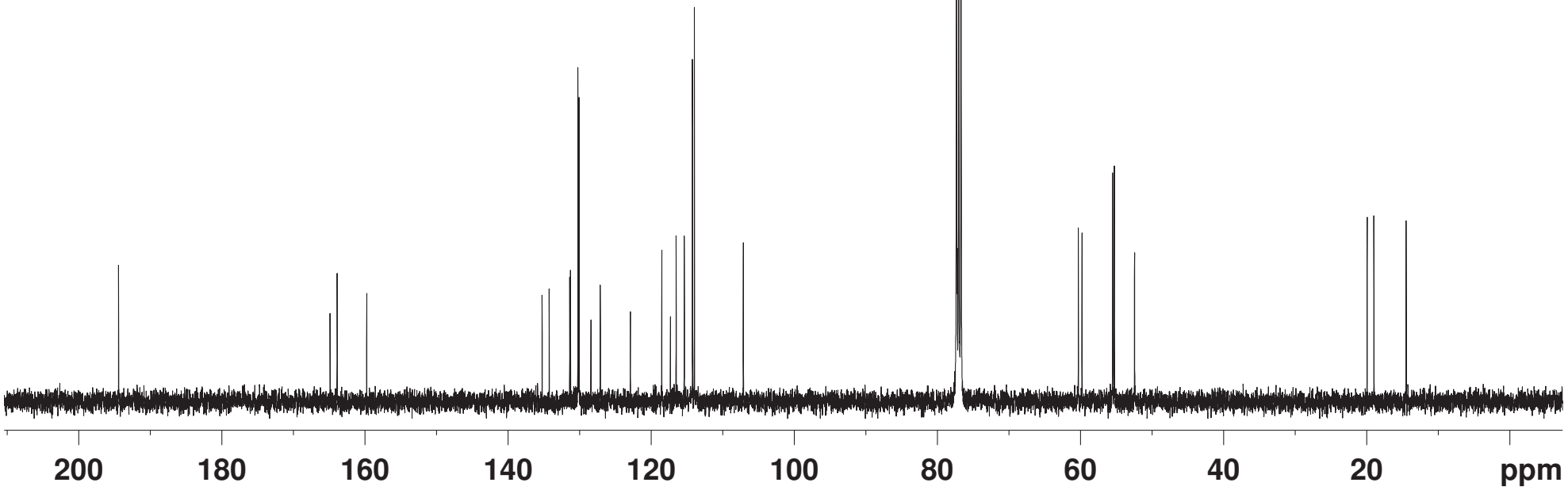
Registry No.:24621

Sample name and description: Bz-B-145 (5f)

p.t. 181-183 °C



Bz-B-145
(5f)

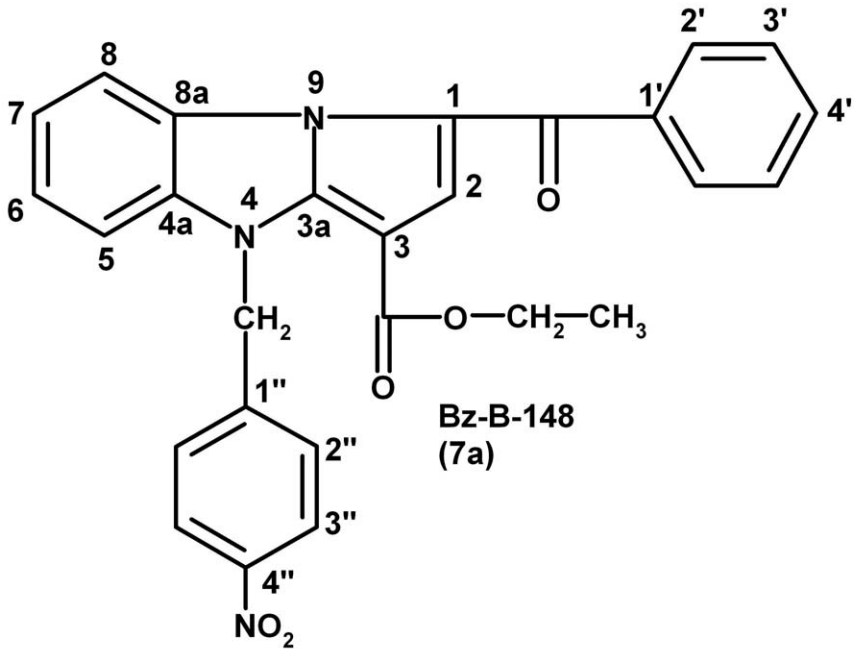


Parameter Set:#H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24876

Sample name and description: Bz-B-148 (7a)

p.t. 270-272 °C



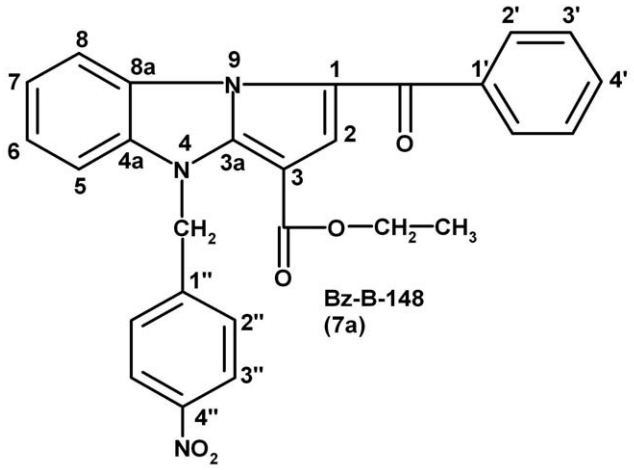
Bz-B-148
(7a)

Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

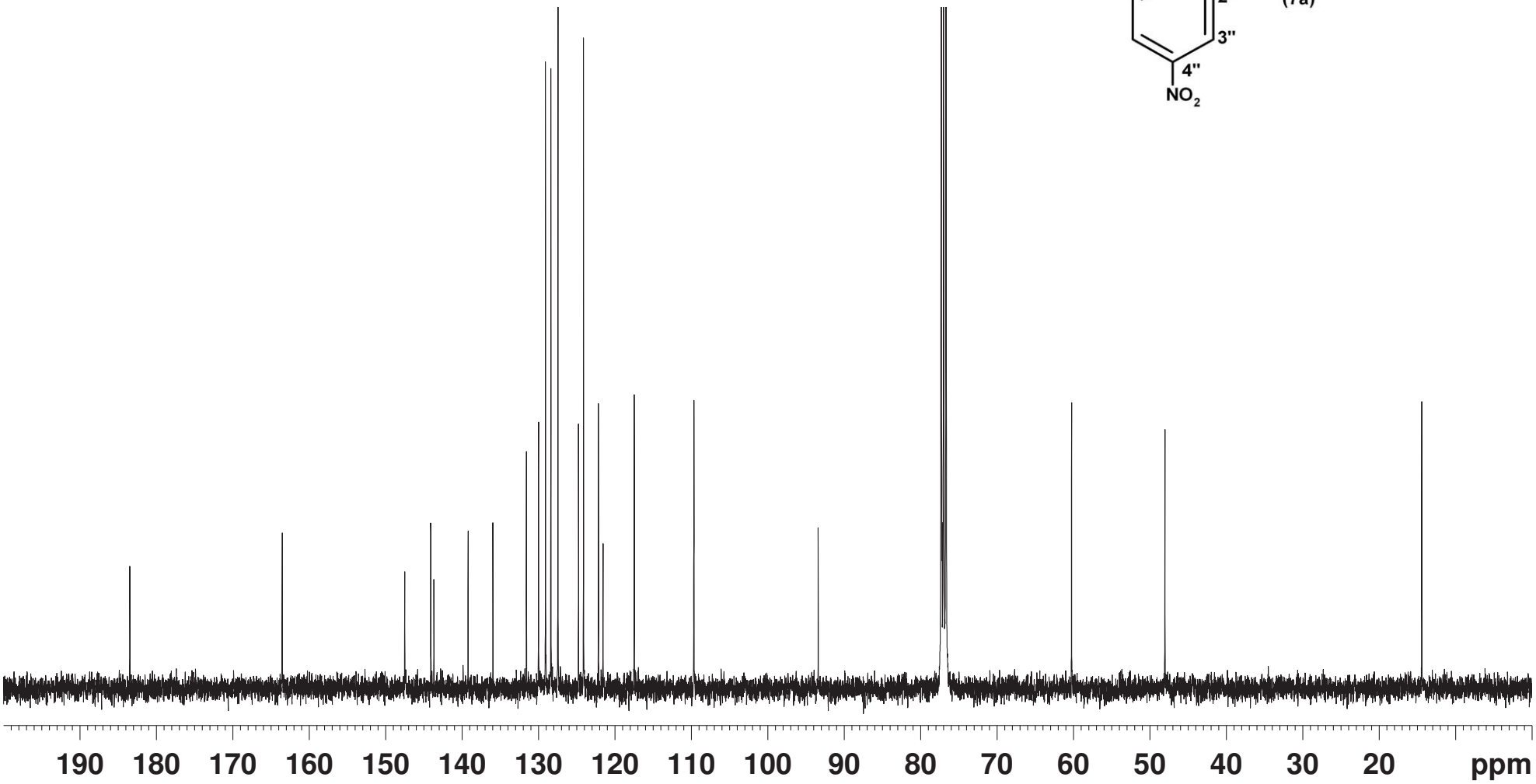
Registry No.:24876

Sample name and description: Bz-B-148 (7a)

p.t. 270-272 °C



Bz-B-148
(7a)

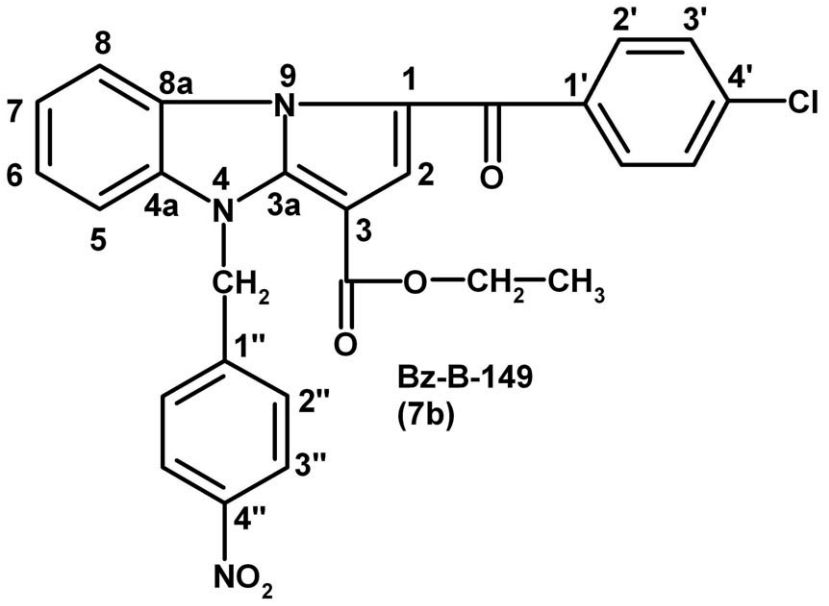


Parameter Set:#H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

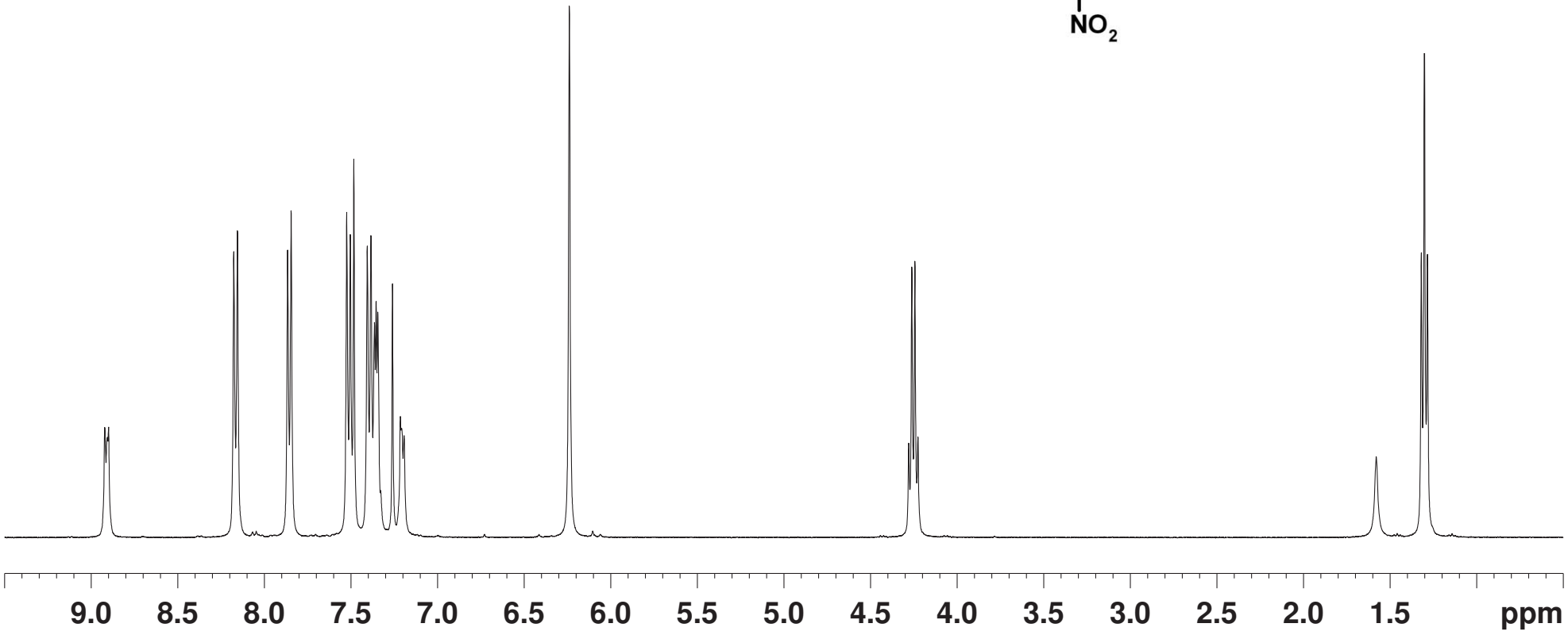
Registry No.:24899

Sample name and description: Bz-B-149 (7b)

p.t. 288-290 °C



Bz-B-149
(7b)

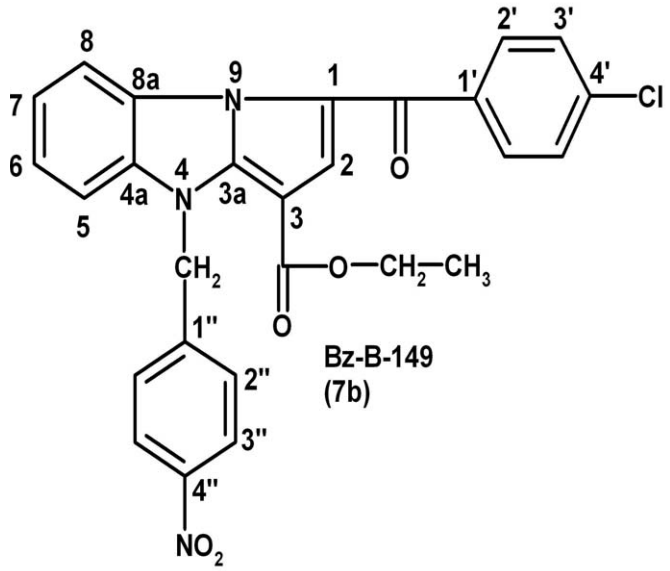


Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

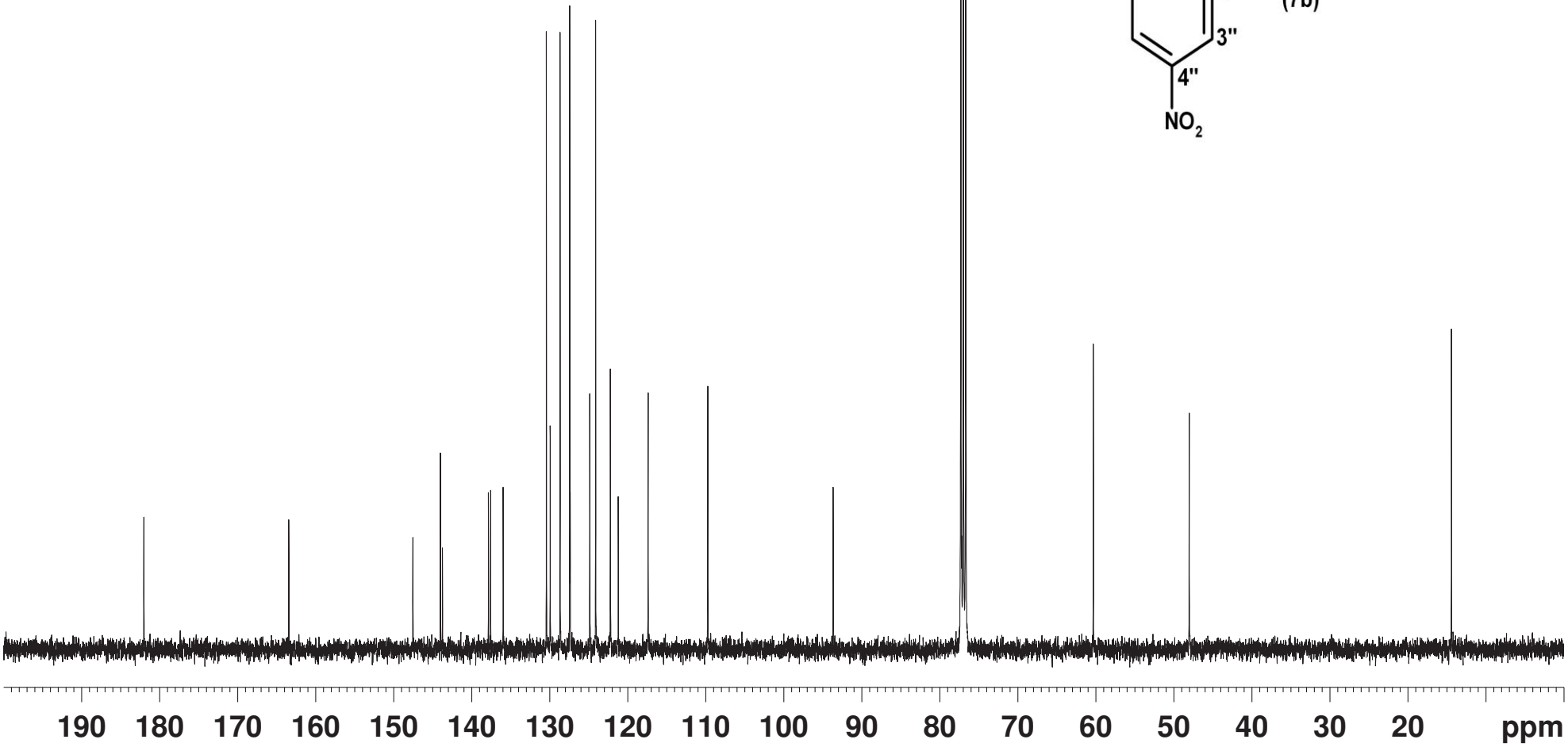
Registry No.:24899

Sample name and description: Bz-B-149 (7b)

p.t. 288-290 °C



Bz-B-149
(7b)

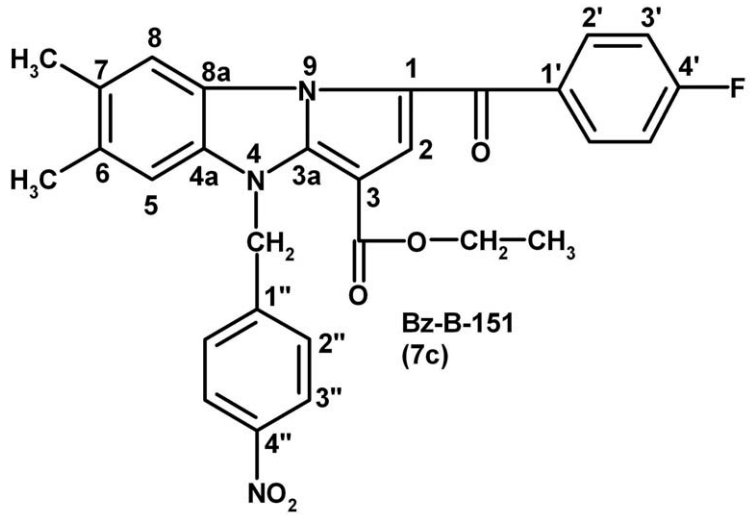


Parameter Set:#H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

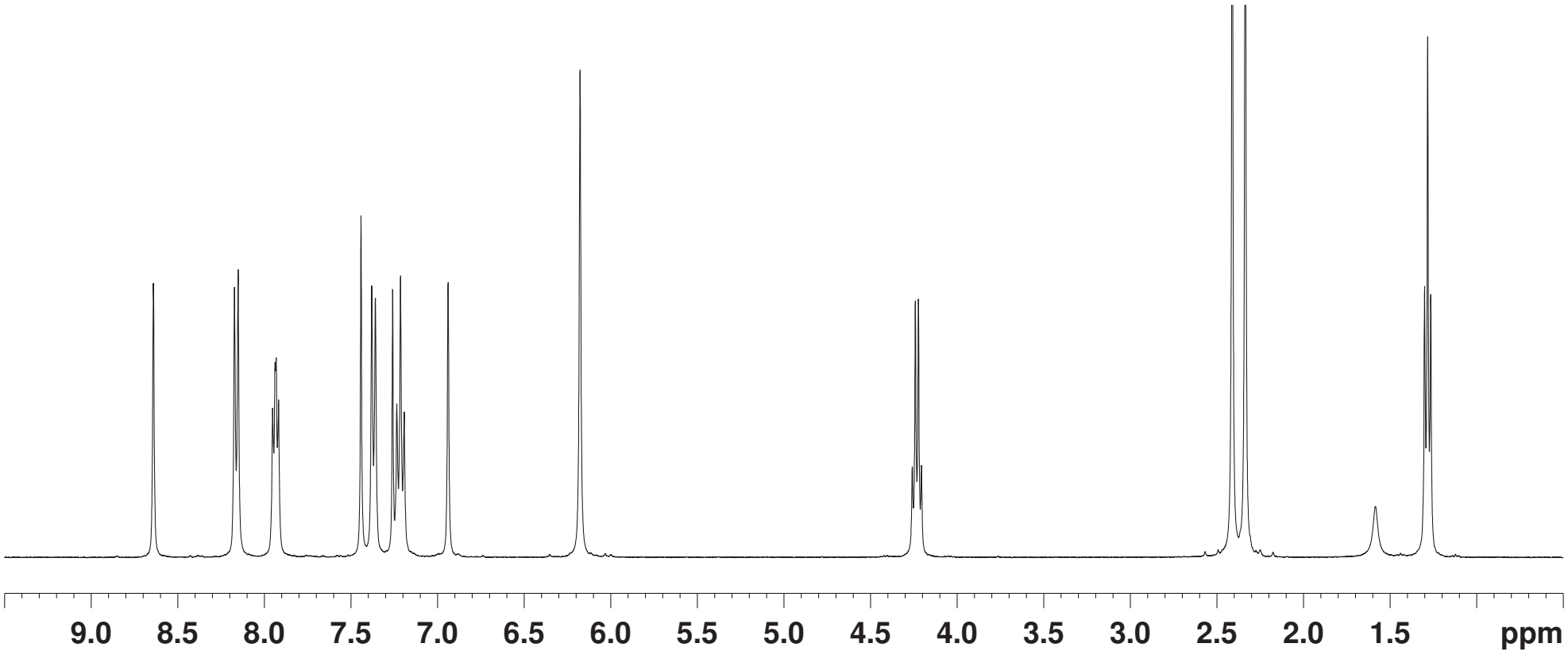
Registry No.:24903

Sample name and description: Bz-B-151 (7c)

p.t. 289-291 °C



Bz-B-151
(7c)

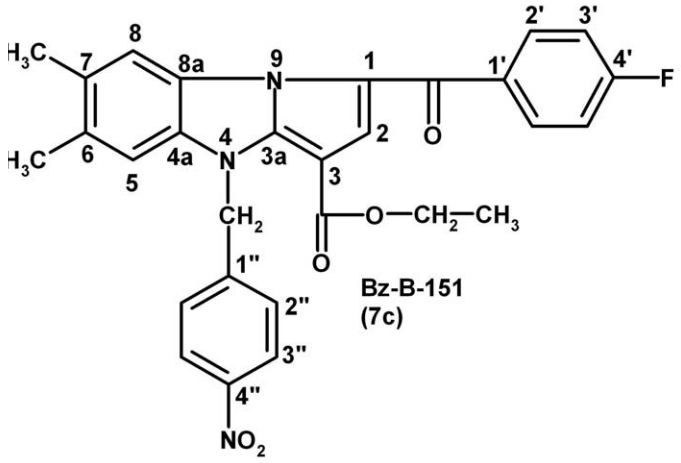


Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

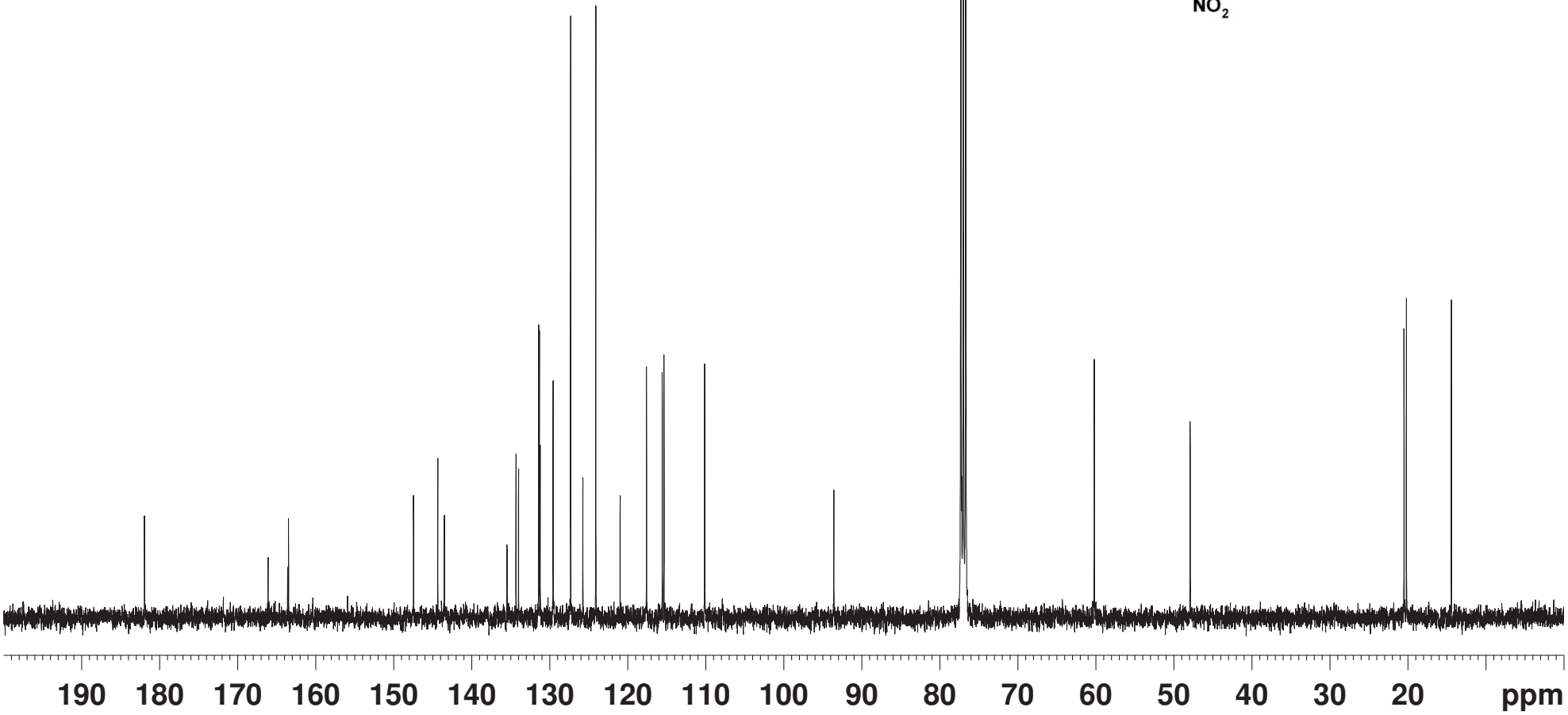
Registry No.:24903

Sample name and description: Bz-B-151 (7c)

p.t. 289-291 °C



Bz-B-151
(7c)

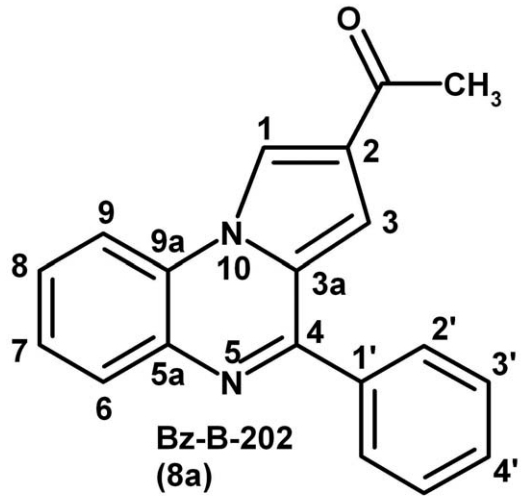


Parameter Set: !H1-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:28371

Sample name and description: Bz-B-202 (8a)

p.t. 189-191 °C



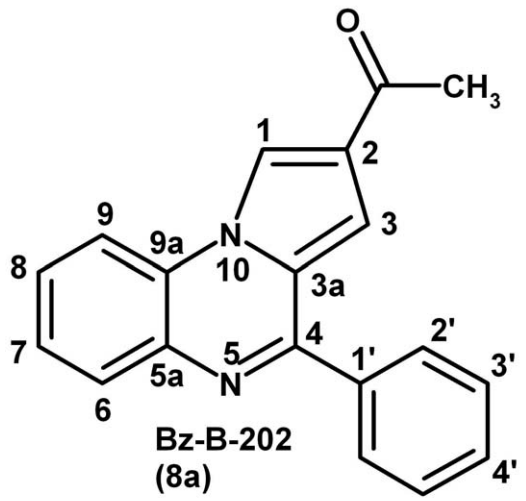
Bz-B-202
(8a)

Parameter Set: !C13-CPD-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

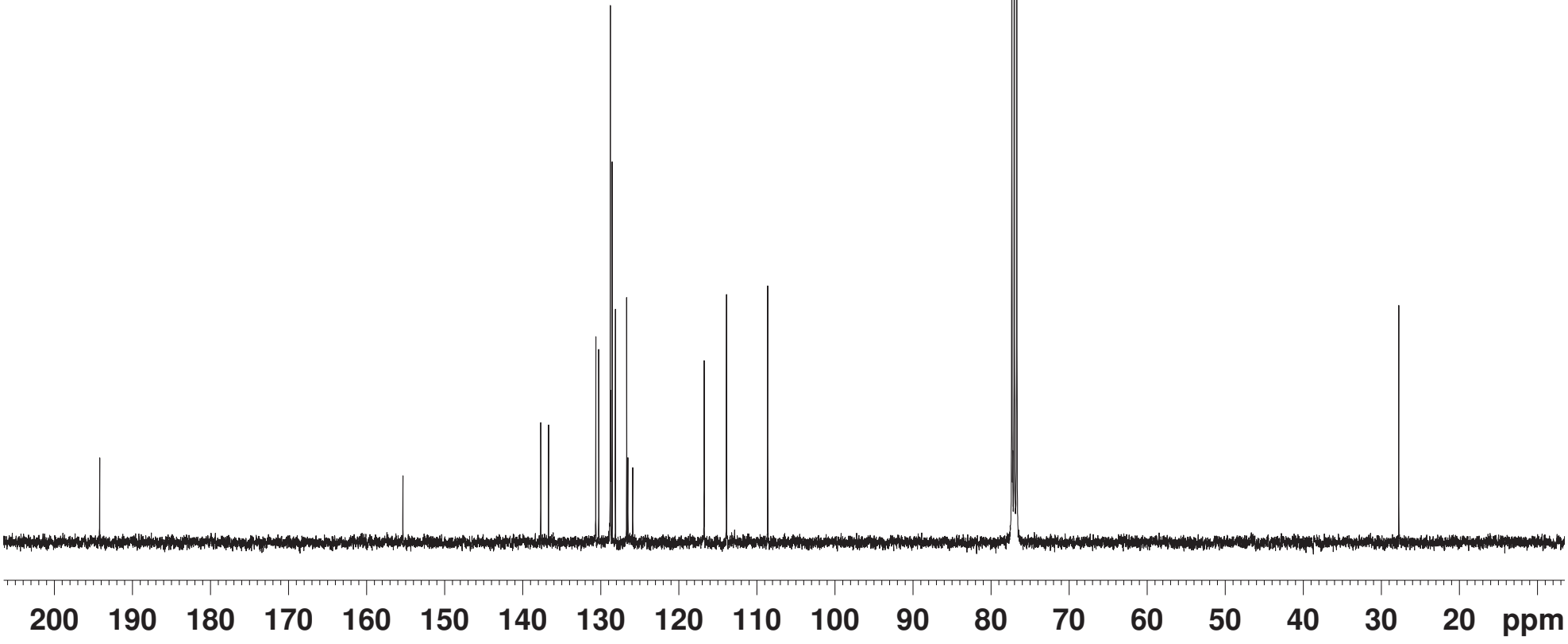
Registry No.:28371

Sample name and description: Bz-B-202 (8a)

p.t. 189-191 °C



Bz-B-202
(8a)

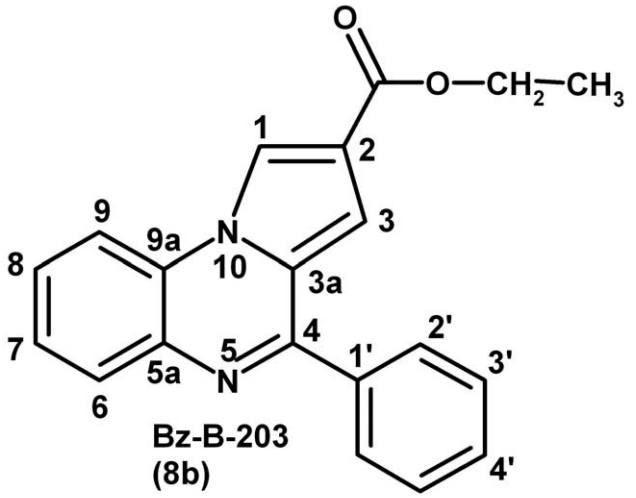


Parameter Set: !H1-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

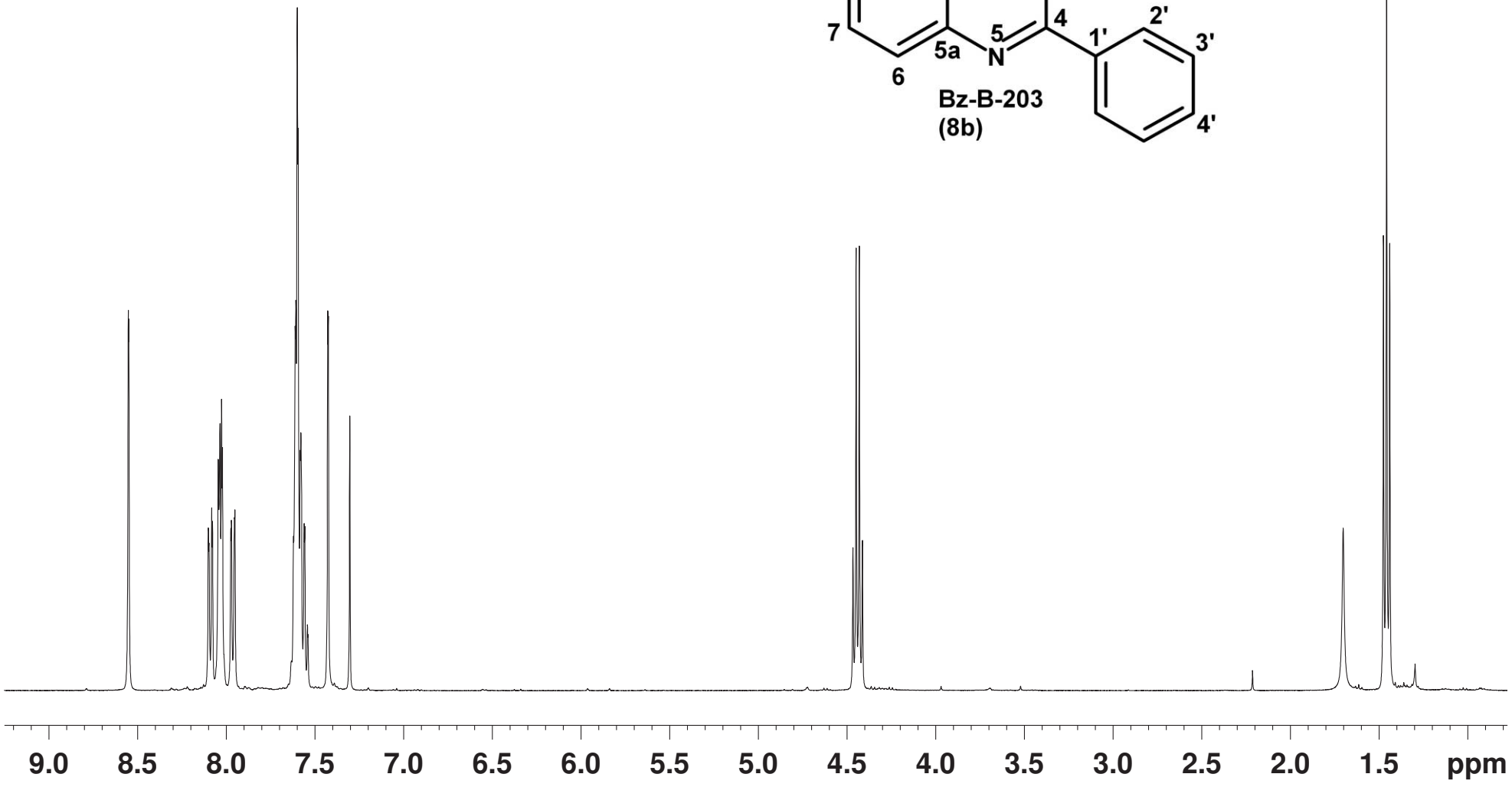
Registry No.:28162

Sample name and description: Bz-B-203 (8b)

p.t. 204-206 °C



Bz-B-203
(8b)

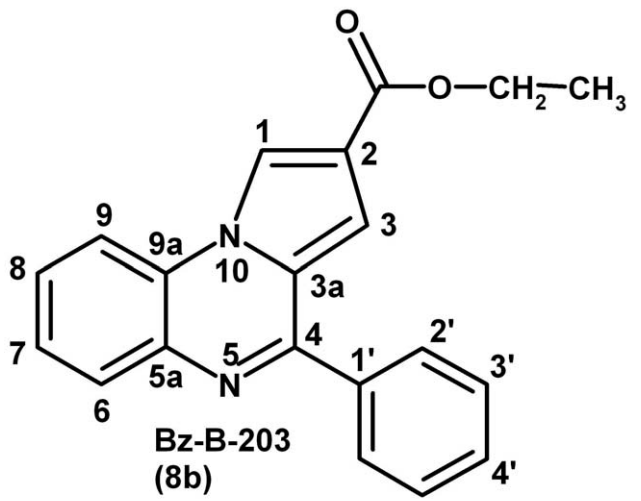


Parameter Set: !C13-CPD-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

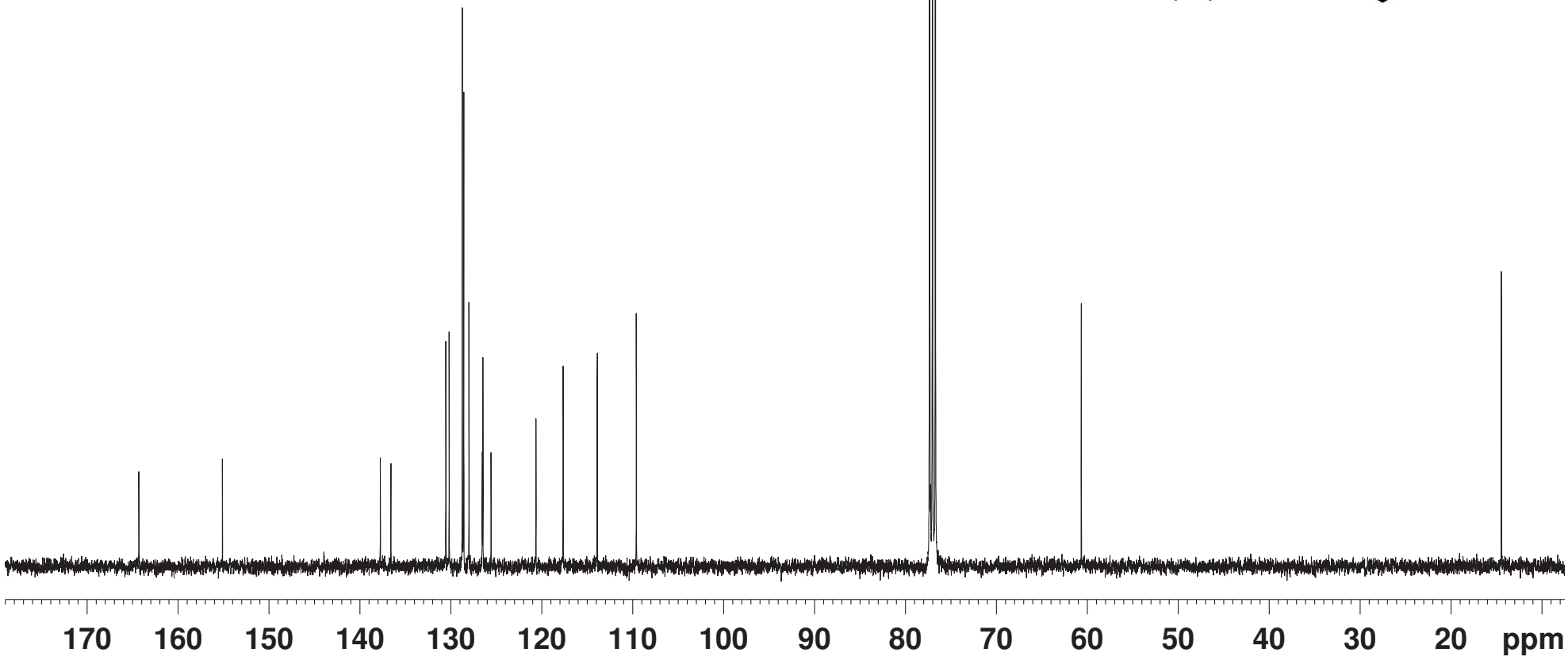
Registry No.:28162

Sample name and description: Bz-B-203 (8b)

p.t. 204-206 °C



Bz-B-203
(8b)

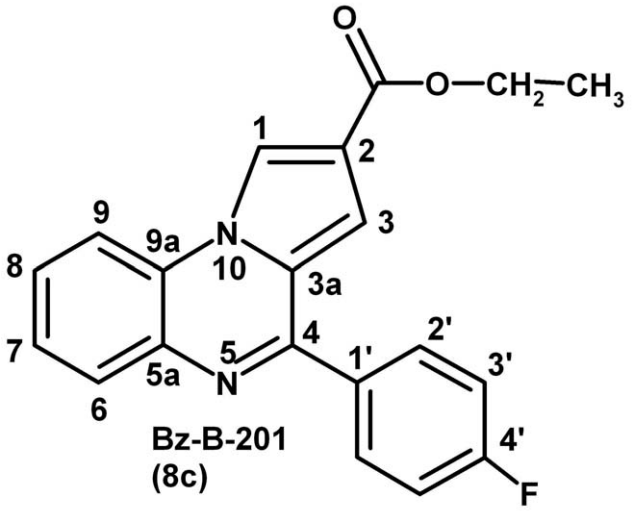


Parameter Set: !H1-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:27987

Sample name and description: Bz-B-201 (8c)

p.t. 189-190 °C



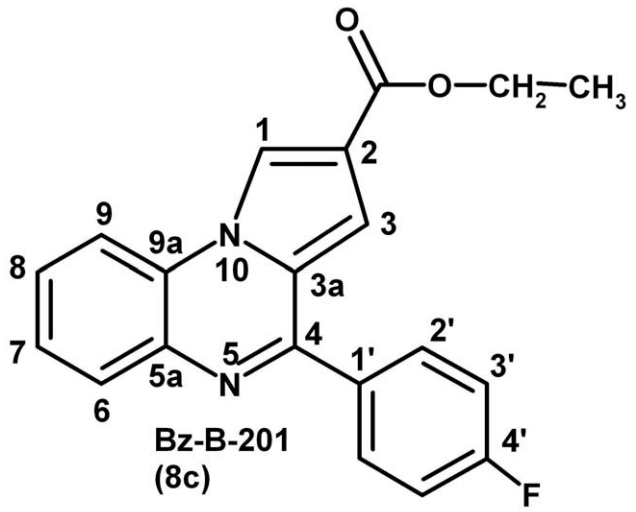
Bz-B-201
(8c)

Parameter Set: !C13-CPD-BBFOa-44 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

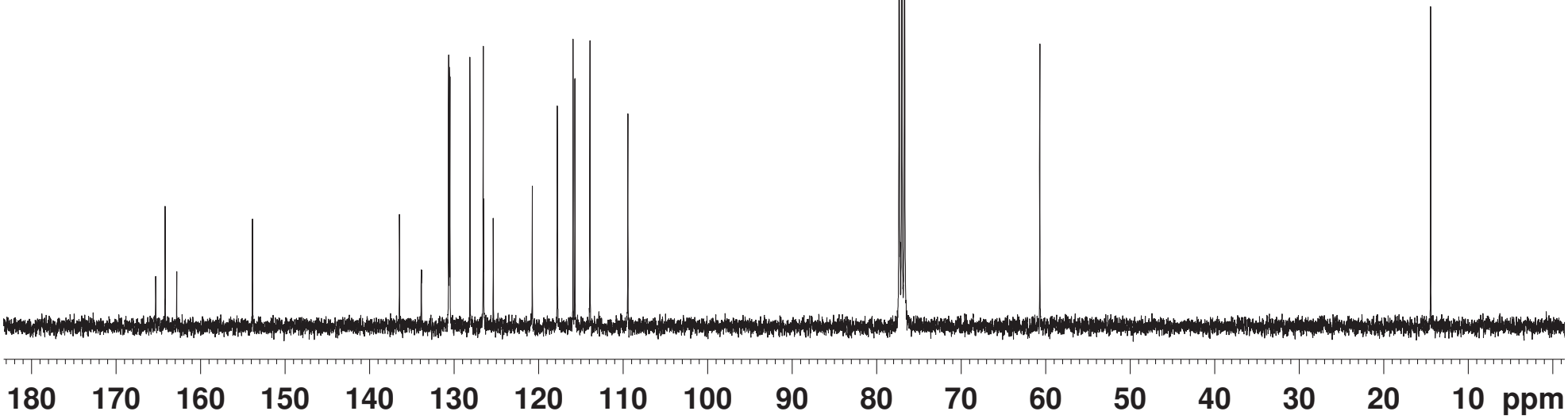
Registry No.:27987

Sample name and description: Bz-B-201 (8c)

p.t. 189-190 °C



Bz-B-201
(8c)

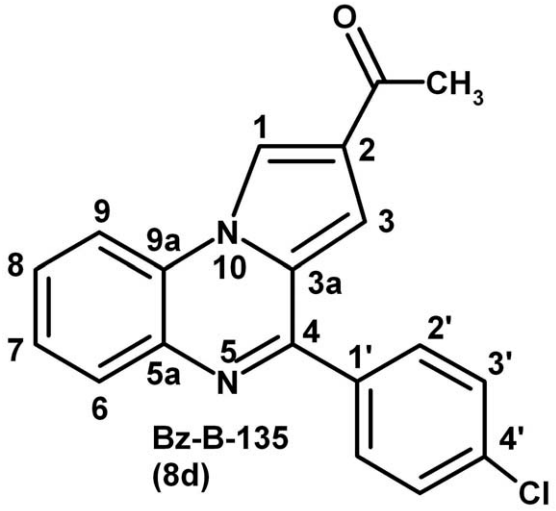


Parameter Set: #H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24943

Sample name and description: Bz-B-135 (8d)

p.t. 225-226 °C



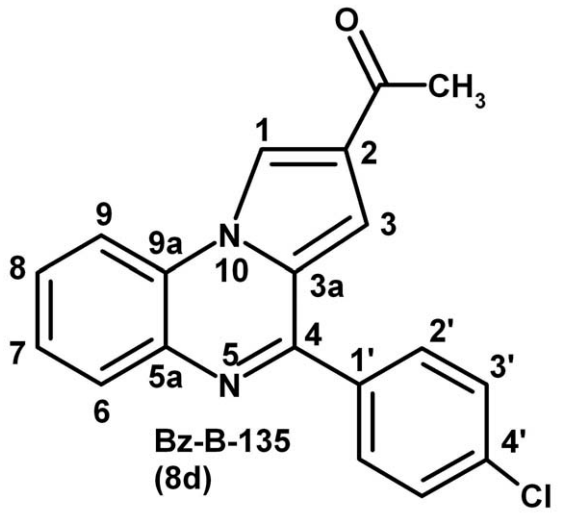
Bz-B-135
(8d)

Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

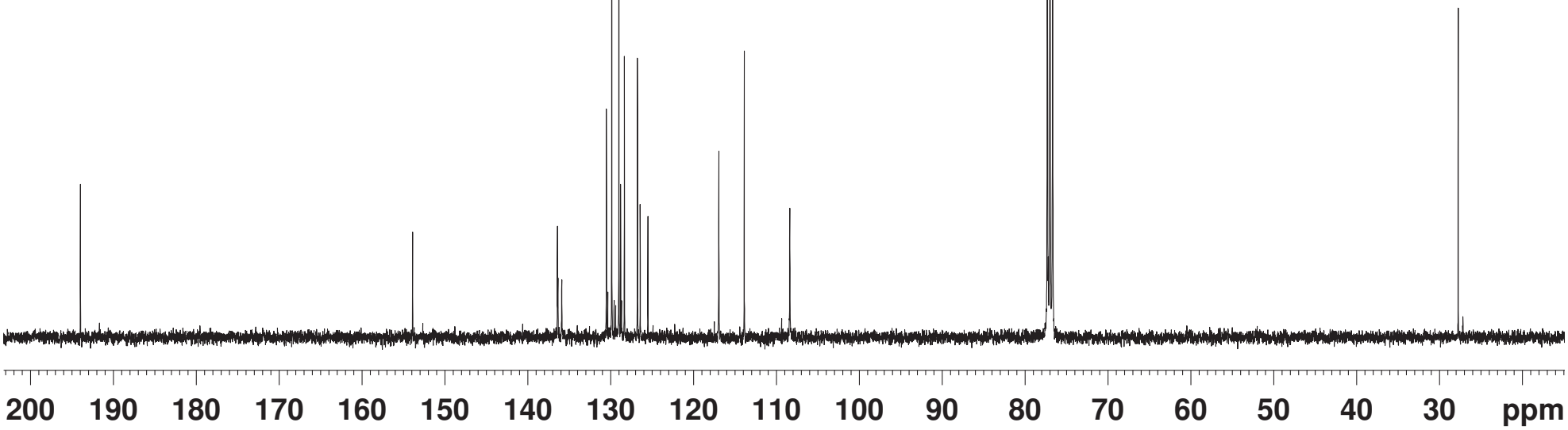
Registry No.:24943

Sample name and description: Bz-B-135 (8d)

p.t. 225-226 °C



Bz-B-135
(8d)

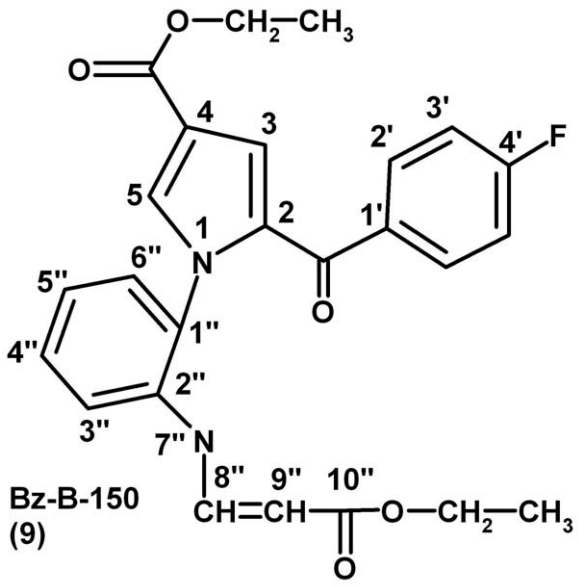


Parameter Set: #H1-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24900

Sample name and description: Bz-B-150 (9)

p.t. 158-160 °C



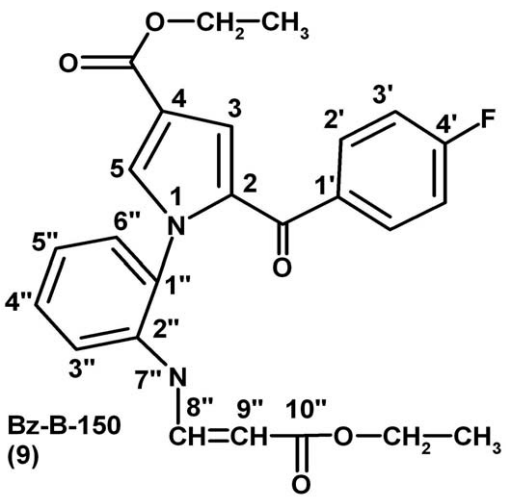
Bz-B-150
(9)

Parameter Set: #C13-CPD-QNP-34 TS1.3PL8.
Instrument: Bruker Avance DRX 400 (ICMPP)

Registry No.:24900

Sample name and description: Bz-B-150 (9)

p.t. 158-160 °C



Bz-B-150
(9)