Supplementary Material

Halogen-bonding in 3-nitrobenzaldehyde-derived dichlorodiazadienes

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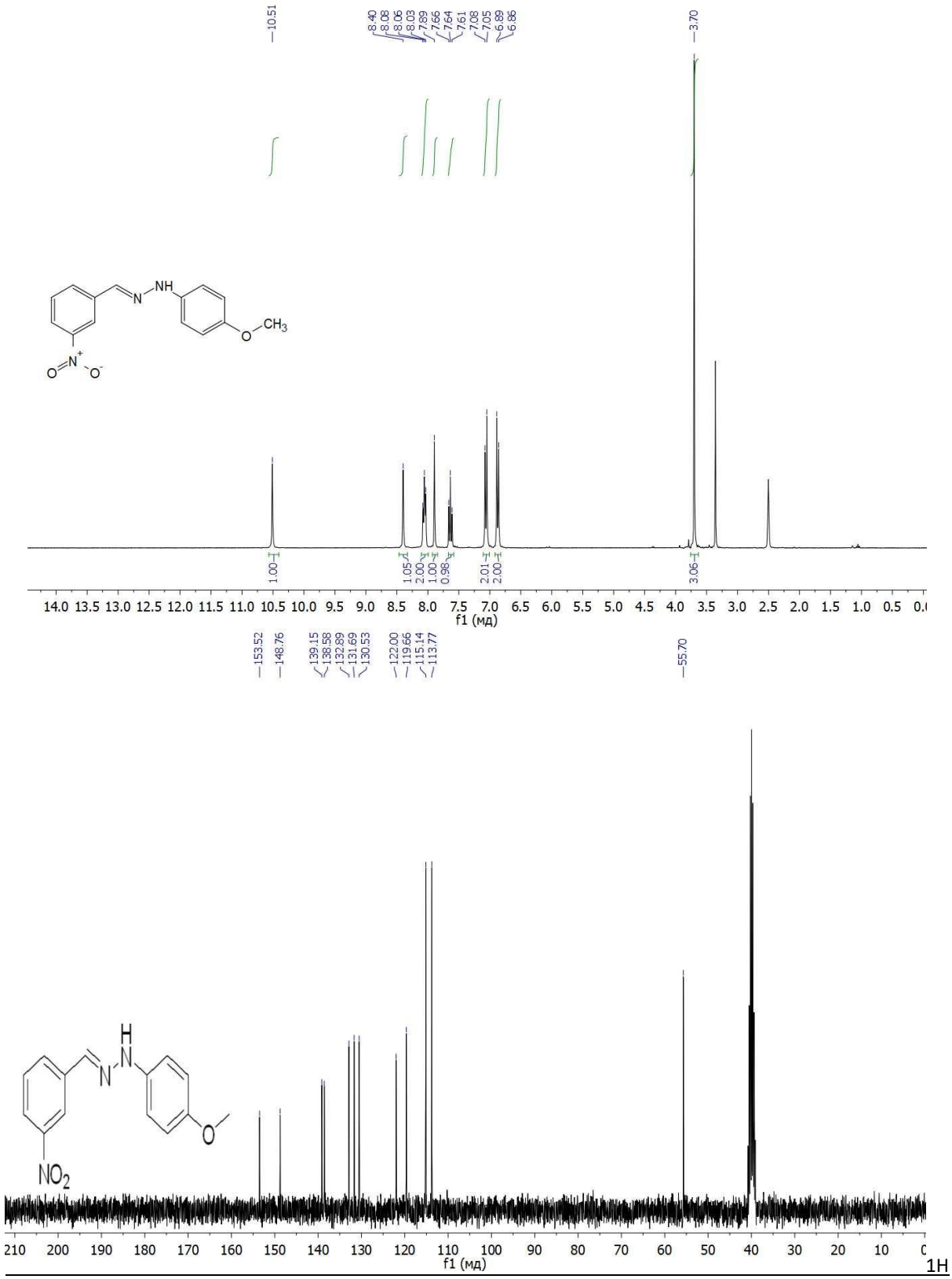
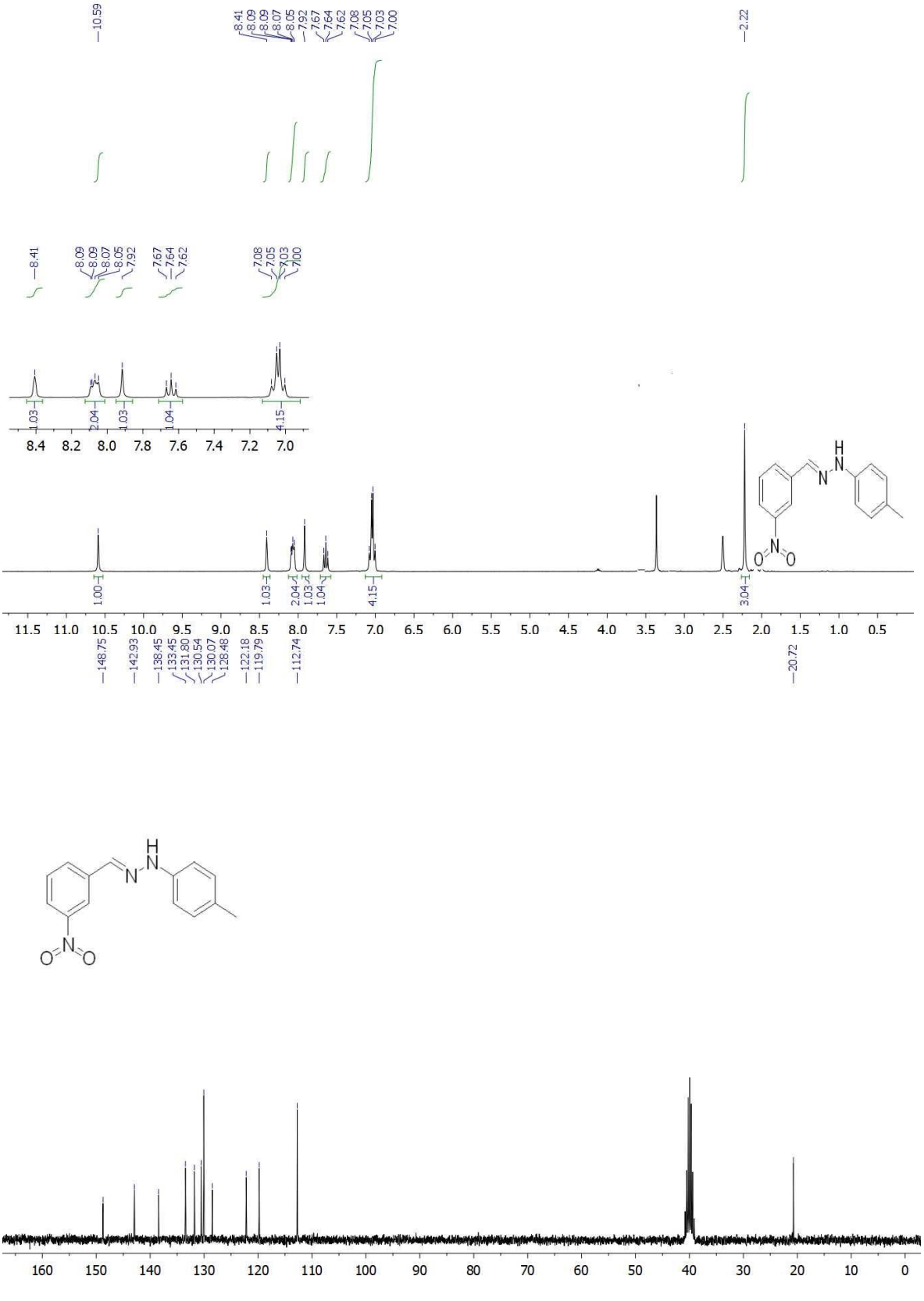
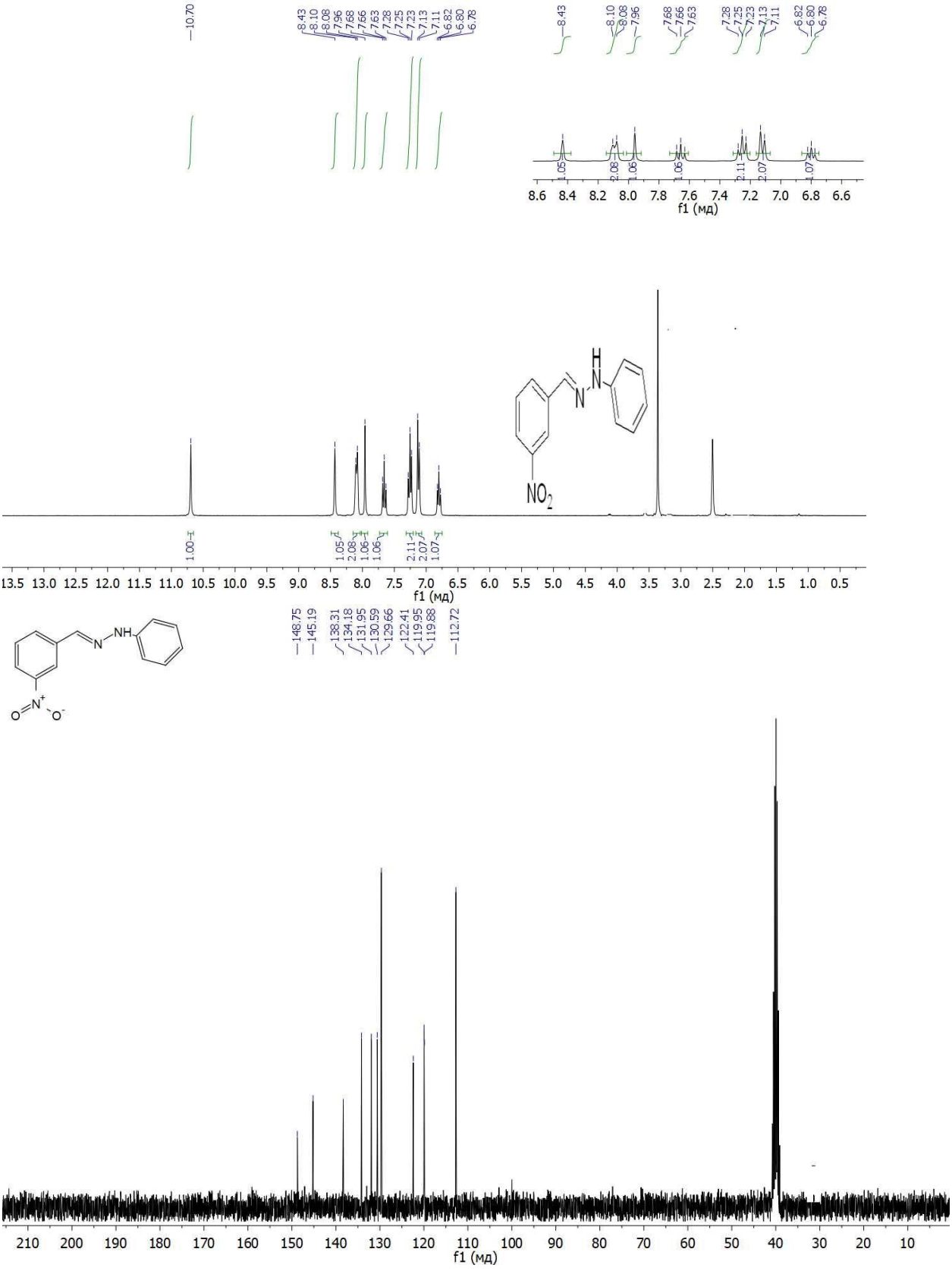


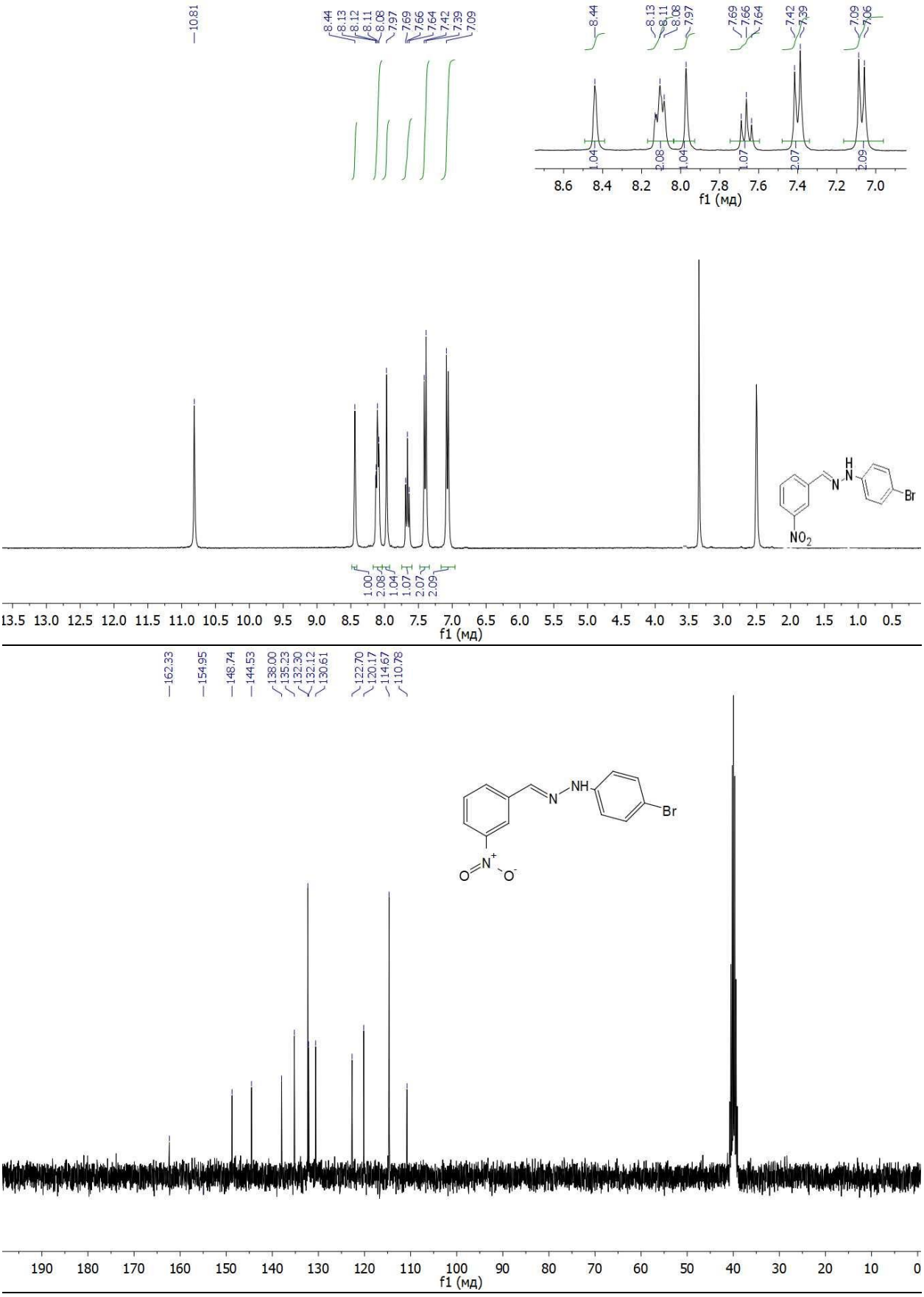
1H and 13C spectra for compound 1



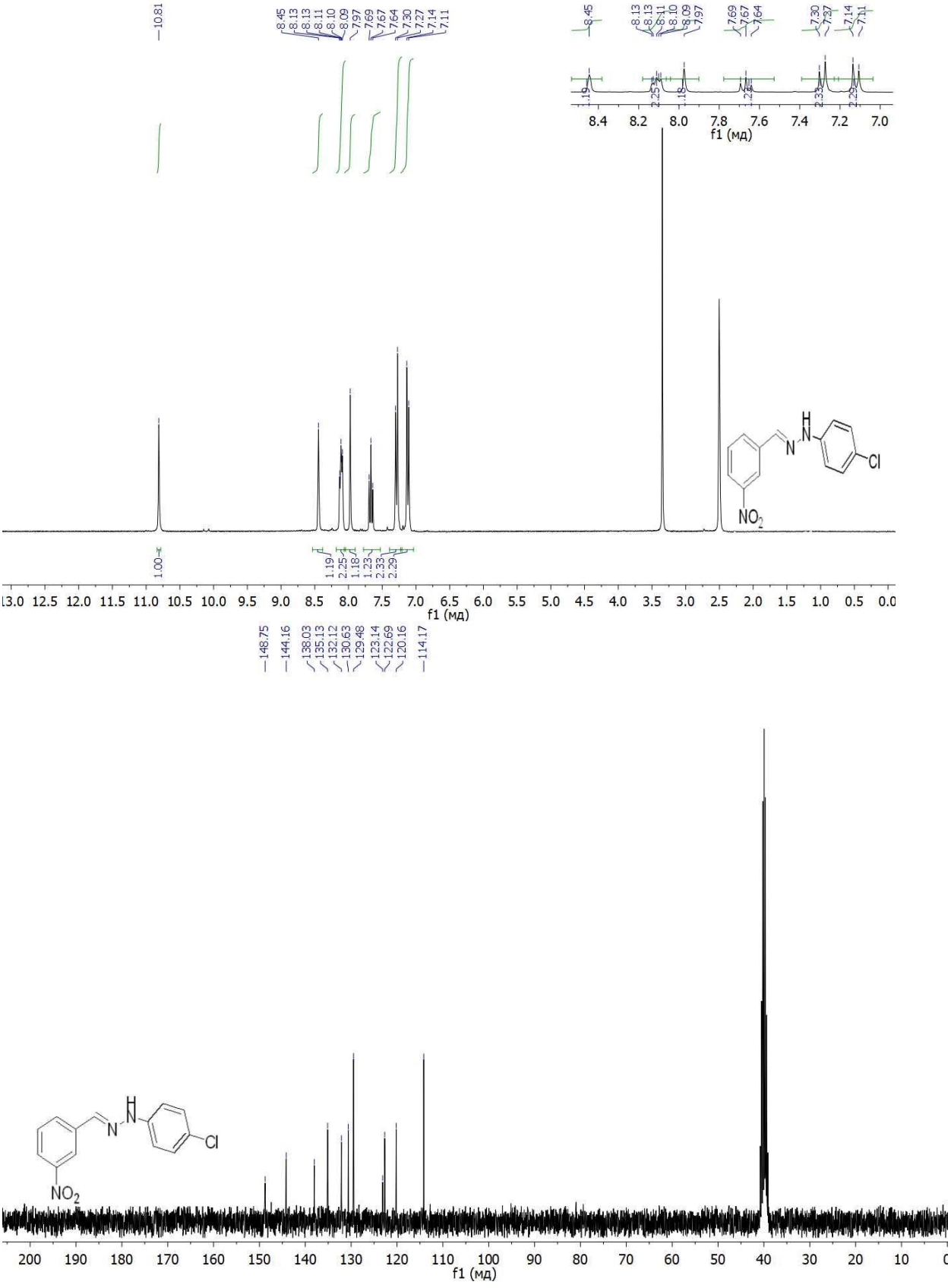
1H and 13C spectra for compound 2



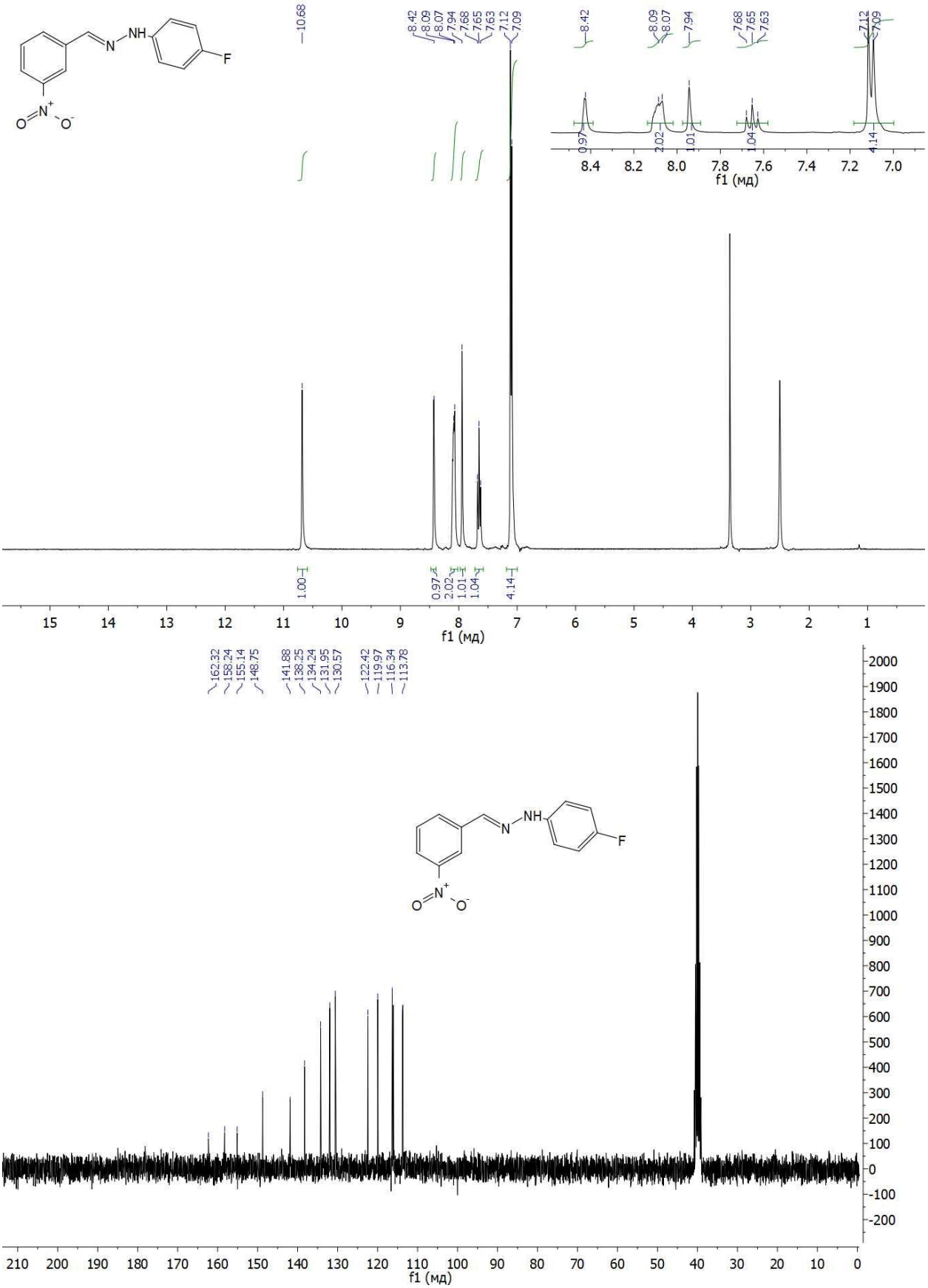
1H and 13C spectra for compound 3



1H and 13C spectra for compound 4



1H and 13C spectra for compound 5



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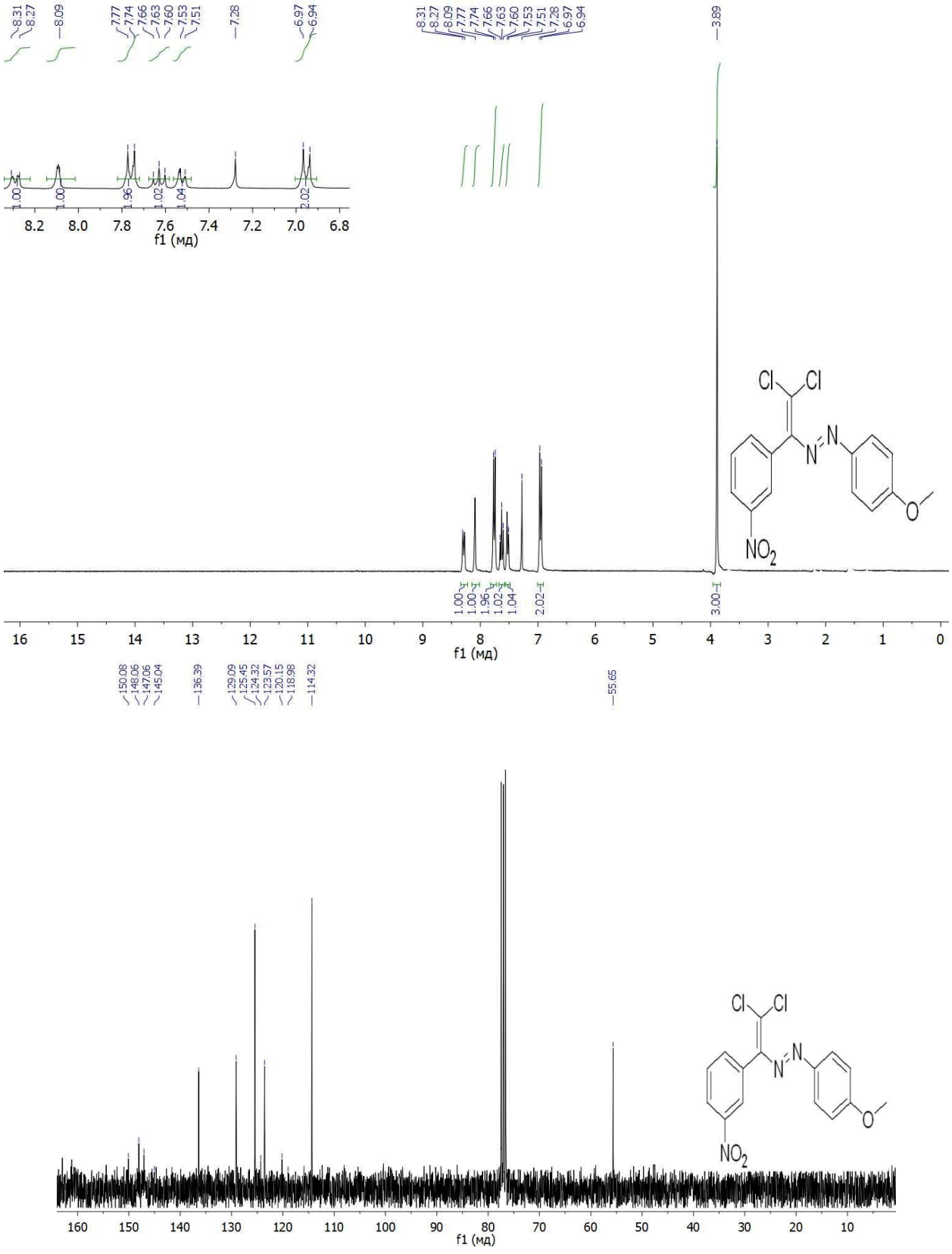
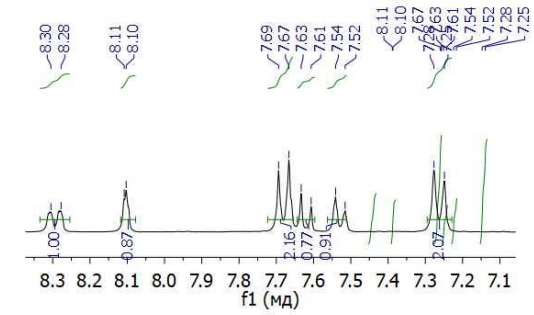
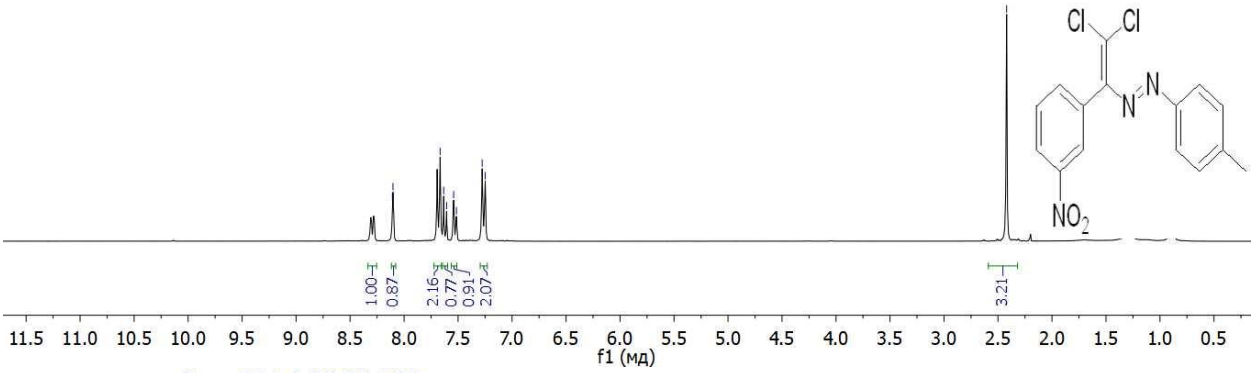
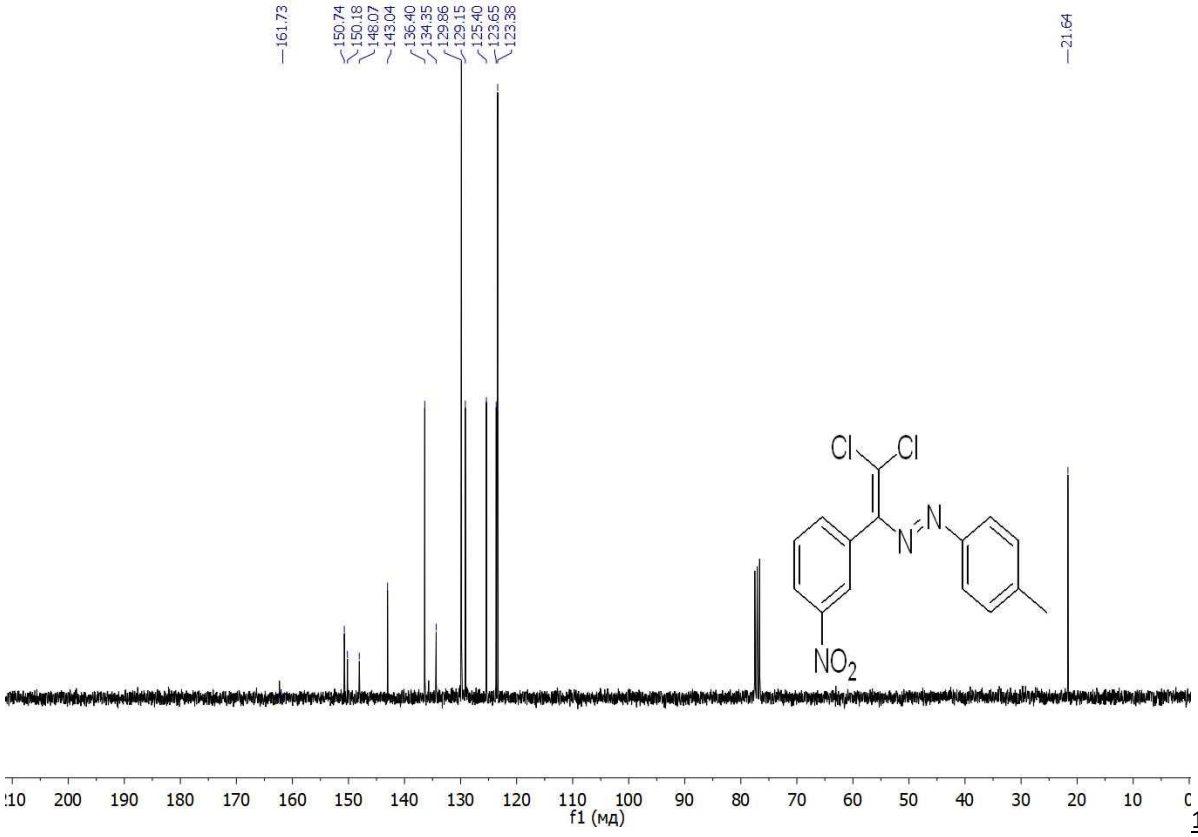
1H and 13C spectra for compound 6



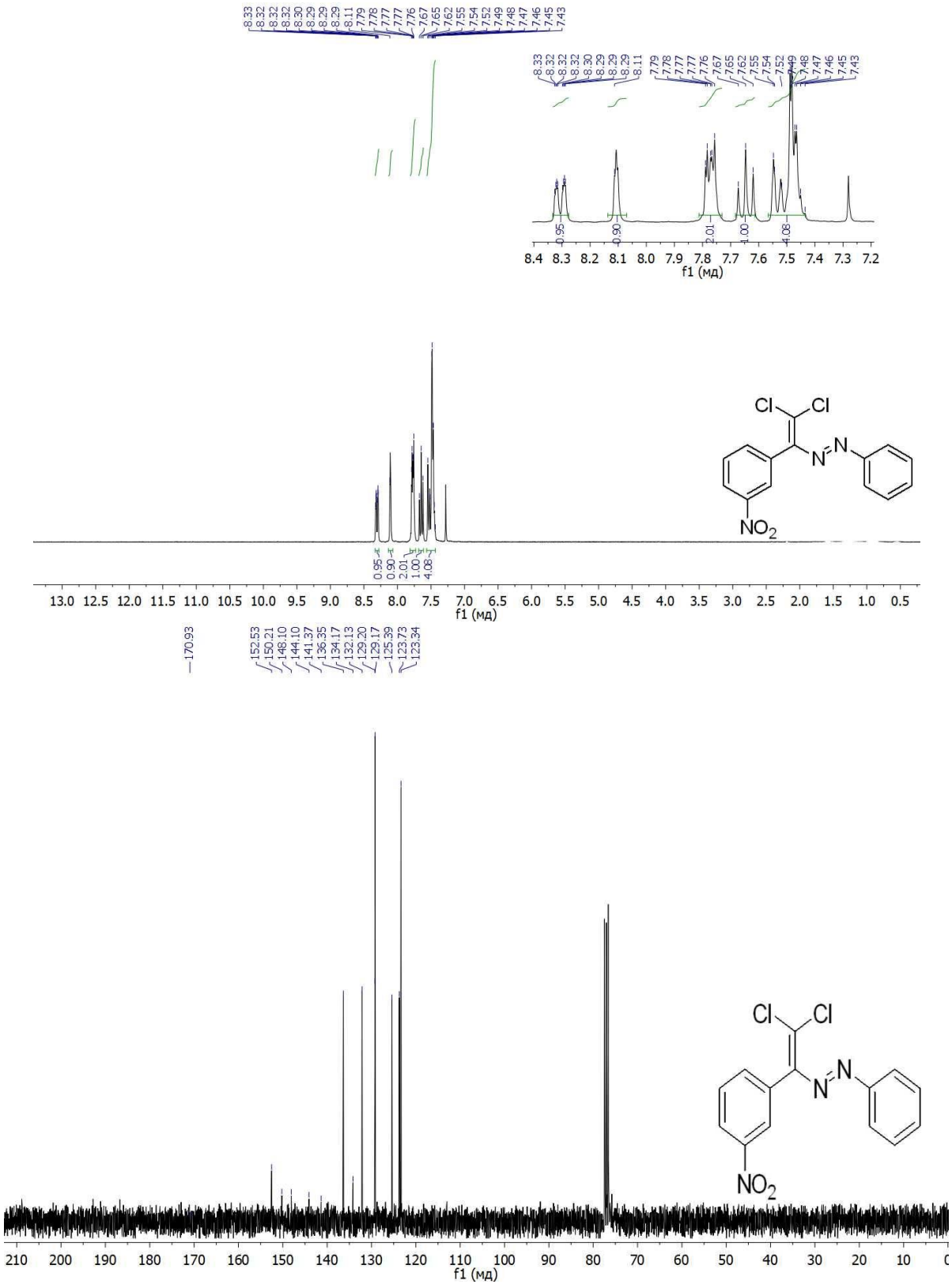
1H and 13C spectra for compound 7



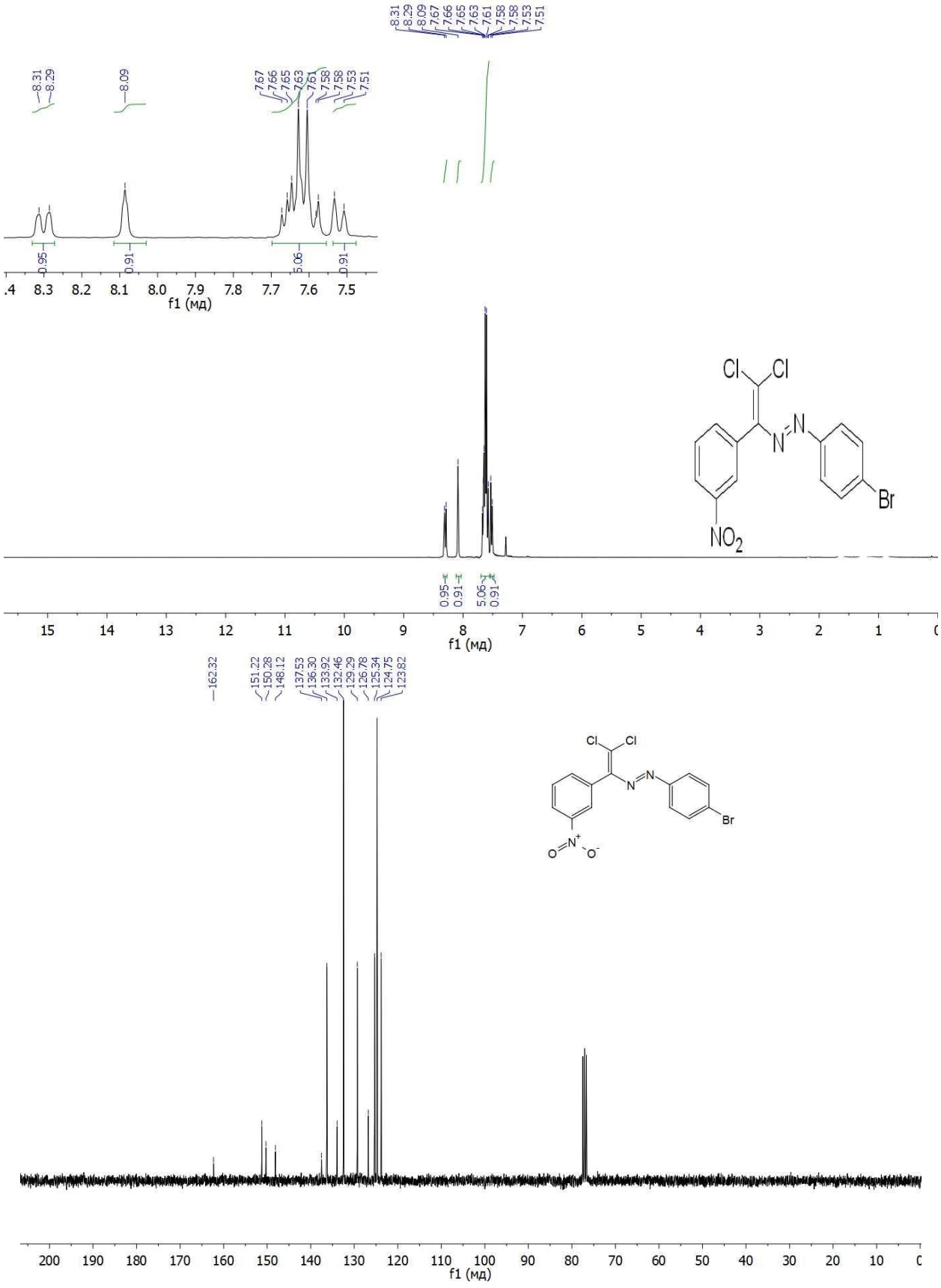




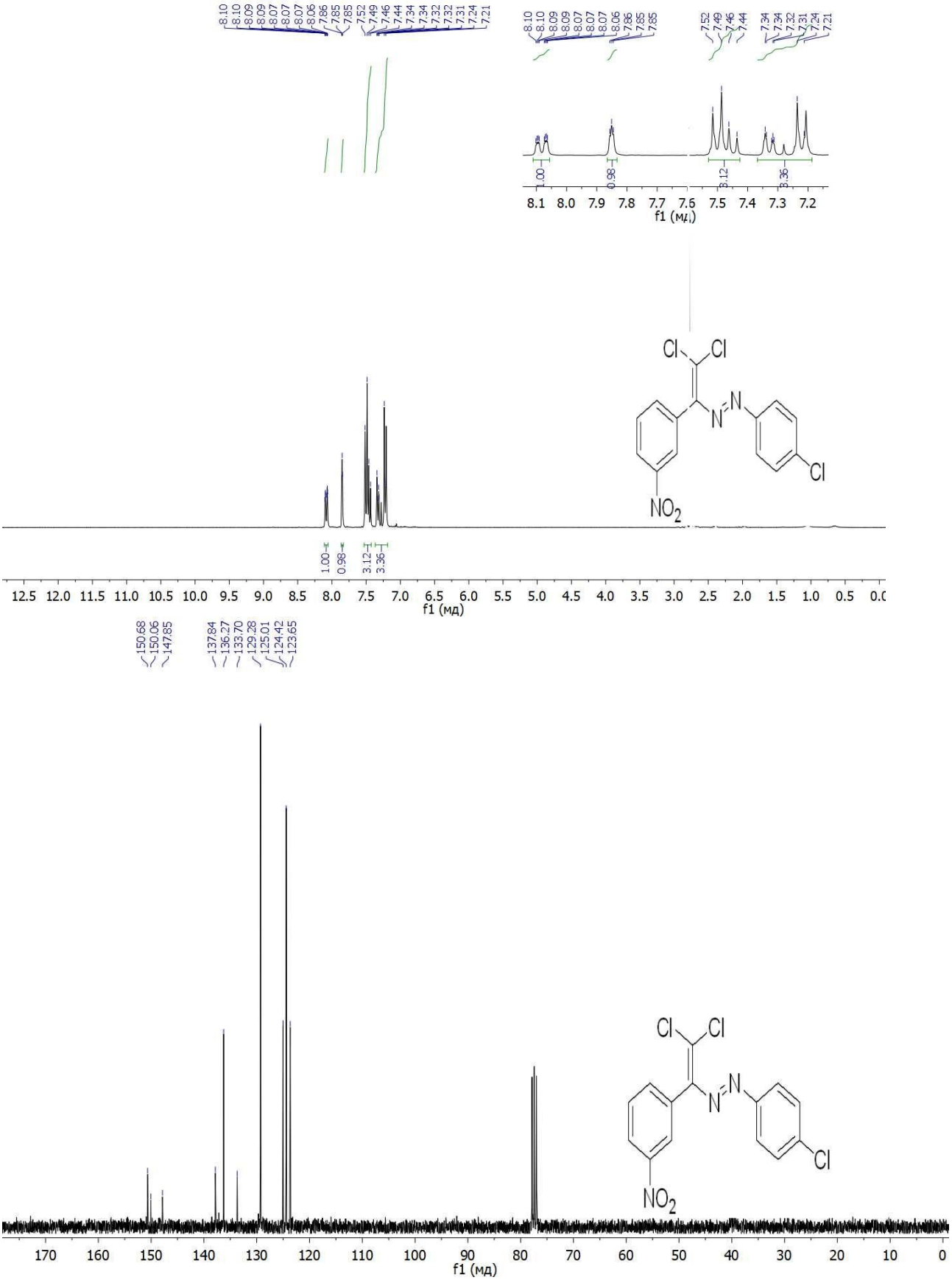
1H and 13C spectra for compound 8



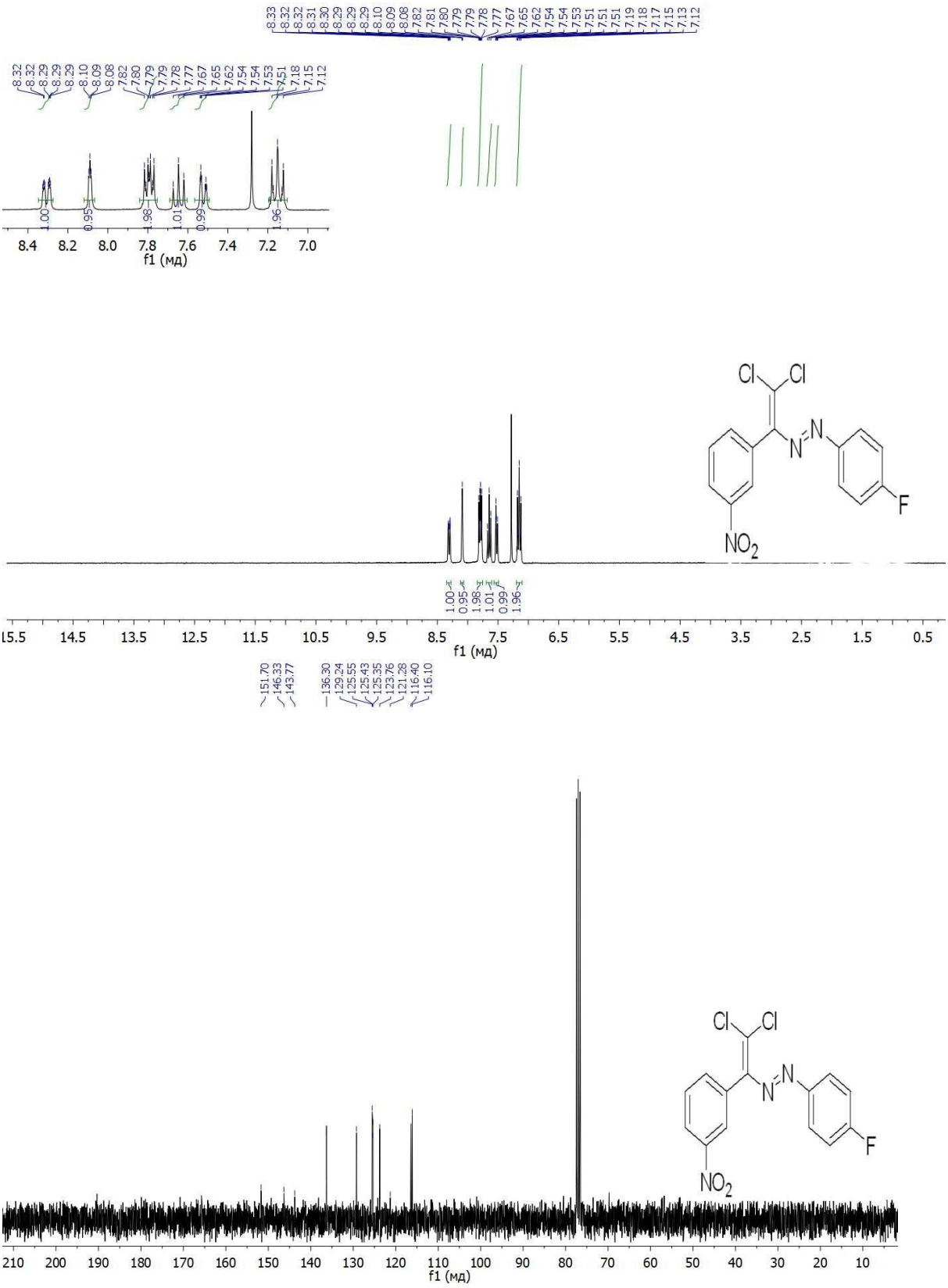
1H and 13C spectra for compound 9



1H and 13C spectra for compound 10



1H and 13C spectra for compound 11



1H and 13C spectra for compound 12

Table S1. Crystallographic data and structure refinement details for **8**, **10** and **11**

	8	**10**	**11**
Empirical formula	$C_{15}H_{11}Cl_2N_3O_2$	$C_{14}H_8BrCl_2N_3O_2$	$C_{14}H_8Cl_3N_3O_2$
fw	336.17	401.04	356.58
Temperature (K)	296(2)	296(2)	296(2)
Cryst. Syst.	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/c$	P-1	P-1
a (Å)	7.971(3)	8.5664(9)	8.4857(7)
b (Å)	29.176(9)	9.6577(10)	9.5516(8)
c (Å)	7.083(2)	10.2478(10)	10.3250(9)
α, °	90°	68.386(4)°	68.031(3)°
β, °	111.510(12)°	79.545(4)°	79.064(3)°
γ, °	90°	87.299(4)°	87.923(3)°
V (Å^3)	1532.4(8)	774.94(14)	761.45(11)
Z	4	2	2
ρ_{calc} *(g cm^{-3})*	1.457	1.719	1.555
μ(Mo Kα) (mm^{-1})	0.433	3.006	0.610
F (000)	688	396	360
R1[a] *($I \geq 2\sigma$)*	0.433	0.0349	0.0409
wR2[b] *($I \geq 2\sigma$)*	0.1638	0.0846	0.1023
GOOF	1.087	1.046	1.051

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

[s1] SMART & SAINT Software Reference Manuals, Version 6.22, Bruker AXS Analytic X-ray Systems, Inc., Madison, WI, 2000.

[s2] Sheldrick GM. SADABS Software for Empirical Absorption Correction, University of Göttingen, Germany, 2000.

[s3] Sheldrick GM. SHELXTL V5.1, Software Reference Manual, Bruker AXS Inc., Madison, Wisconsin, 1997.

