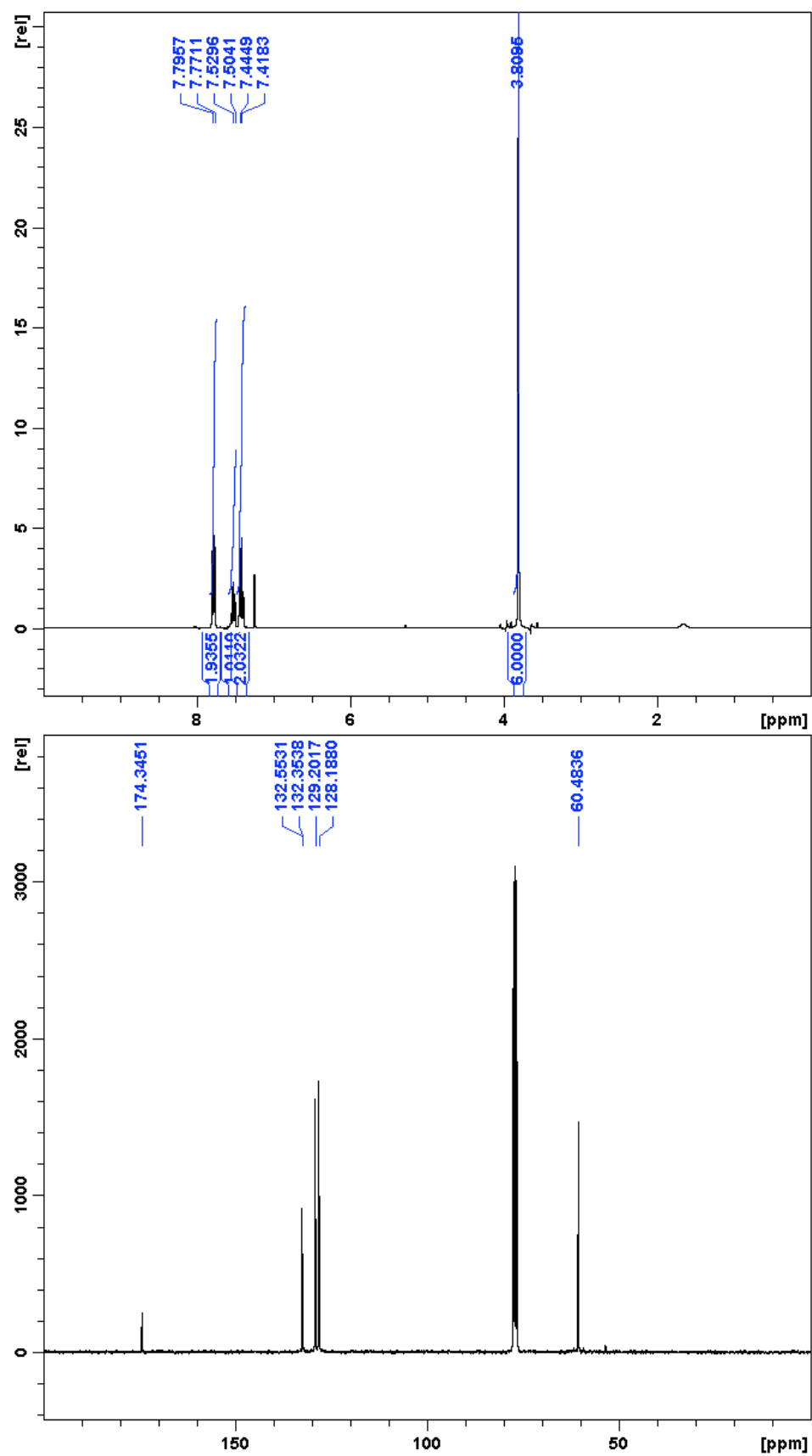


Synthesis and thermal decomposition of *N,N*-dialkoxyamides – Supplementary Material

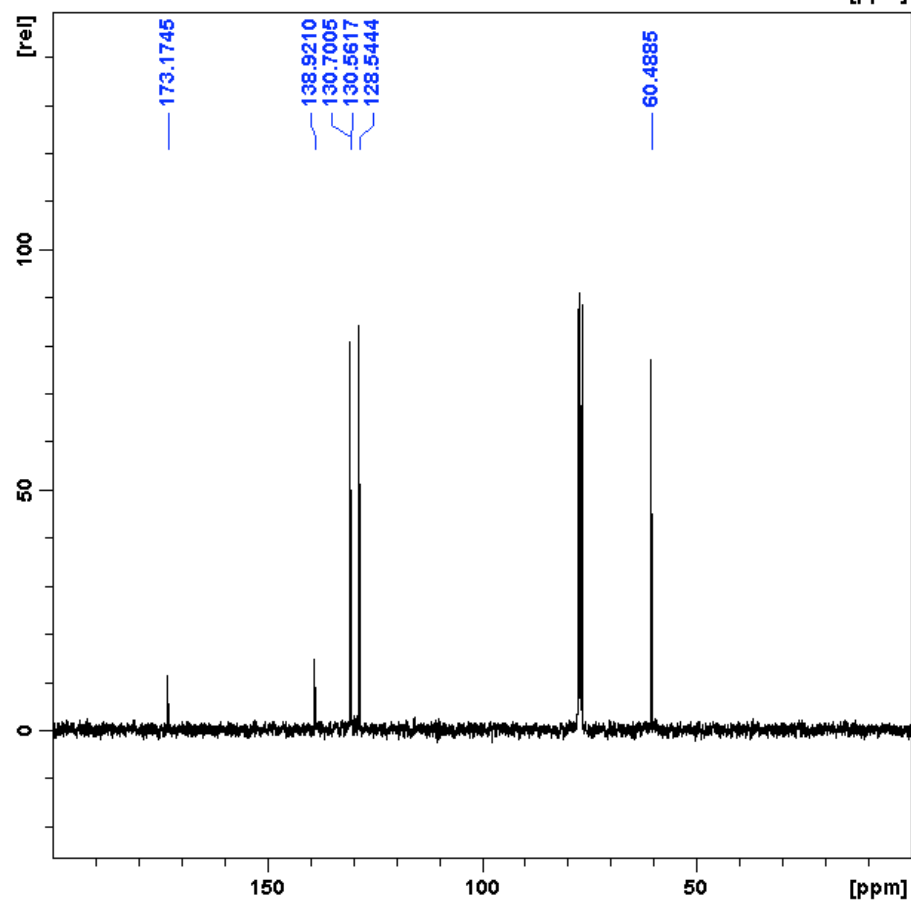
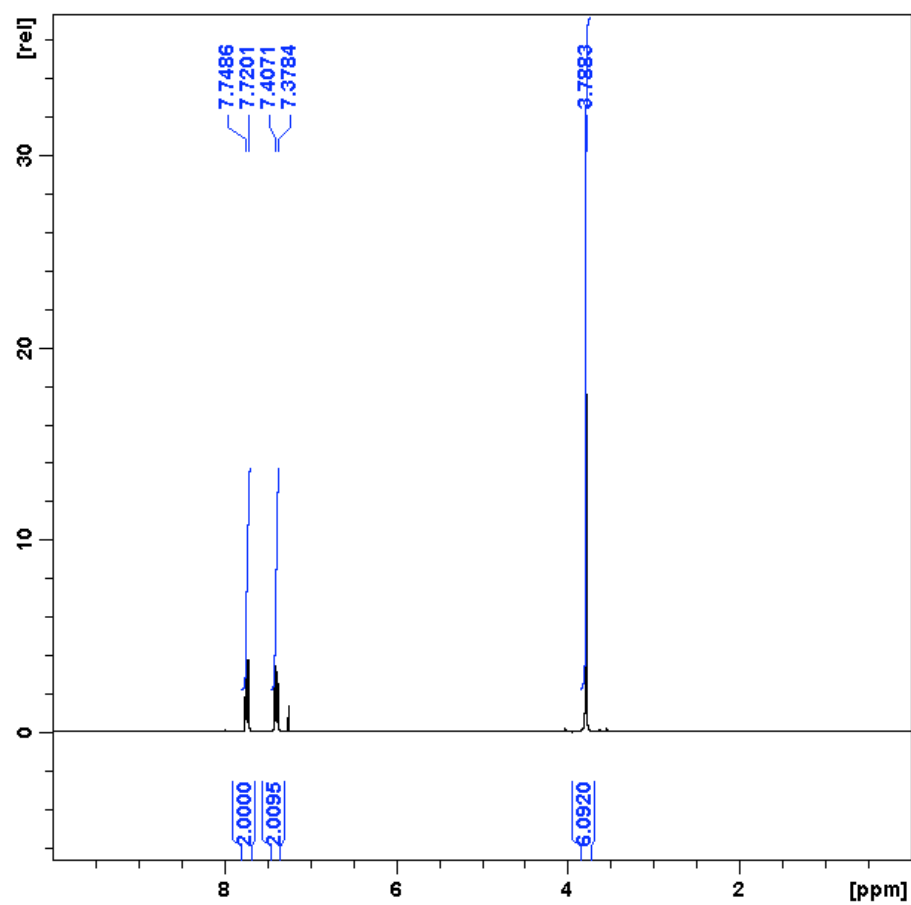
Katherine M. Digianantonio^a, Jennifer P. Johns^a, Stephen A. Glover^{a*} and Adam A. Rosser^a.

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New South Wales 2351, Australia.

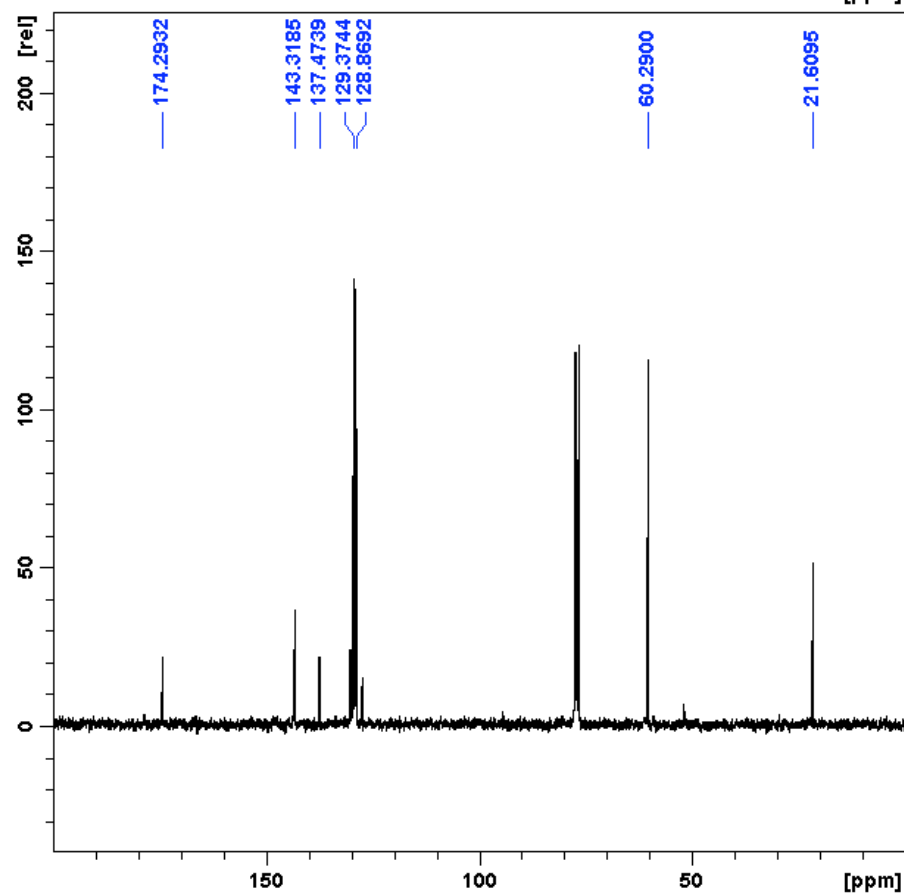
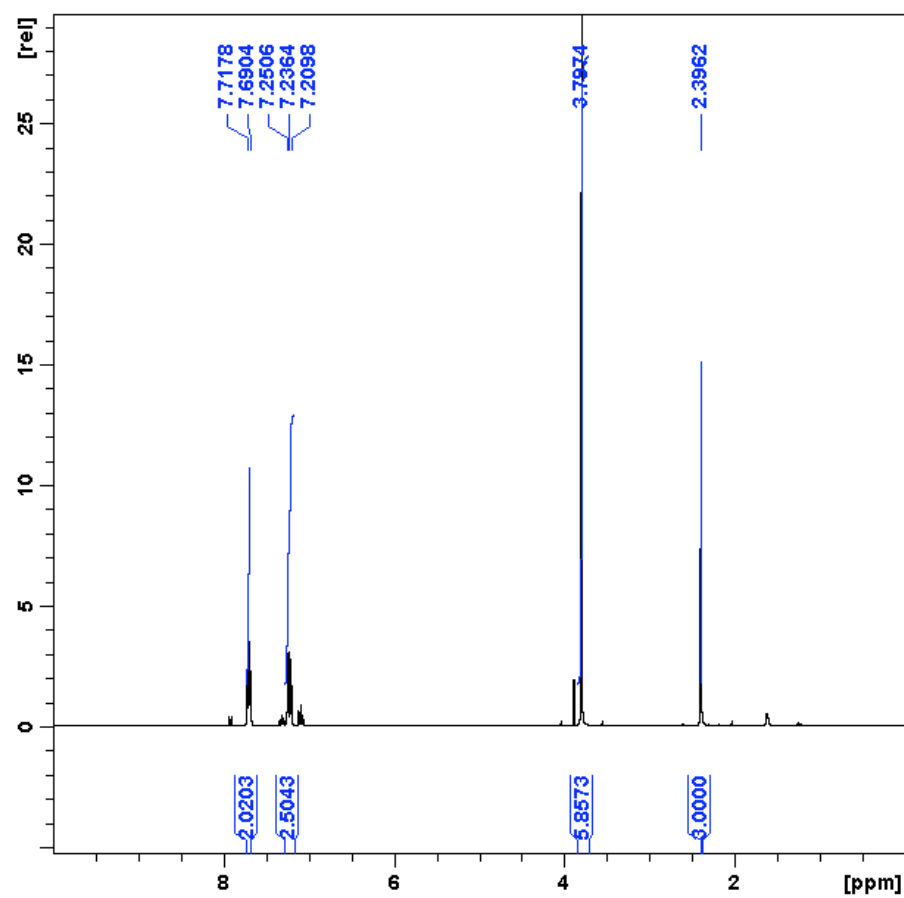
***N,N*-Dimethoxybenzamide 2a**



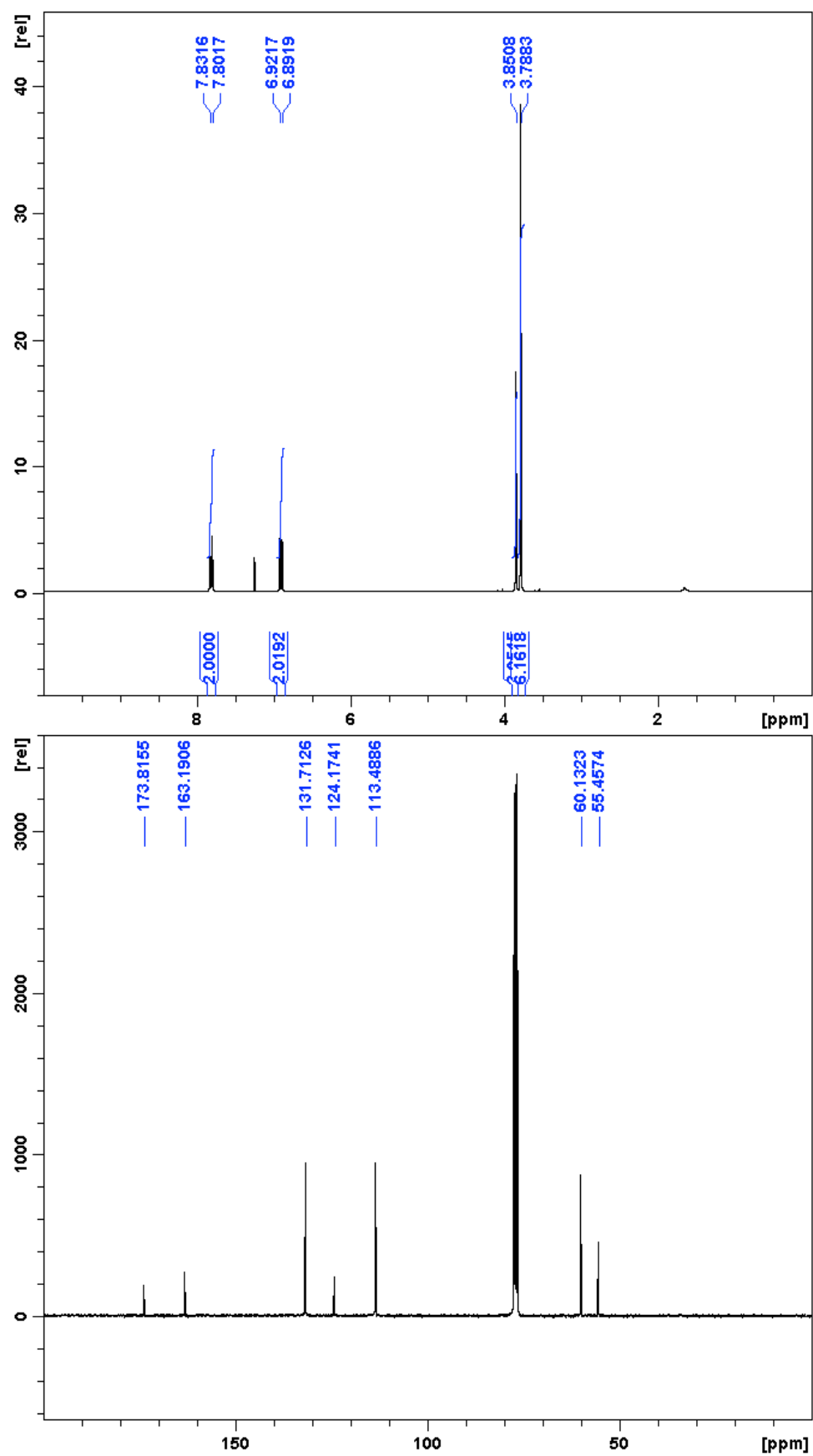
***N,N*-Dimethoxy-4-chlorobenzamide 2b**



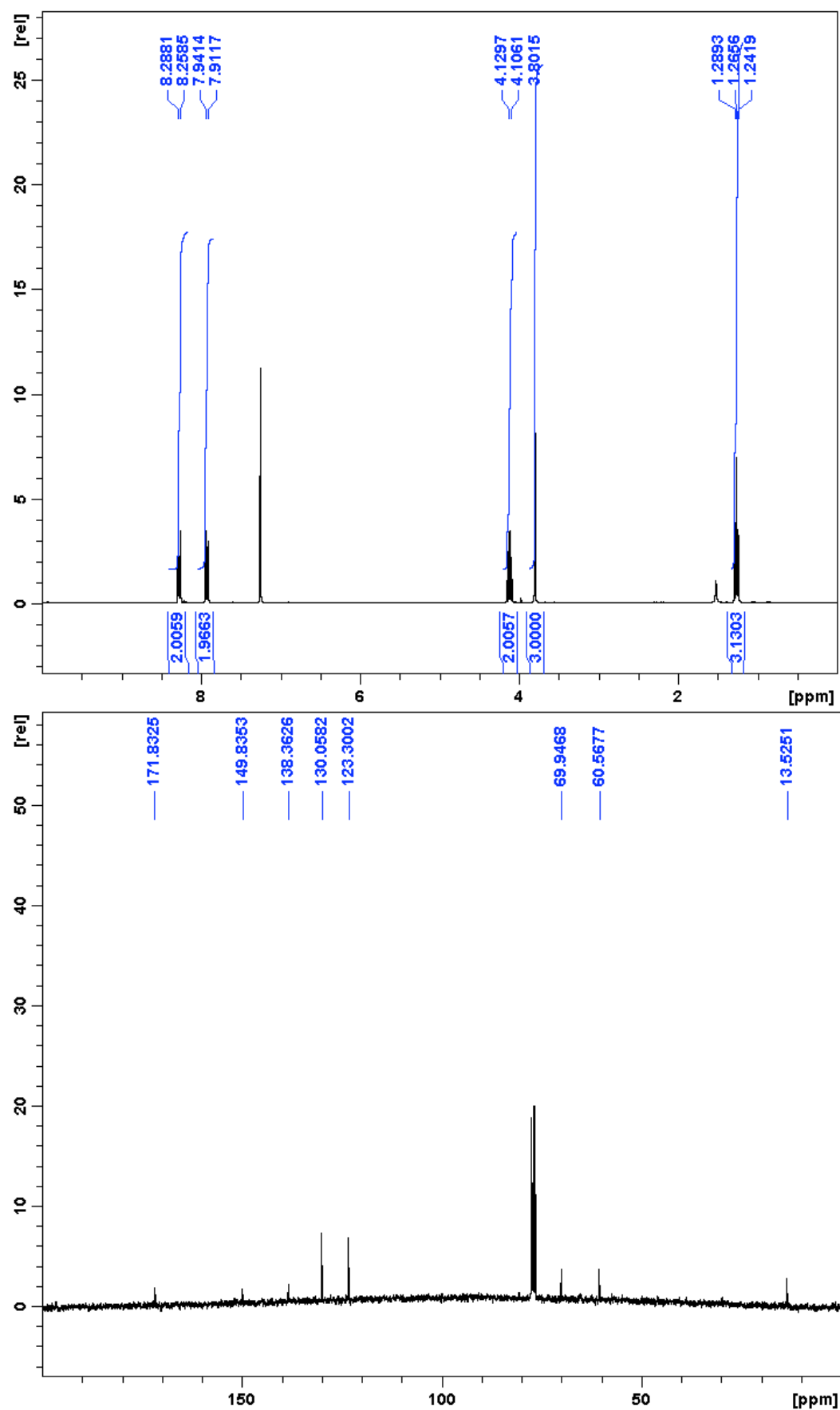
***N,N*-Dimethoxy-4-methylbenzamide 2c**



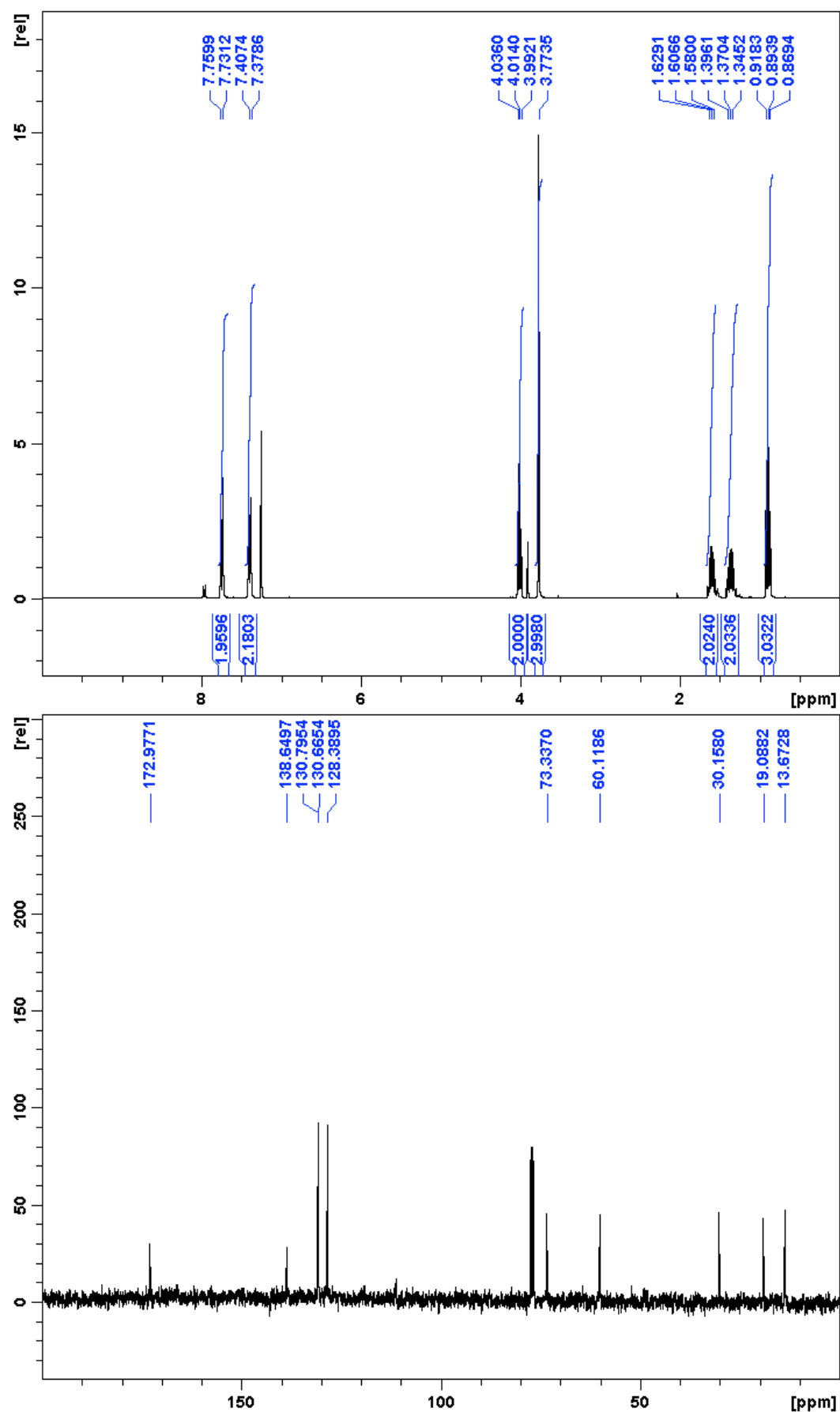
***N,N*-Dimethoxy-4-methoxybenzamide 2d**



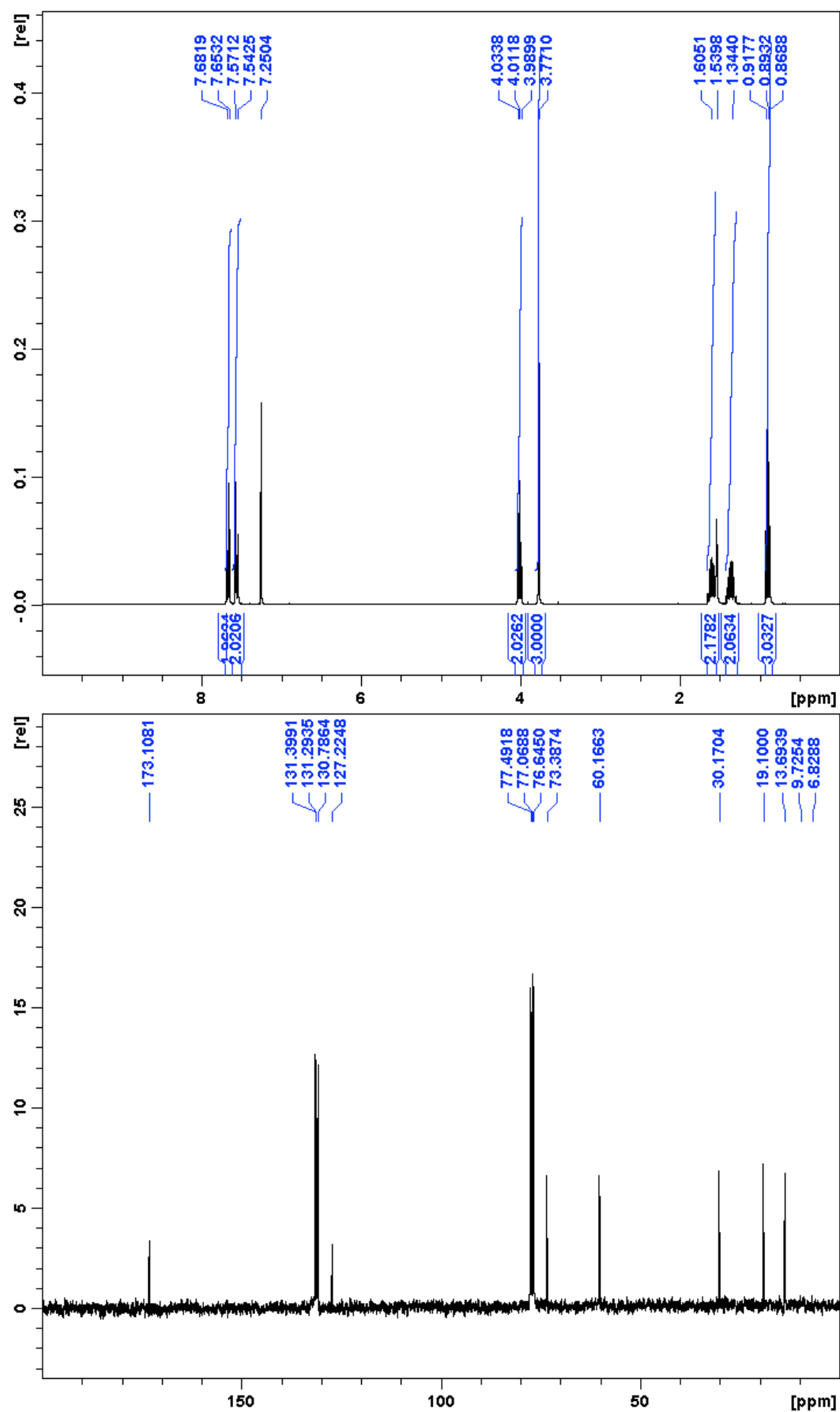
***N*-Ethoxy-*N*-methoxy-4-nitrobenzamide 3a**



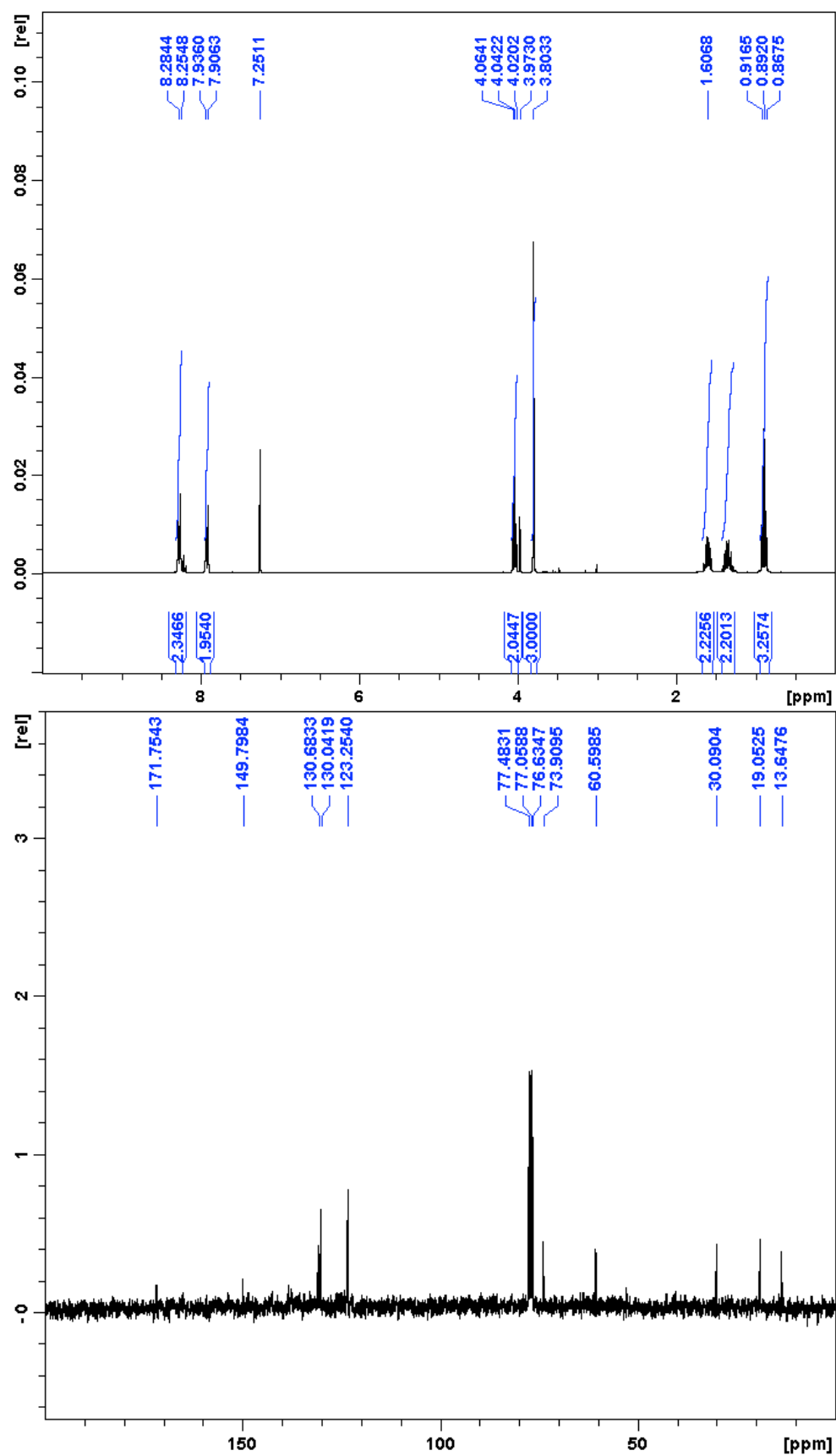
***N*-Ethoxy-*N*-methoxy-4-chlorobenzamide 3b**



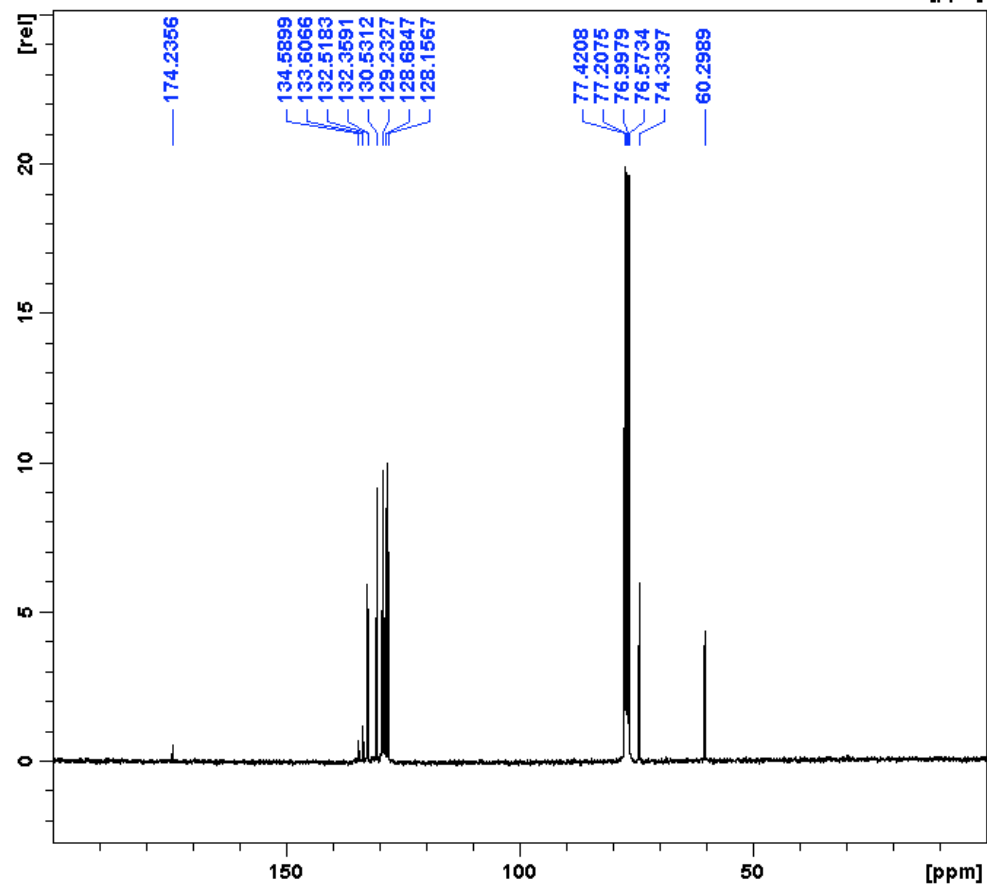
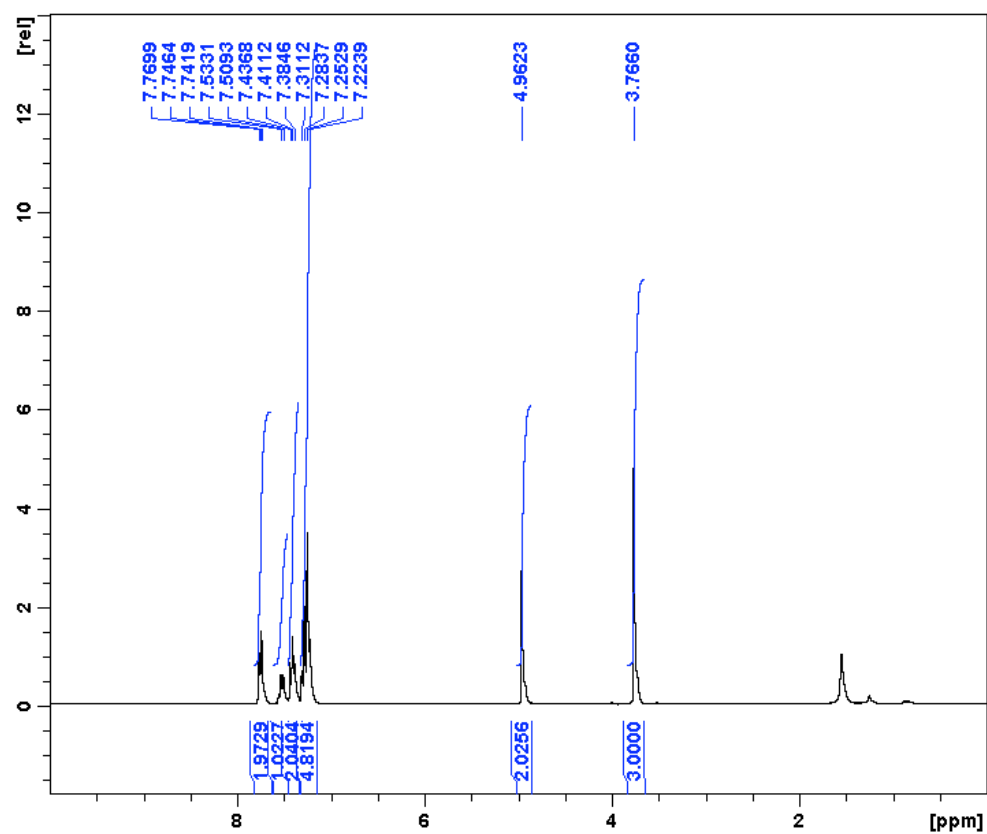
***N*-Butoxy-*N*-methoxy-4-bromobenzamide 3c**



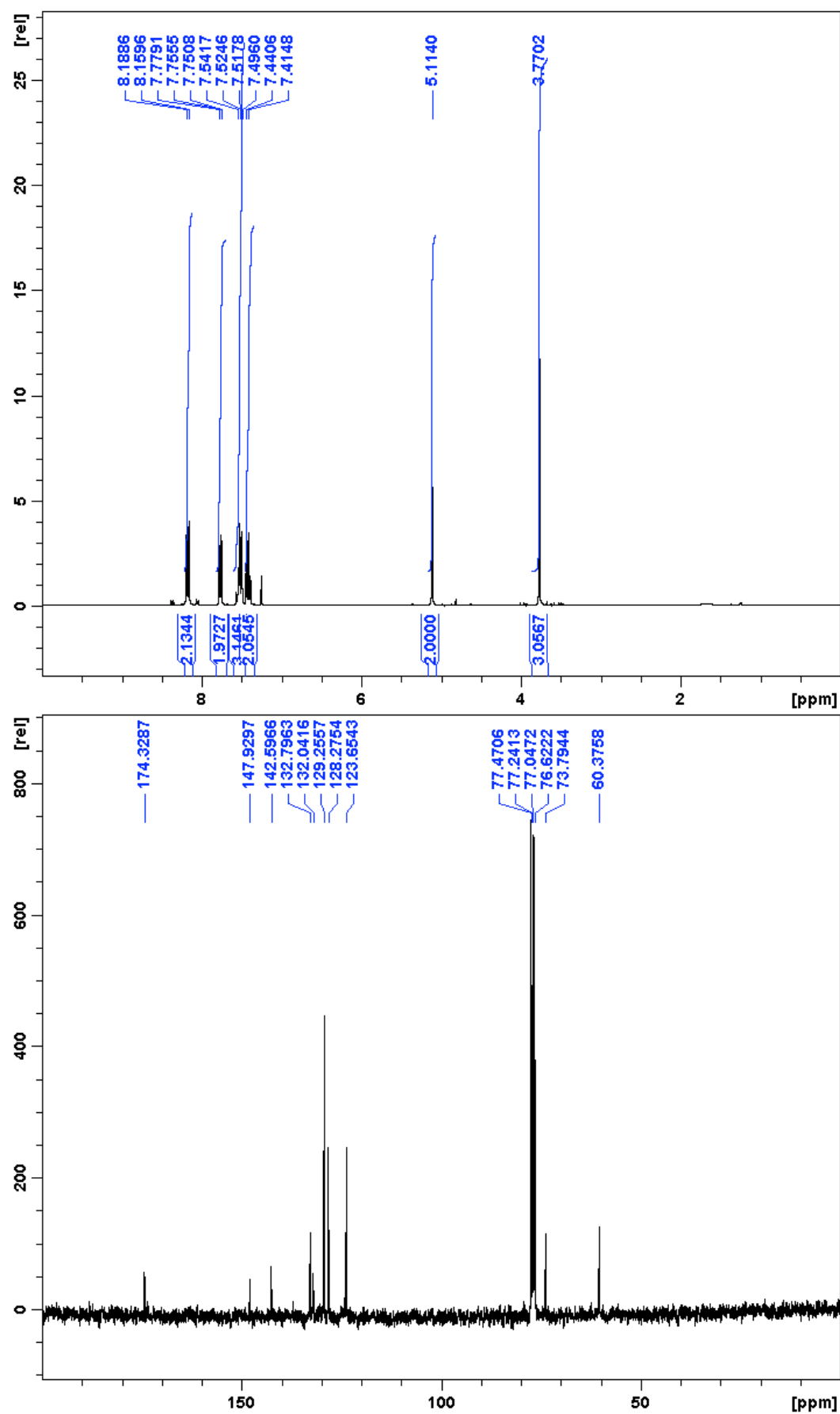
***N*-Butoxy-*N*-methoxy-4-nitrobenzamide 3d**



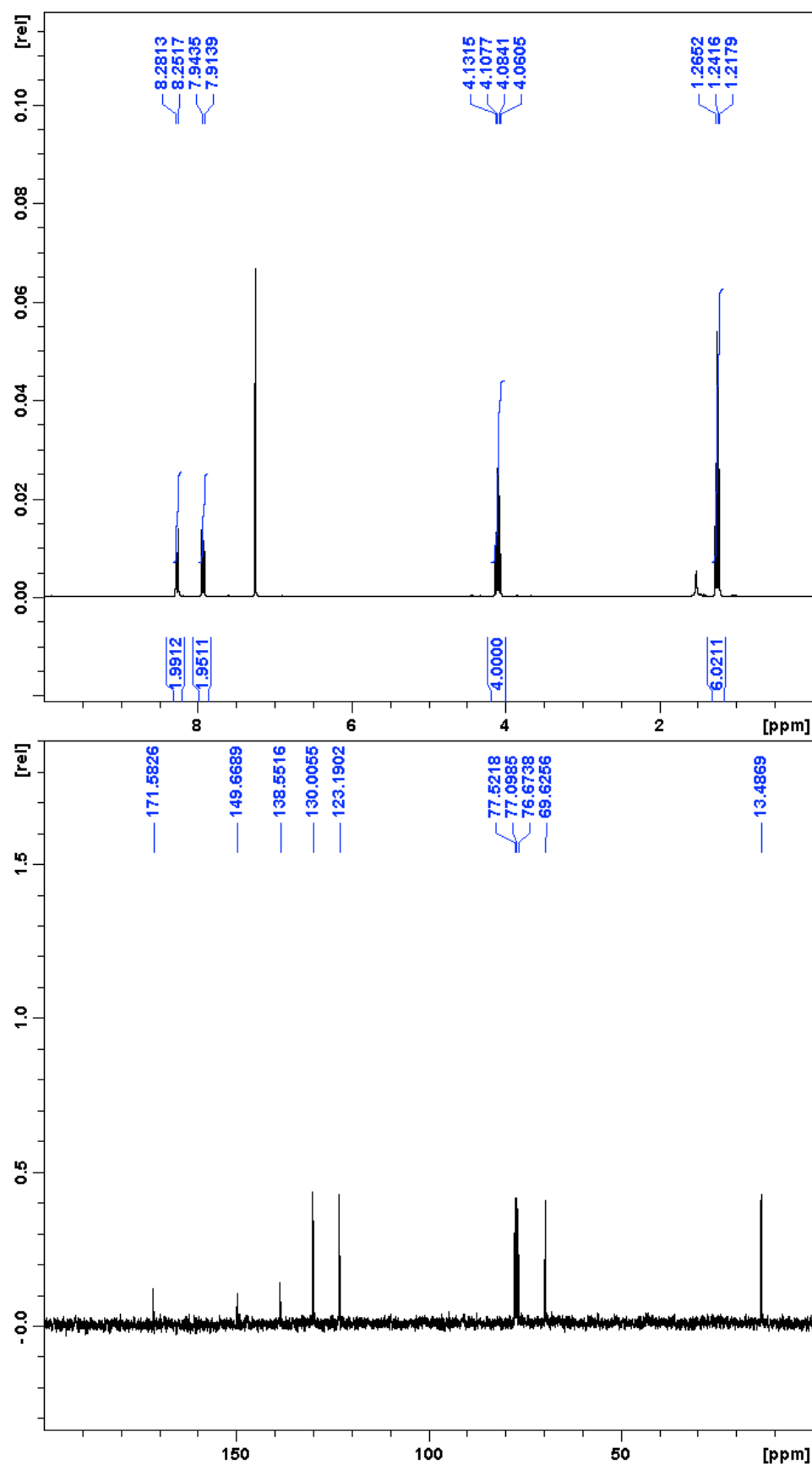
***N*-(4-Chlorobenzyloxy)-*N*-methoxybenzamide 3e**



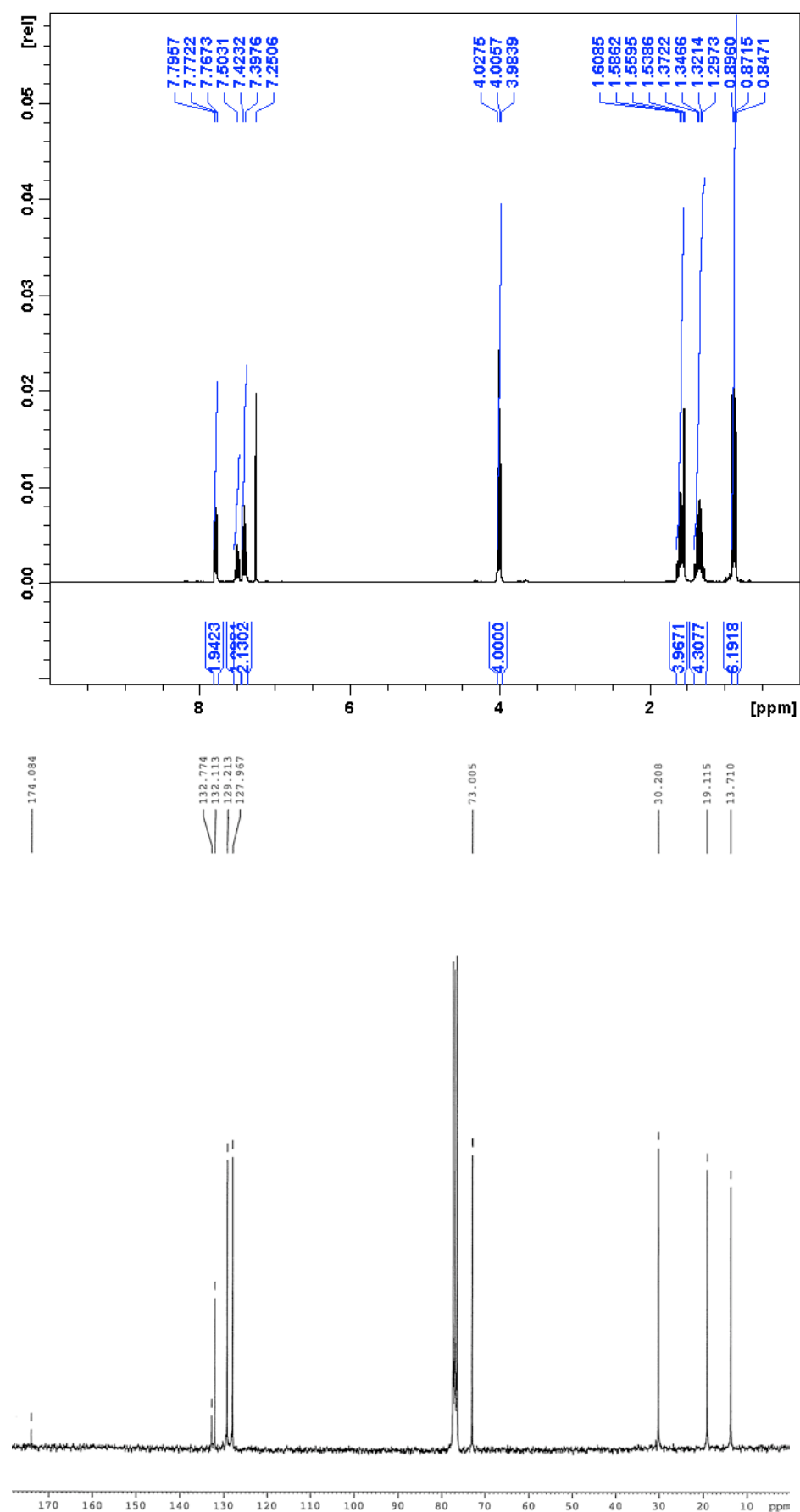
***N*-Methoxy-*N*-(4-nitrobenzyloxy)benzamide 3f**



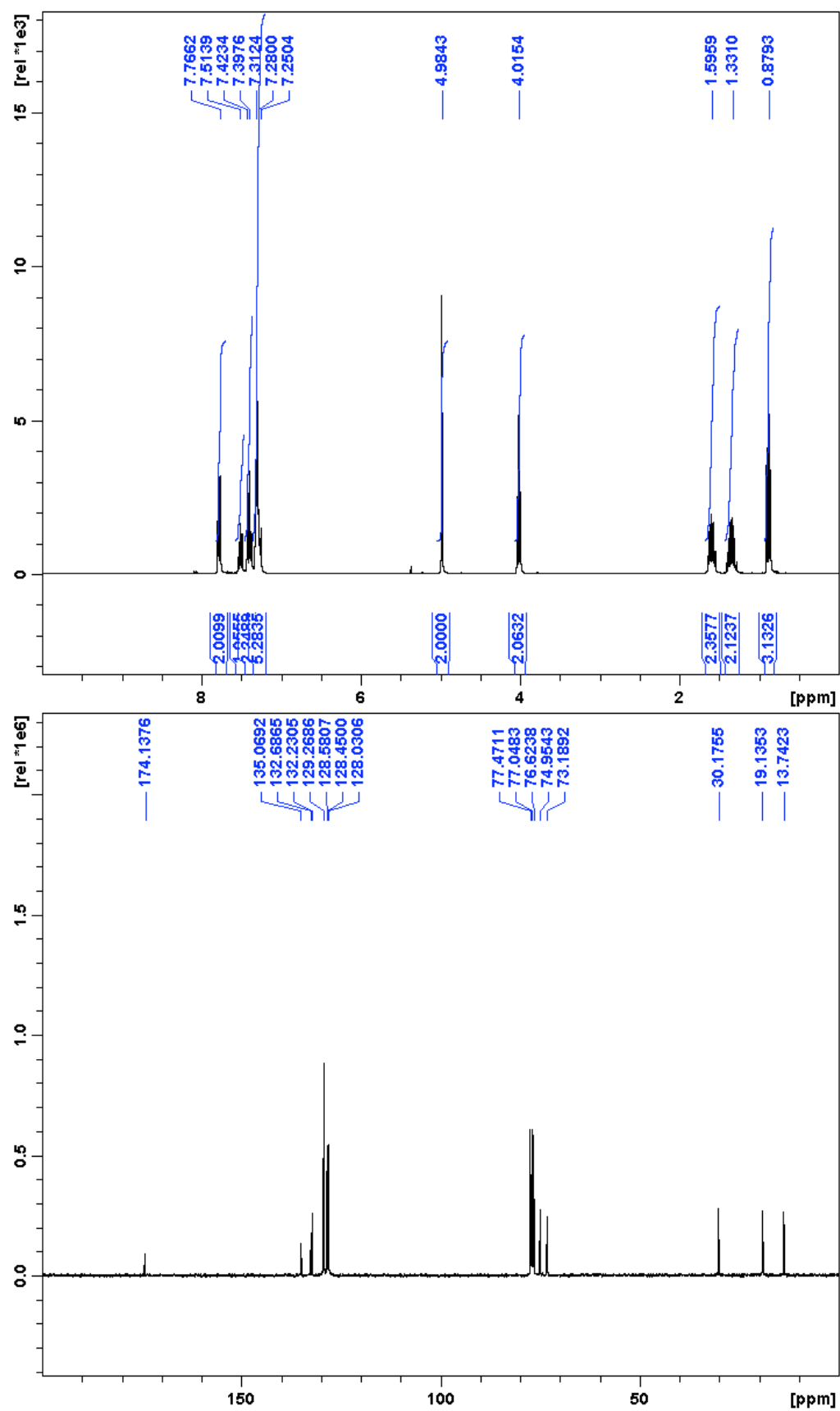
***N,N*-Diethoxy-4-nitrobenzamide 4a**



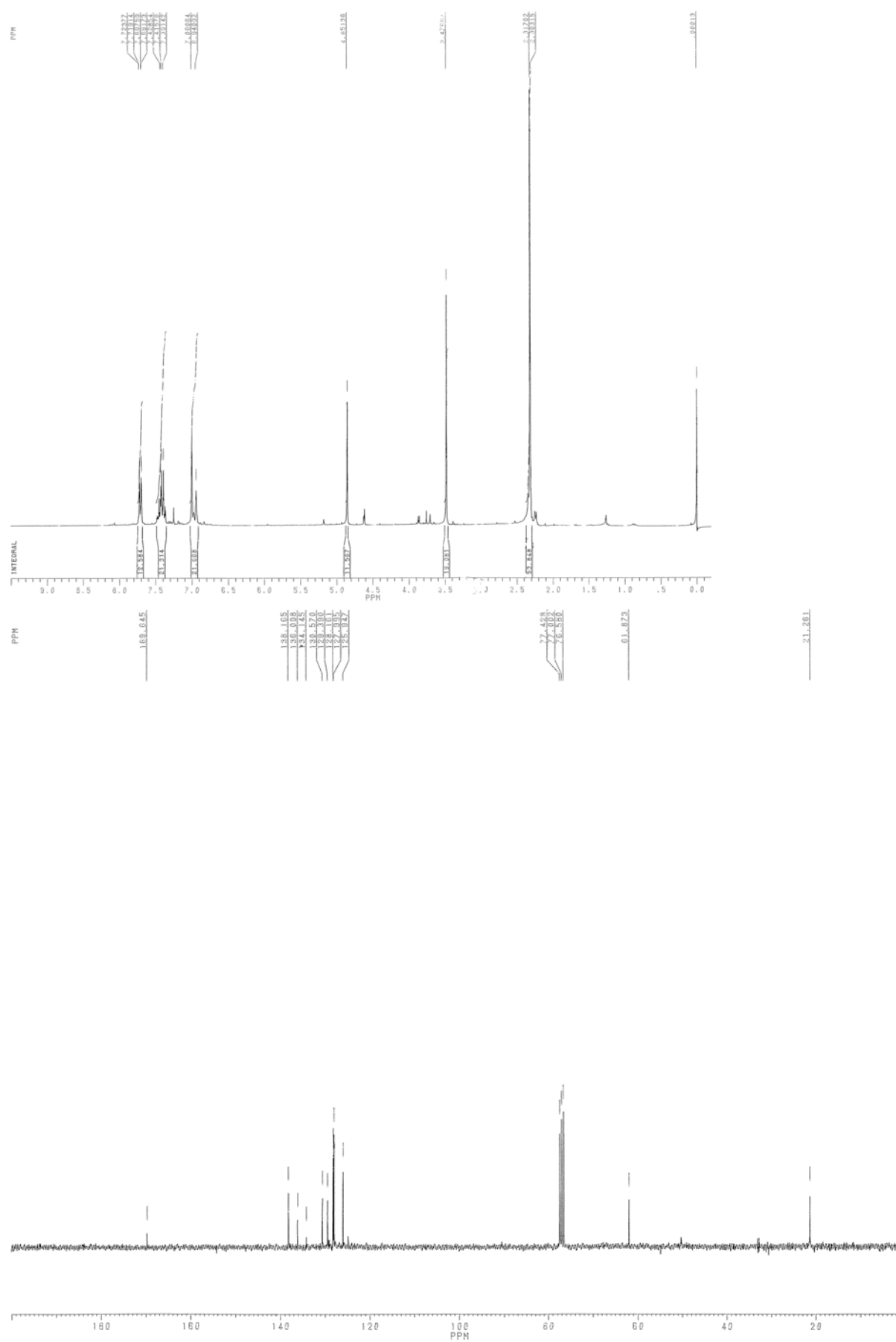
***N,N*-Dibutoxybenzamide 4b**



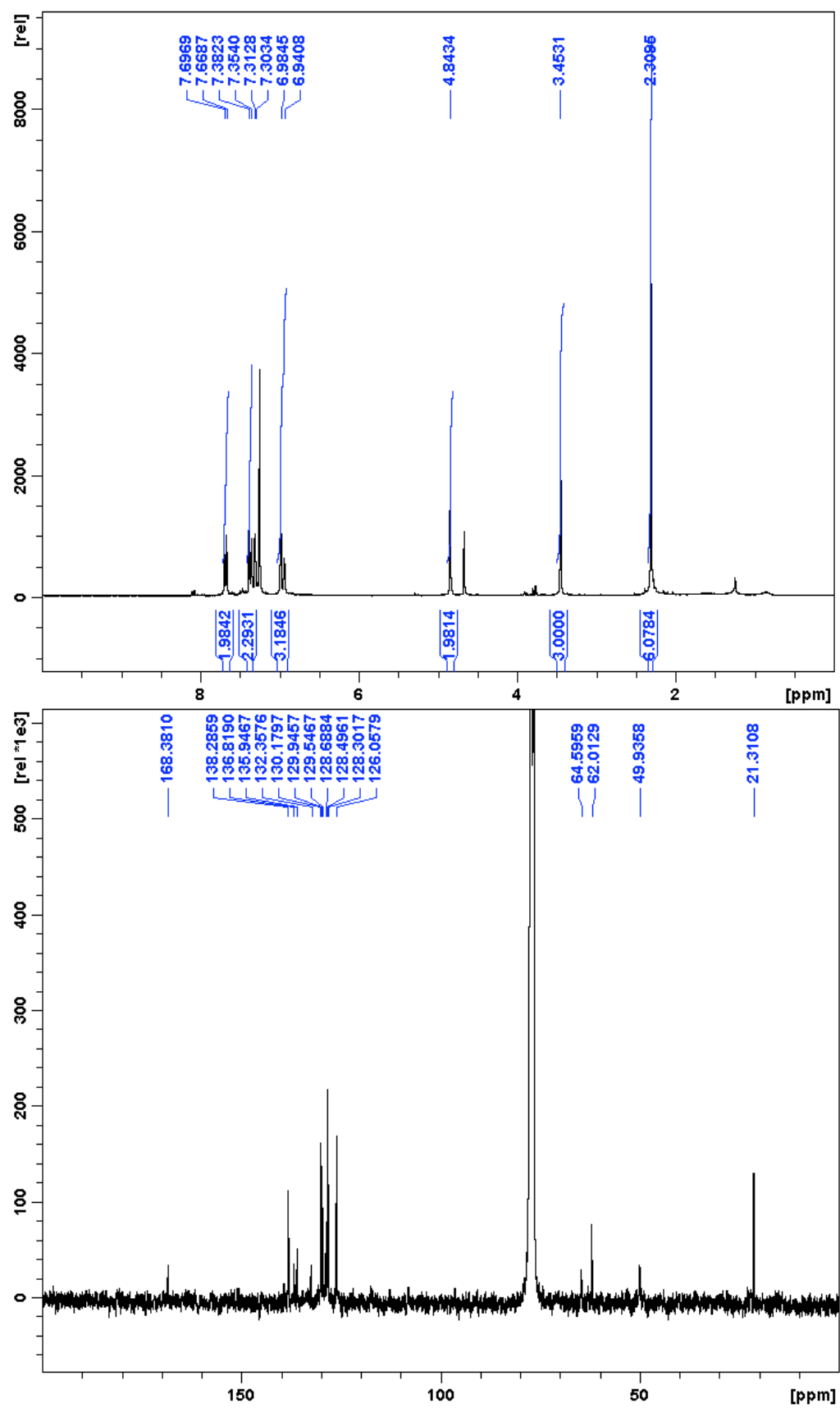
***N*-Benzyloxy-*N*-butoxybenzamide 4c**



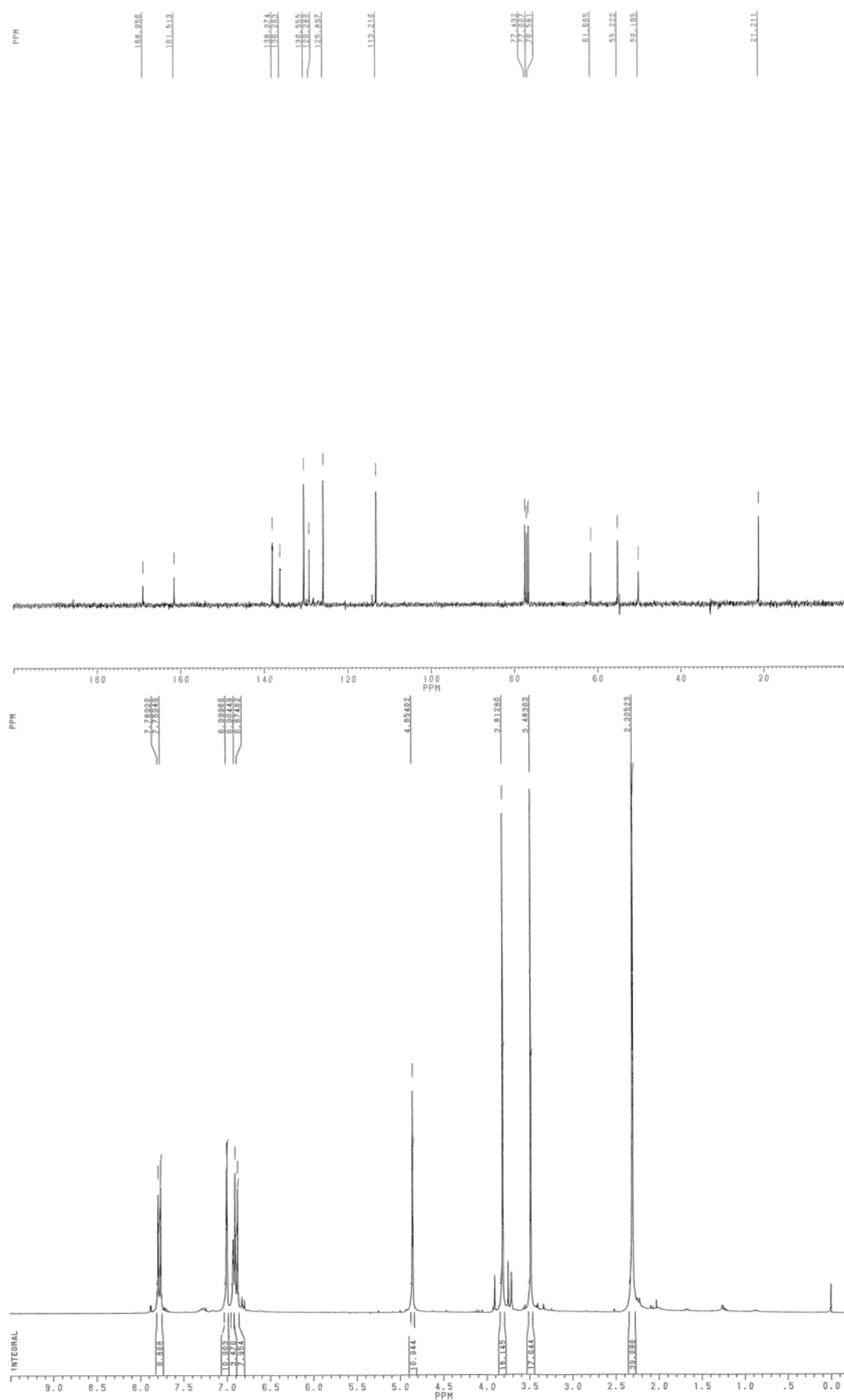
***N*-(3,5-Dimethylbenzyl)-*N*-methoxybenzamide 18a**



***N*-(3,5-dimethylbenzyl)-*N*-methoxy-4-chlorobenzamide 18b**



***N*-(3,5-Dimethylbenzyl)-*N*-methoxy-4-methoxybenzamide 18d**



B3LYP/6-31g(d) optimised geometry of *N*-methoxyacetamidyl radical calculated using Spartan08.¹

Energy: -323.036717 au,

ZPE: 244.9007 kJmol⁻¹;

Enthalpy: 266.3712 kJmol⁻¹;

Entropy: 348.6580 JK⁻¹mol⁻¹

Geometry:

XYZ format:

H	-0.890221	-1.765635	0.879960
C	-1.333189	-1.287032	0.000063
H	-0.890749	-1.765584	-0.880127
H	-2.413608	-1.437436	0.000334
C	-1.059905	0.203186	0.000014
O	-1.944449	1.049737	-0.000163
O	1.119757	-0.365059	-0.000187
C	2.479738	0.099325	-0.000035
H	2.667946	0.696566	-0.896166
H	3.095632	-0.801281	0.001198
H	2.667113	0.698467	0.894988
N	0.263079	0.686372	0.000338

1 Spartan '08 for Macintosh, Wavefunction inc., Irvine, CA, version 1.2.1 , 2008.