Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

SUPPLEMENTARY DATA

Candida tenuis Xylose Reductase Catalysed Reduction of Acetophenones: The Effect of Ring-Substituents on Catalytic Efficiency

Michael Vogl [a], Regina Kratzer [b], Bernd Nidetzky [b] and Lothar Brecker *[a]

a *University of Vienna, Department of Organic Chemistry, Währinger Straße 38, A-1090 Wien, Austria. E-Mail: lothar.brecker@univie.ac.at*

b *Graz University of Technology, Institute of Biotechnology and Biochemical Engineering, Petersgasse 12, A-8010 Graz, Austria*

Content:

Table S1:

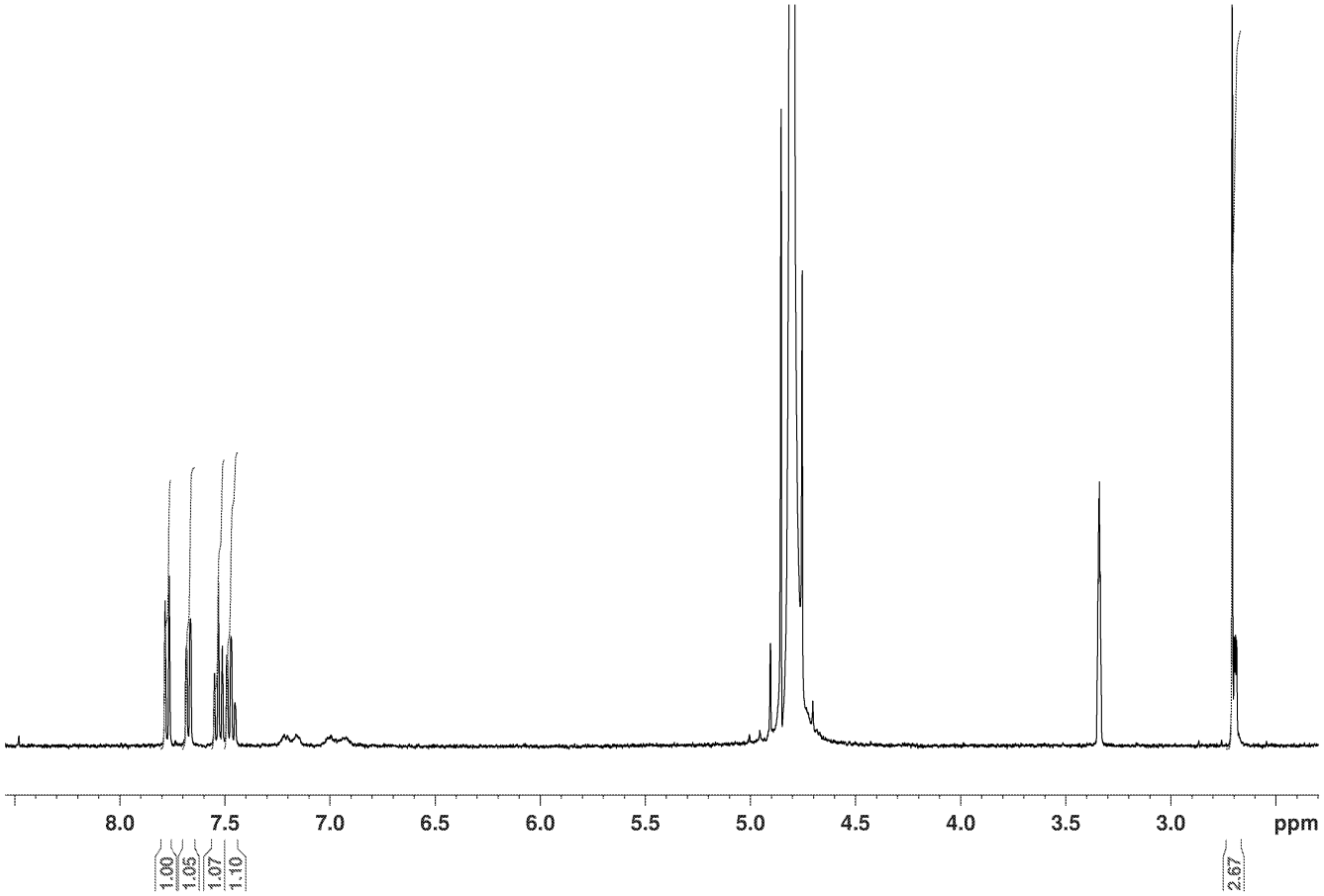
^{1}H NMR Spectra:

Table S1: Values and parameters used for calculation of Figure 1.

Substanz	**σH**	**log*P***	***p&m&o***	**cat $_{eff}$**	**log*P*-acph**	**log cat $_{eff}$**	**log cat $_{eff}$ -acph**
acetophenone [**27**]		1.665	0	0.5	0	-0.301	0.000
ortho-chloro acetophenone [**1**]	0.68	2.09	2	340	0.425	2.531	2.833
ortho-bromo acetophenone [**4**]	0.70	2.277	2	261	0.612	2.417	2.718
ortho-iodo acetophenone [**7**]	0.63	2.275	2	61	0.610	1.785	2.086
ortho-fluoro acetophenone [**9**]	0.54	1.295	2	17	-0.370	1.230	1.531
ortho-cyano acetophenone [**10**]	1.32	0.872	2	135	-0.793	2.130	2.431
ortho-hydroxy acetophenone [**16**]	0.04	1.964	2	4.5	0.299	0.653	0.954
ortho-methoxy acetophenone [**22**]	0.00	1.88	2	14	0.215	1.146	1.447
ortho-acetoxy acetophenone [**24**]	-0.38	0.817	2	1.8	-0.848	0.255	0.556
para-chloro acetophenone [**3**]	0.23	2.35	1	6.6	0.685	0.820	1.121
para-bromo acetophenone [**6**]	0.23	2.43	1	3.2	0.765	0.505	0.806
para-cyano acetophenone [**12**]	0.66	1.22	1	1.8	-0.445	0.255	0.556
meta-chloro acetophenone [**2**]	0.37	2.51	0	0.8	0.845	-0.097	0.204
meta-bromo acetophenone [**5**]	0.39	2.577	0	1.3	0.912	0.114	0.415
meta-iodo acetophenone [**8**]	0.35	2.898	0	0.3	1.233	-0.523	-0.222
meta-cyano acetophenone [**11**]	0.56	1.16	0	1.4	-0.505	0.146	0.447
meta-hydroxy acetophenon [**17**]	0.12	1.39	0	2.4	-0.275	0.380	0.681
meta-amino acetophenone [**20**]	-0.21	0.691	0	2.2	-0.974	0.342	0.643
ortho-nitro acetophenone [**13**]	1.40	1.28	2	18	-0.385	1.255	1.556
meta-nitro acetophenone [**14**]	0.71	1.49	0	37	-0.175	1.568	1.869
para-nitro acetophenone [**15**]	0.78	1.42	1	224	-0.245	2.350	2.651

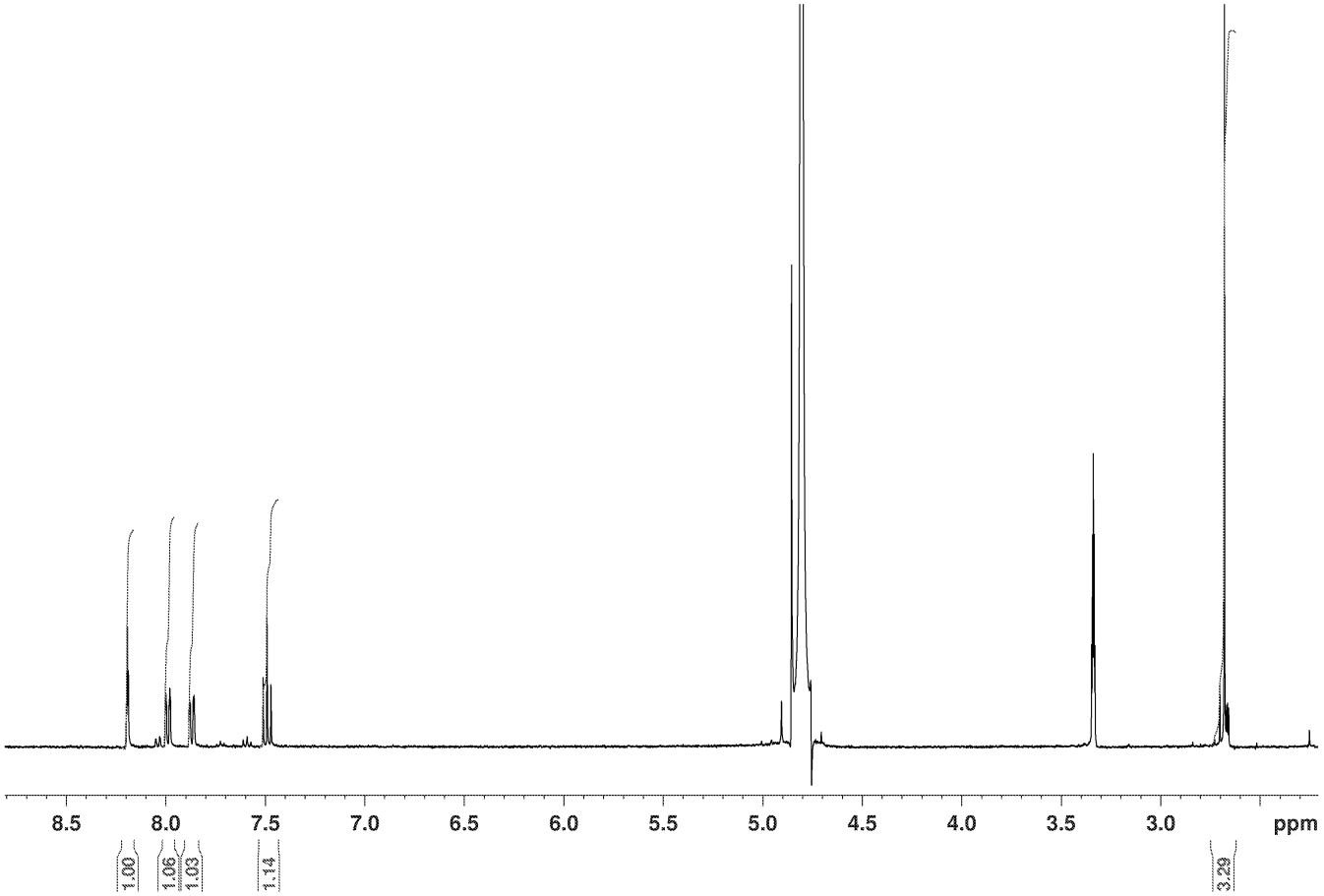
ortho-bromo acetophenone [**4**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



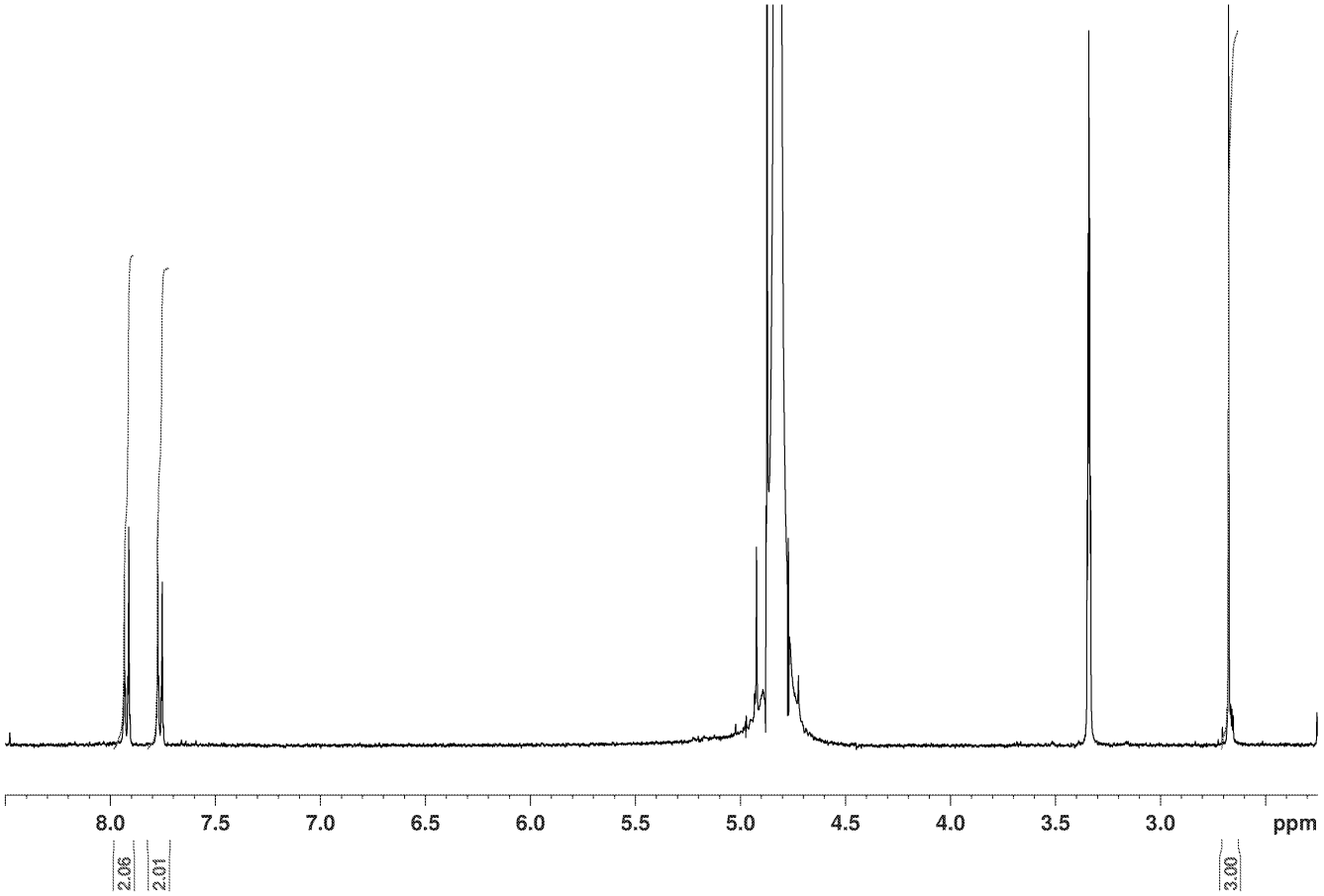
meta-bromo acetophenone [**5**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



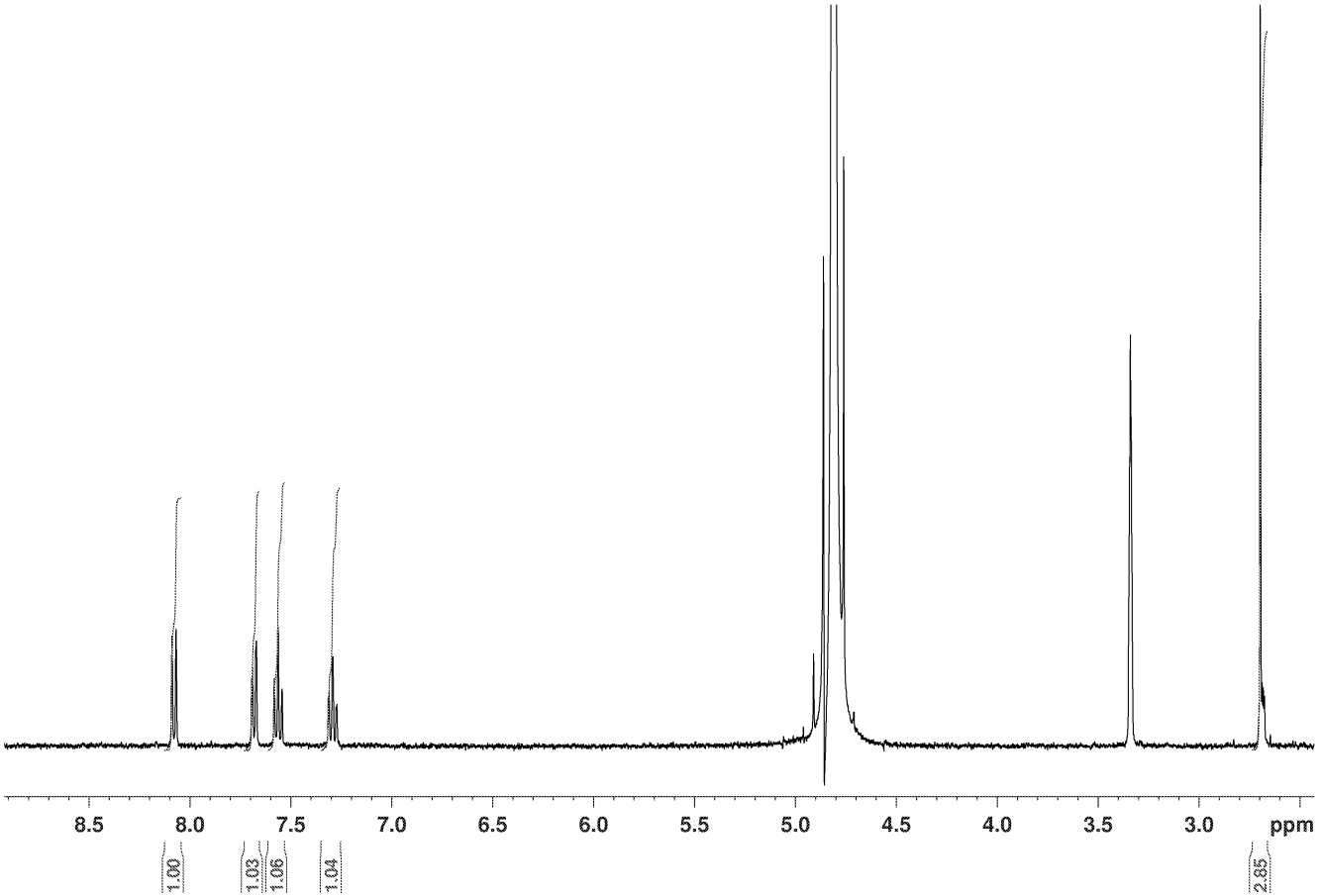
para-bromo acetophenone [**6**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



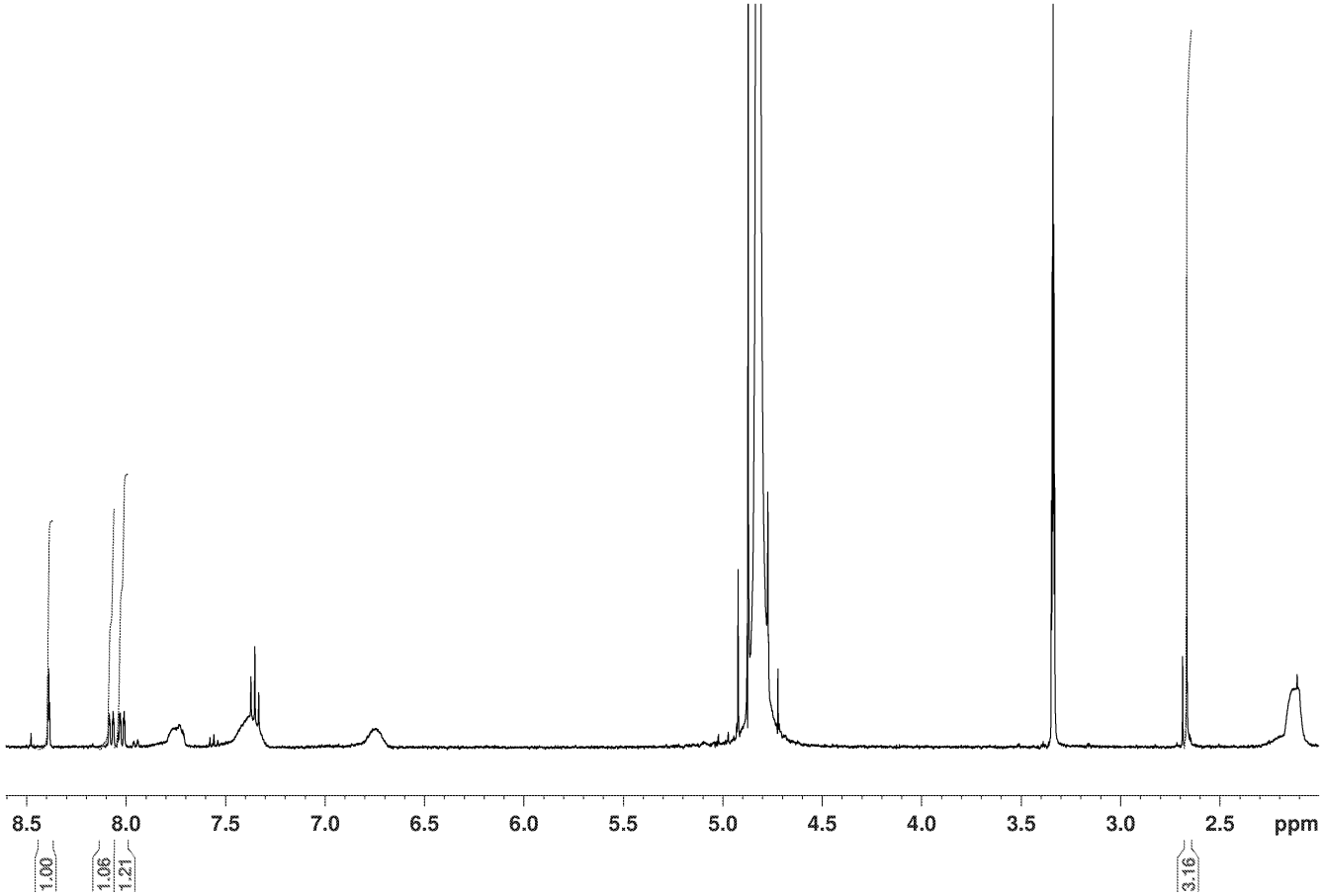
ortho-iodo acetophenone [**7**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



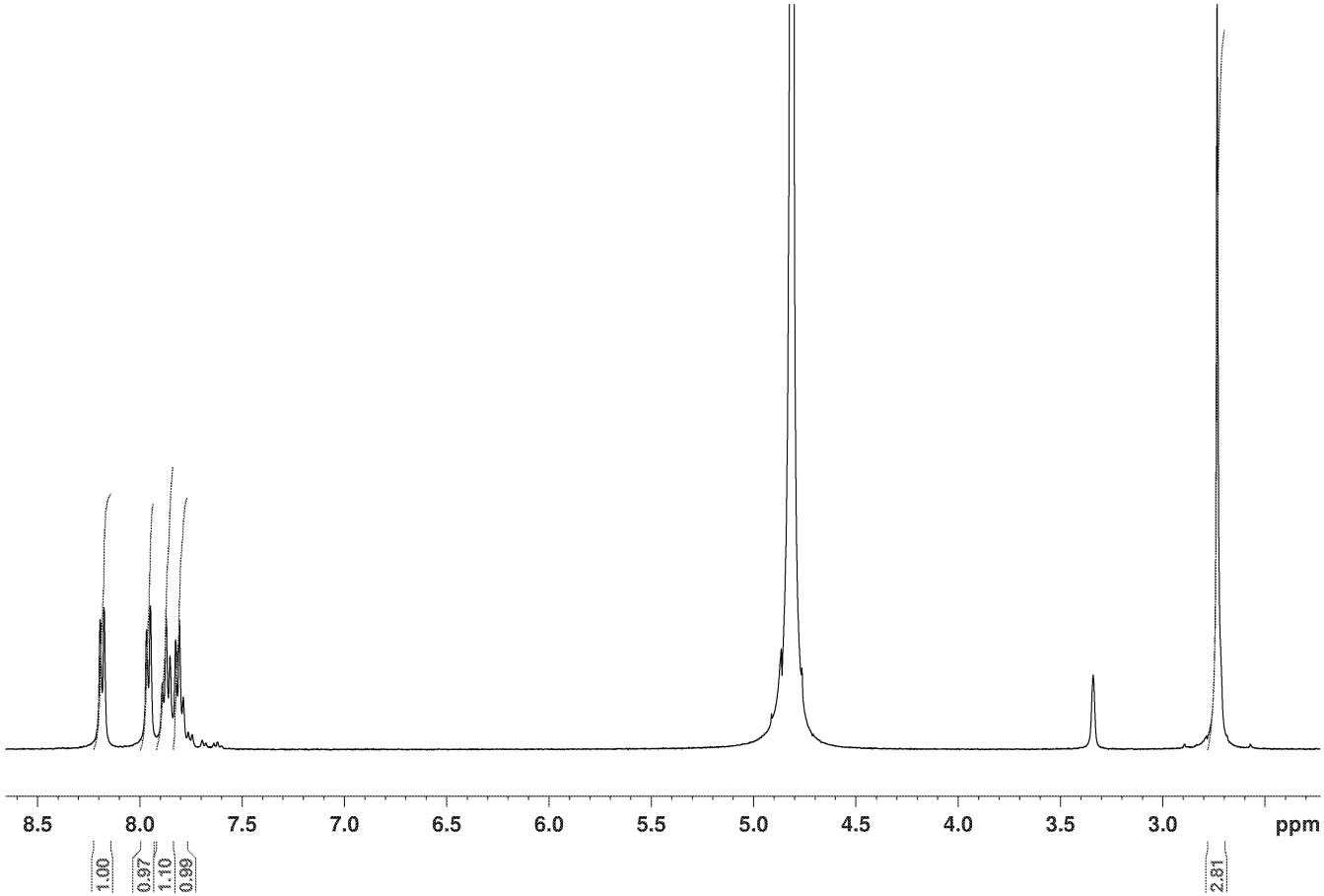
meta-iodo acetophenone [**8**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



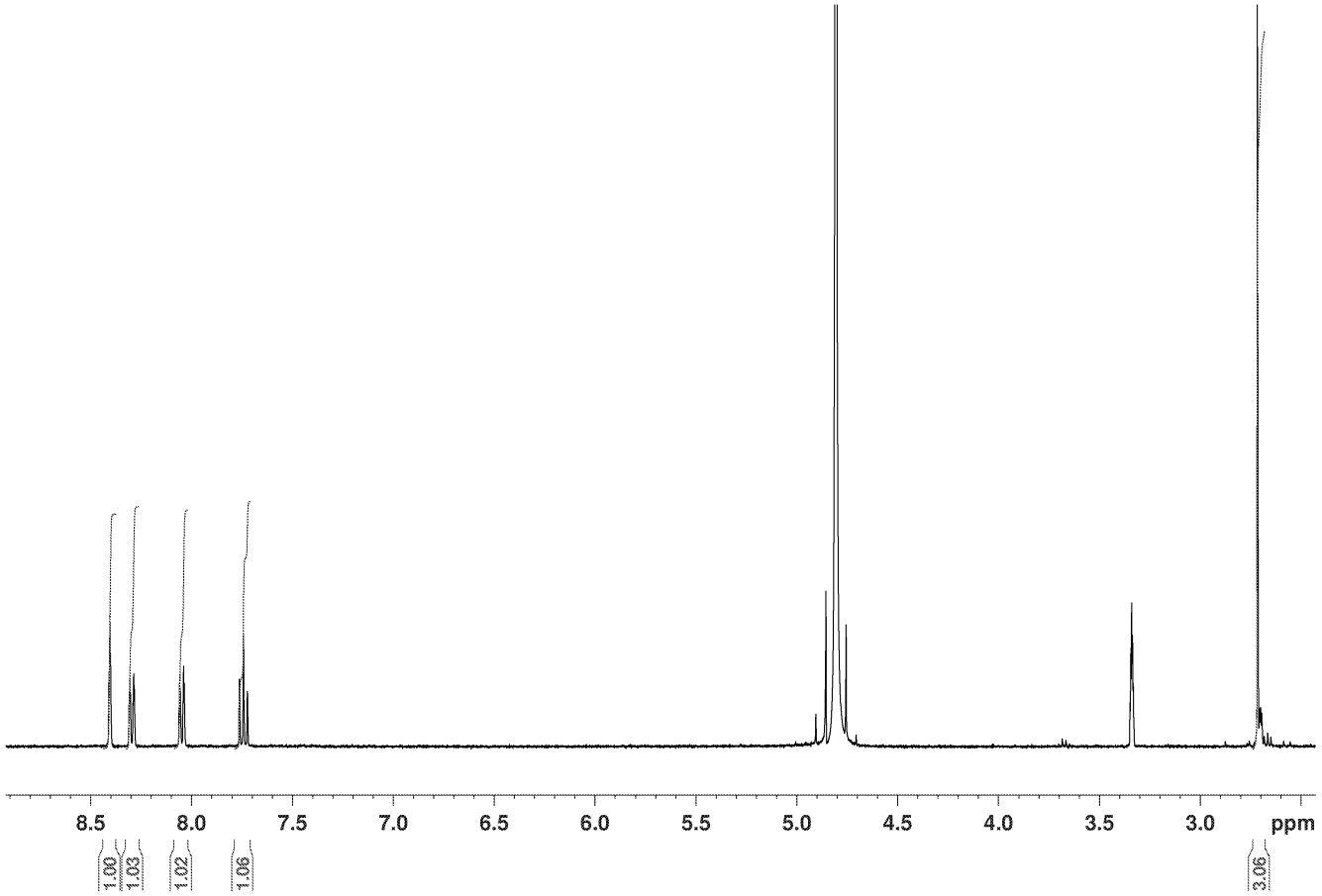
ortho-cyano acetophenone [**10**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



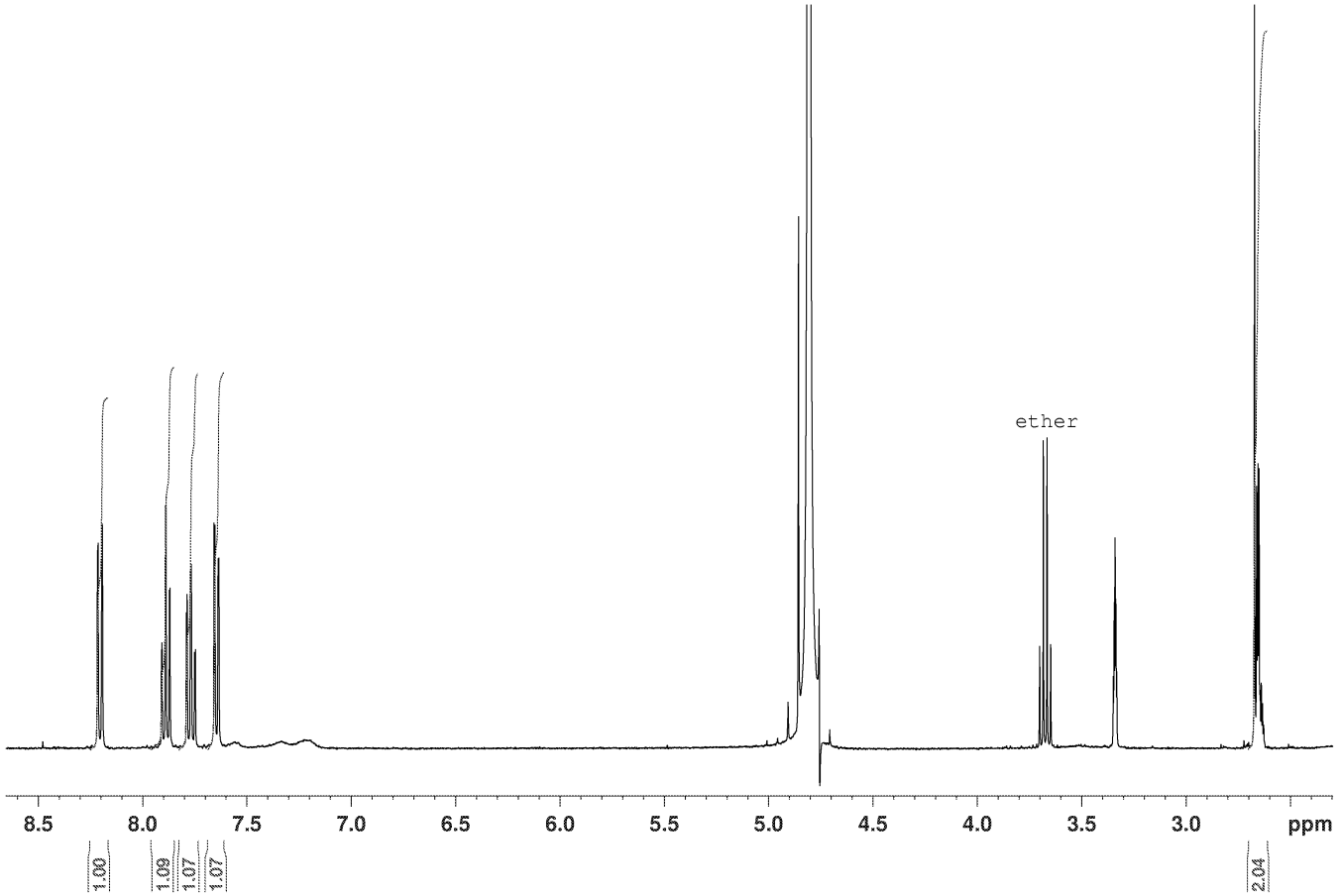
meta-cyano acetophenone [**11**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



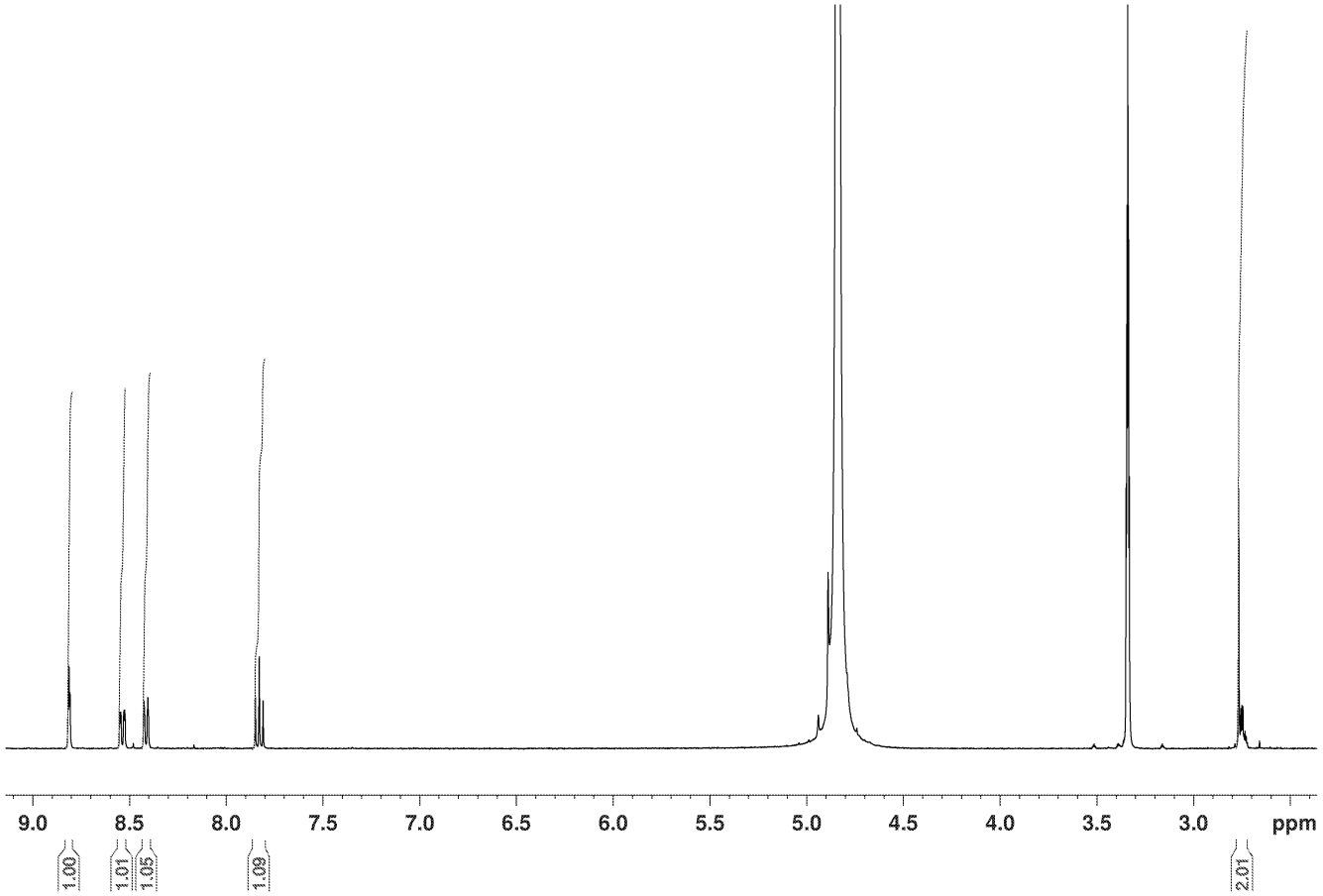
ortho-nitro acetophenone [**13**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



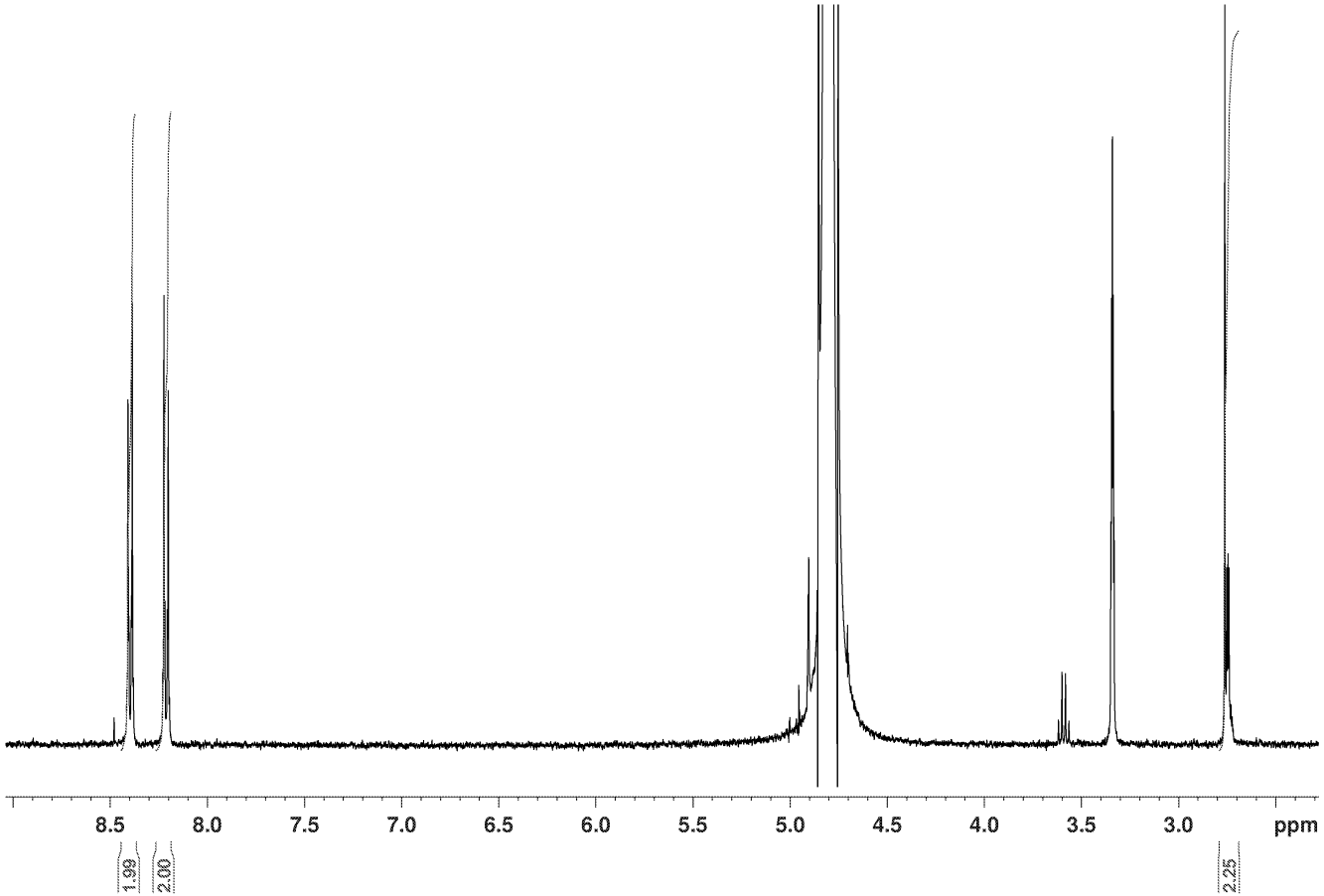
meta-nitro acetophenone [**14**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



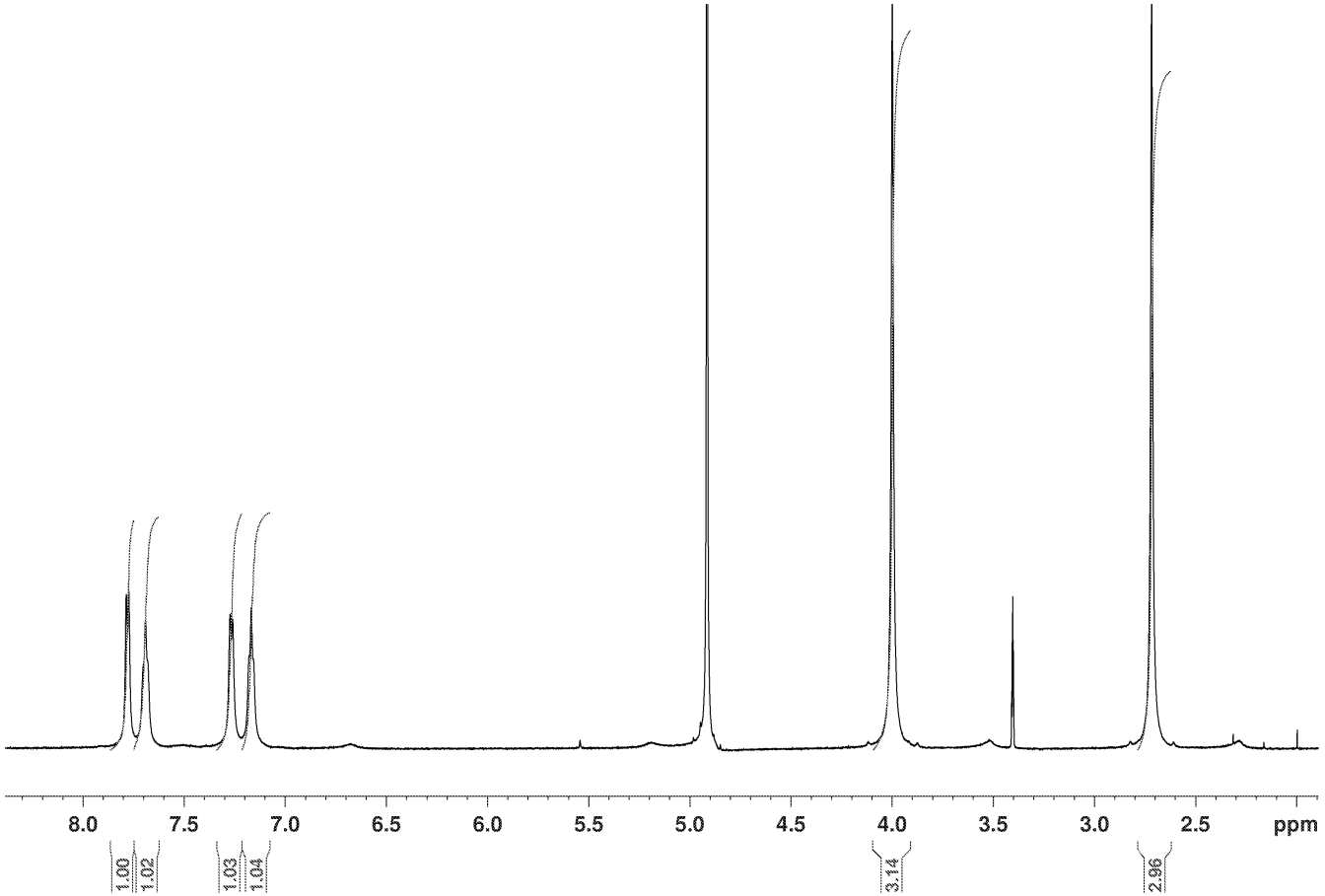
para-nitro acetophenone [**15**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



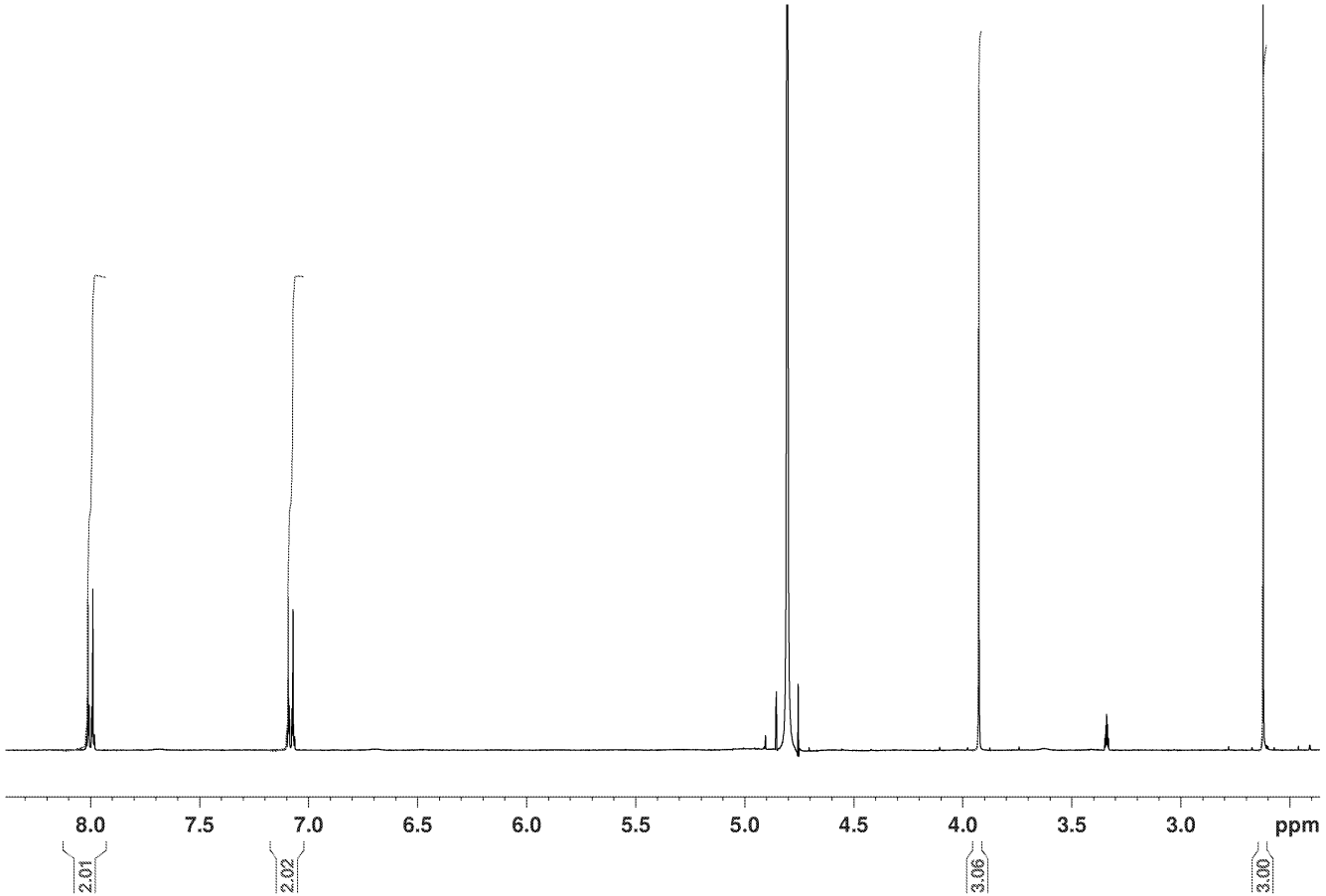
ortho-methoxy acetophenone [**22**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



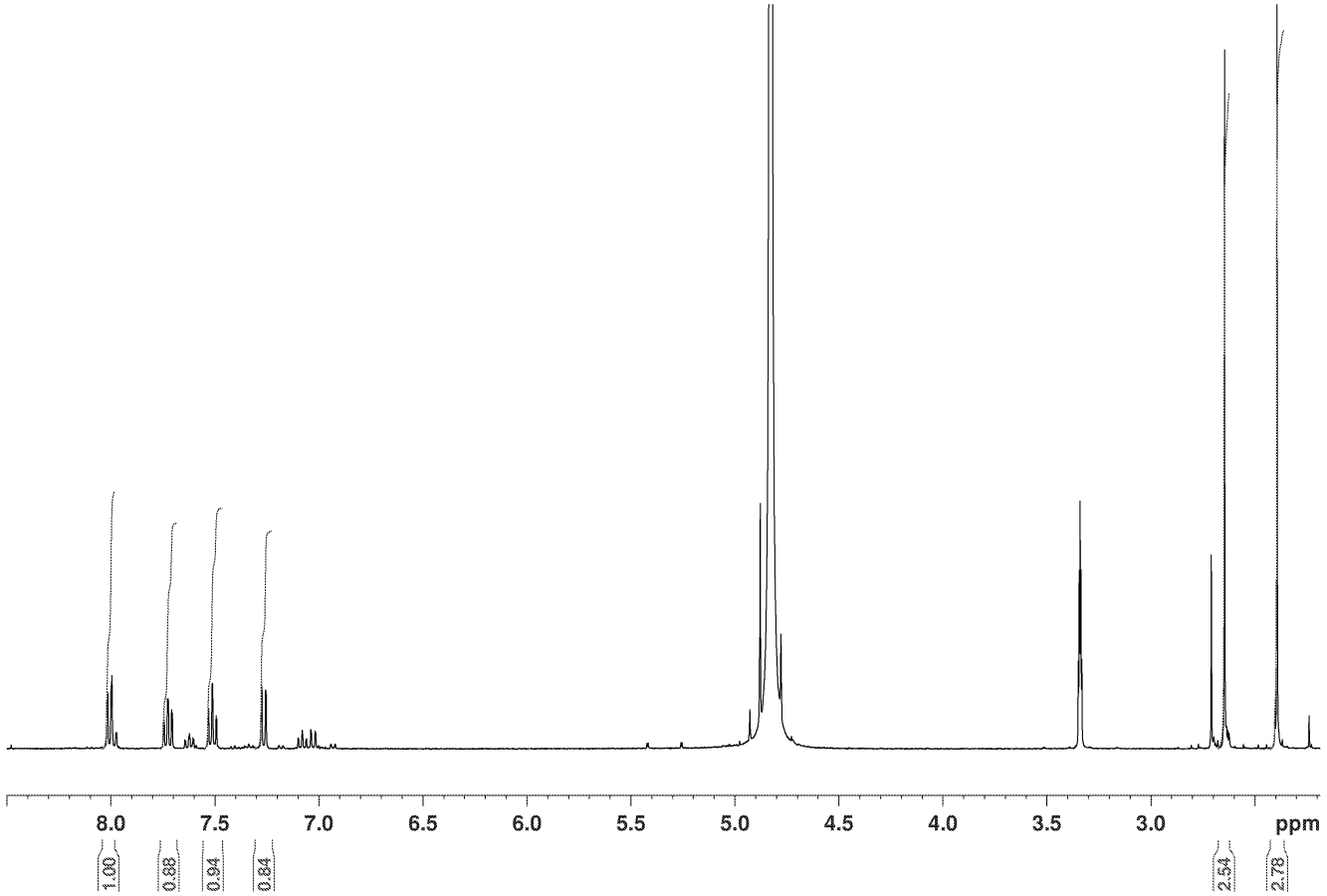
para-methoxy acetophenone [**23**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



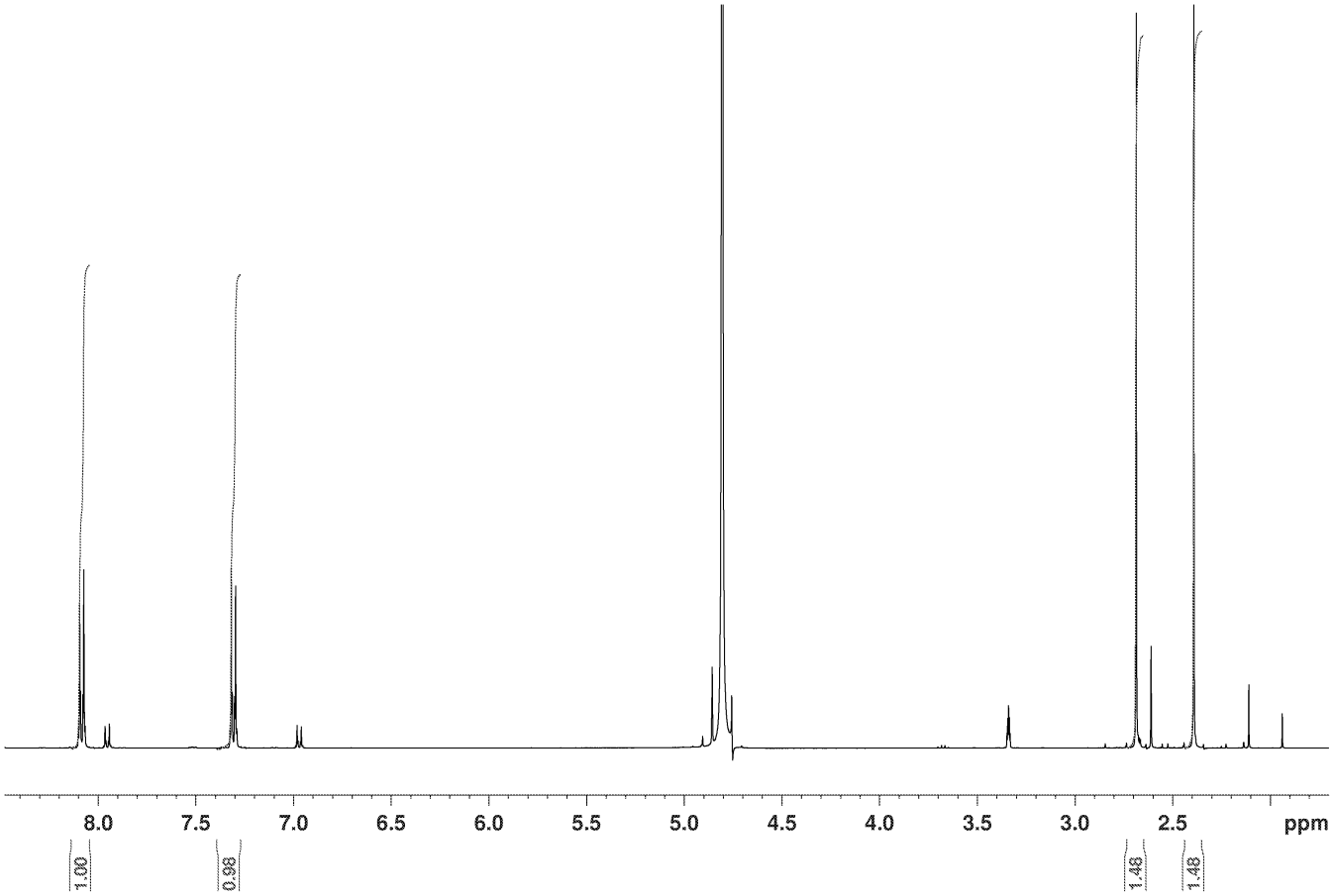
ortho-acetoxy acetophenone [**24**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



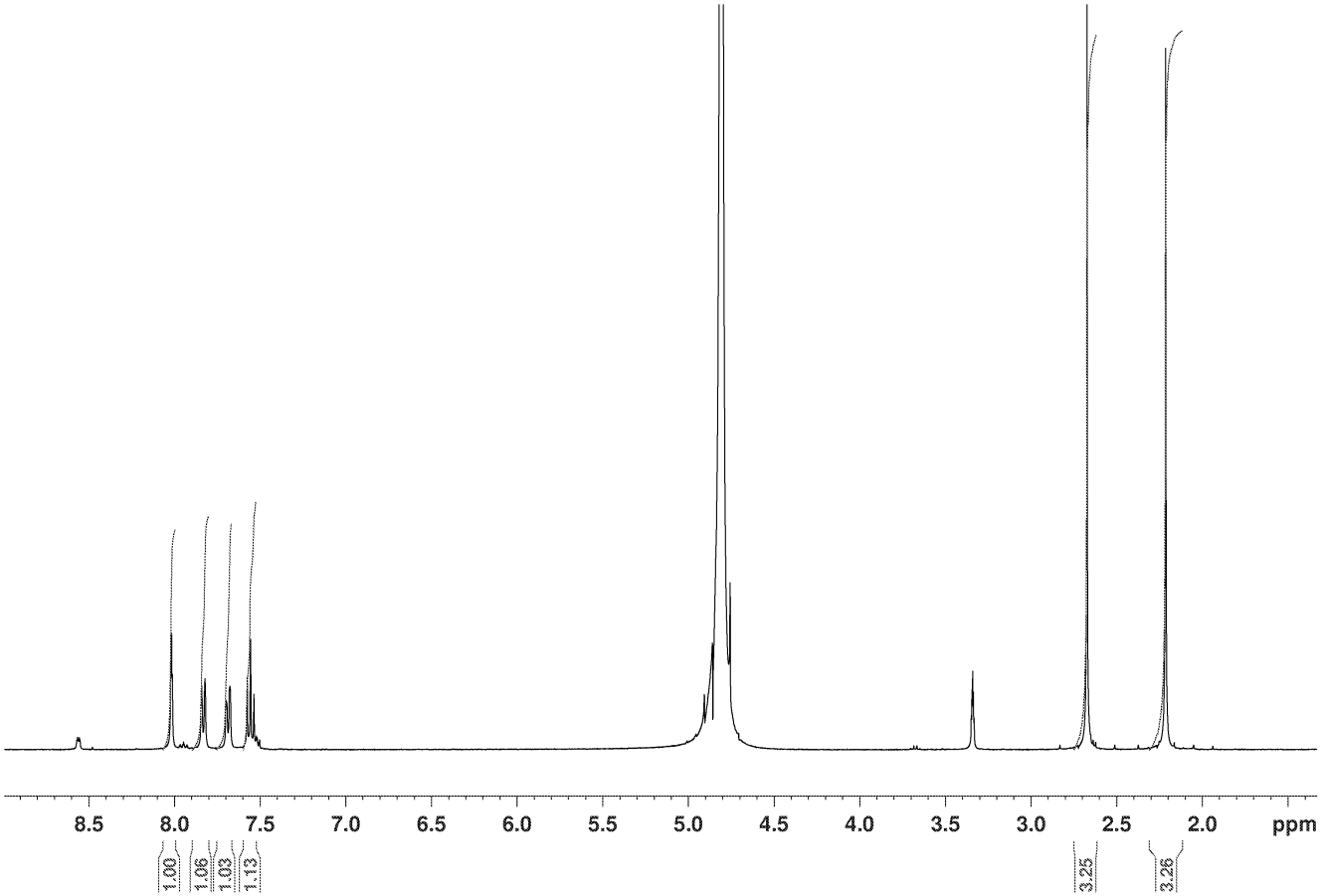
para-acetoxy acetophenone [**25**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



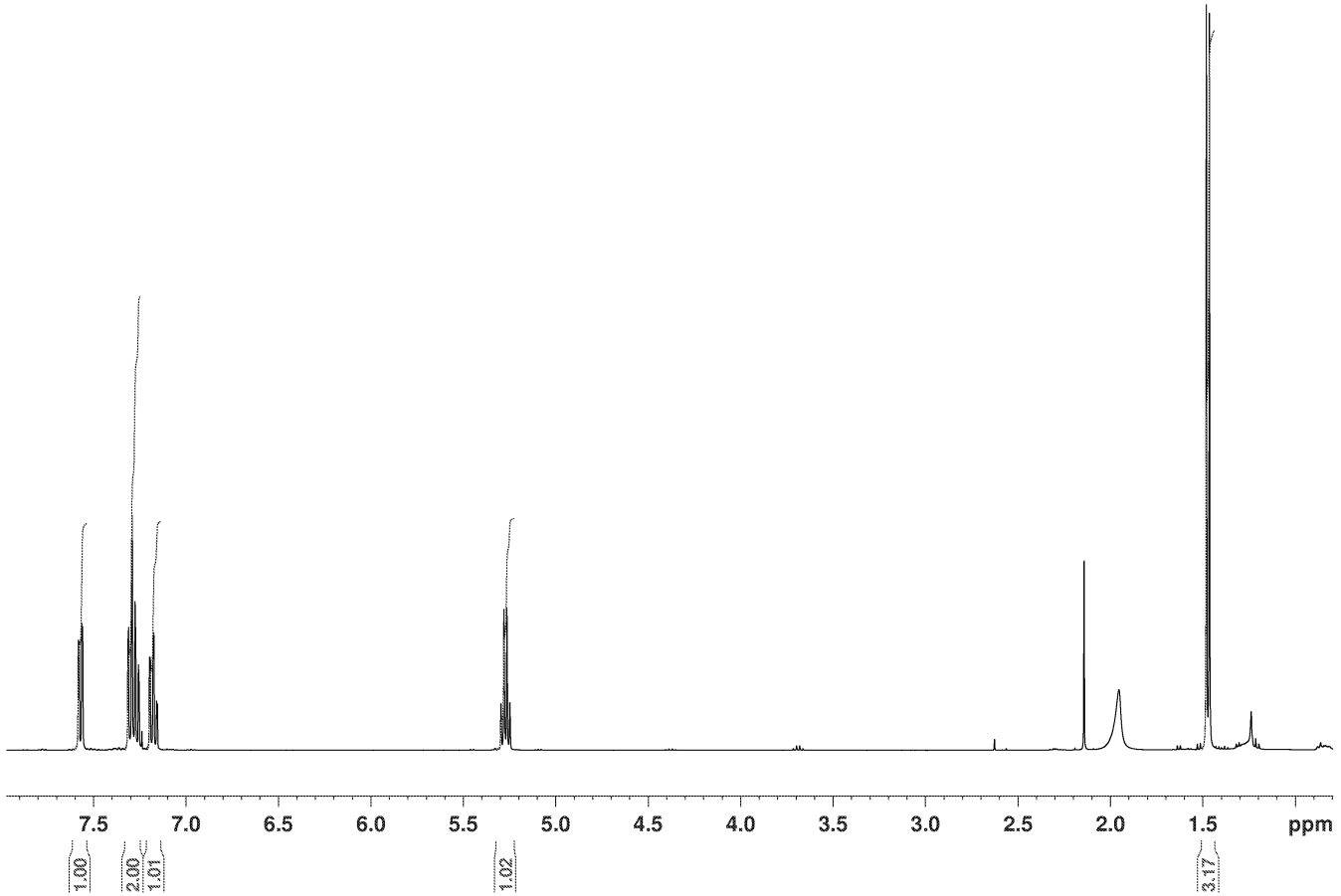
meta-acetamino acetophenone [**26**]

^{1}H-NMR (D_2O/CD_3OD 9:1)



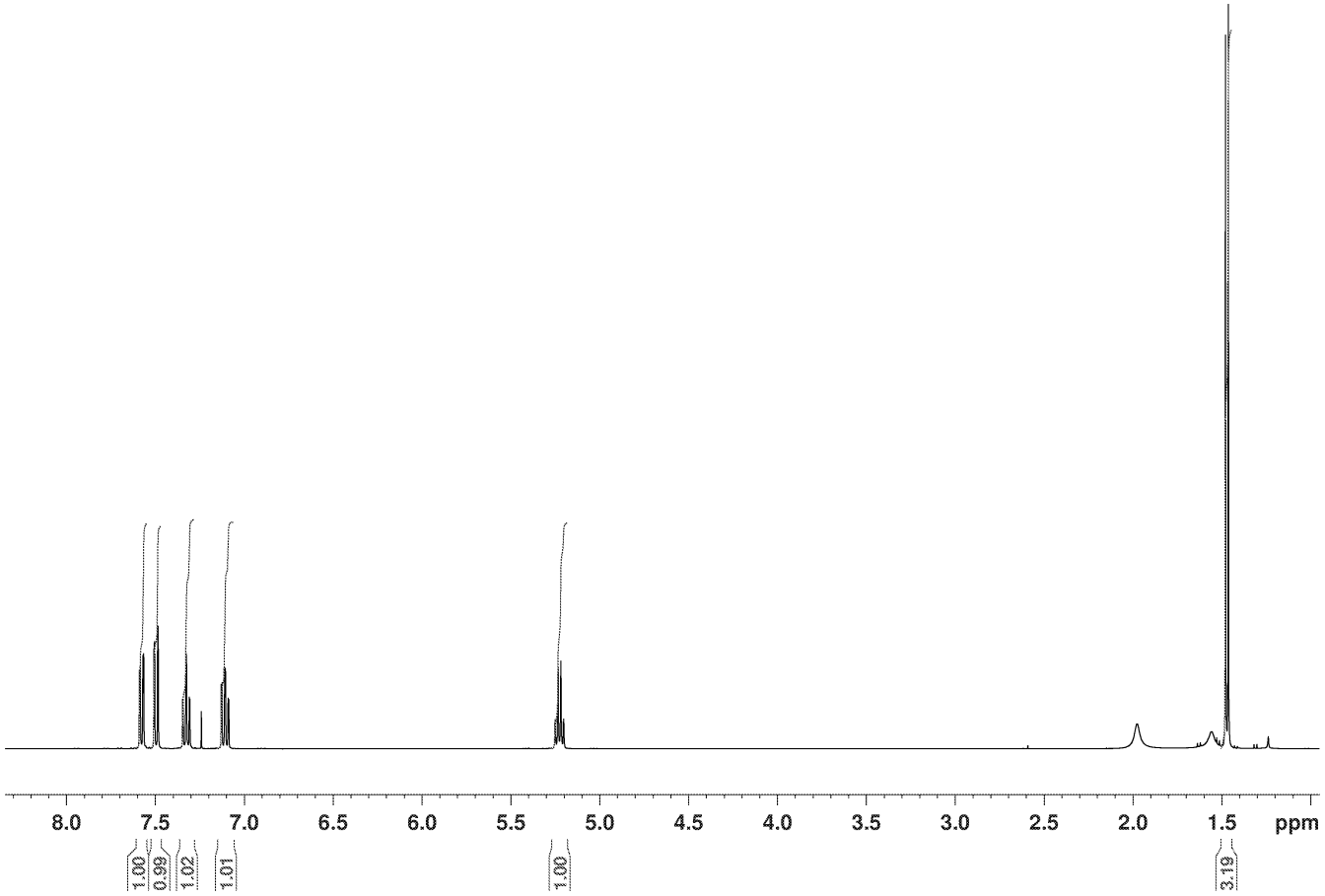
1-(*ortho*-chloro-phenyl) ethanol [**28**]

^{1}H-NMR ($CDCl_3$)



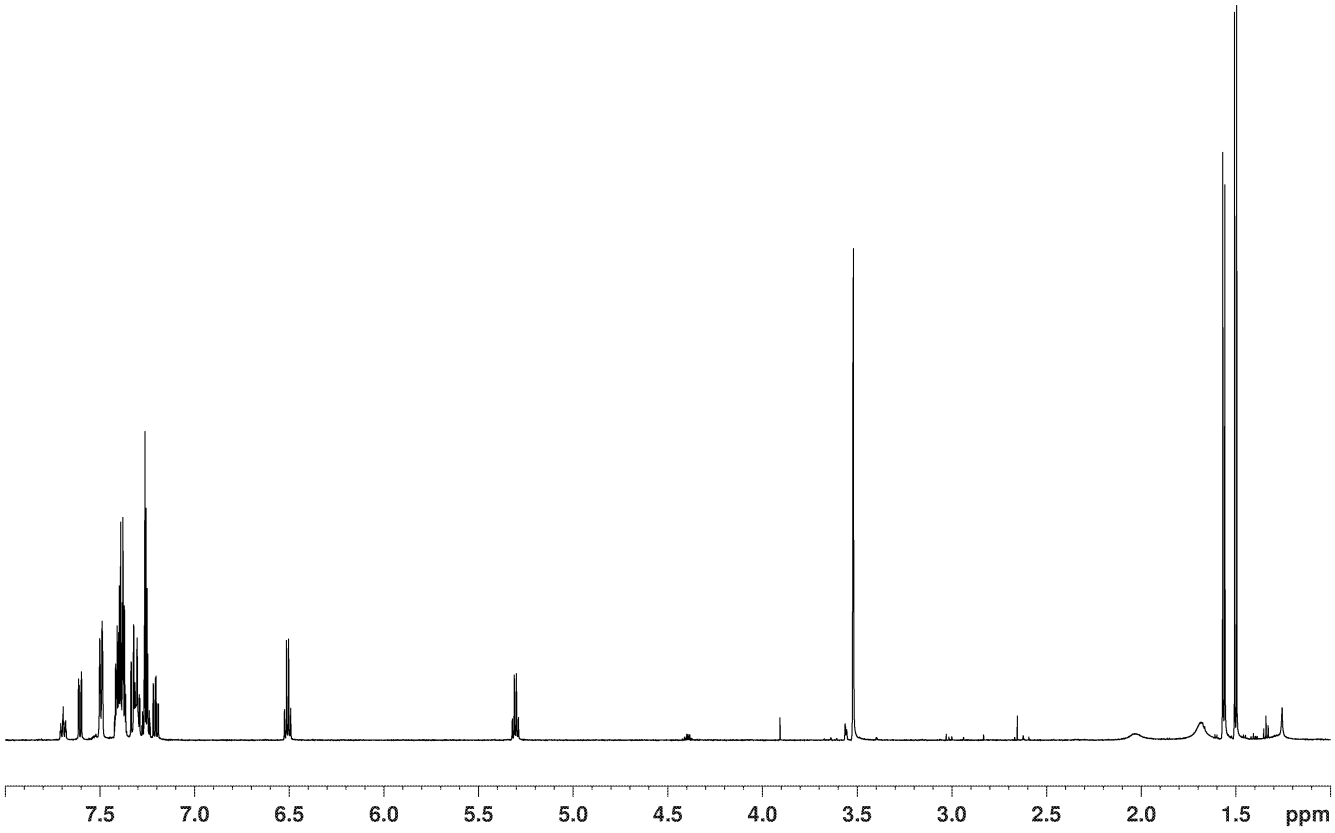
1-(*ortho*-bromo-phenyl) ethanol [**29**]

^{1}H-NMR ($CDCl_3$)



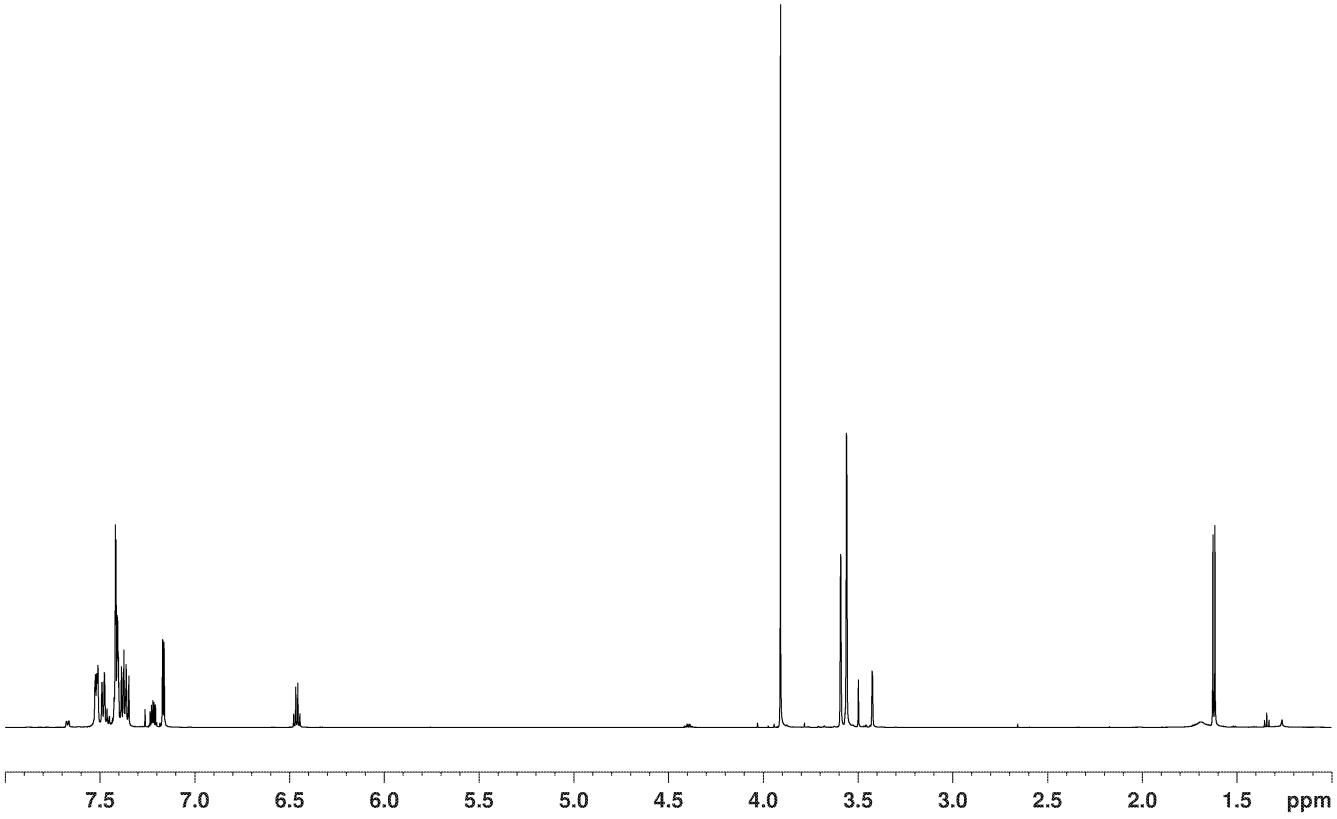
(*S*)-1-(*ortho*-Chlorophenyl) ethyl-(*S*)-α-methoxy-α-trifluoromethylphenylacetate [**30**] & 1-(*ortho*-chloro-phenyl) ethanol [**28**]

^{1}H-NMR ($CDCl_3$)



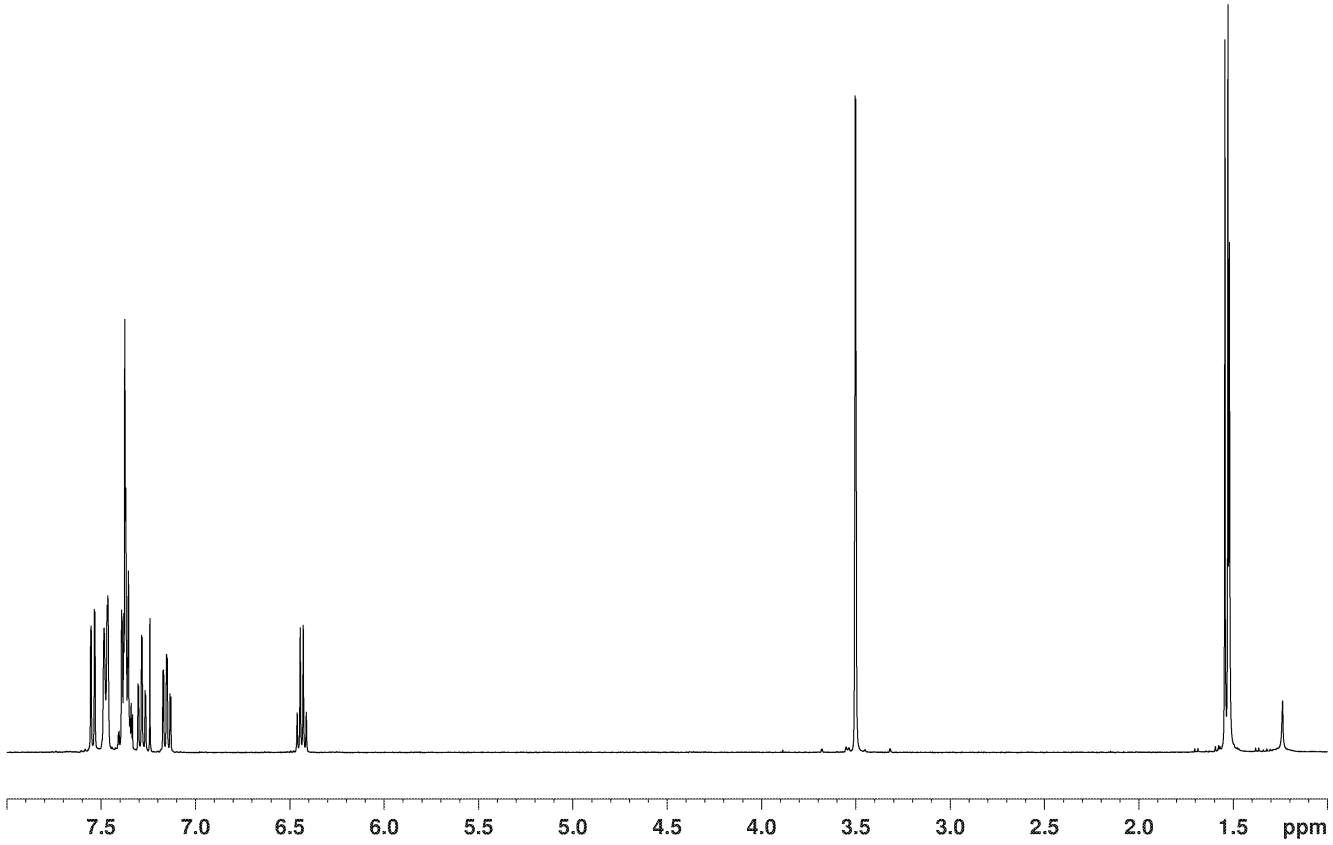
(*S*)-1-(*ortho*-Chlorophenyl) ethyl-(*R*)-α-methoxy-α-trifluoromethylphenylacetate [**31**]

^{1}H-NMR ($CDCl_3$)



(*S*)-1-(*ortho*-bromophenyl) ethyl-(*S*)-α-methoxy-α-trifluoromethylphenylacetate [**32**]

^{1}H-NMR ($CDCl_3$)



(*S*)-1-(*ortho*-bromophenyl) ethyl-(*R*)-α-methoxy-α-trifluoromethylphenylacetate [**33**]

^{1}H-NMR ($CDCl_3$)