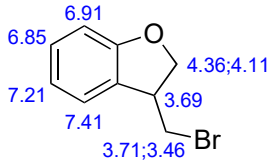
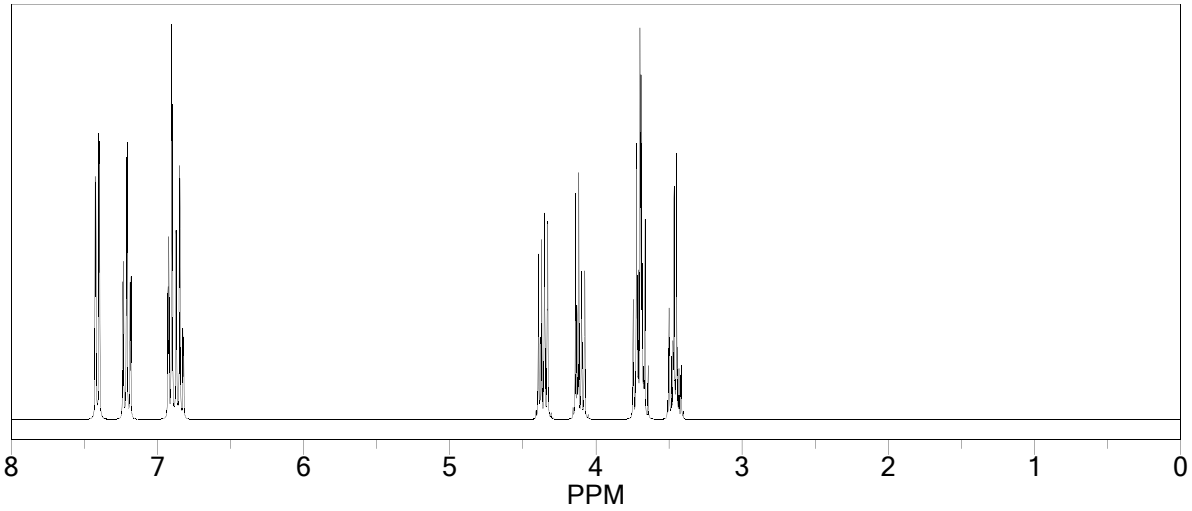
ChemNMR ^{1}H Estimation



Estimation quality is indicated by color: good, medium, rough



Protocol of the H-1 NMR Prediction:

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
CH2	4.36,4.105000	1.37	methylene
		2.61	1 alpha -O-1:C*C*C*C*C*C*1
		0.29	1 beta -1:C*C*C*C*C*C*1
		-0.04	1 beta -C
CH	3.69	1.50	methine
		1.28	1 alpha -1:C*C*C*C*C*C*1
		0.50	1 beta -O-1:C*C*C*C*C*C*1
		0.41	1 beta -Br
CH	6.91	7.26	1-benzene
		-0.49	1 -O-C
		-0.08	1 -C(C)C
		0.22	general corrections
CH	7.41	7.26	1-benzene
		-0.11	1 -O-C
		-0.13	1 -C(C)C
		0.39	general corrections
CH	6.85	7.26	1-benzene
		-0.11	1 -O-C
		-0.18	1 -C(C)C
		-0.12	general corrections
CH	7.21	7.26	1-benzene
		-0.44	1 -O-C
		-0.08	1 -C(C)C
		0.47	general corrections
CH2	3.71,3.465000	1.37	methylene
		1.97	1 alpha -Br
		0.29	1 beta -1:C*C*C*C*C*C*1
		-0.04	1 beta -C

1H NMR Coupling Constant Prediction

shift	atom index	coupling partner, constant and vector
4.23	8	diastereotopic -12.4 H-C-H
	7	7.0 H-CH-C-H
3.69	7	
	8	7.0 H-C-CH-H
	10	7.0 H-C-CH-H

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6.91        6
                    1   7.5  H-C*C-H
                    2   1.5  H-C*CH*C-H
7.41        3
                    2   7.5  H-C*C-H
                    1   1.5  H-C*CH*C-H
6.85        1
                    6   7.5  H-C*C-H
                    2   7.5  H-C*C-H
                    3   1.5  H-C*CH*C-H
7.21        2
                    3   7.5  H-C*C-H
                    1   7.5  H-C*C-H
                    6   1.5  H-C*CH*C-H
3.59       10 diastereotopic -12.4  H-C-H
                    7   7.0  H-CH-C-H
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