

Supporting Information:

Table 1. Experimental and Computed Chemical Shifts for ^{13}C

	Atom #	Exp	GIPAW RPBE			
			X/N D	DFT-D2*	NMR	PW91
Naphthalene NAPHTHA06	1	208.5	-38.8	-33.4	-38.9	-41.5
		202.2	-33.9	-28.6	-29.8	-36.3
	2	-5.9	194.1	189.7	178.4	175.4
		227.6	-56.4	-54.5	-55.3	-59.0
		139.3	28.8	32.8	29.2	25.0
		11.1	196.9	173.9	163.0	159.7
	3	224.7	-55.2	-52.0	-50.3	-53.4
		140.3	28.2	30.5	27.3	24.8
		22.8	178.7	162.1	151.3	146.7
	4	223.9	-54.7	-50.7	-51.0	-54.3
		145.6	22.1	24.5	31.2	27.5
		20.5	184.8	164.8	147.8	144.1
4a	227.6	-59.2	-54.3	-56.5	-60.9	
	138.2	31.4	33.0	30.2	27.8	
Methyl β -D-Xylopyranoside XYLOBM02	1	10.4	194.3	175.0	162.9	158.7
		119.0	49.1	45.6	50.1	-
		102.8	72.0	70.0	70.5	-
	2	90.7	85.0	85.3	83.3	-
		91.9	79.2	77.6	78.0	-
		71.9	101.5	102.7	100.1	-
	3	52.8	123.8	128.8	120.0	-
		89.5	81.9	81.1	84.0	-
		79.0	93.0	94.1	91.0	-
	4	66.1	112.5	114.0	106.1	-
		90.6	79.6	78.7	81.0	-
		71.7	102.7	104.0	102.0	-
	5	46.3	130.6	131.6	124.8	-
		96.1	76.1	75.8	74.4	-
		80.9	92.6	93.0	90.4	-
	6	23.6	154.7	157.5	149.8	-
		90.0	88.8	80.9	83.2	-
		74.6	104.3	98.3	100.6	-
Methyl α -D-Glucopyranoside MGLUCP	1	7.4	189.1	178.2	162.2	-
		119.5	48.3	47.1	51.5	-
		95.1	78.0	77.9	78.3	-
	2	88.2	83.4	85.6	84.2	-
		87.2	82.5	81.4	82.5	-
		77.9	97.6	98.5	94.2	-
	3	51.7	127.1	129.8	121.7	-
		93.8	75.3	75.9	75.6	-
		72.9	102.3	103.1	100.7	-
	4	57.0	120.4	122.6	115.2	-
		88.0	83.6	83.4	84.5	-
		78.2	96.1	96.3	94.2	-
	5	51.2	125.4	127.4	119.3	-
		96.6	75.1	74.7	73.0	-
		73.3	101.8	102.2	97.6	-
	6	56.1	120.0	123.3	116.4	-
		89.2	79.6	79.4	80.3	-
		69.6	107.4	108.0	103.0	-

		32.5	149.1	150.5	140.6	-
	7	88.3	88.5	85.7	82.5	-
		70.0	105.2	101.9	101.3	-
		11.2	178.3	174.2	158.7	-
Sucrose	1	123.8	44.6	44.5	44.1	-
SUCROS04		89.1	83.7	85.3	87.6	-
		69.1	105.0	108.4	106.0	-
	2	94.2	75.8	75.4	77.3	-
		74.5	100.1	102.9	97.5	-
		53.6	121.9	126.0	119.3	-
	3	91.8	78.0	76.9	76.0	-
		73.3	100.4	101.5	100.4	-
		53.6	125.9	128.9	119.5	-
	4	86.0	85.5	83.0	85.0	-
		77.1	95.4	98.9	98.9	-
		40.7	137.4	140.9	132.0	-
	5	93.7	75.8	75.7	74.4	-
		82.8	91.6	93.3	92.8	-
		44.2	131.0	133.5	126.1	-
	6	86.3	83.8	83.3	84.4	-
		67.2	107.7	109.1	101.6	-
		28.1	151.6	154.8	144.9	-
	7	120.6	47.7	45.9	46.8	-
		97.7	74.8	74.3	77.7	-
		89.9	83.3	82.6	85.8	-
	8	104.1	65.6	65.5	66.2	-
		77.4	96.4	98.9	97.3	-
		68.5	106.5	111.3	106.3	-
	9	103.6	67.4	67.8	63.6	-
		66.1	107.6	110.4	104.9	-
		46.7	131.1	133.0	129.1	-
	10	105.5	67.4	68.7	70.3	-
		92.2	78.3	81.3	77.4	-
		48.4	127.1	132.0	122.7	-
	11	84.3	86.2	86.1	83.7	-
		69.8	103.4	105.5	104.0	-
		29.8	149.7	151.7	141.2	-
	12	87.1	84.2	85.0	80.6	-
		74.4	101.9	104.8	100.1	-
		38.0	139.6	143.7	132.6	-
Acetaminophen	1	228.9	-56.1	-46.4	-50.5	-
HXACAN01		133.4	39.9	35.7	33.1	-
		36.8	141.2	139.9	130.9	-
	2	203.5	-36.1	-35.7	-34.5	-
		150.4	19.7	22.8	21.5	-
		16.2	185.9	173.3	164.2	-
	3	193.5	-26.2	-23.3	-24.0	-
		130.0	41.9	44.1	40.6	-
		25.4	174.5	163.7	151.2	-
	4	238.1	-64.6	-59.3	-62.3	-
		154.2	13.7	11.8	9.5	-
		64.6	111.1	110.7	105.9	-
	5	188.8	-20.9	-22.3	-19.9	-
		133.4	44.5	46.4	40.7	-
		24.7	176.9	160.5	143.0	-
	6	194.8	-31.7	-31.7	-27.1	-
		139.4	37.0	38.3	33.4	-
		27.5	177.4	161.8	147.9	-
	7	245.8	-69.8	-67.1	-76.5	-

	174.8	7.3	4.9	-4.1	-
	88.8	88.1	85.1	84.1	-
8	46.5	152.2	136.4	117.9	-
	27.5	156.0	148.3	146.0	-
	-2.5	216.5	182.3	173.7	-
