

Reorganized, Weak C-H...O Interactions Directly Modify the Mechanical Properties and Compaction Performance of a Series of Nitrobenzoic Acids

Aditya B. Singaraju¹, Kyle Nguyen¹, Dale C. Swenson², Mamta Iyer³, Rahul V. Haware³ and Lewis L. Stevens^{1,}*

1. Division of Pharmaceutics and Translational Therapeutics, College of Pharmacy, The University of Iowa, Iowa City, IA 52242

2. X-Ray Diffraction Facility, Department of Chemistry, The University of Iowa, Iowa City, IA 52242

3. Division of Pharmaceutical Sciences, College of Pharmacy & Health Sciences, Campbell University, Buies Creek, NC 27506

L. L. Stevens, corresponding author. Tel: (319)-335-8823; e-mail: lewis-stevens@uiowa.edu

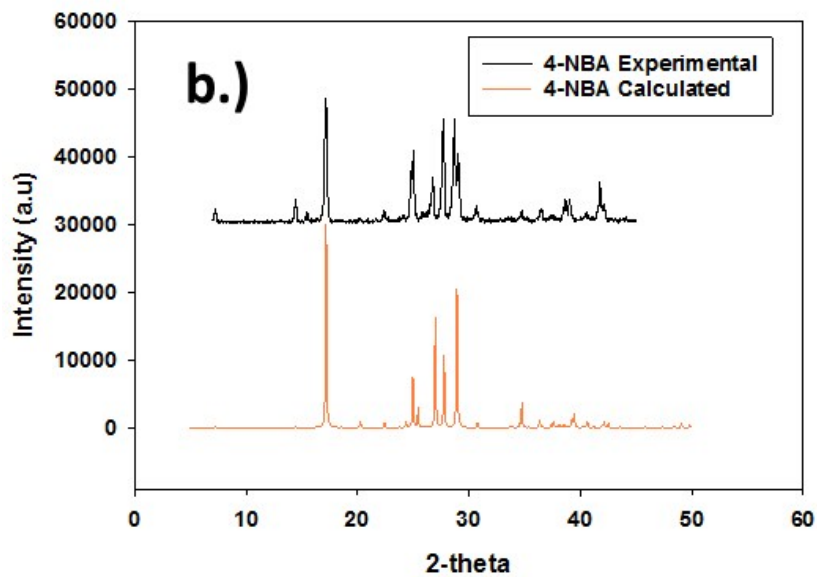
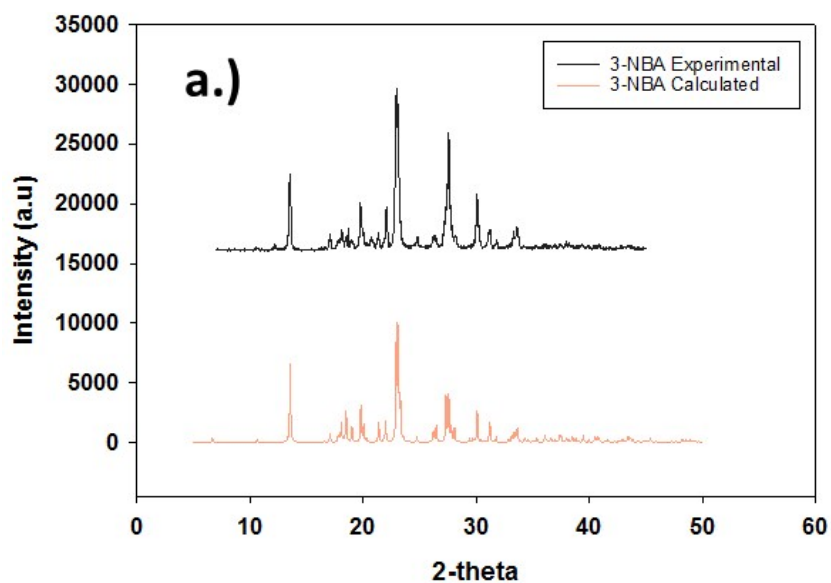
Supporting Information

Table S1. Geometrical parameters for all interactions (C-H...O, p-p and halogen short contacts) across the NBA series.

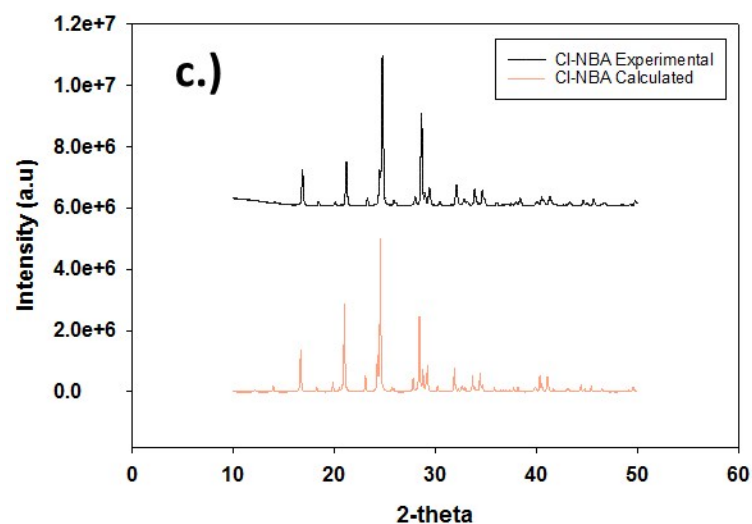
Material	Interaction	A-X (Å)	D-A (Å)	Angle (deg.)	Motif
4-NBA	C2-H2...O3	2.555	3.445	156	1-d tape
	C5-H4...O1	2.489	3.374	155	1-d tape
	C6-H5...O2	2.577	3.416	147	1-d tape
	C3-H3...O4	2.515	3.384	152	Inter-tape
	π - π	---	5.187	---	Ring-to-ring
3-NBA	C8-H4...O7	2.474	3.275	144	1-d tape
	C7-H3...O8	2.661	3.455	145	1-d tape
	C9-H5...O6	2.507	3.353	129	1-d tape
	C3-H1...O8	2.540	3.393	155	Inter-tape
	C10-H6...O1	2.465	3.418	152	Inter-tape
Cl-NBA	C5-H2...O2	2.555	3.406	151	1-d tape
	C6-H3...O1	2.515	3.475	153	1-d tape
	C2-H1...O4	2.612	3.326	134	Inter-tape
	C4-Cl1...O4	2.897	2.977	70	Intramolecular short contact
	π - π	---	4.559	---	Ring-to-ring
Br-NBA	C5-H5...O4	2.570	3.435	152	1-d tape
	C6-H6...O3	2.499	3.383	155	1-d tape
	C3-H3...O1	2.612	3.306	130	Inter-tape
	C1-Br1...O1	3.231	5.050	70	Inter-tape short contact
	π - π	---	4.485	---	Ring-to-ring
Me-NBA	C16-H16...O4	2.498	3.491	158	1-d tape
	C5-H5...O17	2.860	3.569	155	1-d tape
	C6-H6...O8	2.793	3.672	130	1-d tape
	π - π	---	4.683	---	Ring-to-ring

Figure S1. PXRD overlay of experimental and predicted patterns for a.) 3-NBA, b.) 4-NBA, c.) Cl-NBA, d.) Br-NBA and e.) Me-NBA.

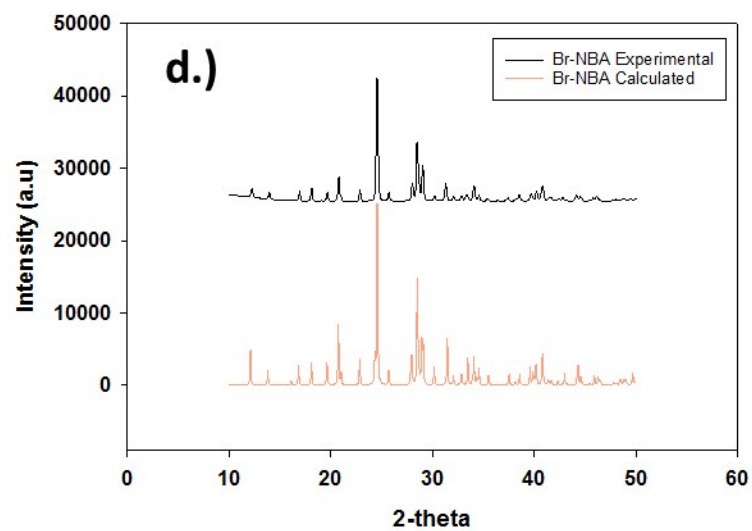
Experimental and Calculated Powder Patterns for 3-NBA



Experimental and Calculated Powder Patterns for Cl-NBA



Experimental and Calculated Powder Patterns for Br-NBA



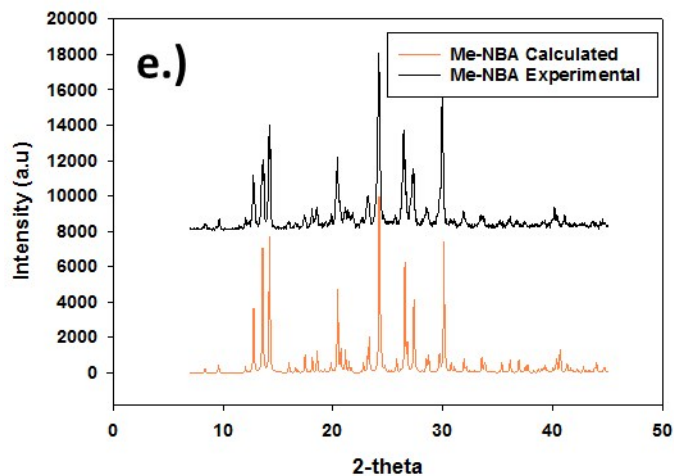


Figure S2. In-Die Heckel Plots for a.) 3-NBA, b.) 4-NBA, c.) Cl-NBA, d.) Br-NBA and e) Me-NBA

Figure S2a.)

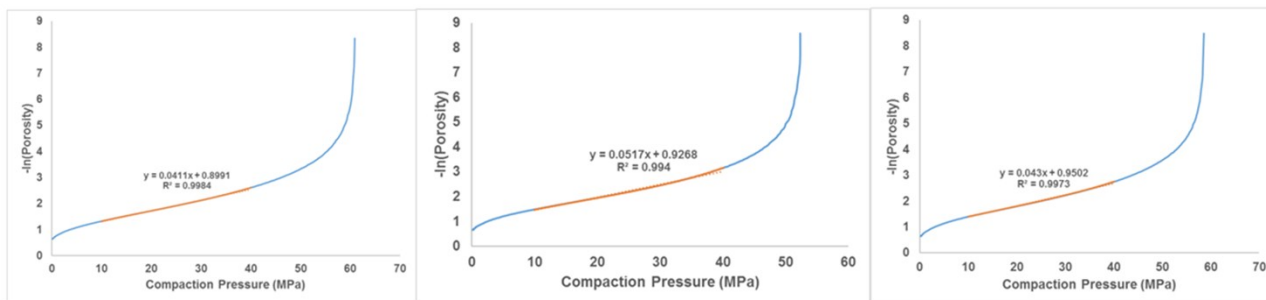


Figure S2b.)

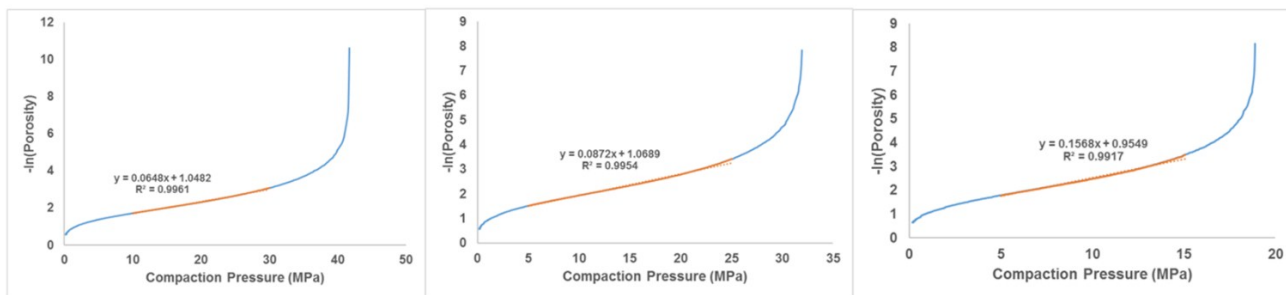


Figure S2c.)

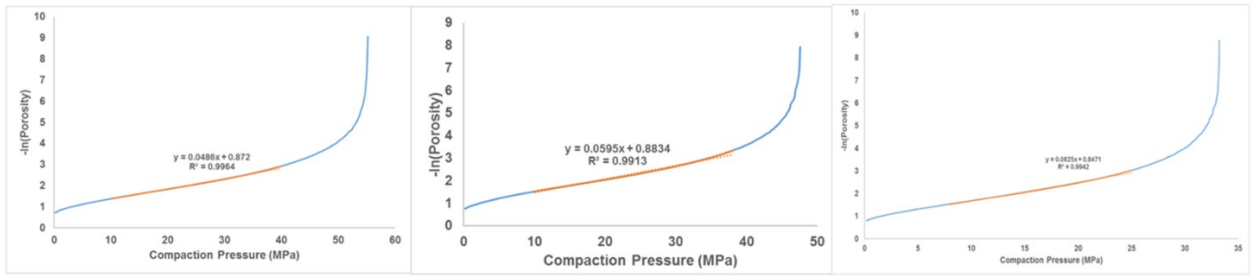


Figure S2d.)

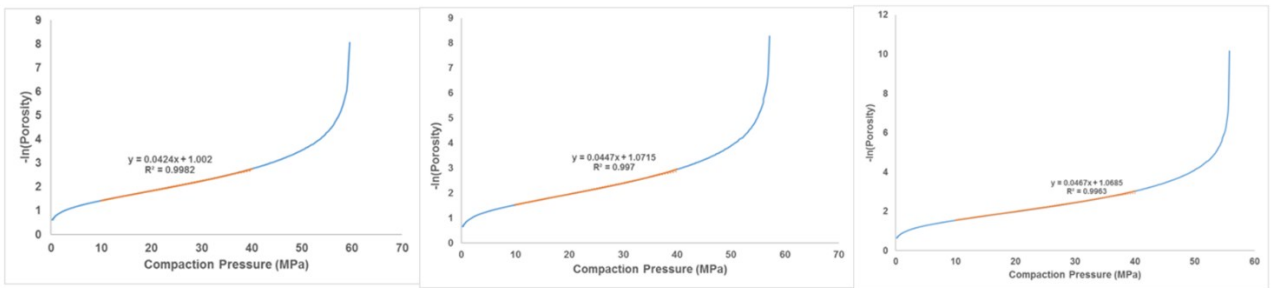


Figure S2e.)

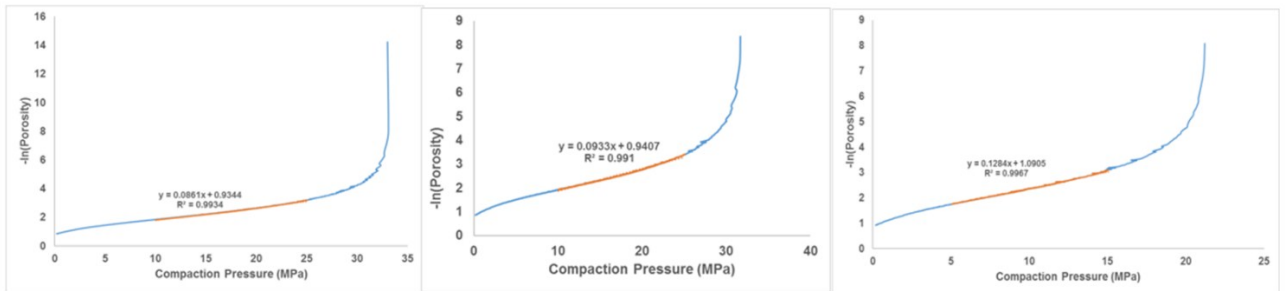


Figure S3. SEM Images for a.) 3-NBA, b.) 4-NBA, c.) Cl-NBA, d.) Br-NBA and e) Me-NBA
Figure S3a.)

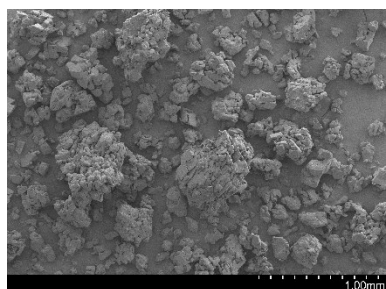


Figure S3b.)

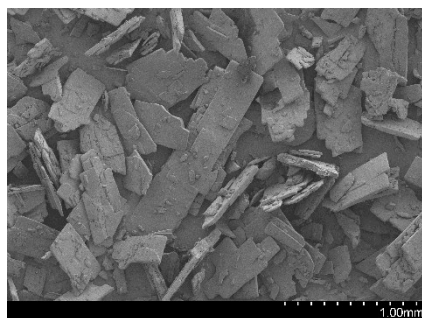


Figure S3c.)

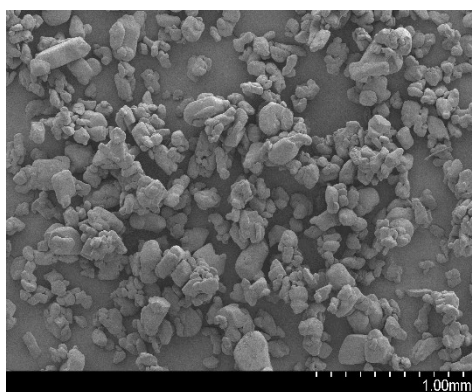


Figure S3d.)



Figure S3e.)

