New Drug-Drug and Drug-Nutraceutical Salts of Anti-emetic Drug Domperidone: Structural and Physicochemical Aspects of New Salts

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Table S1: The geometries of hydrogen bond interaction in DOM salts.

DOM-NCA-I				
D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1W^{i}	0.85 (3)	1.98 (3)	2.825 (3)	173 (2)
N3—H3N···O3	0.94 (3)	1.92 (3)	2.831 (4)	165 (2)
N3—H3N···O4	0.94 (3)	2.47 (3)	3.172 (6)	132.2 (19)
N5—H5N···O2^{ii}	0.92 (4)	1.87 (4)	2.790 (3)	172 (3)
O1W—H1W···O2W	0.88 (1)	1.86 (2)	2.686 (4)	156 (5)
O2W—H3W···O2^{iii}	0.86 (1)	1.92 (1)	2.772 (4)	172 (6)
O2W—H4W···O4	0.86 (1)	1.73 (3)	2.532 (7)	156 (7)
Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+4, −*y*+1, −*z*+2; (iii) *x*−1, *y*, *z*.				
DOM-NCA-II				
N1—H1N···N6^{i}	0.86	1.98	2.830 (3)	170
N3—H3N···O3	0.98 (3)	1.76 (3)	2.735 (5)	172 (2)
N5—H5N···O1W^{ii}	0.86	2.05	2.821 (3)	149
O1W—H2W···O4^{iii}	0.86 (1)	2.46 (5)	3.085 (5)	131 (6)
O1W—H1W···O2	0.86 (1)	1.96 (1)	2.804 (3)	169 (5)
O2W—H3W···O3W	0.87 (1)	2.01 (4)	2.792 (8)	149 (7)
O2W—H4W···O2	0.88 (1)	2.10 (4)	2.851 (4)	144 (7)
Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*, *y*+1/2, −*z*+1/2.				
DOM-MAA-I				
O2W—H4W···O5^{i}	0.86 (1)	2.06 (2)	2.902 (4)	166 (5)
N1—H1N···O2W^{ii}	0.86 (2)	2.02 (2)	2.857 (3)	165 (3)
N3—H3N···O3	0.86 (3)	2.63 (2)	3.226 (3)	127 (2)
N3—H3N···O4	0.86 (3)	1.90 (3)	2.754 (2)	173 (3)
N5—H5N···O2^{iii}	0.92 (2)	1.88 (2)	2.799 (2)	171 (4)
O5—H5O···O4	0.87 (1)	1.98 (9)	2.589 (3)	127 (9)
O5—H5O···O3W	0.87 (1)	2.45 (10)	2.928 (17)	116 (8)
O1W—H1W···O3	0.86 (1)	1.92 (2)	2.749 (4)	164 (6)
O1W—H2W···O2^{iv}	0.85 (1)	2.01 (2)	2.846 (3)	167 (6)
O2W—H3W···O1W	0.86 (1)	1.93 (2)	2.763 (4)	163 (6)
Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*; (iv) *x*+1, *y*, *z*.				
DOM-MAA-II				
N1—H1N···O1W^{i}	0.91 (2)	1.92 (2)	2.830 (3)	171 (2)
N5—H5N···O1^{ii}	0.90 (3)	2.07 (3)	2.961 (3)	174 (3)
O3—H3A···O2^{iii}	0.82	1.86	2.604 (4)	151
O1W—H2W···O1^{iv}	0.86 (1)	2.06 (2)	2.902 (3)	165 (7)
O2W—H3W···O4^{v}	0.87 (1)	1.96 (1)	2.826 (3)	173 (4)
N3—H3N···O4	0.84 (3)	2.41 (3)	3.069 (3)	136 (2)
N3—H3N···O5	0.84 (3)	2.00 (3)	2.820 (3)	164 (2)
O1W—H1W···O2W	0.86 (1)	1.96 (1)	2.817 (3)	173 (4)
O2W—H4W···O5	0.87 (1)	2.09 (2)	2.936 (3)	162 (4)
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) *x*−1, *y*, *z*; (v) −*x*+1/2, *y*−1/2, −*z*+1/2.				
DOM-MAA				
N1—H1···O1^{i}	0.88	1.98	2.823 (3)	160
N5—H5A···O2^{ii}	0.88	1.95	2.775 (4)	155
O5—H5O···O4^{iii}	0.84	2.28	2.927 (5)	134

N3—H3N···O3	0.91 (2)	1.71 (2)	2.618 (4)	179 (4)
N3—H3N···O4	0.91 (2)	2.55 (3)	3.126 (4)	122 (3)
O5—H5O···O4	0.84	2.18	2.665 (4)	116
Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+2; (iii) −*x*+2, −*y*+1, −*z*+2.				
DOM-SLA				
N1—H1N···O2W^{i}	0.87 (2)	1.97 (2)	2.828 (2)	168 (2)
N5—H5N···O2^{ii}	0.82 (2)	1.99 (3)	2.794 (2)	165 (3)
O1W—H2W···O3^{iii}	0.88 (2)	1.99 (2)	2.826 (3)	158 (4)
O2W—H4W···O5^{iv}	0.87 (2)	2.10 (3)	2.925 (4)	157 (5)
O5—H5O···O4	0.90 (2)	1.95 (5)	2.511 (4)	118 (4)
N3—H3N···O3	0.95 (2)	1.83 (2)	2.719 (2)	155.7 (18)
O1W—H1W···O2	0.86 (2)	1.94 (2)	2.791 (3)	166 (4)
O2W—H3W···O1W	0.89 (2)	1.86 (2)	2.734 (3)	167 (5)
O3W—H6W···O4	0.87 (2)	2.16 (3)	3.004 (6)	163 (7)
Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*, −*y*+2, −*z*+2; (iii) *x*−1, *y*, *z*; (iv) *x*−1, *y*+1, *z*.				
DOM-OTA				
N1—H1N···O5^{i}	0.82 (3)	2.03 (3)	2.821 (4)	162 (3)
N5—H5N···O6^{ii}	0.90 (4)	1.94 (4)	2.832 (3)	175 (4)
N6—H6N···O4^{iii}	0.90 (3)	1.97 (3)	2.843 (3)	166 (3)
N7—H7N···O2^{iv}	0.77 (2)	2.05 (3)	2.811 (3)	177 (3)
N3—H3N···O3	0.94 (3)	1.72 (3)	2.658 (3)	174 (2)
Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) *x*+1, *y*−1, *z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*−1, *y*+1, *z*.				
DOM-ASP				
N5—H5N···O4^{i}	0.95 (3)	1.92 (3)	2.798 (2)	153 (2)
N5—H5N···O5^{i}	0.95 (3)	2.65 (3)	3.290 (2)	125.5 (18)
N1—H1N···O3^{ii}	0.82 (2)	2.17 (2)	2.9510 (19)	159.9 (19)
N3—H3N···O3	0.88 (2)	1.81 (2)	2.6842 (19)	171.7 (18)
N3—H3N···O4	0.88 (2)	2.646 (19)	3.288 (2)	130.5 (15)
Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) *x*, *y*−1, *z*.				

Table S2: The percentage weight loss comparison in DOM salts with theoretical weight loss.

Compound name	Theoretical weight loss for H_2O molecules	Observed weight loss between 30-150 °C	Decomposition temperature (°C)
DOM	--	0.51%	250
DOM-NCA II	7.58%	6.74%	160
DOM-MAA II	5.86%	6.1%	200
DOM-MAA	--	0.50%	200
DOM-SLA	7.38%	7.25%	200
DOM-OTA	--	0.58%	275
DOM-ASP	--	0.18%	190

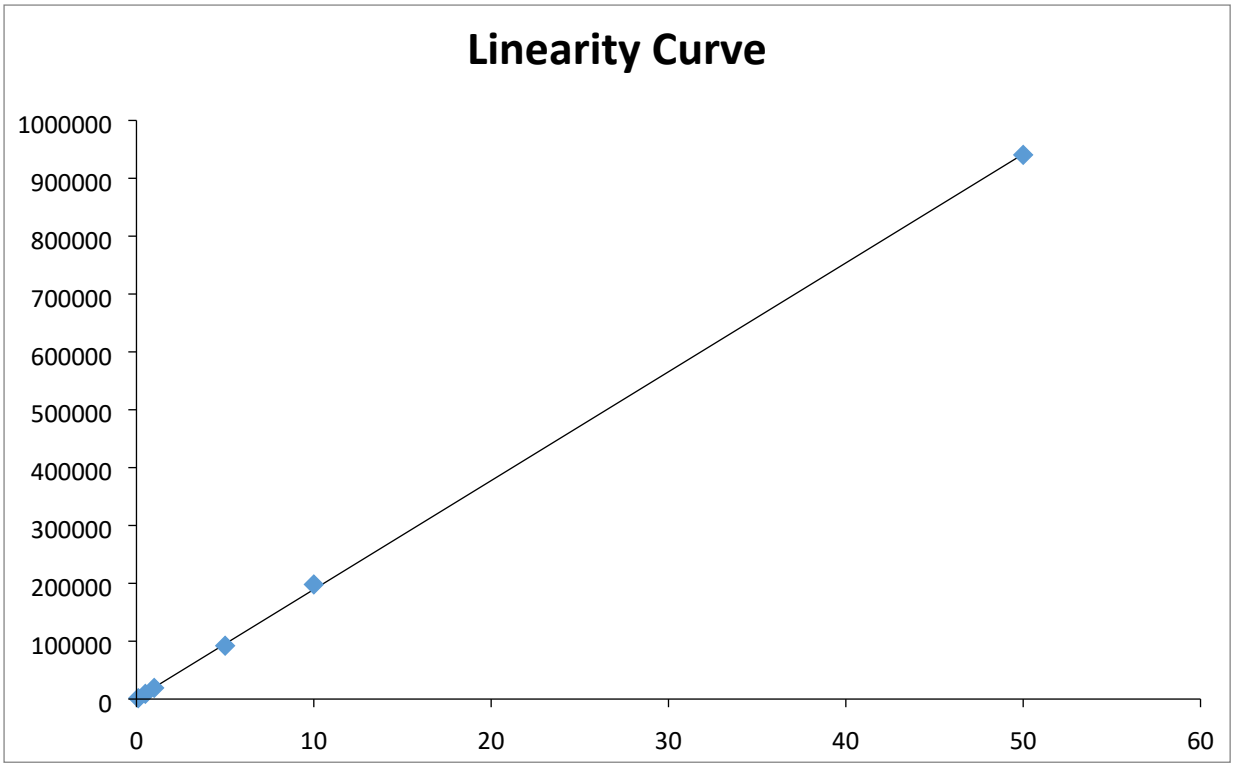

Figure S1: Standard Linearity curve of DOM.

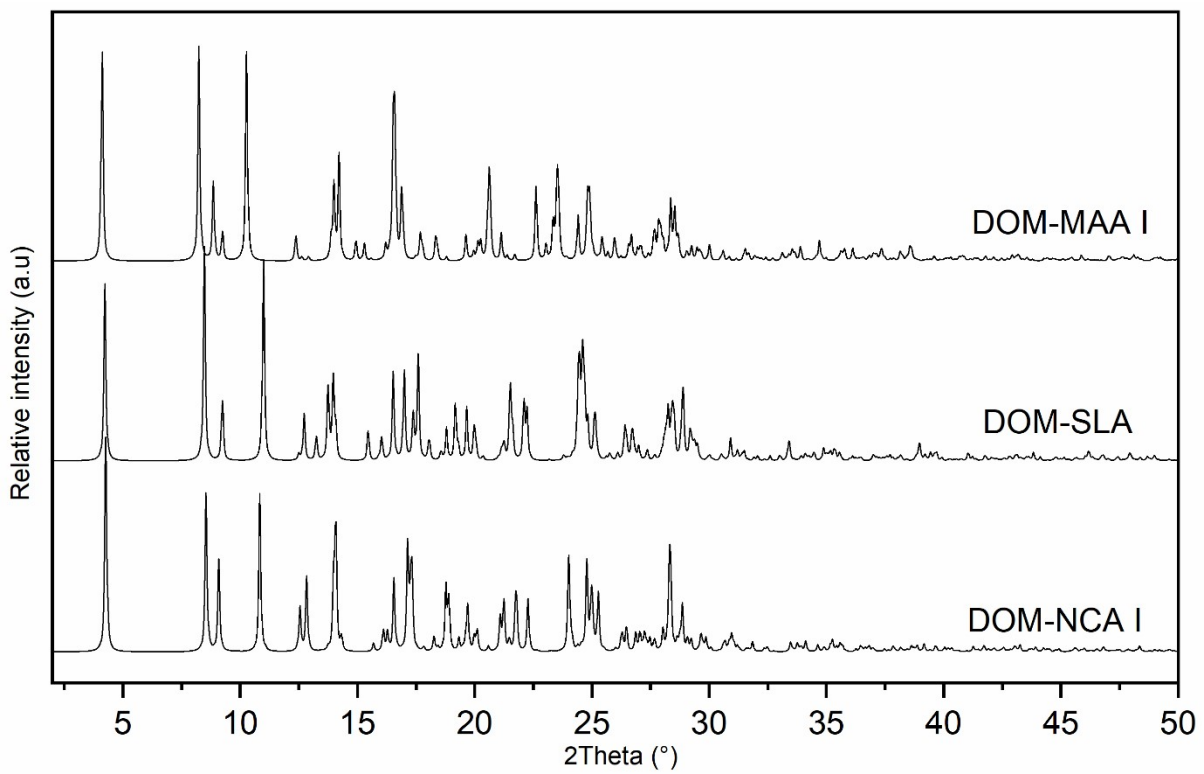

Figure S2: PXRD overlay of DOM-NCA I, DOM-SLA, and DOM-MAA I salt shows the PXRD patterns' similarity.

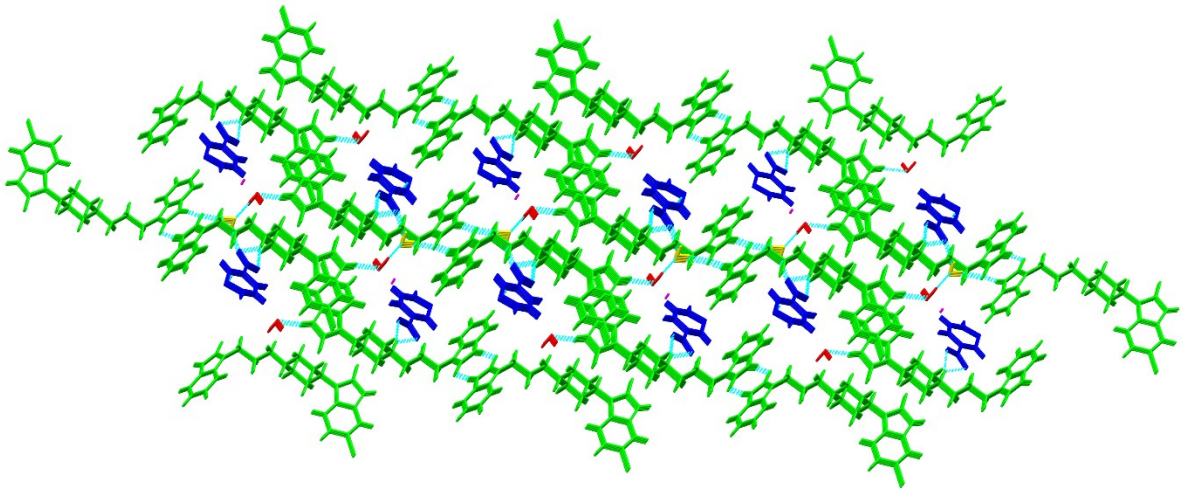

Figure S3: 3D Packing of DOM-NCA I (Green color: DOM, Blue color: NCA)

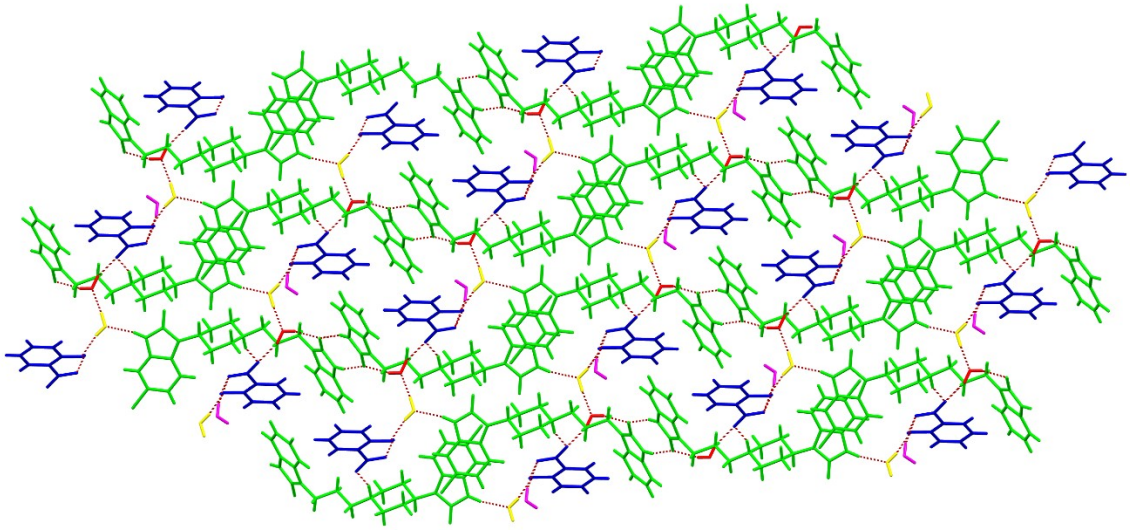

Figure S4: 3D Packing of DOM-SLA (Green color: DOM, Blue color: SLA).

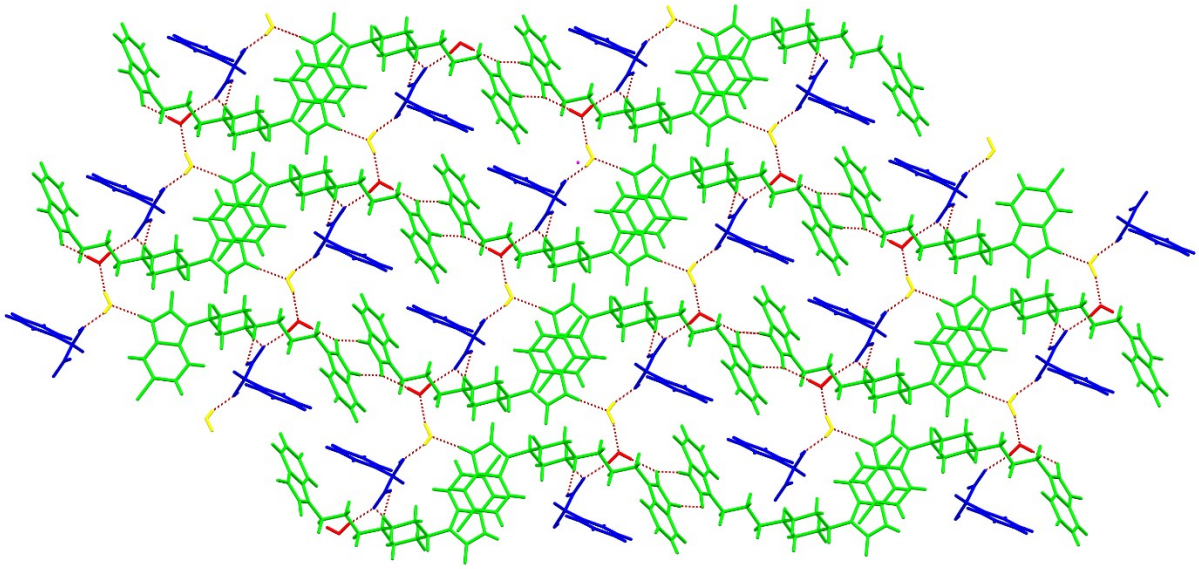

Figure S5: 3D Packing of DOM-MAA I (Green color: DOM, Blue color: MAA).

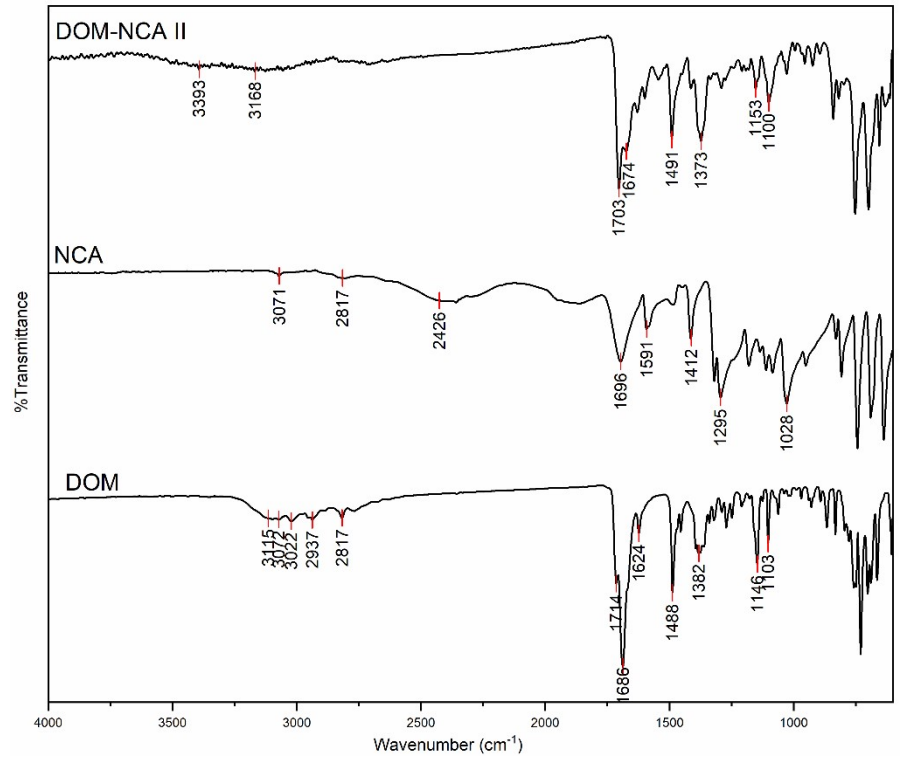

Figure S6: FT-IR comparison plot of DOM-NCA II with DOM and NCA.

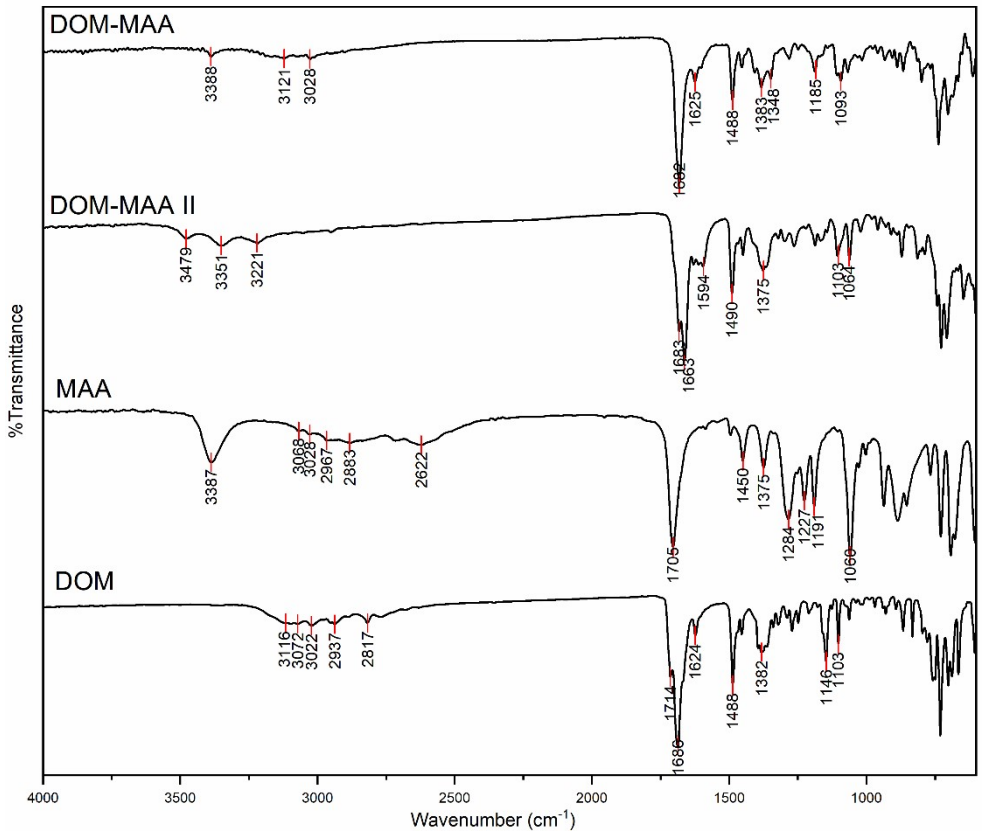

Figure S7: FT-IR comparison plot of DOM-MAA II and DOM-MAA with DOM and MAA.

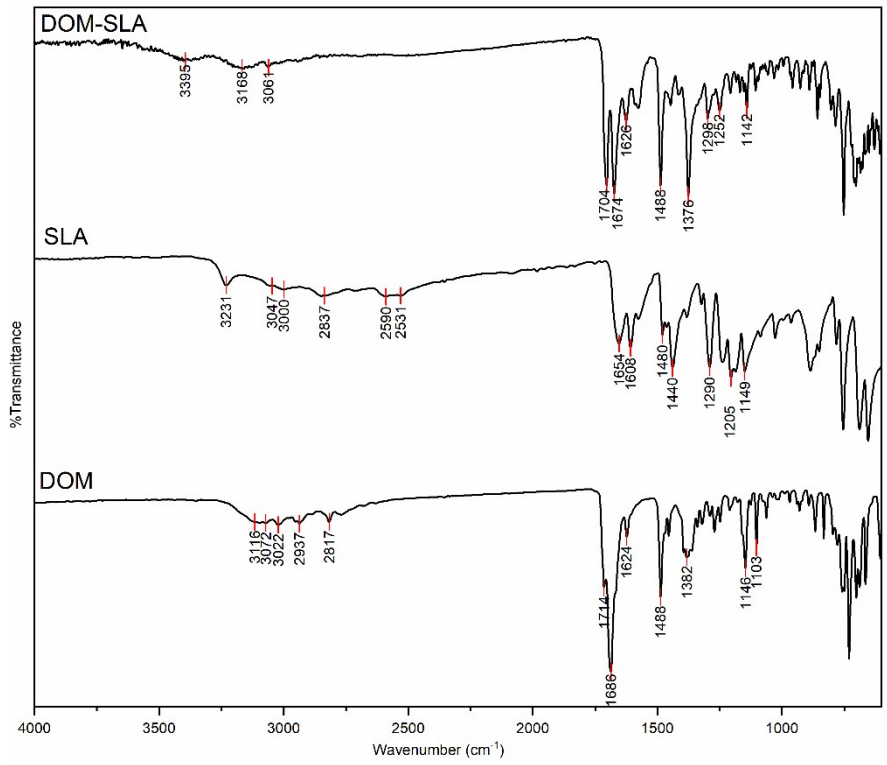

Figure S8: FT-IR comparison plot of DOM-SLA with DOM and SLA.

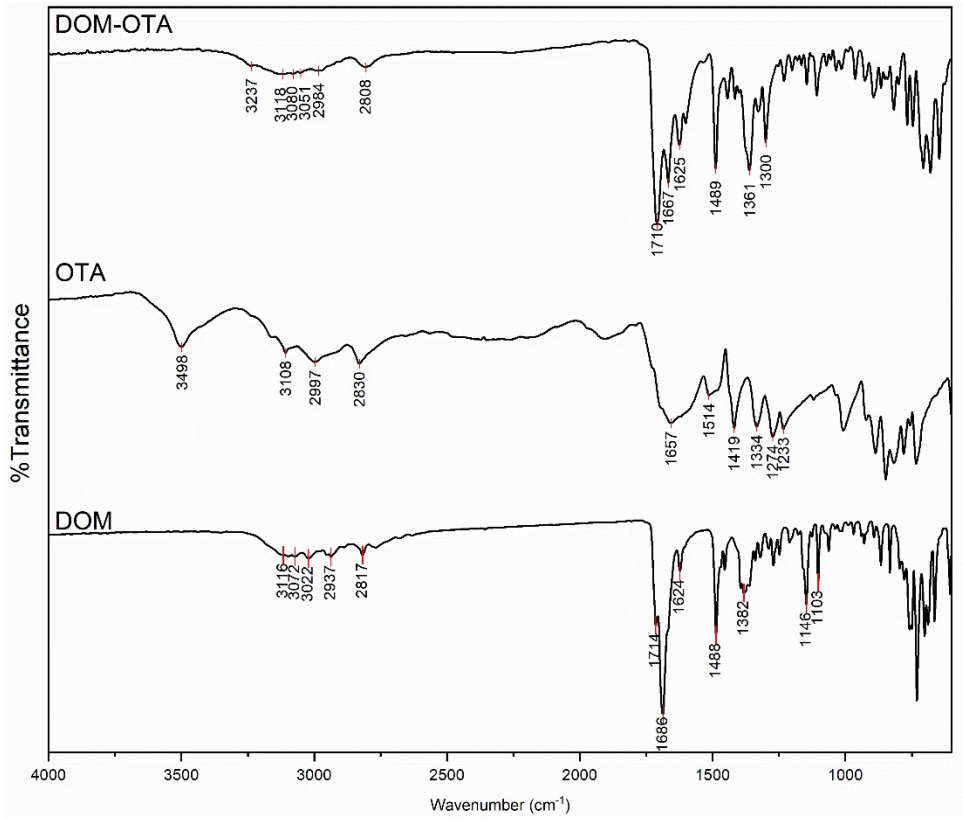

Figure S9: FT-IR comparison plot of DOM-OTA with DOM and OTA.

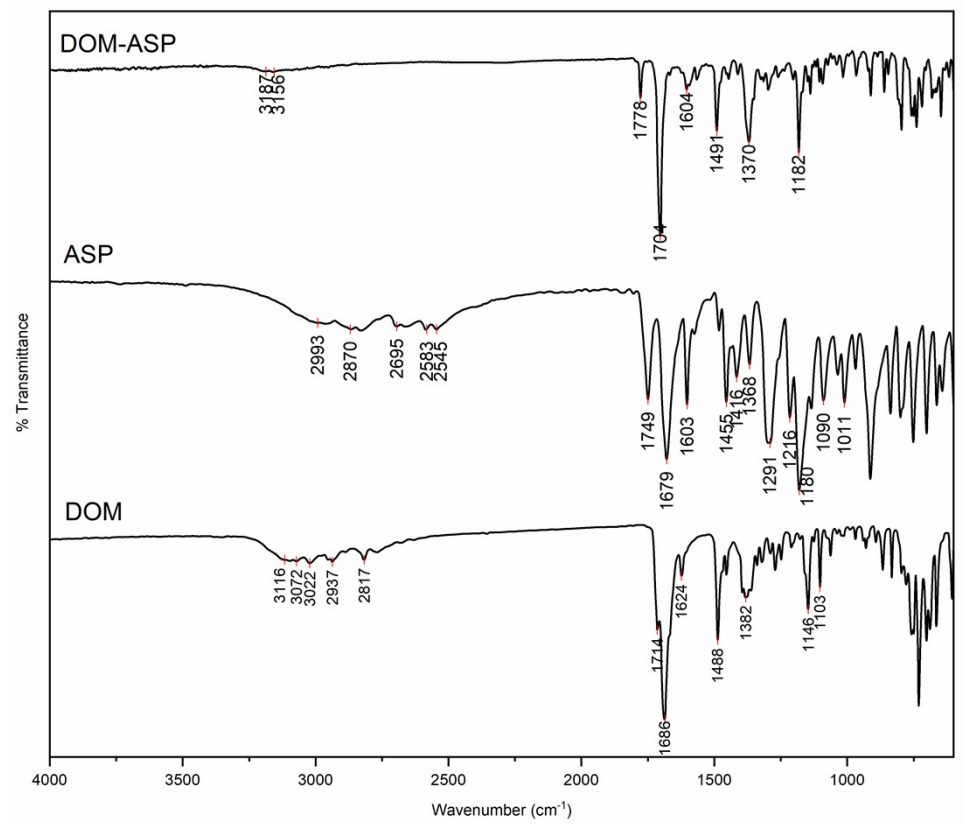

Figure S10: FT-IR comparison plot of DOM-ASP with DOM and ASP.

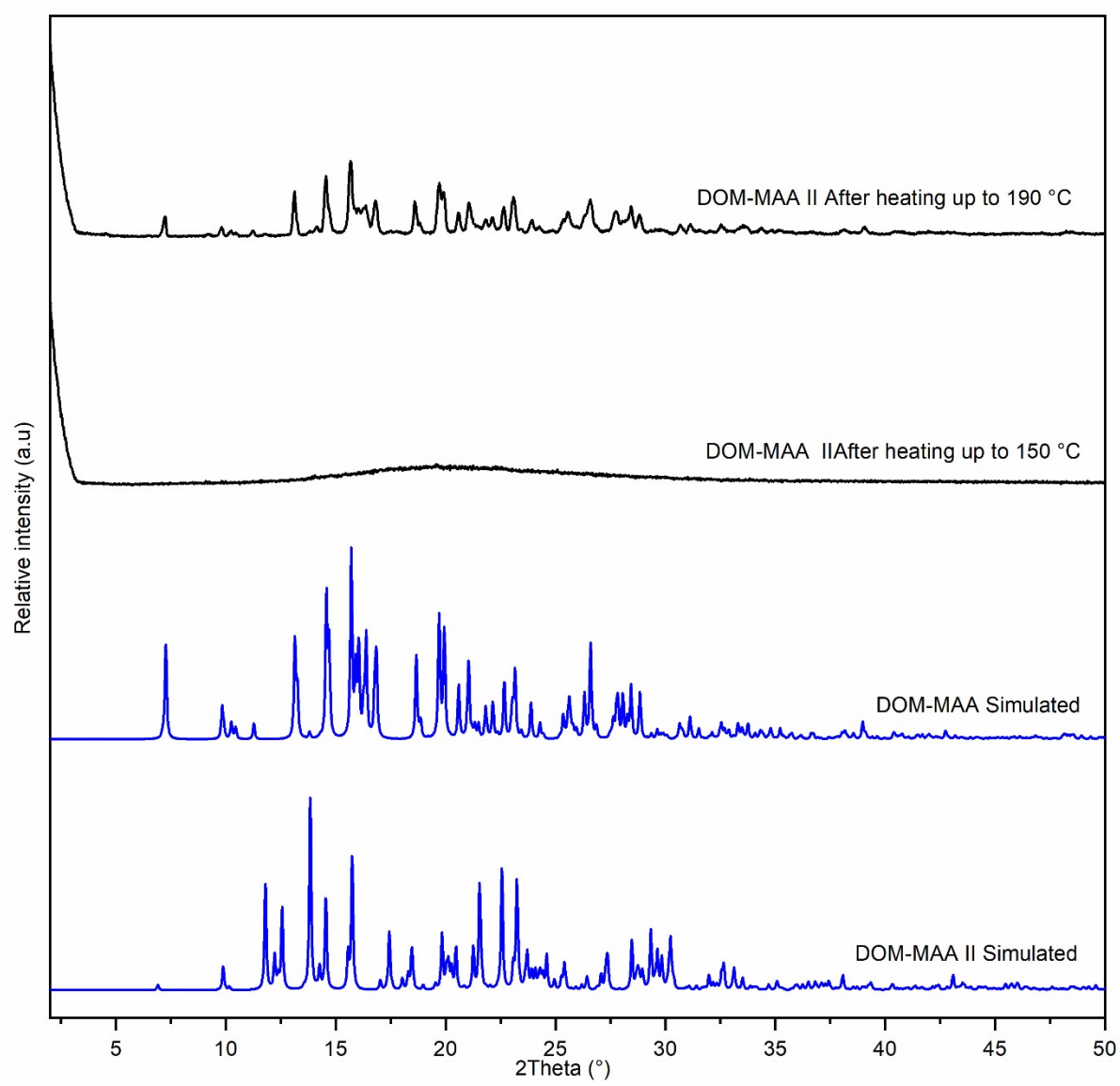

Figure S11: PXRD overlay of DOM-MAA II after heating with simulated patterns.

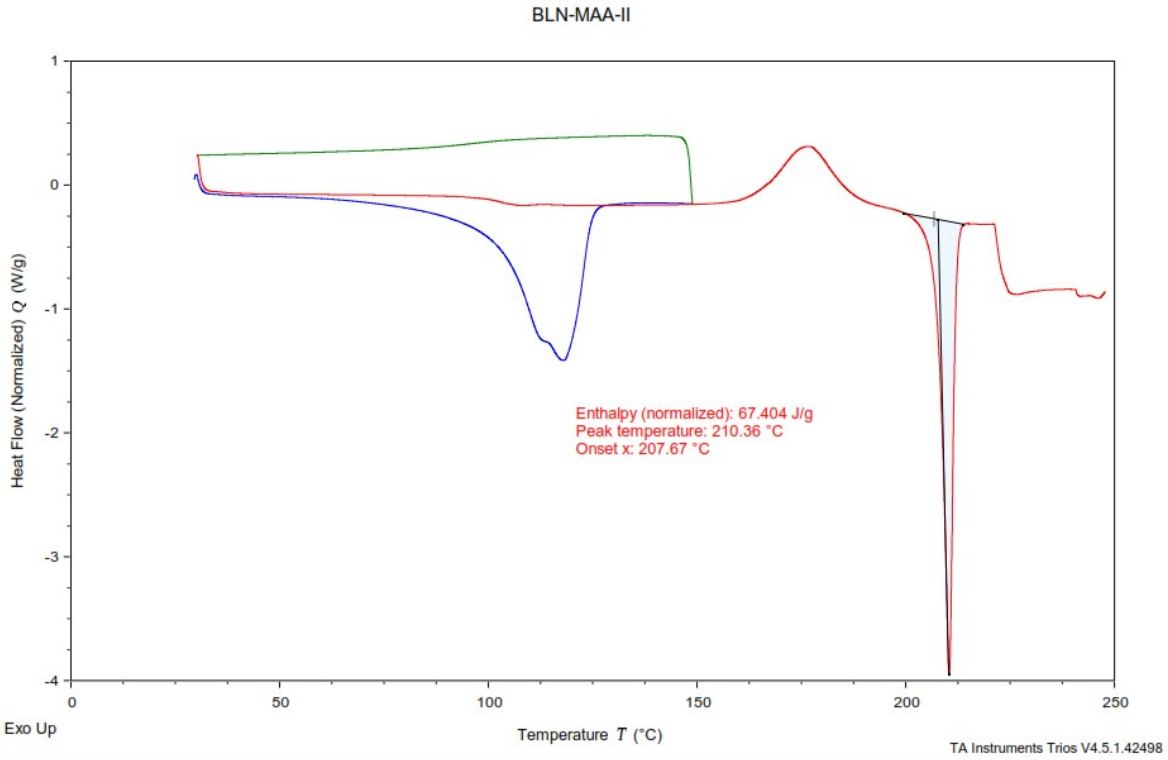

Figure S12: DSC thermogram of DOM-MAA II heat-cool experiment.

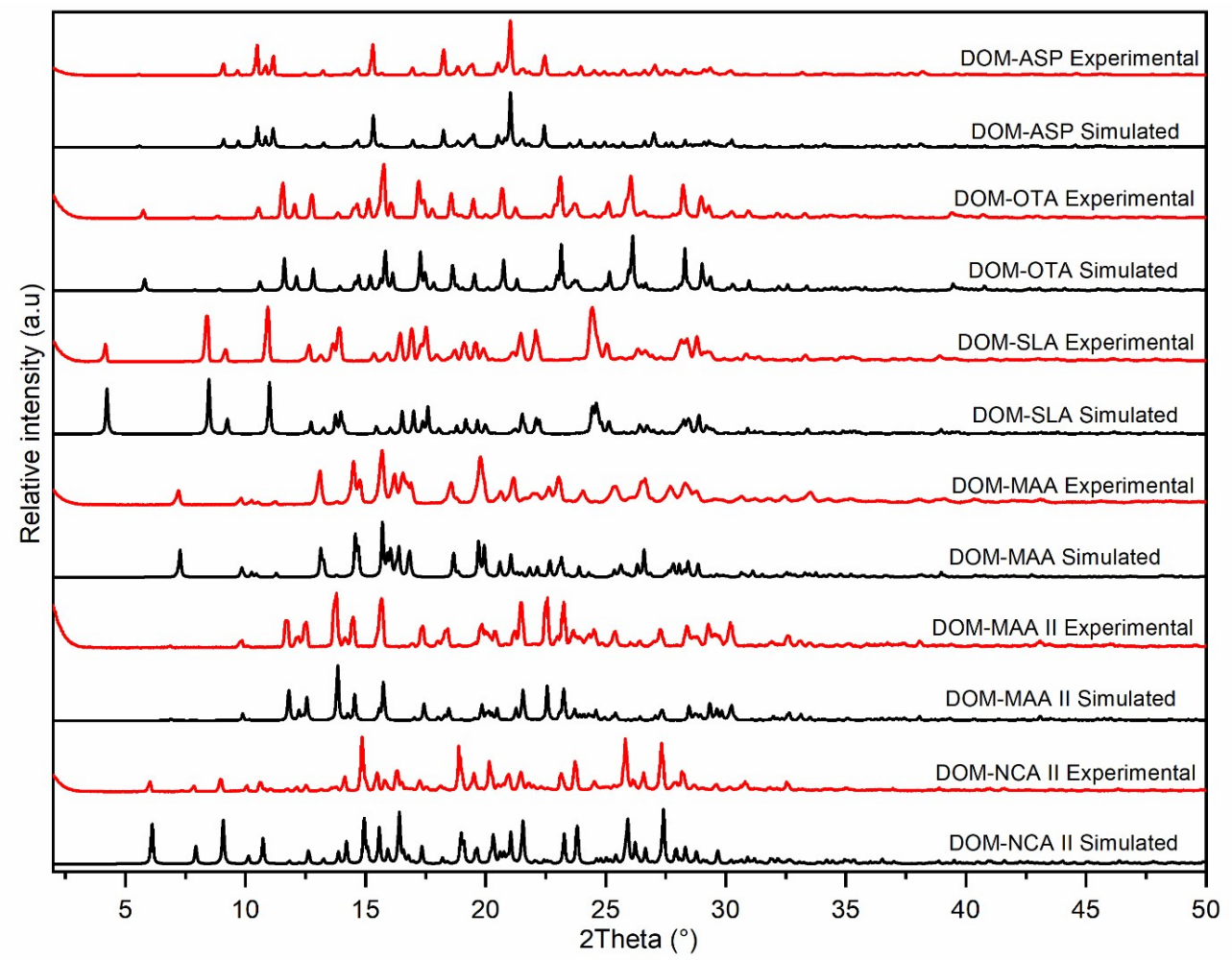

Figure S13: Comparison of PXRD of simulated and experimental patterns.

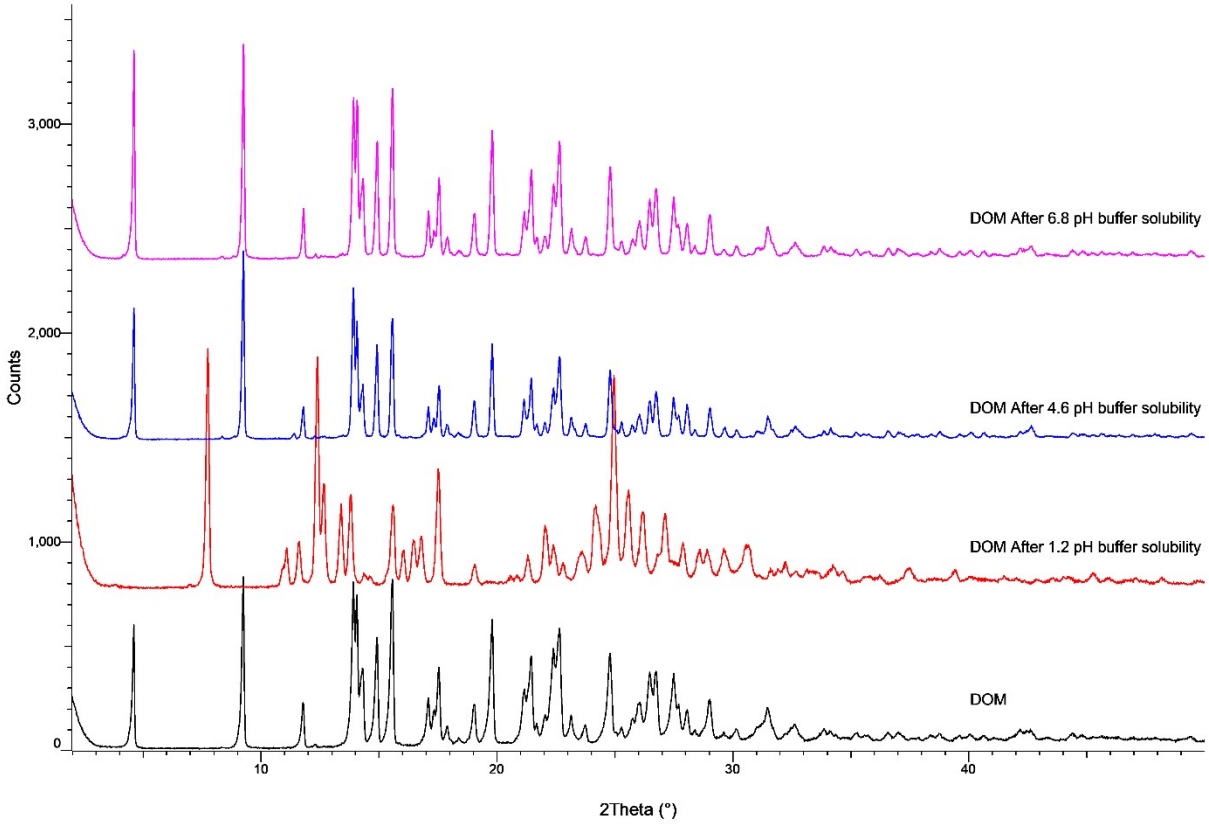

Figure S14: PXRD overlay of DOM after equilibrium solubility study.

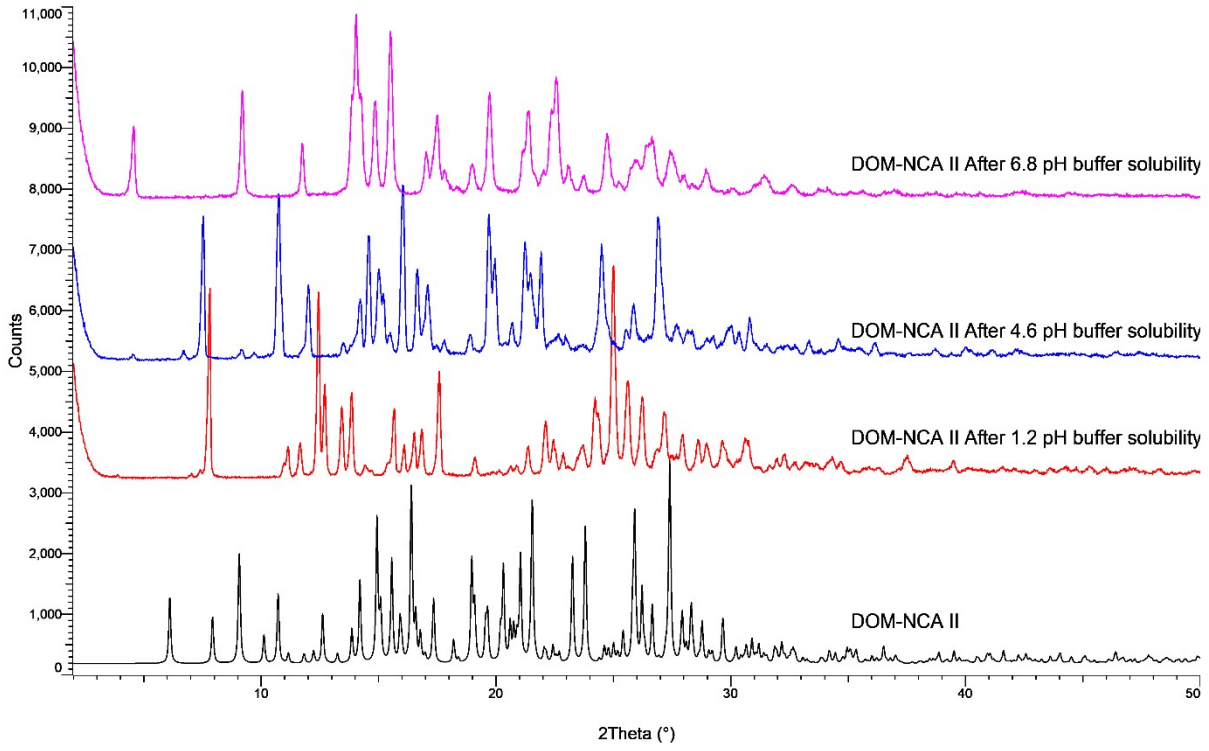

Figure S15: PXRD overlay of DOM-NCA II salt after equilibrium solubility study.

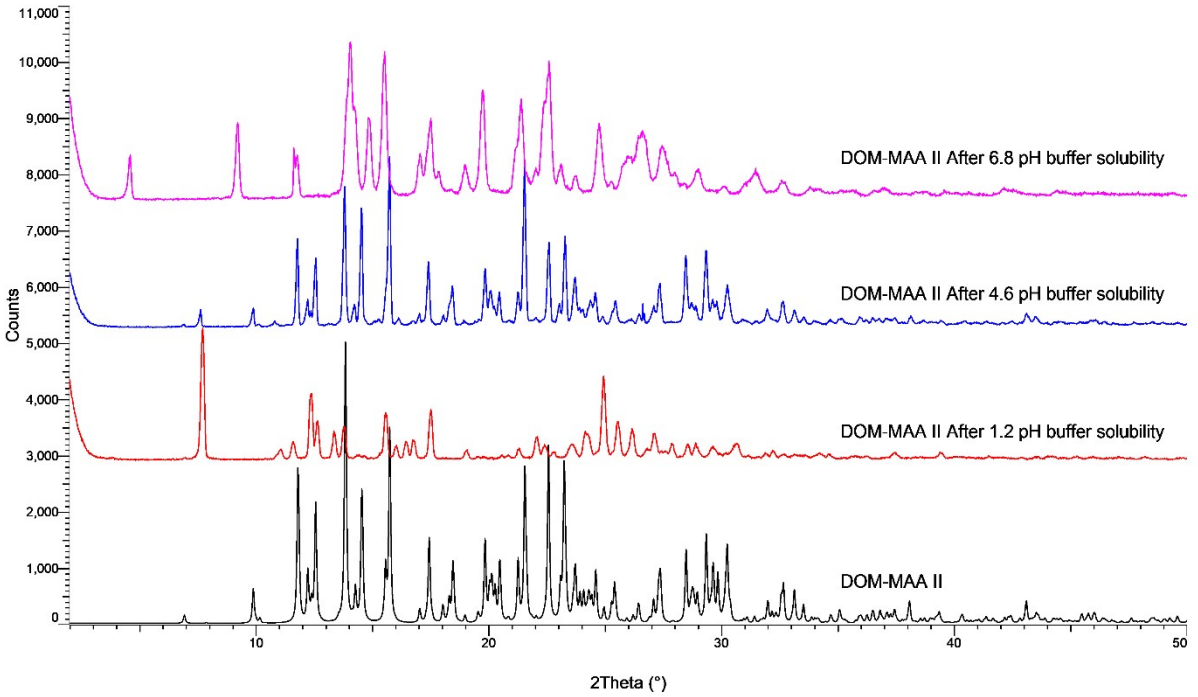

Figure S16: PXRD overlay of DOM-MAA II salt after equilibrium solubility study.

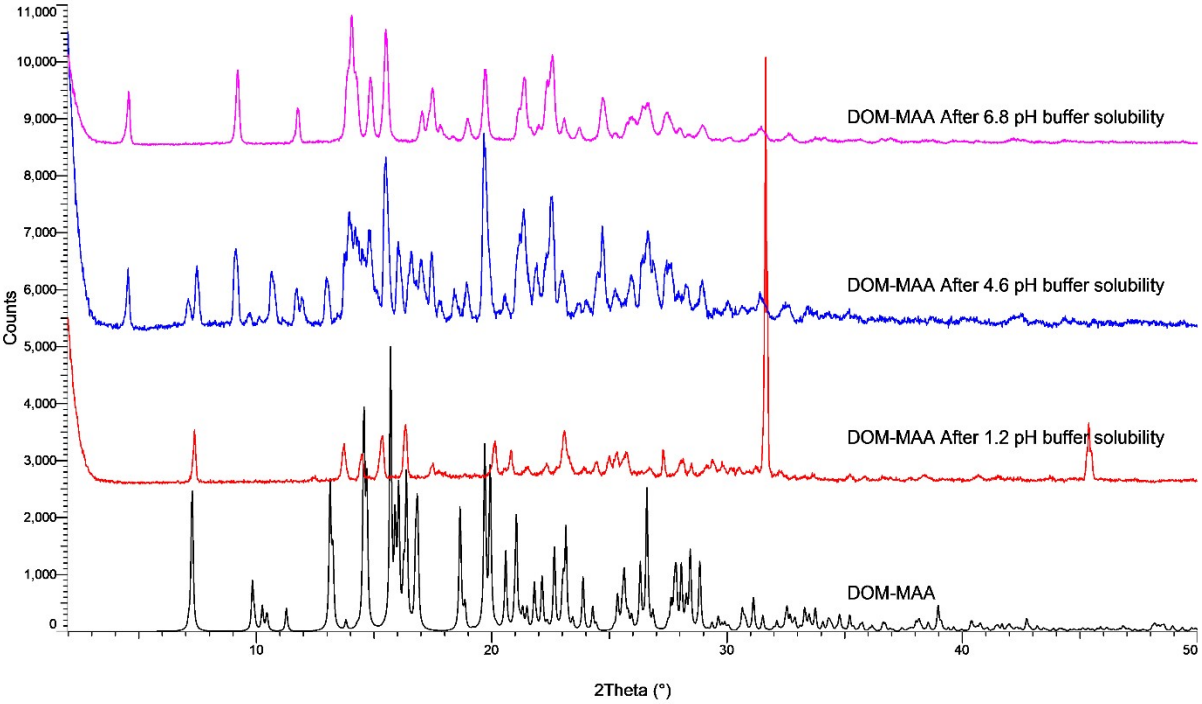

Figure S17: PXRD overlay of DOM-MAA salt after equilibrium solubility study.

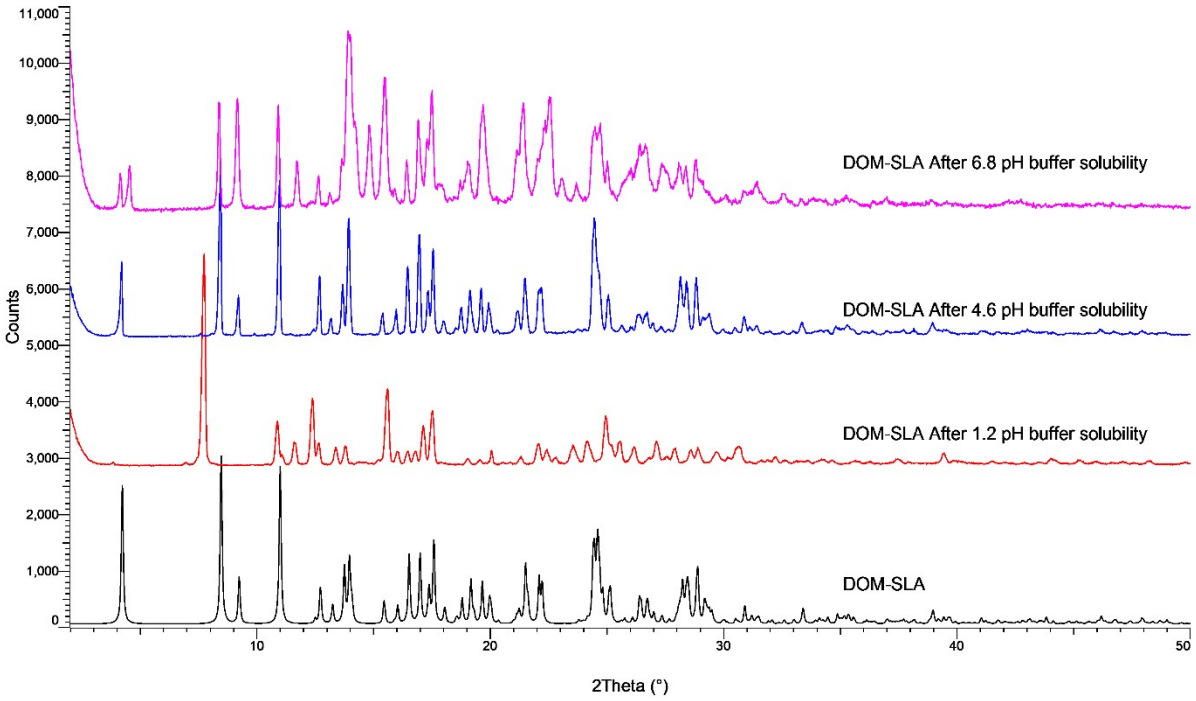

Figure S18: PXRD overlay of DOM-SLA salt after equilibrium solubility study.

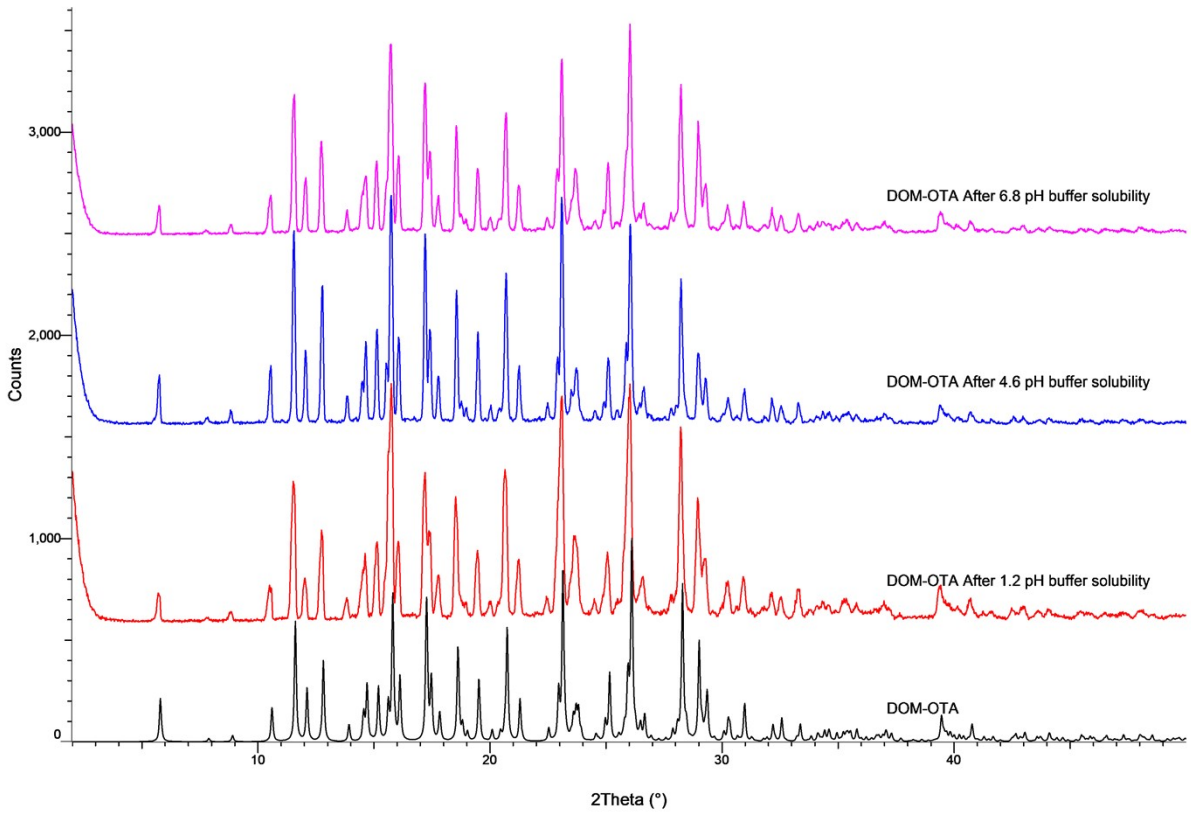

Figure S19: PXRD overlay of DOM-OTA salt after equilibrium solubility study.

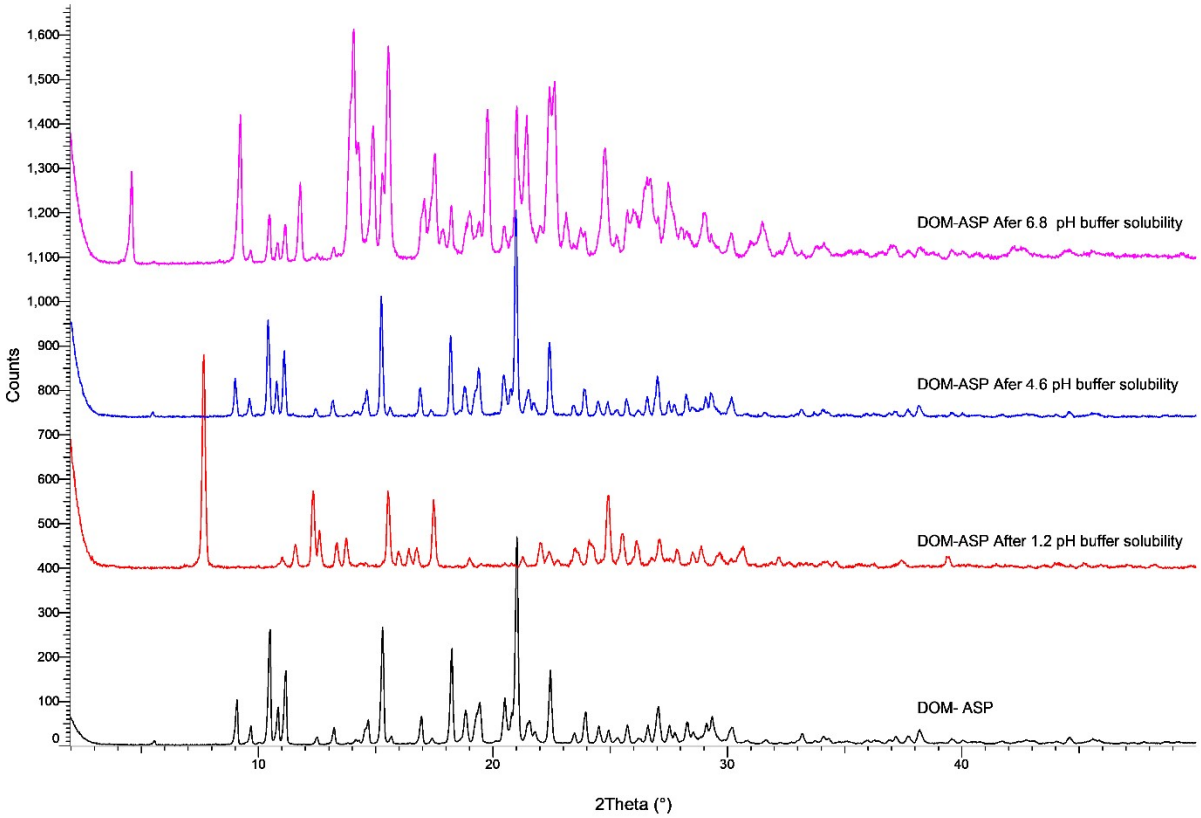

Figure S20: PXRD overlay of DOM-ASP salt after equilibrium solubility study.