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Role of halogen-involved intermolecular interactions and existence of isostructurality in the crystal packing of —CF3 and halogen (Cl or Br or I) substituted benzamides

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Table S1

Table S2 The possible intermolecular interactions and interaction energies (kJ/mol) for the different molecular pair of the benzamides obtained from the PIXEL method.

Motifs	Symmetry code	Centroid–centroid distance (Å)	E_{Coul}	E_{Pol}	E_{Disp}	E_{Rep}	E_{Tot}	Involved interactions	Geometry (Å/deg)
			kJ/mol						
PC22									
I	x-1,y,z	4.757	-33.4	-16.9	-46.5	51.5	-45.3	N1–H1···O1 F3···π(C6)	1.90, 158 3.103(2), 155
II	-x,-y,1-z	6.576	-9.1	-4.7	-40.9	24.9	-29.7	π(C3)···π(C10)	3.463(2)
III	x-1,-y+1/2,z-1/2	8.530	-12.3	-4.9	-22.3	16.5	-23.0	C4–H4···O1 C13–H13···π(C4–C5) C4–H4···F2 C3–H3···F2	2.43, 167 2.75, 157 2.73, 117 2.70, 119
IV	-x-1,-y,-z+1	8.279	-6.2	-4.1	-29.3	21.5	-18.1	Cl1···Cl1 C2–H2···Cl1	3.356(1), 151, 151 2.88, 133
V	x,-y+1/2,z-1/2	7.715	-0.8	-2.5	-19.5	9.9	-13.0	C5–H5···π(C13)	2.71, 136
VI	-x,y-1/2,-z+1.5	10.961	-1.9	-0.6	-6.1	2.3	-6.2	C10–H10···F1 C10–H10···F2	2.76, 116 2.81, 157
VII	-x+1,y+1/2,-z+1.5	11.433	-2.4	-0.4	-4.0	1.0	-5.8	C11–H11···F1 C11–H11···F3	2.87, 137 2.90, 146
VIII	-x+1,-y,-z+2	12.838	-0.5	-1.5	-9.4	5.8	-5.6	H11···H12	2.38
PC23									
I	x-1,y,z	4.808	-27.9	-12.1	-43.7	38.7	-45.0	N1–H1···O1 F1A···F2A	2.00, 147 3.000(6), 116, 139

II	-x,1-y,-z	6.708	-9.0	-3.3	-39.2	20.8	-30.8	Cl1···π(C2) Cl1···π(C7)	3.633(2), 82 3.582(2), 121
III	1-x,-y,-z	7.606	-13.9	-7.2	-26.2	18.5	-28.8	H6···H12 H13···H13 C12–H12···O1	2.17 2.27 2.62, 128
IV	-x,-y,-z	6.168	-4.3	-1.8	-37.6	17.4	-26.3	π(C6)···π(C12)	3.631(3)
V	-1-x,1-y,-z	8.451	-7.5	-6.2	-30.2	25.8	-18.0	Cl1···Cl1 C2–H2···Cl1	3.336(1), 148, 148 2.77, 146
VI	-x+1/2,y+1/2,-z+1/2	10.937	-5.1	-1.0	-6.5	3.0	-9.6	C4–H4···F2A	2.62, 118
VII	-x-1/2,y-1/2,-z+1/2	11.268	-2.0	-0.7	-5.5	2.9	-5.4	C4–H4···F1A C3–H3···F1A	2.61, 123 2.68, 121
VIII	x-1/2,-y+1/2,z-1/2	13.993	-1.9	-0.6	-5.4	3.0	-4.9	C10–H10···F3A C11–H11···F3A	2.61, 123 2.69, 119
PC24									
I	x-1,y,z	4.819	-51.9	-19.7	-50.1	91.0	-30.7	N1–H1···O1 F1···F2 O1···π(C2)	1.99, 148 2.881(2), 160, 116 3.178(2)
II	-x+2,-y+1,-z+1	6.174	-25.5	-8.9	-47.0	54.9	-26.5	Cl1···C7 π(C2)···π(C10)	3.403(1), 120 3.555(2)
III	-x+3,-y,-z+1	9.214	-10.6	-6.9	-21.6	18.8	-20.3	C12–H12···O1 H13···H13 H6···H12	2.57, 135 2.25 2.35
IV	-x+1,-y+1,-z+1	7.618	-9.0	-6.3	-26.1	27.4	-14.0	Cl1···Cl1 C2–H2···Cl1	3.258(1), 150, 150 2.94, 152
V	-x+2,-y,-z	10.157	-3.9	-2.5	-11.1	8.2	-9.2	H5···H5 C6–H6···F3	2.22 2.91, 120

								C5–H5···F3	2.81, 124
VI	-x+2,-y,-z+1	7.277	-19.4	-8.5	-41.3	60.3	-8.9	π(C13)···π(C13)	3.486(2)
VII	-x+1,-y+1,-z	11.321	-3.6	-0.4	-5.6	3.3	-6.3	F2···F2	3.087(2), 109, 109
VIII	x,y,z-1	14.028	-3.4	-0.9	-6.6	5.0	-5.9	C10–H10···F1 C11–H11···F1	2.53, 131 2.93, 114
IX	x-1,y,z-1	14.560	-2.8	-0.7	-5.0	3.1	-5.4	C11–H11···F2 C11–H11···F3	2.75, 146 2.74, 139
X	2-x,1-y,-z	10.783	0.2	-0.3	-3.9	3.1	-0.9	F1···F1	3.062(2), 121, 121
PC32									
I	-x+1.5,y,z+1/2	4.424	-61.1	-28.0	-58.8	105.2	-42.7	N1–H1···O1 C9–H9···O1 N1–H1···π(C13) C2–H2···π(C12)	1.93, 149 2.48, 128 2.65, 126 2.75, 162
II	-x+1/2,y,z-1/2	8.744	-6.4	-4.4	-15.5	14.2	-12.1	C3–H3···π(C1) C3–H3···O1 C4–H4···F3	2.89, 156 2.80, 136 2.72, 120
III	-x+2.5,y,z-1/2	9.127	-5.4	-2.8	-13.4	12.2	-9.3	C10–H10···Cl1 C10–H10···π(C11) C10–H10···π(C12)	2.96, 137 3.08, 116 3.09, 140
IV	x-1/2,-y+1,z	10.404	-5.5	-4.1	-13.7	14.4	-8.9	C11–H11···Cl1	2.64, 167
V	-x+1,-y,z-1/2	11.082	-4.0	-1.1	-5.6	4.1	-6.6	C4–H4···F1 C5–H5···F3	2.57, 132 2.94, 138
VI	x-1/2,-y,z	10.245	0.2	-1.2	-5.8	5.5	-1.3	C5–H5···F1	2.58, 118
PC33									
I	x,-y+1/2,z+1/2	4.696	-61.8	-23.2	-45.5	88.9	-41.6	N1–H1···O1 C2–H2···O1 C9–H9···O1 F1···π(C5)	1.89, 162 2.54, 124 2.61, 122 3.108(2), 173

II	x,y-1,z	5.335	-15.1	-8.1	-39.2	43.9	-18.5	C4–H4···F2 π(C9)···π(C12) π(C3)···π(C6)	2.62, 139 3.411(2) 3.482(2)
III	-x+2,-y+1,-z	13.817	-6.1	-2.2	-14.9	11.4	-11.7	C11–H11···Cl1	3.09, 122
IV	x,-y+1.5,z-1/2	7.155	-5.7	-4.1	-15.7	14.8	-10.7	C12–H12···Cl1	2.74, 161
V	x,-y-1/2,z-1/2	7.060	-6.1	-3.4	-14.2	13.2	-10.5	C3–H3···F1 C3–H3···π(C5)	2.57, 131 2.84, 139
VI	-x+1,-y,-z	12.358	-6.3	-1.0	-8.8	8.2	-8.0	F2···F3 C4–H4···F2	3.053(2), 105, 126 2.77, 149
VII	-x+2,y+1/2,-z-1/2	15.199	-2.5	-1.4	-9.3	8.4	-4.7	Cl1···Cl1 C11–H11···Cl1	3.613(1), 102, 154 3.17, 137
PC34									
I	x-1,y,z	5.156	-37.4	-13.6	-47.5	49.9	-48.6	N1–H1···O1 C9–H9···O1 Cl1···π(C10)	2.02, 156 2.69, 119 3.384(3), 83
II	-x+2,-y+1,-z	4.973	-16.2	-7.8	-46.5	34.7	-35.8	C6–H6···π(C8-C9) C5–H5···π(C10)	2.69, 129 2.87, 144
III	-x+1,-y,-z	8.041	-16.8	-7.1	-39.2	27.7	-35.5	C2–H2···Cl1 N1···Cl1	2.80, 155 3.499(3), 99
IV	-x+1,-y+1,-z	5.557	-9.0	-5.9	-39.5	27.7	-26.7	C10–H10···F2 C9–H9···π(C6)	2.63, 160 2.76, 160
V	-x+1,-y+1,-z+1	9.231	-6.1	-2.6	-16.2	8.0	-16.8	H3···H3 C3–H3···F1	2.3 2.76, 131
VI	-x+2,-y,-z	9.072	-6.3	-5.2	-24.3	19.3	-16.5	C13–H13···Cl1 O1···Cl1	2.75, 173 3.366(3), 145
VII	-x+2,-y+1,-z+1	8.658	0.6	-0.4	-8.8	1.6	-7.1	F1···π(C2)	3.482(4), 157
VIII	x+1,y+1,z+1	14.561	-2.0	-0.4	-4.9	1.7	-5.6	C11–H11···F2	2.66, 130

IX	x,y+1,z+1	14.605	-0.3	-0.7	-7.1	4.0	-4.1	C11–H11···F3	2.65, 148
PC42									
a…a									
I	-x+1,-y,-z+1	7.018	-8.6	-2.1	-16.3	7.6	-19.5	C10–H10···F3	2.42, 161
II	x,-y+1/2,z+1/2	9.616	-5.4	-2.2	-14.8	8.1	-14.4	C5–H5···π(C12) F2···π(C13)	2.73, 172 3.375(3), 147
III	-x+1,-y+1,-z+1	9.949	1.6	-2.0	-16.7	15.1	-2.0	π(C3)···π(C3)	3.167(3)
a…b									
IV	x,y,z	4.910	-42.9	-17.6	-45.0	51.3	-54.2	N1–H1···O2 C9–H9···π(C16–C15–C20)	1.95, 152 2.59, 146
V	x-1,y,z	5.018	-44.6	-18.0	-44.9	55.3	-52.1	N2–H2···O1 C23–H23···π(C2–C1)	1.91, 153 2.66, 155
VI	-x+1,-y,-z+1	7.610	-16.0	-4.9	-31.0	18.1	-33.8	C17–H17···O1 C16–H16···π(C11)	2.51, 154 2.79, 138
VII	-x+1,-y+1,-z+1	7.809	-16.5	-5.6	-31.1	21.6	-31.6	C3–H3···π(C27–C22) C2–H2A···π(C25)	2.72, 145 2.79, 129
VIII	-x+1,y+1/2,-z+1/2	11.295	-0.4	-0.9	-7.7	6.6	-2.4	F2···Cl2 F3···Cl2	3.132(2), 100, 173 3.373(1), 89, 149
IX	-x+1,y+1/2,-z+1.5	13.251	-0.7	-0.1	-0.3	0.0	-1.1	F4···Cl1 F5···Cl1	3.084(2), 108, 162 3.397(2), 94, 146
b…b									
X	-x+2,-y+1,-z+1	7.246	-6.2	-1.5	-13.4	3.2	-17.9	C24–H24···F6	2.65, 165

XI	x,-y+1/2,z-1/2	9.584	-6.1	-2.3	-16.3	8.8	-15.9	C19–H19···π(C25) C18–H18···Cl2	2.82, 145 3.11, 122
XII	-x+2,-y,-z+1	9.804	2.5	-1.9	-15.7	10.6	-4.5	π(C17)···π(C17)	3.401(3)
PC43									
I	x,-y+1/2,z+1/2	4.882	-60.6	-25.2	-42.5	85.0	-43.3	N1–H1···O1 C2–H2···O1	1.92, 162 2.28, 132
II	-x+1,-y+1,-z+1	8.560	-39.7	-13.4	-51.3	85.8	-18.6	π(C8)···π(C10) π(C9)···π(C11) Cl1···π(C7)	3.408(2) 3.417(3) 3.546(2), 99
III	-x,-y,-z+1	8.302	-15.5	-3.6	-20.0	25.7	-13.4	F3A···π(C2)	3.199(3), 123
IV	x,-y+1.5,z-1/2	11.146	-3.6	-1.9	-12.5	7.9	-10.1	C12–H12···π(C10) C10–H10···Cl1	2.99, 144 3.20, 141
V	x,y+1,z	10.386	-10.3	-3.9	-17.6	23.7	-8.1	π(C3)···π(C12) Cl···π(C2)	3.438(3) 3.614(3), 100
VI	-x,y-1/2,-z+1.5	8.724	-5.9	-1.6	-10.4	10.2	-7.7	C6–H6···F3A O1···F3A	2.37, 139 3.195(2), 132
VII	-x+1,y-1/2,-z+1/2	10.950	-2.2	-2.1	-8.9	5.5	-7.7	C9–H9···Cl1	2.90, 145
VIII	x,-y-1/2,z-1/2	11.796	-2.7	-1.2	-6.2	5.8	-4.3	C4–H4···F2A	2.39, 131
IX	1-x,2-y,1-z	16.779	-1.4	-1.1	-6.5	6.1	-2.9	Cl1···Cl1	3.531(1), 156, 156
PC44									
a…a									
I	x,y-1,z	5.252	-37.8	-12.5	-45.1	45.3	-50.0	N1–H1···O1 C9–H9···O1	2.11, 153 2.48, 125
II	-x+2,y-1/2,-z+1/2	7.949	-10.1	-5.8	-39.2	25.3	-29.8	C13–H13···π(C12-C13) C2–H2A···Cl1 C12–H12···N1	2.67, 147 2.96, 147 2.73, 135
a…b									

III	x,y,z	5.271	-17.8	-8.4	-47.7	34.4	-39.5	C6–H6···π(C23-C24) C20–H20···π(C9-C10)	2.59, 155 2.62, 156
IV	x,y-1,z	5.314	-9.3	-7.1	-46.5	30.4	-32.6	C10–H10···π(C19-C20) C24–H24···π(C5-C6) F6···Cl1	2.73, 144 2.71, 146 3.479(2), 108, 140
V	x,-y+1/2,z-1/2	10.425	-2.4	-1.0	-11.0	4.5	-10.0	C3–H3···F5	2.52, 148
VI	x,-y+1.5,z-1/2	10.84	-3.1	-0.8	-5.8	3.4	-6.3	C17–H17···F1	2.41, 157
VII	2-x,1-y,1-z	15.989	-0.4	-0.5	-5.9	4.2	-2.6	F5···Cl1	3.161(2), 173, 107
VIII	1-x,1-y,-z	16.150	-0.2	-0.4	-5.9	4.0	-2.4	F1···Cl2	3.223(2), 174, 105
b…b									
IX	x,y-1,z	5.252	-36.3	-12.1	-43.7	44.1	-48.0	N2–H2···O2 C23–H23···O2	2.12, 153 2.47, 126
X	-x+1,y+1/2,-z+1/2	8.096	-10.3	-5.6	-38.7	25.8	-28.9	C27–H27···π(C26-C27) C26–H26···N2 C16–H16···Cl2	2.66, 145 2.73, 136 3.00, 151
PB23									
I	1+x,y,z	4.799	-29.5	-12.2	-44.8	42.5	-43.8	N1–H1···O1 C2···O1 F1A···C4	1.98, 149 3.214(1) 3.151(1), 129
II	2-x,1-y,2-z	6.084	-6.9	-2.3	-39.4	19.5	-29.1	C11–H11···F2A	2.76, 130
III	2-x,-y,2-z	5.956	-9.7	-2.7	-35.0	19.5	-27.9	C2···Br1	3.669(1), 85
IV	1-x,1-y,2-z	7.874	-11.8	-8.9	-27.8	23.5	-25.0	H12···H6 C12–H12···O1 H13···H13	2.14 2.56, 128 2.22
V	3-x,-y,2-z	7.520	-10.7	-6.5	-29.8	38.2	-8.8	C2–H2···Br1	2.83, 143

								Br1⋯Br1	3.401(1), 146, 146
VI	2.5-x,1/2+y,1.5-z	11.816	-4.4	-0.8	-5.4	1.8	-8.8	C4–H4⋯F2A C3–H3⋯F3A	2.75, 132 2.75, 146
VII	1/2+x,1/2-y,1/2+z	13.850	-2.3	-0.6	-5.1	1.9	-6.1	C10–H10⋯F3A	2.61, 143
PB24									
I	1+x,y,z	4.806	-32.1	-13.6	-49.9	51.3	-44.3	N1–H1⋯O1 C2⋯O1 F1A⋯F2A	1.98, 151 3.149(1) 2.878(1), 160, 111
II	1-x,-y,1-z	5.322	-13.3	-3.3	-41.2	27.6	-30.1	C2⋯Br1 C7⋯Br1	3.623(1), 85 3.601(1), 124
III	1-x,-y,2-z	7.141	-4.5	-2.9	-40.9	25.9	-22.4	π(C7-N1-C8-C13-C12)⋯ π(C7-N1-C8-C13-C12)	3.536
IV	-x,-y,2-z	9.323	-8.9	-5.3	-21.0	12.8	-22.4	C12–H12⋯O1	2.59, 135
V	2-x,-y,1-z	6.750	-9.8	-4.1	-24.5	28.0	-10.2	C2–H2⋯Br1 Br1⋯Br1	3.02, 147 3.410(1), 148, 148
VI	1/2+x,1/2-y,-1/2+z	11.725	-4.6	-1.1	-7.8	4.2	-9.3	C5–H5⋯F2A C5–H5⋯F1A	2.66, 131 2.55, 130
VII	1.5-x,1/2+y,1.5-z	14.049	-2.7	-0.7	-6.5	3.5	-6.4	C10–H10⋯F3A C11–H11⋯F1A	2.56, 126 2.76, 147
PB32									
I	1/2-x,y,1/2+z	4.425	-44.3	-21.1	-59.0	70.1	-54.3	C13–H13⋯O1 N1–H1⋯O1 N1–H1⋯C9 C6–H6⋯C10	2.47, 128 1.92, 150 2.68, 126 2.73, 162
II	1.5-x,y,1/2+z	9.128	-2.7	-2.7	-14.4	6.9	-12.9	C5–H5⋯C1 C4–H4⋯F2	2.92, 157 2.73, 120

III	-1/2-x,y,1/2+z	8.815	-3.1	-1.6	-13.6	7.7	-10.6	C12–H12···Br1	3.05, 134
IV	1/2+x,2-y,z	9.545	-4.3	-2.8	-13.0	12.7	-7.3	C11–H11···Br1 Br1···Br1	2.78, 165 4.093(1), 112, 89
V	-x,2-y,1/2+z	10.454	-1.4	-1.1	-11.1	7.6	-6.0	C11···Br1	3.519(1), 173
VI	1-x,1-y,1/2+z	12.180	-2.2	-0.8	-5.5	2.5	-6.0	C4–H4···F1	2.57, 132
VII	1/2+x,1-y,z	11.286	1.2	-0.7	-5.7	2.8	-2.4	C3–H3···F1	2.58, 118
PB34									
I	x,1+y,z	4.994	-43.0	-16.1	-47.7	54.7	-52.0	N1–H1···O1 C3···C6	1.92, 161 3.368(1)
II	1+x,y,z	4.859	-5.5	-4.4	-49.8	28.3	-31.4	C12···C9 C13–H13···C8 N1···C2 C5···F2	3.384(1) 2.94, 116 3.326(1) 3.266(1), 99
III	1+x,1+y,z	6.968	-5.3	-5.4	-22.9	13.3	-20.2	C6–H6···F1 H3···H6 C3–H3···O1 H12···H9 C12–H12···Br1	2.50, 135 2.15 2.87, 132 2.25 3.25, 148
IV	3-x,1/2+y,1-z	14.140	-2.3	-0.7	-5.7	2.8	-5.8	C11–H11···Br1	3.08, 172
V	1-x,1/2+y,-z	14.090	-1.8	-0.5	-5.1	2.3	-5.2	C5–H5···F3 F3···F3 F2···F3	2.61, 144 3.129(1), 97, 157 3.078(1), 100, 161
VI	2-x,1/2+y,1-z	12.767	-4.9	-1.4	-9.4	12.9	-2.8	Br1···Br1	3.569(1), 99, 172
PB43									
I	x,1/2-y,-1/2+z	5.207	-48.1	-20.7	-42.7	62.2	-49.2	C2–H2···O1 N1–H1···O1	2.29, 132 1.91, 163

								H1⋯H6	2.27
II	2-x,1-y,-1-z	7.217	-17.9	-5.5	-47.9	36.8	-34.5	C9⋯C11	3.409(1)
III	1-x,-y,1-z	9.900	-7.2	-1.2	-19.4	5.8	-22.0	F2⋯C2	3.301(1), 118
IV	x,-1+y,z	10.488	-4.4	-1.7	-16.2	10.4	-11.8	C12–H12⋯C3 Br1⋯C2	3.10,104 3.768(1), 97
V	x,1.5-y,-1/2+z	9.911	-2.3	-1.2	-12.2	4.8	-10.9	C12–H12⋯C10 C10–H10⋯Br1 C12–H12⋯Br1	3.11, 147 3.27, 144 3.47, 109
VI	1-x,-1/2+y,1.5-z	9.559	-3.5	-1.1	-9.9	5.7	-8.9	O1⋯F2 C6–H6⋯F2	3.172(1), 132 2.37, 138
VII	2-x,-1/2+y,1/2-z	10.439	-2.4	-1.4	-8.4	4.7	-7.5	C9–H9⋯Br1	3.01, 141
VIII	x,-1/2-y,-1/2+z	13.266	-1.1	-0.9	-6.0	3.9	-4.2	C4–H4⋯F3	2.43, 133
IX	2-x,2-y,1-z	15.271	-2.6	-0.9	-7.5	10.0	-1.1	Br1⋯Br1	3.565(1), 154, 154
PB44									
a…a									
I	-x,1/2+y,1/2-z	5.242	-39.5	-13.1	-46.1	47.2	-51.4	C13–H13⋯C12 C13–H13⋯C13	2.73, 158 2.77, 135
II	x,1+y,z	6.450	-10.6	-5.9	-39.9	26.7	-29.7	C9–H9⋯O1 N1–H1⋯O1	2.44, 126 2.12, 152
a…b									
III	x,1+y,z	4.767	-18.2	-8.4	-48.3	36.1	-38.8	C20–H20⋯C9 C20–H20⋯C10 C6–H6⋯C23 C6–H6⋯C24	2.71, 164 2.70, 145 2.71, 162 2.67, 143
IV	x,y,z	4.668	-9.7	-7.7	-47.7	32.9	-32.1	C24–H24⋯C5 C24–H24⋯C6 C10–H10⋯C19	2.75, 155 2.80, 135 2.76, 154

V	x,1.5-y,1/2+z	12.309	-3.8	-1.0	-10.5	4.3	-11.0	C3–H3···F5	2.52, 148
VI	x,1/2-y,1/2+z	12.685	-2.6	-0.7	-5.2	2.8	-5.7	C17–H17···F1	2.45, 159
VII	-x,1-y,-z	16.172	-1.5	-0.5	-5.8	4.8	-2.9	Br1A···F5	3.220(1), 171, 108
VIII	1-x,1-y,1-z	16.343	-1.1	-0.4	-5.8	4.6	-2.6	Br2A···F1	3.257(1), 175, 106
b…b									
IX	x,1+y,z	5.242	-37.4	-12.8	-44.7	46.6	-48.3	C23–H23···O2 N2–H2···O2	2.43, 126 2.10, 152
X	1-x,1/2+y,1/2-z	6.576	-11.3	-5.7	-39.7	27.9	-28.8	C27–H27···C26 C27–H27···C27	2.70, 156 2.78, 133
PI22									
I	x,-y+1/2,z-1/2	4.858	-57.4	-26.6	-54.6	104.2	-34.5	N1–H1···O1 C13–H13···π(C2–C3)	1.92, 155 2.72, 134
II	x,-y+1.5,z-1/2	8.082	-13.1	-4.0	-14.7	13.5	-18.3	C3–H3···O1 C4–H4···F2	2.61, 166 2.51, 129
III	-x+2,-y+1,-z+1	12.046	-11.5	-2.9	-12.4	11.5	-15.4	C4–H4···F3	2.60, 127
IV	x,y+1,z	6.597	-19.2	-7.7	-31.0	44.2	-13.7	π(C2)···π(C13) F1···π(C4) C12–H12···O1	3.277(6) 3.165(6), 128 2.80, 133
V	-x+1,-y,-z+1	10.451	-5.9	-2.4	-12.1	11.3	-9.2	C10–H10···I1	3.30, 148
VI	x,-y-1/2,z+1/2	8.302	-2.4	-2.5	-14.1	10.8	-8.2	C12–H12···π(C9) C11–H11···I1	3.05, 133 3.47, 132
VII	-x+2,y-1/2,-z+1/2	12.298	-3.3	-1.1	-5.7	3.9	-6.3	C5–H5···F3	2.63, 127
VIII	-x+1,y+1/2,-z+1/2	9.988	-3.2	-2.2	-10.9	10.2	-6.1	H10···H11 C11–H11···I1	2.41 3.50, 118
PI23									

I	-x+1,-y,-z	8.184	-19.2	-9.2	-26.9	25.2	-30.2	C12–H12···O1 H6···H12 H13···H13	2.54, 132 2.20 2.29
II	x,y-1,z	4.736	-50.6	-19.6	-50.8	96.4	-24.5	F2A···F3A N1–H1···O1	2.824(7), 144, 122 1.96, 144
III	-x+1,-y+1,-z	6.228	-22.0	-7.5	-42.5	51.4	-20.6	C11–H11···F2A π(C6)···π(C12)	2.83, 146 3.553(5)
IV	-x,-y+1,-z	5.838	-12.7	-3.7	-23.2	23.3	-16.3	I1···π(C2)	3.978(4), 98
V	-x,-y+2,-z	7.124	-17.9	-9.2	-32.7	46.9	-12.9	I1···I1 C2–H2···I1	3.813(1), 145, 145 3.09, 138
VI	x,-y+1/2,z+1/2	13.610	-5.3	-1.1	-7.1	5.8	-7.8	C11–H11···F3A C11–H11···F2A π(C10)···F1A	2.77, 134 2.90, 130 3.436(9), 110
VII	x,-y+1.5,z-1/2	13.397	-1.5	-0.5	-4.2	1.3	-4.9	C10–H10···F2A	2.92, 133
VIII	-x,y-1/2,-z-1/2	11.569	-0.9	-1.6	-8.6	6.8	-4.3	C3–H3···F1A	2.48, 127
PI24									
I	x,-y+1/2,z-1/2	4.791	-72.0	-27.9	-54.5	108.3	-46.1	N1–H1···O1 C2–H2···O1 C9–H9···π(C1-C2)	1.91, 166 2.54, 127 2.78, 127
II	x,-y-1/2,z-1/2	9.693	-13.1	-5.1	-16.7	16.9	-18.0	C10–H10···O1 C10–H10··· π(C13)	2.44, 148 2.96, 137
III	-x+2,-y,-z+1	10.744	-9.4	-3.6	-14.4	15.1	-12.2	C12–H12···I1	3.24, 145
IV	x,y+1,z	7.181	-5.4	-6.6	-27.7	27.6	-12.1	C2–H2···π(C9-C10) C6–H6···F3	2.78, 139 2.72, 107
V	-x+1,-y+1,-z+1	11.857	-3.6	-1.8	-11.4	6.7	-10.1	C5–H5···F2	2.67, 138
VI	x,-y+1.5,z-1/2	7.421	-7.2	-2.3	-13.4	15.5	-7.4	F1···π(C3) C5–H5···F3	3.156(10), 126 2.75, 122

								C3–H3⋯ π(C5)	3.11, 136
VII	-x+2,y-1/2,-z+1/2	10.708	-2.9	-1.9	-10.2	8.6	-6.3	C11–H11⋯I1	3.54, 119
PI32									
I	-x+1/2,y,z+1/2	4.448	-67.1	-29.9	-62.1	117.8	-41.3	N1–H1⋯O1 C9–H9⋯O1 N1–H1⋯π(C13) C2–H2⋯π(C12)	1.89, 151 2.46, 126 2.73, 125 2.70, 164
II	-x-1/2,y,z-1/2	9.540	-4.7	-3.4	-13.6	10.5	-11.2	C4–H4⋯F3	2.75, 121
III	-x+1.5,y,z-1/2	8.659	-6.4	-3.2	-15.1	15.7	-9.1	C10–H10⋯I1 C10–H10⋯π(C11) C10–H10⋯π(C12)	3.24, 130 3.13, 115 3.16, 139
IV	x+1/2,-y+1,z	9.020	-13.8	-5.6	-16.4	28.5	-7.4	C11–H11⋯I1 I1⋯I1	3.03, 162 4.175(3), 112, 90
V	-x,-y,z-1/2	13.146	-4.3	-1.1	-5.6	4.5	-6.6	C4–H4⋯F2	2.57, 130
VI	-x+1,-y+1,z-1/2	9.856	-8.4	-3.7	-15.1	21.6	-5.6	I1⋯π(C11)	3.613(3), 171
VII	x-1,y,z	7.950	4.5	-3.7	-14.4	11.1	-2.5	H2⋯H10 C9–H9⋯π(C3)	2.41 3.00, 146
VIII	x-1/2,-y,z	12.207	0.0	-1.2	-5.5	5.0	-1.8	C5–H5⋯F2	2.61, 118
PI33									
I	x,-y+1/2,z-1/2	4.754	-63.6	-24.1	-44.2	90.6	-41.4	N1–H1⋯O1 C2–H2⋯O1	1.85, 167 2.53, 121
II	x,y-1,z	5.290	-18.5	-9.4	-42.9	50.6	-20.3	C4-H4⋯F2 π(C9)⋯π(C12)	2.64, 135 3.373(3)
III	x,-y-1/2,z-1/2	7.154	-7.0	-3.5	-14.6	13.7	-11.4	C3–H3⋯π(C5) C3–H3⋯π(C6) C3–H3⋯F3	2.85, 139 2.86, 159 2.59, 129

IV	-x+1,-y+1,-z+1	12.121	-8.7	-3.3	-14.3	16.3	-10.1	C11–H11···I1	3.25, 140
V	x,-y+1.5,z-1/2	7.069	-7.8	-5.3	-18.9	22.3	-9.7	C12–H12···I1	3.01, 143
VI	-x,-y,-z+1	15.386	-6.0	-1.0	-8.6	7.8	-7.8	C4–H4···F2 F1···F2	2.79, 151 3.054(2), 126, 106
VII	-x+1,y-1/2,-z+1/2	13.332	-10.4	-3.2	-10.1	18.2	-5.5	I1···I1	3.973(1), 113, 162
PI34									
I	x,y-1,z	4.964	-66.1	-24.6	-50.5	98.8	-42.5	N1–H1···O1 π(C3)···π(C6) I1···π(C11) C4–H5···F3	1.91, 160 3.374(5) 3.679(4), 89 2.69, 137
II	x+1,y-1,z	6.981	-6.7	-7.5	-25.3	20.8	-18.7	C6–H6···F1 H3···H6 H9···H12 C3–H3···O1 C12–H12···I1	2.46, 135 2.14 2.19 2.82, 132 3.43, 142
III	x-1,y,z	4.908	-26.6	-10.7	-52.8	76.0	-14.2	π(C9)···π(C12) N1···π(C2)	3.382(5) 3.348(4)
IV	-x+1,y+1/2,-z	12.067	-15.9	-5.0	-12.4	26.4	-6.9	I1···I1	3.841(1), 106, 171
V	-x,y-1/2,-z	13.258	-2.4	-1.3	-7.0	5.4	-5.3	C11–H11···I1	3.30, 172
VI	-x+2,y+1/2,-z+1	15.459	-2.9	-0.7	-5.2	5.0	-3.8	C5–H5···F3 F2···F3 F3···F3	2.59, 145 3.105(3), 160, 100 3.141(4), 98, 157
PI43									
I	x,-y+1/2,z+1/2	5.757	-61.7	-24.9	-43.2	87.8	-42.0	N1–H1···O1 C2–H2···O1	1.91, 161 2.34, 132

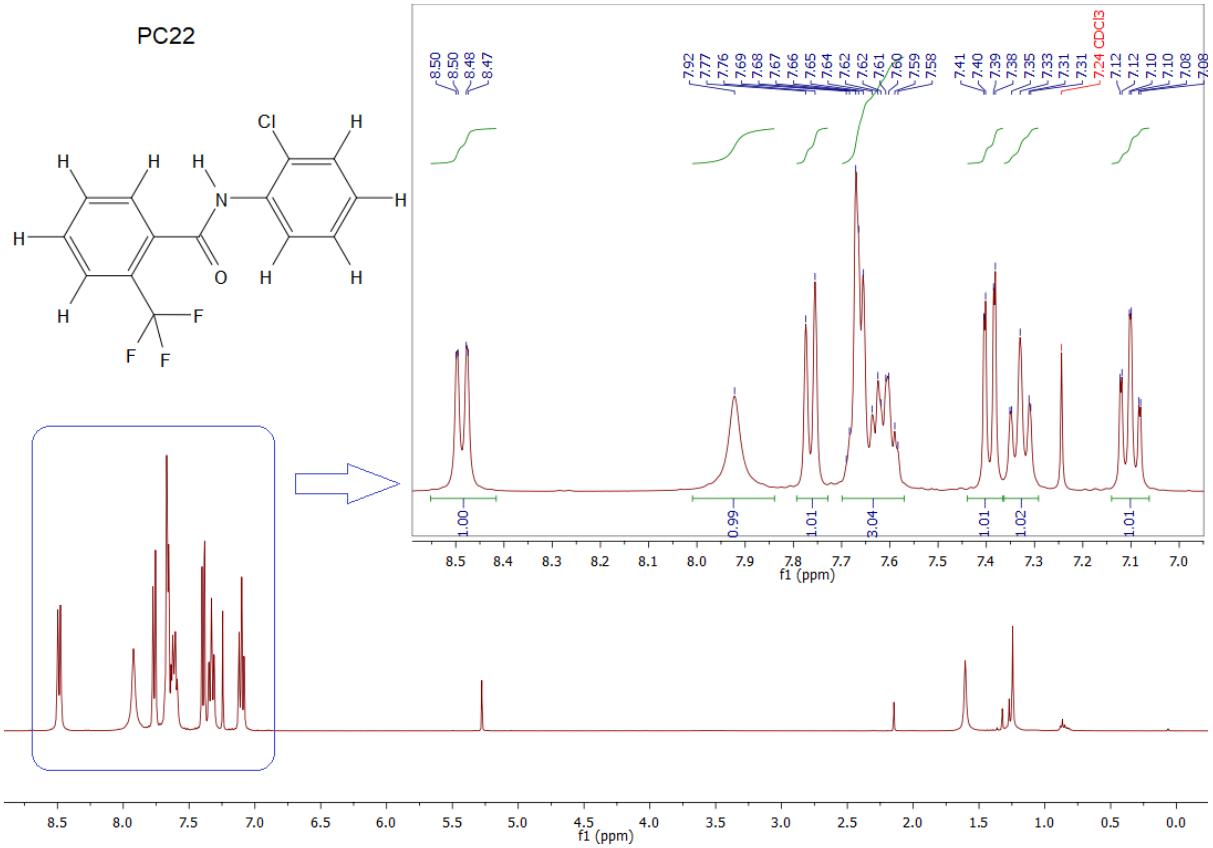
								C9–H9···O1 H1···H6	2.67, 127 2.28
II	-x,-y,-z	6.309	-41.5	-14.7	-52.1	89.5	-18.8	π(C9)···π(C11)	3.466(3)
III	-x+1,-y+1,-z	11.316	-17.2	-3.9	-20.6	26.3	-15.5	F1···π(C2)	3.309(3), 113
IV	x,-y-1/2,z+1/2	9.079	-6.0	-2.8	-14.8	13.8	-9.7	C10–H10···I1	3.39, 147
V	x,y-1,z	10.708	-9.6	-3.8	-16.3	20.8	-9.0	C12–H12···π(C3) I1···π(C3)	3.15, 108 3.941(3), 75
VI	-x,y-1/2,-z+1/2	10.151	-4.5	-2.4	-9.3	8.8	-7.4	C9–H9···I1	3.22, 138
VII	-x+1,y-1/2,-z-1/2	10.395	-5.3	-1.5	-9.7	10.0	-6.6	C6–H6···F1	2.35, 143
VIII	-x,-y-1,-z	14.274	-12.5	-5.7	-13.1	27.0	-4.3	I1···I1	3.732(1), 152, 152
IX	x,-y+1.5,z+1/2	14.601	-2.6	-1.3	-5.8	5.4	-4.2	C4–H4···F3	2.43, 132
PI44									
I	x,y-1,z	5.252	-58.0	-18.5	-46.9	78.3	-45.0	N1–H1···O1 C9–H9···O1	2.12, 151 2.39, 126
II	-x+1,-y+1,-z+1	4.904	-33.4	-14.7	-51.8	68.5	-31.3	C6–H6···π(C10) C5–H5···I1	2.69, 143 3.15, 146
III	-x+1,-y,-z+1	4.645	-26.0	-13.1	-50.2	62.8	-26.6	C10–H10···π(C5–C6)	2.67, 149
IV	-x+1,y-1/2,-z+1.5	5.598	-23.9	-10.8	-42.7	56.0	-21.4	C13–H13···π(C12) C12–H12···N1 C2–H2···I1	2.71, 145 2.82, 138 3.20, 148
V	-x,-y,-z+1	14.134	-8.1	-1.8	-10.4	7.9	-12.4	C3–H3···F3	2.56, 159
VI	x-1,-y+1/2,z-1/2	16.682	-5.3	-1.6	-7.5	11.1	-3.3	F3···I1 F2···I1	3.369(4), 172, 103 3.628(4), 151, 93

Table S3 Lattice Energy (kJ/mol) obtain from PIXELC method

Sample code	E_{coul}	E_{pol}	E_{disp}	E_{rep}	E_{tot}	Density (g/cm^3)
PC22	-62.2	-29.5	-144.5	107.4	-128.8	1.581
PC23	-52.3	-23.3	-135.5	89.1	-122.1	1.535
PC24	-95.4	-38.5	-147.6	187.3	-94.2	1.573
PC32	-86.4	-41.5	-142.7	177.6	-93.0	1.516
PC33	-100.8	-44.1	-145.6	183.9	-106.7	1.562
PC34	-67.2	-30.1	-153.9	115.0	-136.2	1.570
PC42	-67.3	-30.3	-128.1	99.8	-125.9	1.468
PC43	-112.9	-44.6	-144.4	197.7	-104.2	1.536
PC44	-62.4	-26.7	-154.6	111.1	-132.5	1.561
PB23	-56.1	-23.0	-135.6	97.8	-116.9	1.734
PB24	-60.8	-23.5	-140.8	106.9	-118.2	1.739
PB32	-58.8	-28.5	-142.2	117.3	-112.2	1.716
PB34	-64.6	-27.5	-151.4	115.3	-128.3	1.810
PB43	-74.9	-31.8	-140.5	118.1	-129.0	1.726
PB44	-66.0	-27.9	-156.7	117.1	-133.5	1.773
PI22	-111.3	-51.2	-150.7	199.6	-113.5	1.965
PI23	-92.4	-37.8	-141.2	184.3	-87.1	1.894
PI24	-115.0	-48.6	-148.7	196.3	-116.0	1.937
PI32	-108.6	-47.8	-153.6	214.7	-95.2	1.882
PI33	-120.3	-51.6	-153.1	212.6	-112.5	1.924
PI34	-122.6	-47.8	-164.7	235.7	-99.4	1.994
PI43	-124.3	-49.5	-150.1	218.6	-105.3	1.881
PI44	-118.6	-44.8	-165.7	217.9	-111.2	1.944

Figure S1 ^{1}H-NMR Spectra of the newly synthesized bulk benzamide compounds

PC22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7.60
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7.58
7.41
7.40
7.39
7.38
7.35
7.33
7.31
7.31
7.24 CDCl3
7.12
7.12
7.10
7.10
7.08
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1.01
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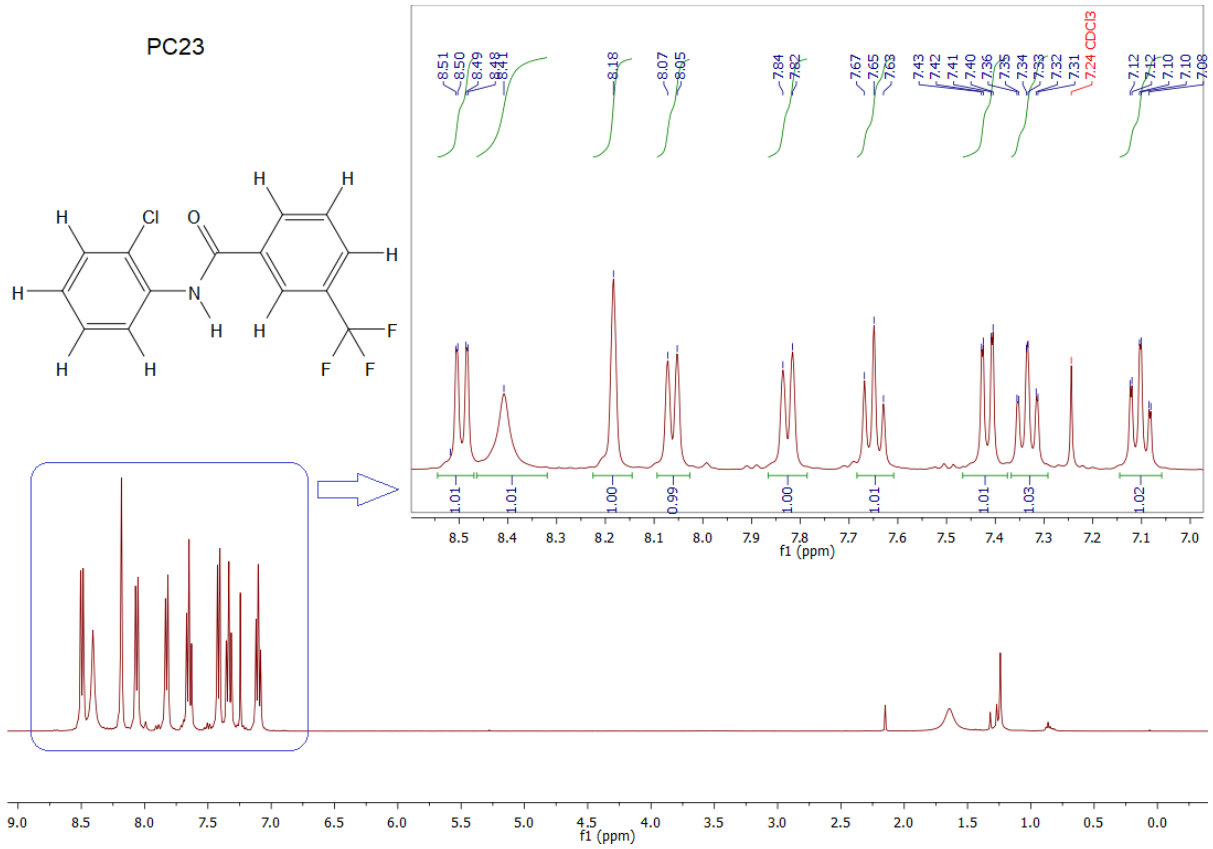
1.01
1.02
1.01
f1 (ppm)

PC23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7.35
7.34
7.33
7.32
7.31
7.24 CDCl3
7.12
7.12
7.10
7.10
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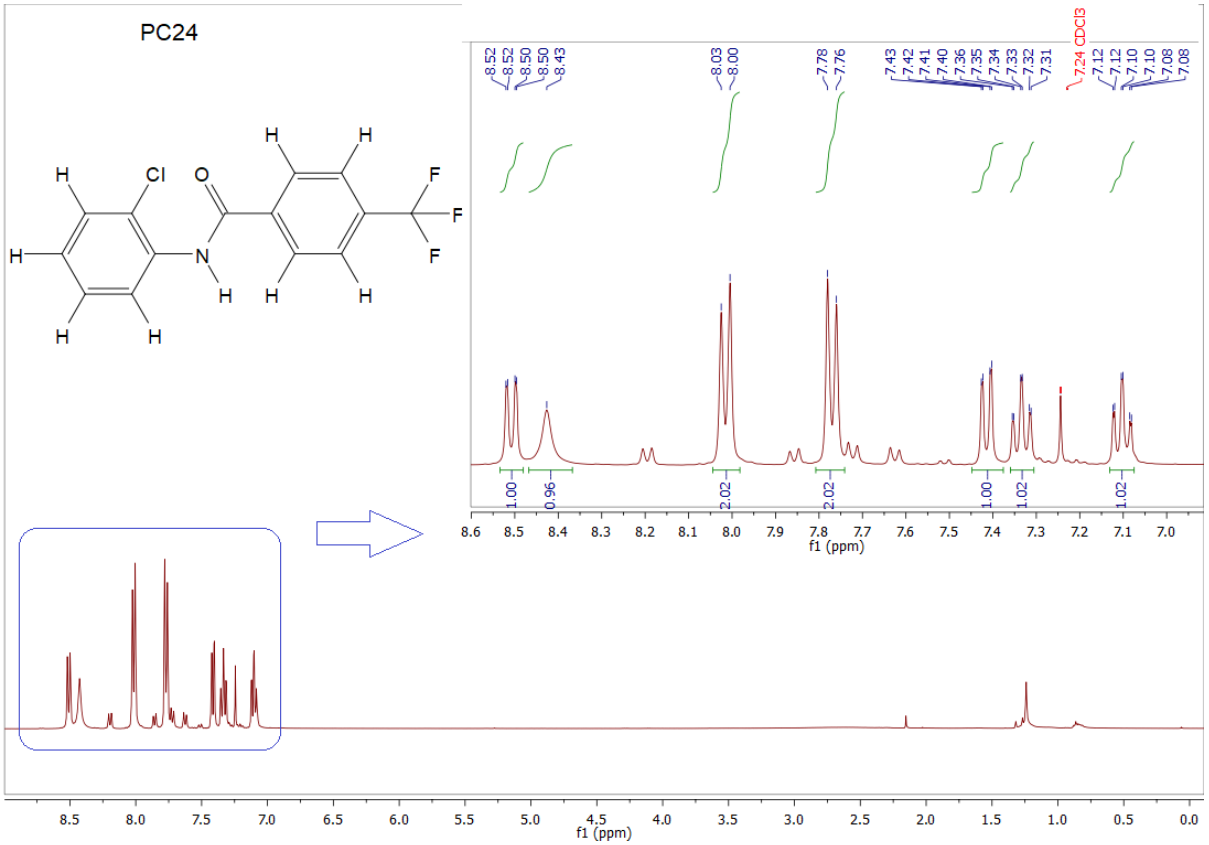
1.03
1.02
f1 (ppm)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7.33
7.32
7.31
7.24 CDCl3
7.12
7.12
7.10
7.10
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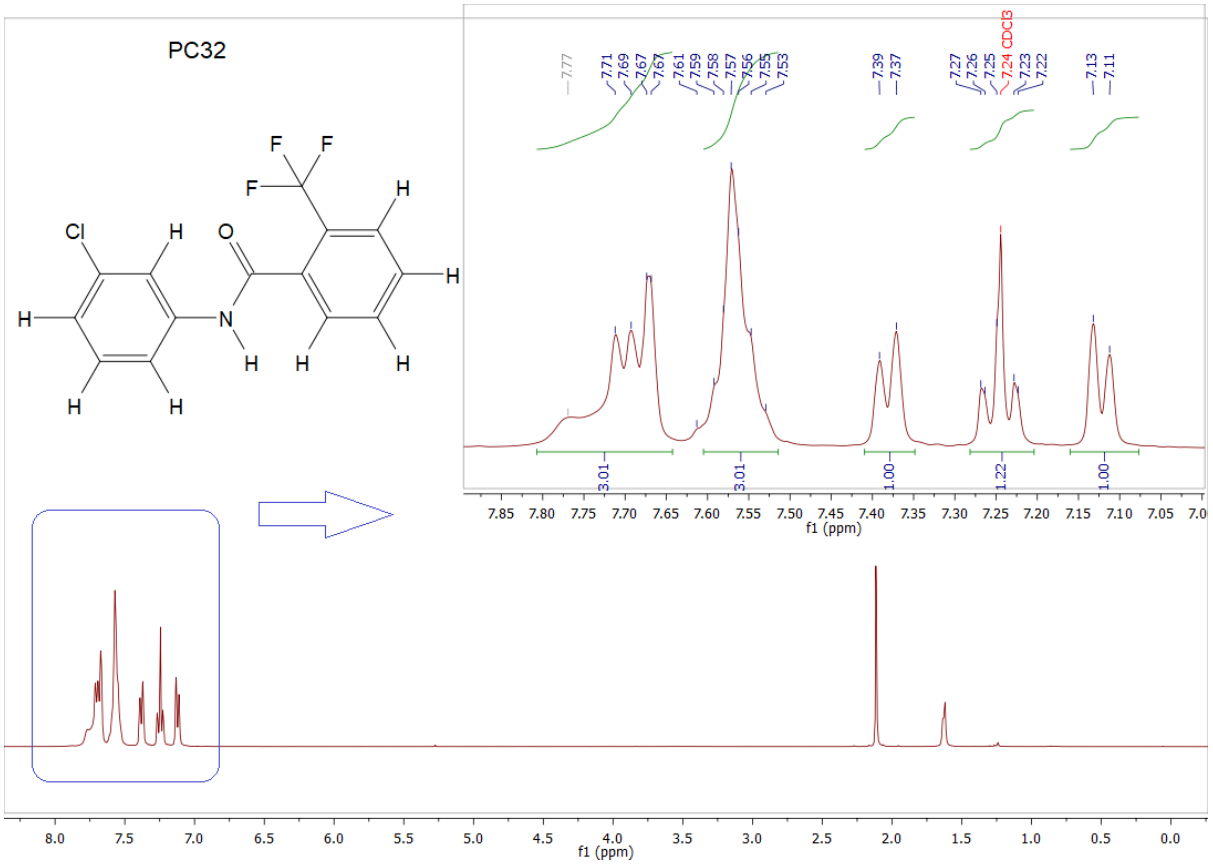
1.02
1.02
f1 (ppm)
f1 (ppm)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7.25
7.24 CDCl3
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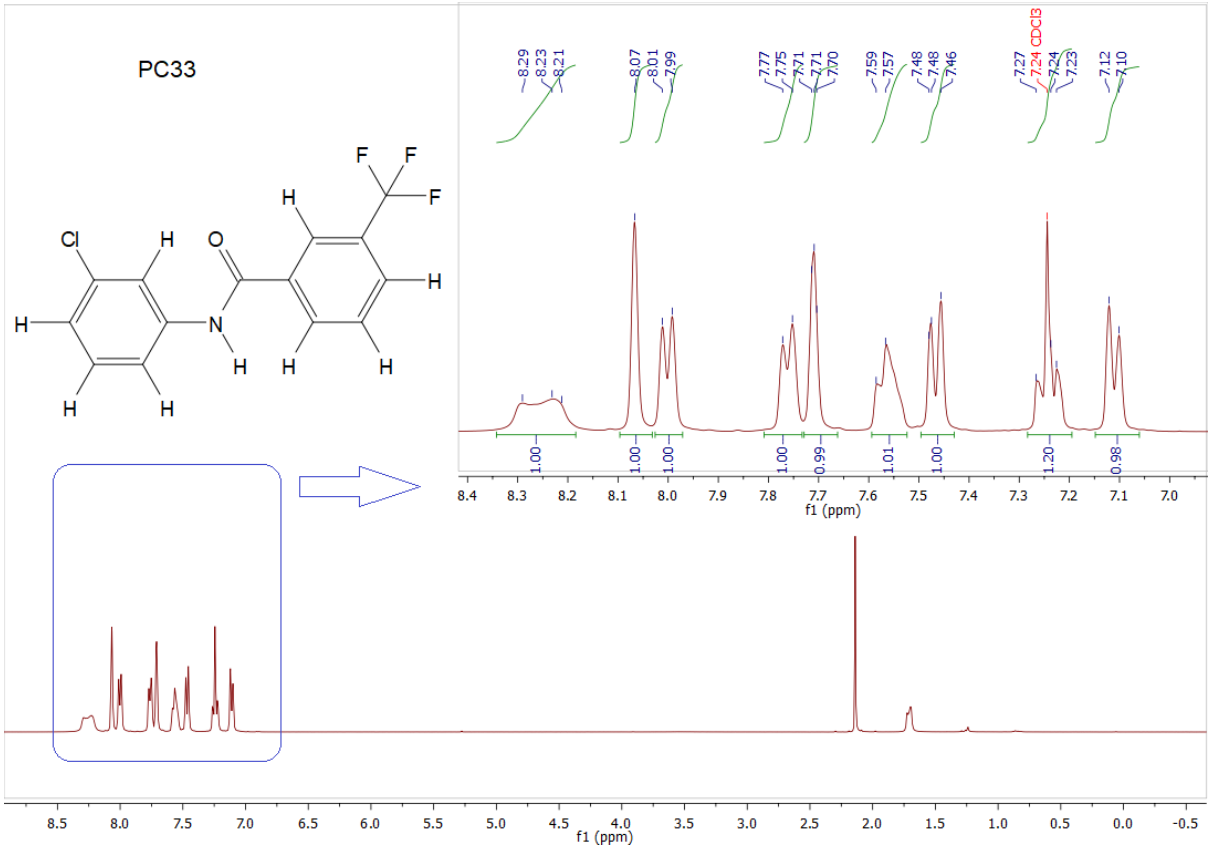
f1 (ppm)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7.46
7.27
7.24 CDCl3
7.24
7.23
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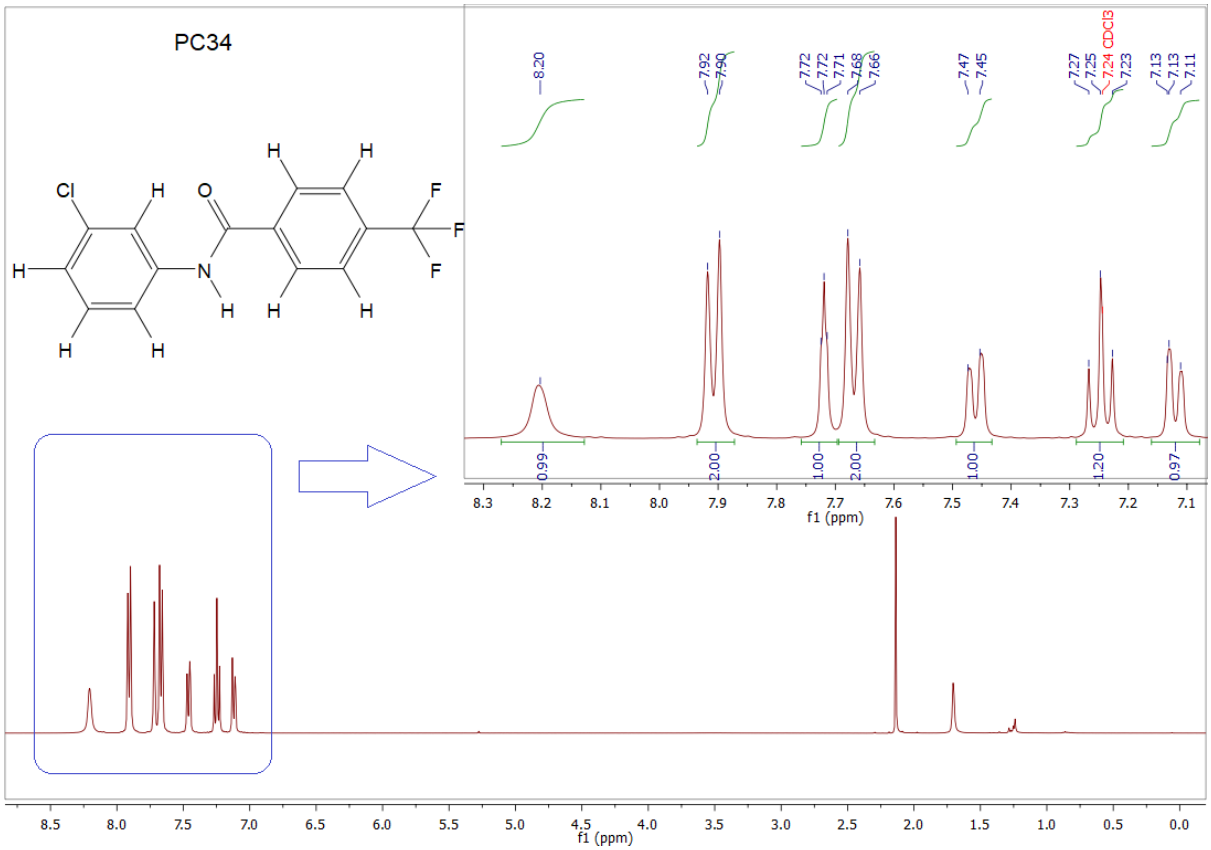
1.20
0.98
f1 (ppm)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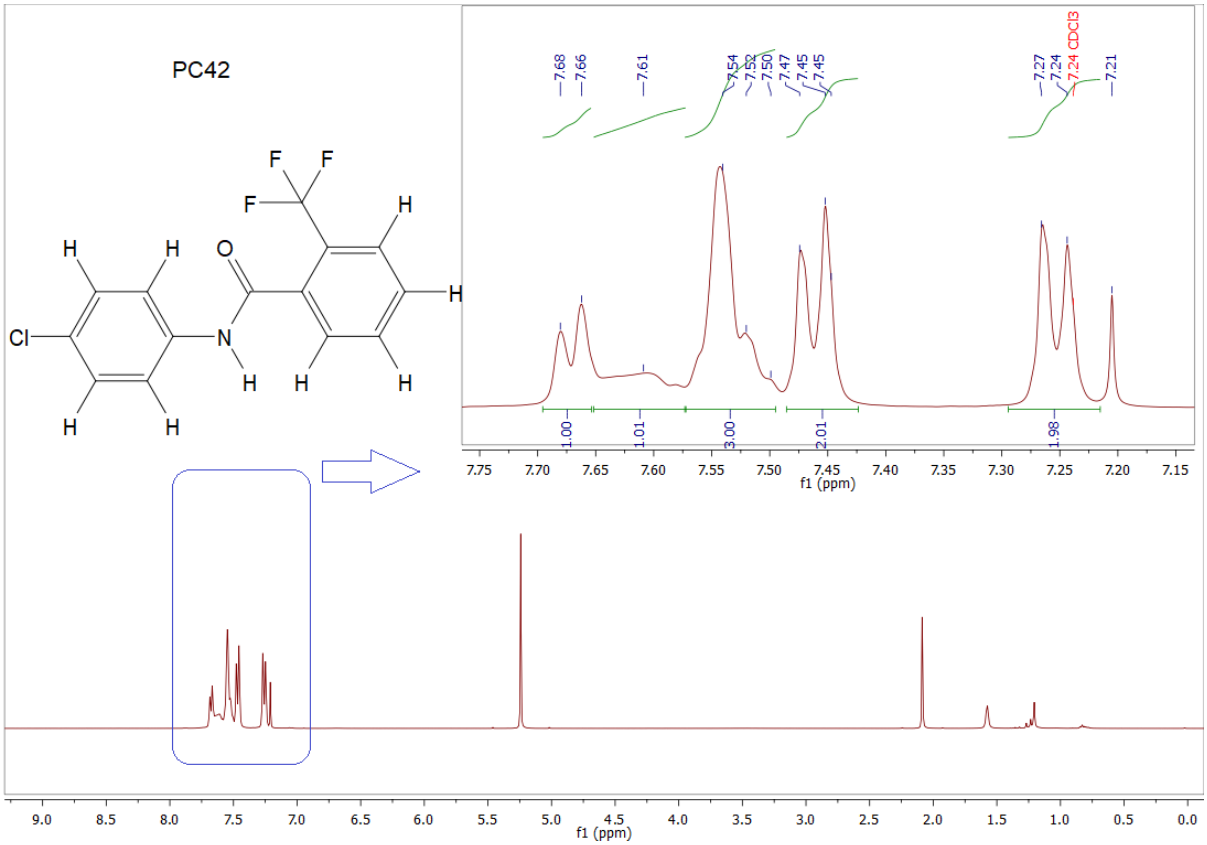
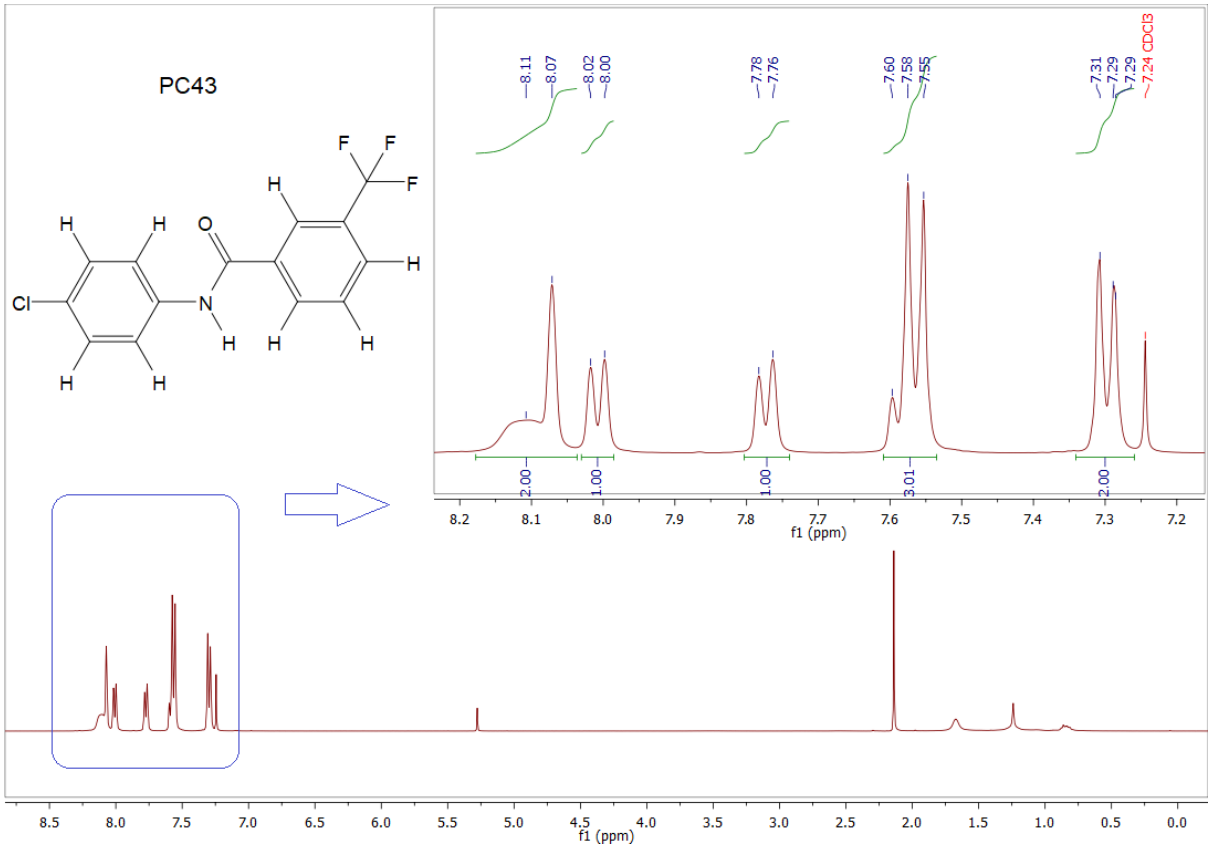
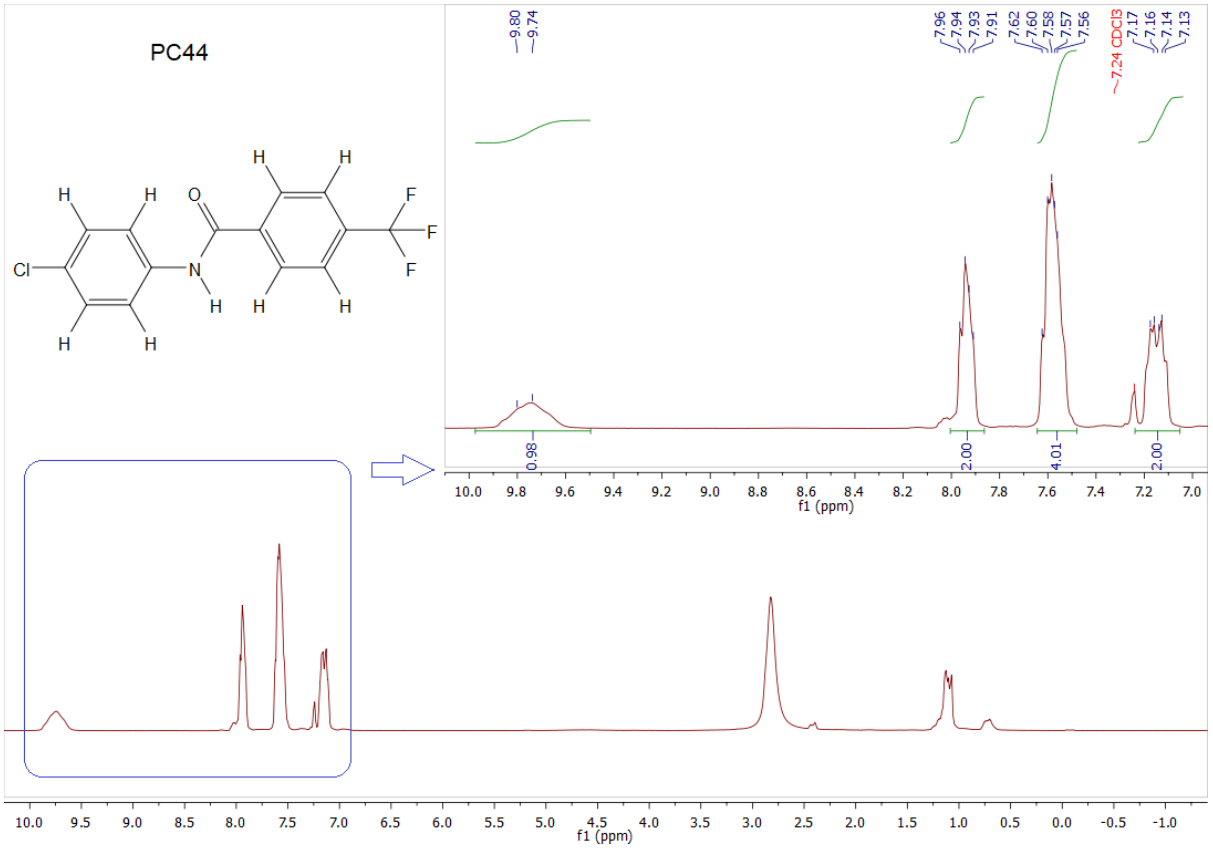
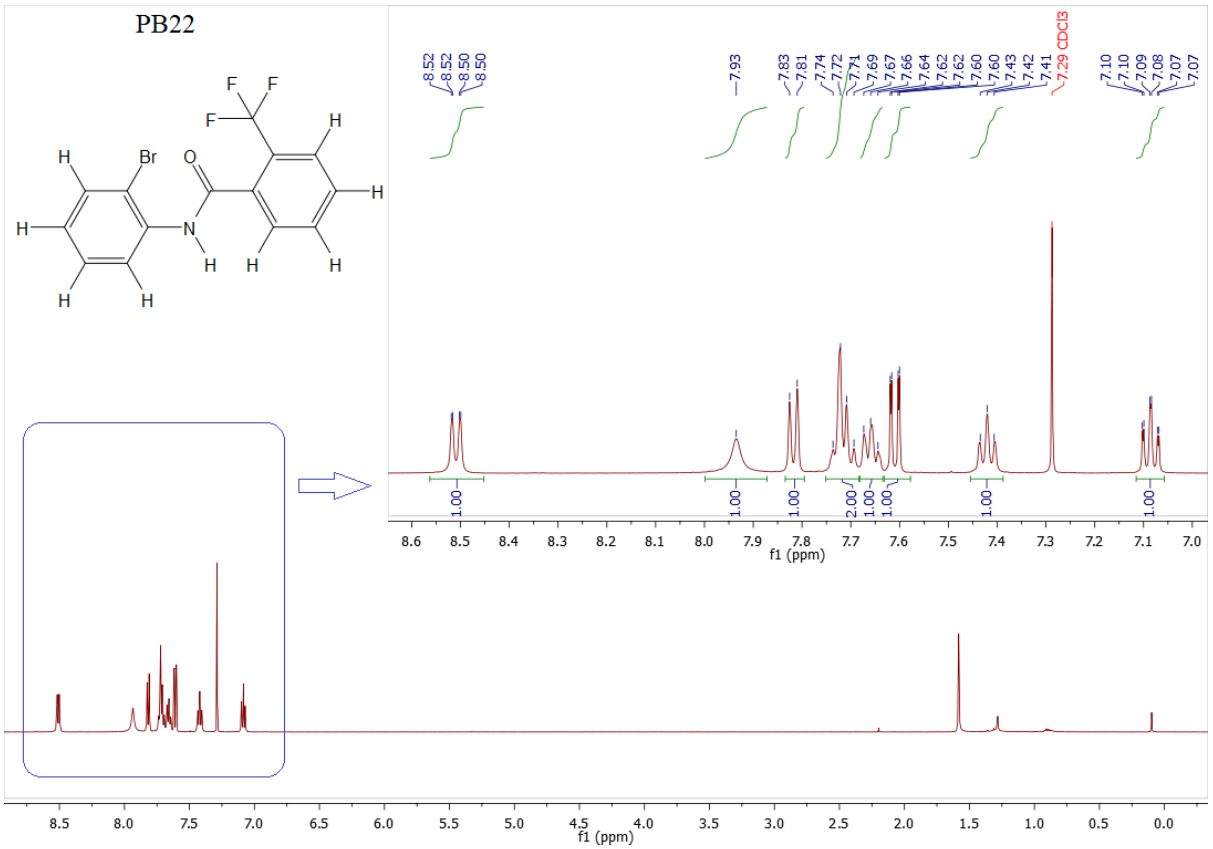
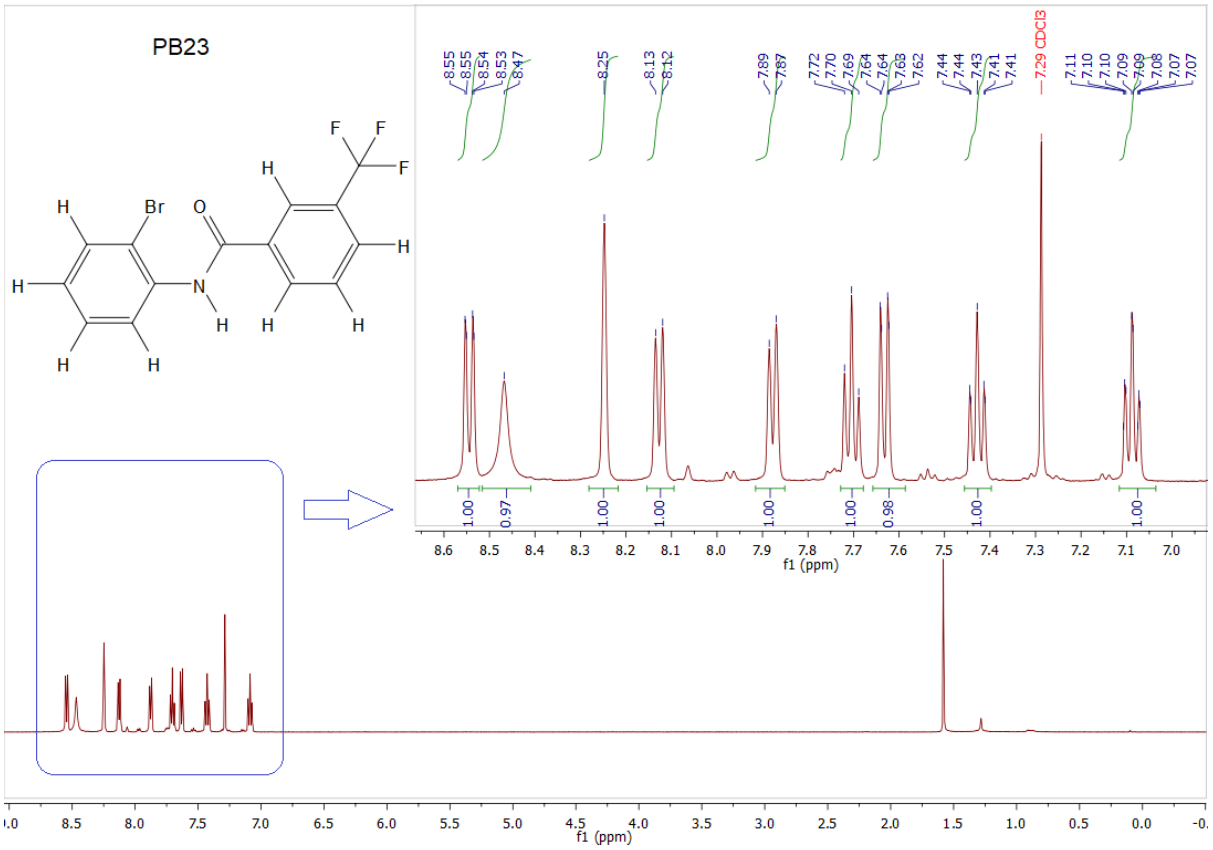
7.25
7.24 CDCl3
7.23
7.13
7.13
7.11
0.99
2.00
1.00
2.00
1.00
1.20
0.97
f1 (ppm)

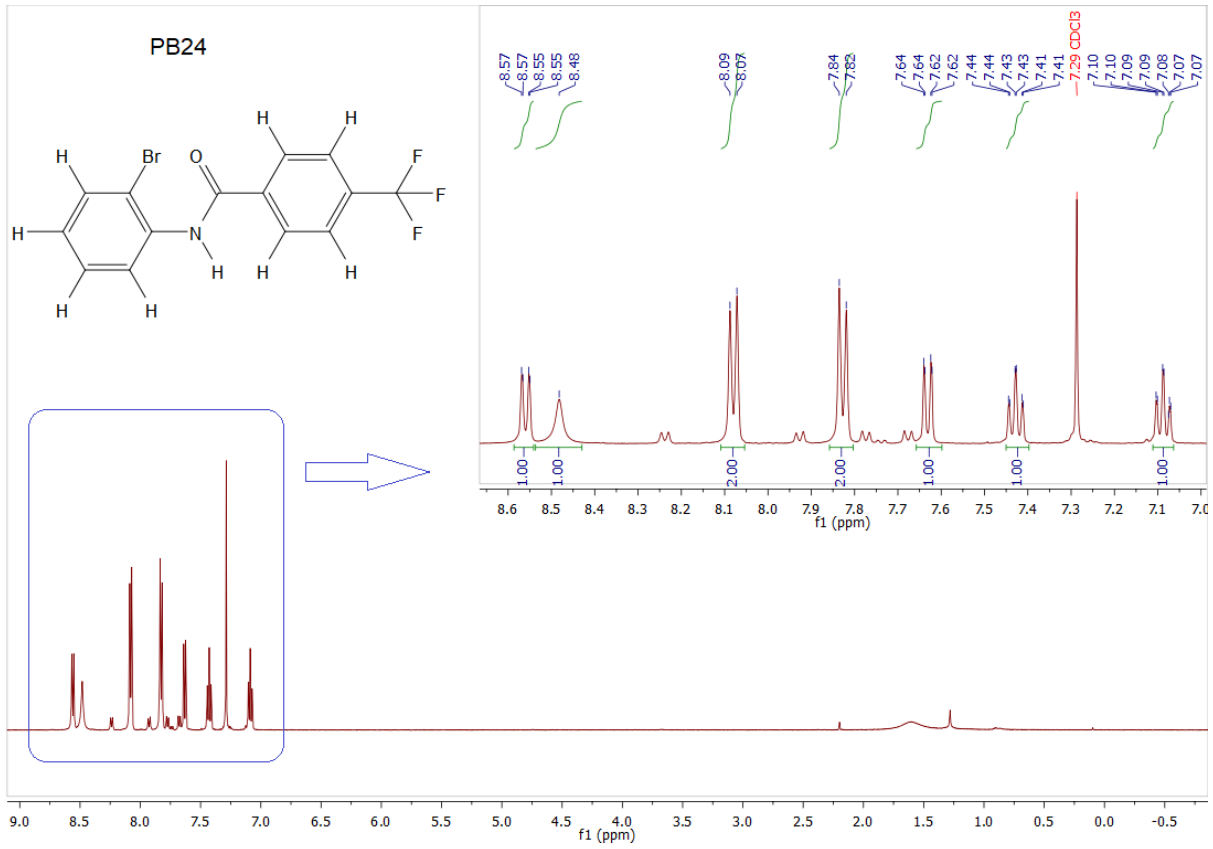

PC42
F
F
F
H
H
H
O
H
Cl
N
H
H
H
H
H
H
7.68
7.66
7.61
7.54
7.52
7.50
7.47
7.45
7.45
7.27
7.24 CDCl3
7.21
1.00
1.01
3.00
2.01
1.98
7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15
f1 (ppm)
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

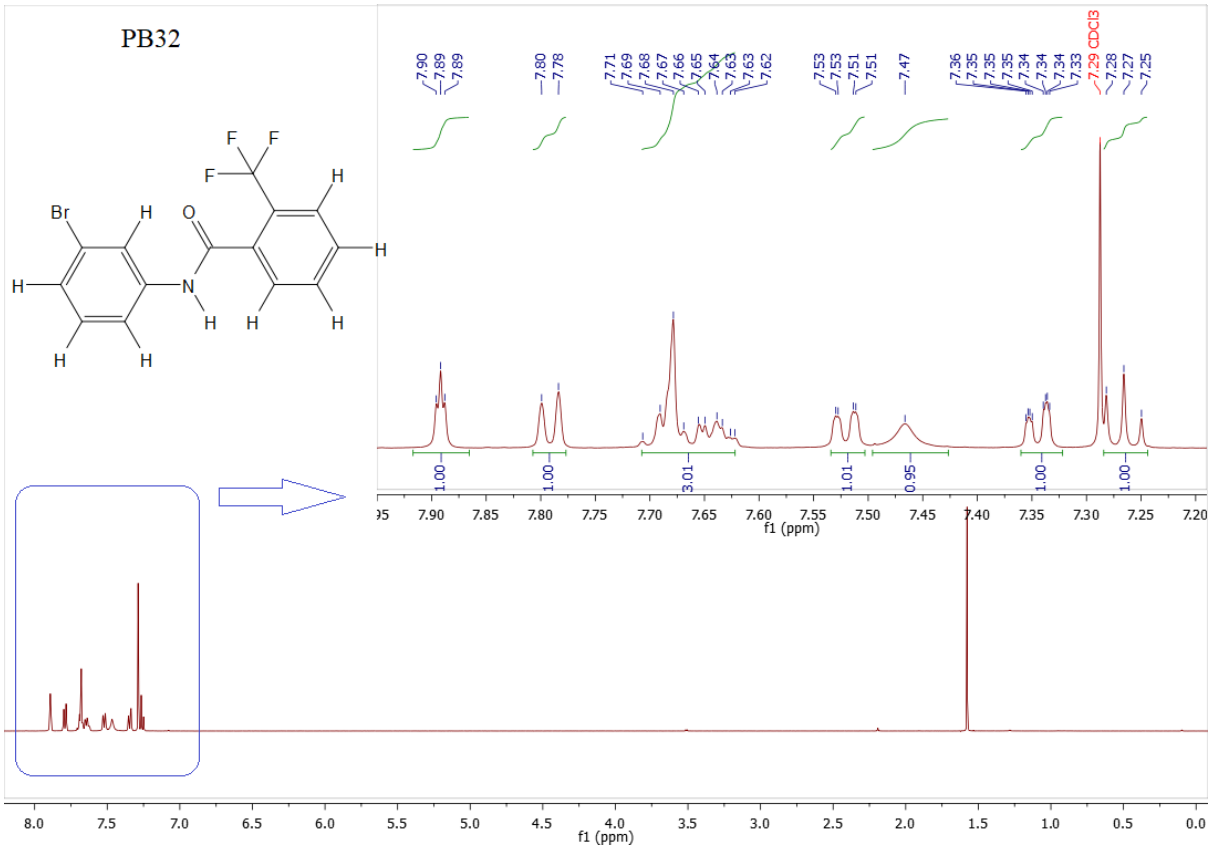

PC43
F
F
F
H
H
H
O
H
Cl
N
H
H
H
H
H
H
8.11
8.07
8.02
8.00
7.78
7.76
7.60
7.58
7.55
7.31
7.29
7.29
7.24 CDCl3
2.00
1.00
1.00
3.01
2.00
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

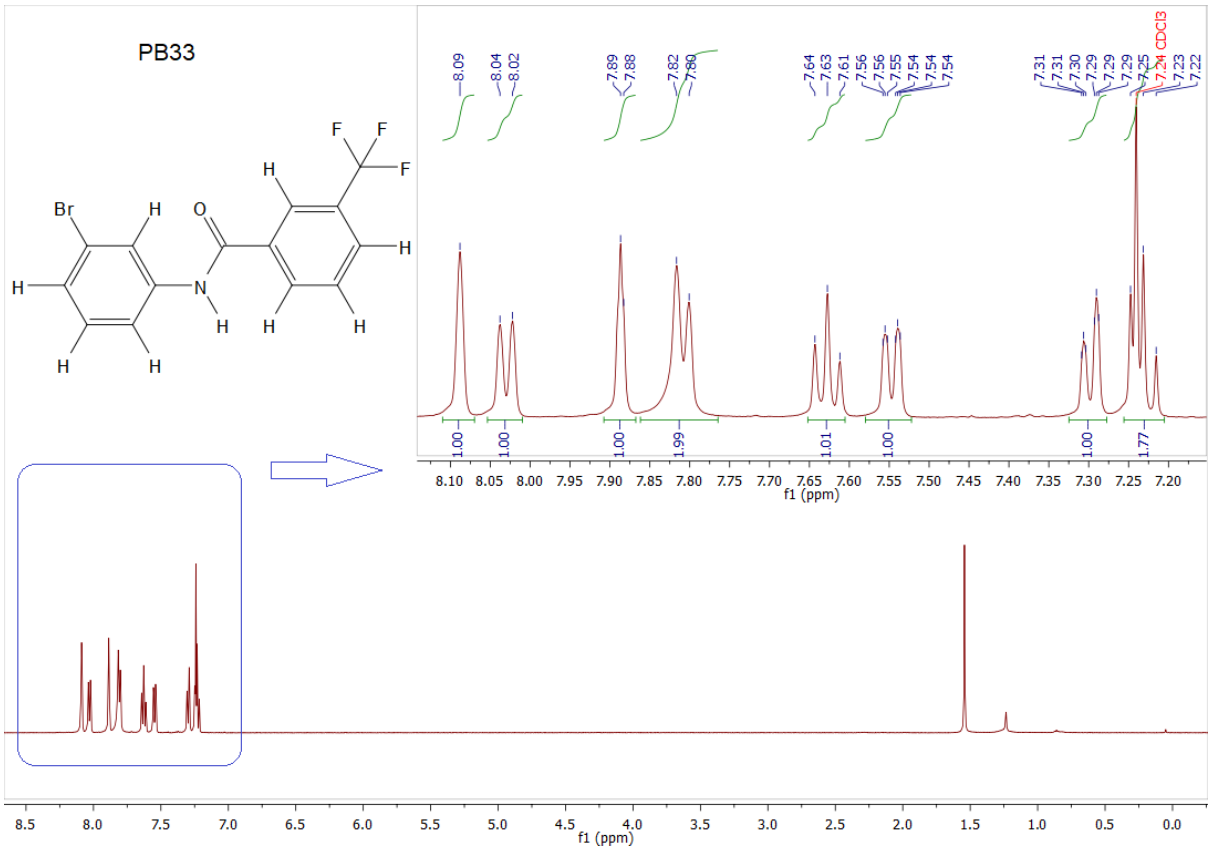

PC44
9.80
9.74
7.96
7.94
7.93
7.91
7.62
7.60
7.58
7.57
7.56
7.24 CDCl3
7.17
7.16
7.14
7.13
0.98
2.00
4.01
2.00
f1 (ppm)

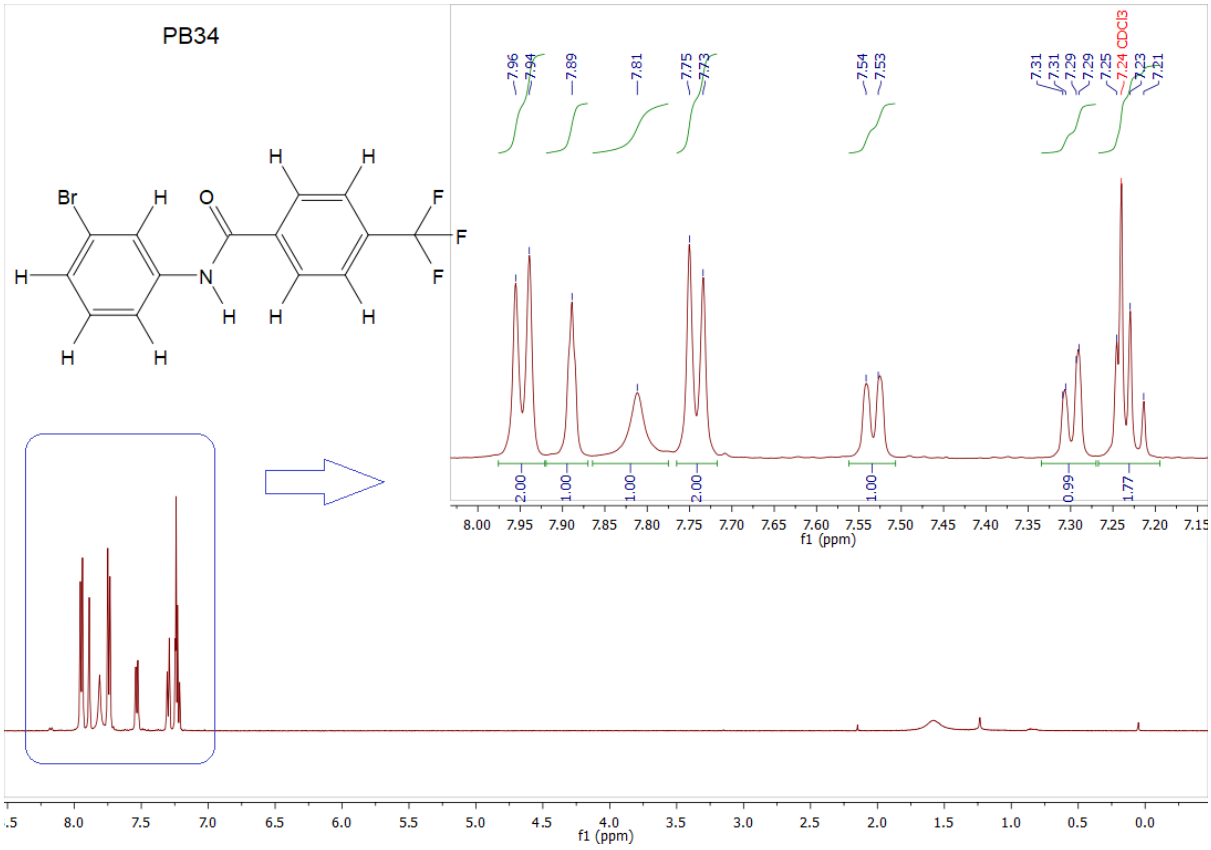

PB22
8.52
8.52
8.50
8.50
7.93
7.83
7.81
7.74
7.72
7.71
7.69
7.67
7.66
7.64
7.62
7.62
7.60
7.60
7.43
7.42
7.41
7.29 CDCl3
7.10
7.10
7.09
7.08
7.07
7.07
1.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
f1 (ppm)

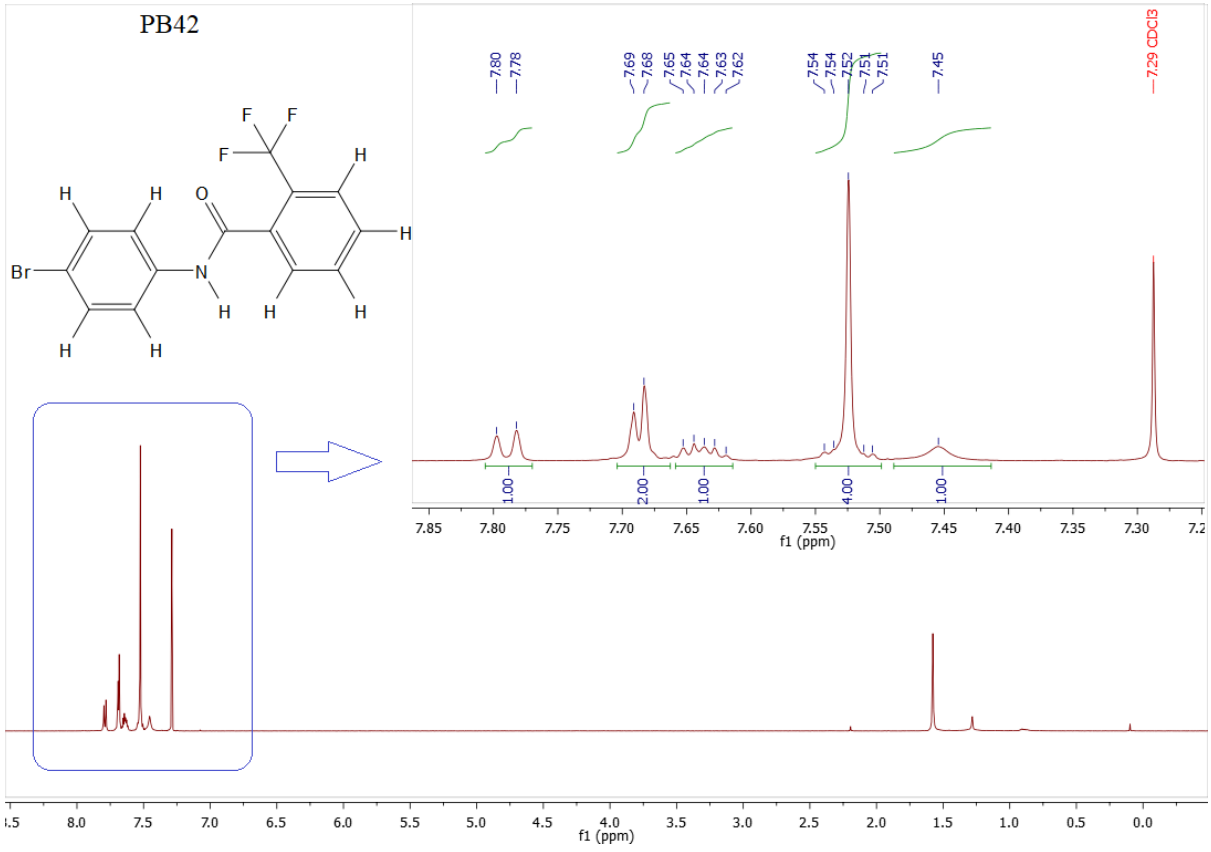

PB23
f1 (ppm)

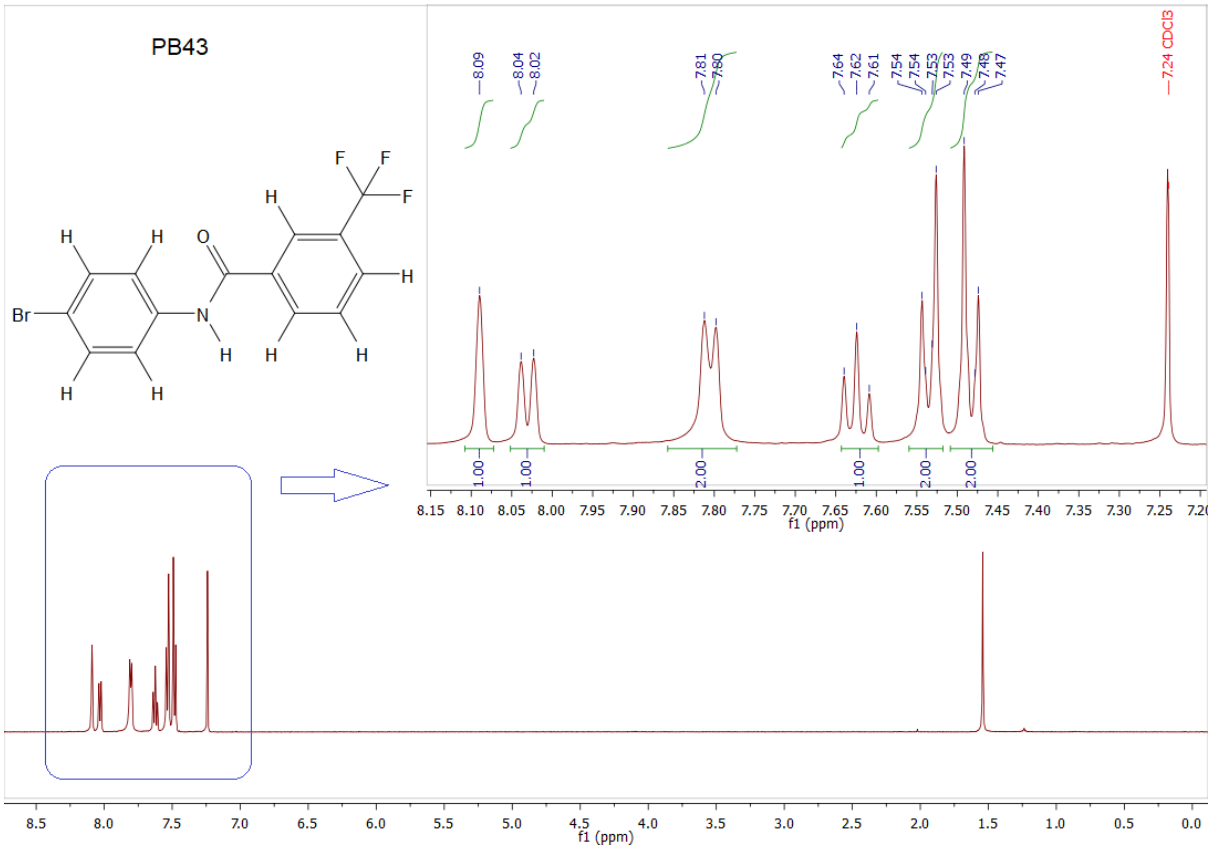

PB24
f1 (ppm)

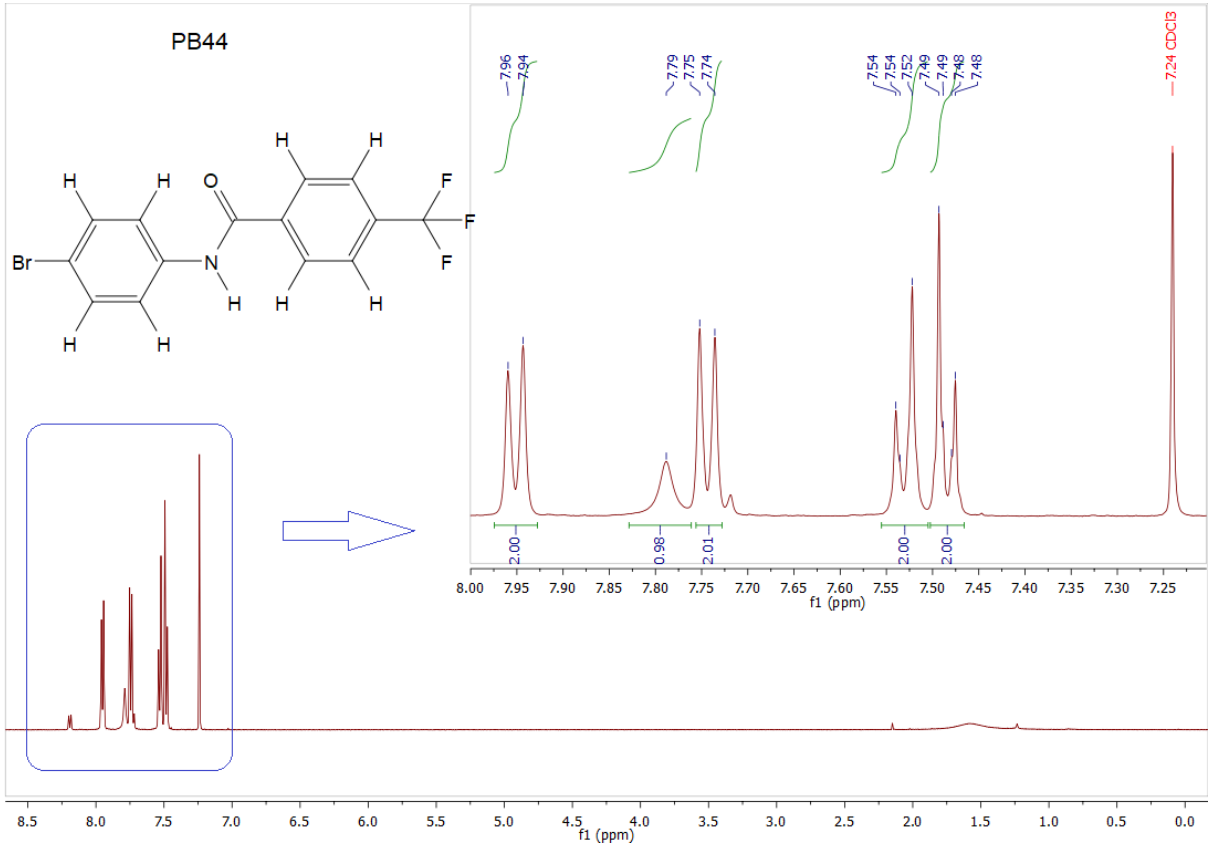

PB32
7.90
7.89
7.89
7.80
7.78
7.71
7.69
7.68
7.67
7.66
7.65
7.64
7.63
7.63
7.62
7.53
7.53
7.51
7.51
7.47
7.36
7.35
7.35
7.35
7.34
7.34
7.34
7.33
7.29 CDCl3
7.28
7.27
7.25
1.00
1.00
3.01
1.01
0.95
1.00
1.00
f1 (ppm)

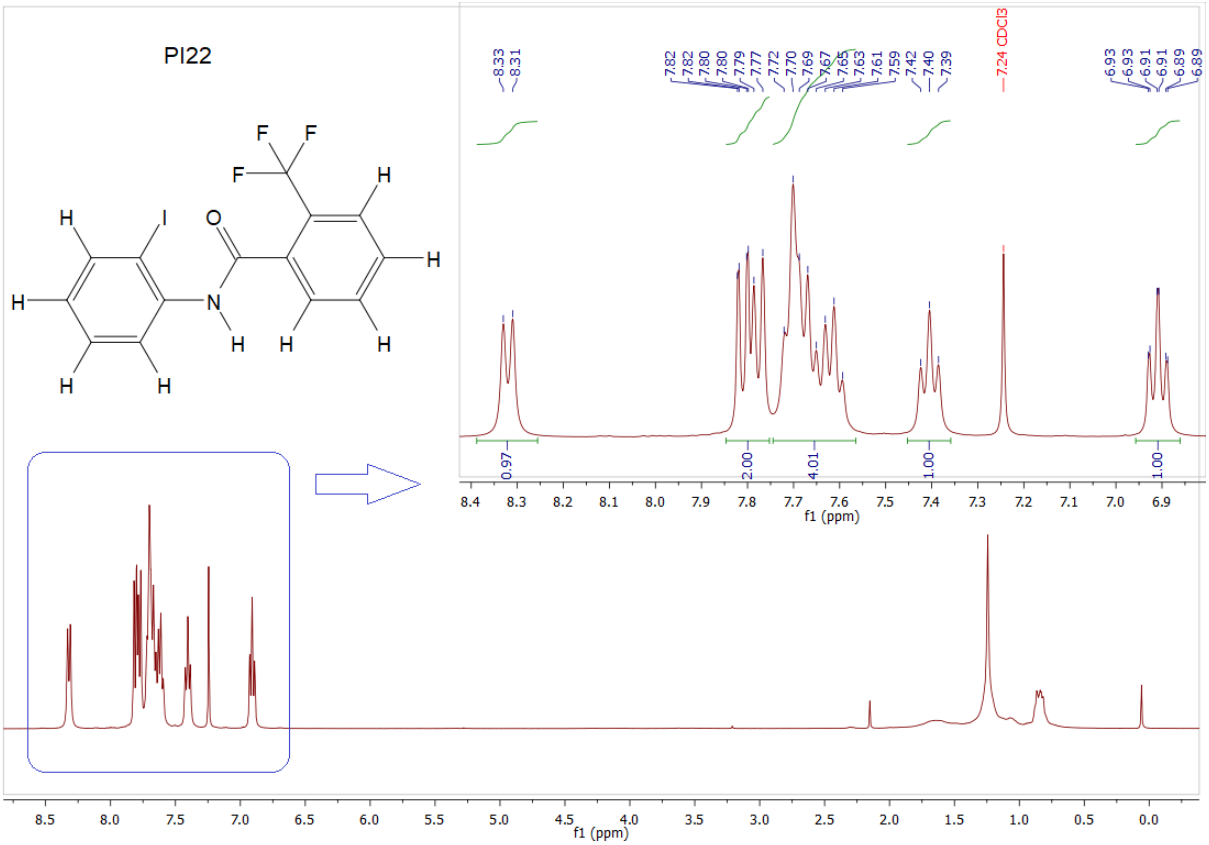

PB33
8.09
8.04
8.02
7.89
7.88
7.82
7.80
7.64
7.63
7.61
7.56
7.55
7.54
7.54
7.54
7.31
7.31
7.30
7.29
7.29
7.29
7.25
7.24 CDCl3
7.23
7.22
1.00
1.00
1.00
1.99
1.01
1.00
1.00
1.77
f1 (ppm)

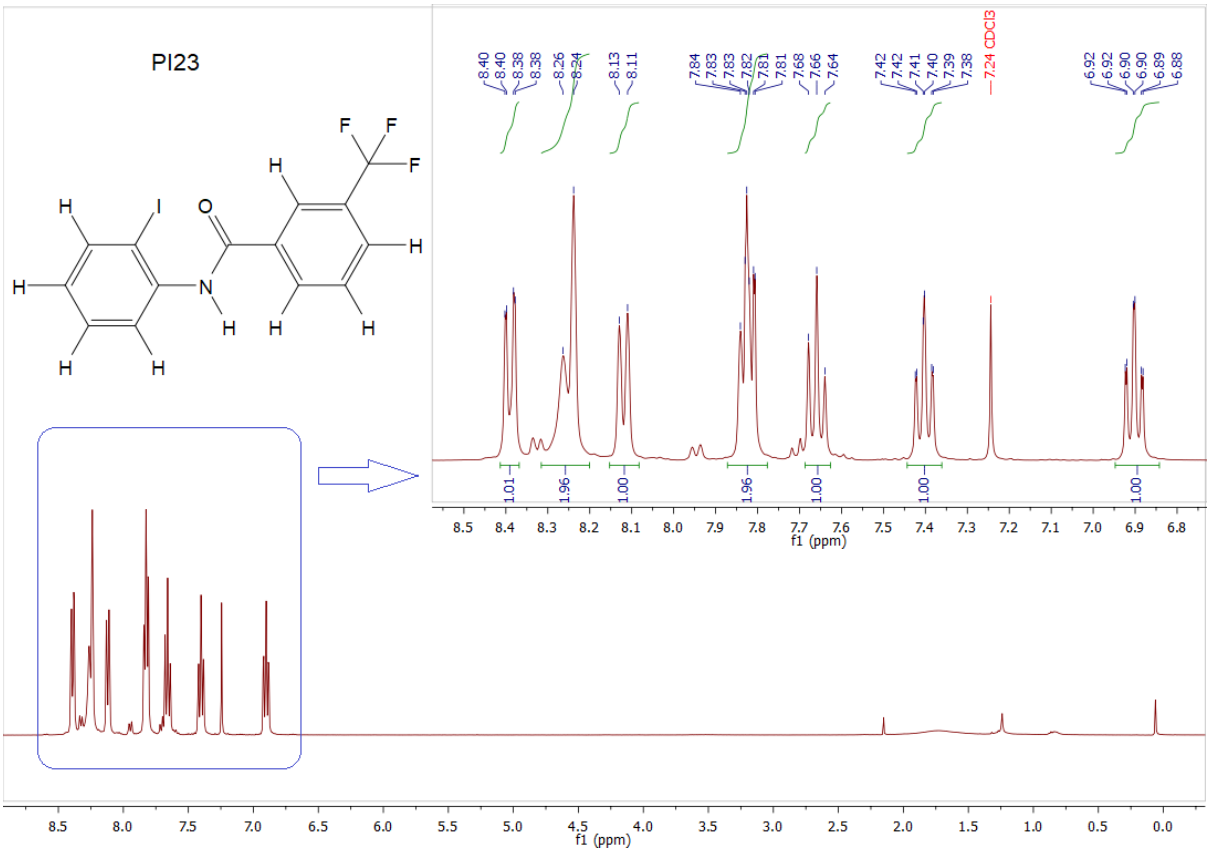

PB34
Br
H
O
F
F
F
N
H
7.96
7.94
7.89
7.81
7.75
7.73
7.54
7.53
7.31
7.31
7.29
7.29
7.25
7.24 CDCl3
7.23
7.21
2.00
1.00
1.00
2.00
1.00
0.99
1.77
f1 (ppm)

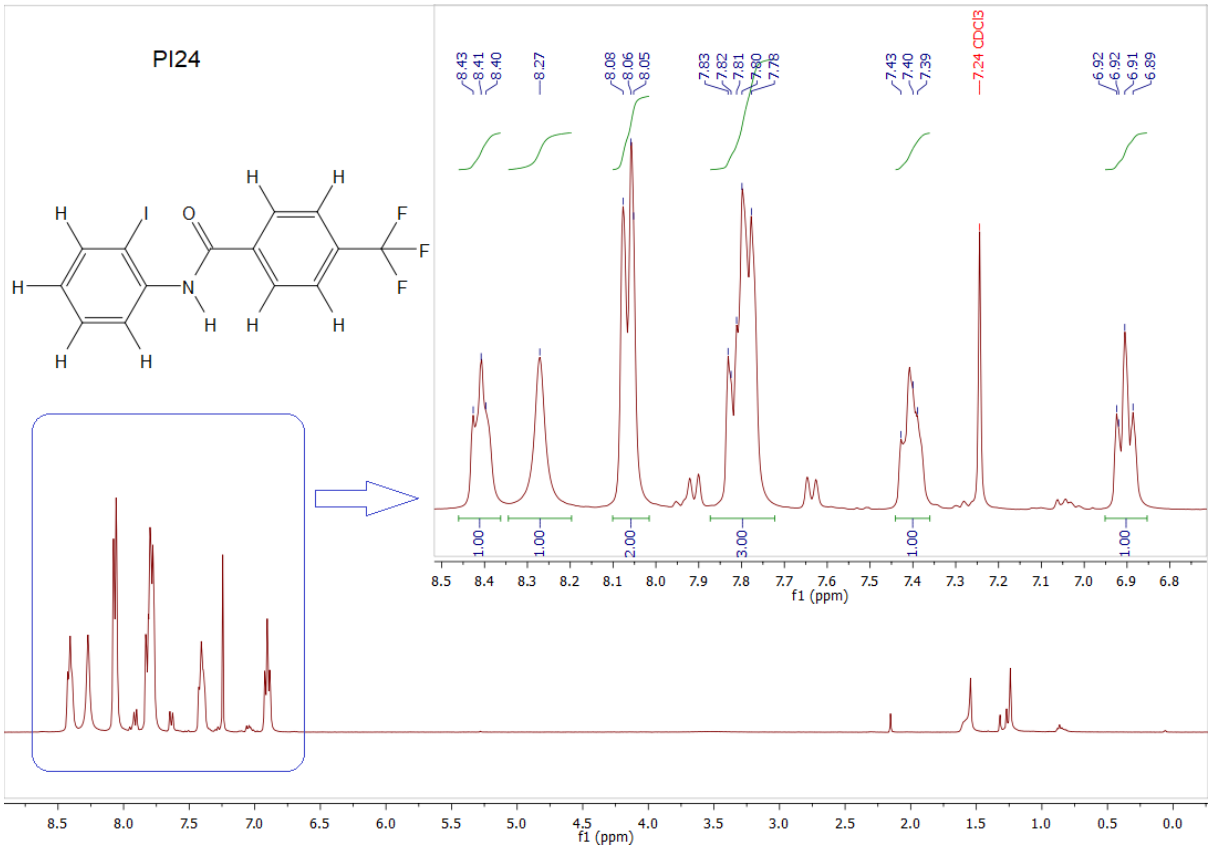

PB42
F
F
F
H
H
O
H
Br
N
H
7.80
7.78
7.69
7.68
7.65
7.64
7.64
7.63
7.62
7.54
7.54
7.52
7.51
7.51
7.45
7.29 CDCl3
1.00
2.00
1.00
4.00
1.00
f1 (ppm)

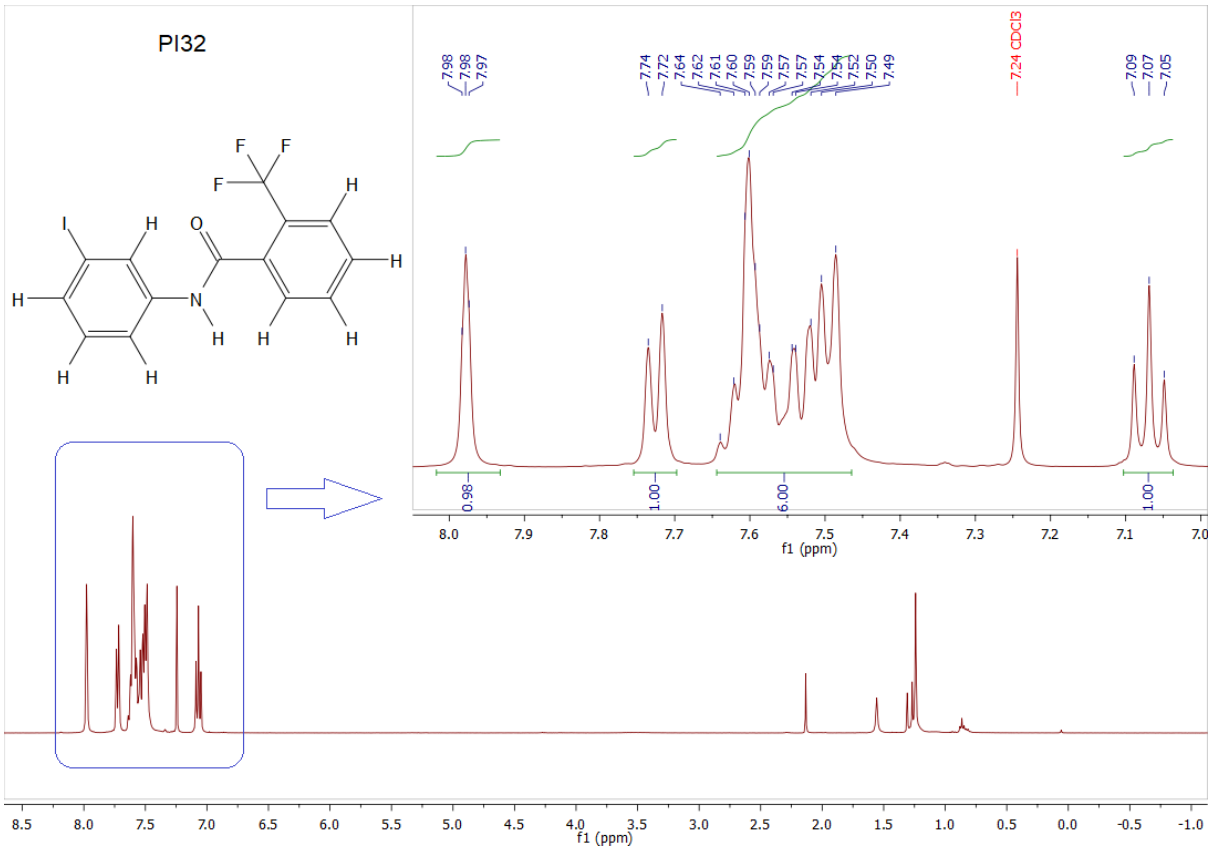

PB43
8.09
8.04
8.02
7.81
7.80
7.64
7.62
7.61
7.54
7.54
7.53
7.53
7.49
7.48
7.47
7.24 CDCl3
1.00
1.00
2.00
1.00
2.00
2.00
f1 (ppm)

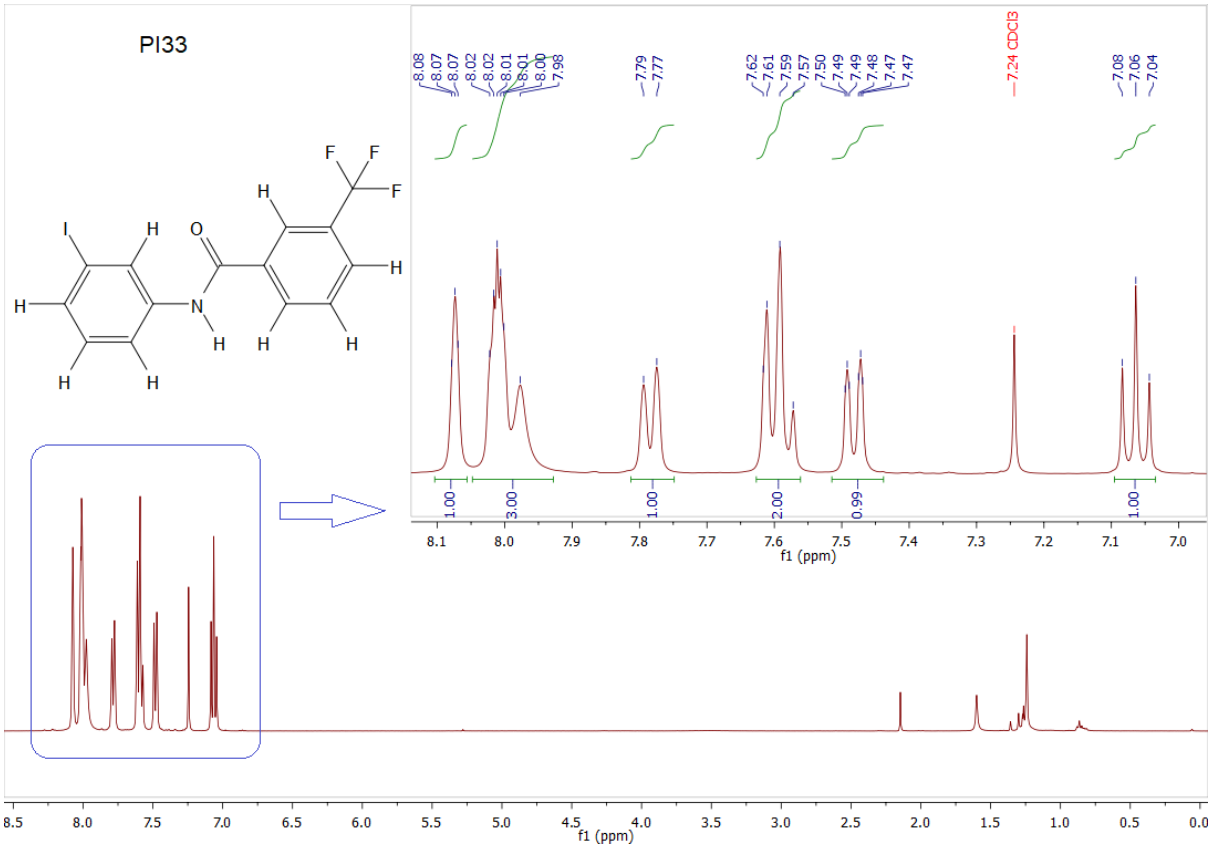

PB44
7.96
7.94
7.79
7.75
7.74
7.54
7.54
7.52
7.49
7.49
7.48
7.48
7.24 CDCl3
2.00
0.98
2.01
2.00
2.00
f1 (ppm)

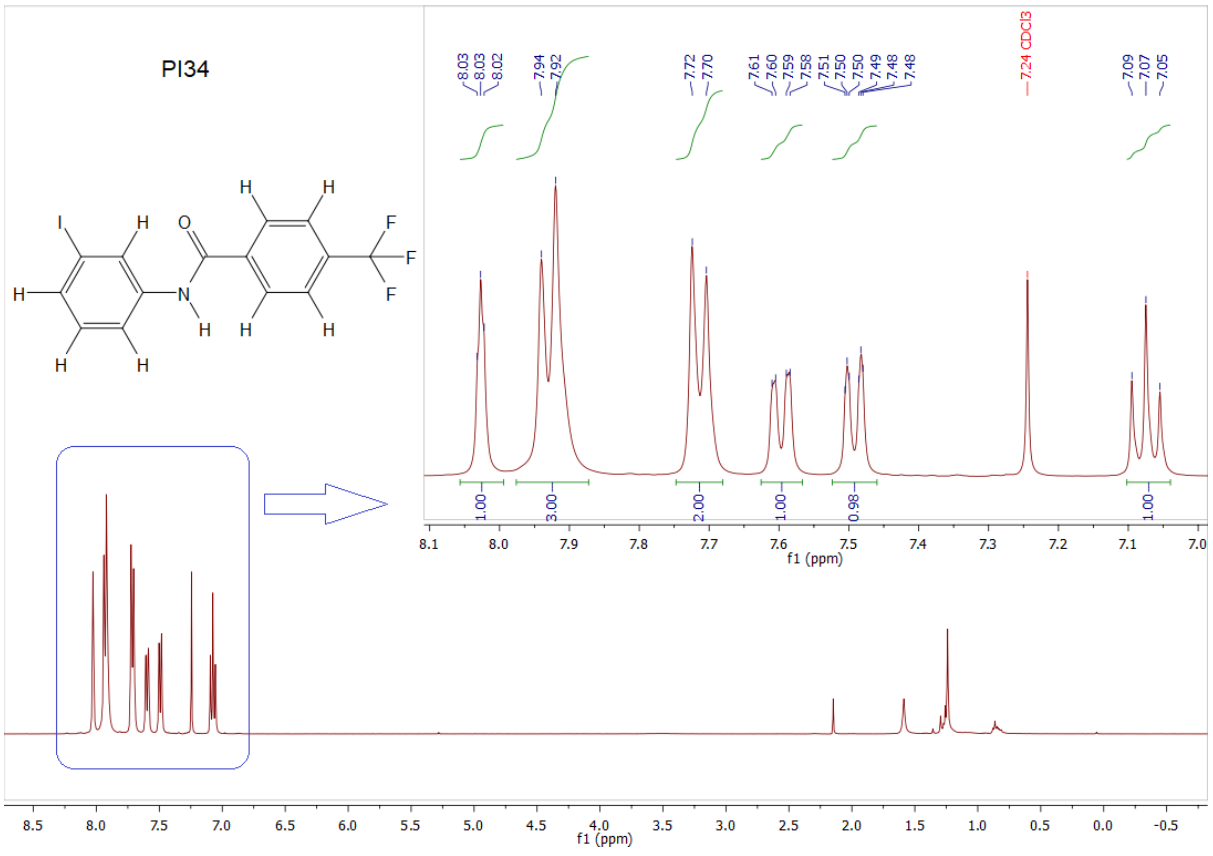

PI22
8.33
8.31
7.82
7.82
7.80
7.80
7.79
7.77
7.72
7.70
7.69
7.67
7.65
7.63
7.61
7.59
7.42
7.40
7.39
7.24 CDCl3
6.93
6.93
6.91
6.91
6.89
6.89
0.97
2.00
4.01
1.00
1.00
f1 (ppm)

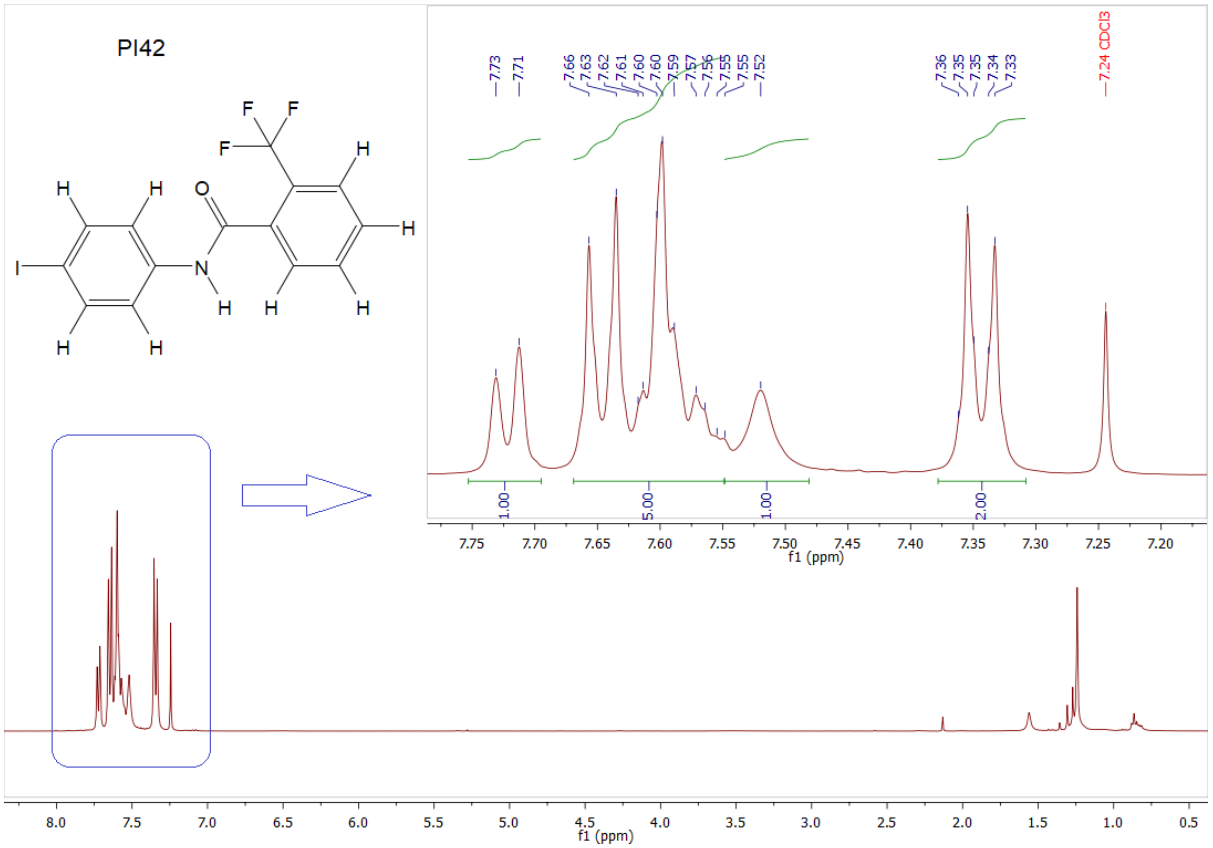

PI23
8.40
8.40
8.38
8.38
8.26
8.24
8.13
8.11
7.84
7.83
7.83
7.82
7.81
7.81
7.68
7.66
7.64
7.42
7.42
7.41
7.40
7.39
7.38
7.24 CDCl3
6.92
6.92
6.90
6.90
6.89
6.88
1.01
1.96
1.00
1.96
1.00
1.00
1.00
f1 (ppm)

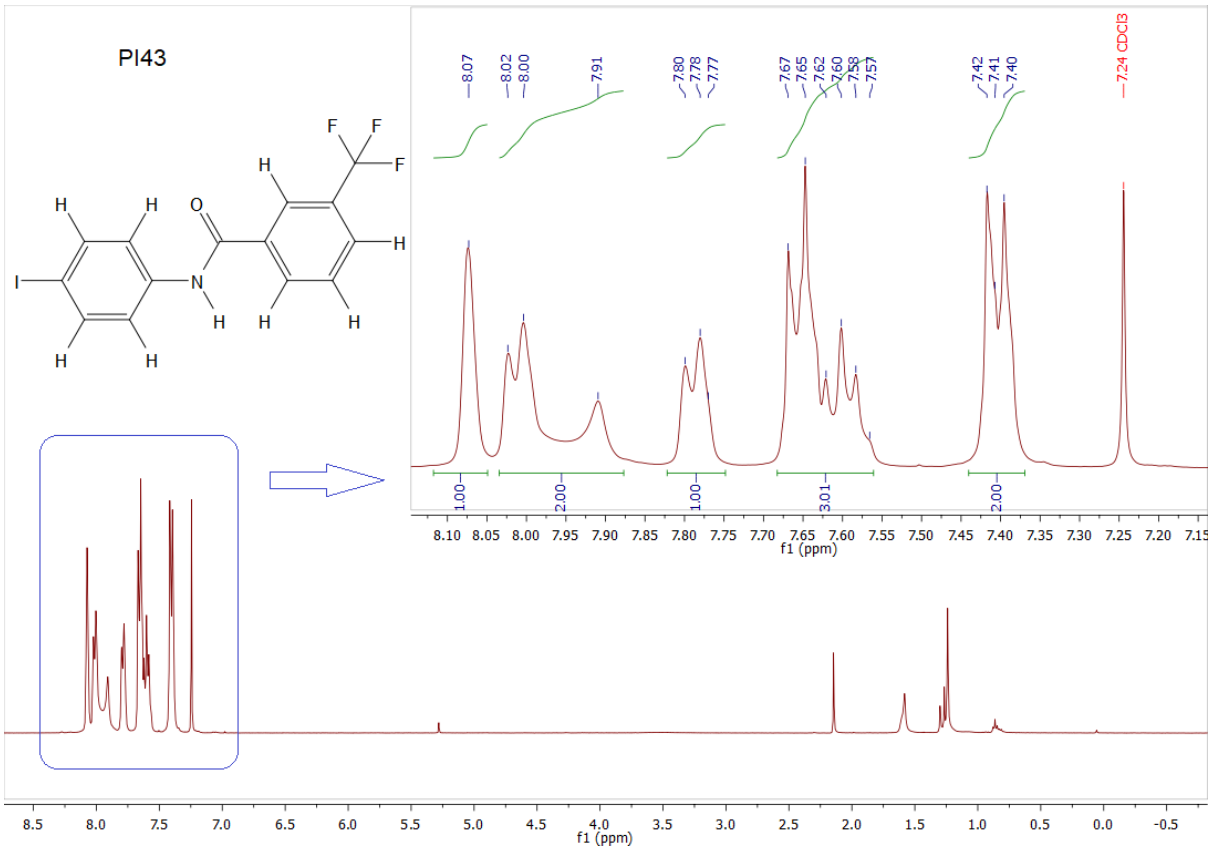

PI24
8.43
8.41
8.40
8.27
8.08
8.06
8.05
7.83
7.82
7.81
7.80
7.78
7.43
7.40
7.39
7.24 CDCl3
6.92
6.92
6.91
6.89
1.00
1.00
2.00
3.00
1.00
1.00
f1 (ppm)


PI32
7.98
7.98
7.97
7.74
7.72
7.64
7.62
7.61
7.60
7.59
7.59
7.57
7.57
7.54
7.54
7.52
7.50
7.49
7.24 CDCl3
7.09
7.07
7.05
0.98
1.00
6.00
1.00
f1 (ppm)


PI33
8.08
8.07
8.07
8.02
8.02
8.01
8.01
8.00
7.98
7.79
7.77
7.62
7.61
7.59
7.57
7.50
7.49
7.49
7.48
7.47
7.47
7.24 CDCl3
7.08
7.06
7.04
1.00
3.00
1.00
2.00
0.99
1.00
f1 (ppm)


PI34
8.03
8.03
8.02
7.94
7.92
7.72
7.70
7.61
7.60
7.59
7.58
7.51
7.50
7.50
7.49
7.48
7.48
7.24 CDCl3
7.09
7.07
7.05
1.00
3.00
2.00
1.00
0.98
1.00
f1 (ppm)


PI42
7.73
7.71
7.66
7.63
7.62
7.61
7.60
7.60
7.59
7.57
7.56
7.55
7.55
7.52
7.36
7.35
7.35
7.34
7.33
7.24 CDCl3
1.00
5.00
1.00
2.00
f1 (ppm)


PI43
8.07
8.02
8.00
7.91
7.80
7.78
7.77
7.67
7.65
7.62
7.60
7.58
7.57
7.42
7.41
7.40
7.24 CDCl3
1.00
2.00
1.00
3.01
2.00
f1 (ppm)

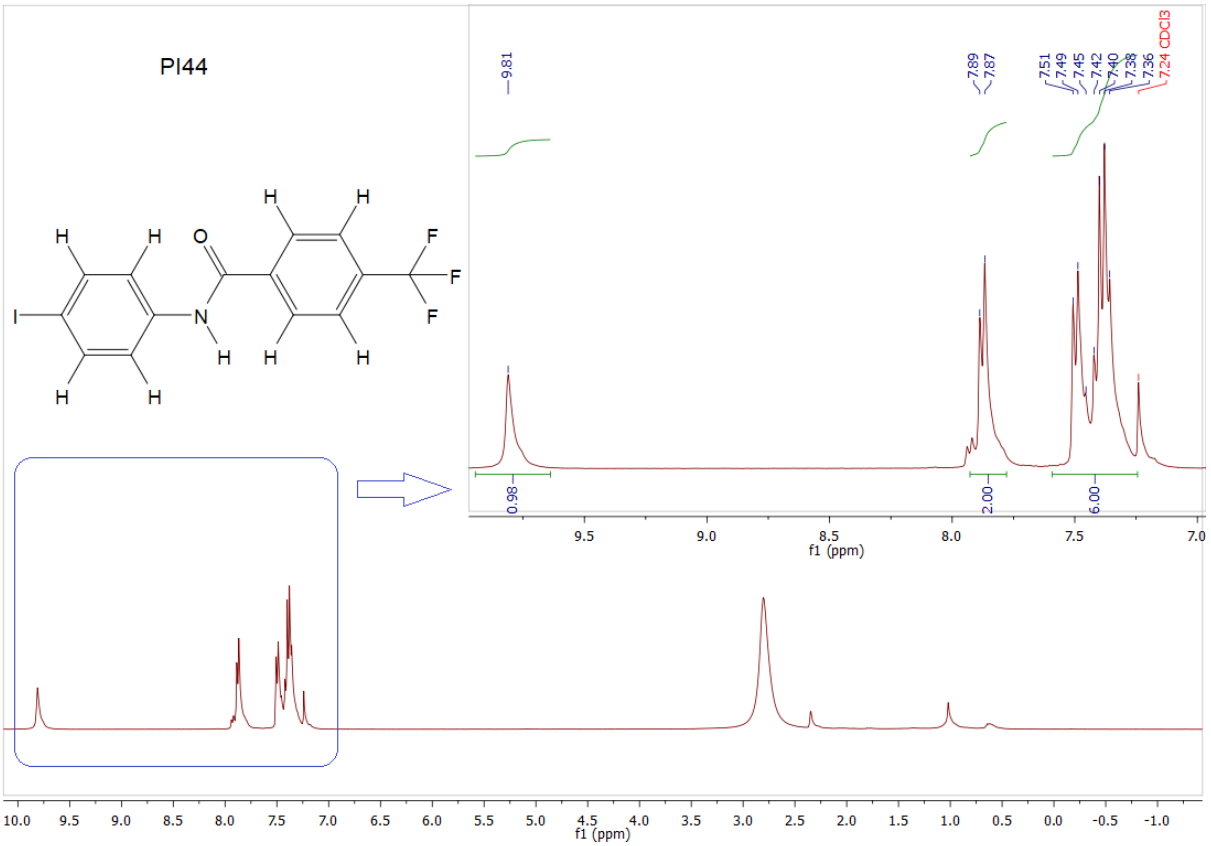
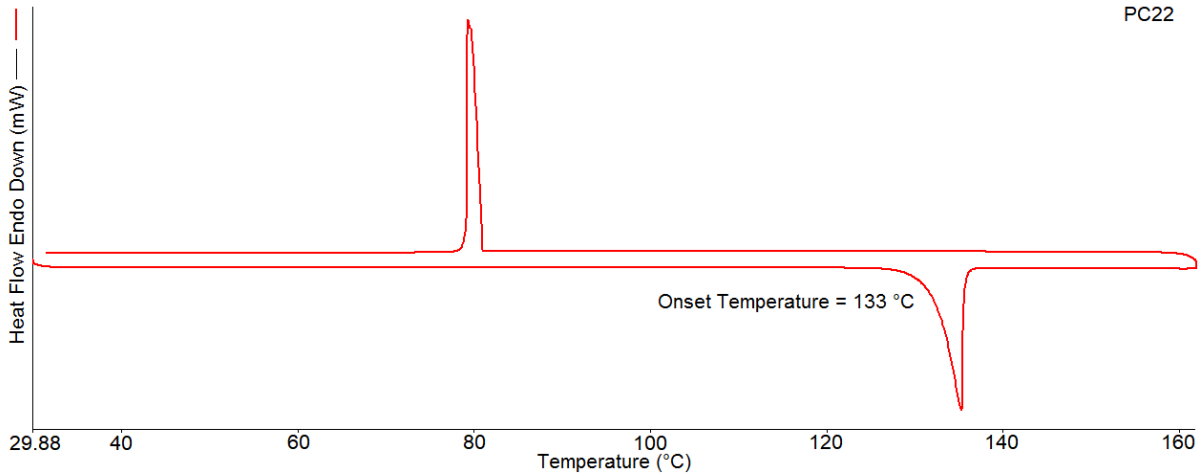
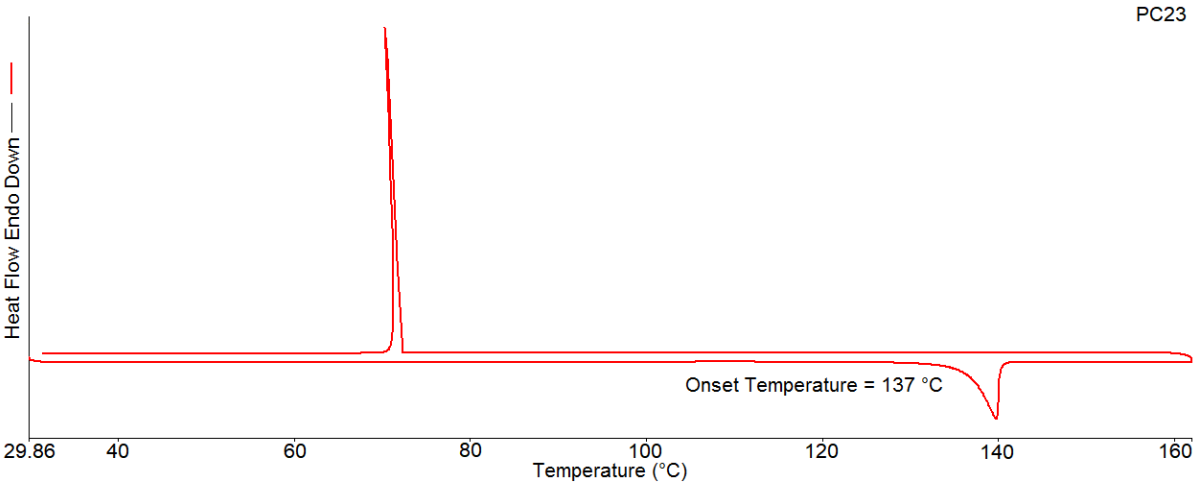
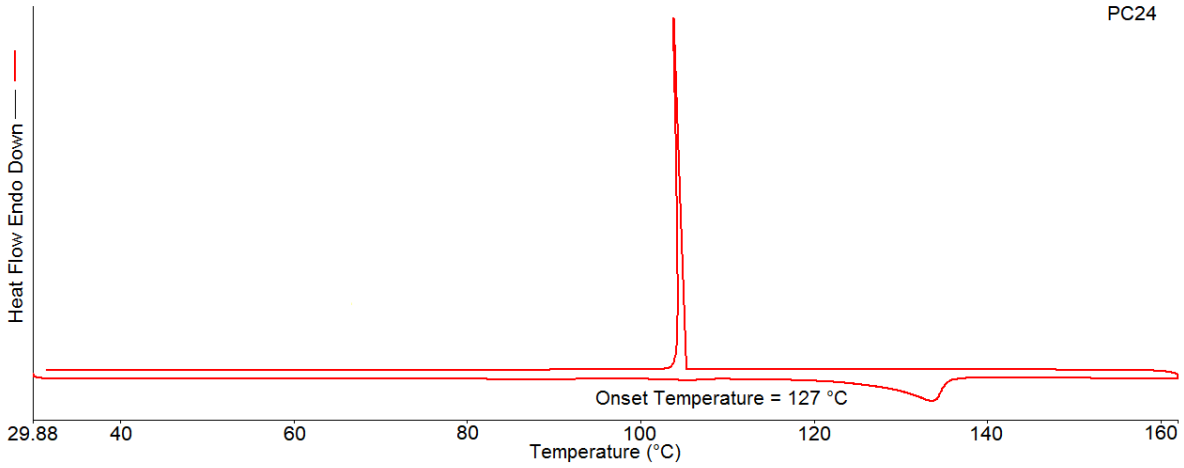
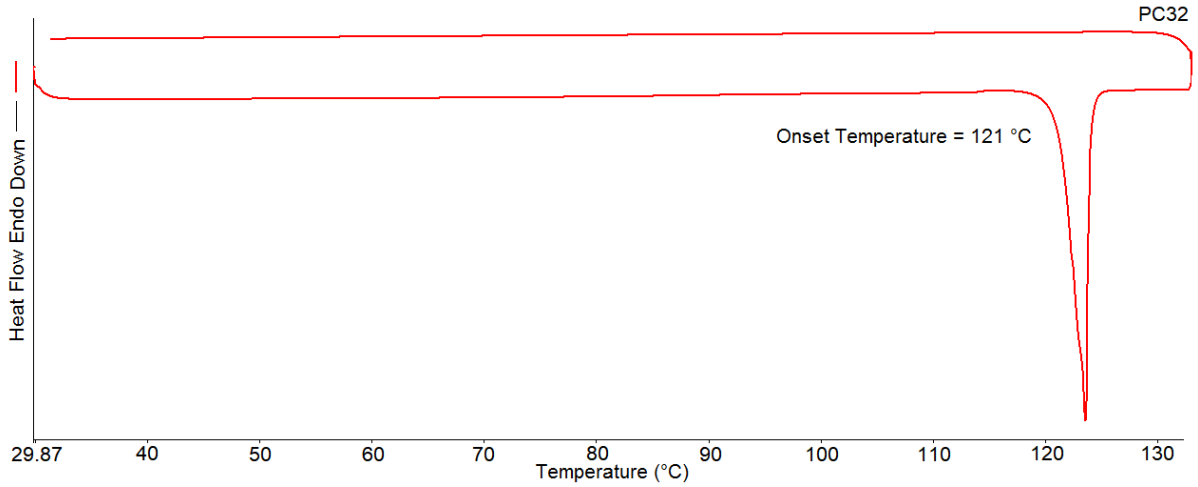


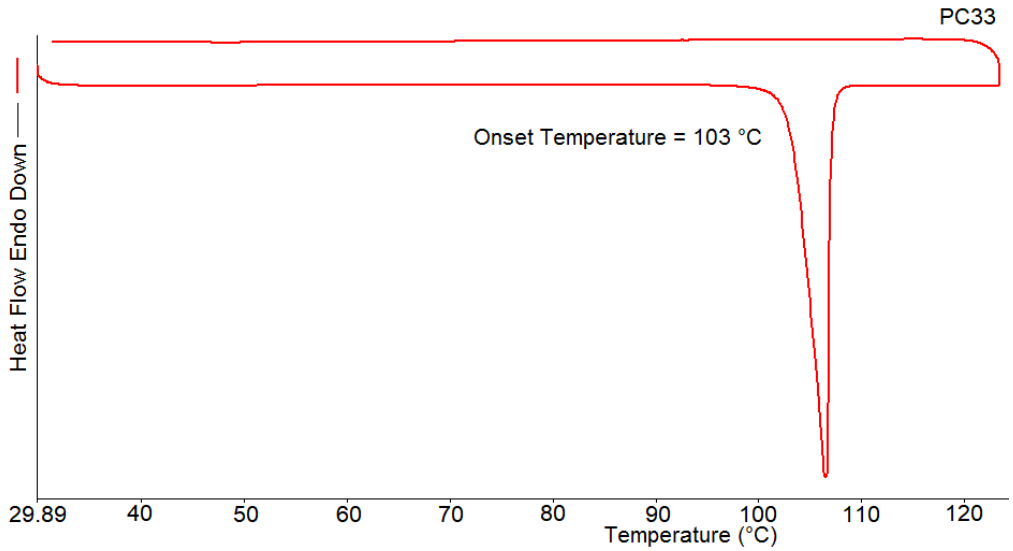
Figure S2 DSC traces of the newly synthesized bulk benzamide compounds @5 °C/min.

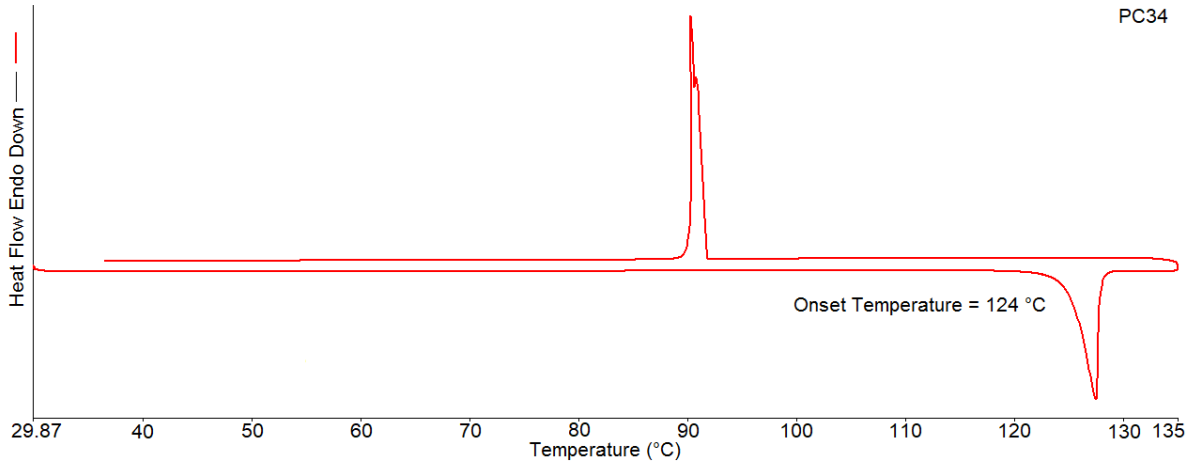


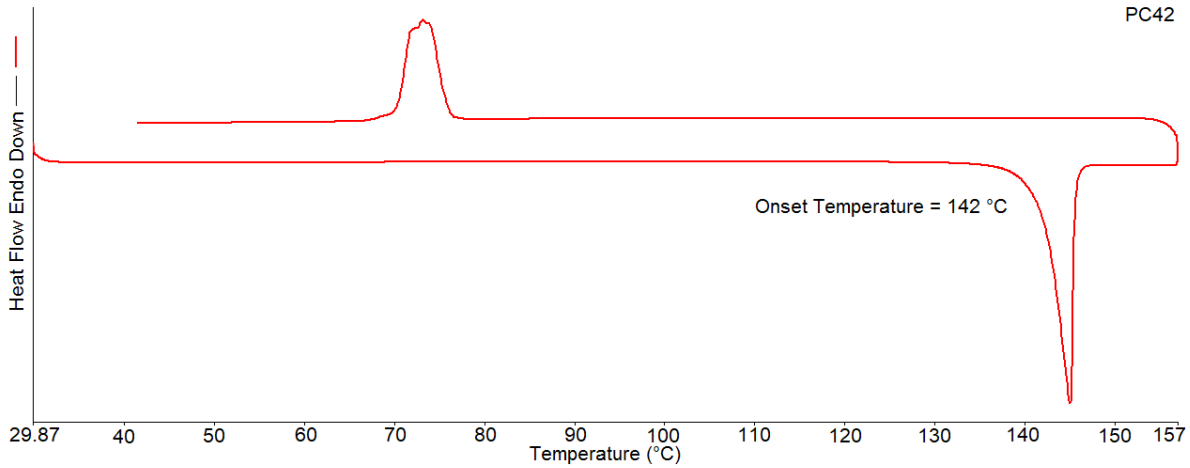

PC23
Heat Flow Endo Down
Onset Temperature = 137 °C
29.86
40
60
80
100
120
140
160
Temperature (°C)

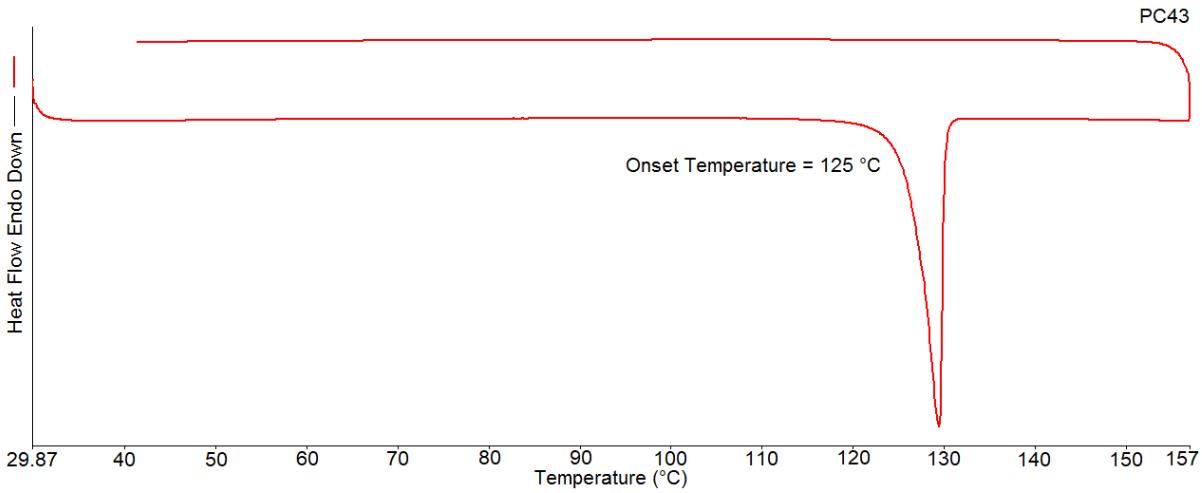

PC24
Heat Flow Endo Down
Onset Temperature = 127 °C
29.88
40
60
80
100
120
140
160
Temperature (°C)

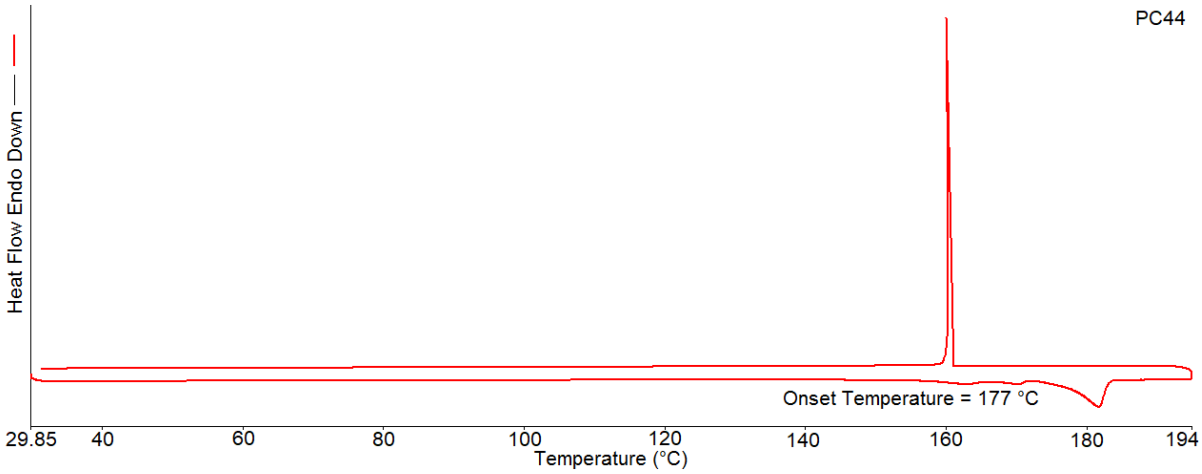

PC32
Heat Flow Endo Down
Onset Temperature = 121 °C
29.87
40
50
60
70
80
90
100
110
120
130
Temperature (°C)

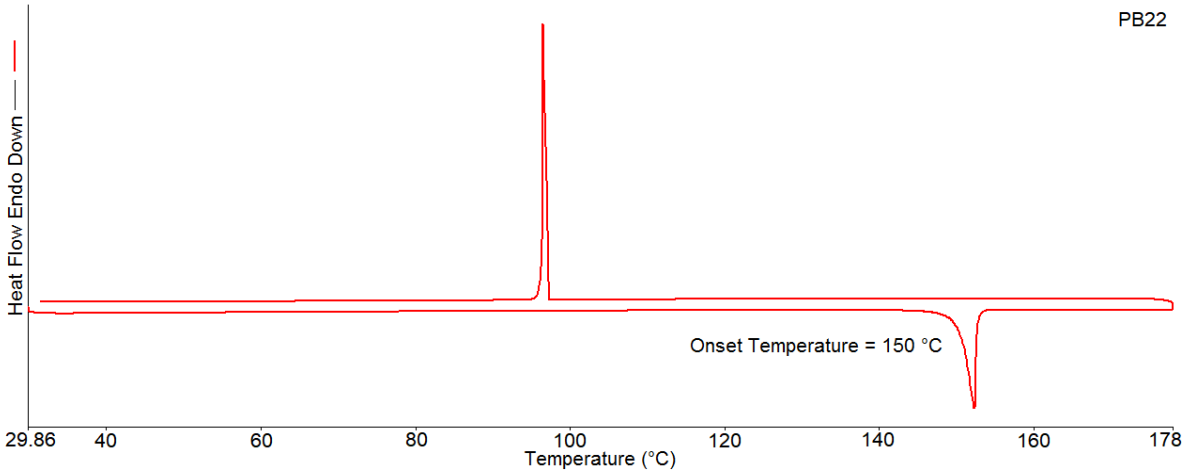

PC33
Onset Temperature = 103 °C
Heat Flow Endo Down
29.89
40
50
60
70
80
90
100
110
120
Temperature (°C)

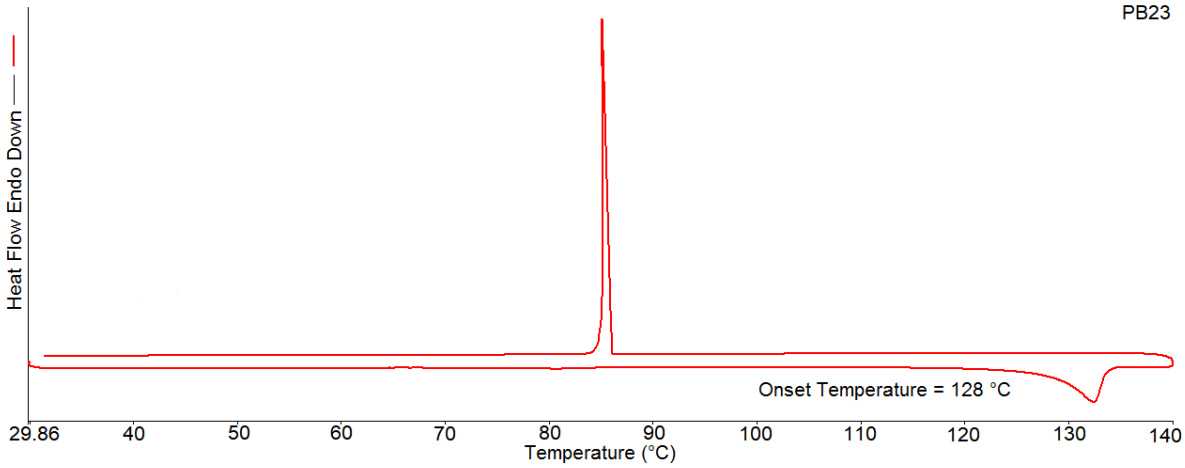

PC34
Onset Temperature = 124 °C
Heat Flow Endo Down
29.87
40
50
60
70
80
90
100
110
120
130
135
Temperature (°C)

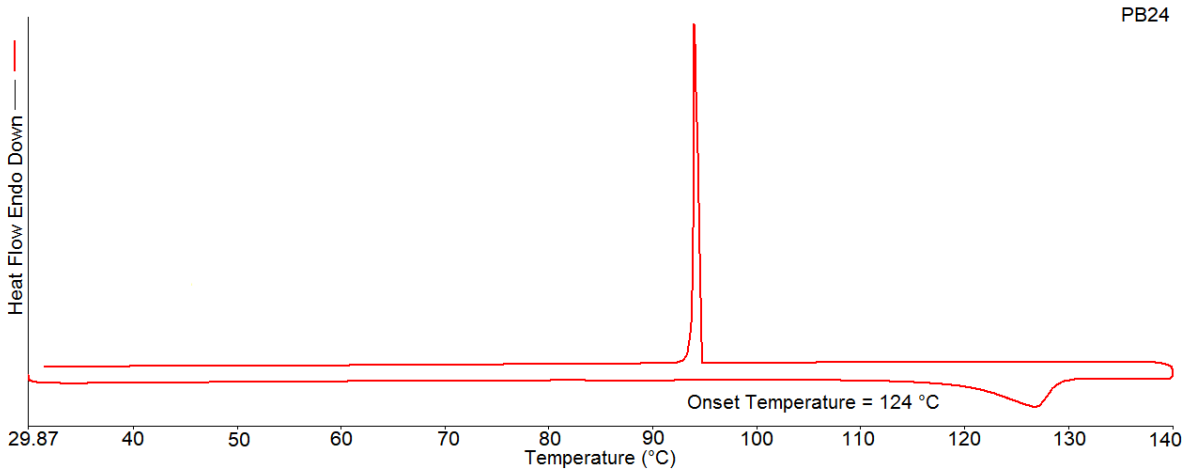

PC42
Onset Temperature = 142 °C
Heat Flow Endo Down
29.87
40
50
60
70
80
90
100
110
120
130
140
150
157
Temperature (°C)

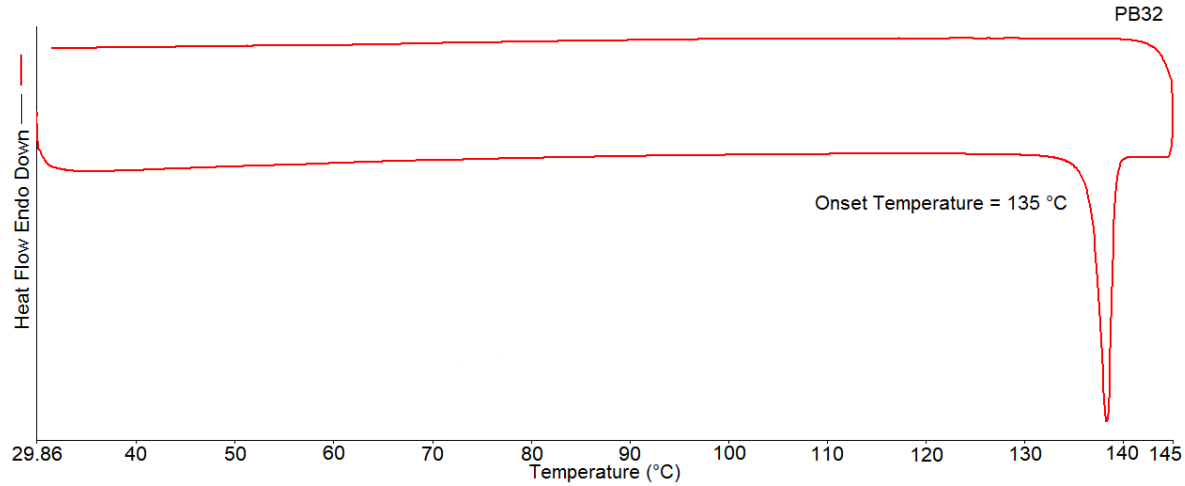

PC43
Heat Flow Endo Down
Onset Temperature = 125 °C
29.87
40
50
60
70
80
90
100
110
120
130
140
150
157
Temperature (°C)

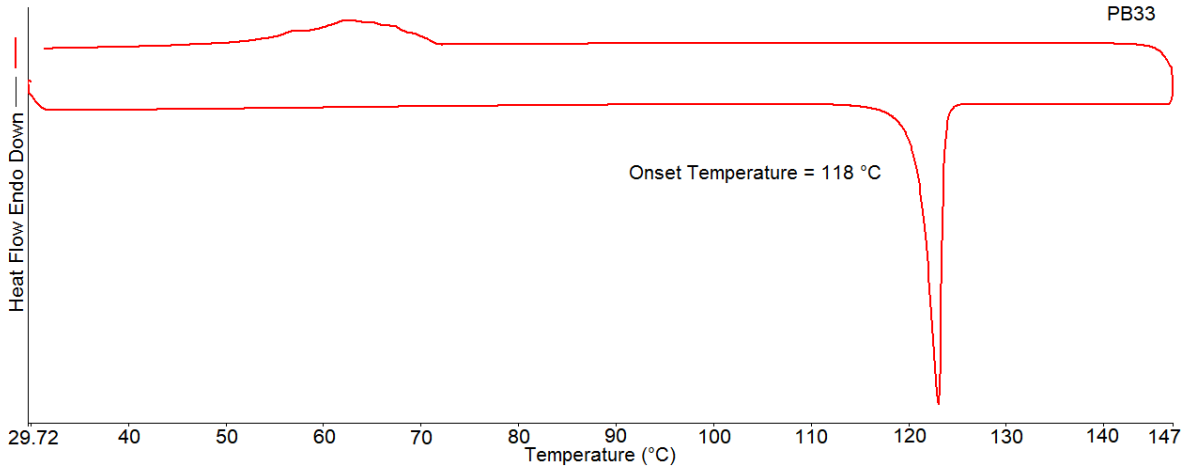

PC44
Heat Flow Endo Down
Onset Temperature = 177 °C
29.85
40
60
80
100
120
140
160
180
194
Temperature (°C)

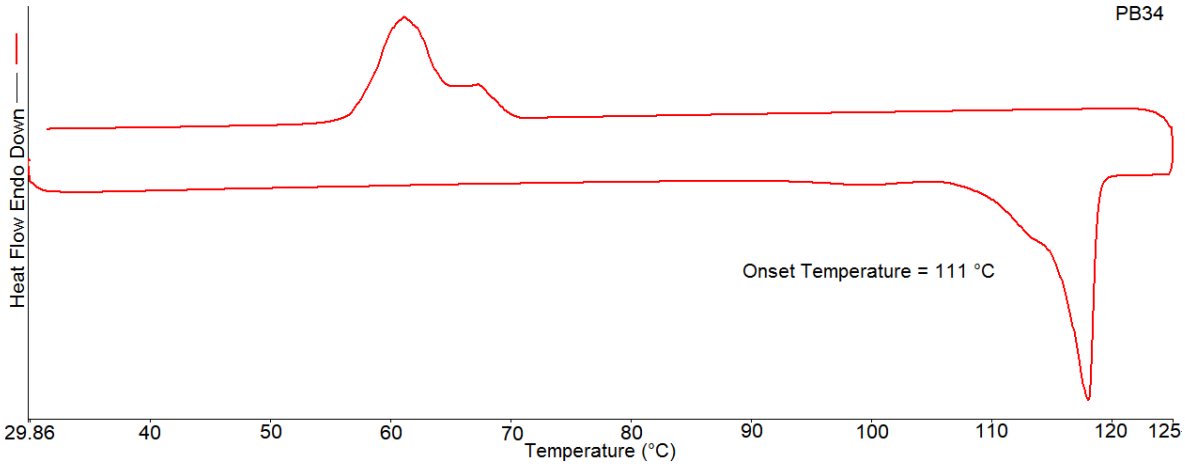

PB22
Heat Flow Endo Down
Onset Temperature = 150 °C
29.86
40
60
80
100
120
140
160
178
Temperature (°C)

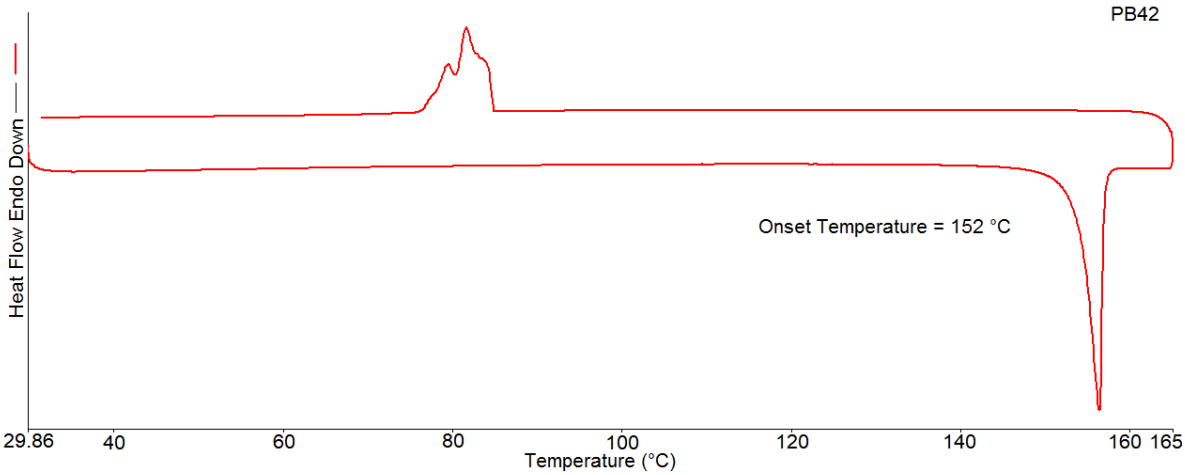

PB23
Heat Flow Endo Down
Onset Temperature = 128 °C
29.86 40 50 60 70 80 90 100 110 120 130 140
Temperature (°C)

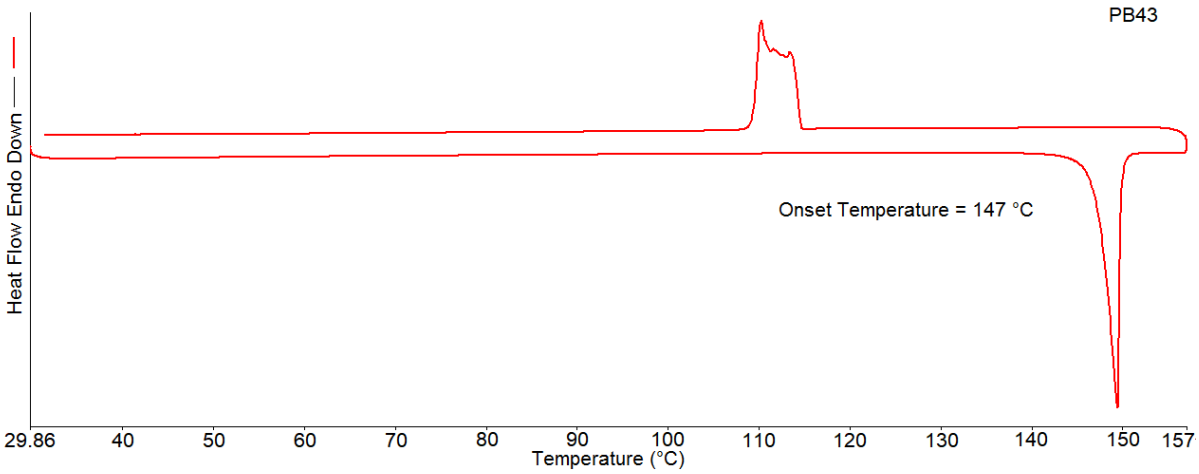

PB24
Heat Flow Endo Down
Onset Temperature = 124 °C
29.87 40 50 60 70 80 90 100 110 120 130 140
Temperature (°C)

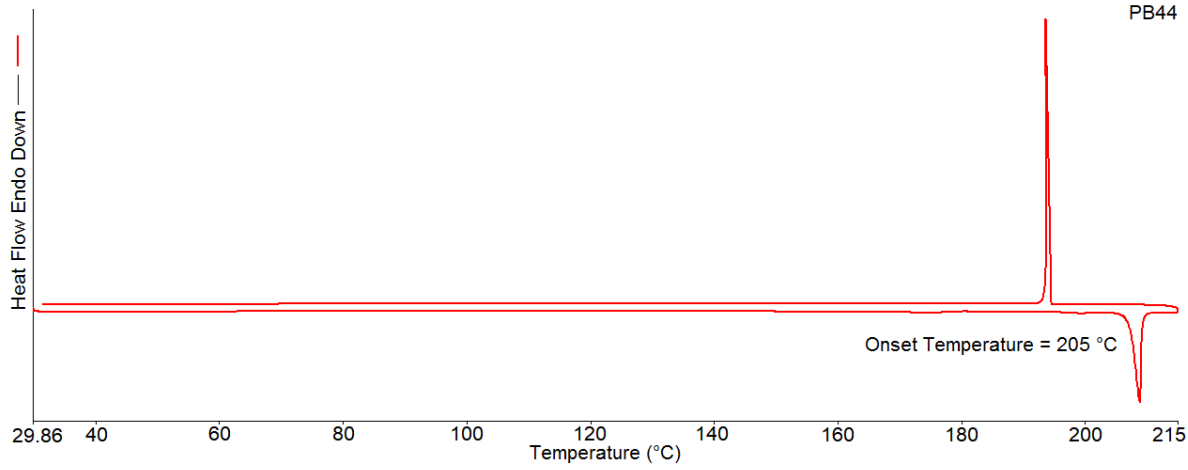

PB32
Heat Flow Endo Down
Onset Temperature = 135 °C
29.86 40 50 60 70 80 90 100 110 120 130 140 145
Temperature (°C)

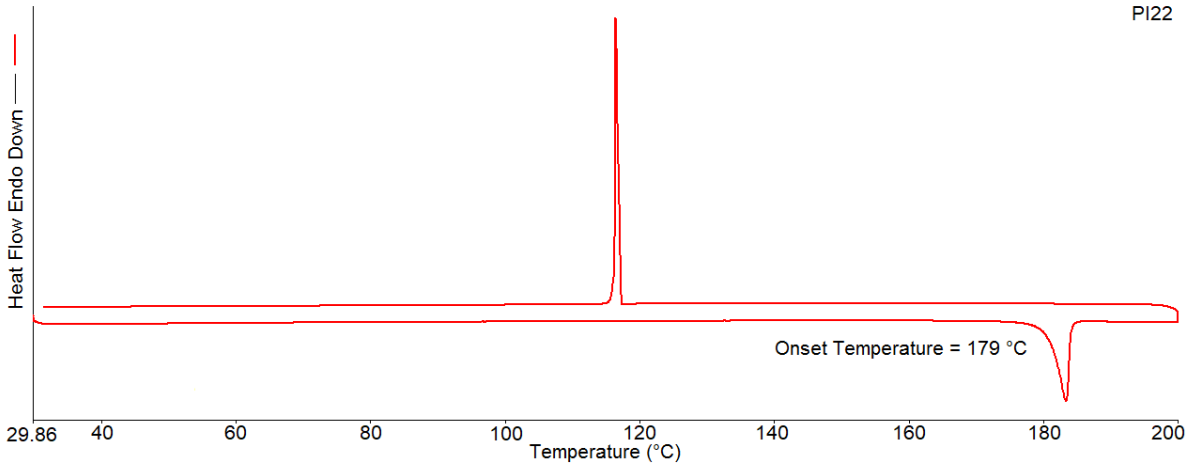

PB33
Heat Flow Endo Down
Onset Temperature = 118 °C
29.72 40 50 60 70 80 90 100 110 120 130 140 147
Temperature (°C)

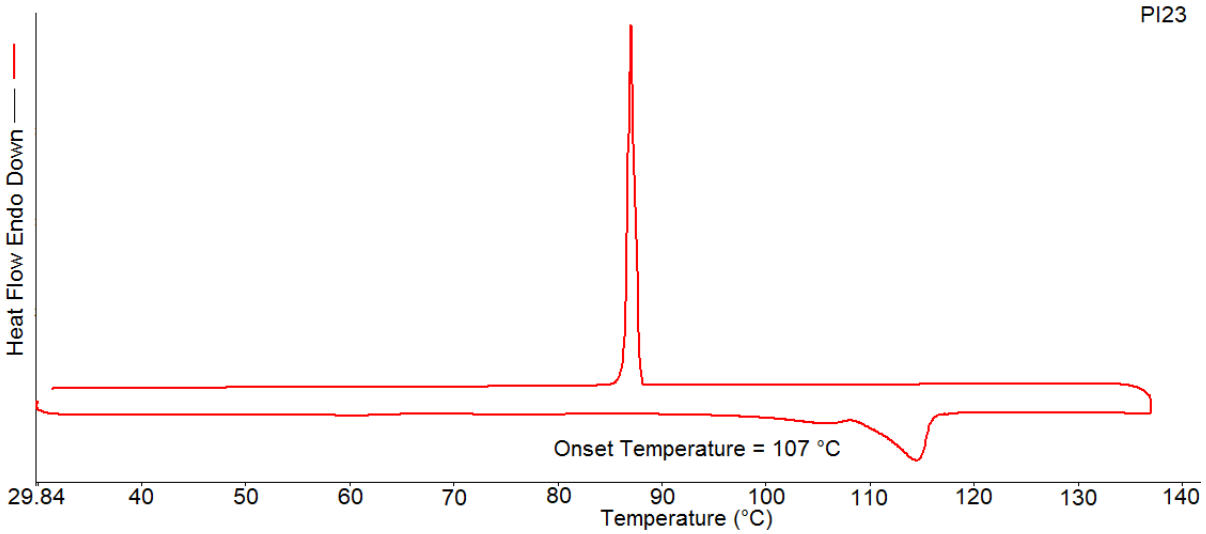

PB34
Heat Flow Endo Down
Onset Temperature = 111 °C
29.86 40 50 60 70 80 90 100 110 120 125
Temperature (°C)

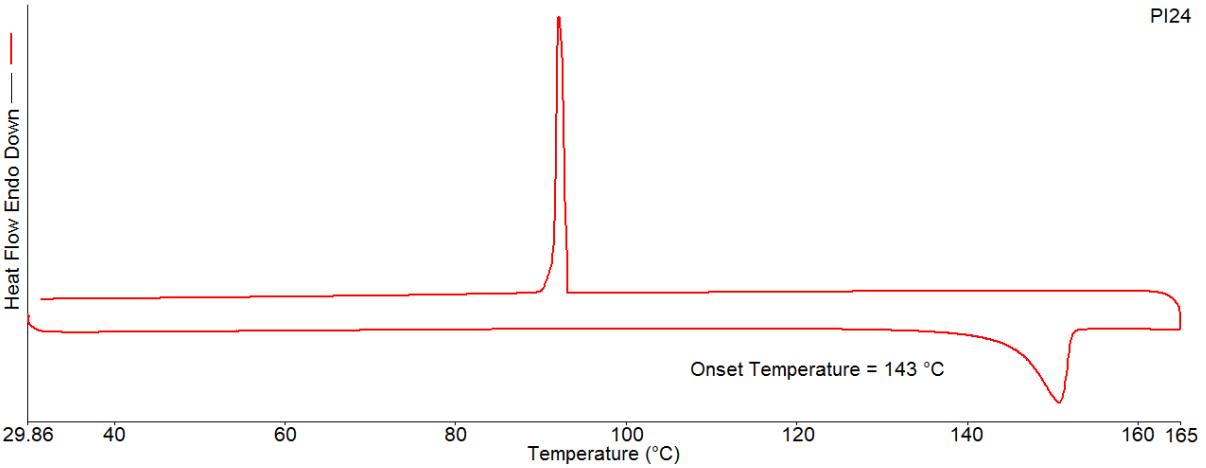

PB42
Heat Flow Endo Down
Onset Temperature = 152 °C
29.86 40 60 80 100 120 140 160 165
Temperature (°C)

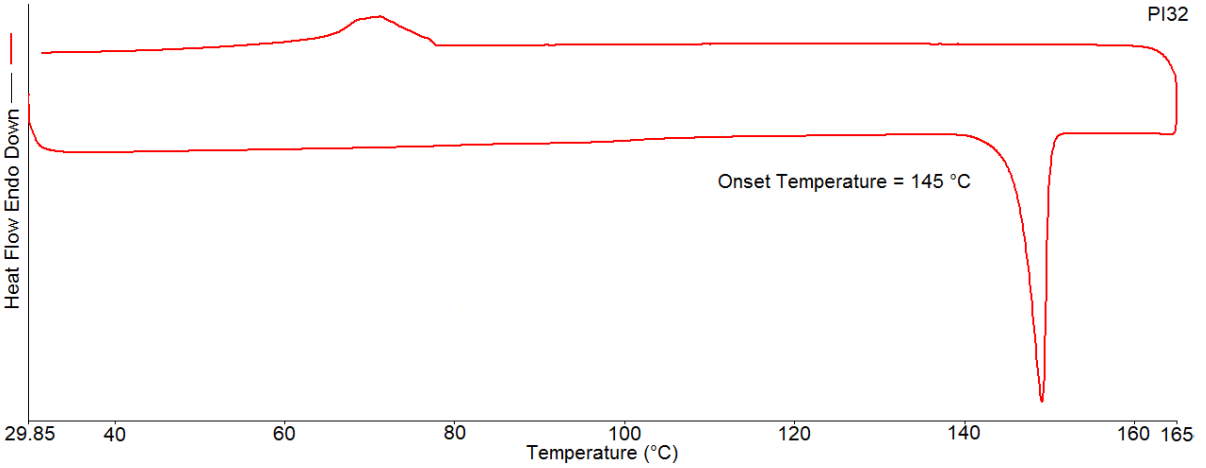

PB43
Heat Flow Endo Down
Onset Temperature = 147 °C
29.86
40
50
60
70
80
90
100
110
120
130
140
150
157
Temperature (°C)

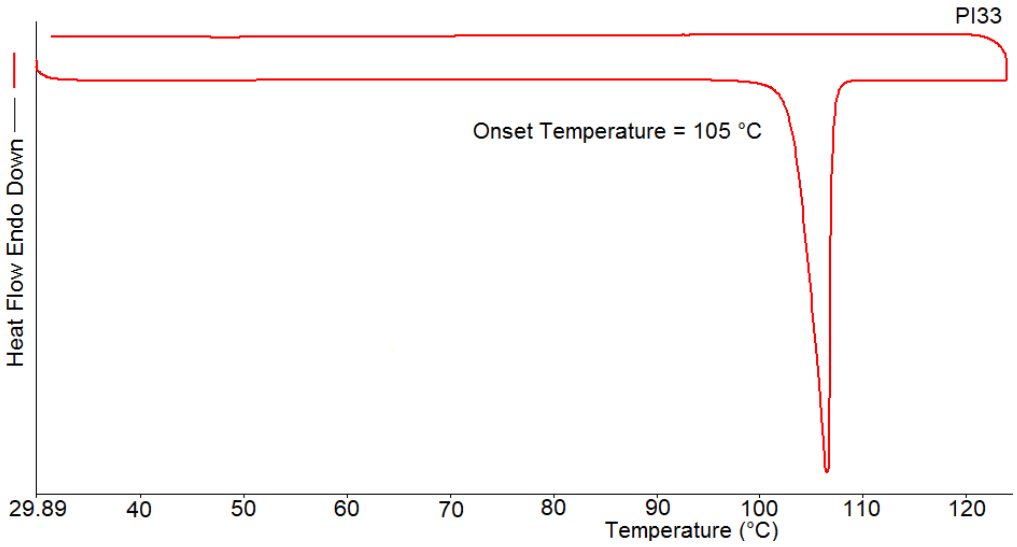

PB44
Heat Flow Endo Down
Onset Temperature = 205 °C
29.86
40
60
80
100
120
140
160
180
200
215
Temperature (°C)

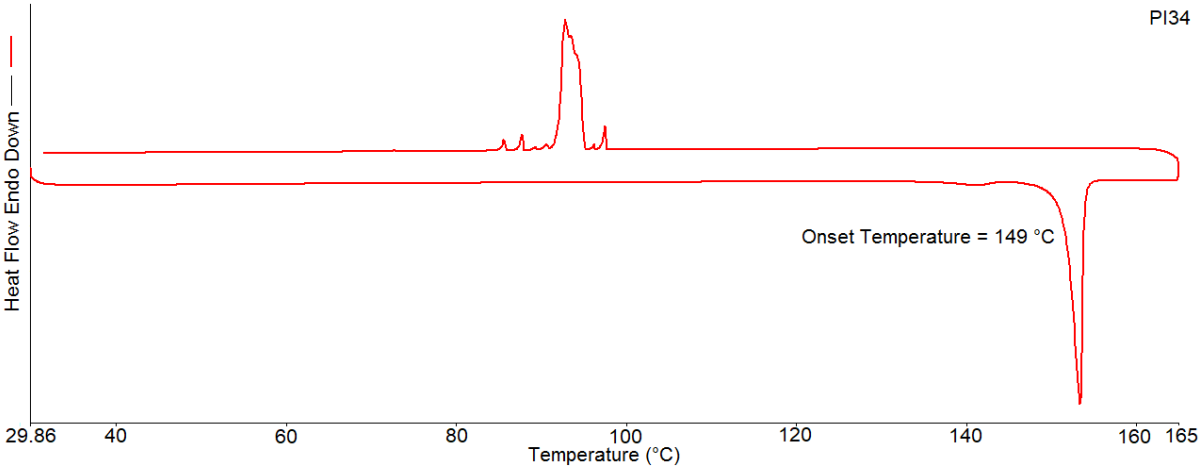

PI22
Heat Flow Endo Down
Onset Temperature = 179 °C
29.86
40
60
80
100
120
140
160
180
200
Temperature (°C)

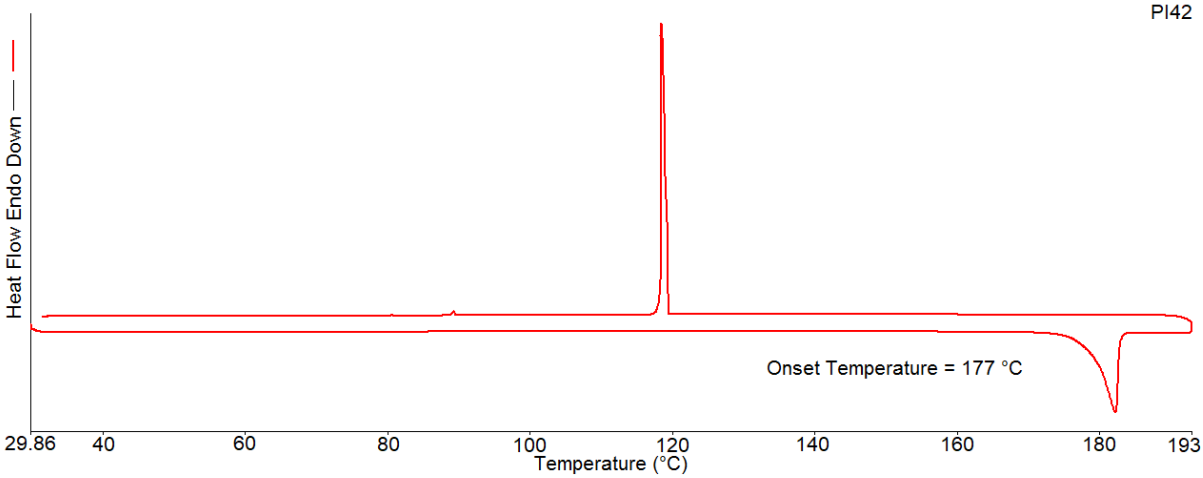

PI23
Heat Flow Endo Down
Onset Temperature = 107 °C
29.84
40
50
60
70
80
90
100
110
120
130
140
Temperature (°C)

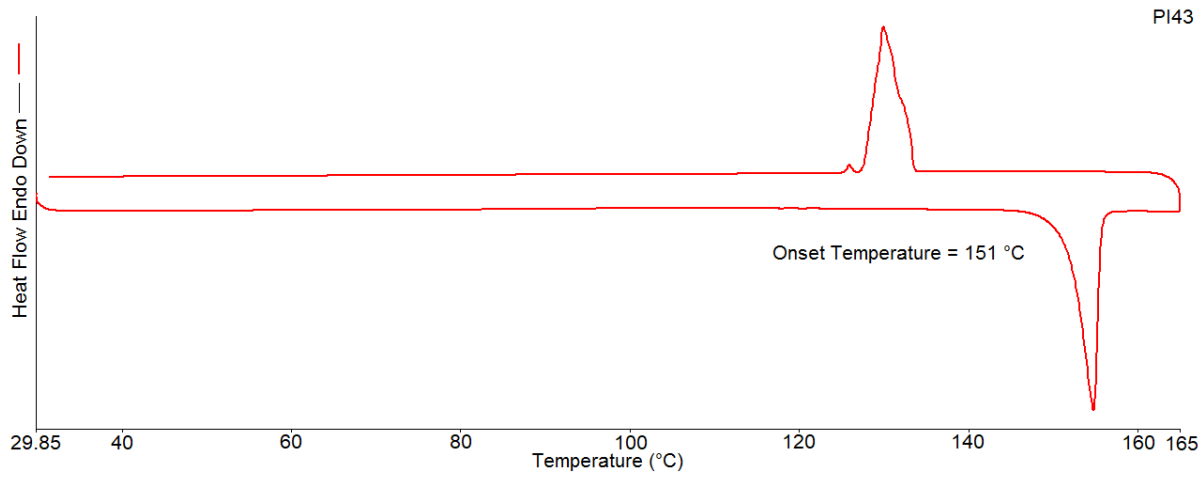

PI24
Heat Flow Endo Down
Onset Temperature = 143 °C
29.86
40
60
80
100
120
140
160
165
Temperature (°C)

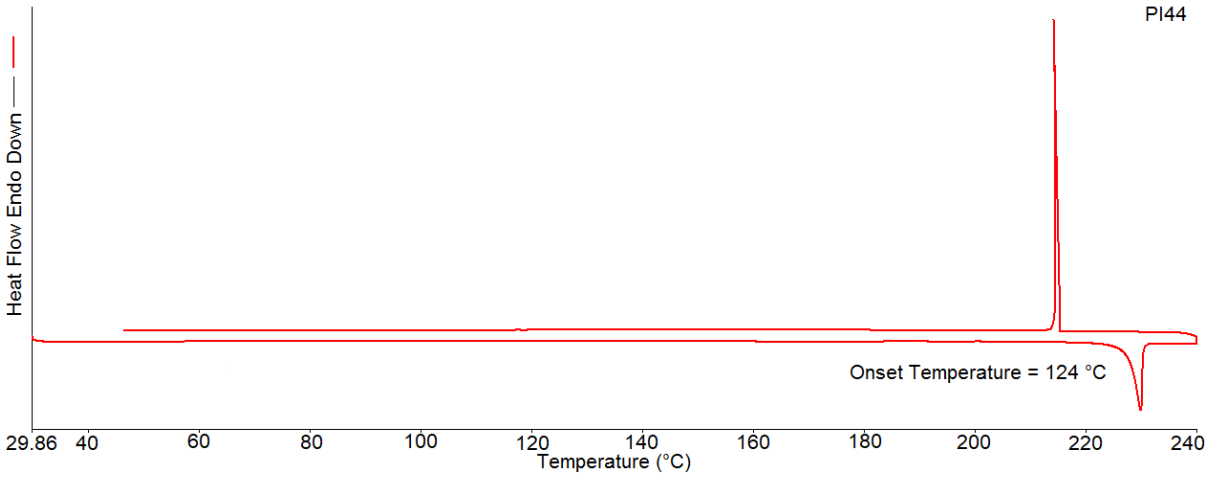

PI32
Heat Flow Endo Down
Onset Temperature = 145 °C
29.85
40
60
80
100
120
140
160
165
Temperature (°C)


PI33
Onset Temperature = 105 °C
Heat Flow Endo Down
29.89
40
50
60
70
80
90
100
110
120
Temperature (°C)


PI34
Onset Temperature = 149 °C
Heat Flow Endo Down
29.86
40
60
80
100
120
140
160
165
Temperature (°C)


PI42
Onset Temperature = 177 °C
Heat Flow Endo Down
29.86
40
60
80
100
120
140
160
180
193
Temperature (°C)


PI43
Heat Flow Endo Down
Onset Temperature = 151 °C
29.85
40
60
80
100
120
140
160
165
Temperature (°C)


PI44
Heat Flow Endo Down
Onset Temperature = 124 °C
29.86
40
60
80
100
120
140
160
180
200
220
240
Temperature (°C)

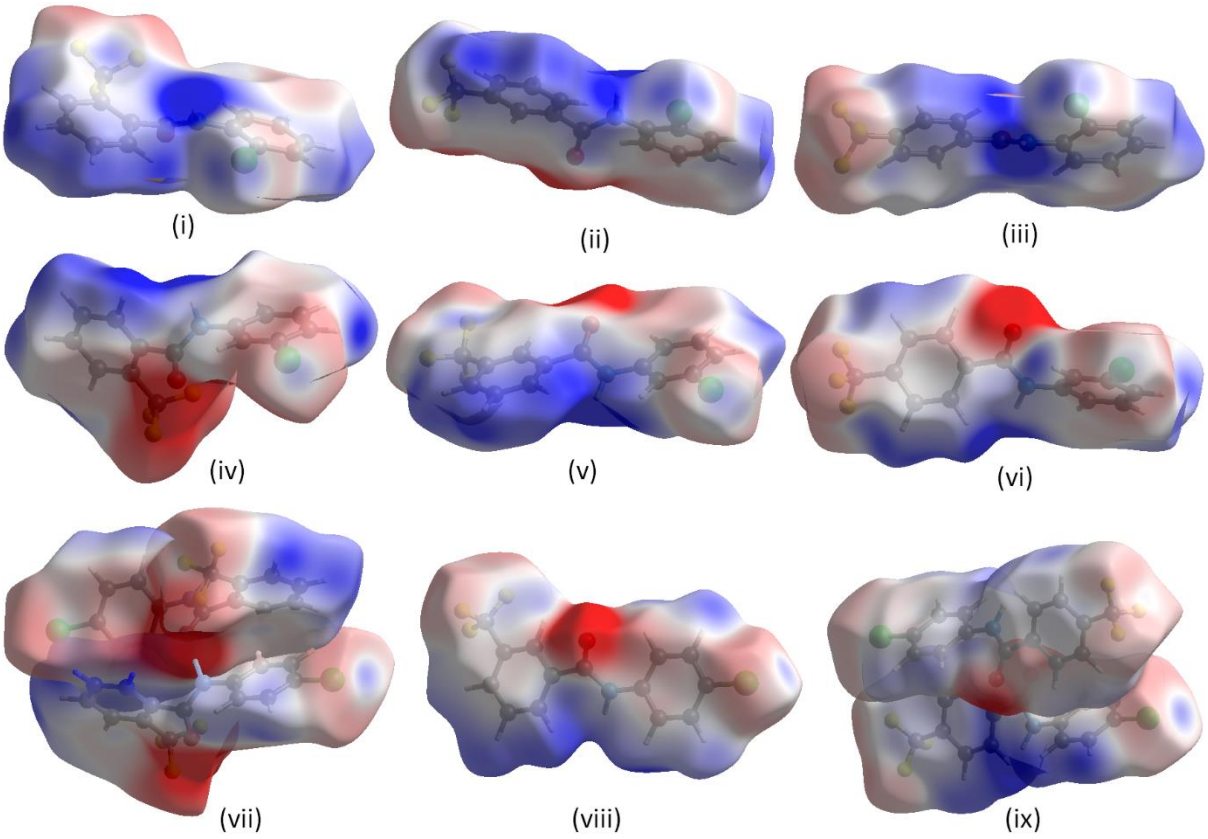


Figure S3 Electrostatic potential map on the Hirshfeld surface of N-chlorophenyl-trifluoromethyl-benzamide. The ranges of ESP are from −0.05 a.u. (red) to 0.05 a.u. (blue). (i) PC22 (ii) PC23 (iii) PC24 (iv) PC32 (v) PC33 (vi) PC34 (vii) PC42 (viii) PC43 (ix) PC44.

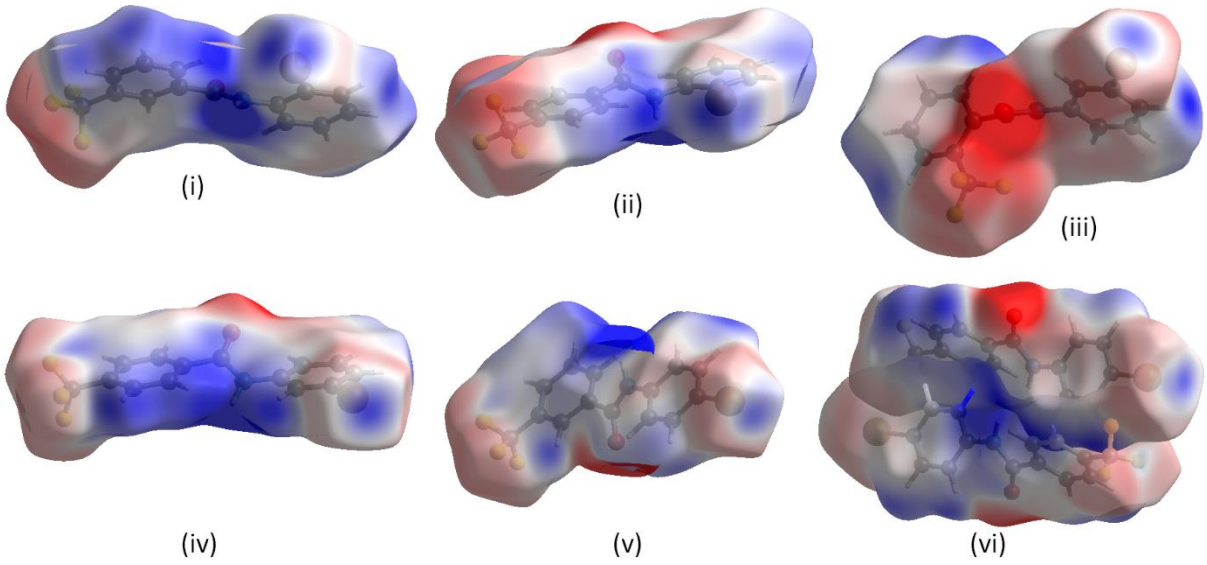


Figure S4 Electrostatic potential map on the Hirshfeld surface of N-bromophenyl-trifluoromethyl-benzamide. The ranges of ESP are from −0.05 a.u. (red) to 0.05 a.u. (blue). (i) PB23 (ii) PB24 (iii) PB32 (iv) PB34 (v) PB43 (vi) PB44.

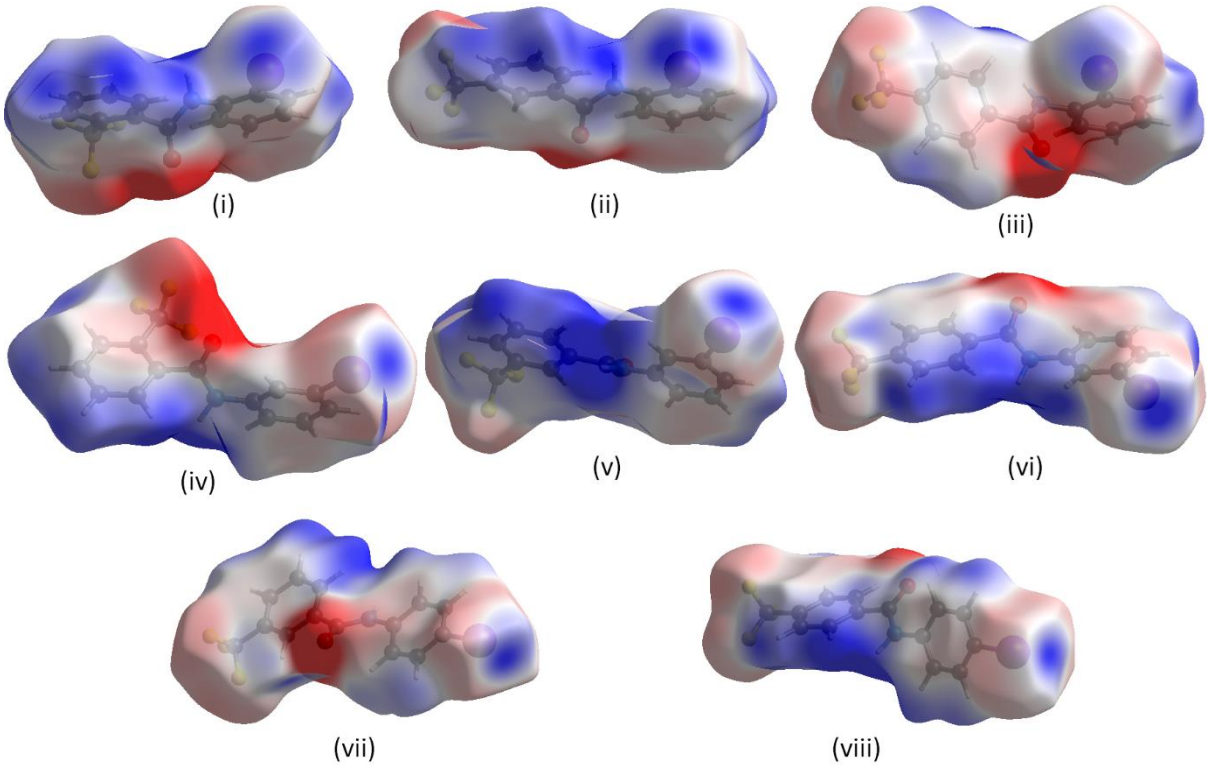
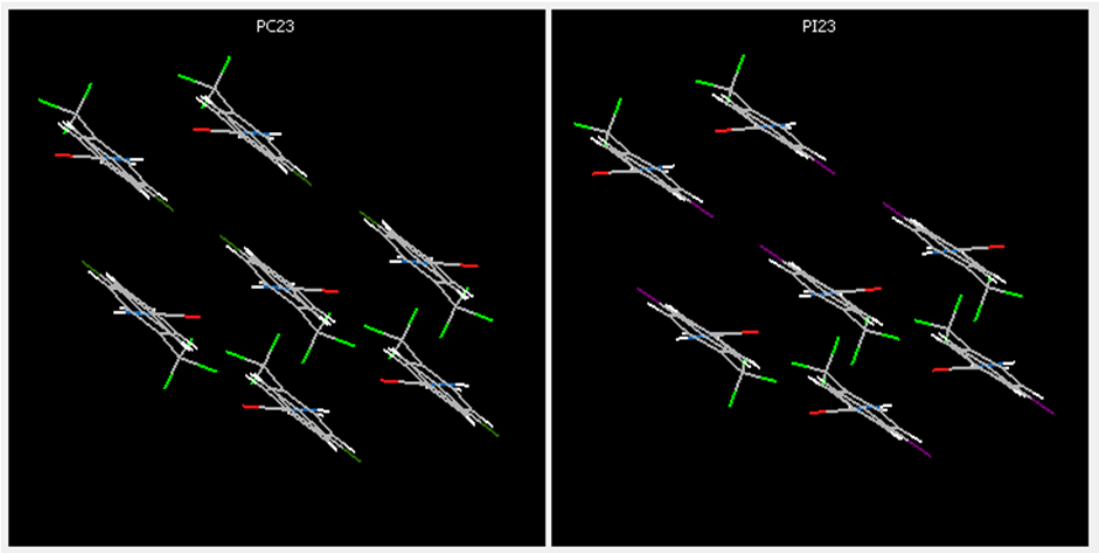
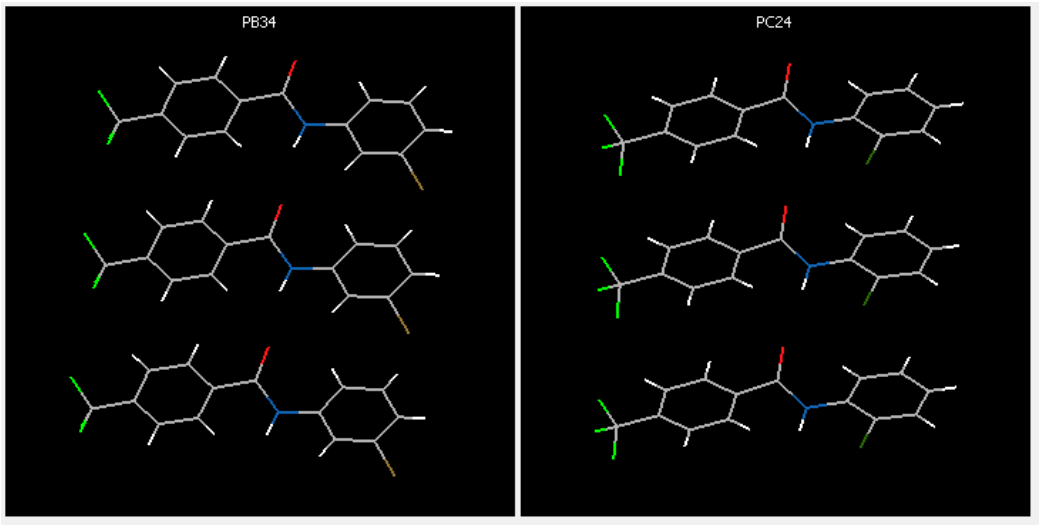


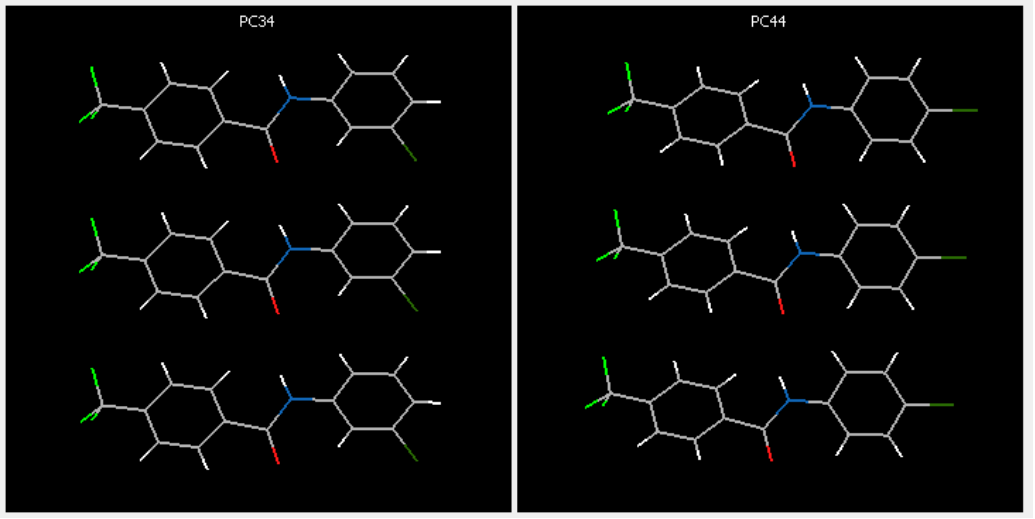
Figure S5 Electrostatic potential map on the Hirshfeld surface of N-iodophenyl-trifluoromethyl-benzamide. The ranges of ESP are from −0.05 a.u. (red) to 0.05 a.u. (blue). (i) PI22 (ii) PI23 (iii) PI24 (iv) PI32 (v) PI33 (vi) PI34 (vii) PI43 (viii) PI44.



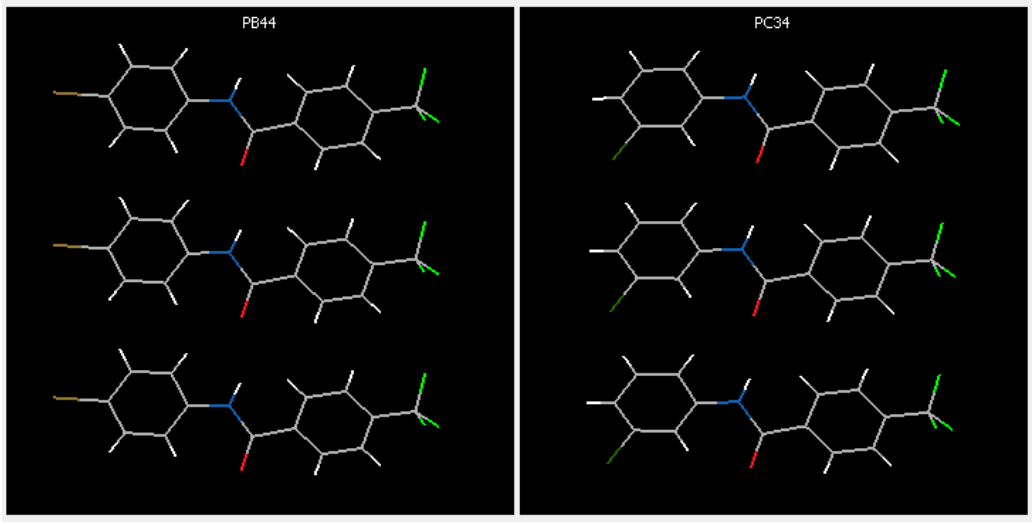
(i)



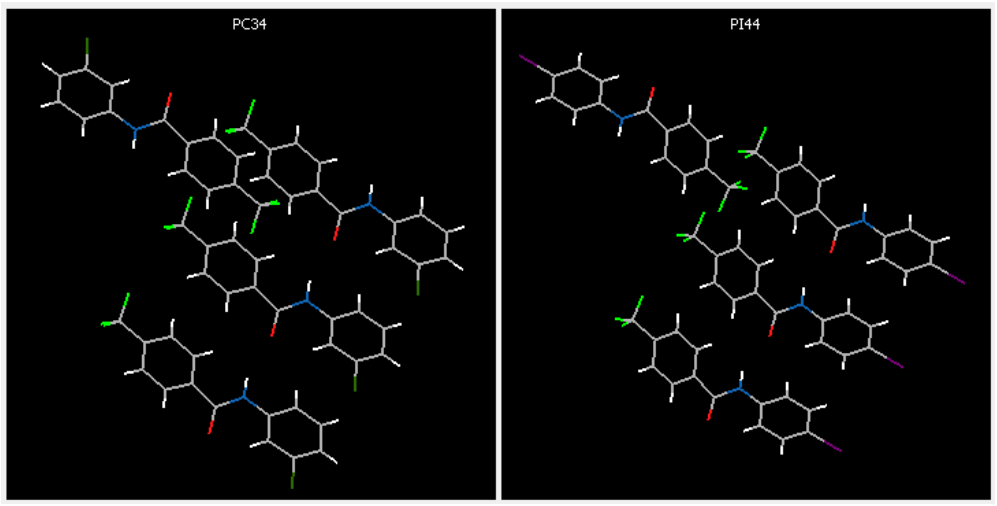
(ii)



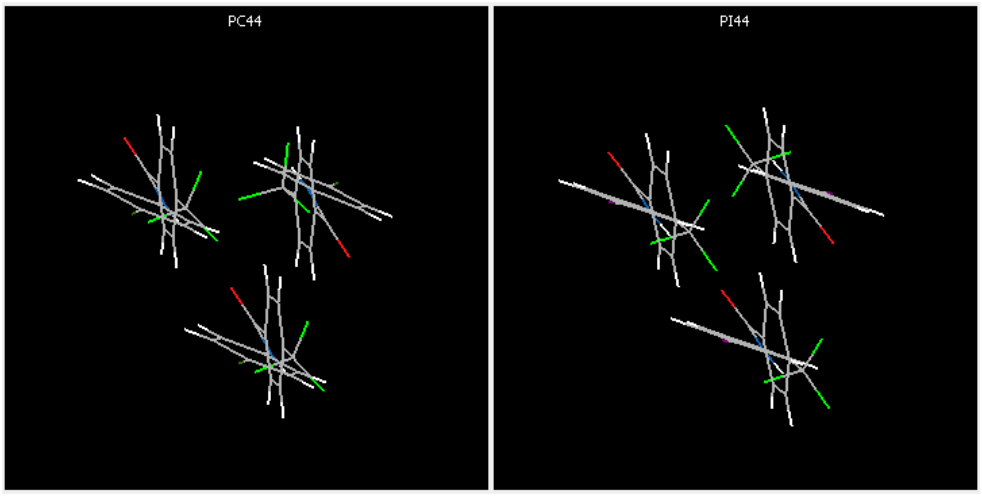
(iii)



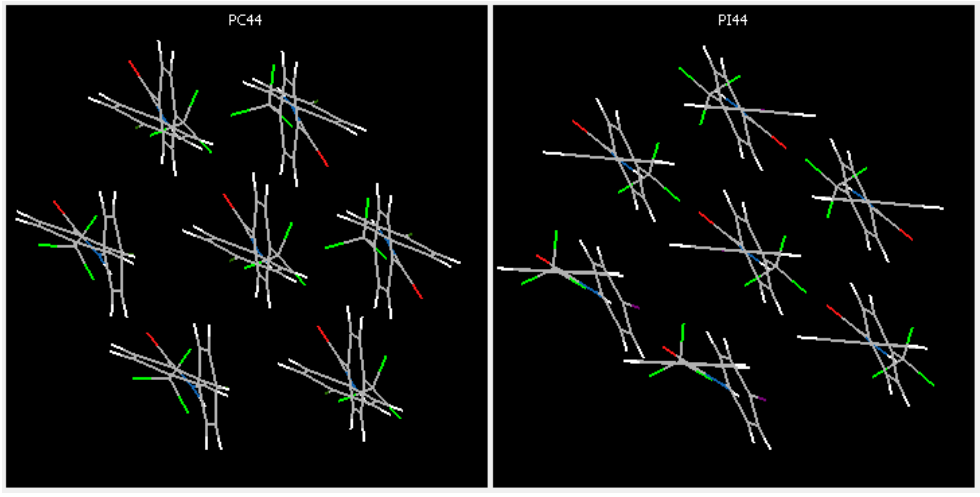
(iv)



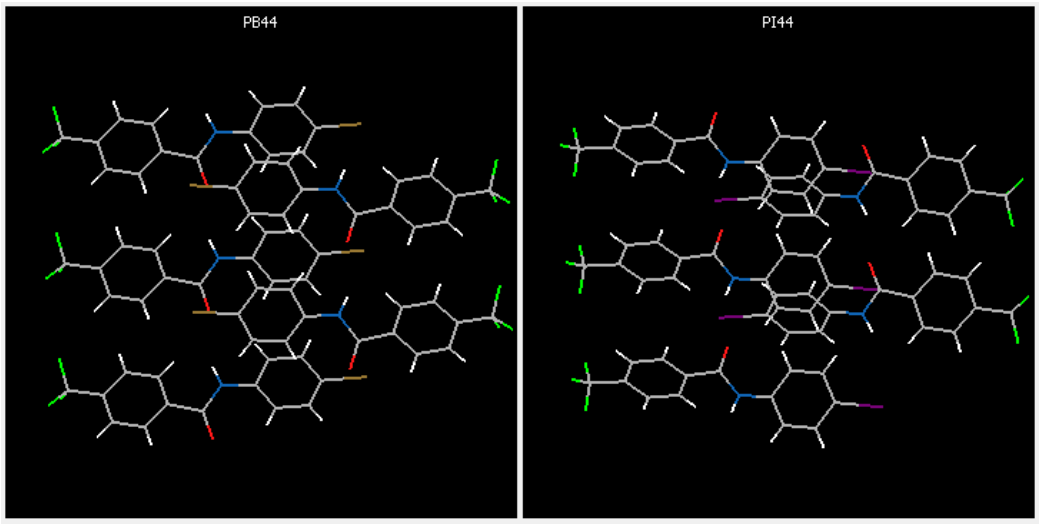
(v)



(vi)



(vii)



(viii)

Figure S6 The 2D and 1D supramolecular constructs obtained from *XPac*analysis for (i) PC23 and PI23, (ii) PB34 and PC24,(iii) PC34 and PC44,(iv) PB44 and PC34,(v) PC34 and PI44,(vi) PC44 and PI44, (two packing diagrams from the 2-1 seed) (vii) PC44 and PI44, (two packing diagrams from the 1-1 seed) (viii)PB44 and PI44 (two packing diagrams from the 1-1 seed).