Structure-based rational design, synthesis, crystal structure, DFT and molecular docking of 1,4 benzene dicarboxamide isomers with application as hardeners

MeenuTeotia[a], NaziaTarannum[a], MohitChauhan[a], and Rakesh Kumar Soni[a]
[a]Department of Chemistry, ChaudharyCharan Singh University, Meerut 250004, India
E-mail: teotiameenu@gmail.com, orcid.org/0000-0001-9833-7821, Phone: 09758154719

New Journal of Chemistry (RSC)
Supplementary files

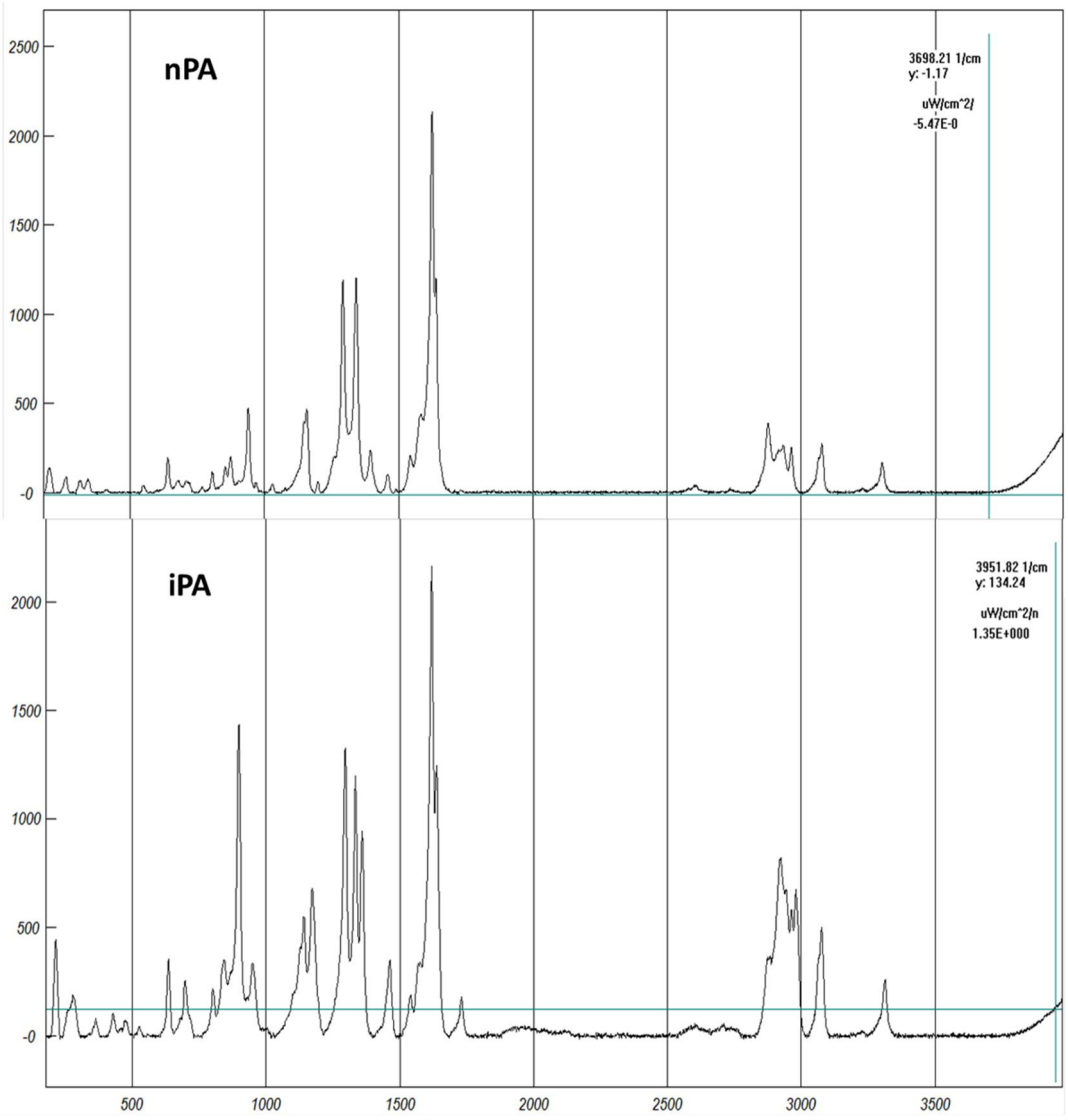

Figure S1: Raman spectra of N, N' di n-propyl and N, N' di-isopropyl 1,4 benzene dicarboxamides

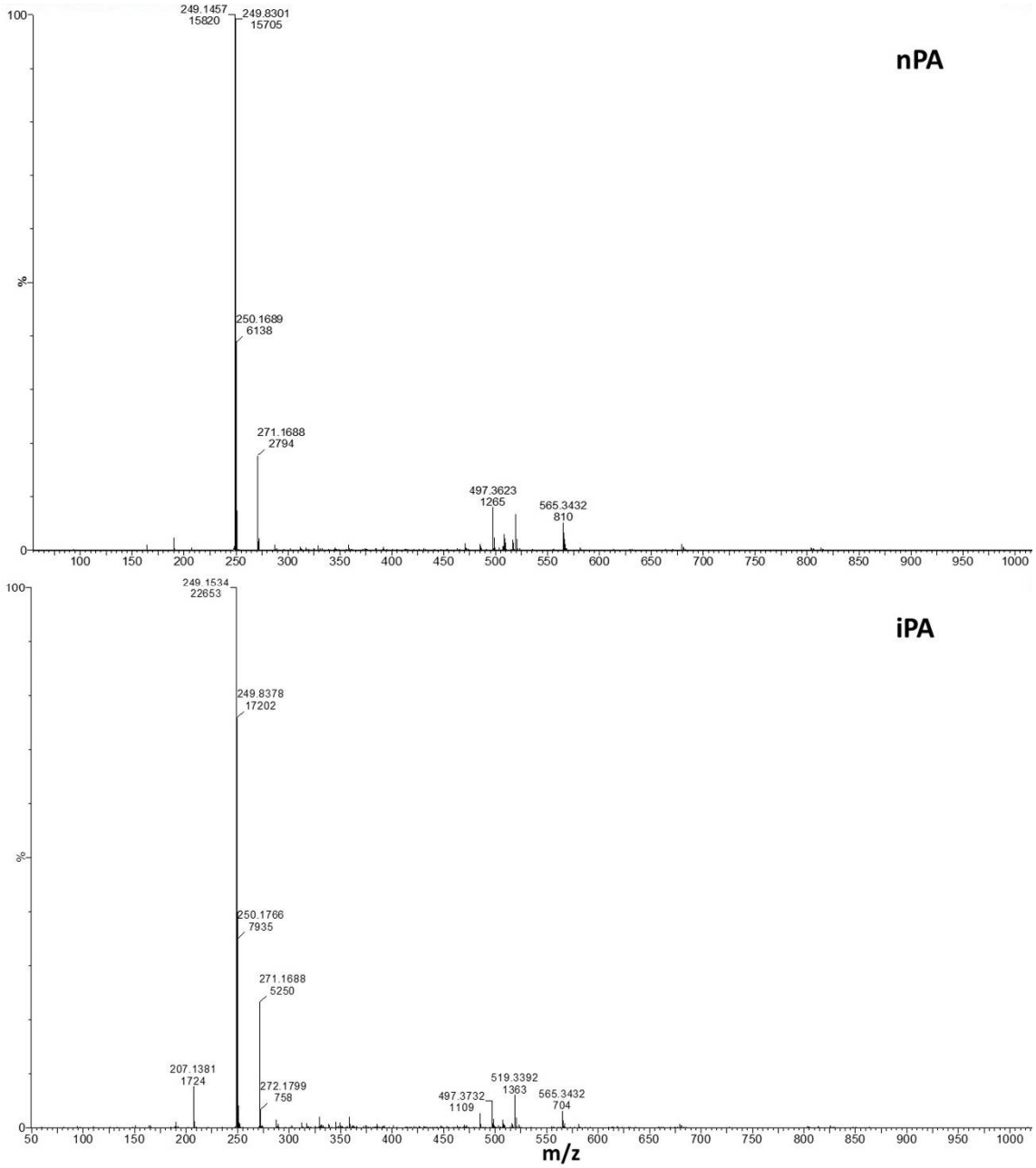

Figure S2: MS spectra of N, N’ di n-propyl and N, N’ di-isopropyl 1,4 benzene dicarboxamides

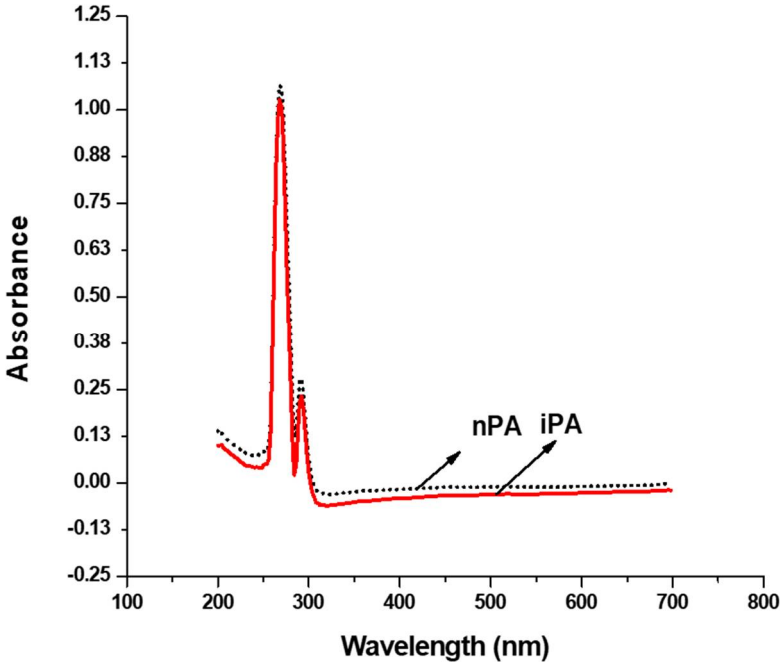

Figure S3: UV-Visible spectra of nPA (N, N' di n-propyl) and iPA (N, N' di-isopropyl) 1,4 benzene dicarboxamides

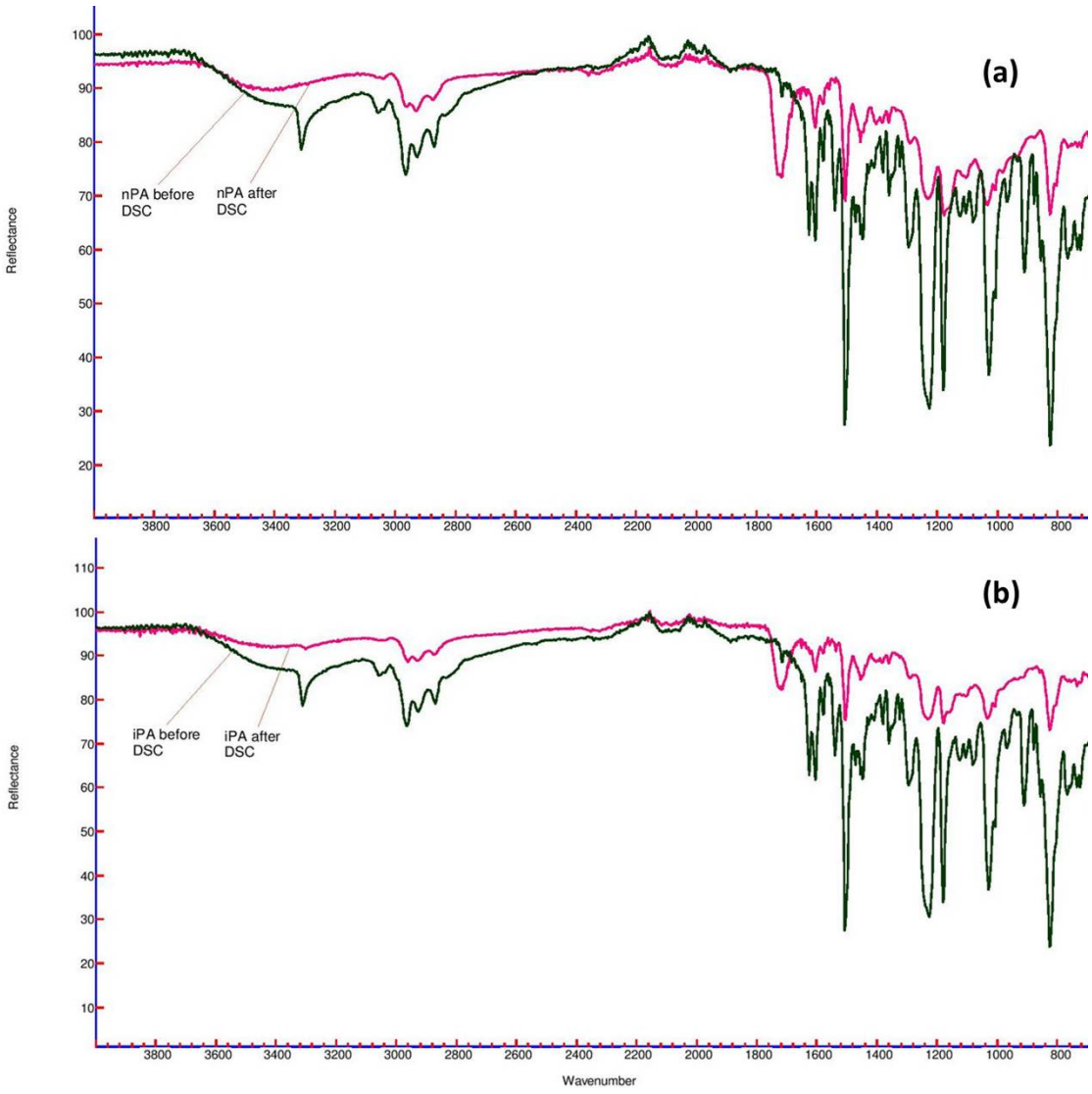

Figure S4: FTIR spectra of uncured and cured FnPA (a) and FiPA (b) formulations

Table S1: Muliken atomic charges

Atom No.	Atom	Charge	Atom No.	Atom	Charge
1	C	-0.1521	1	C	-0.1537
2	C	-0.1519	2	C	-0.1556
3	C	0.0583	3	C	0.5768
4	C	-0.1434	4	C	-0.14542
5	C	-0.1430	5	C	-0.14514
6	C	0.0567	6	C	0.06133
7	H	0.1278	7	H	0.12882
8	H	0.1290	8	H	0.128712
9	H	0.1741	9	H	0.17422
10	H	0.1743	10	H	0.17508
11	C	0.4659	11	C	0.47832
12	C	0.4671	12	C	0.47376
13	O	-0.4733	13	N	-0.64311
14	O	-0.4694	14	N	-0.64425
15	N	-0.6450	15	H	0.31077
16	N	-0.6499	16	O	-0.4761
17	H	0.3138	17	O	-0.4775
18	H	0.3134	18	H	0.3156
19	C	-0.0876	19	C	0.0562
20	C	-0.0904	20	C	0.05146
21	H	0.1930	21	H	0.17681
22	H	0.1387	22	H	0.12493
23	H	0.1825	23	C	-0.41741
24	H	0.1322	24	C	-0.38959
25	C	-0.2312	25	C	-0.39534
26	C	-0.2309	26	C	-0.39678
27	H	0.1168	27	H	0.126488
28	H	0.1448	28	H	0.14818
29	H	0.1579	29	H	0.14732
30	H	0.1185	30	H	0.16875
31	C	-0.4120	31	H	-0.00443
32	H	0.1295	32	H	0.13405
33	H	0.1431	33	H	0.12235
34	H	0.1388	34	H	0.12934
35	C	-0.4116	35	H	0.1267
36	H	0.1333	36	H	0.18349
37	H	0.1437	37	H	0.12942
38	H	0.1381	38	H	0.18474

Table S2: Crystallographic data and refinement parameters

	nPA	iPA
Empirical formula	C14 H20 N2 O2	C14 H20 N2 O2
Formula weight	248.32	248.30
Temperature	296(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic
Space group	2 'P -1'/'-P 1'	2 'P -1' '-P 1'
Z	1	1
Density (calculated)	1.210 Mg/m^3	1.189 Mg/m^3
Absorption coefficient	0.081 mm^{-1}	0.080 mm^{-1}
Theta range for data collection	2.211 to 25.047°	3.076 to 25.048°
Index ranges	5<=h<=5, -8<=k<=9, -11<=l<=11	6<=h<=5, -6<=k<=6, -16<=l<=16
Reflections collected	3419	1191
Independent reflections	1205 [R(int) = 0.0433]	723 [R(int) = 0.0476]
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2014/7 (Sheldrick, 2014)
Data / restraints / parameters	1205/0/83	1191/0/84
Goodness-of-fit on F^2	0.919	1.307
Final R indices [I>2sigma(I)]	R1 = 0.0673, wR2 = 0.1600	R1 = 0.0741, wR2 = 0.1488
R indices (all data)	R1 = 0.1157, wR2 = 0.1922	R1 = 0.1386, wR2 = 0.1720
Largest diff. peak and hole	0.181 and -0.293 $e.Å^{-3}$	0.186 and -0.229 $e.Å^{-3}$