Supplementary Information:









b.
$$[X = -F; o, m, p]$$



c. [X = -F; o, m, p]

Scheme S1: Synthetic procedure.

	Starting materials	Molecular Weight (g)	Weight taken (g)	No of mmoles
DC1	Aniline	93.13 (ρ = 1.023)	0.104 (101.9 µl)	1.12
DCI	o-FluoroBenzoyl Chloride	158.56 (ρ = 1.328)	0.178 (133.7 µl)	1.12
	DMAP	122.7	0.160	1.30
DC2	Aniline	93.13 ($\rho = 1.023$)	0.104 (101.9 µl)	1.12
D 0 -	m-FluoroBenzoyl Chloride	$158.56 (\rho = 1.304)$	0.178 (136.2 µl)	1.12
	DMAP	122.7	0.160	1.30
DC3	Aniline	93.13 ($\rho = 1.023$)	0.104 (102 µl)	1.12
	p-FluoroBenzoyl Chloride	$158.56 (\rho = 1.342)$	0.178 (132.3 µl)	1.12
	DMAP	122.7	0.160	1.30
DC4	o-Fluoroaniline	$111.12 (\rho = 1.151)$	0.128 (111 µl)	1.12
DC4	Benzoyl Chloride	$140.57 (\rho = 1.211)$	0.157 (130 µl)	1.12
	DMAP	122.7	0.160	1.30
DC5	m-Fluoroaniline	111.12 ($\rho = 1.156$)	0.128 (110.6 µl)	1.12
DCS	Benzoyl Chloride	140.57 ($\rho = 1.211$)	0.157 (130 µl)	1.12
	DMAP	122.7	0.160	1.30
DC6	p-Fluoroaniline	111.12 ($\rho = 1.173$)	0.129 (109.0 µl)	1.12
Dev	Benzovl Chloride	140.57(a - 1.211)	0 157 (1201)	1 1 2
	DMAP	140.37 (p - 1.211) 122.7	0.157 (150 μl) 0.160	1.12
		144.1	0.100	1.50
	o-FluoroAniline	11112(0 = 1151)	0 262 (228 µl)	2.36
DC7	o-FluoroBenzovl Chloride	111.12 (p = 1.131) 158 56 (p = 1.328)	$0.202 (228 \mu l)$ 0.374 (282 µl)	2.30
DC7	DMAP	138.30 (p = 1.328) 122 7	$0.374 (202 \mu I)$ 0.320	2.50
		122.1	0.520	2.00
	o-FluoroAniline	11112(0 = 1151)	0 053 (46 11)	0 47
DC8	m-FluoroBenzovl Chloride	158.56(0 = 1.304)	0.075 (57 µl)	0.47
	DMAP	122.7	0.063	0.52
				···· =

Table S1: Amounts of Reactants taken for the synthesis of substituted benzanilides.

Electronic Supplementary Material for CrystEngComm This journal is (c) The Royal Society of Chemistry 2007

	Starting materials	Molecular Weight (g)	Weight taken (g)	No of mmoles
	o-FluoroAniline	$111.12 (\rho = 1.151)$	0.262 (228 µl)	2.36
DC9	p-FluoroBenzoyl Chloride	$158.56 (\rho = 1.342)$	0.374 (279 µl)	2.36
	DMAP	122.7	0.320	2.60
	m-FluoroAniline	$111.12 (\rho = 1.156)$	0.262 (226.6 µl)	2.36
DC10	o-FluoroBenzoyl Chloride	$158.56 (\rho = 1.328)$	0.374 (281.6 µl)	2.36
	DMAP	122.7	0.32	2.60
	m-FluoroAniline	111.12 ($\rho = 1.156$)	0.052 (45 µl)	0.47
DC11	m-FluoroBenzoyl Chloride	158.56 ($\rho = 1.304$)	0.075 (58 µl)	0.47
	DMAP	122.7	0.063	0.52
	m-FluoroAniline	111.12 ($\rho = 1.156$)	0.262 (227 µl)	2.36
DC12	p-FluoroBenzoyl Chloride	$158.56 (\rho = 1.342)$	0.374 (279 µl)	2.36
	DMAP	122.7	0.32	2.60
	p-FluoroAniline	111.12 ($\rho = 1.173$)	0.052 (45 µl)	0.47
DC12	o-FluoroBenzoyl Chloride	158.56 ($\rho = 1.328$)	0.075 (58 µl)	0.47
DCIS	DMAP	122.7	0.063	0.52
	p-FluoroAniline	$111.12 (\rho = 1.173)$	0.052 (45 µl)	0.47
DC14	m-FluoroBenzoyl Chloride	158.56 ($\rho = 1.304$)	0.075 (58 µl)	0.47
	DMAP	122.7	0.063	0.52
	p-FluoroAniline	111.12 (p = 1.173)	0.052 (45 µl)	0.47
DC15	p-FluoroBenzoyl Chloride	158.56 (ρ = 1.342)	0.075 (56 µl)	0.47
	DMAP	122.7	0.063	0.52

Characterization of the prepared compounds:

IR-spectroscopy and Powder Diffraction was used to characterize the synthesized column pure compounds. DSC/ DTA measurements were done to determine the melting points accurately. Nonlinear Optical measurements on both the powdered samples and the crystals were also performed.

IR Measurements:

Powdered samples were pelleted with dry KBr and the IR pattern was recorded on a Mettler Toledo instrument.

Powder Diffraction Measurements:

Powder X-ray diffraction measurements were done on Philips X'Pert Pro X-Ray diffractometer operating at 40kV/30mA using CuK_{α} radiation in reflection mode. All the powder patterns were recorded between the 20 ranges 3 - 50°, step size of 0.01° and time per step is 0.75 sec.

Non Linear Optical property (SHG measurements):

In order to ascertain whether these compounds are good materials for exhibiting SHG property or not, measurements for the presence of non-linear optical property were performed on both the powdered samples and also the crystals. Powder SHG measurements were done in accordance with the Kurtz and Perry technique for NLO measurements on powdered materials using Quanta DCR3 LASER (1064nm) and a Photo Diode used as detector. 1064nm was cut off by a CuSO₄ solution and BG38 filter. The sample was illuminated with a Nd:YAG laser emitting a fundamental wavelength of 1064 nm. A green signal (532nm) was observed proving that the material exhibits SHG activity. The corresponding output was recorded. The nature of the signal in case of both crystal and powder is the same.

Melting Point measurements:

Differential thermal analysis on freshly powdered sample was recorded on a SDTQ600 instrument at 5 °C/min and by differential scanning calorimetry[#] on a Mettler Toledo STAR^e system with heating/cooling rate of 5 °C/min.

Compound (cm ⁻¹)	DC1	DC2	DC3	DC4	DC5	DC6
-C=C- stretch	1535	1535	1530	1532	1526	1520
-C=O	1658, 1600	1656,1590	1655,1599	1655,1607	1661,1604	1650,1609
=C-H stretch	3063	3078	3059	3060	3098	3061
=C-N stretch	1443	1440	1437	1449	1436	1448
-N-H stretch	3374	3345	3349	3314	3348	3347
-C-O stretch	1245	1264	1227	1259	1242	1212
-N-H bend	632	633	648	641	645	644
Compound (cm ⁻¹)	DC7	DC8	DC9	DC10	DC11	DC12
-C=C- stretch	1541	1536	1535	1558	1535	1538
-C=O	1667,1614	1657,1589	1652, 1605	1658,1608	1655,1594	1661, 1605
=C-H stretch	3049	3071	3067	3073	3075	3093
=C-N stretch	1454	1451	1541	1488	1485	1438
-N-H stretch	3408	3299	3309	3227	3306	3357
-C-O stretch	1209	1261	1260	1260	1269	1280
-N-H bend	-	644	655	648	-	648

Table S2: Important Vibrational Spectroscopic Assignments.

Compound (cm ⁻¹)	DC13	DC14	DC15
-C=C- stretch	1538	1513	1521
-C=O	1654, 1613	1651, 1587	1654, 1605
=C-H stretch	3060	3082	3075
=C-N stretch	1451	1439	1404
-N-H stretch	3351	3337	3360
-C-O stretch	1280	1268	1247
-N-H bend	645	649	623

Table S3: Melting point of the prepared compounds:

Compound	M. P(°C)	Compound	M. P(°C)
DC1	101.2	DC9	130.2
$\mathbf{DC2}^{\#}$	153.6	DC10	96.8
DC3	186.8	DC11	129.6
DC4 [#]	112.9	DC12	144.3
DC5 [#]	144.5	DC13	117.1
DC6 [#]	186.1	DC14	149.8
DC7	89.61	DC15 [#]	186.8
DC8	116.1		