Supporting Information

Experimental and computational insights into the nature of weak intermolecular interactions in trifluoromethyl substituted isomeric crystalline *N*-methyl-*N*-phenylbenzamides.

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Section1. List of synthesized compounds along with their synthesized yields (after column), melting points (from DSC, onset value), and spectroscopic characterization (FTIR, ^{1}H NMR):

1. ***N*-methyl-*N*-phenyl-2-(trifluoromethyl)benzamide (NM01):** Colourless thick oil; yield = 78%; M.P. = not determined; FTIR (in cm^{-1}: KBr): 3066, 2930, 1660; ^{1}H NMR (400MHz, $CDCl_3$): δ 7.56 (d, *J* = 6.67Hz, 1H), 7.30 (m, 2H), 7.20 (t, *J* = 7.06 Hz, 2H), 7.11 (m, 4H), 3.53 (s, 3H).

(a) ***N*-methyl-*N*-phenyl-3-(trifluoromethyl)benzamide (NM02):** White solid**;** yield = 84%; M.P. = 65°C; FTIR (in cm^{-1}: NaCl round cell plate): 3066, 2930, 1651; ^{1}H NMR (400MHz, $CDCl_3$): δ7.58 (s, 1H), 7.49 (t, *J* = 7.43 Hz, 2H), 7.28 (m, 3H), 7.19 (tt, *J* = 7.43 Hz, 1.44 Hz, 1H), 7.05 (d, *J* = 7.43 Hz, 2H), 3.53 (s, 3H)

2. ***N*-methyl-*N*-phenyl-4-(trifluoromethyl)benzamide (NM03):** White solid**;** yield = 91%; M.P. = 86°C; FTIR (in cm^{-1}: NaCl round cell plate): 3064, 2932, 1658; ^{1}H NMR (400MHz, $CDCl_3$): δ 7.43 (dt, *J* = 10.87 Hz, 4.25Hz, 4H), 7.27 (tt, *J* = 7.26 Hz, 1.70 Hz, 2H), 7.19 (tt, *J* = 7.35Hz, 1.43 Hz, 1H), 7.05 (d, *J* = 7.35 Hz, 2H), 3.53 (s, 3H).

3. ***N*-methyl-*N*-(2-(trifluoromethyl)phenyl)benzamide (NM10):** White solid**;** yield = 88%; M.P. 74°C =; FTIR (in cm^{-1}: NaCl round cell plate): 3066, 2925, 1658; ^1H NMR (400MHz, $CDCl_3$): δ 7.65 (d, *J* = 7.44 Hz, 2H), 7.45 (m, 3H), 7.36 (t, *J* = 7.44 Hz, 1H), 7.21 (d, *J* = 6.65 Hz, 1H), 7.16 (d, *J* = 7.00 Hz,3H), 3.45 (s, 3H).
4. ***N*-methyl-*N*-(3-(trifluoromethyl)phenyl)benzamide (NM20):** Colourless **t**hick oil; yield = 81%; M.P. = not determined; FTIR (in cm^{-1}: NaCl round cell plate): 3063, 2930, 1659; ^1H NMR (400MHz, $CDCl_3$): δ 7.41 (d, *J* = 7.76 Hz, 1H), 7.35 (m, 2H), 7.29 (m, 2H), 7.22 (d, *J* = 7.42, 3H), 3.54 (s, 3H).
5. ***N*-methyl-*N*-(4-(trifluoromethyl)phenyl)benzamide (NM30):** White low melting solid; yield = 86 %; M.P. = 39°C; FTIR (in cm^{-1}: NaCl round cell plate): 3062, 2931, 1659; ^1H NMR (400MHz, $CDCl_3$): 7.51 (d, *J* = 8.29 Hz, 2H), 7.31 (m, 3H), 7.23 (m, 2H), 7.17 (d, *J* = 8.29 Hz, 2H), 3.54 (s, 3H).
6. ***N*-methyl-2-(trifluoromethyl)-*N*-(2-(trifluoromethyl)phenyl)benzamide (NM11):** White solid; yield = 93 %; M.P. = 88°C; FTIR (in cm^{-1}: NaCl round cell plate): 3074, 2923, 1667; ^1H NMR (400MHz, $CDCl_3$): δ7.81 (d, *J* = 7.95Hz, 1H), 7.78 (d, *J* = 7.95Hz, 1H), 7.70 (qn, *J* = 9.00Hz, 2H), 7.60 (d, *J* = 7.73 Hz,1H), 7.55 (q, *J* = 7.45, 2H), 7.45 (d, *J* = 7.73Hz, 1H), 3.11 (s, 3H).
7. ***N*-methyl-3-(trifluoromethyl)-*N*-(2-(trifluoromethyl)phenyl)benzamide (NM12):** White solid; yield = 91 %; M.P. = 58°C; FTIR (in cm^{-1}: NaCl round cell plate): 3076, 2944, 1661; ^1H NMR (400MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.70 Hz, 1H), 7.54 (s, 1H), 7.49 (t, *J* = 6.80 Hz, 3H), 7.41 (t, *J* = 7.43 Hz, 1H), 7.30 (t, *J* = 7.42 Hz, 1H), 7.22 (d, *J* = 7.77 Hz, 1H), 3.47 (s, 3H).
8. ***N*-methyl-4-(trifluoromethyl)-*N*-(2-(trifluoromethyl)phenyl)benzamide (NM13):** Colourless **t**hick oil; yield = 81%; M.P. = not determined; FTIR (in cm^{-1}: NaCl round cell plate): 3069, 2930, 1652; ^1H NMR (400MHz, $CDCl_3$): δ 7.48 (m, 3H), 7.40 (t, *J* = 7.73 Hz, 3H), 7.36 (d, *J* = 7.72 Hz, 1H), 7.21 (d, *J* = 7.72 Hz, 1H), 3.55 (s, 3H).
9. ***N*-methyl-2-(trifluoromethyl)-*N*-(3-(trifluoromethyl)phenyl)benzamide (NM21):** Colourless **t**hick oil; yield = 88%; M.P. = not determined; FTIR (in cm^{-1}: NaCl round cell plate): 3072, 2926, 1664; ^1H NMR (400MHz, $CDCl_3$): δ 7.68 (s, 1H), 7.57 (m, 2H), 7.34 (m, 4H), 7.15 (s, 1H), 3.56 (s, 3H).

10. ***N*-methyl-3-(trifluoromethyl)-*N*-(3-(trifluoromethyl)phenyl)benzamide (NM22):** White solid; yield = 89 %; M.P. = 60°C; FTIR (in cm^{-1}: NaCl round cell plate): 3070, 2930, 1660; ^1H NMR (400MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.42 Hz, 2H), 7.48 (t, *J* = 9.05 Hz, 2H), 7.38 (m, 3H), 7.23 (d, *J* = 7.96Hz, 1H), 3.56 (s, 3H).
11. ***N*-methyl-4-(trifluoromethyl)-*N*-(3-(trifluoromethyl)phenyl)benzamide (NM23):** White solid; yield = 93 %; M.P. = 67°C; FTIR (in cm^{-1}: NaCl round cell plate): 3069, 2932, 1660; ^1H NMR (400MHz, $CDCl_3$): δ 7.48 (m, 3H), 7.40 (t, *J* = 7.01 Hz, 3H), 7.36 (d, *J* = 7.43 Hz, 1H), 7.21 (d, *J* = 7.85 Hz, 1H), 3.55 (s, 3H).
12. ***N*-methyl-2-(trifluoromethyl)-*N*-(4-(trifluoromethyl)phenyl)benzamide (NM31):** White solid; yield = 87 %; M.P. = 72°C; FTIR (in cm^{-1}: NaCl round cell plate): 3071, 2931, 1667; ^1H NMR (400MHz, $CDCl_3$): δ 7.61 (d, J = 7.84Hz, 2H), 7.48 (d, J = 6.90Hz, 2H), 7.36 (t, J = 6.93Hz, 2H), 7.20 (d, J = 6.90Hz, 2H), 3.56 (s, 3H).
13. ***N*-methyl-3-(trifluoromethyl)-*N*-(4-(trifluoromethyl)phenyl)benzamide (NM32):** Colourless **t**hick oil; yield = 90%; M.P. = not determined; FTIR (in cm^{-1}: NaCl round cell plate): 3075, 2930, 1660; ^1H NMR (400MHz, $CDCl_3$): δ 7.59 (s, 1H), 7.55 (t, *J* = 9.11Hz, 3H), 7.48 (d, *J* = 7.56Hz, 1H), 7.36 (t, *J* = 7.83Hz, 1H), 7.18 (d, *J* = 7.90Hz, 2H), 3.56 (s, 3H).
14. ***N*-methyl-4-(trifluoromethyl)-*N*-(4-(trifluoromethyl)phenyl)benzamide (NM33):** White solid; yield = 93 %; M.P. = 66°C; FTIR (in cm^{-1}: NaCl round cell plate): 3066, 2931, 1659; ^1H NMR (400MHz, $CDCl_3$): δ 7.54 (t, *J* = 7.65 Hz, 3H), 7.50 (s, 1H), 7.44 (d, *J* = 8.31 Hz, 2H), 7.18 (d, *J* = 8.02 Hz, 2H), 3.55 (s, 3H).

Table S1: Details of Crystallization Experiments:

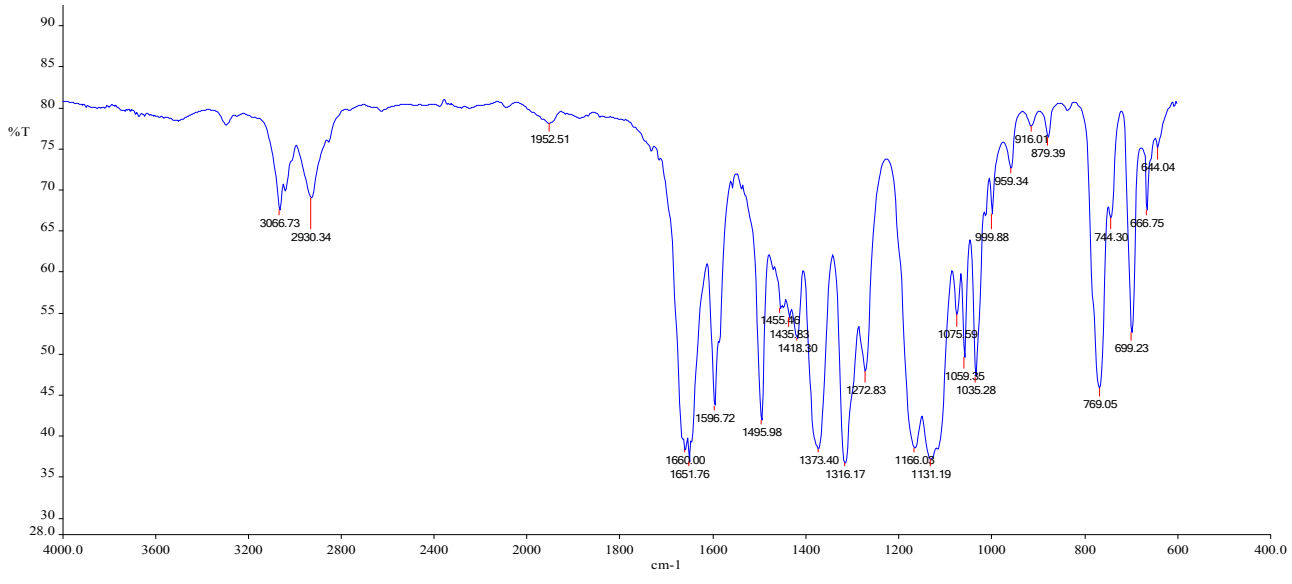
Sl. No.	Compound Code	Solvent and Crystallization conditions [a]
1.	NM02	Hexane (5°C), Chloroform (5°C),
2.	NM03	Hexane (5°C)
3.	NM10	Hexane (5°C), Ether (-20°C), Dichloromethane (5°C), Chloroform (5°C), Benzene (5°C)
4.	NM30[b]	--------

5.	NM11	Hexane (5°C), Ether (-20°C), Methanol (RT), Dichloromethane + cyclohexane (1:1, 5°C)
6.	NM12	Hexane (5°C), Ether (-20°C)
7.	NM22	Dichloromethane (5°C), Hexane (5°C)
8.	NM23	Hexane (5°C)
9.	NM31	Hexane (5°C), Dichloromethane (5°C)
10.	NM33	Hexane (5°C), Dichloromethane + cyclohexane (1:1, 5°C)

[a] All crystals, crystallized from different solvents or conditions for a particular compound, were found to be of the same phase. [b] No solid aggregate could be obtained after crystallization from any solvent. Single crystal of **NM30** was observed directly in the sample vial.

Figure S1: IR-Spectra of the compounds: All IR spectra were recorded on NaCl round cell plate on Perkin Elmer instrument.

(a) NM01:



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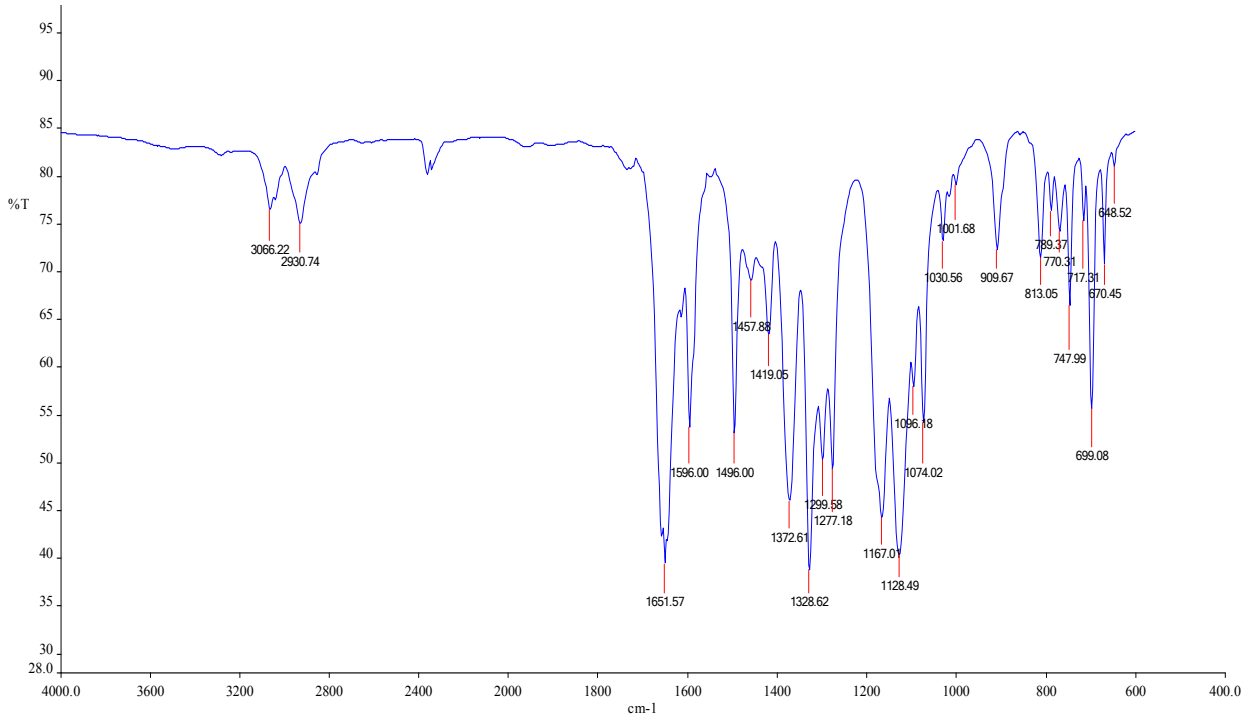
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1277.18
1167.01
1128.49
1096.18
1074.02
1030.56
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699.08
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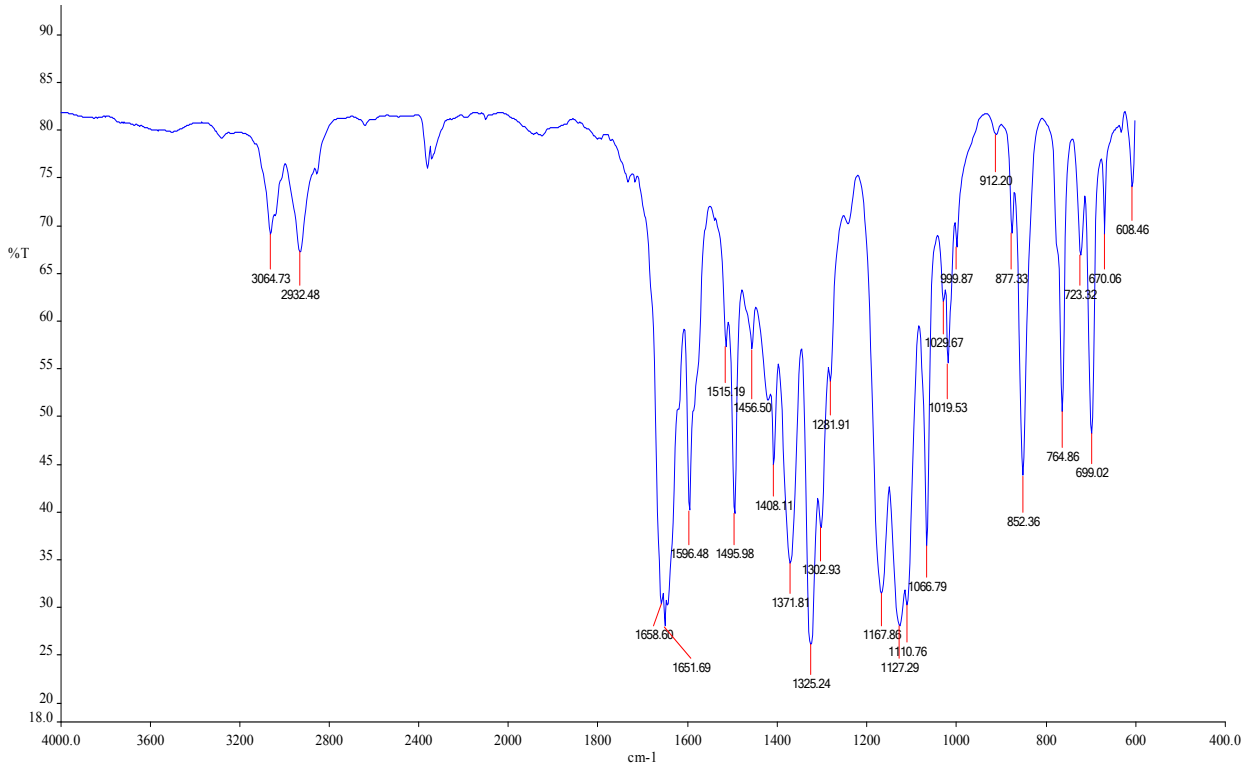
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1325.24
1302.93
1281.91
1167.86
1127.29
1110.76
1066.79
1029.67
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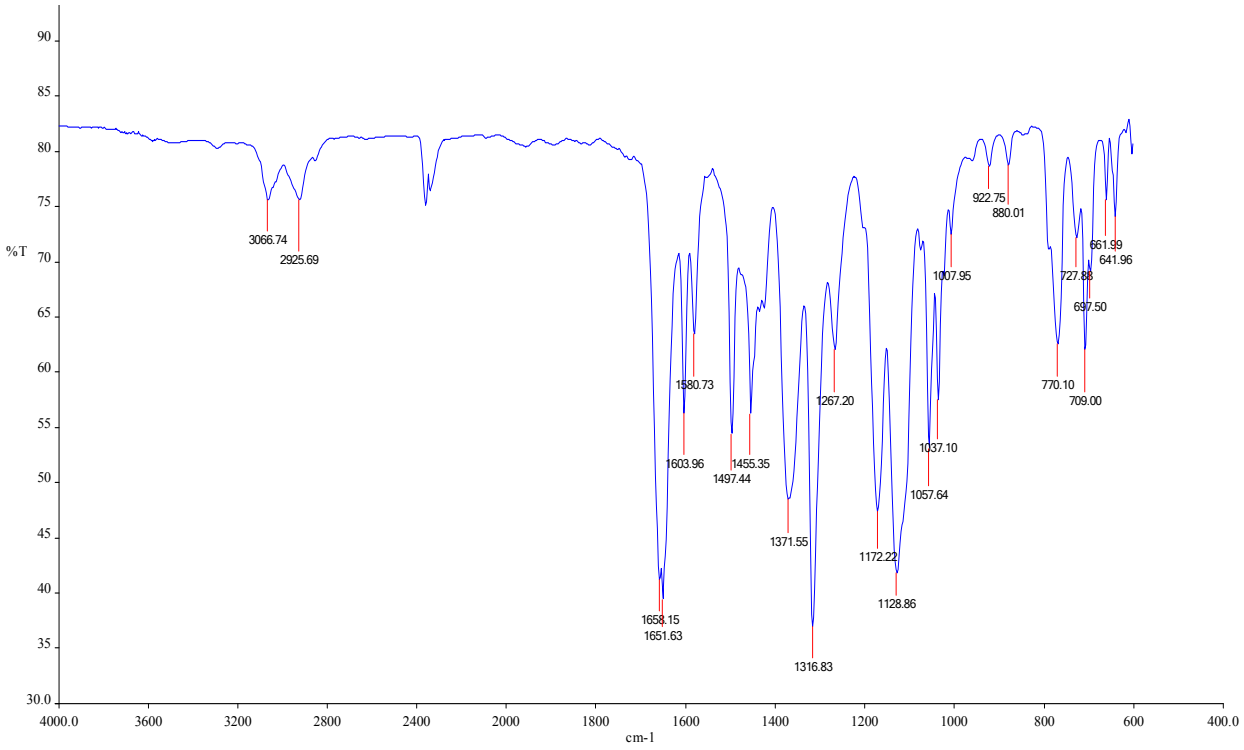
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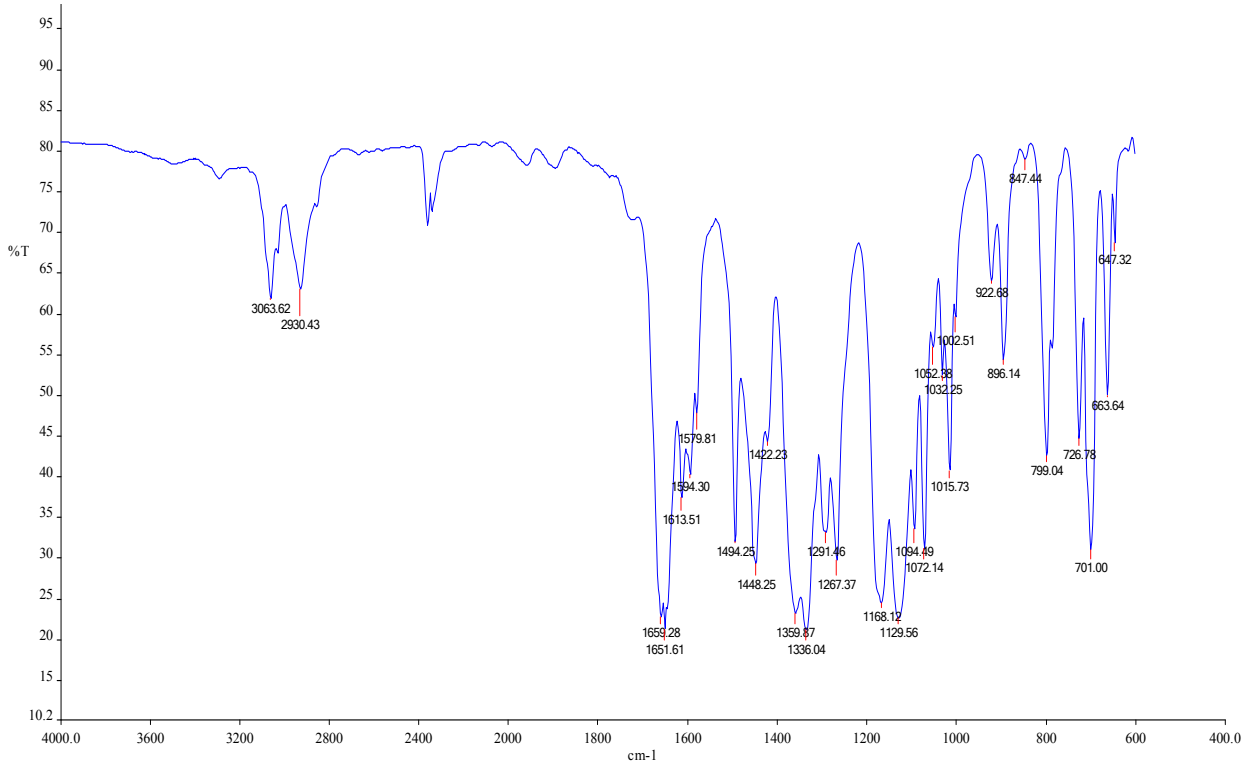
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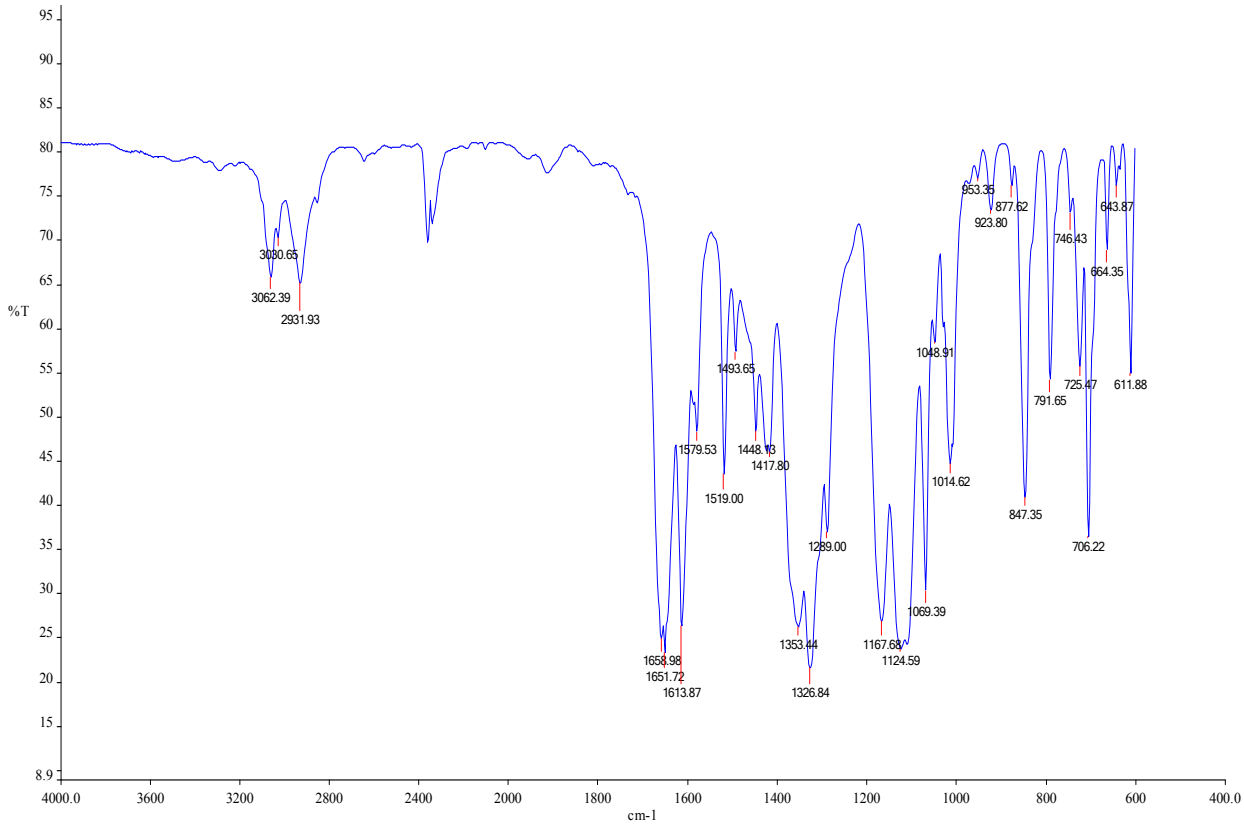
(f) NM30: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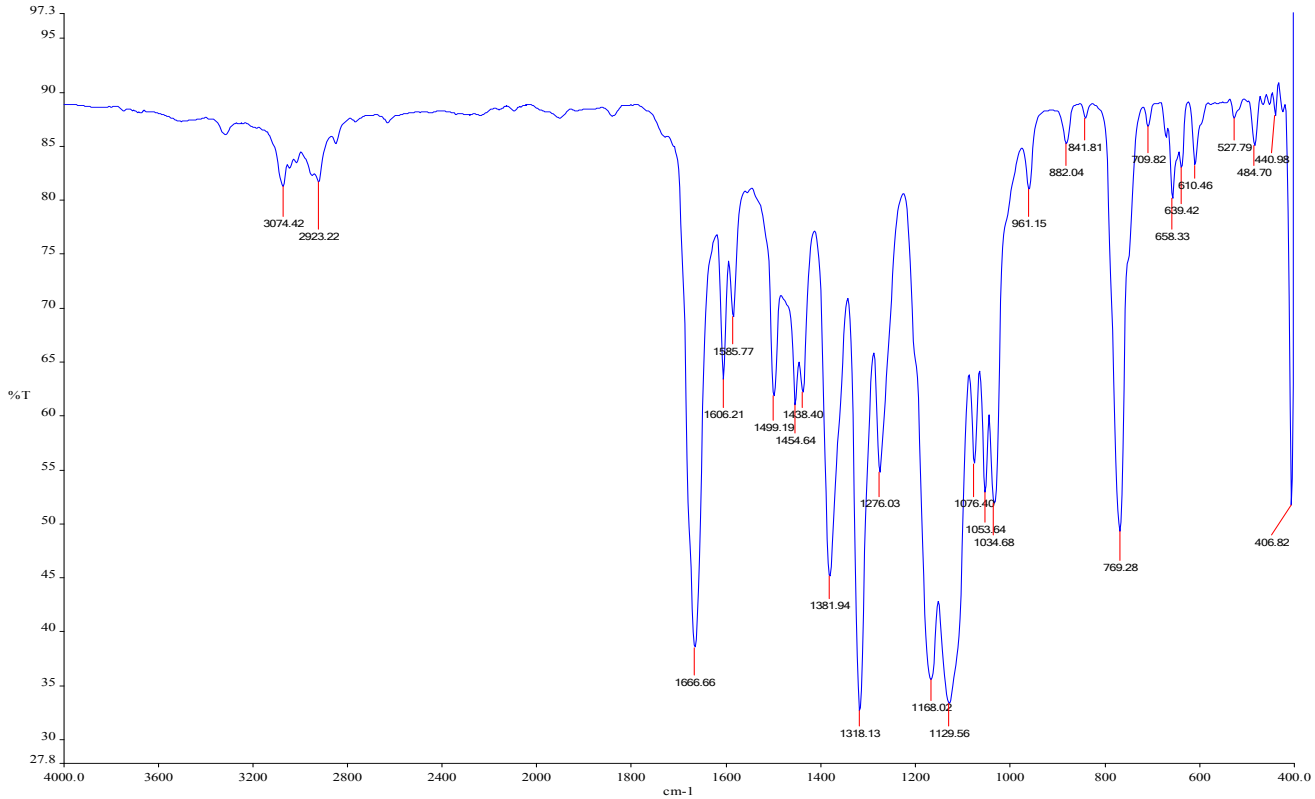
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1076.40
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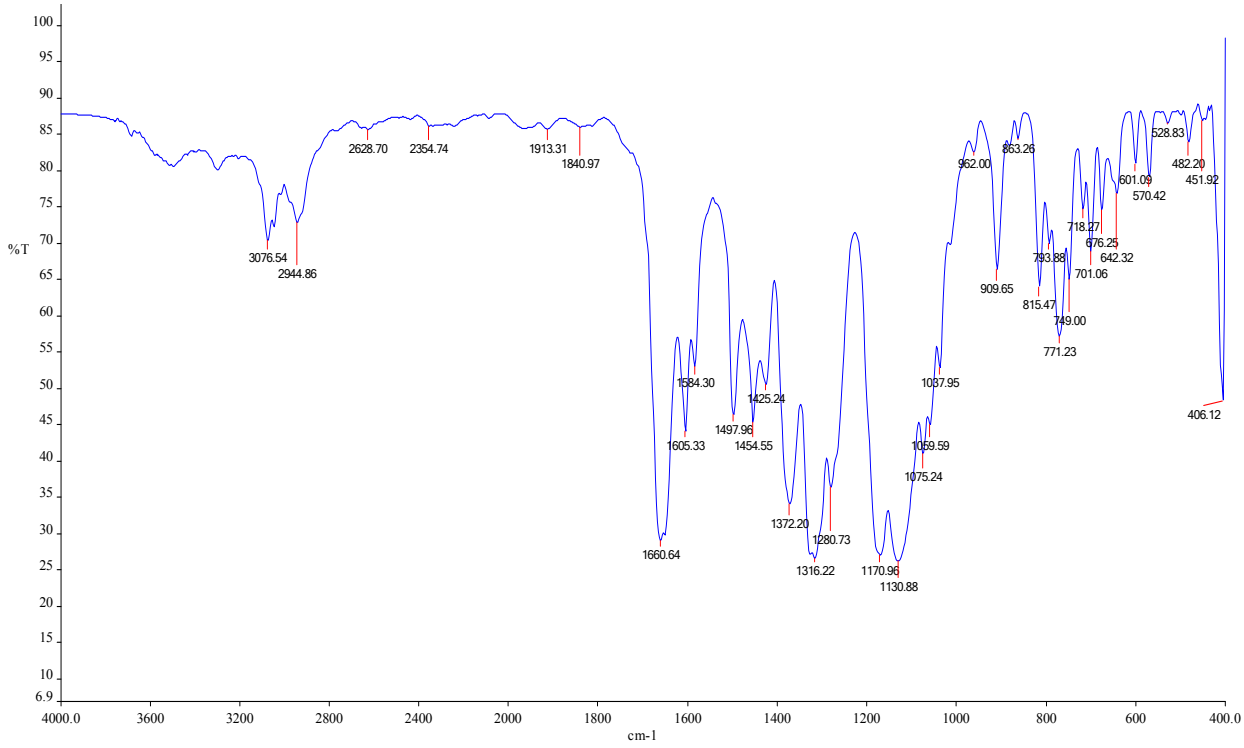
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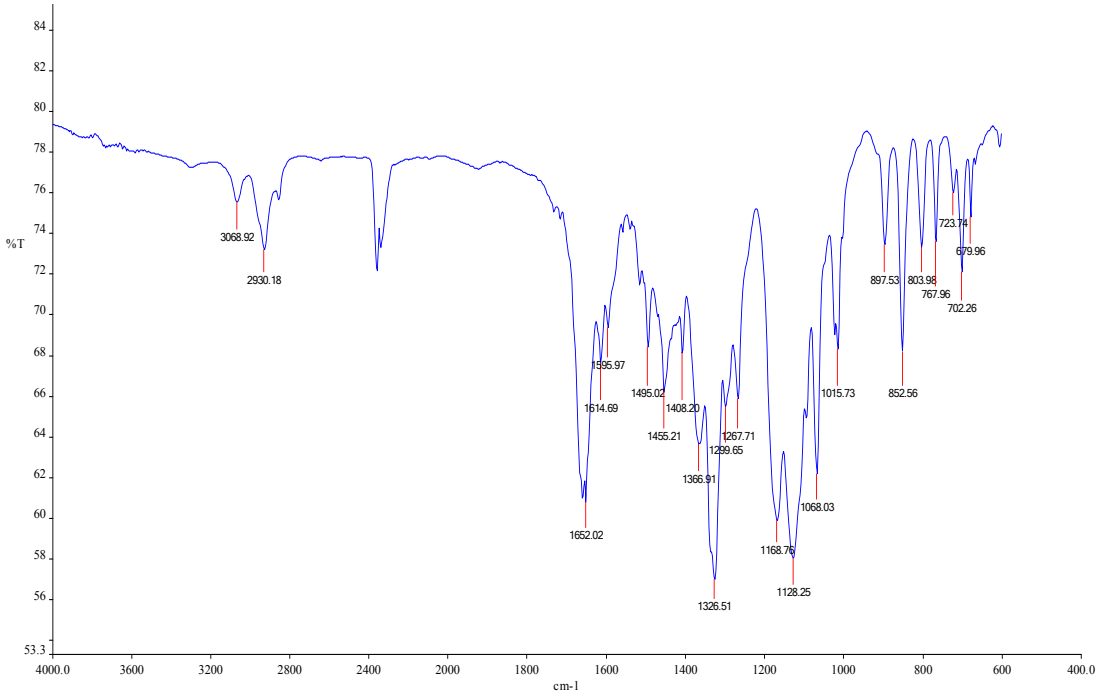
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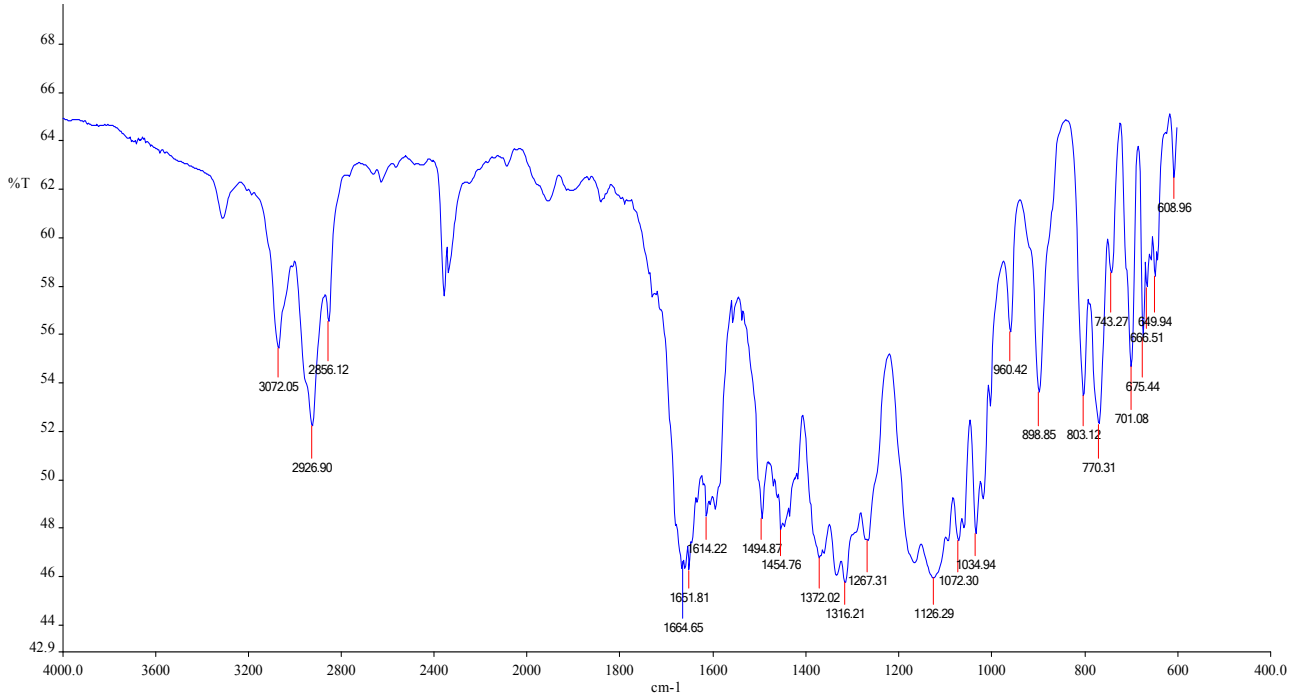
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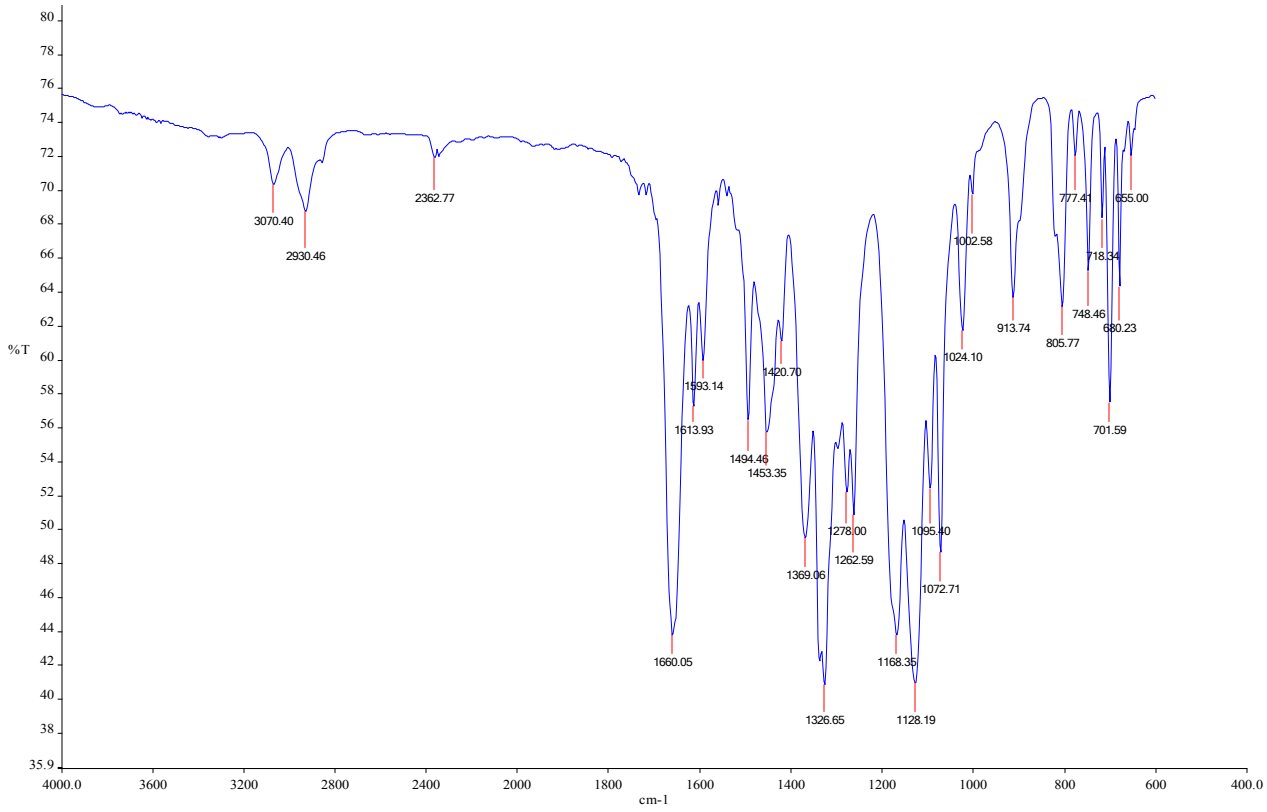
(k) NM22: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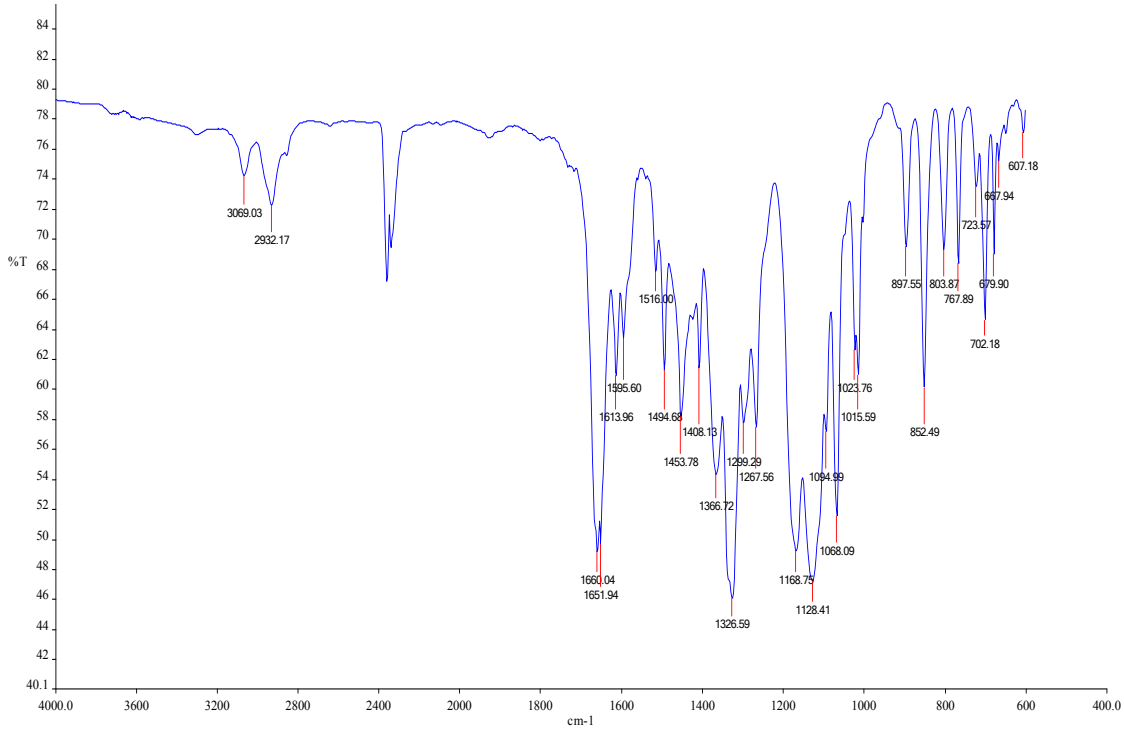
(l) NM 23: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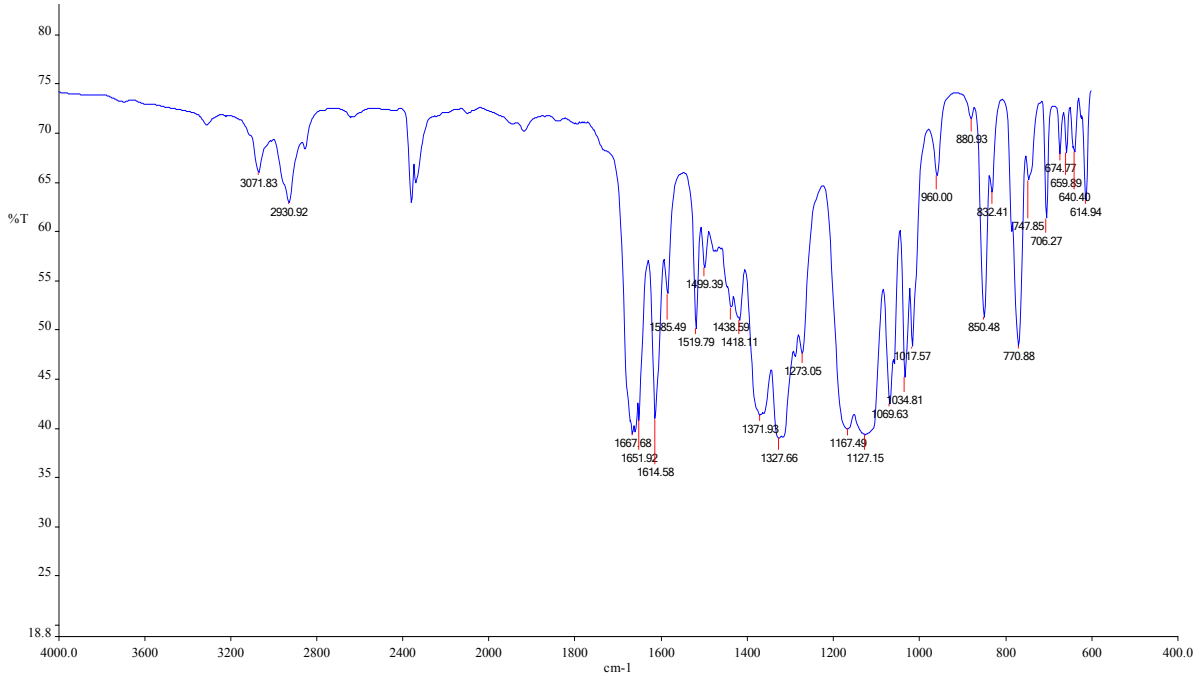
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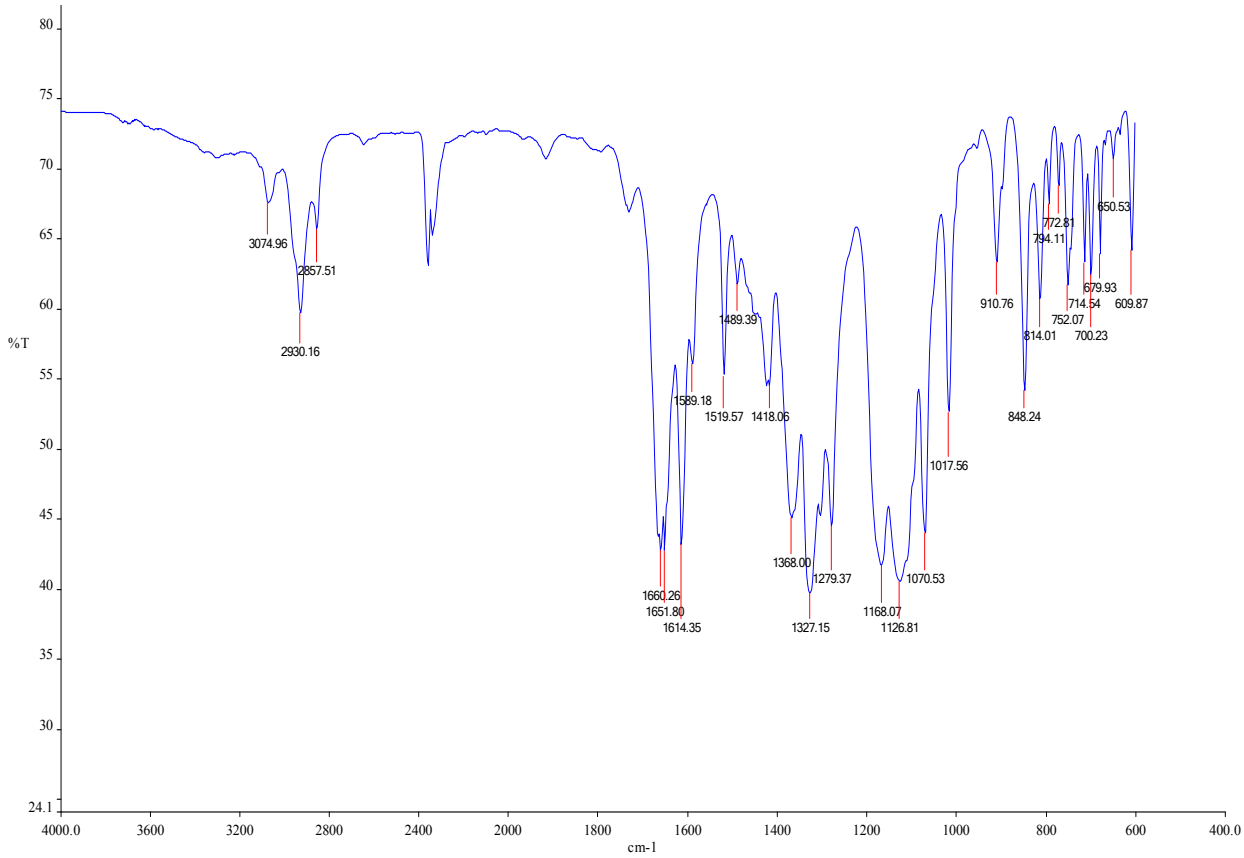
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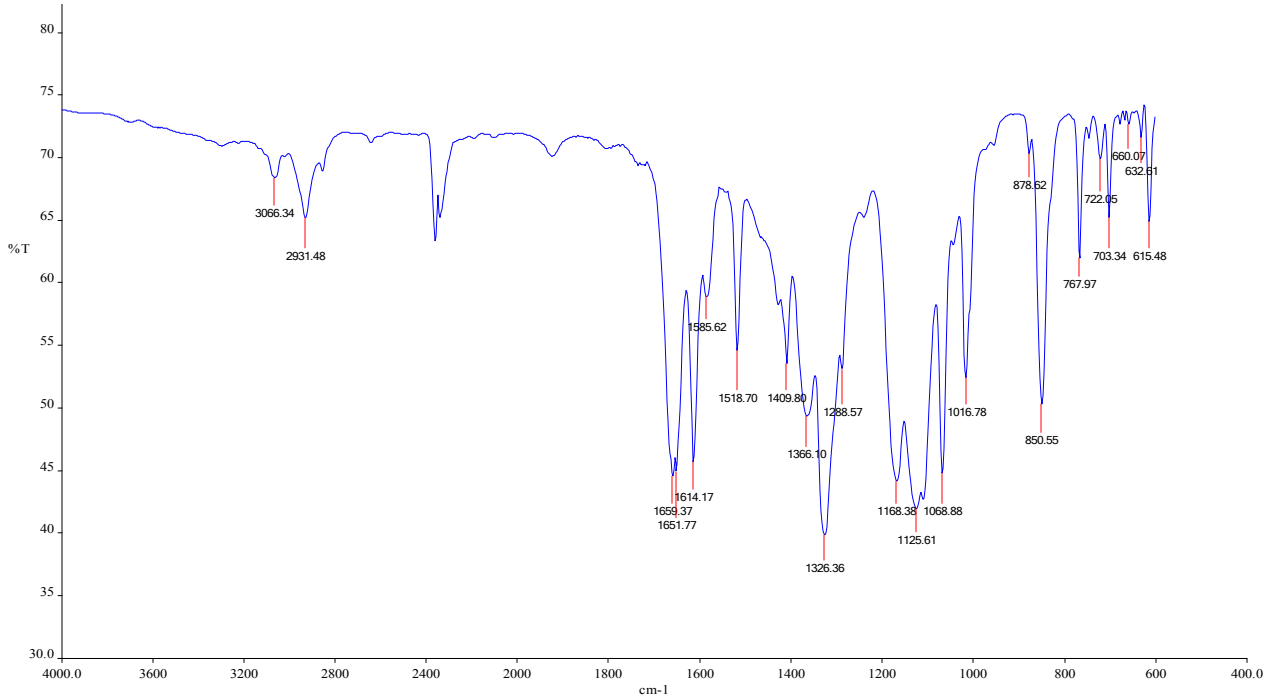
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1125.61
1068.88
1016.78
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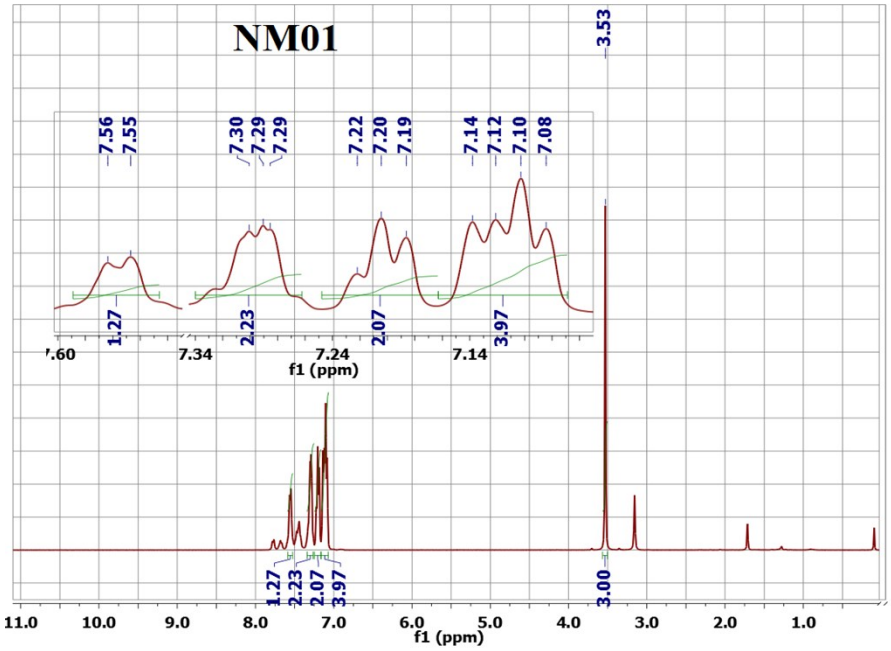
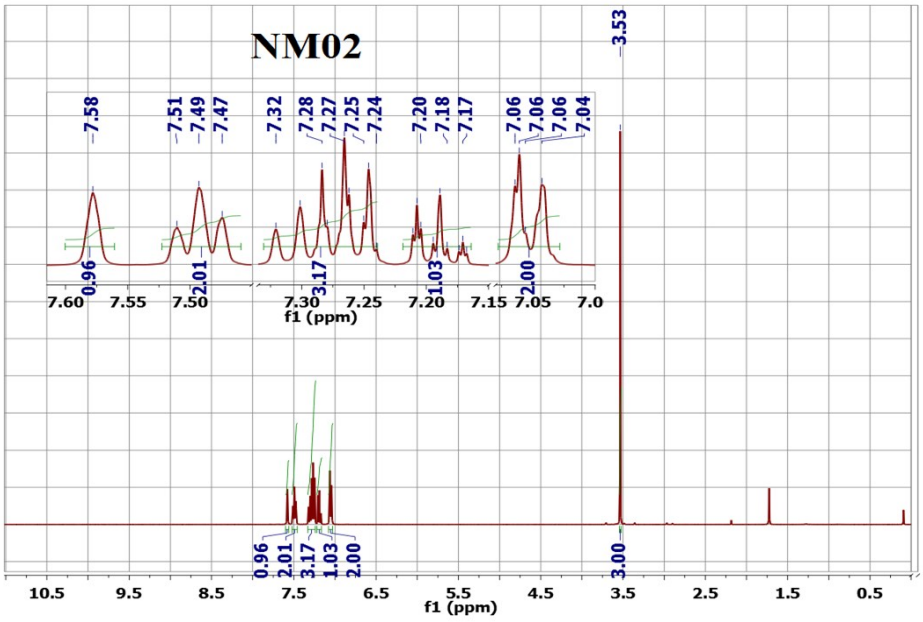
850.55
767.97
722.05
703.34
660.07
632.81
615.48

Figure S2: ^{1}HNMR of all compounds: All NMR spectra were recorded on a 400MHz spectrometer (from Bruker) in $CDCl_3$ as solvent.

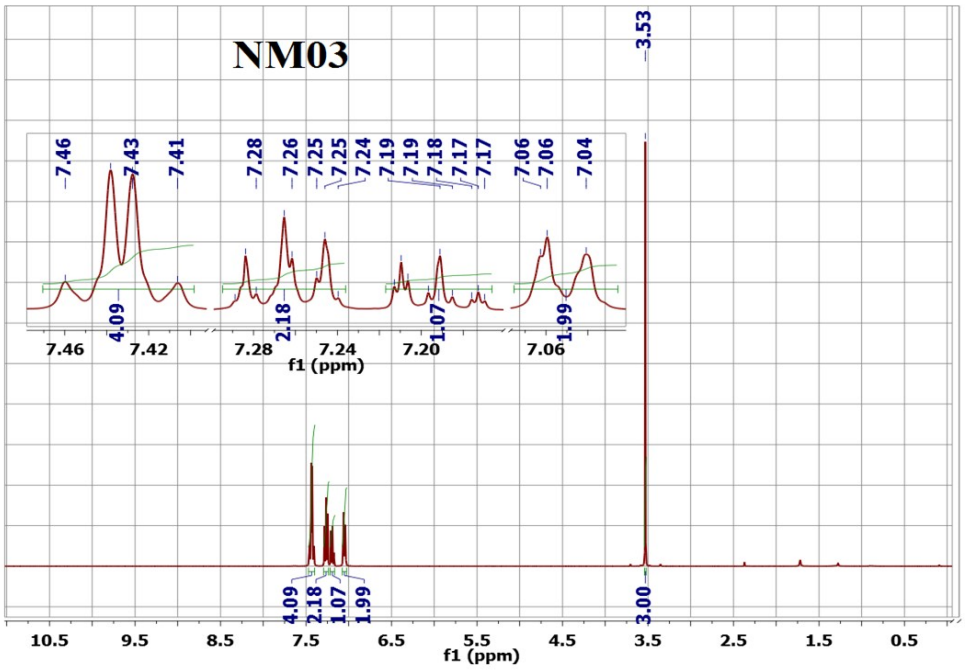
(a) NM01 (12 H)**:** δ 7.56 (d, *J* = 6.67Hz, 1H), 7.30 (m, 2H), 7.20 (t, *J* = 7.06 Hz, 2H), 7.11 (m, 4H), 3.53 (s, 3H).



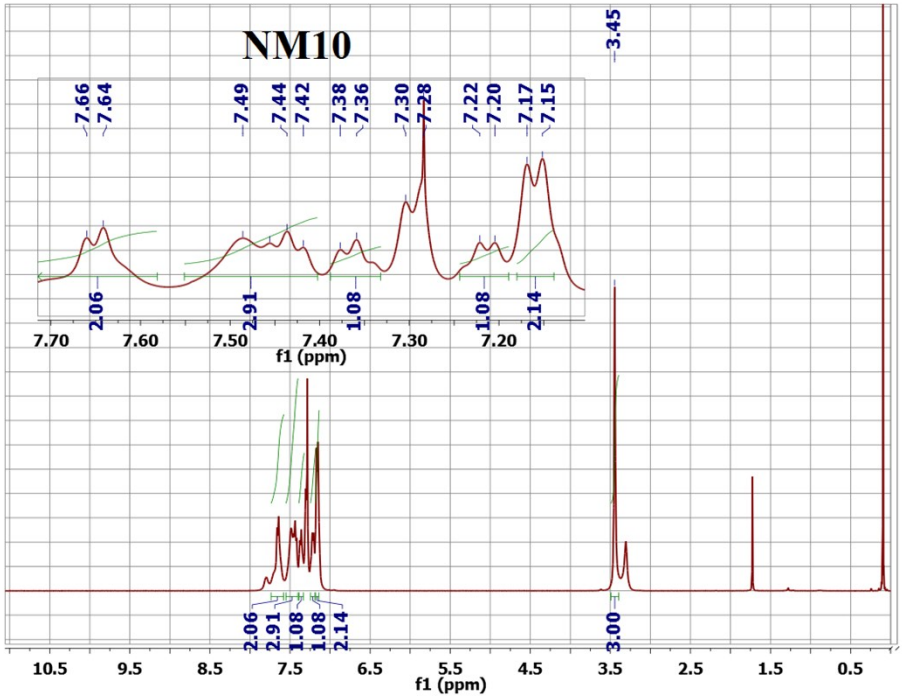
(b) NM02 (12 H)**:** δ7.58 (s, 1H), 7.49 (t, *J* = 7.43 Hz, 2H), 7.28 (m, 3H), 7.19 (tt, *J* = 7.43 Hz, 1.44 Hz, 1H), 7.05 (d, *J* = 7.43 Hz, 2H), 3.53 (s, 3H)



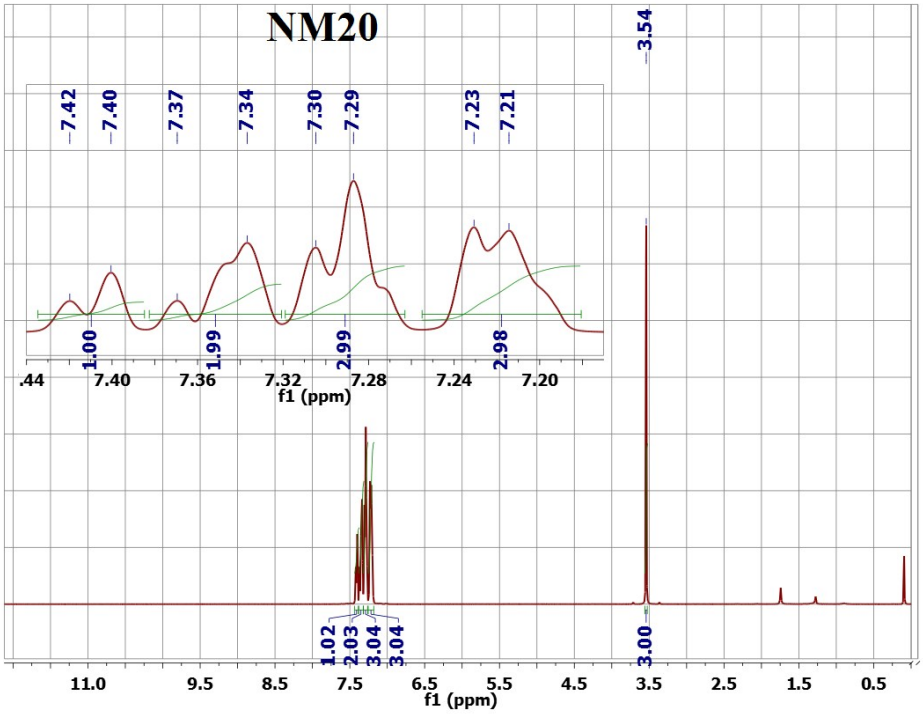
(c) NM03 (12 H)**:** δ 7.43 (td, *J* = 10.87 Hz, 4.25Hz, 4H), 7.27 (tt, *J* = 7.26 Hz, 1.70 Hz, 2H), 7.19 (tt, *J* = 7.35Hz, 1.43 Hz, 1H), 7.05 (d, *J* = 7.35 Hz, 2H), 3.53 (s, 3H)



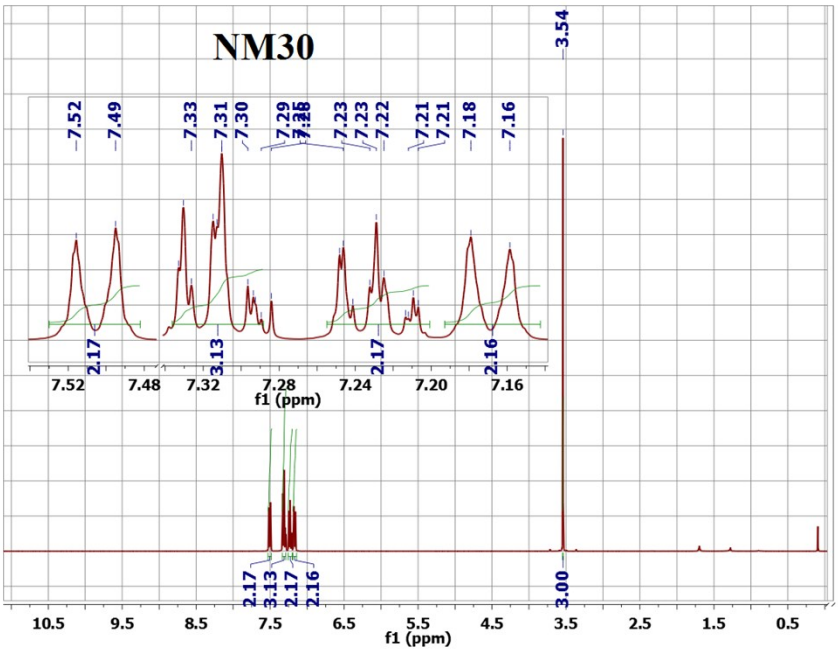
(d) NM10 (12 H)**:** δ 7.65 (d, *J* = 7.44 Hz, 2H), 7.45 (m, 3H), 7.36 (t, *J* = 7.44 Hz, 1H), 7.21 (d, *J* = 6.65 Hz, 1H), 7.16 (d, *J* = 7.00 Hz,2H), 3.45 (s, 3H)



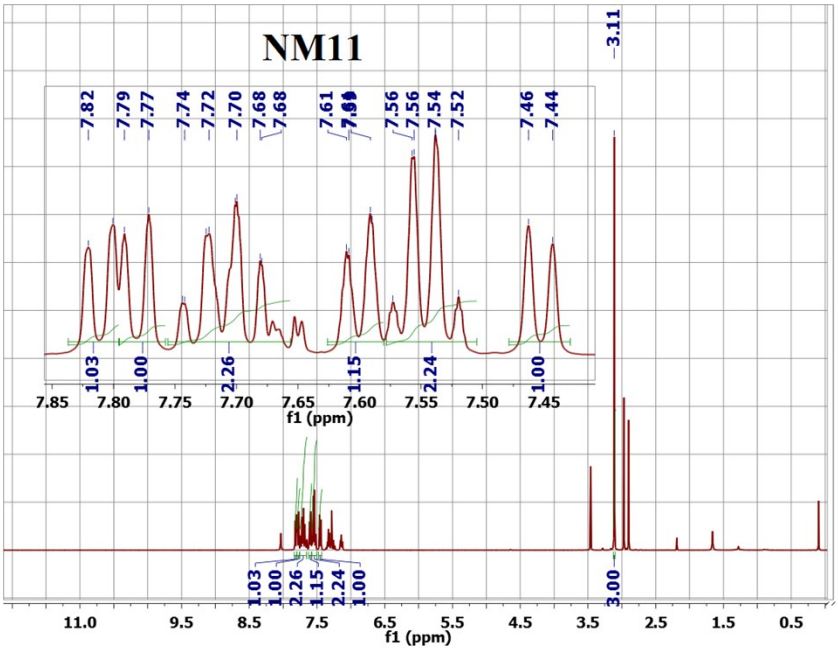
(e) NM20 (12 H)**:** δ 7.41 (d, *J* = 7.76 Hz, 1H), 7.35 (m, 2H), 7.29 (m, 3H), 7.22 (d, *J* = 7.42, 3H), 3.54 (s, 3H).



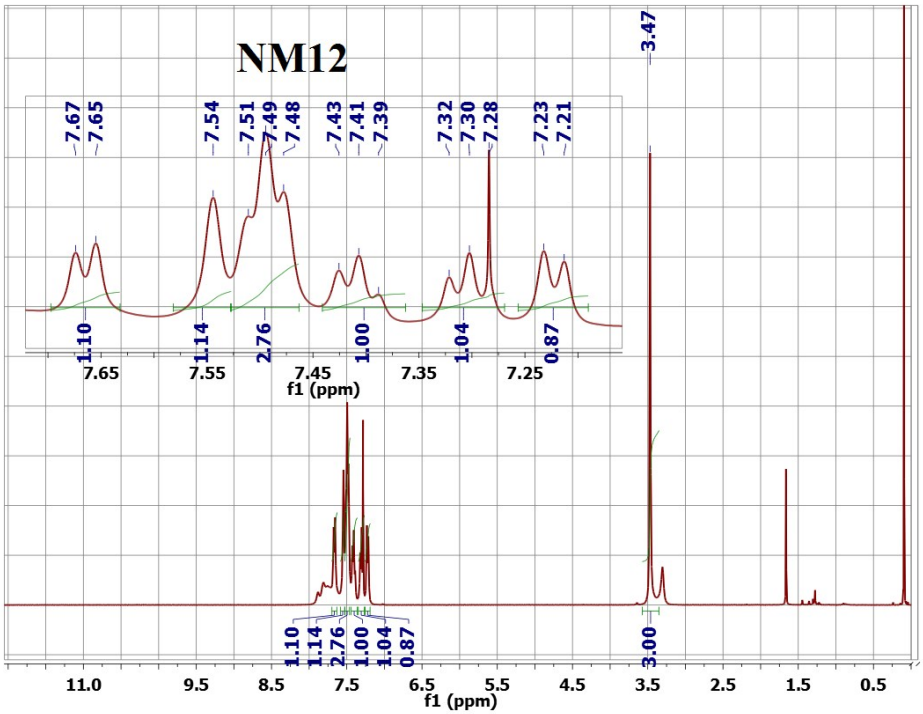
(f) NM30 (12 H)**:** 7.51 (d, *J* = 8.29 Hz, 2H), 7.31 (m, 3H), 7.23 (m, 2H), 7.17 (d, *J* = 8.29 Hz, 2H), 3.54 (s, 3H).



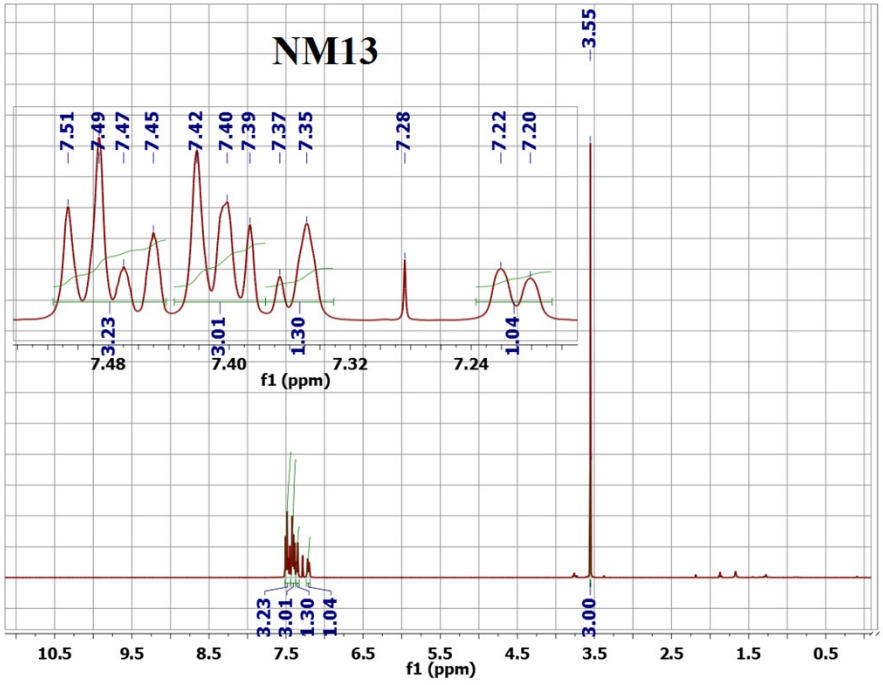
(g) NM11 (11 H)**:** δ7.81 (d, *J* = 7.95Hz, 1H), 7.78 (d, *J* = 7.95Hz, 1H), 7.70 (qn, *J* = 9.00Hz, 2H), 7.60 (d, *J* = 7.73 Hz,1H), 7.55 (q, *J* = 7.45, 2H), 7.45 (d, *J* = 7.73Hz, 1H), 3.11 (s, 3H).



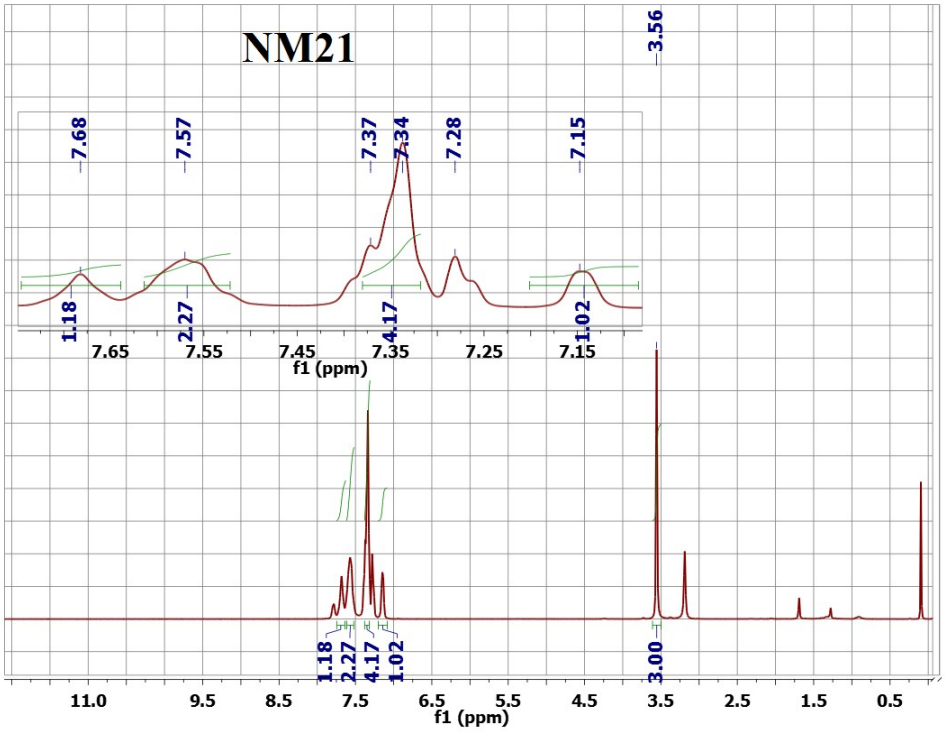
(h) NM12 (11 H)**:** δ 7.66 (d, *J* = 7.70 Hz, 1H), 7.54 (s, 1H), 7.49 (t, *J* = 6.80 Hz, 3H), 7.41 (t, *J* = 7.43 Hz, 1H), 7.30 (t, *J* = 7.42 Hz, 1H), 7.22 (d, *J* = 7.77 Hz, 1H), 3.47 (s, 3H).



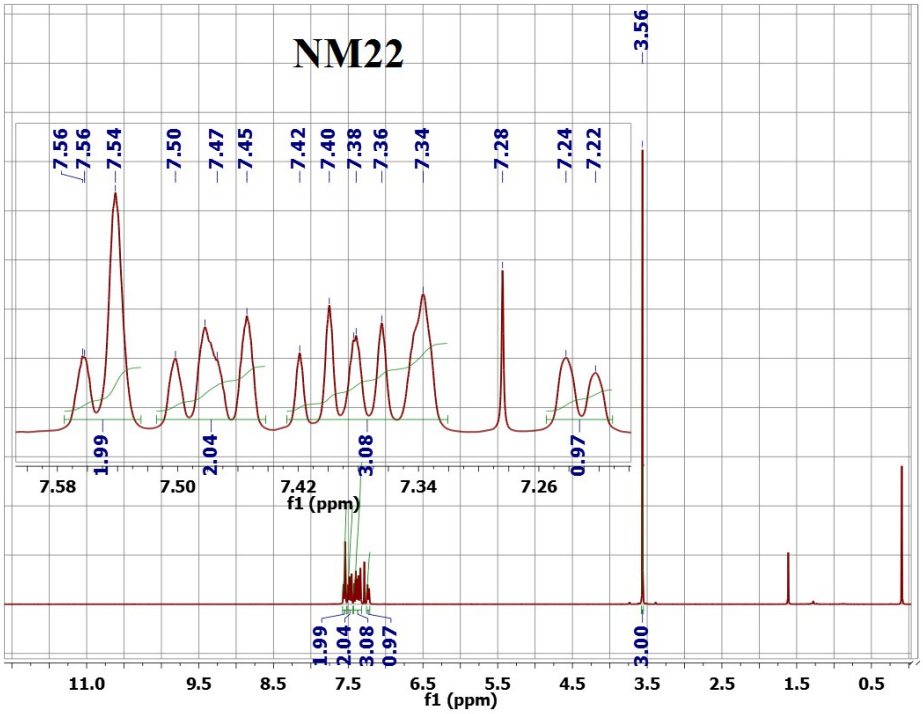
(i) NM13 (11 H**):** δ 7.48 (m, 3H), 7.40 (t, *J* = 7.73 Hz, 3H), 7.36 (d, *J* = 7.72 Hz, 1H), 7.21 (d, *J* = 7.72 Hz, 1H), 3.55 (s, 3H).



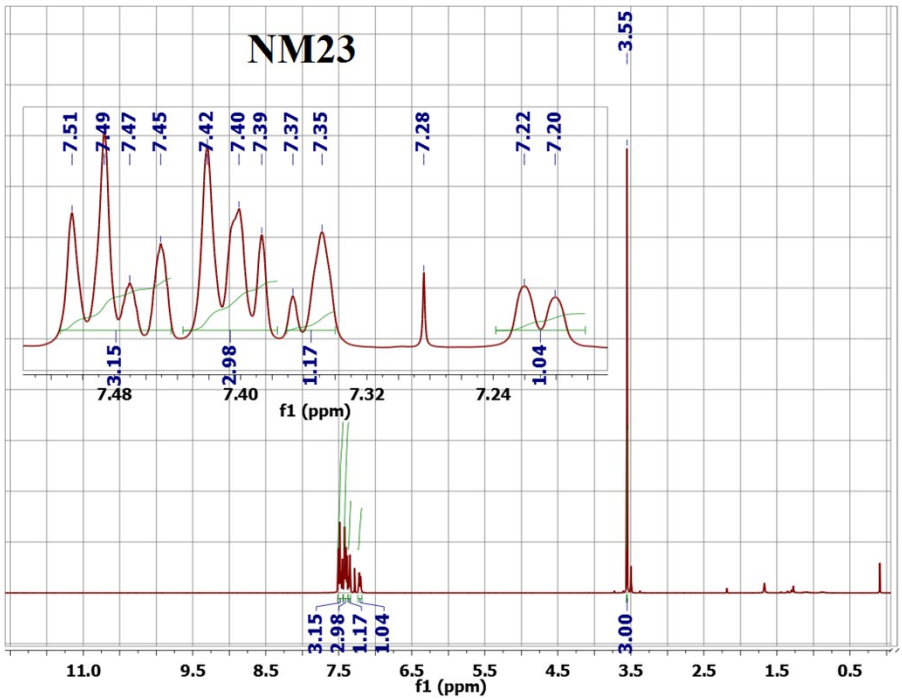
(j) NM21 (11H**):** δ 7.68 (s, 1H), 7.57 (m, 2H), 7.34 (m, 4H), 7.15 (s, 1H), 3.56 (s, 3H)



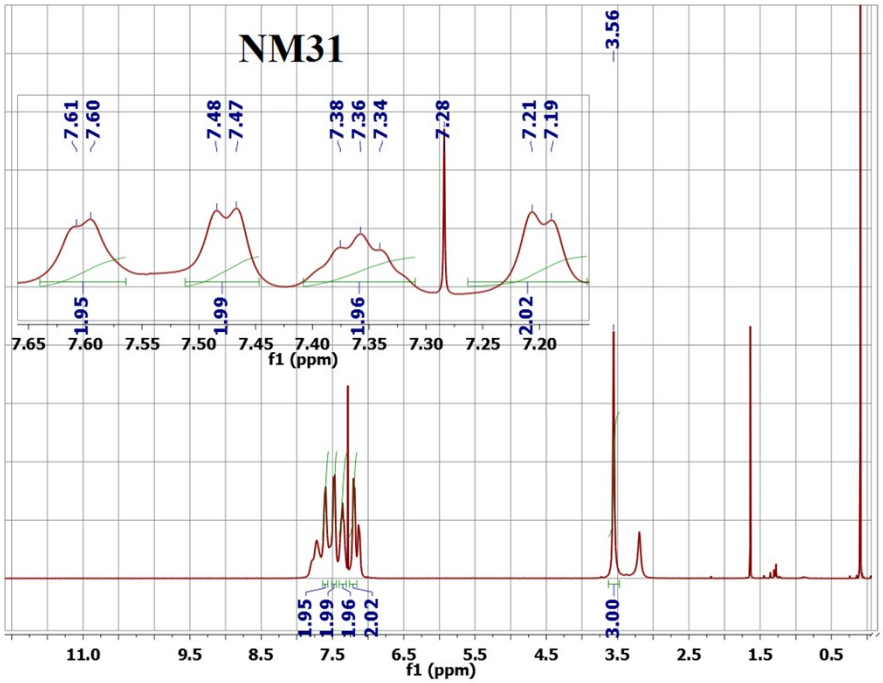
(k) NM22 (11H**):** δ 7.55 (d, *J* = 8.42 Hz, 2H), 7.48 (t, *J* = 9.05 Hz, 2H), 7.38 (m, 3H), 7.23 (d, *J* = 7.96Hz, 1H), 3.56 (s, 3H).



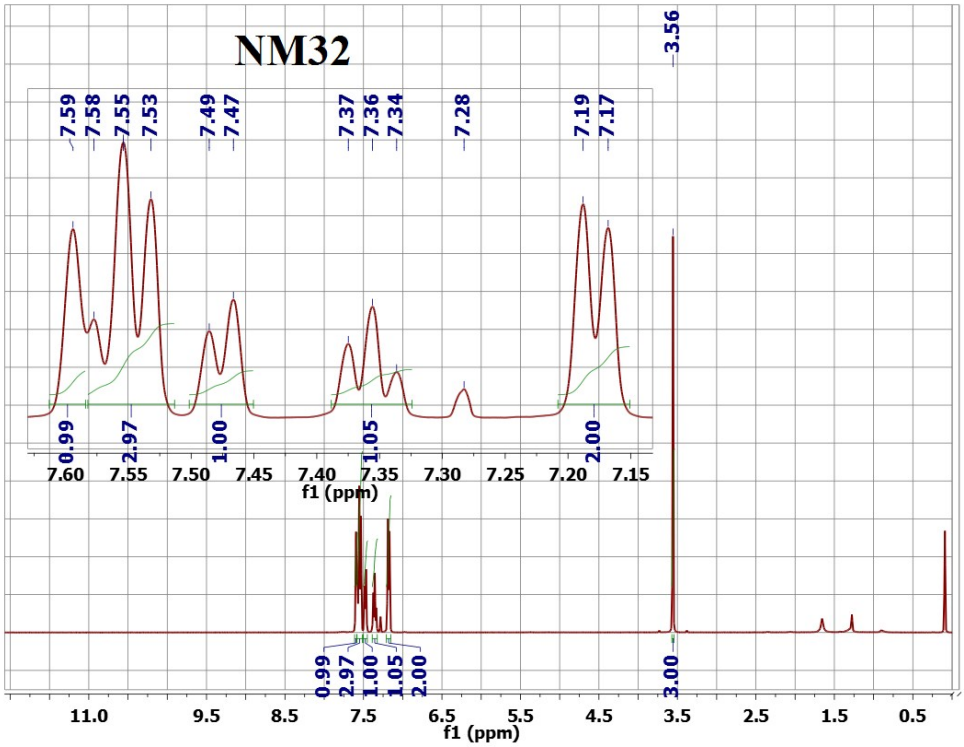
(l) NM23 (11H**):** δ 7.48 (m, 3H), 7.40 (t, *J* = 7.01 Hz, 3H), 7.36 (d, *J* = 7.43 Hz, 1H), 7.21 (d, *J* = 7.85 Hz, 1H), 3.55 (s, 3H).



(m) NM31 (11H**):** δ 7.61 (d, J = 7.84Hz, 2H), 7.48 (d, J = 6.90Hz, 2H), 7.36 (t, J = 6.93Hz, 2H), 7.20 (d, J = 6.90Hz, 2H), 3.56 (s, 3H).



(n) NM32 (11H**):** δ 7.59 (s, 1H), 7.55 (t, *J* = 9.11Hz, 3H), 7.48 (d, *J* = 7.56Hz, 1H), 7.36 (t, *J* = 7.83Hz, 1H), 7.18 (d, *J* = 7.90Hz, 2H), 3.56 (s, 3H).



(o) NM33 (11H**):** δ 7.54 (t, *J* = 7.65 Hz, 3H), 7.50 (s, 1H), 7.44 (d, *J* = 8.31 Hz, 2H), 7.18 (d, *J* = 8.02 Hz, 2H), 3.55 (s, 3H).

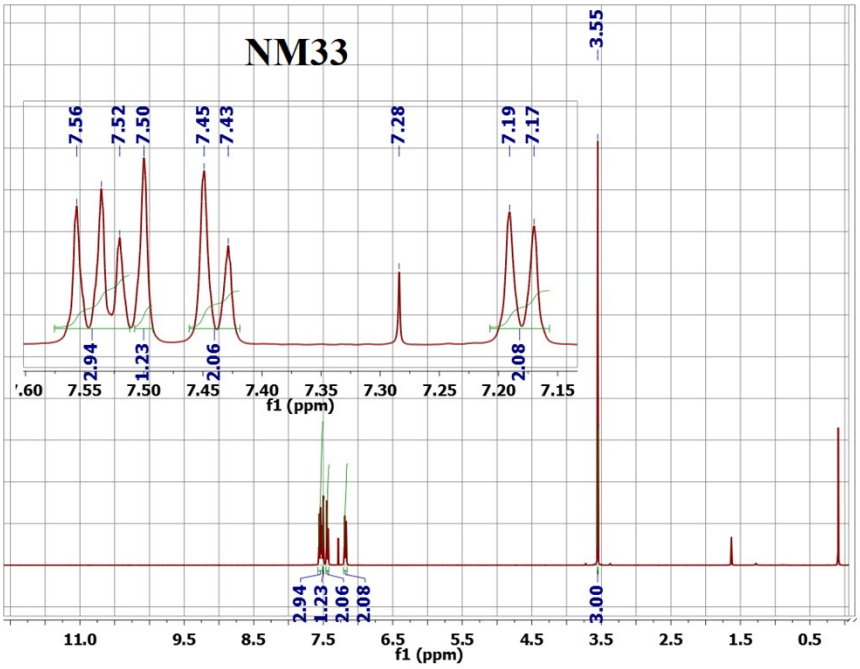
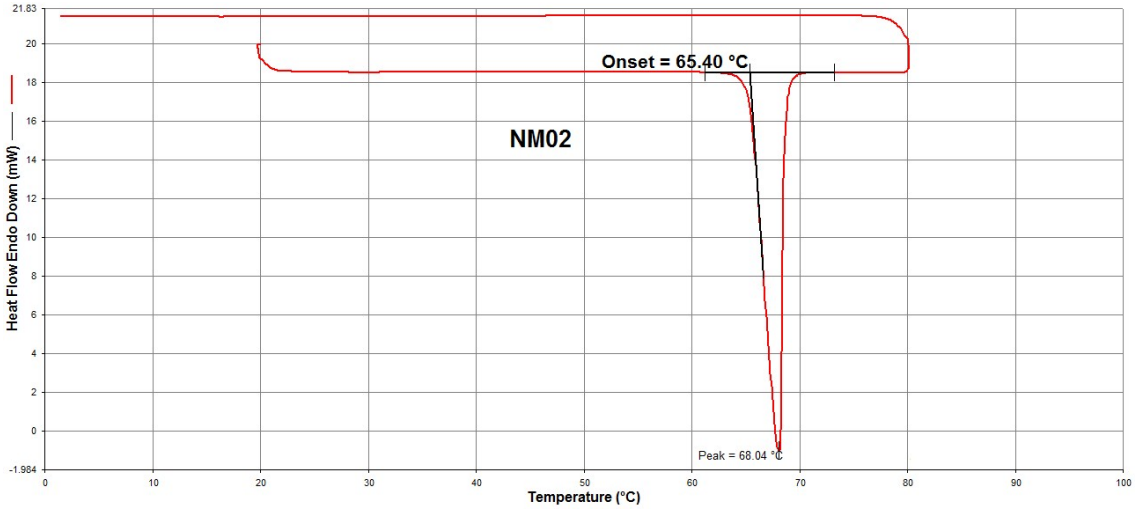
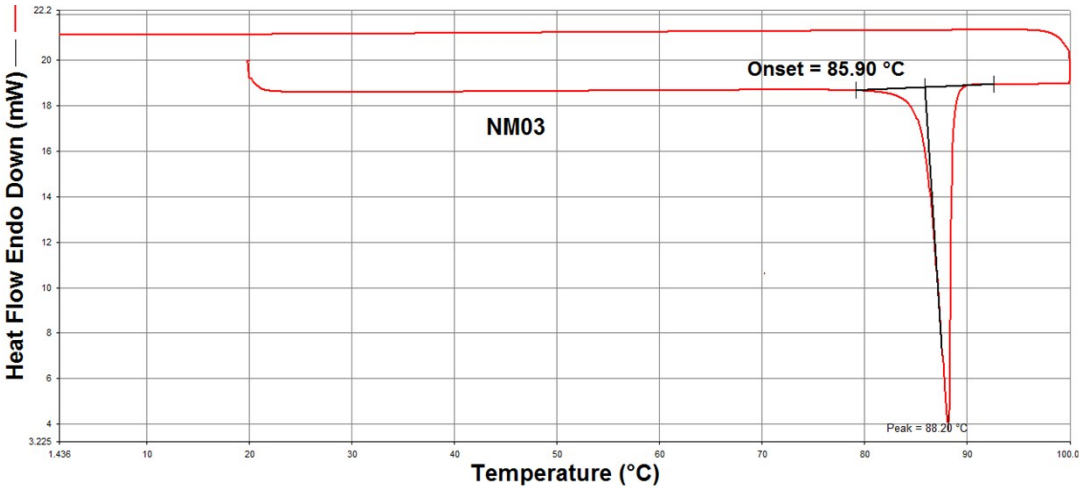


Figure S3: DSC curves of solids (@ 5°C/min) recorded on Perkin Elmer DSC 6000.

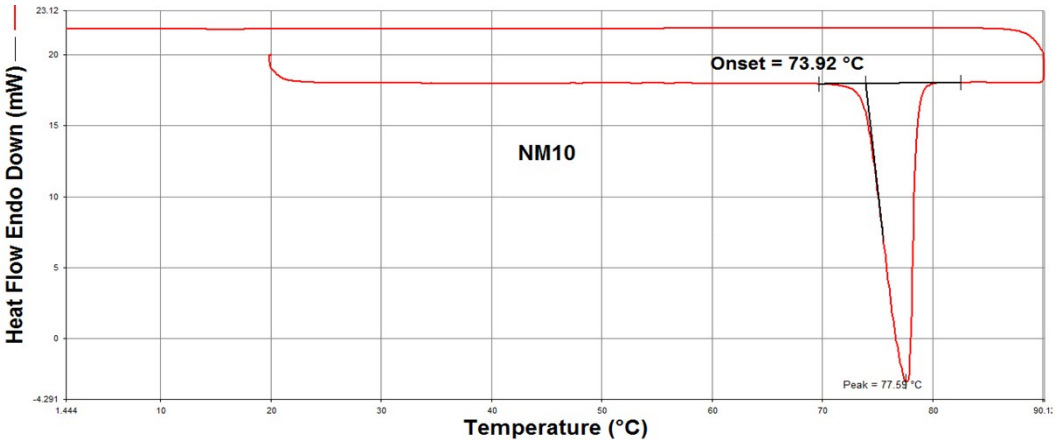
(a) NM02



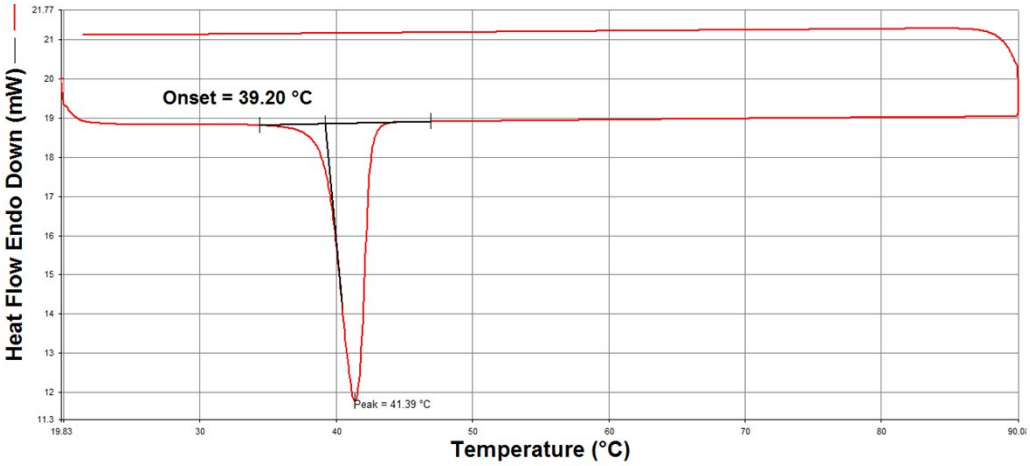
(b) NM03:



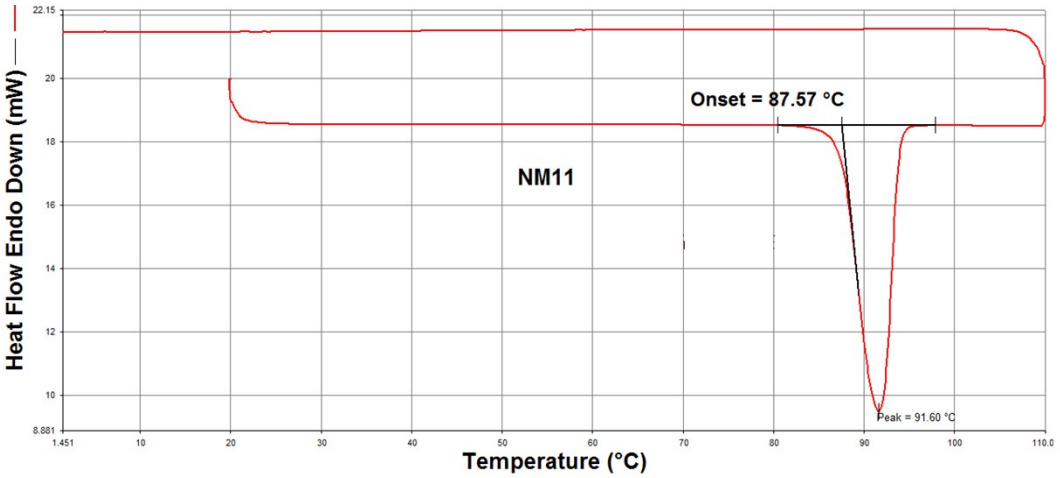
(c) NM10:



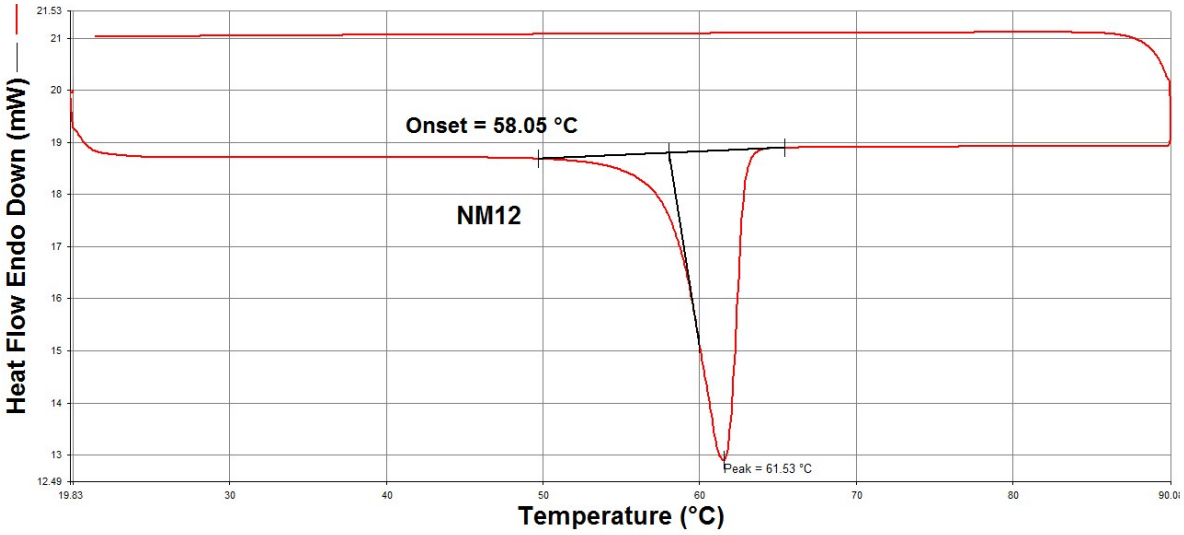
(d) NM30:



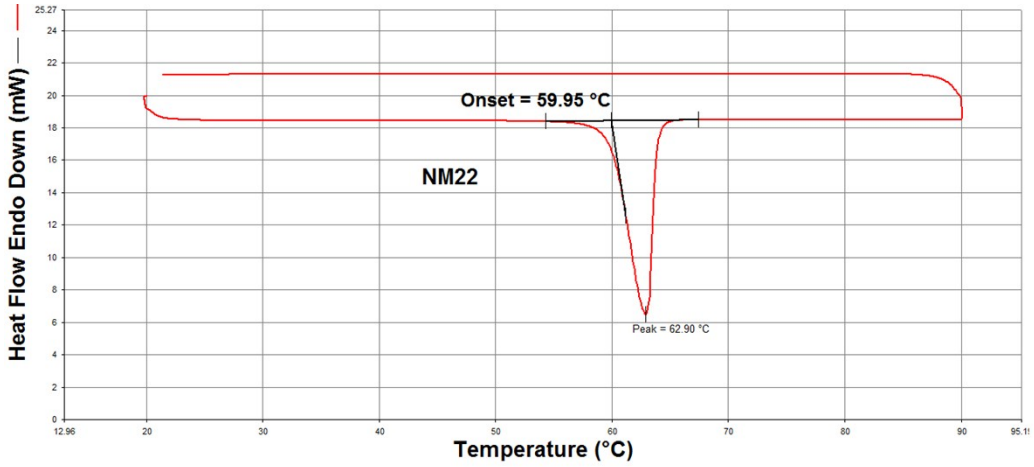
(e) NM11:



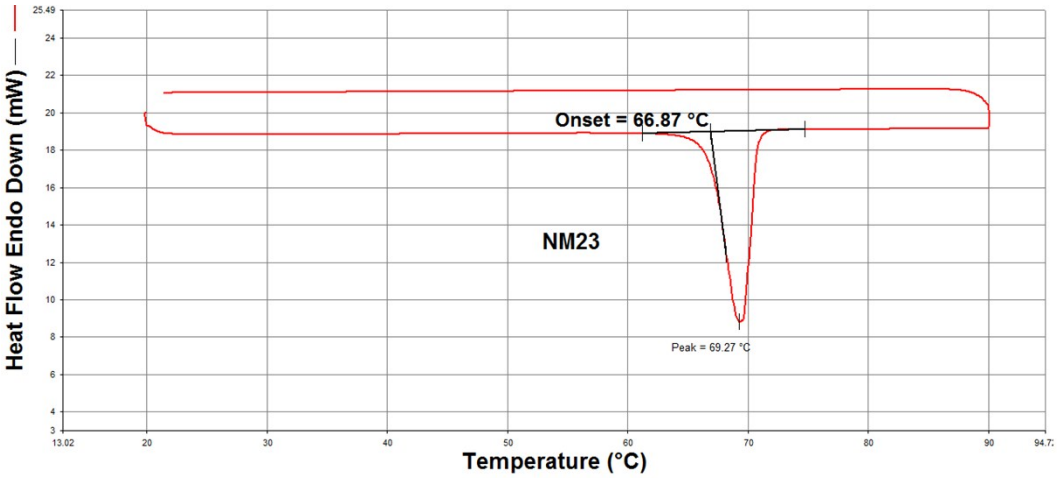
(f) NM12:



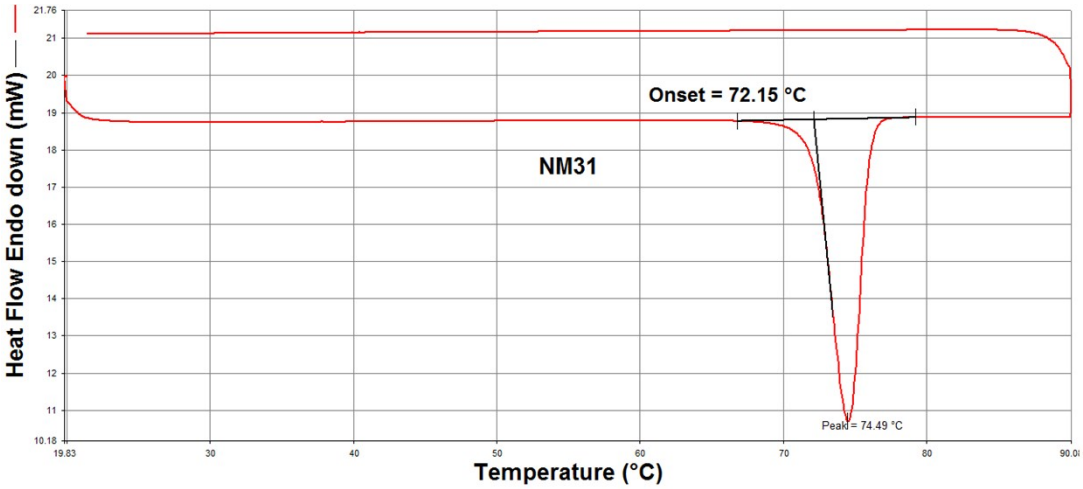
(g) NM22:



(h) NM23:


Heat Flow Endo Down (mW)
Onset = 66.87 °C
NM23
Peak = 69.27 °C
Temperature (°C)

(i) NM31:


Heat Flow Endo down (mW)
Onset = 72.15 °C
NM31
Peak = 74.49 °C
Temperature (°C)

(j) NM33:

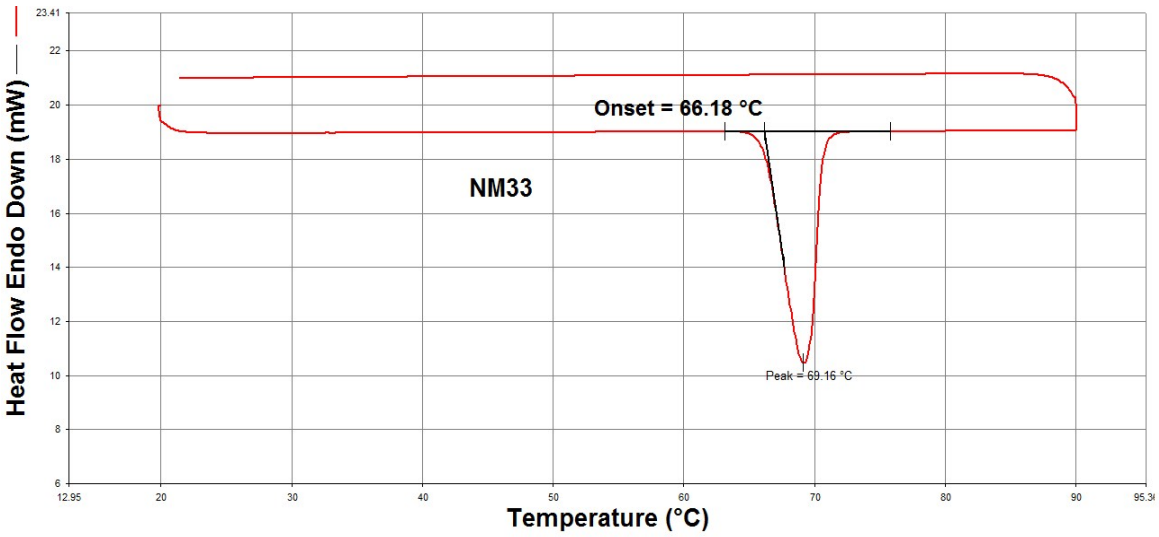
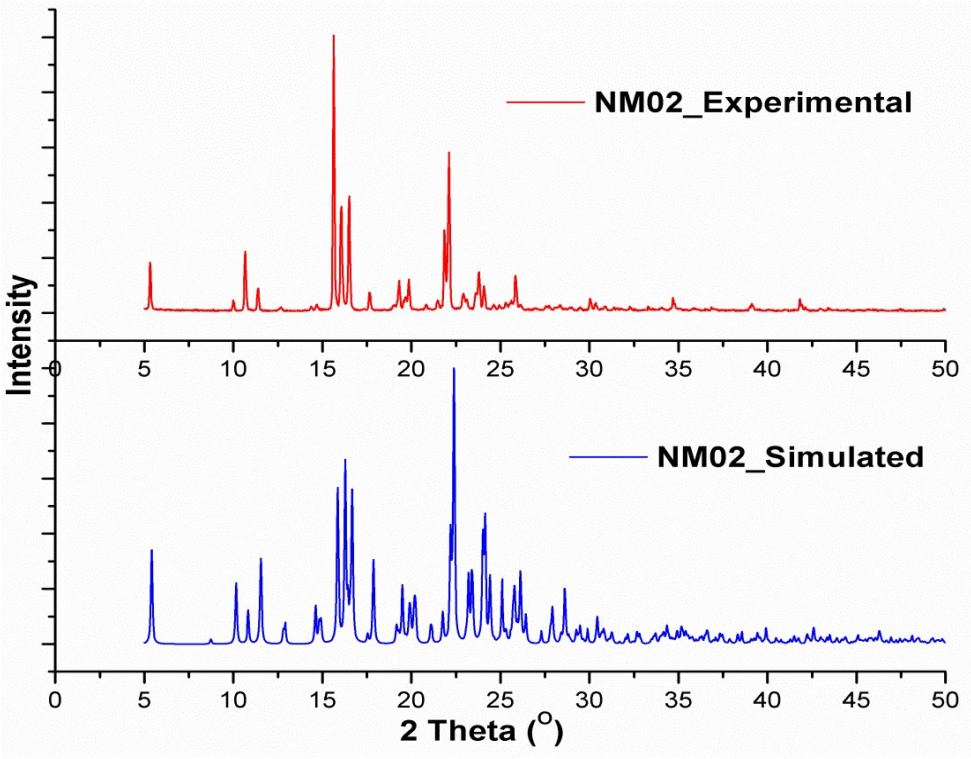
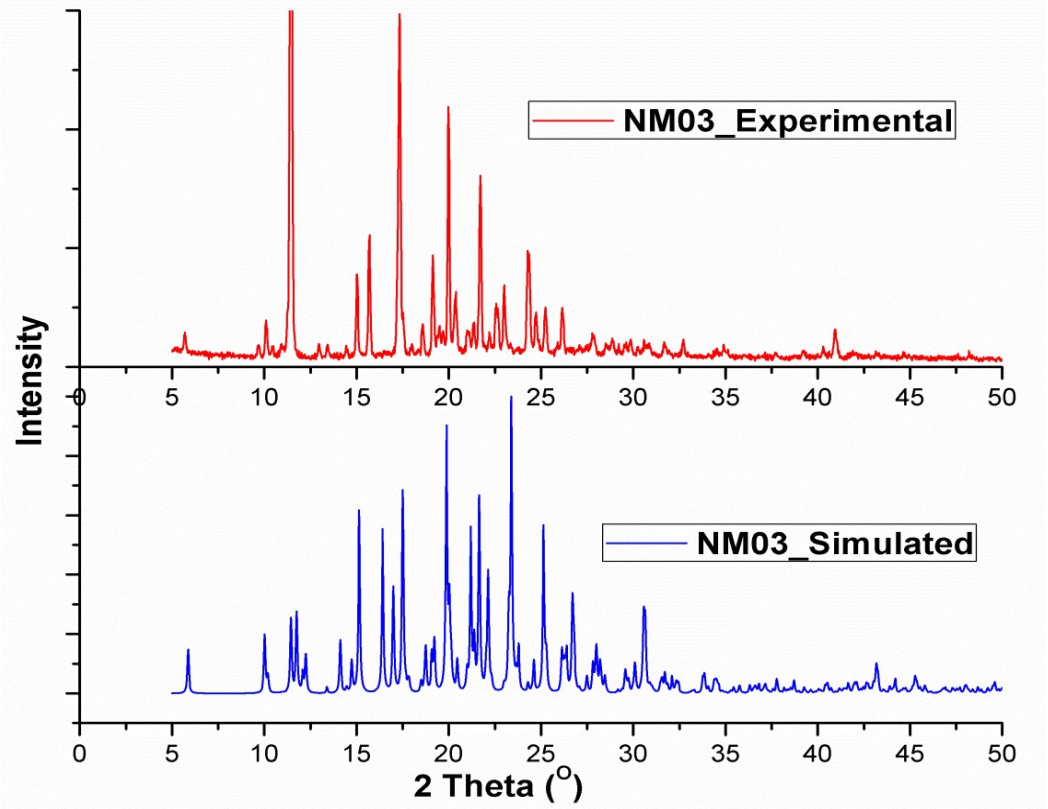

Heat Flow Endo Down (mW)
Onset = 66.18 °C
NM33
Peak = 69.16 °C
Temperature (°C)

Figure S4: Experimental powder pattern for all solid compounds and its comparison with the simulated powder pattern.

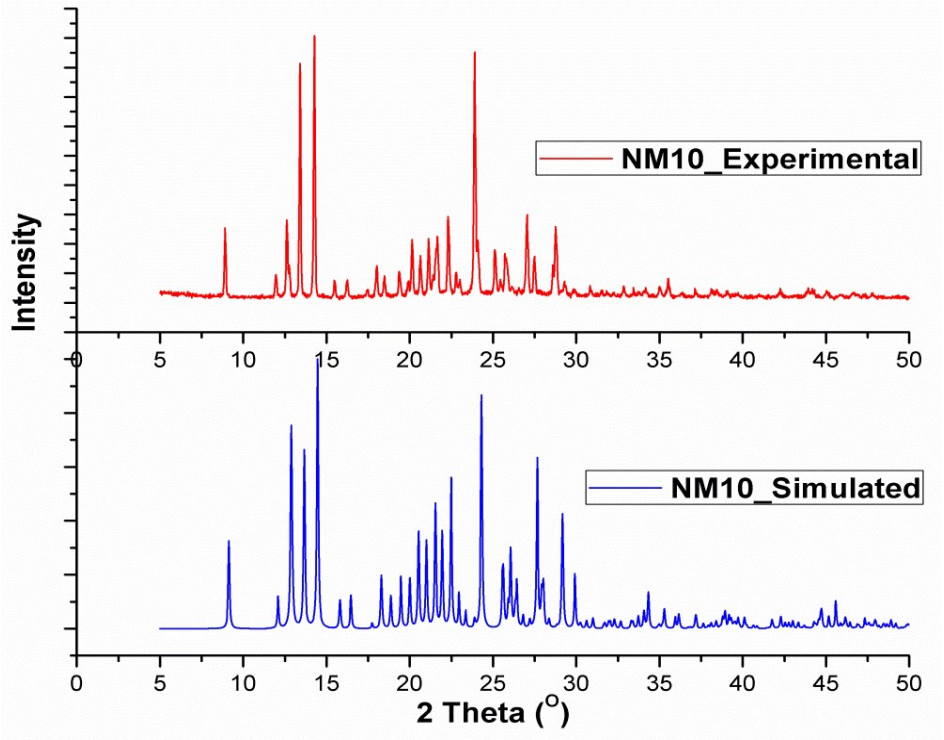
(a) NM02:



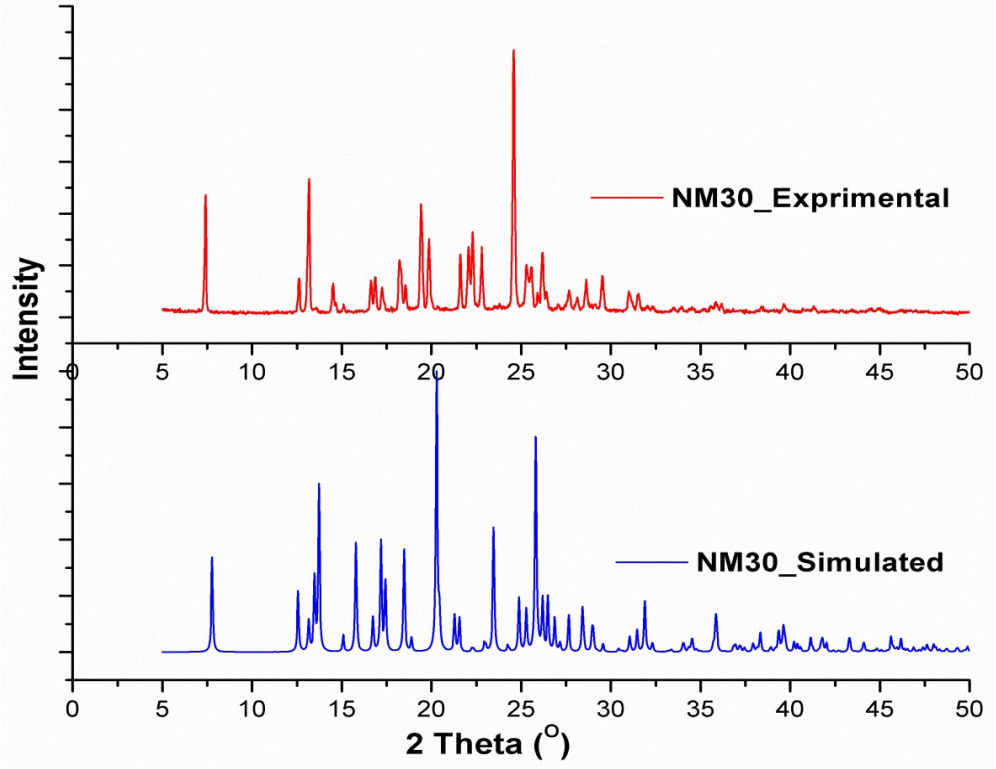


(b) NM03

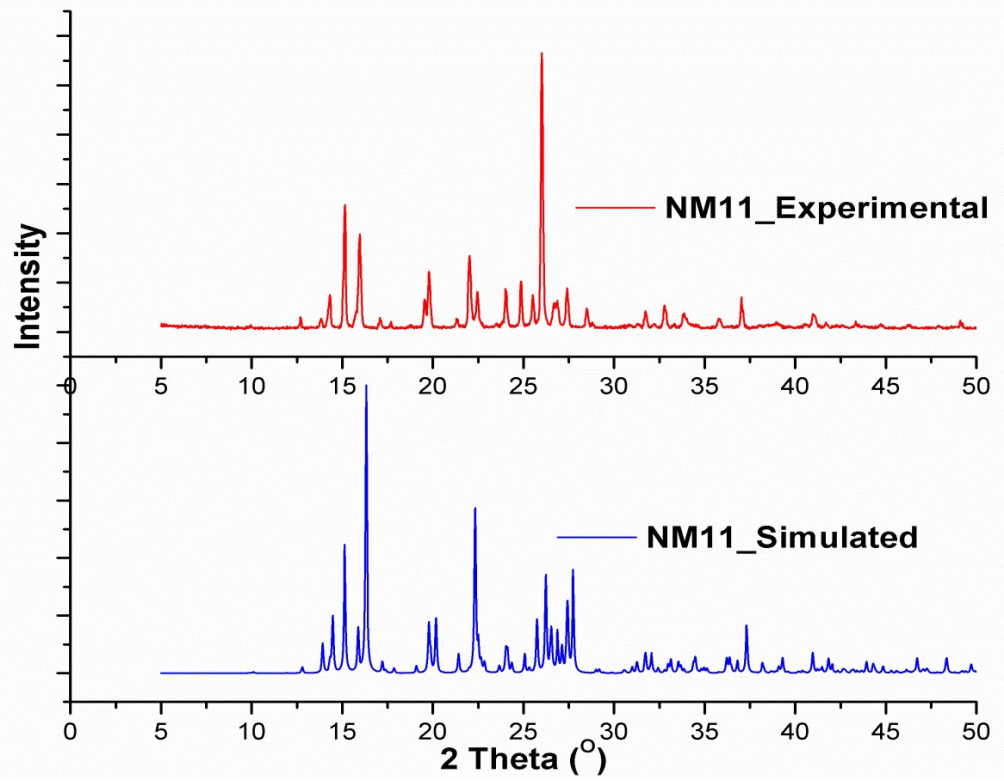
(c) NM10:



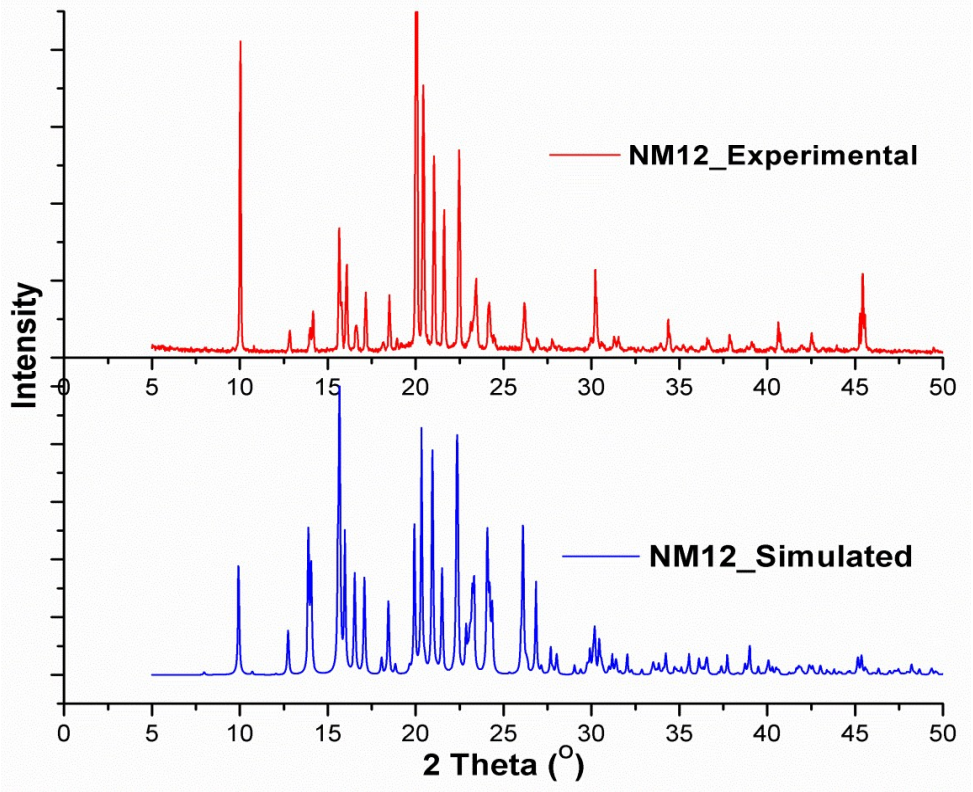
(d) NM30:


NM30_Exprimental
NM30_Simulated
Intensity
2 Theta (°)
0
5
10
15
20
25
30
35
40
45
50

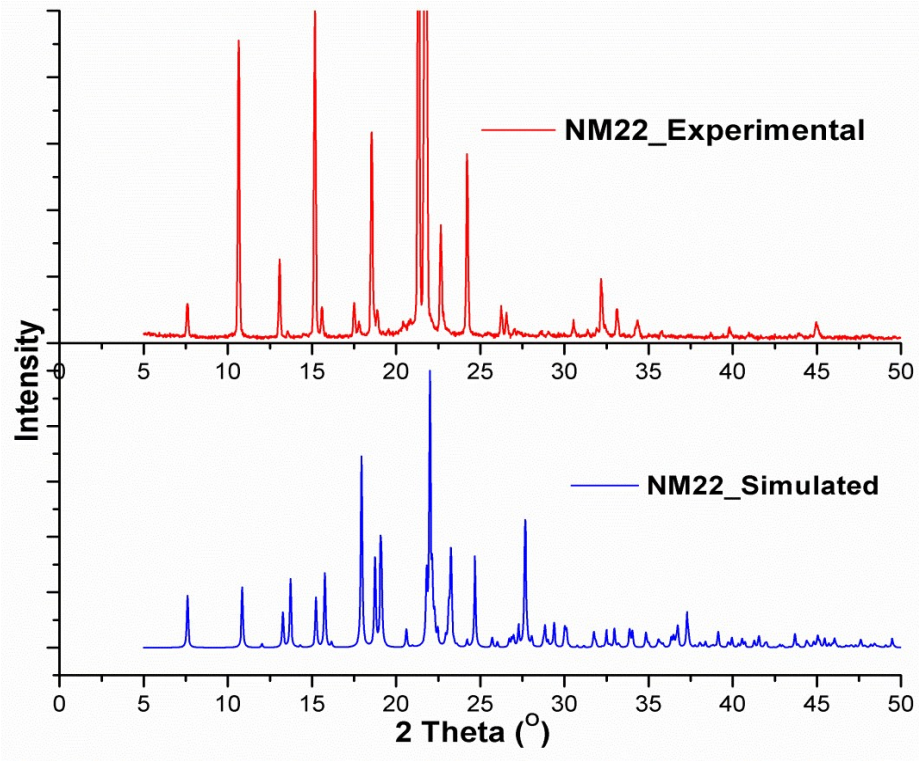
(e) NM11:


NM11_Experimental
NM11_Simulated
Intensity
2 Theta (°)
0
5
10
15
20
25
30
35
40
45
50

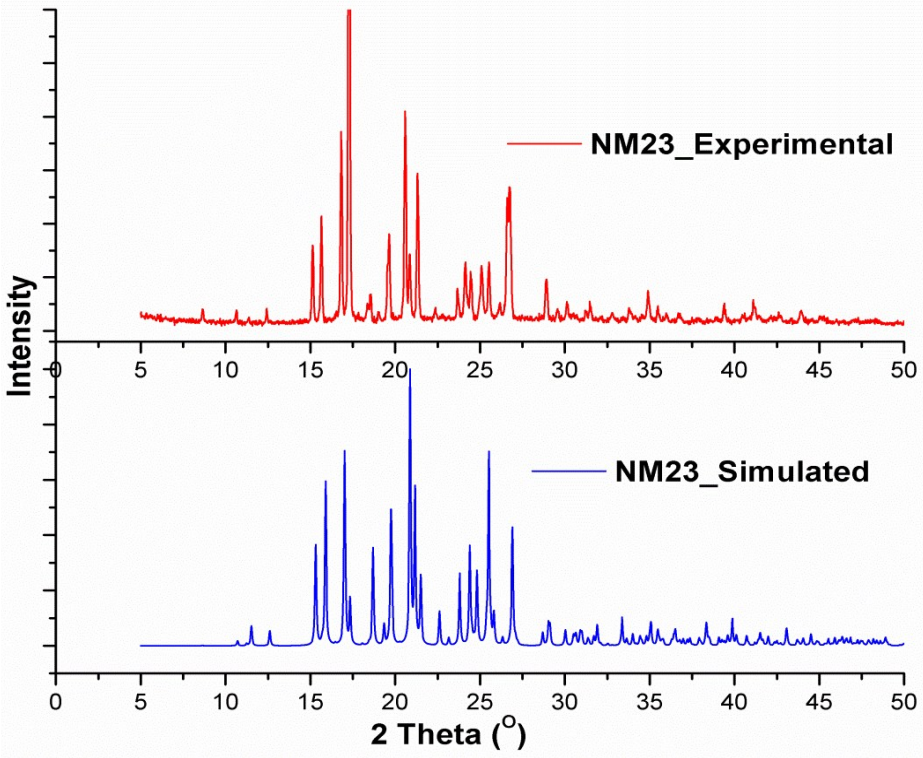
(f) NM12:


NM12_Experimental
NM12_Simulated
Intensity
2 Theta (°)
0
5
10
15
20
25
30
35
40
45
50

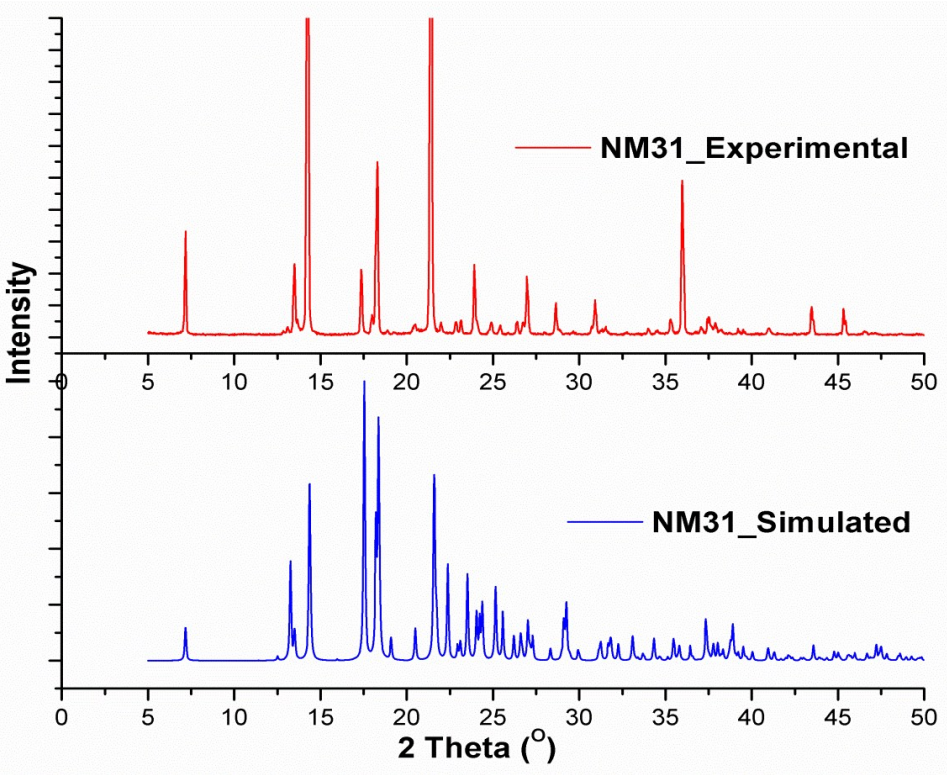
(g) NM22:


NM22_Experimental
NM22_Simulated
Intensity
2 Theta (°)
0
5
10
15
20
25
30
35
40
45
50

(h) NM23:


NM23_Experimental
NM23_Simulated
Intensity
2 Theta (O)

(i) NM31:


NM31_Experimental
NM31_Simulated
Intensity
2 Theta (O)

(j) NM33:

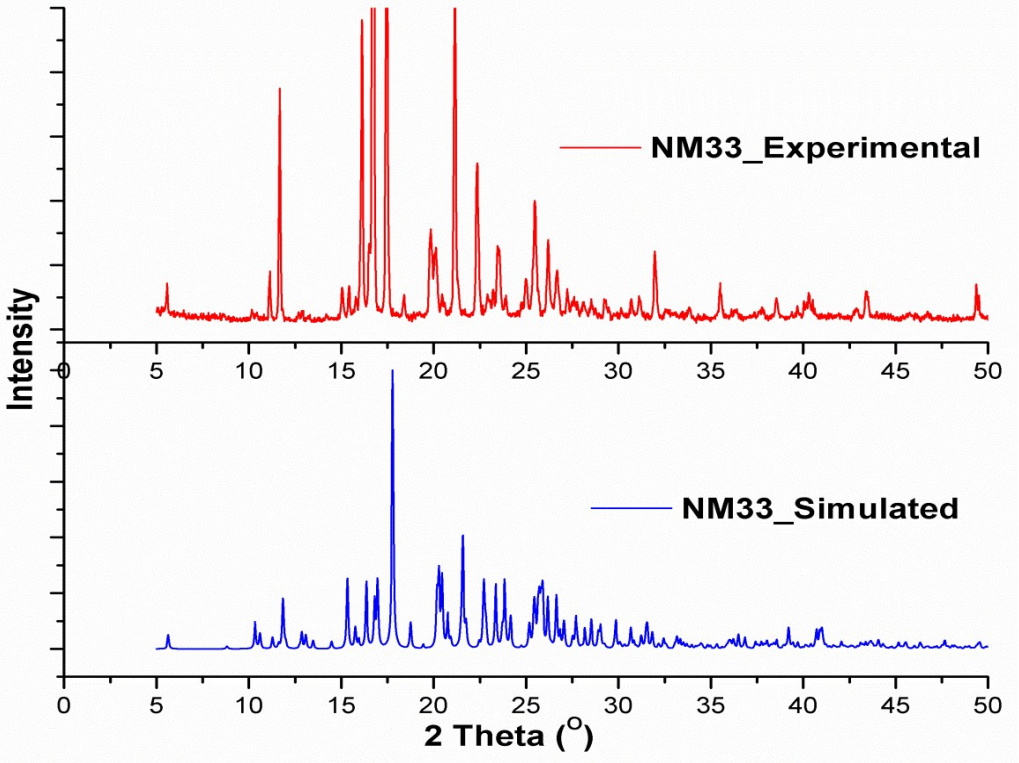
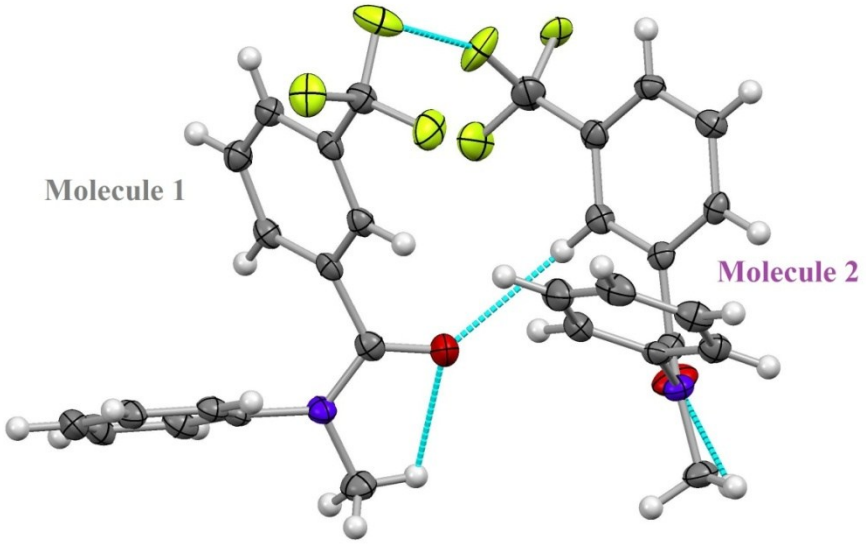
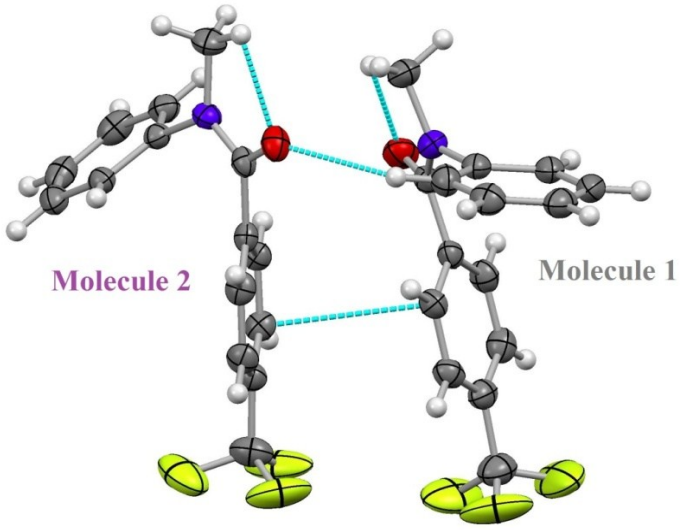


Figure S5: *ORTEP* of all compounds drawn with 50% ellipsoidal probability with atom-numbering scheme. Only the major component was shown in case of disorder for clarity. The dotted lines indicate presence of intra or intermolecular interactions.

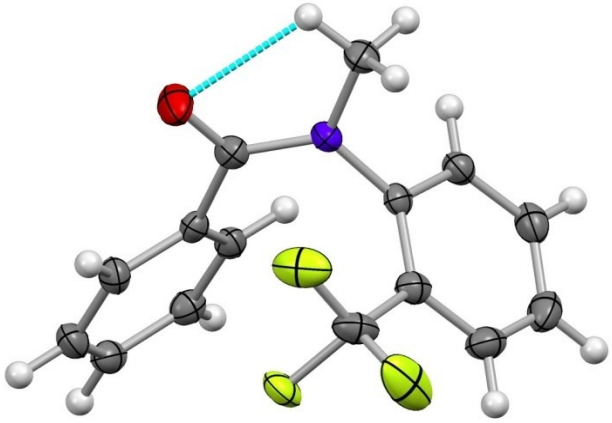
(a) NM02:



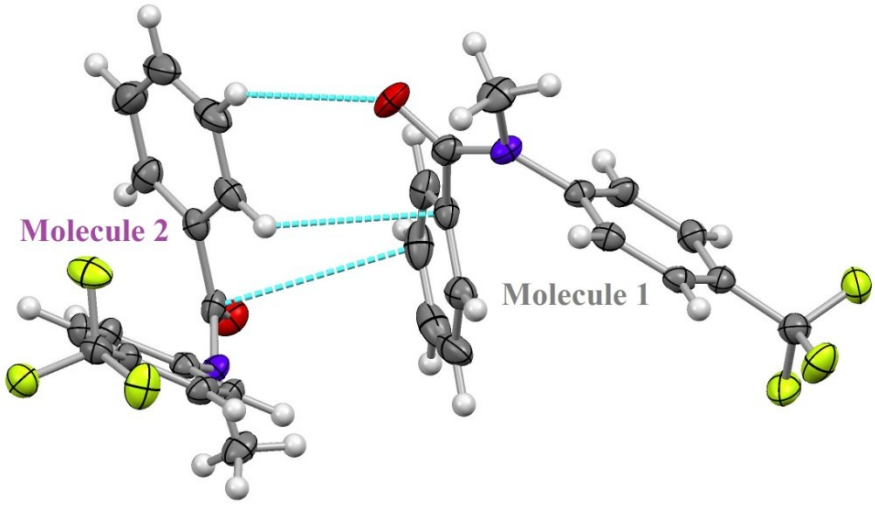
(b) NM03:



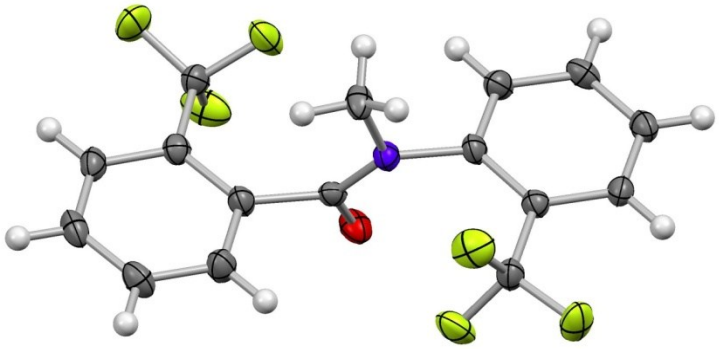
(c) NM10:



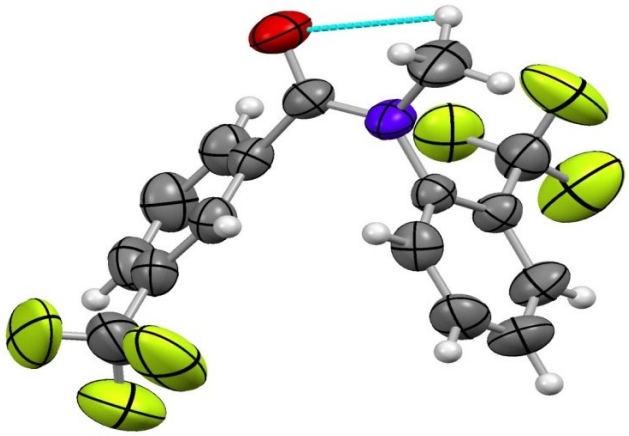
(d) NM30:



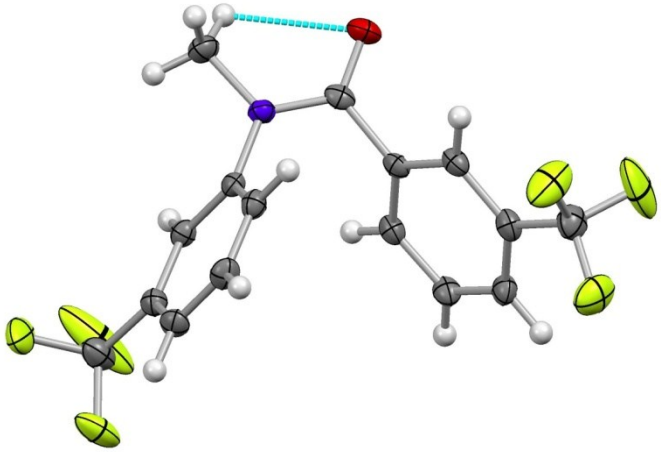
(e) NM11



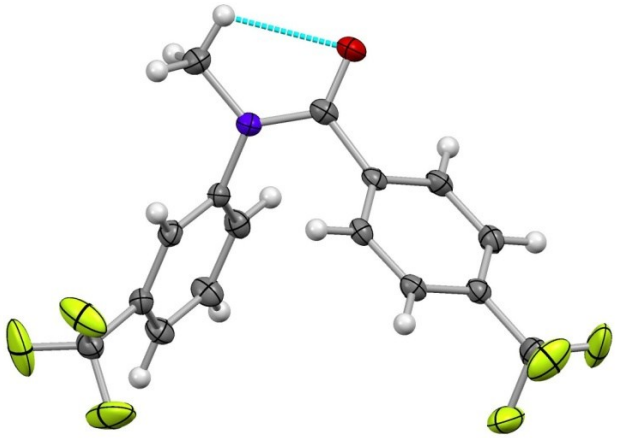
(f) NM12:



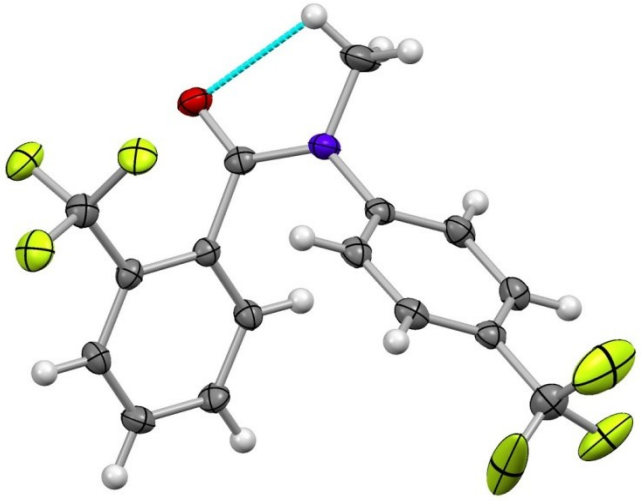
(g) NM22:



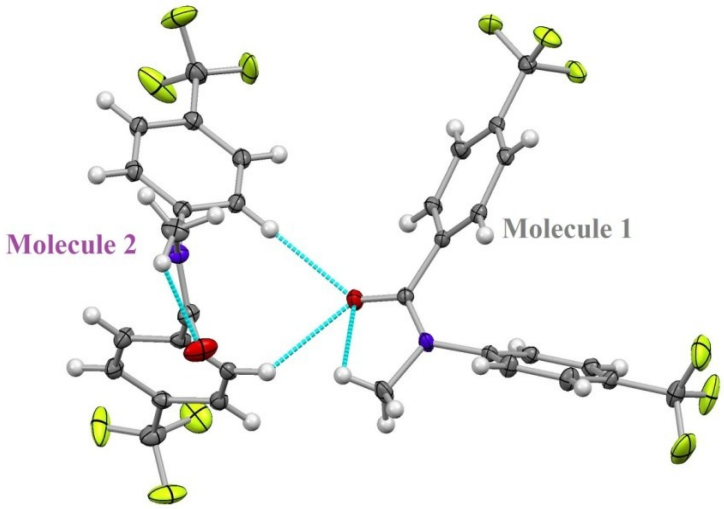
(h) NM23:



(i) NM31:



(j) NM33:



Section 2: XPac analysis: Comparison of Crystal Sructures

For XPAC analysis, the circled atoms, were consider for the 'corresponding ordered sets of points' (COSPs) [Fig S6]. The filter setting was set to 'High': a/p/d: 12/18/1.50 for all comparisons.The results of the analysis are presented in Table S2 and S3. The observed Supramolecular constructs (SC) are shown in the Figures S7 – S11.

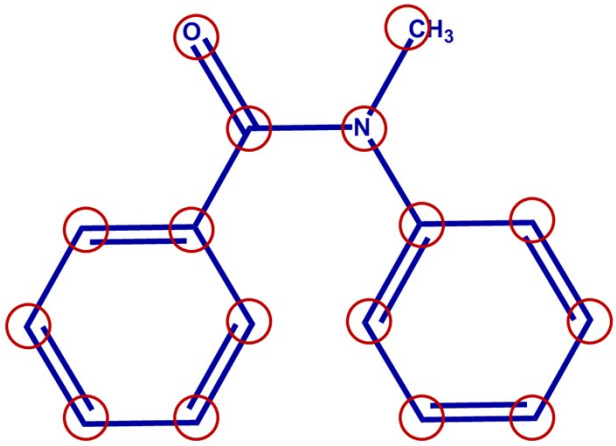


Figure S6: Molecule structure representing COSPs (in red circle), considered for XPac analysis.

Table S2: Result of XPac analysis. 'An', 'Bn' and 'Cn' (n = integer) represents presence of 0D SC, 1D SC and 2D SC respectively. Numbers in bracket represent corresponding dissimilarity index, 'X'. The blank boxes correspond to no similarity observed.

NM00	**NM00**											
NM02_1		**NM02_1**										
NM02_2			**NM02_2**									
NM03_1			**B1 (12.4)**	**NM03_1**								
NM03_2	**A3 (15.0)**	**C1 (6.7)**			**NM03_2**							
NM10	**A1 (18.0)**		**B1 (12.7)**	**B2 (13.2)**		**NM10**						
NM30_1						**A2 (15.2)**	**NM30_1**					
NM30_2						**A2 (15.2)**		**NM30_2**				
NM12				**A1 (13.4)**		**A1 (10.5)**			**NM12**			
NM22						**A2 (16.6)**	**A2 (8.5)**	**A2 (8.5)**	**B3 (11.8)**	**NM22**		
NM23				**A1 (7.5)**		**A1 (19.0)**	**A4 (14.6)**	**A4 (14.6)**	**A1 (18.2)**	**B4 (14.1)**	**NM23**	
NM31												**NM31**
NM33_1	**A3 (12.5)**		**A2 (17.1)**		**A3 (7.3)**						**A6 (8.2)**	
NM33_2							**A5 (11.7)**	**A5 (11.7)**			**B5 (8.2)**	**B6 (9.**

Figure S7: Presence of 2D supramolecular constructs (SC) in NM02_1 / NM03_2

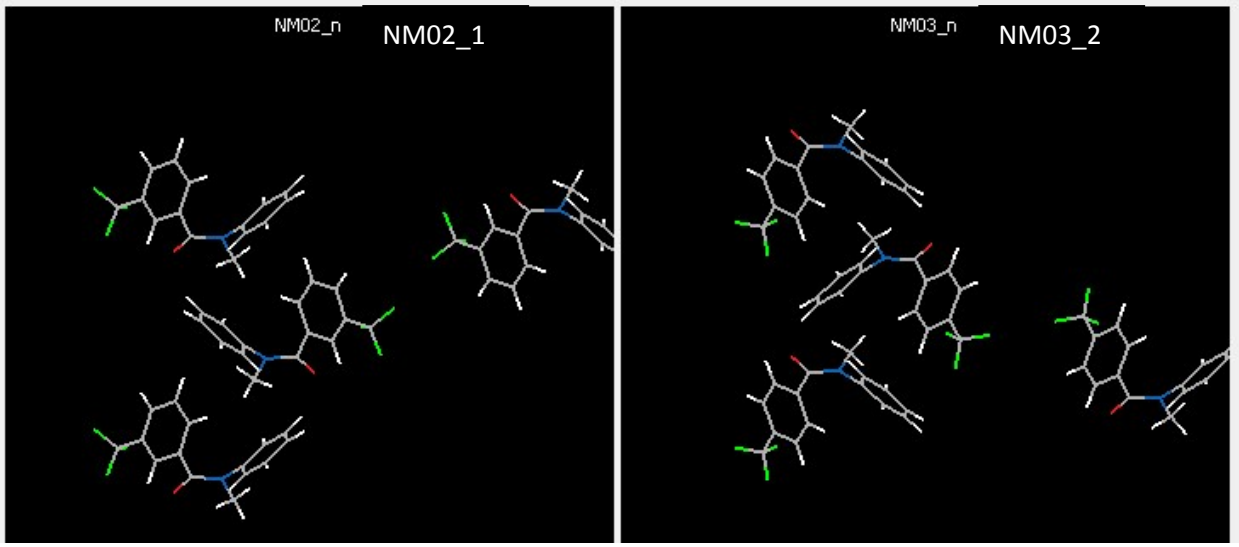
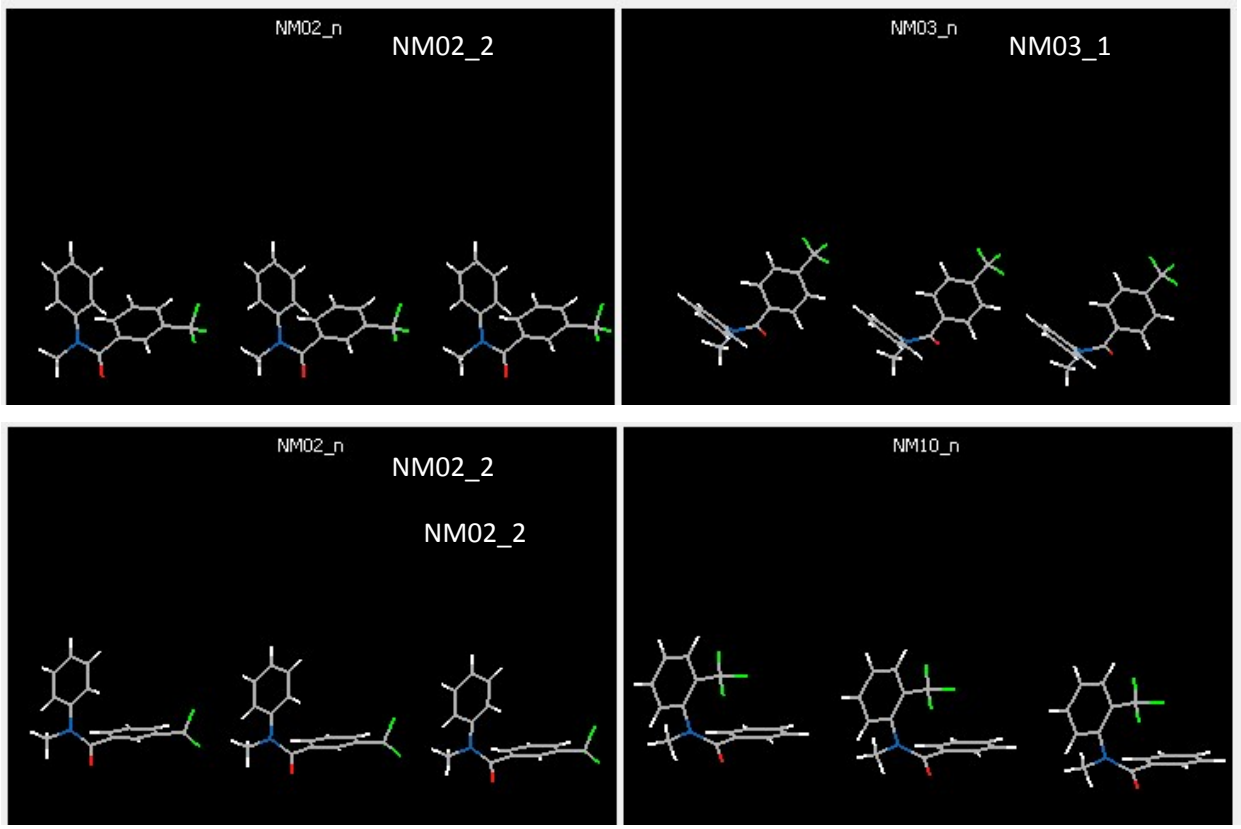
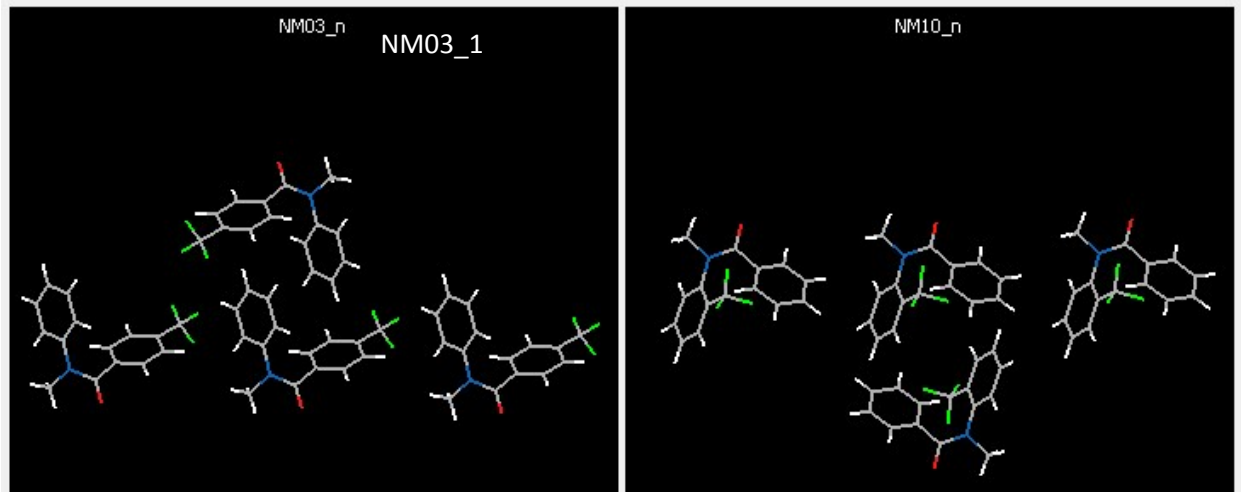


Figure S8: Presence of 1D supramolecular constructs (SC)

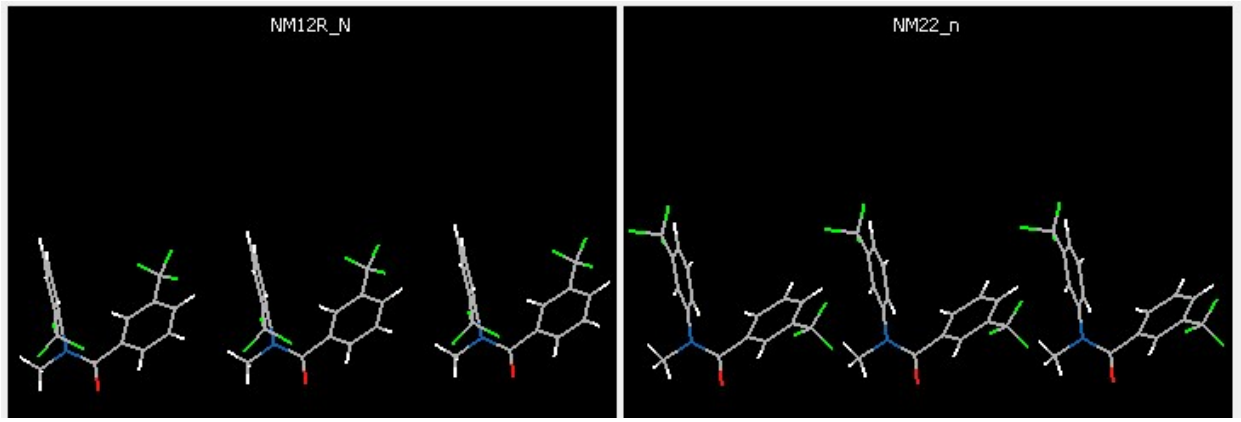
(a) **B1**



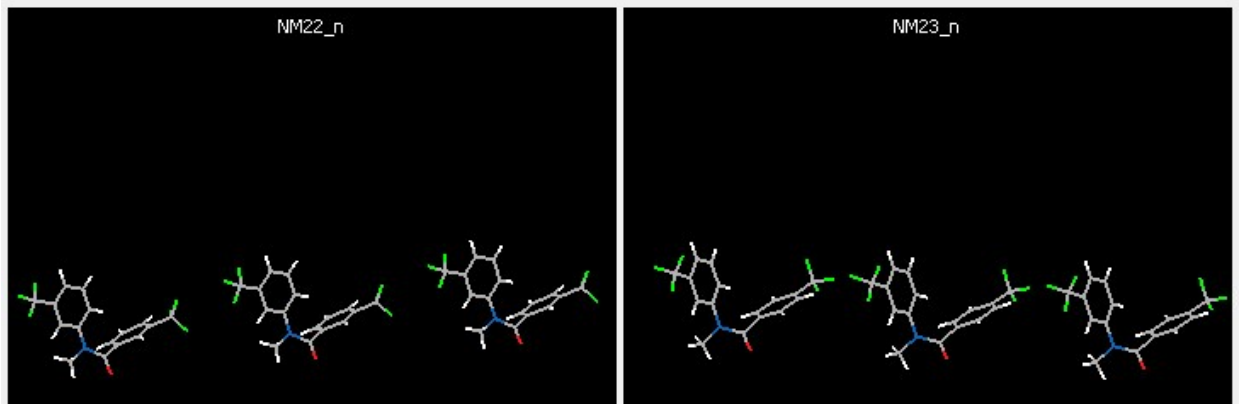
(b) **B2**



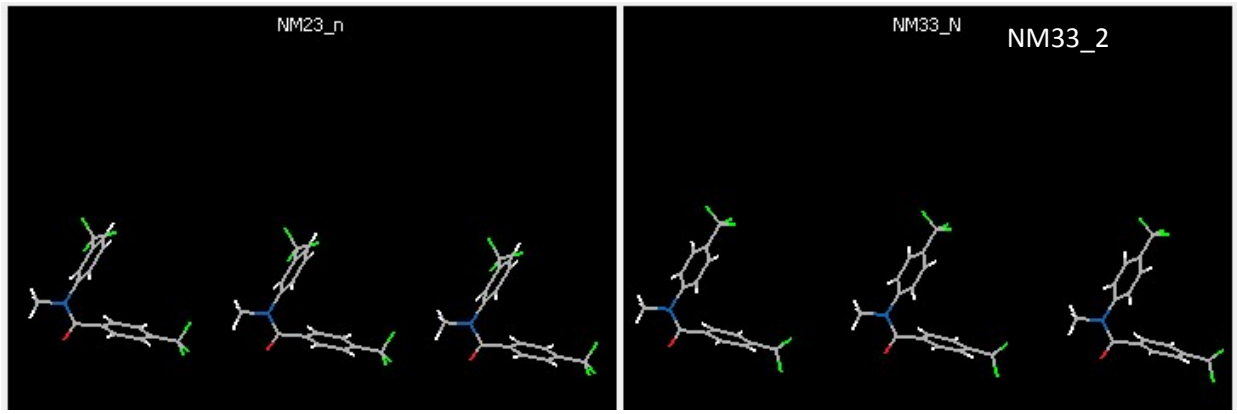
(c) **B3:**



(d) **B4:**



(e) **B5:**



(f) **B6:**

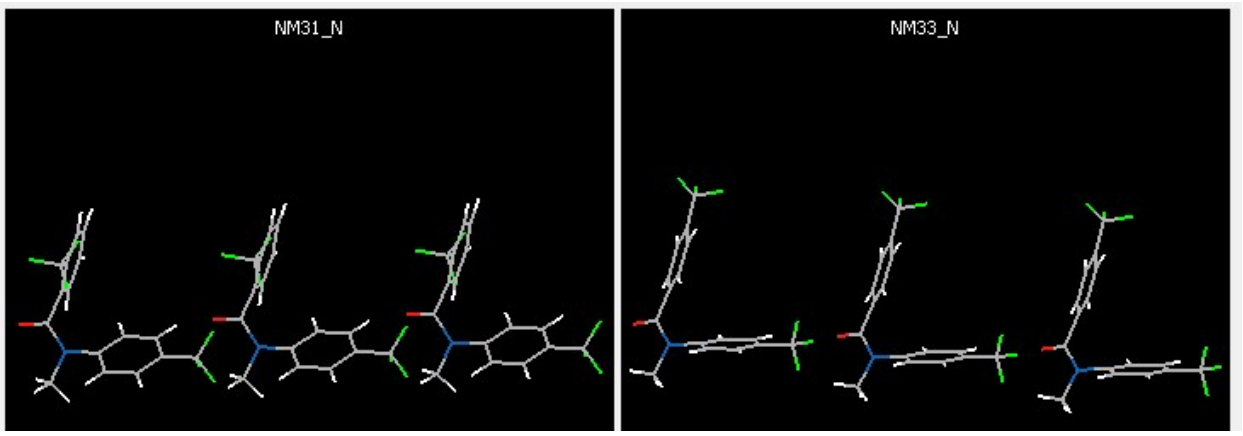
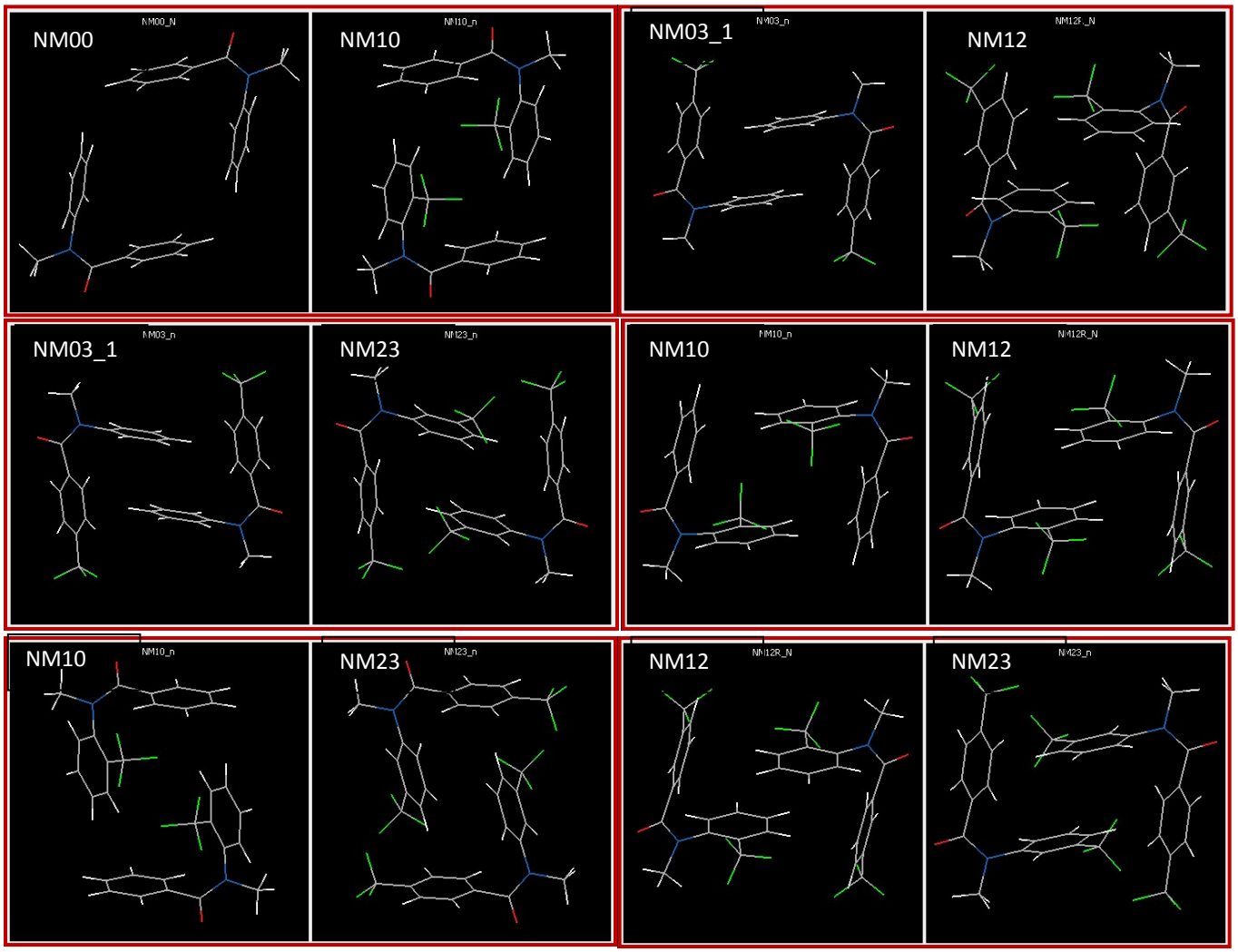
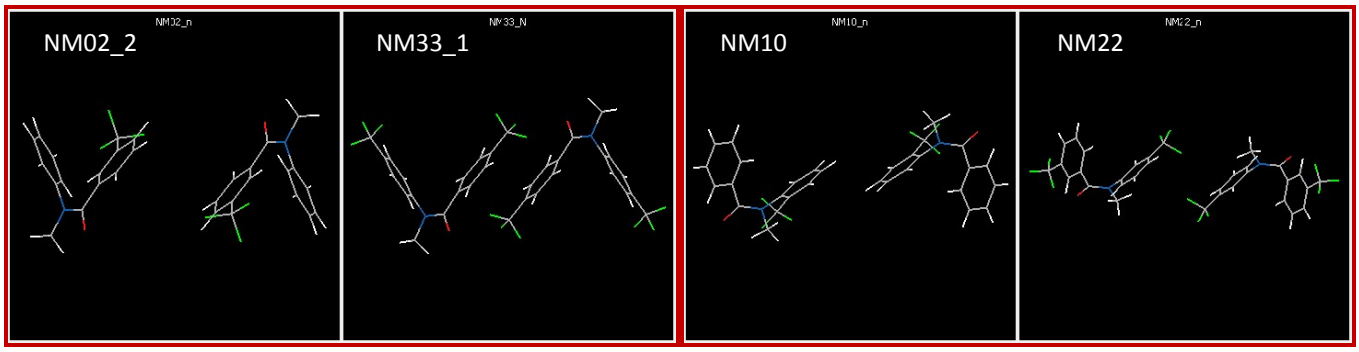


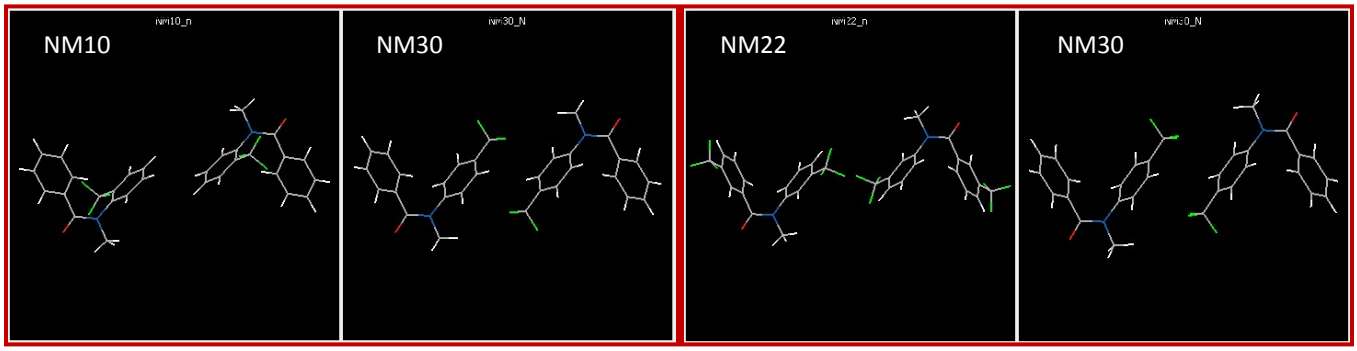
Figure S9: Presence of 0D supramolecular constructs (SC)

(a) A1:

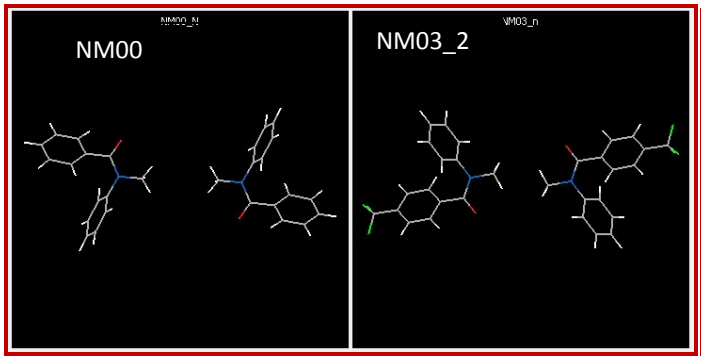

NM00
NM10
NM03_1
NM12
NM03_1
NM23
NM10
NM12
NM10
NM23
NM12
NM23

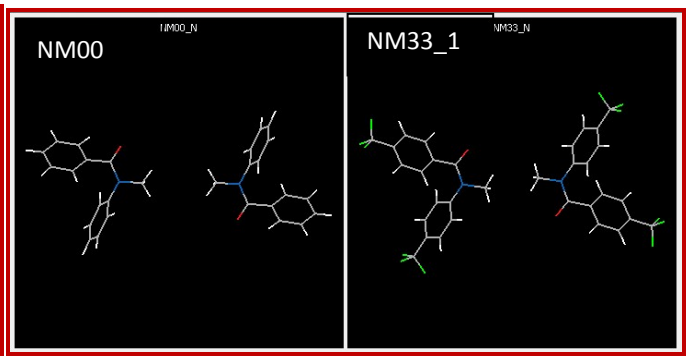
(b) A2:

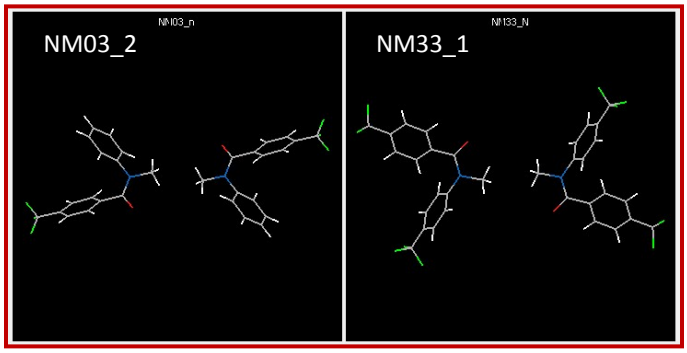

NM02_2
NM33_1
NM10
NM22


NM10
NM30
NM22
NM30

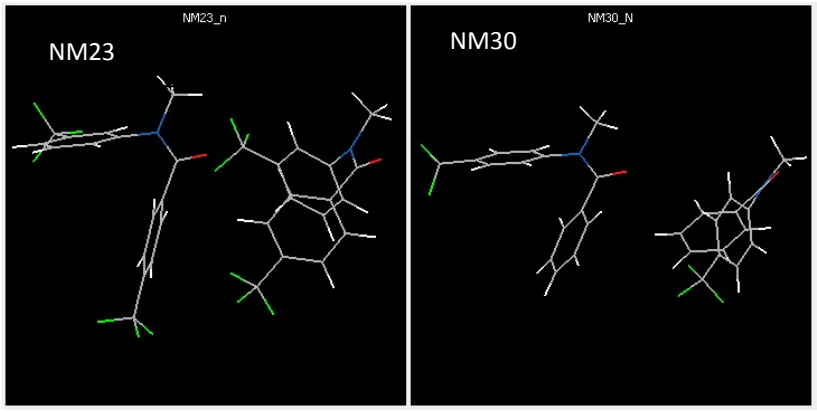
(c) A3:


NM00
NM03_2

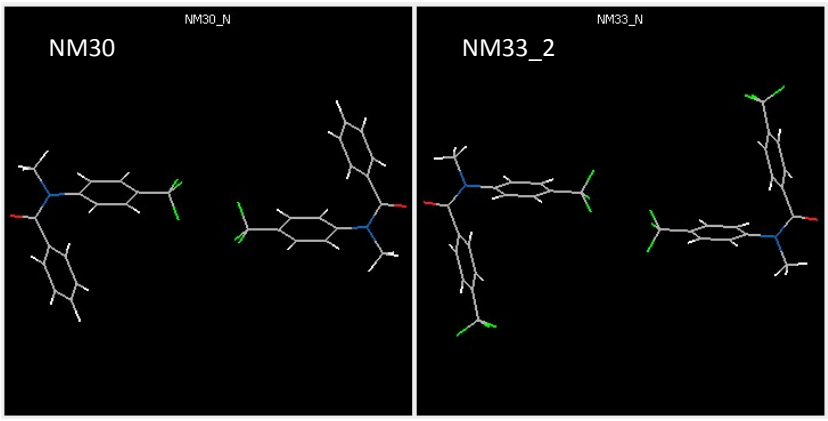

NM00
NM33_1


NM03_2
NM33_1

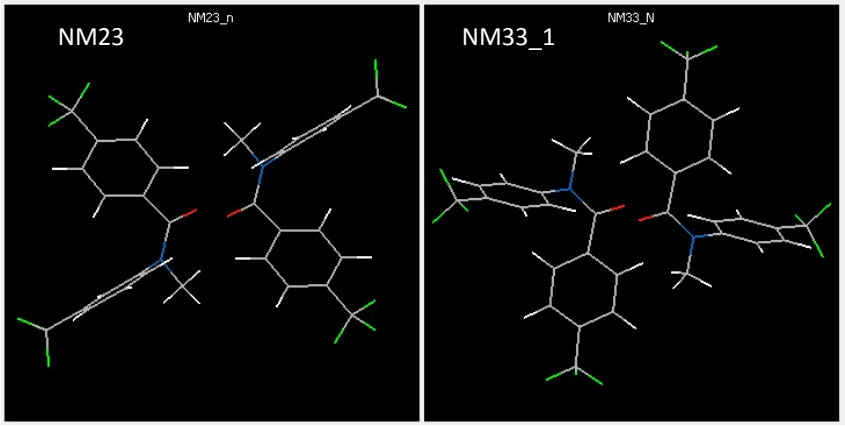
(d) A4:



(e) A5:



(f) A6:



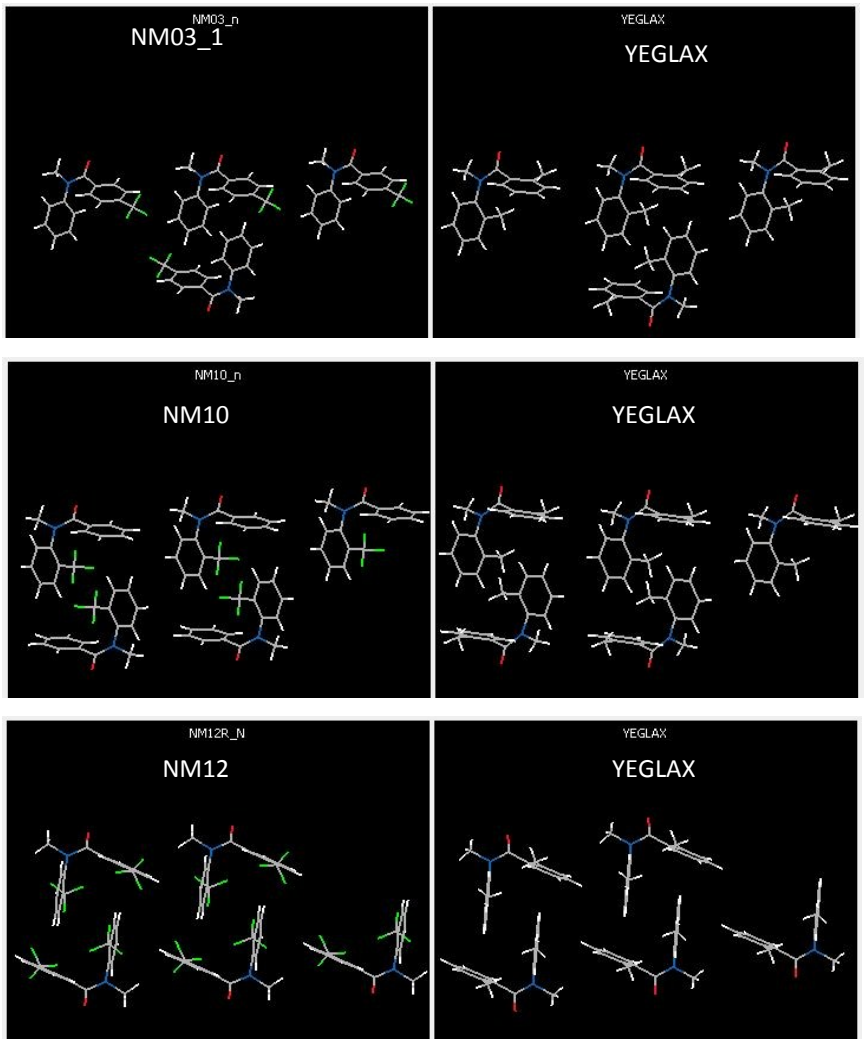
Comparison of crystal structure reported in CSD with the present series by XPac

Table S2: Result of XPac analysis with crystal structure reported in CSD

	NM00	NM02_1	NM02_2	NM03_1	NM03_2	NM10	NM30_1	NM30_1	NM12	NM22	NM23	NM31	NM33_
YEGKEA	---	---	---	**0D (12.1)**	---	**0D (8.7)**	---	---	**0D (6.5)**	---	**0D (17.0)**	---	---
YEGKIE	---	---	---	---	---	---	---	---	---	---	---	---	---
YEGKOK	---	**0D (10.5)**	---	---	---	**0D (16.6)**	---	---	**0D (16.2)**	**0D (18.9)**	---	---	---
YEGLAX	---	**0D (8.3)**	---	**1D (9.7)**	---	**1D (15.0)**	---	---	**1D (7.1)**	**1D (7.5)**	---	**0D (14.9)**	---

Figure S10: Presence of 1D supramolecular constructs (SC)

(a)



(b)

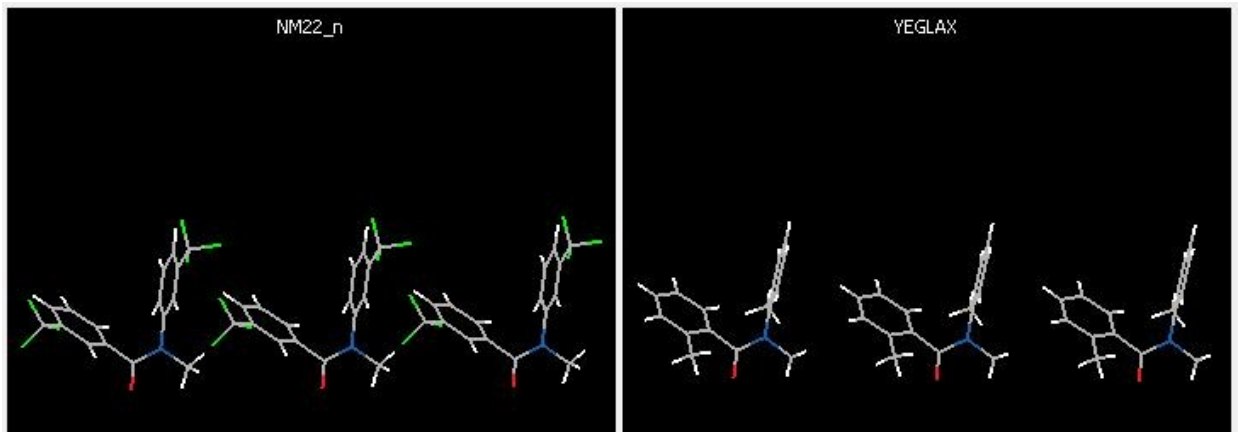
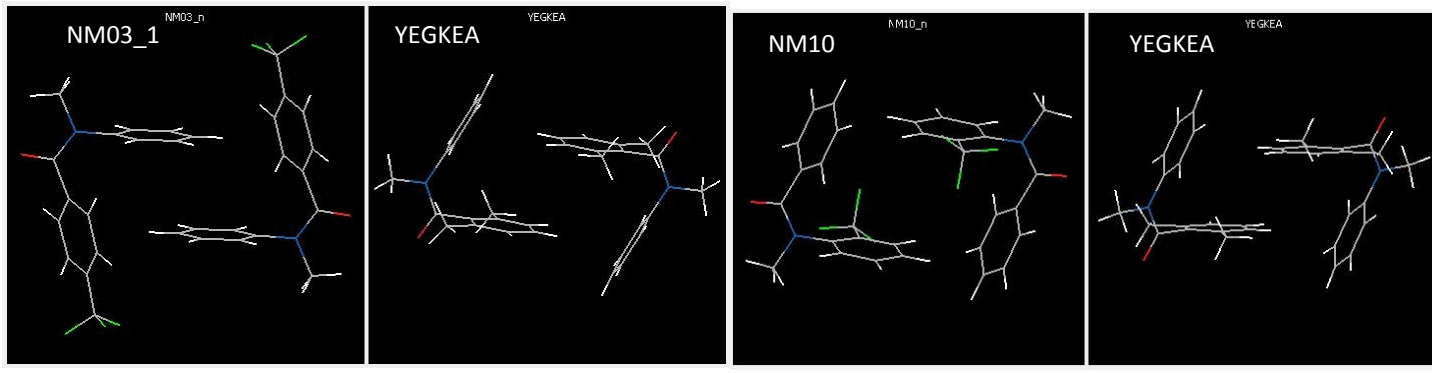
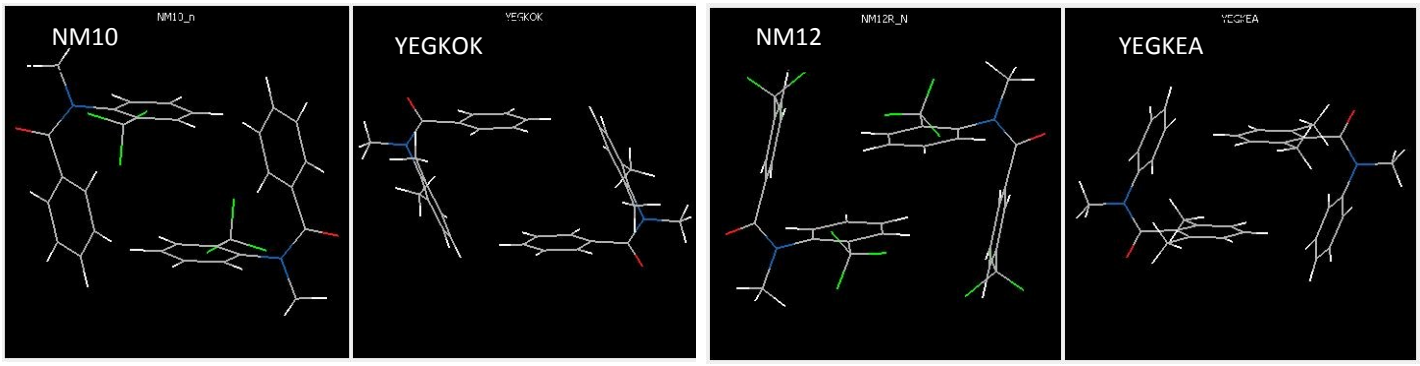
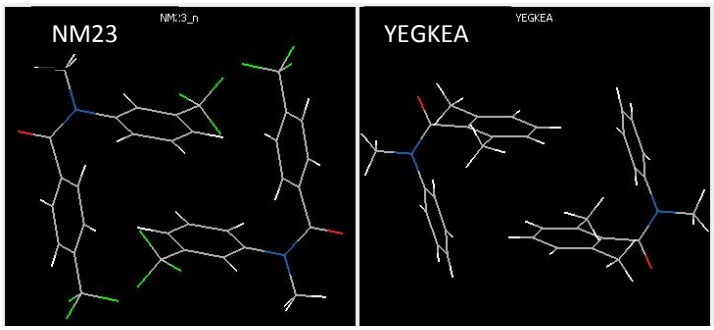


Figure S11: Presence of 0D supramolecular constructs (SC)

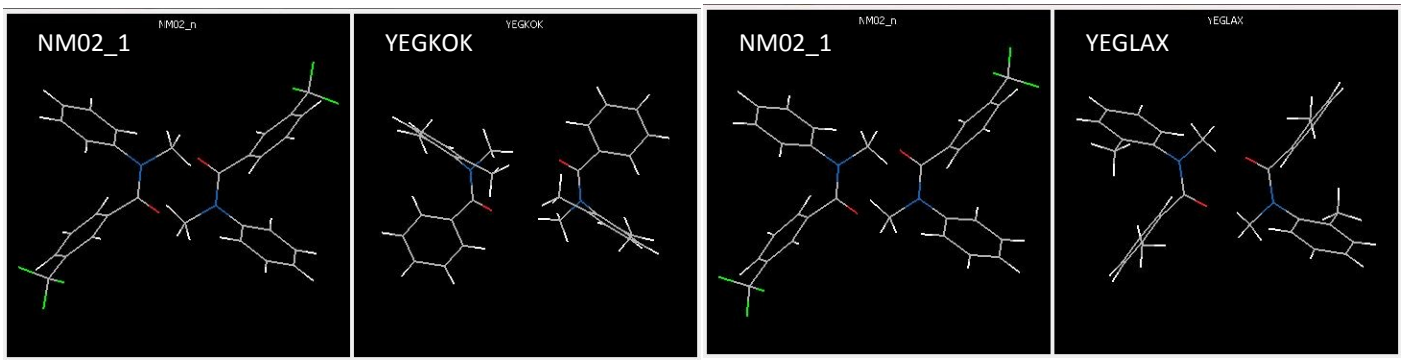
(a)



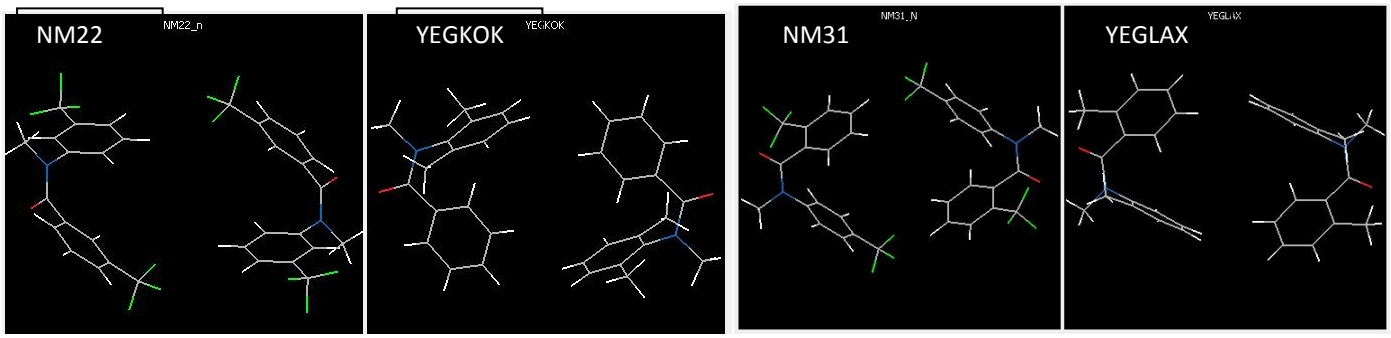




(b)



(c)



(d)

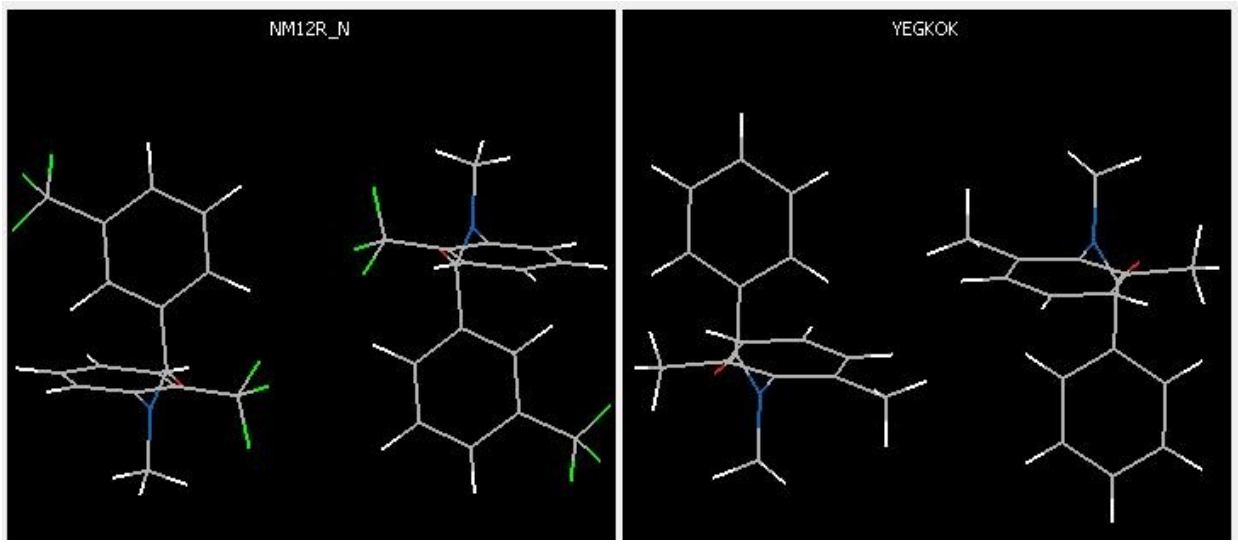
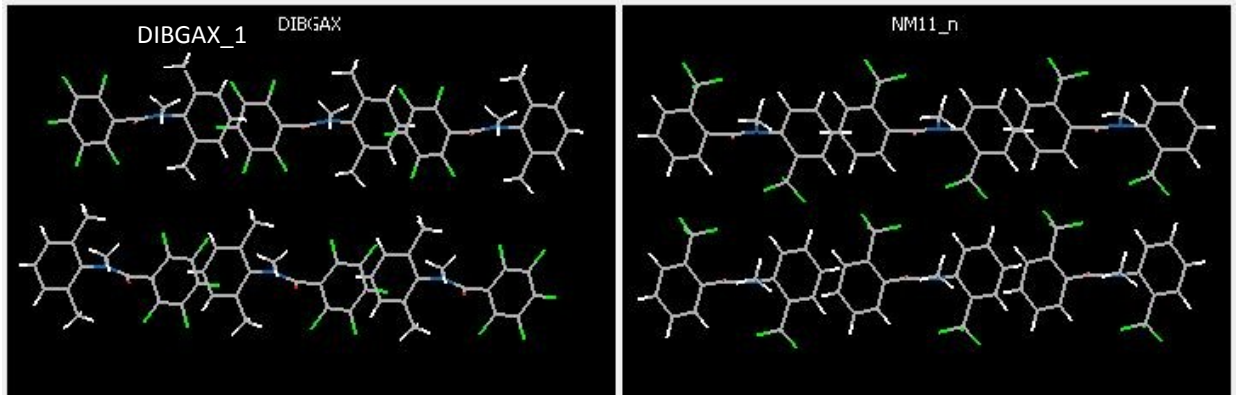


Figure S12: XPac result for comparison of NM11 with molecules reported in CSD having *trans*-geometry (Ref code: YEGJEY, DIBGIF and DIBGAX)

(a) NM11 with DIBGAX_1 (Dissimilarity index, X = 13.3)



(b) NM11 with DIBGAX_4 (Dissimilarity index, X = 13.3)