**Supplementary data**

**2.5 Generation of morphology from calculated modified attachment energy**

The surface docking method as a prediction tool was employed to simulate the impact of additives on the crystal morphology.[1] If an additive has a strong interaction on one particular face, the growth rate of this particular face will be slowed down. Thus, this face will be bigger relative to the other facets, therefore guiding the absolute morphology. For the solid surface consideration, the crystal morphology was computed using attachment energy and the morphologically importance (MI) faces were determined. The attachment energy method generated possible crystal faces where the morphology was controlled by {0 0 1}, {0 1 0}, {0 1 1}, {1 0 0}, {1 1 1}, {0 0 2}, and {1 1 0} crystal facets. These seven faces of the upmost morphological significance were picked individually and provided the necessary lattice values for the generation of amorphous cell. The liquid side modeling requires the construction of amorphous cells which comprised solvents and additive molecules.[2] The amorphous cell was constructed containing definite number of solvent and additive molecules and then the structure was refined by MD technique. Nif crystal was sliced parallel to the respective (hkl) plane. A crystal segment was created as a periodic superstructure. This crystal segment was optimized by the molecular dynamics. An amorphous cell was created, which enclosed calculated number of solvent and additive molecules. It was impossible to place the total polymer chains in a vacuum box during simulation, hence a representative HPMC chain length was taken as per the molar ratio present during the experimental crystallization.[3, 4] This amorphous cell was additionally refined by MD technique. The subsequent task involved optimization of this amorphous cell. These amorphous cells were then minimized at 10,000 iteration steps. Newton method was used for the energy minimization. The succeeding equilibration on this cell comprised of 100 ps NVE and 10 ps NPT runs.

Double-layer interfacial method was used for MD calculation to study the impact of the polymer additive on the crystal shape. One part of this model was the crystal segment and the solvent (DCM) + additive (HPMC) layer occupied another. Vacuum slab of 10 Å thick was built over the solvent + additive layer. The energy minimization was carried out before the molecular dynamics simulation. NVT calculations were carried out for 10 ps with a time step of 1 fs. The attained potential energy containing both crystal surface and amorphous structure was denoted as $E_{total}$. Consequently, the energies of the divided structures of the crystal surface and amorphous layer were determined and denoted as $E_{surface}$ and $E_{amorphous}$ correspondingly. MAE (Modified attachment energy) was calculated by the method[5, 6]:

$$^{mod}E_{att} = E_{total} - (E_{surface} + E_{amorphous}) \quad (1)$$

Where $^{mod}E_{att}$ stands for the attachment energy (modified) of the selected additive and solvent with a particular crystal face and $E_{total}$ symbolizes the energy of layer. $E_{surface}$ stands for the energy of crystal surface and $E_{amorphous}$ represents the energy of additives and solvents. The habit was created based on the Hartman and Bennema equation.[7]

$$R_g \sim [^{mod}E_{att}] \quad (2)$$

Where $R_g$ stand for the growth rate in a specific direction, which is directly comparative to the modified attachment energy.

### 3.1 Crystallization experiments and computational simulation

Crystal facets {1 0 0}showed equal abundance of non-polar functional groups (4 methyl) and polar functional groups (2 carboxyl), facet{1 1 0} showed dominance of non polar functional groups (2 methyl), facet {0 0 2} demonstrated the abundance of non polar functional groups (2 methyl and 2 aromatic rings) when compared to polar functional groups (1 nitro and 1 carboxyl), facet {(0 1 1}showed an abundance of polar functional moieties (1 nitro,1 carboxyl and 1 amine) when compared to non-polar functional moieties (2 methyl), while {1 1 -1} facet demonstrated an abundance of polar functional moieties (two carboxyl with two amine) in comparison to non-polar functional moieties (2 methyl and 1 aromatic ring), and a profusion of non polar functional groups (four methyl and one aromatic ring) when compared to the polar functional groups (two carboxyl and one amine) that was observed on facet {1 1 1}.

## References


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**Supplementary Table 1.** Percent surface area of important facets of Nif by BFDH and layer docking (LD) models

| hkl | % Surface area | | | | |
|---|---|---|---|---|---|
| | ***BFDH*** | ***Layer Docking*** | | | |
| | | Nif-0 | Nif-2 | Nif-4 | Nif-6 |
| { 1 0 0 } | 35.61 | | | | |
| { 0 1 1 } | 41.04 | | 11.28 | 8.23 | 4.88 |
| { 1 1 0 } | 7.39 | 21.35 | 44.84 | 49.76 | 67.45 |
| { 0 0 2 } | 13.62 | 10.95 | 15.47 | 18.68 | 22.23 |
| { 1 1 1 } | 1.087 | 50.33 | 13 | 14.14 | 3.90 |
| { 1 0 -2 } | 1.23 | 17.34 | 12.21 | | |

**Supplementary Table 2.** Particle size distribution of Nif crystals with different HPMC concentration

| | $D_{10}$(µm) | $D_{50}$(µm) | $D_{90}$(µm) |
|---|---|---|---|
| **Nif-0** | 1142.68 ± 2.32 | 1278.26 ± 6.62 | 1434.78 ± 4.48 |
| **Nif-2** | 1157.24 ± 3.62 | 1328.76 ± 4.46 | 1464.84 ± 5.40 |
| **Nif-4** | 1153.45 ± 4.68 | 1274.60 ± 7.48 | 1476.72 ± 8.86 |
| **Nif-6** | 1164.34 ± 3.80 | 1312.62 ± 8.94 | 1481.44 ± 11.26 |

**Supplementary Table 3.** Nif-0 PXRD

| No. | Pos. [°2Th.] | d-spacing [Å] | Rel. Int. [%] | FWHM [°2Th.] | Area [cts*°2Th.] | Backgr.[cts] | Height [cts] |
|---|---|---|---|---|---|---|---|
| 1 | 8.2015 | 10.77185 | 62.83 | 0.0836 | 1335.20 | 175.50 | 15412.31 |
| 2 | 10.5338 | 8.39149 | 12.26 | 0.0836 | 260.51 | 169.46 | 3007.04 |
| 3 | 11.8861 | 7.43963 | 36.76 | 0.0669 | 624.94 | 165.95 | 9017.18 |
| 4 | 12.0397 | 7.34507 | 11.95 | 0.0669 | 203.20 | 165.55 | 2932.01 |
| 5 | 13.0956 | 6.75510 | 3.25 | 0.0836 | 69.13 | 162.81 | 797.95 |
| 6 | 14.9102 | 5.93684 | 17.23 | 0.0669 | 293.00 | 158.11 | 4227.68 |
| 7 | 16.3191 | 5.42733 | 100.00 | 0.1338 | 3400.17 | 154.45 | 24530.24 |
| 8 | 17.2132 | 5.14737 | 14.43 | 0.1004 | 368.08 | 152.13 | 3540.62 |
| 9 | 18.4442 | 4.80649 | 7.41 | 0.1338 | 252.00 | 148.94 | 1818.06 |
| 10 | 19.1150 | 4.63932 | 4.76 | 0.1673 | 202.17 | 147.20 | 1166.81 |
| 11 | 19.6898 | 4.50517 | 19.54 | 0.1004 | 498.36 | 145.71 | 4793.81 |
| 12 | 19.8829 | 4.46184 | 11.52 | 0.0836 | 244.74 | 145.21 | 2825.06 |
| 13 | 20.7852 | 4.27014 | 4.58 | 0.1171 | 136.27 | 142.87 | 1123.57 |
| 14 | 21.2192 | 4.18377 | 3.00 | 0.1338 | 102.15 | 141.75 | 736.92 |
| 15 | 21.9790 | 4.04083 | 15.36 | 0.1338 | 522.30 | 139.78 | 3768.10 |
| 16 | 22.5219 | 3.94463 | 13.45 | 0.1506 | 514.54 | 138.37 | 3299.66 |
| 17 | 22.8161 | 3.89443 | 21.23 | 0.1338 | 721.86 | 137.60 | 5207.83 |
| 18 | 23.7859 | 3.73779 | 2.76 | 0.1338 | 93.69 | 135.09 | 675.88 |
| 19 | 24.5129 | 3.62856 | 63.32 | 0.1171 | 1883.87 | 133.20 | 15532.62 |
| 20 | 24.7568 | 3.59336 | 24.17 | 0.0836 | 513.53 | 132.57 | 5927.75 |
| 21 | 25.0196 | 3.55621 | 14.27 | 0.1004 | 363.87 | 131.89 | 3500.19 |
| 22 | 25.9889 | 3.42573 | 25.48 | 0.2007 | 1299.54 | 129.38 | 6250.28 |
| 23 | 26.4660 | 3.36506 | 18.00 | 0.1673 | 765.12 | 128.14 | 4415.90 |
| 24 | 27.1104 | 3.28651 | 19.25 | 0.0669 | 327.33 | 126.47 | 4723.03 |
| 25 | 27.9105 | 3.19409 | 8.77 | 0.1338 | 298.11 | 124.39 | 2150.71 |
| 26 | 29.2614 | 3.04962 | 2.85 | 0.1338 | 96.84 | 120.89 | 698.65 |
| 27 | 29.6939 | 3.00619 | 3.14 | 0.1673 | 133.43 | 119.77 | 770.07 |
| 28 | 29.9848 | 2.97768 | 2.20 | 0.1338 | 74.76 | 119.01 | 539.33 |
| 29 | 30.4549 | 2.93278 | 1.99 | 0.2007 | 101.38 | 117.80 | 487.58 |
| 30 | 31.1476 | 2.86912 | 2.84 | 0.1338 | 96.60 | 116.00 | 696.91 |
| 31 | 31.5166 | 2.83636 | 3.54 | 0.2007 | 180.60 | 115.04 | 868.60 |
| 32 | 31.9314 | 2.80046 | 3.97 | 0.1673 | 168.66 | 113.97 | 973.43 |
| 33 | 32.8434 | 2.72475 | 13.63 | 0.1506 | 521.56 | 111.60 | 3344.66 |
| 34 | 33.4215 | 2.67893 | 2.03 | 0.1338 | 69.19 | 110.10 | 499.14 |
| 35 | 34.8333 | 2.57351 | 2.24 | 0.1673 | 95.32 | 106.44 | 550.14 |
| 36 | 35.5085 | 2.52611 | 3.33 | 0.2007 | 169.68 | 104.69 | 816.11 |
| 37 | 35.9646 | 2.49512 | 6.53 | 0.0669 | 111.01 | 103.51 | 1601.77 |
| 38 | 36.3399 | 2.47020 | 2.14 | 0.2007 | 108.98 | 102.53 | 524.14 |
| 39 | 36.9049 | 2.43367 | 1.61 | 0.1338 | 54.71 | 101.07 | 394.67 |
| 40 | 37.9199 | 2.37083 | 2.22 | 0.3346 | 188.29 | 98.44 | 543.38 |
| 41 | 38.7886 | 2.31971 | 2.61 | 0.2007 | 133.31 | 96.18 | 641.15 |
| 42 | 39.4169 | 2.28417 | 1.78 | 0.2007 | 90.93 | 94.55 | 437.32 |
| 43 | 42.3001 | 2.13491 | 3.29 | 0.2676 | 223.98 | 87.08 | 807.95 |
| 44 | 43.0020 | 2.10167 | 1.85 | 0.1673 | 78.72 | 85.26 | 454.36 |
| 45 | 43.7044 | 2.06951 | 3.25 | 0.1004 | 82.87 | 83.44 | 797.14 |
| 46 | 44.4823 | 2.03510 | 3.91 | 0.1338 | 133.07 | 81.42 | 960.03 |
| 47 | 47.1345 | 1.92659 | 1.44 | 0.2676 | 98.00 | 74.54 | 353.49 |
| 48 | 47.5511 | 1.91068 | 1.67 | 0.1673 | 70.77 | 73.46 | 408.46 |
| 49 | 48.5478 | 1.87375 | 1.64 | 0.2856 | 160.52 | 70.89 | 401.47 |

**Supplementary Table 4.** Nif-2 PXRD

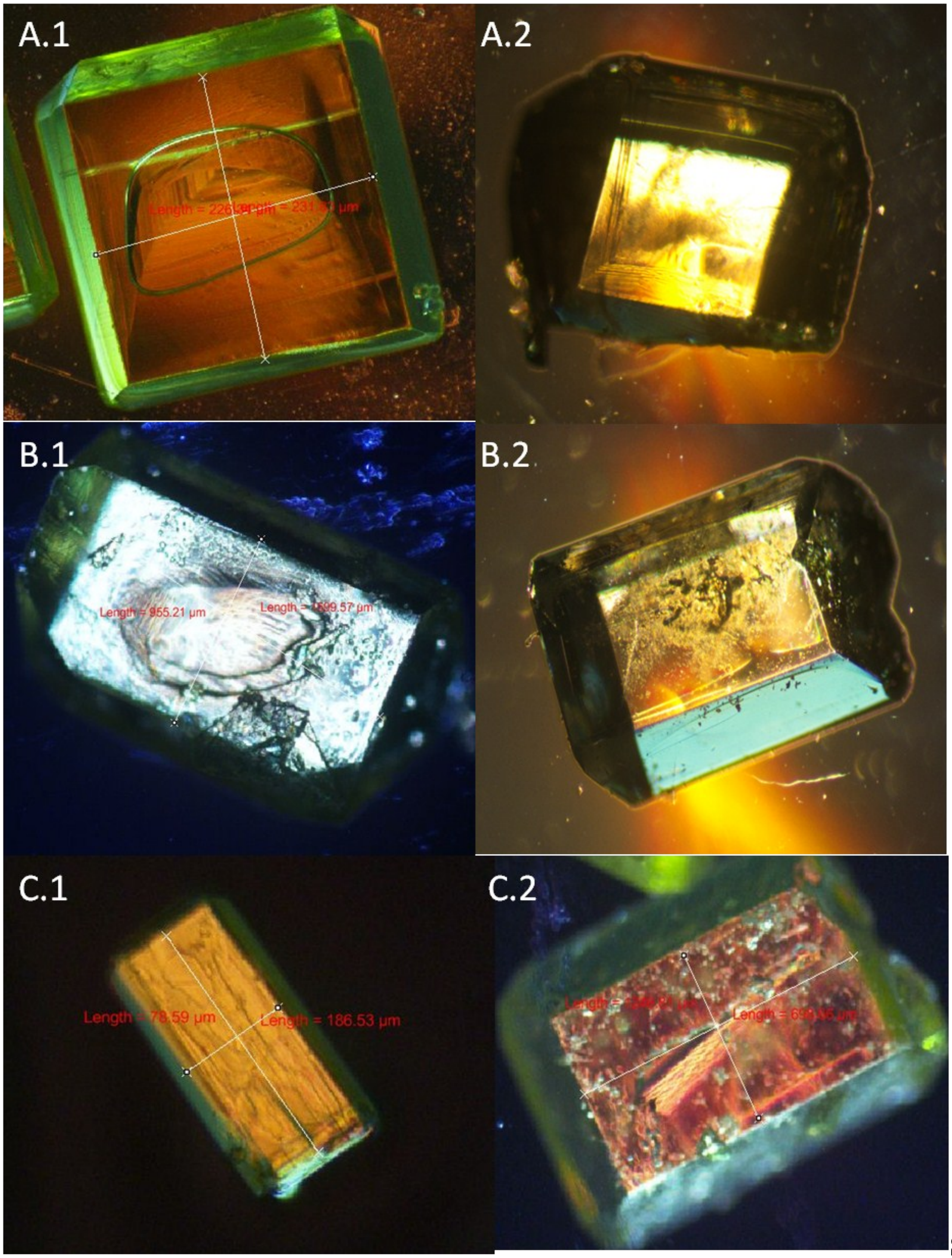
| No. | Pos. [°2Th.] | d-spacing [Å] | Rel. Int. [%] | FWHM [°2Th.] | Area [cts*°2Th.] | Backgr.[cts] | Height [cts] |
|---|---|---|---|---|---|---|---|
| 1 | 8.2127 | 10.75711 | 51.47 | 0.0669 | 846.88 | 148.44 | 12219.50 |
| 2 | 10.5568 | 8.37323 | 7.53 | 0.0669 | 123.95 | 139.67 | 1788.53 |
| 3 | 11.8951 | 7.43401 | 24.10 | 0.0836 | 495.69 | 134.66 | 5721.74 |
| 4 | 13.0737 | 6.76639 | 1.19 | 0.2007 | 58.76 | 130.25 | 282.63 |
| 5 | 14.7815 | 5.98822 | 10.51 | 0.1171 | 302.57 | 123.86 | 2494.68 |
| 6 | 14.9291 | 5.92935 | 9.83 | 0.0669 | 161.74 | 123.31 | 2333.66 |
| 7 | 16.3245 | 5.42552 | 100.00 | 0.0836 | 2056.84 | 118.09 | 23742.23 |
| 8 | 17.2583 | 5.13402 | 13.87 | 0.0669 | 228.28 | 114.60 | 3293.78 |
| 9 | 18.4129 | 4.81460 | 7.81 | 0.1171 | 224.76 | 110.28 | 1853.13 |
| 10 | 19.1197 | 4.63818 | 4.28 | 0.1673 | 176.21 | 107.64 | 1016.98 |
| 11 | 19.6781 | 4.50781 | 19.62 | 0.1673 | 807.26 | 105.55 | 4659.14 |
| 12 | 19.8927 | 4.45966 | 9.58 | 0.1004 | 236.53 | 104.75 | 2275.27 |
| 13 | 20.1835 | 4.39606 | 3.35 | 0.0836 | 68.89 | 103.66 | 795.20 |
| 14 | 20.8135 | 4.26439 | 5.89 | 0.1171 | 169.67 | 101.30 | 1398.94 |
| 15 | 21.2274 | 4.18218 | 2.61 | 0.2007 | 128.65 | 99.75 | 618.77 |
| 16 | 22.0267 | 4.03218 | 14.03 | 0.0669 | 230.82 | 96.76 | 3330.43 |
| 17 | 22.5367 | 3.94208 | 11.87 | 0.0836 | 244.09 | 94.86 | 2817.59 |
| 18 | 22.8468 | 3.88927 | 9.45 | 0.1673 | 388.78 | 93.70 | 2243.86 |
| 19 | 24.5125 | 3.62862 | 63.55 | 0.1171 | 1830.08 | 87.46 | 15089.08 |
| 20 | 24.7932 | 3.58816 | 15.70 | 0.1338 | 516.57 | 86.41 | 3726.73 |
| 21 | 25.8590 | 3.44264 | 43.77 | 0.1004 | 1080.29 | 82.43 | 10391.58 |
| 22 | 26.4715 | 3.36436 | 11.18 | 0.2007 | 552.12 | 80.14 | 2655.47 |
| 23 | 27.1353 | 3.28355 | 17.59 | 0.0836 | 361.70 | 77.65 | 4175.18 |
| 24 | 27.9696 | 3.18747 | 10.38 | 0.1171 | 298.84 | 74.53 | 2463.97 |
| 25 | 29.2837 | 3.04736 | 3.98 | 0.0836 | 81.76 | 69.62 | 943.82 |
| 26 | 29.7132 | 3.00428 | 3.76 | 0.2007 | 185.73 | 68.01 | 893.30 |
| 27 | 31.1251 | 2.87114 | 5.63 | 0.1506 | 208.30 | 62.73 | 1335.82 |
| 28 | 31.8516 | 2.80729 | 9.69 | 0.1004 | 239.20 | 60.01 | 2300.90 |
| 29 | 32.8372 | 2.72524 | 12.45 | 0.0836 | 256.02 | 56.32 | 2955.24 |
| 30 | 33.4135 | 2.67955 | 2.28 | 0.1338 | 75.12 | 54.17 | 541.97 |
| 31 | 34.8731 | 2.57067 | 2.32 | 0.1673 | 95.30 | 48.71 | 550.03 |
| 32 | 35.5586 | 2.52266 | 10.13 | 0.0836 | 208.44 | 46.15 | 2406.07 |
| 33 | 35.9673 | 2.49493 | 3.72 | 0.1338 | 122.55 | 44.62 | 884.11 |
| 34 | 36.3344 | 2.47056 | 3.62 | 0.2007 | 178.83 | 43.24 | 860.10 |
| 35 | 37.5186 | 2.39526 | 2.85 | 0.2007 | 140.86 | 38.81 | 677.48 |
| 36 | 37.9769 | 2.36740 | 1.85 | 0.2007 | 91.17 | 37.10 | 438.51 |
| 37 | 38.8274 | 2.31748 | 5.91 | 0.1506 | 218.77 | 33.92 | 1402.93 |
| 38 | 39.4623 | 2.28164 | 1.65 | 0.1673 | 67.69 | 31.54 | 390.68 |
| 39 | 40.8674 | 2.20638 | 1.01 | 0.2676 | 66.67 | 26.29 | 240.50 |
| 40 | 41.3510 | 2.18169 | 0.85 | 0.1338 | 27.93 | 24.48 | 201.51 |
| 41 | 41.8740 | 2.15564 | 2.38 | 0.2007 | 117.62 | 22.52 | 565.71 |
| 42 | 42.3117 | 2.13435 | 5.10 | 0.0669 | 83.93 | 20.88 | 1211.08 |
| 43 | 43.0213 | 2.10077 | 1.85 | 0.1673 | 76.07 | 18.23 | 439.06 |
| 44 | 44.2962 | 2.04322 | 3.37 | 0.2007 | 166.58 | 13.46 | 801.20 |
| 45 | 44.5316 | 2.03297 | 3.85 | 0.2007 | 189.97 | 12.58 | 913.70 |
| 46 | 46.2641 | 1.96079 | 0.53 | 0.6528 | 116.08 | 6.12 | 127.02 |
| 47 | 47.0728 | 1.92897 | 1.69 | 0.2856 | 160.73 | 3.10 | 401.99 |

**Supplementary Table 5.** Nif-4 PXRD

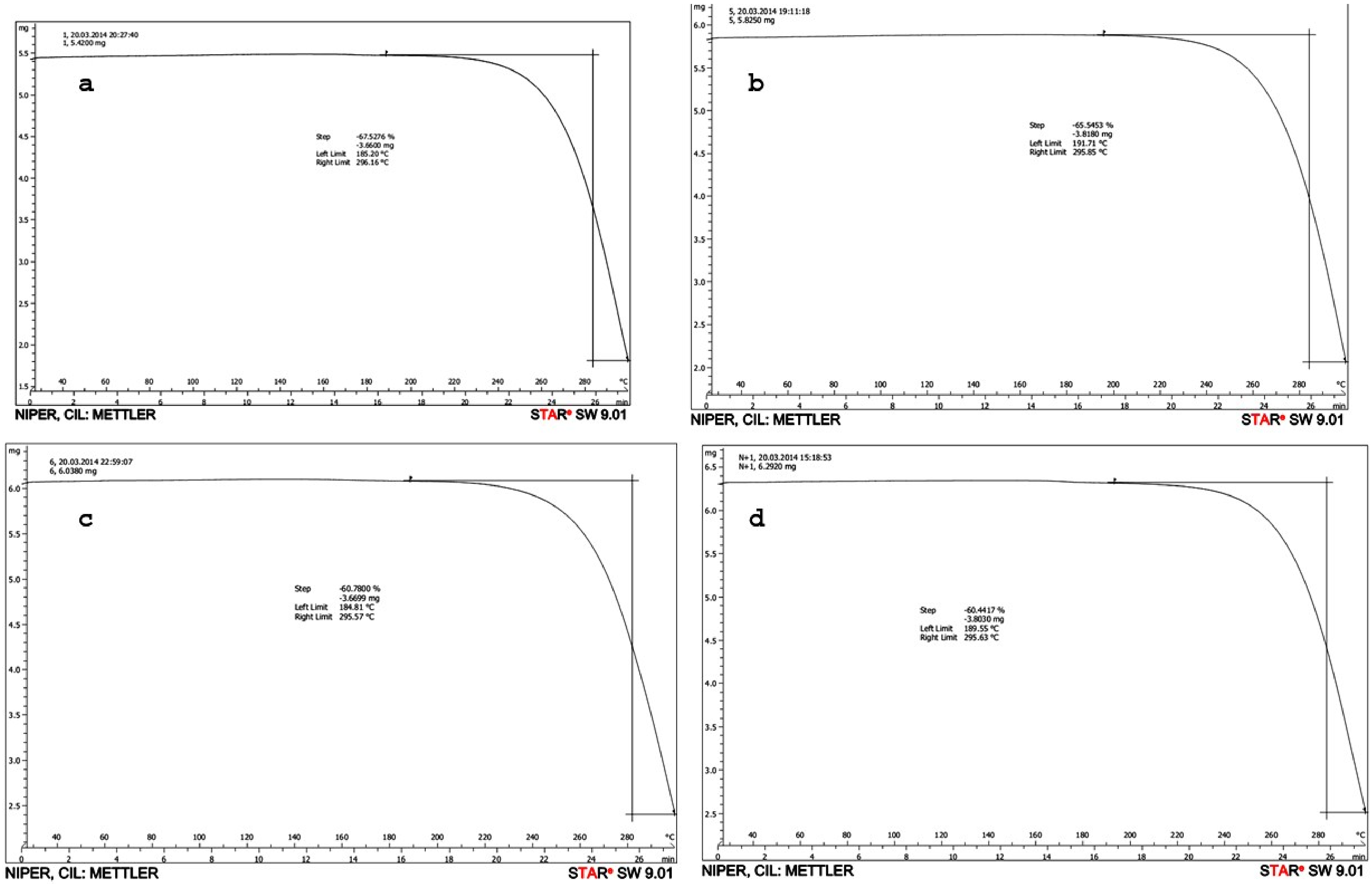
| No. | Pos. [°2Th.] | d-spacing [Å] | Rel. Int. [%] | FWHM [°2Th.] | Area [cts*°2Th.] | Backgr.[cts] | Height [cts] |
|---|---|---|---|---|---|---|---|
| 1 | 8.2860 | 10.67094 | 48.32 | 0.0836 | 1111.51 | 166.30 | 13471.72 |
| 2 | 10.6420 | 8.31330 | 6.44 | 0.1338 | 236.93 | 158.97 | 1794.76 |
| 3 | 11.9804 | 7.38742 | 15.95 | 0.1338 | 587.00 | 154.81 | 4446.61 |
| 4 | 12.1342 | 7.29410 | 10.05 | 0.0669 | 184.94 | 154.33 | 2801.97 |
| 5 | 13.1761 | 6.71957 | 4.23 | 0.0836 | 97.30 | 151.09 | 1179.33 |
| 6 | 14.9745 | 5.91638 | 15.85 | 0.1171 | 510.27 | 145.49 | 4417.58 |
| 7 | 16.4056 | 5.40337 | 100.00 | 0.1338 | 3680.42 | 141.04 | 27879.74 |
| 8 | 17.2994 | 5.12615 | 8.99 | 0.1171 | 289.51 | 138.25 | 2506.39 |
| 9 | 18.5604 | 4.78062 | 8.63 | 0.0669 | 158.76 | 134.33 | 2405.29 |
| 10 | 19.2212 | 4.61774 | 3.29 | 0.1338 | 121.26 | 132.27 | 918.54 |
| 11 | 19.7561 | 4.49390 | 12.59 | 0.2342 | 810.66 | 130.61 | 3509.07 |
| 12 | 19.9544 | 4.44969 | 10.41 | 0.0836 | 239.43 | 129.99 | 2901.98 |
| 13 | 20.2394 | 4.38768 | 4.10 | 0.1004 | 113.29 | 129.11 | 1144.25 |
| 14 | 22.0708 | 4.02756 | 11.16 | 0.1171 | 359.29 | 123.41 | 3110.49 |
| 15 | 22.6349 | 3.92844 | 24.65 | 0.0669 | 453.67 | 121.65 | 6873.18 |
| 16 | 22.9139 | 3.88124 | 11.52 | 0.1171 | 370.87 | 120.78 | 3210.70 |
| 17 | 24.5973 | 3.61930 | 65.78 | 0.1338 | 2420.81 | 115.55 | 18337.99 |
| 18 | 24.8570 | 3.58207 | 25.28 | 0.1004 | 697.69 | 114.74 | 7046.82 |
| 19 | 25.9682 | 3.43126 | 14.32 | 0.0669 | 263.43 | 111.28 | 3991.08 |
| 20 | 26.1024 | 3.41392 | 16.88 | 0.1171 | 543.73 | 110.86 | 4707.25 |
| 21 | 26.5613 | 3.35597 | 7.39 | 0.2342 | 475.80 | 109.43 | 2059.59 |
| 22 | 27.1810 | 3.28085 | 11.15 | 0.1338 | 410.40 | 107.51 | 3108.85 |
| 23 | 28.0244 | 3.18400 | 5.05 | 0.2342 | 325.24 | 104.88 | 1407.85 |
| 24 | 29.2239 | 3.05598 | 4.91 | 0.2676 | 361.15 | 101.15 | 1367.88 |
| 25 | 29.7310 | 3.00500 | 3.22 | 0.1338 | 118.49 | 99.57 | 897.57 |
| 26 | 31.2558 | 2.86180 | 2.24 | 0.2007 | 123.62 | 94.83 | 624.30 |
| 27 | 31.6401 | 2.82791 | 4.34 | 0.1004 | 119.82 | 93.63 | 1210.25 |
| 28 | 32.0306 | 2.79432 | 2.95 | 0.2007 | 162.75 | 92.41 | 821.91 |
| 29 | 32.9162 | 2.72114 | 12.73 | 0.0836 | 292.89 | 89.66 | 3549.95 |
| 30 | 34.9539 | 2.56704 | 2.01 | 0.1338 | 73.94 | 83.32 | 560.10 |
| 31 | 36.0537 | 2.49121 | 4.55 | 0.0836 | 104.61 | 79.90 | 1267.93 |
| 32 | 38.0662 | 2.36401 | 1.49 | 0.3011 | 122.97 | 73.63 | 414.02 |
| 33 | 38.9330 | 2.31335 | 2.64 | 0.2007 | 145.67 | 70.94 | 735.67 |
| 34 | 39.5433 | 2.27904 | 1.35 | 0.1673 | 61.91 | 69.04 | 375.16 |
| 35 | 40.9443 | 2.20424 | 1.22 | 0.2676 | 89.84 | 64.68 | 340.27 |
| 36 | 41.4158 | 2.18023 | 1.51 | 0.1673 | 69.64 | 63.21 | 422.03 |
| 37 | 42.5720 | 2.12366 | 2.64 | 0.4015 | 291.47 | 59.61 | 735.97 |
| 38 | 44.5683 | 2.03306 | 2.74 | 0.1338 | 100.81 | 53.40 | 763.65 |
| 39 | 47.2591 | 1.92339 | 1.03 | 0.4015 | 113.46 | 45.03 | 286.48 |
| 40 | 48.6605 | 1.87123 | 1.49 | 0.0836 | 34.24 | 40.67 | 414.99 |
| 41 | 49.2987 | 1.84696 | 0.38 | 0.2448 | 34.14 | 38.68 | 104.61 |

**Supplementary Table 6.** Nif-6 PXRD

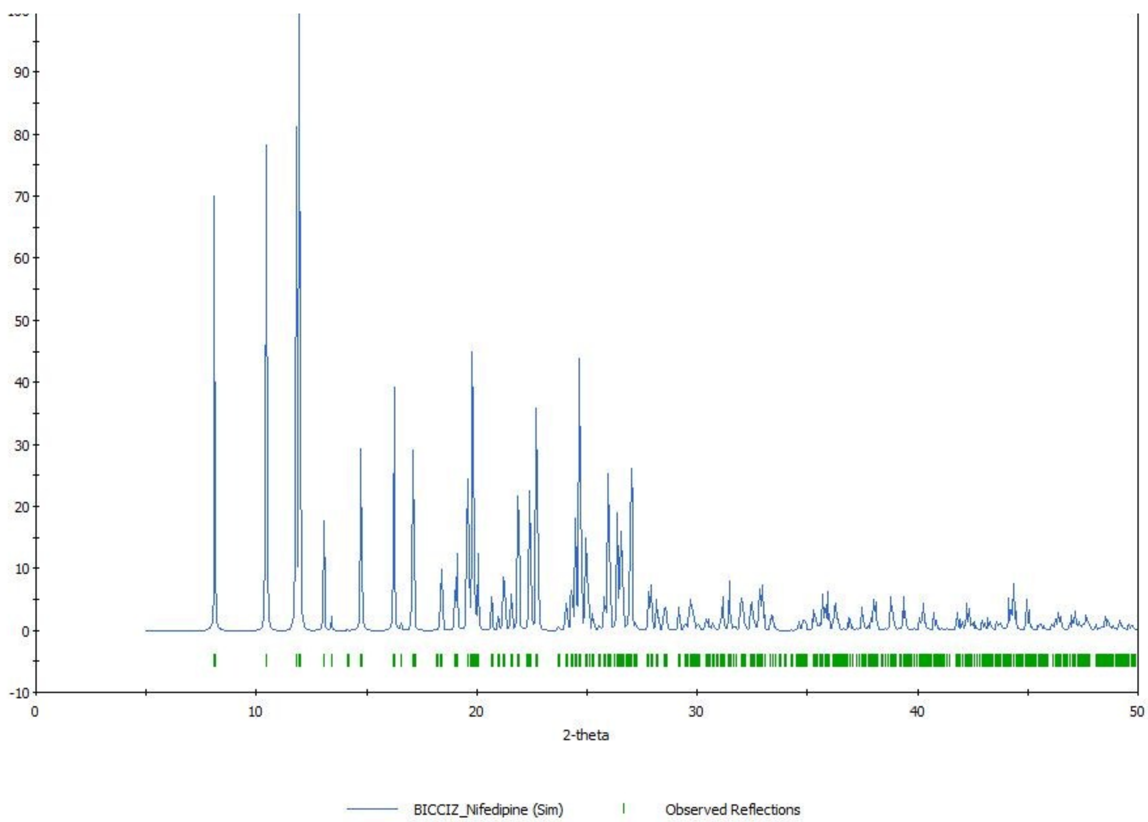
| No. | Pos. [°2Th.] | d-spacing [Å] | Rel. Int. [%] | FWHM [°2Th.] | Area [cts*°2Th.] | Backgr.[cts] | Height [cts] |
|---|---|---|---|---|---|---|---|
| 1 | 8.3269 | 10.60986 | 46.45 | 0.0836 | 420.26 | 111.34 | 4851.10 |
| 2 | 10.6560 | 8.29554 | 16.60 | 0.1506 | 270.29 | 111.24 | 1733.33 |
| 3 | 11.9855 | 7.37817 | 26.51 | 0.1171 | 335.83 | 111.18 | 2768.92 |
| 4 | 12.2149 | 7.24012 | 10.01 | 0.0836 | 90.61 | 111.17 | 1045.87 |
| 5 | 13.2561 | 6.67370 | 2.70 | 0.2007 | 58.72 | 111.13 | 282.42 |
| 6 | 14.9072 | 5.93801 | 17.68 | 0.1506 | 287.89 | 111.06 | 1846.17 |
| 7 | 16.2552 | 5.44851 | 53.09 | 0.1171 | 672.53 | 111.00 | 5545.06 |
| 8 | 16.4595 | 5.38134 | 100.00 | 0.0836 | 904.85 | 110.99 | 10444.76 |
| 9 | 17.3633 | 5.10321 | 12.97 | 0.0836 | 117.34 | 110.95 | 1354.42 |
| 10 | 18.5268 | 4.78524 | 13.25 | 0.1506 | 215.80 | 110.90 | 1383.87 |
| 11 | 19.2237 | 4.61332 | 14.75 | 0.1004 | 160.19 | 110.87 | 1540.95 |
| 12 | 19.8154 | 4.47688 | 38.92 | 0.0836 | 352.19 | 110.84 | 4065.31 |
| 13 | 19.9781 | 4.44080 | 31.83 | 0.1004 | 345.64 | 110.84 | 3324.82 |
| 14 | 20.1902 | 4.39462 | 19.93 | 0.0669 | 144.27 | 110.83 | 2081.59 |
| 15 | 20.8237 | 4.26232 | 4.34 | 0.2007 | 94.18 | 110.80 | 452.95 |
| 16 | 21.2954 | 4.16896 | 4.43 | 0.2007 | 96.30 | 110.78 | 463.15 |
| 17 | 22.0922 | 4.02038 | 24.37 | 0.1338 | 352.85 | 110.74 | 2545.64 |
| 18 | 22.9184 | 3.87727 | 34.93 | 0.1673 | 632.06 | 110.71 | 3647.94 |
| 19 | 24.4436 | 3.63870 | 51.79 | 0.1338 | 749.87 | 110.64 | 5409.85 |
| 20 | 24.6519 | 3.60842 | 66.88 | 0.0836 | 605.16 | 110.63 | 6985.40 |
| 21 | 24.8989 | 3.57317 | 48.73 | 0.1004 | 529.17 | 110.62 | 5090.25 |
| 22 | 26.1164 | 3.40929 | 51.71 | 0.1338 | 748.67 | 110.57 | 5401.23 |
| 23 | 26.5737 | 3.35166 | 25.18 | 0.1171 | 318.92 | 110.55 | 2629.48 |
| 24 | 27.2279 | 3.27259 | 44.26 | 0.1004 | 480.60 | 110.52 | 4622.96 |
| 25 | 27.9403 | 3.19075 | 12.68 | 0.1673 | 229.42 | 110.49 | 1324.09 |
| 26 | 28.5796 | 3.12081 | 3.82 | 0.3346 | 138.23 | 110.46 | 398.89 |
| 27 | 29.3816 | 3.03742 | 5.28 | 0.2342 | 133.72 | 110.43 | 551.28 |
| 28 | 29.8049 | 2.99524 | 5.06 | 0.2007 | 109.87 | 110.41 | 528.42 |
| 29 | 30.4996 | 2.92858 | 5.92 | 0.2007 | 128.63 | 110.38 | 618.65 |
| 30 | 31.3001 | 2.85549 | 5.27 | 0.2007 | 114.34 | 110.35 | 549.93 |
| 31 | 31.6795 | 2.82215 | 13.51 | 0.0669 | 97.79 | 110.33 | 1411.00 |
| 32 | 32.0687 | 2.78878 | 6.16 | 0.2007 | 133.76 | 110.31 | 643.34 |
| 33 | 32.9745 | 2.71421 | 16.25 | 0.1338 | 235.30 | 110.27 | 1697.54 |
| 34 | 34.9213 | 2.56723 | 7.70 | 0.1673 | 139.39 | 110.19 | 804.48 |
| 35 | 35.6824 | 2.51419 | 11.89 | 0.1004 | 129.13 | 110.16 | 1242.12 |
| 36 | 35.9351 | 2.49709 | 9.49 | 0.0836 | 85.83 | 110.15 | 990.79 |
| 37 | 36.5371 | 2.45732 | 9.23 | 0.0669 | 66.85 | 110.12 | 964.50 |
| 38 | 38.0543 | 2.36276 | 3.14 | 0.2007 | 68.11 | 110.05 | 327.60 |
| 39 | 38.9926 | 2.30804 | 11.35 | 0.1004 | 123.27 | 110.01 | 1185.77 |
| 40 | 40.3974 | 2.23096 | 1.85 | 0.2676 | 53.64 | 109.95 | 193.50 |
| 41 | 40.9701 | 2.20109 | 1.58 | 0.2676 | 45.73 | 109.93 | 164.94 |
| 42 | 42.3882 | 2.13067 | 3.26 | 0.3346 | 117.82 | 109.87 | 340.00 |
| 43 | 43.0794 | 2.09807 | 4.35 | 0.1673 | 78.72 | 109.84 | 454.34 |
| 44 | 44.4941 | 2.03459 | 2.78 | 0.2676 | 80.46 | 109.77 | 290.23 |
| 45 | 46.5255 | 1.95038 | 1.46 | 0.2007 | 31.77 | 109.69 | 152.80 |
| 46 | 47.4065 | 1.91617 | 2.41 | 0.5712 | 201.70 | 109.65 | 252.23 |
| 47 | 47.9086 | 1.89725 | 7.29 | 0.2856 | 304.30 | 109.63 | 761.06 |



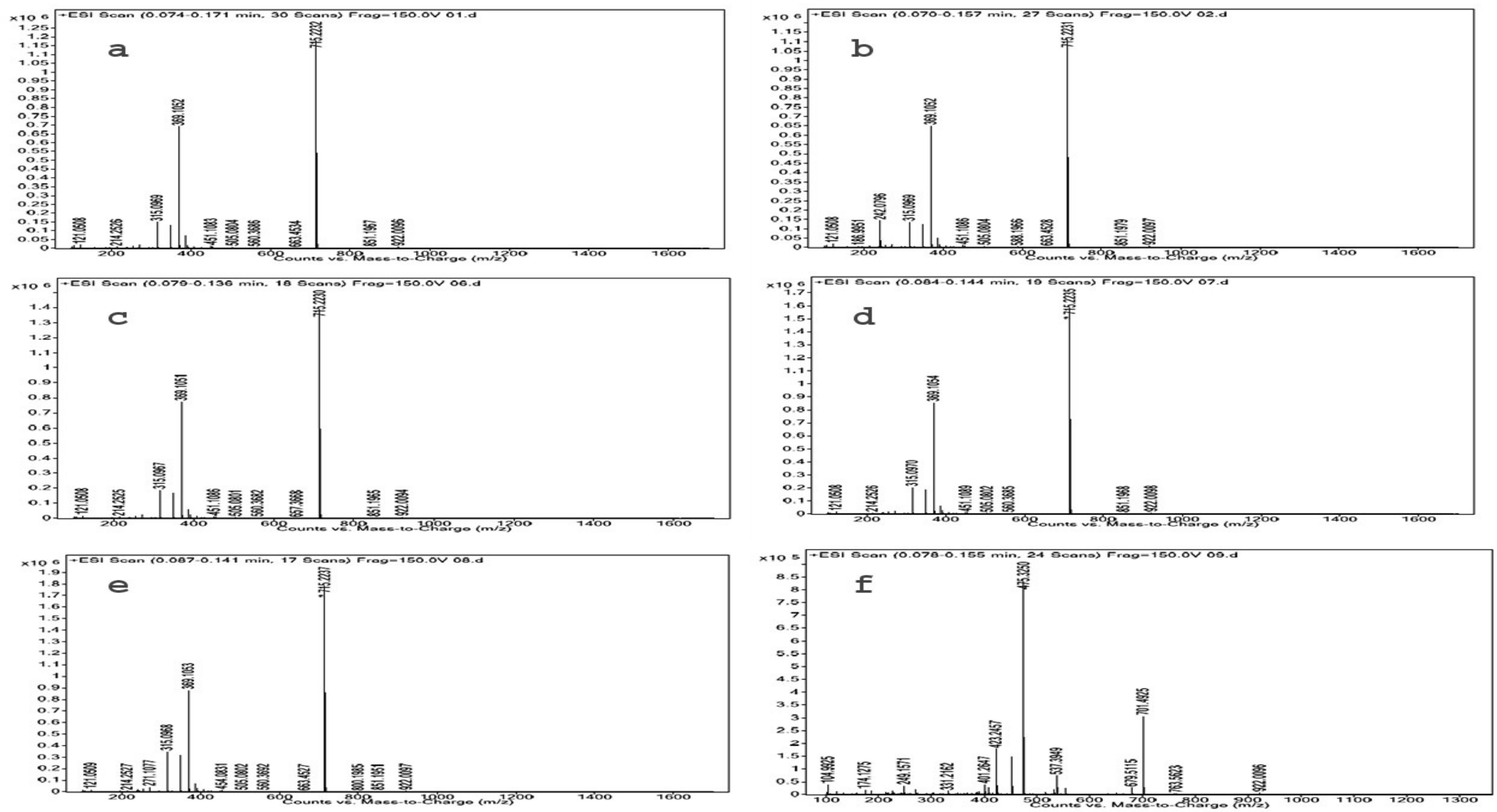

**Supplementary figure 1.** Modified crystal habits of Nif with DCM as solvent and HPMC as additive (a) Experimental Nif-2 habit (b) Experimental Nif-4 habit (c) Experimental Nif-6 habit




**Supplementary figure 2.** TGA of a. Nif -0, b. Nif-2, c. Nif-4, d. Nif-6




**Supplementary figure 3.** Nif simulated p-XRD




**Supplementary figure 4.** Mass spectra of a. Nif b. Nif-0 c. Nif-2 d. Nif-4 e. Nif-6 f. HPMC