Electronic supplementary information (ESI) file of the paper

Rationalization of liquid assisted grinding intercalation yields of organic molecules into layered double hydroxides by multivariate analysis

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achieve the best fit of the non-superimposed peaks the yield resulted to be, quite confidently, about 50%.

Anyway, performing the fit restraining the peak positions and CS_L (Crystallite Size) to the (003) and (006) peak of the starting LDH_NO

Figure S11: Complete dataset. In red the variables excluded from the analysis after the variable screening data mining procedure (the suffix "_c" means "prepared in capillary", as detailed in the experimental section).

In Figure S12 the peak falling at about 10.4° is more intense than the (001) peak of LDH_COUM since it is formed by three superimposed peaks, namely the (002) peak of the LDH_COUM phase, the (003) peak of LDH_NO2 and the partially superimposed (003) peak of the LDH_CO2 phase. The intercalation of complex organic molecules inside LDH layers instead of simple inorganic anions (such as nitrate, chloride, or carbonate) causes a lowering of the symmetry from R-3m to P-1. For this reason we indexed the lamellar peaks of the organic intercalated LDHs as (001), (002), (003) etc. while the lamellar peaks of LDH_CO3 and LDH_NO2 are indexed as (003), (006), (009) etc.
Figure SI3: XRPD pattern (in black) and Single peak fit (in red) of LDH_FLUR obtained by LAG intercalation. The peaks of the intercalated phase are visible up to the seventh order (at 3.69° and multiples). The peaks of LDH_NO₃ falling at 9.90° (003) and 19.81° (006) are almost invisible.

Figure SI4: XRPD pattern (in green) and Single peak fit (in red) of LDH_TIAP obtained by LAG intercalation. Peak assignment: 4.10°, 8.15° and 12.10° LDH_TIAP, 10° and 20° LDH_NO₃
Figure SI5: a) Loading plot reporting variables projection on PC1 vs. PC3. b) Score plot reporting the samples on the PC1 vs. PC3 axes. Sample color codes were used to highlight the fully intercalated ones (green) the partially intercalated (yellow) and the poorly or not intercalated (red).
Figure S16: a) Loading plot reporting variables projection on PC1 vs. PC4. b) Score plot reporting the samples on the PC1 vs. PC4 axes.
Figure SI7: a) Loading plot reporting variables projection on PC2 vs. PC4. b) Score plot reporting the samples on the PC2 vs. PC4 axes.
Figure SI8: a) Loading plot reporting variables projection on PC3 vs. PC4. b) Score plot reporting the samples on the PC3 vs. PC4 axes.
Figure SI9: XRPD pattern (in blue) and Single peak fit (in red) of LDH_PABA obtained by LAG intercalation.

Peak attribution: 8.14° and 16.298° LDH_PABA, 9.58°, 13.95°, 14.82° and 15.41° PABA, 9.95° and 19.90° LDH_NO₃

Figure SI10: XRPD pattern (in blue) and Single peak fit (in red) of LDH_TOLU obtained by LAG intercalation.

Peak attribution: 4.38° and 8.77° LDH_TOLU, 12.57°, 13.9°, 14.64° and 17.32° TOLU, 9.90° and 19.81° LDH_NO₃