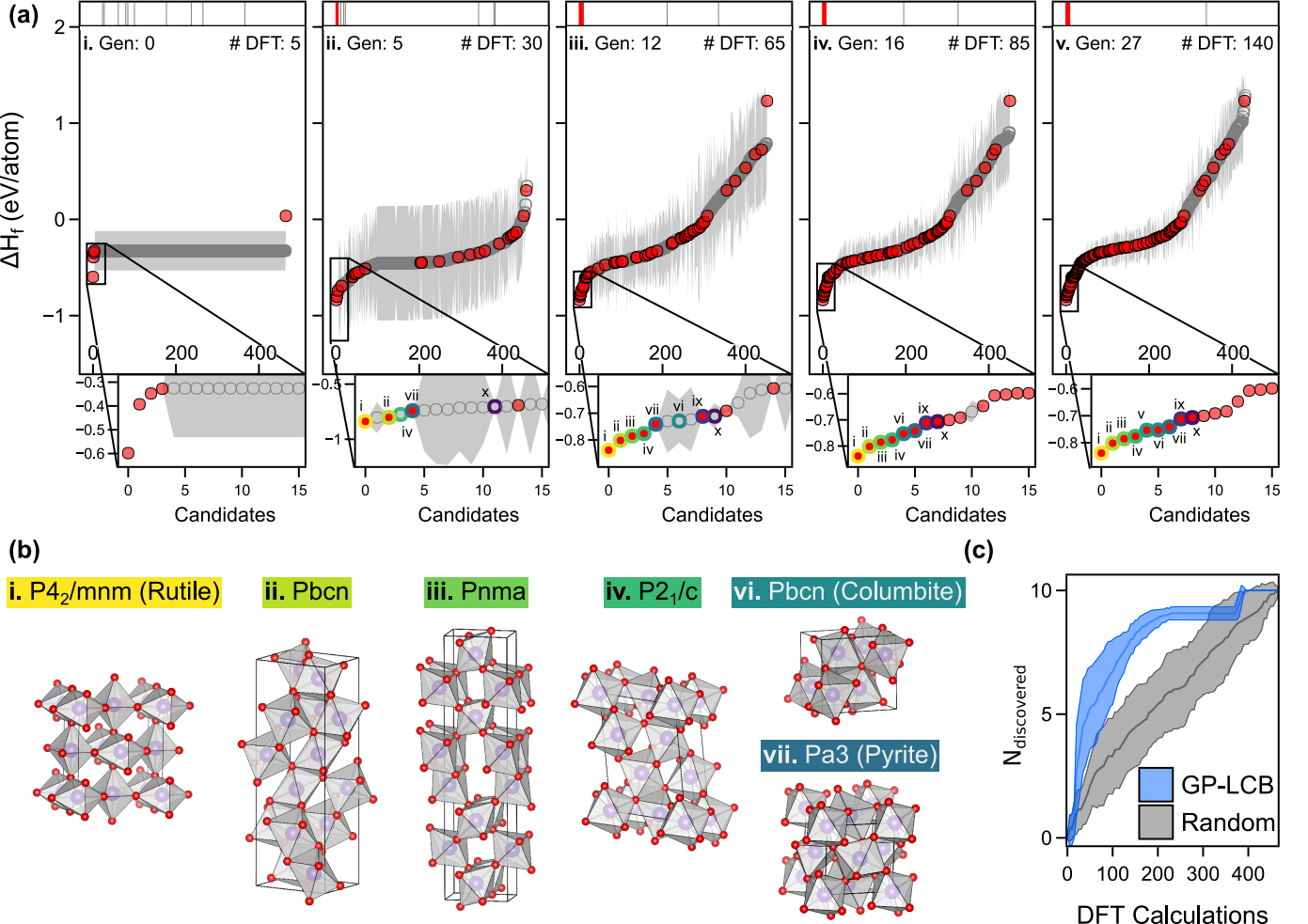
(a)
i. Gen: 0
DFT: 5
ii. Gen: 5
DFT: 30
iii. Gen: 12
DFT: 65
iv. Gen: 16
DFT: 85
v. Gen: 27
DFT: 140
ΔHf (eV/atom)
Candidates
(b)
i. P42/mnm (Rutile)
ii. Pbcn
iii. Pnma
iv. P21/c
vi. Pbcn (Columbite)
vii. Pa3 (Pyrite)
(c)
Ndiscovered
GP-LCB
Random
DFT Calculations