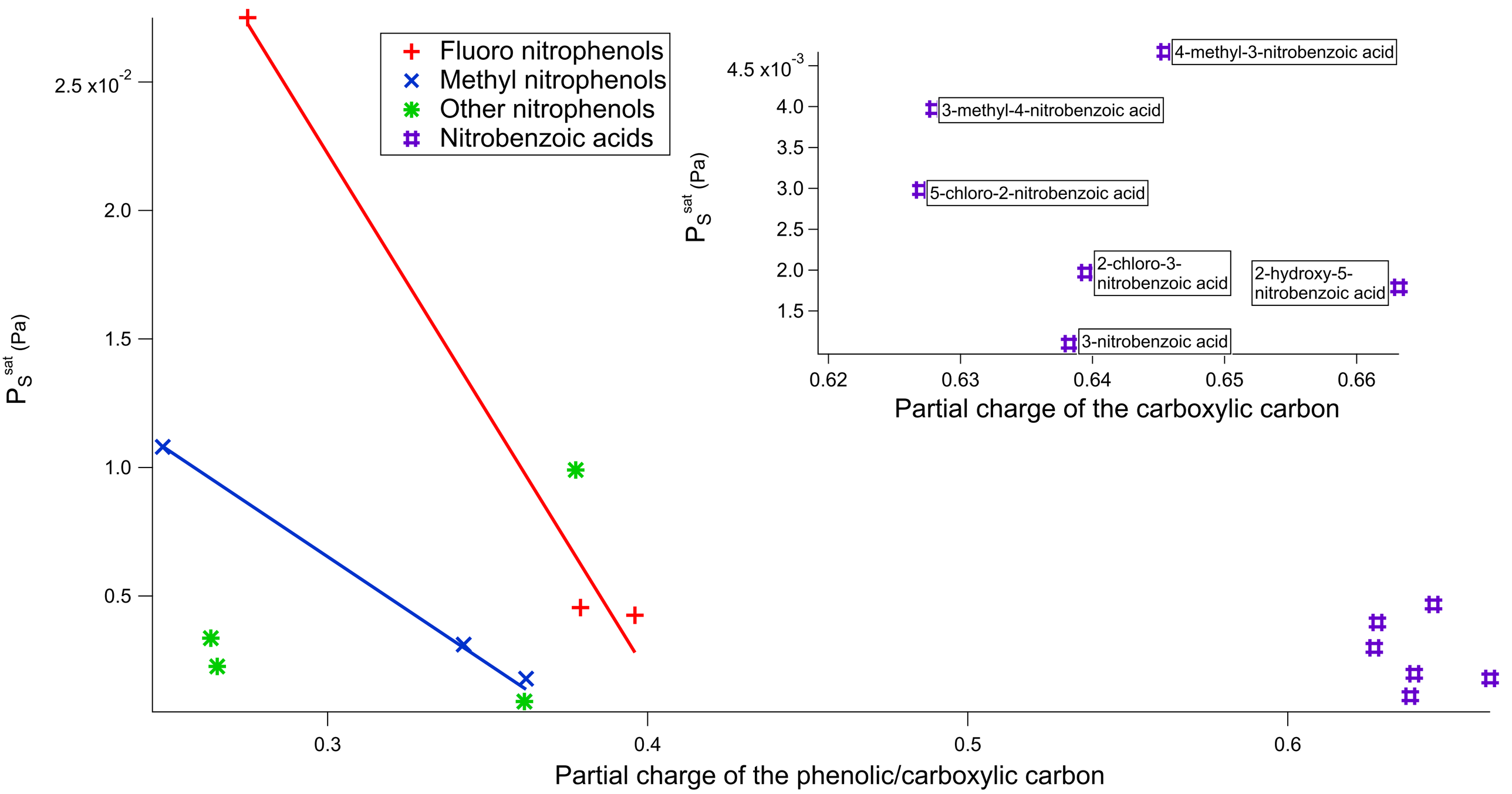
Fluoro nitrophenols
Methyl nitrophenols
Other nitrophenols
Nitrobenzoic acids
2.5 x10^-2
2.0
1.5
1.0
0.5
P_S^sat (Pa)
0.3
0.4
0.5
0.6
Partial charge of the phenolic/carboxylic carbon
4.5 x10^-3
4.0
3.5
3.0
2.5
2.0
1.5
P_S^sat (Pa)
4-methyl-3-nitrobenzoic acid
3-methyl-4-nitrobenzoic acid
5-chloro-2-nitrobenzoic acid
2-chloro-3-nitrobenzoic acid
2-hydroxy-5-nitrobenzoic acid
3-nitrobenzoic acid
0.62
0.63
0.64
0.65
0.66
Partial charge of the carboxylic carbon