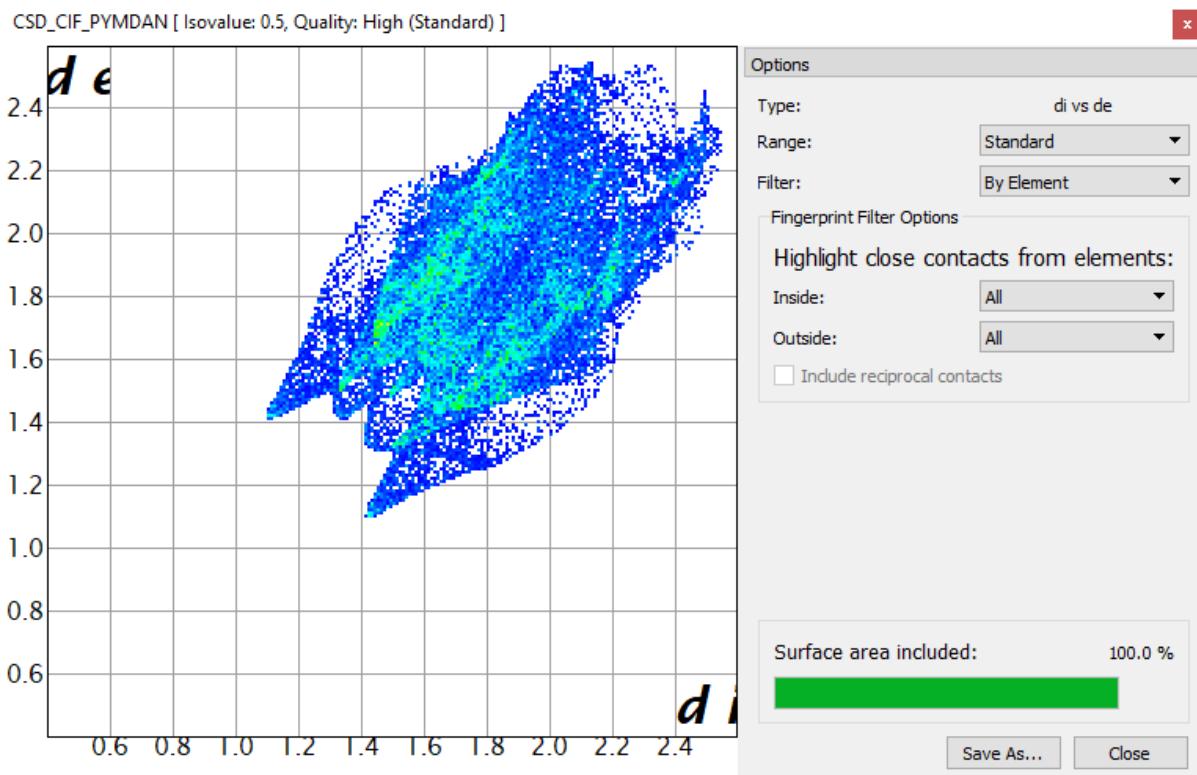
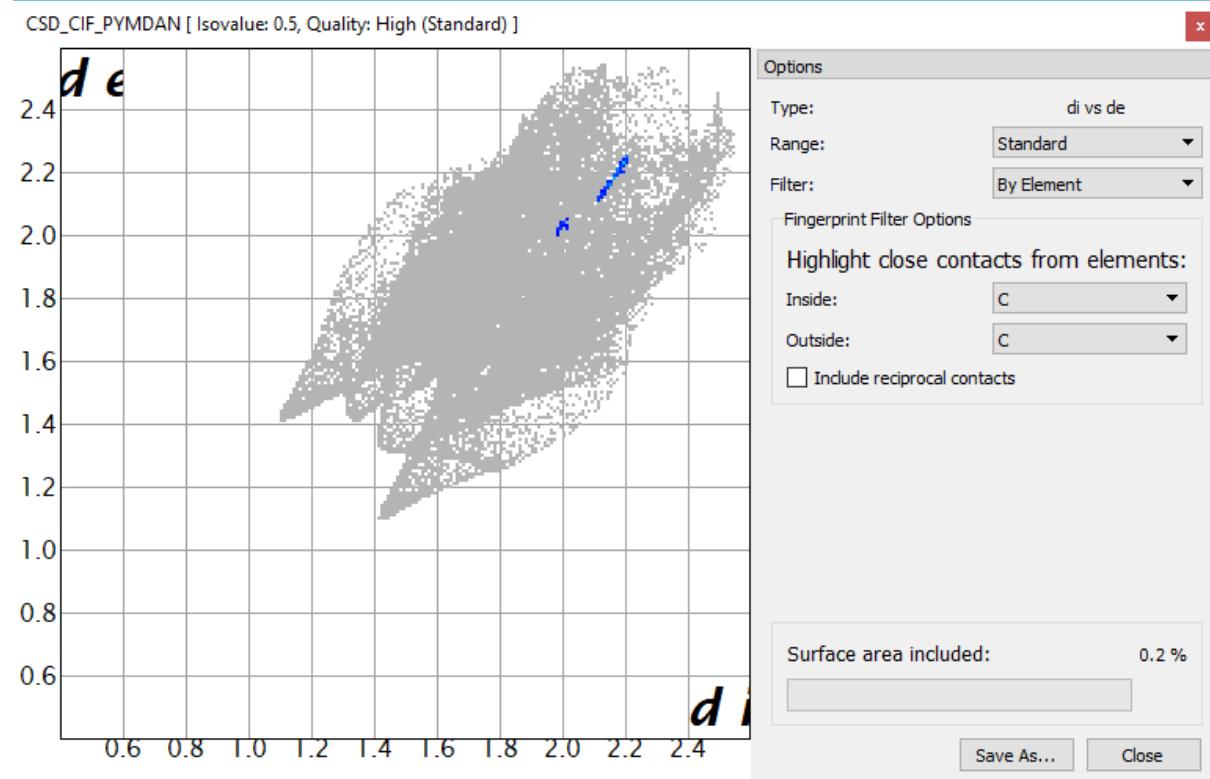


## PYMDAN

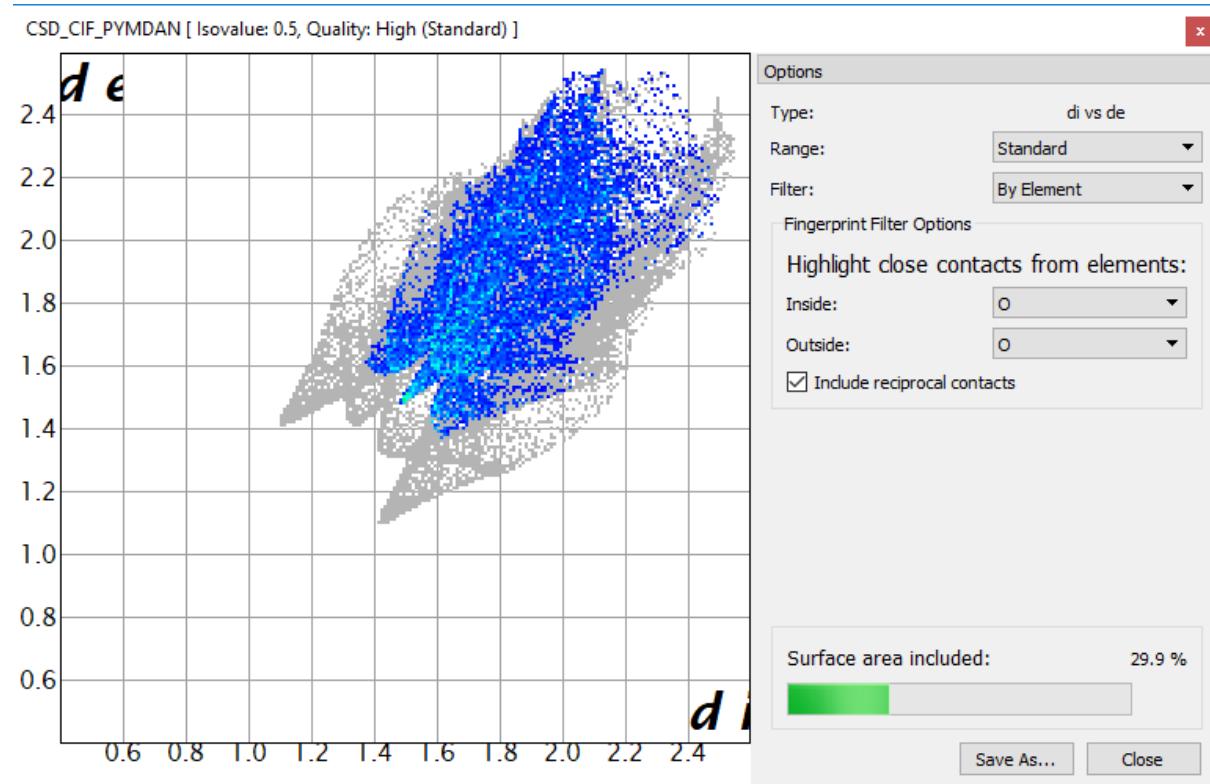
ALL: 100 %



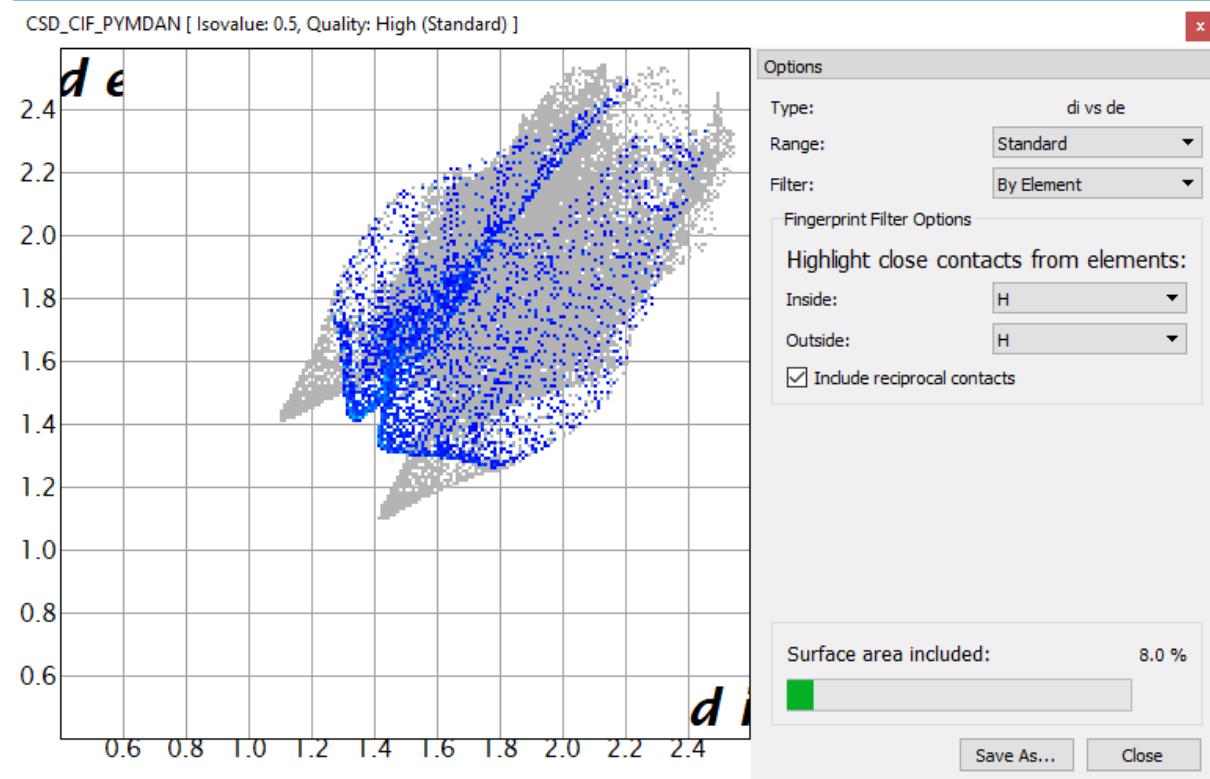
C-C: 0.2 %



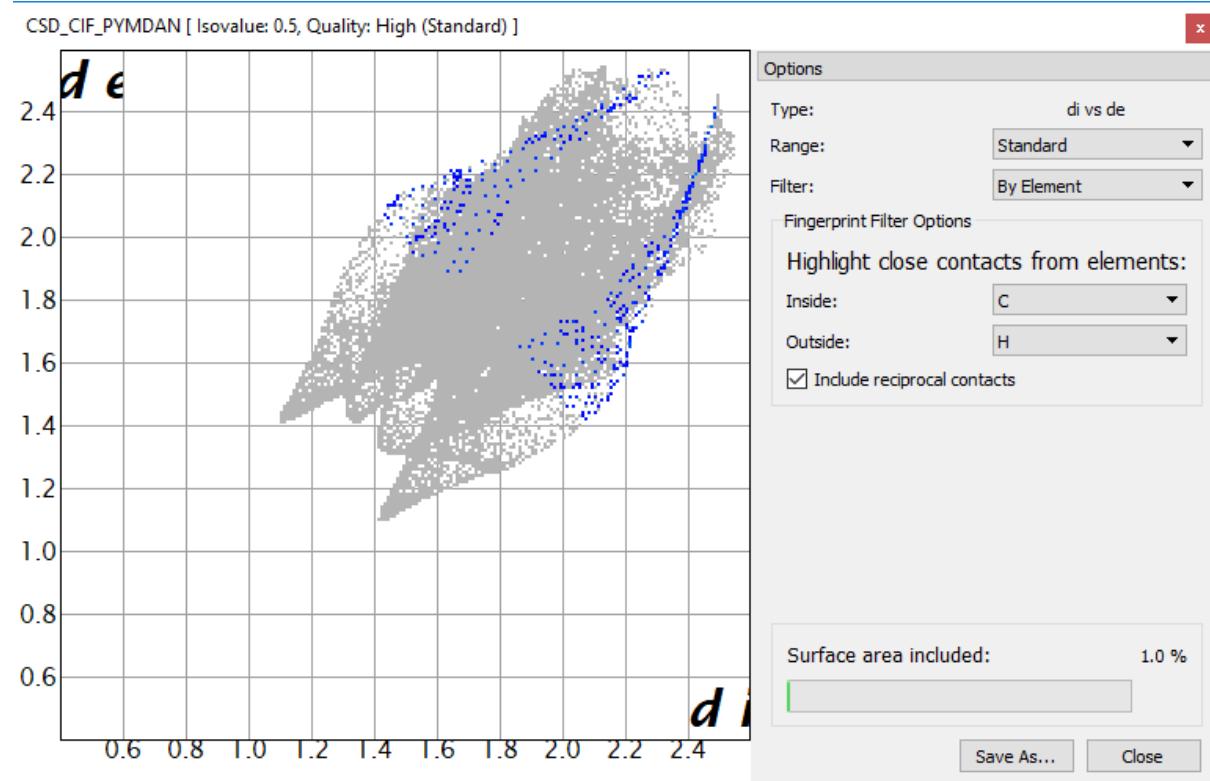
O-O: 29.9 %



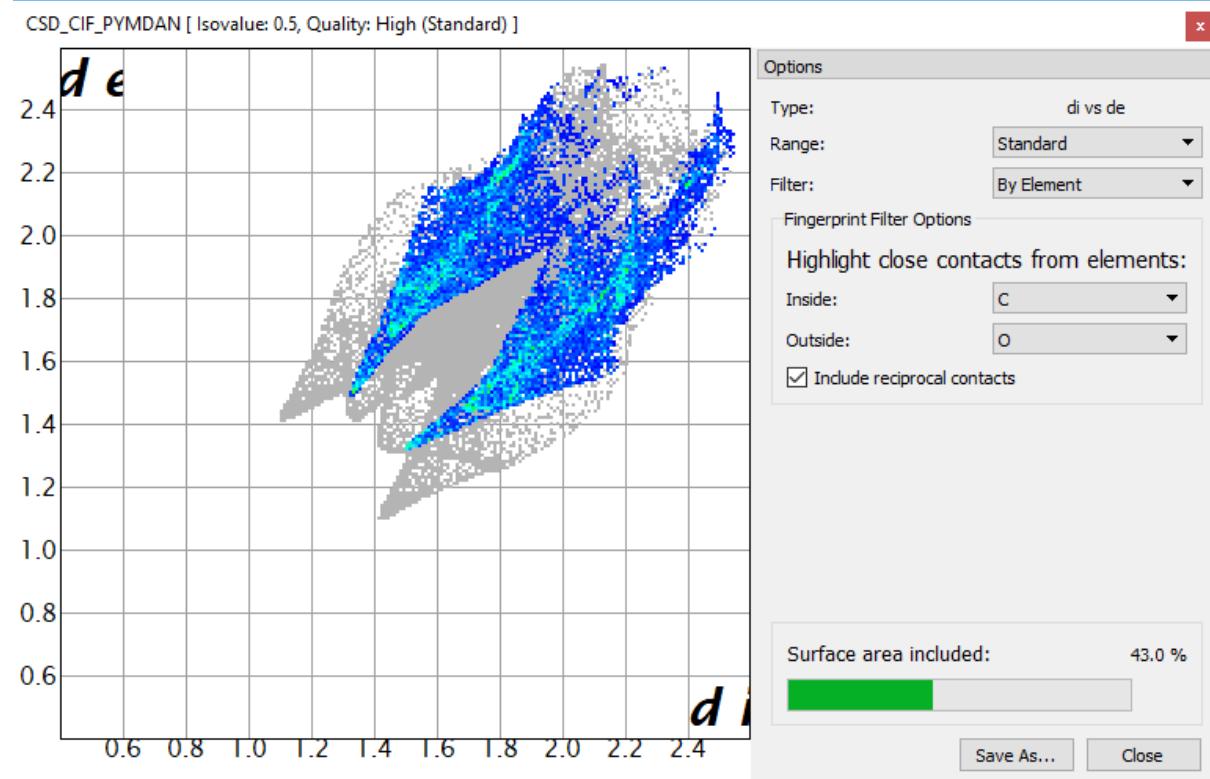
H-H: 8.0 %



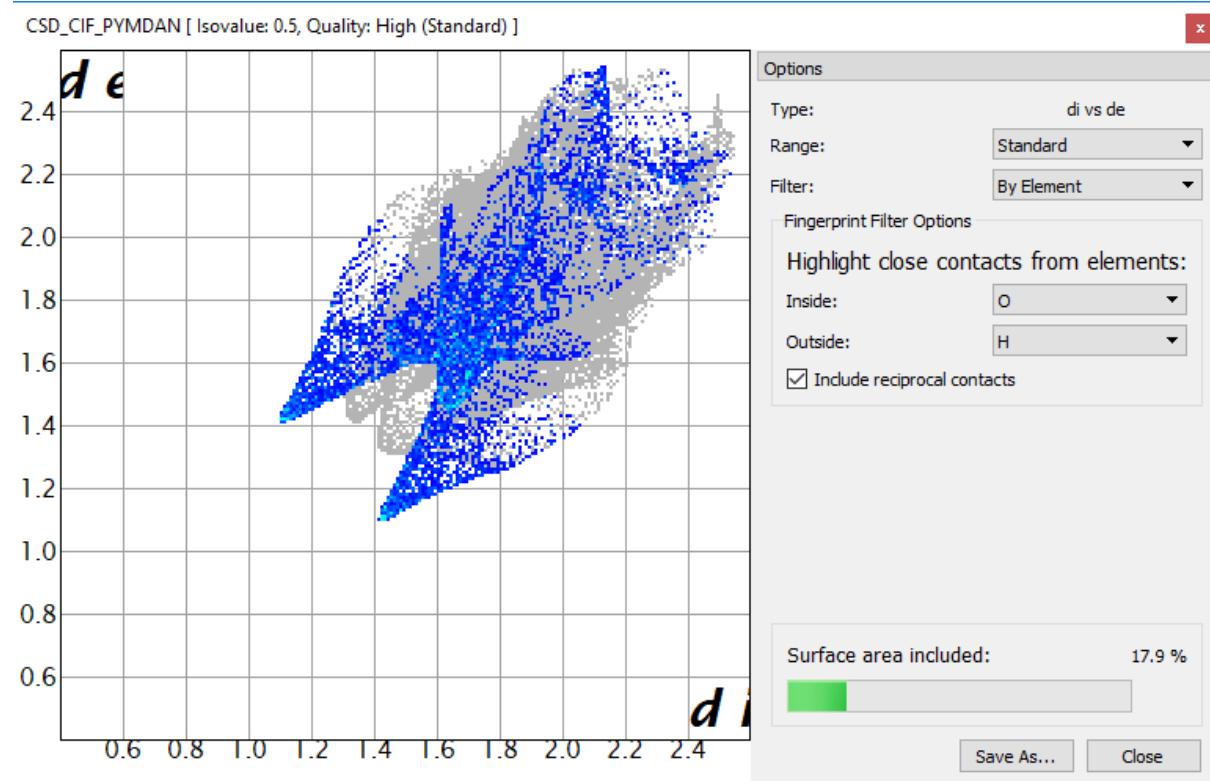
C-H: 1.0 %



C-O: 43.0 %



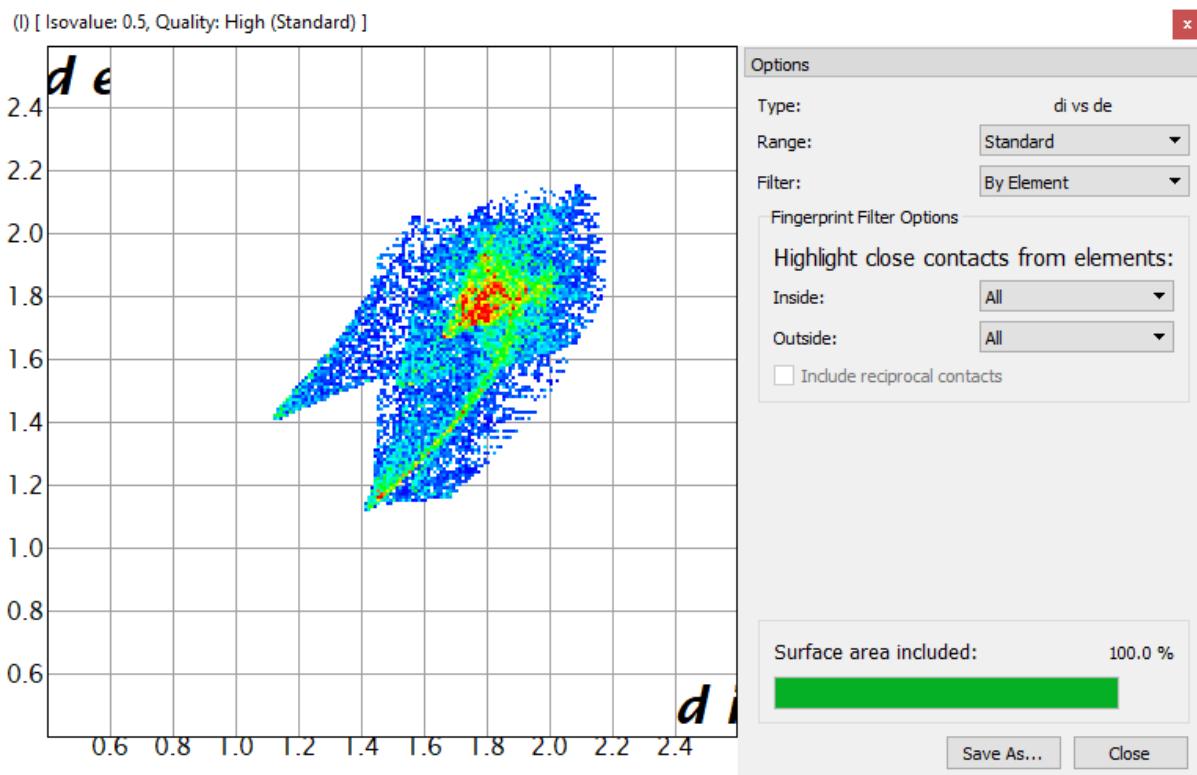
O-H: 17.9 %



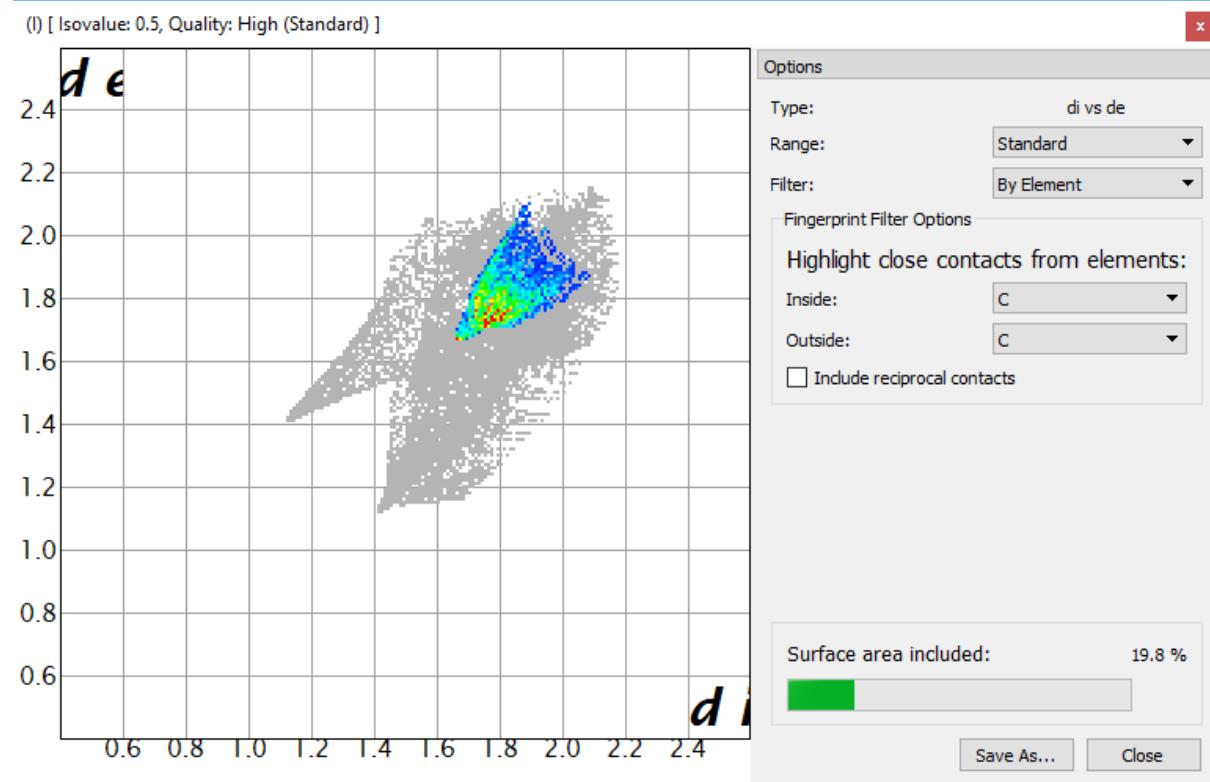


(I)

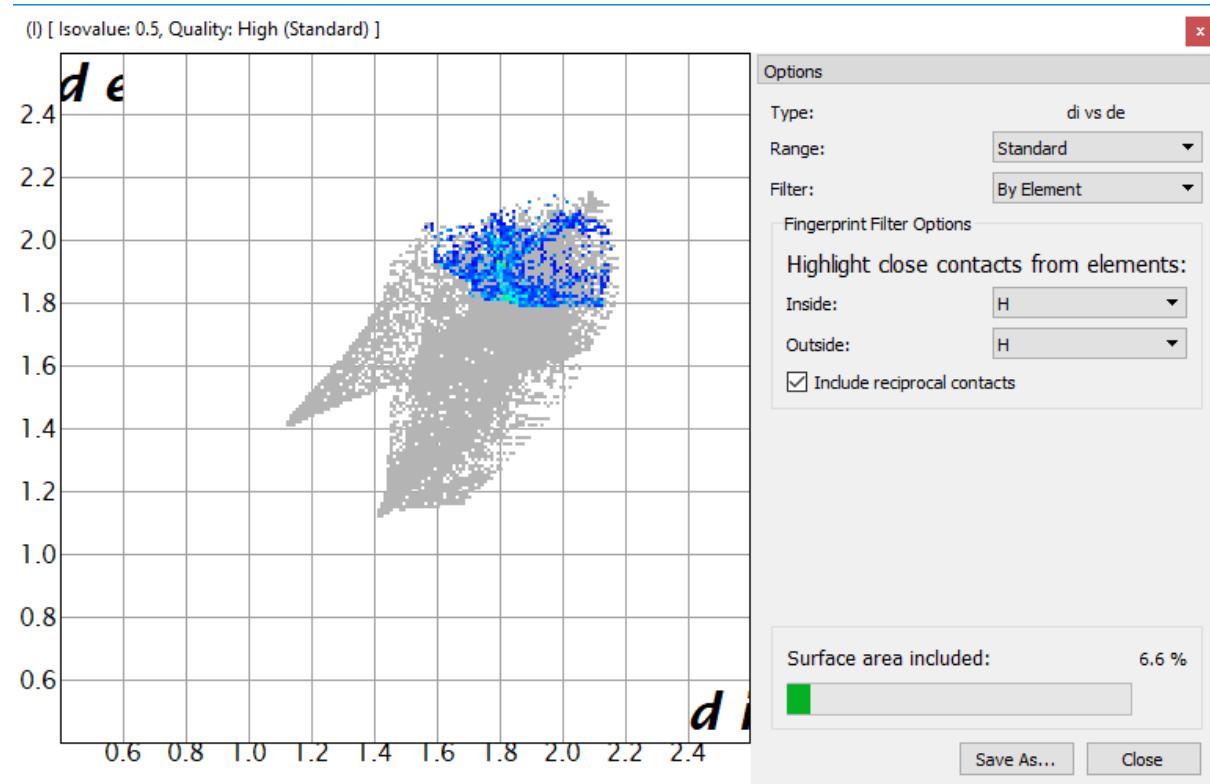
ALL: 100 %



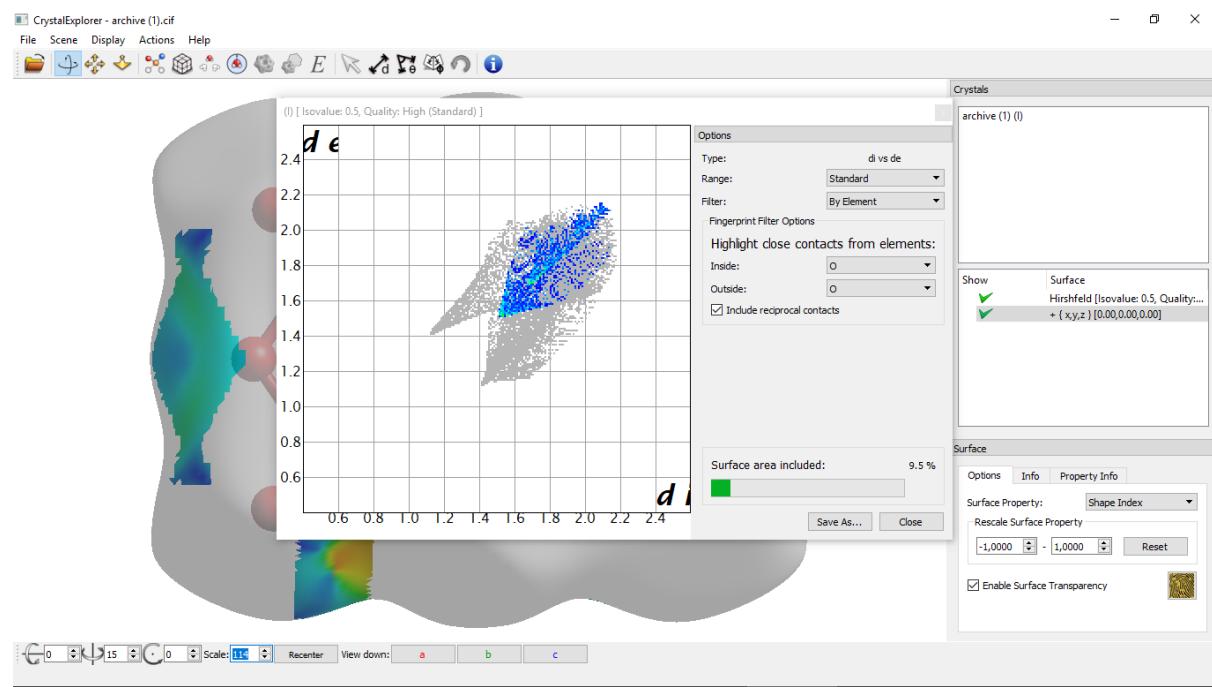
C-C: 19.8 %



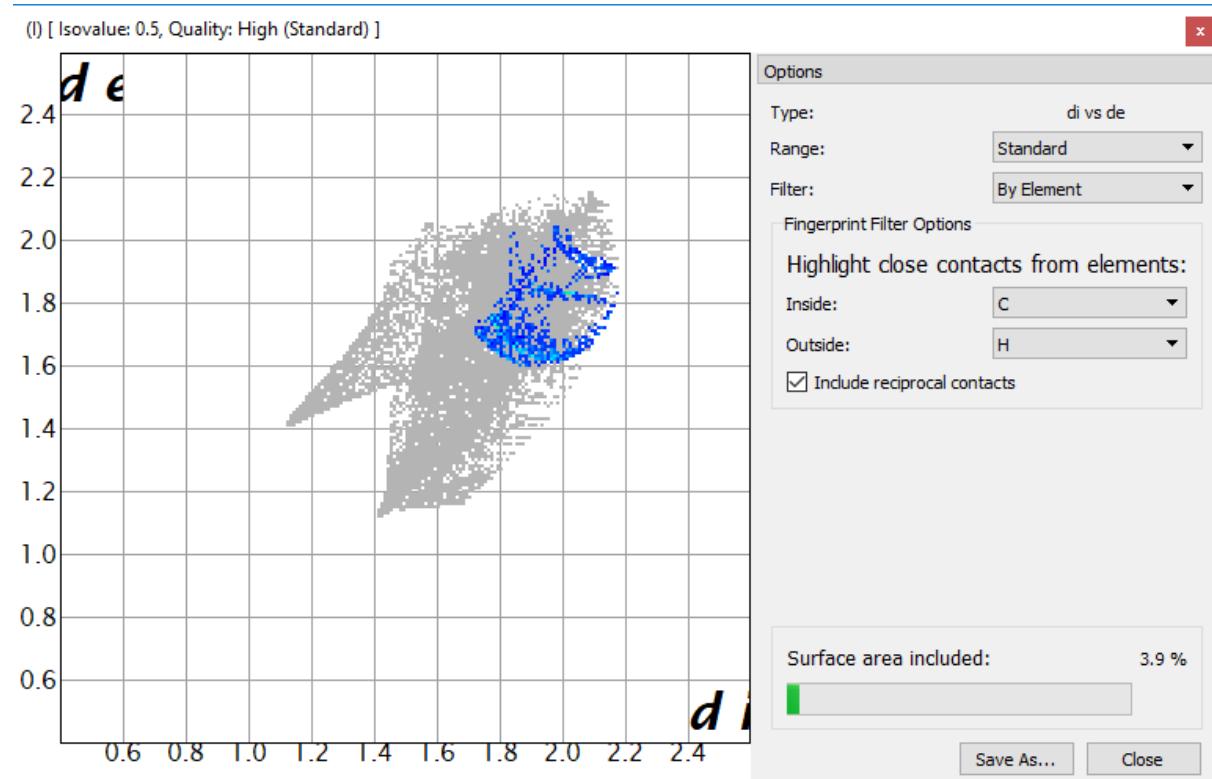
H-H: 6.6 %



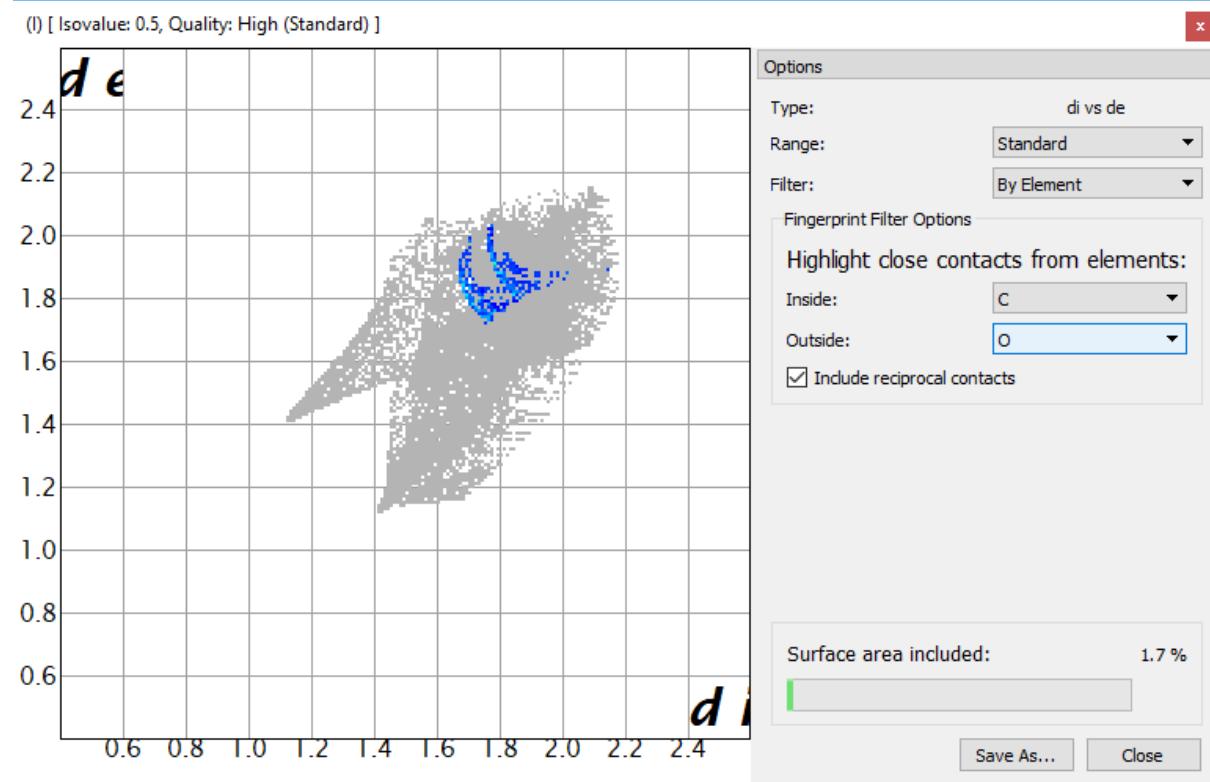
O-O: 9.5 %



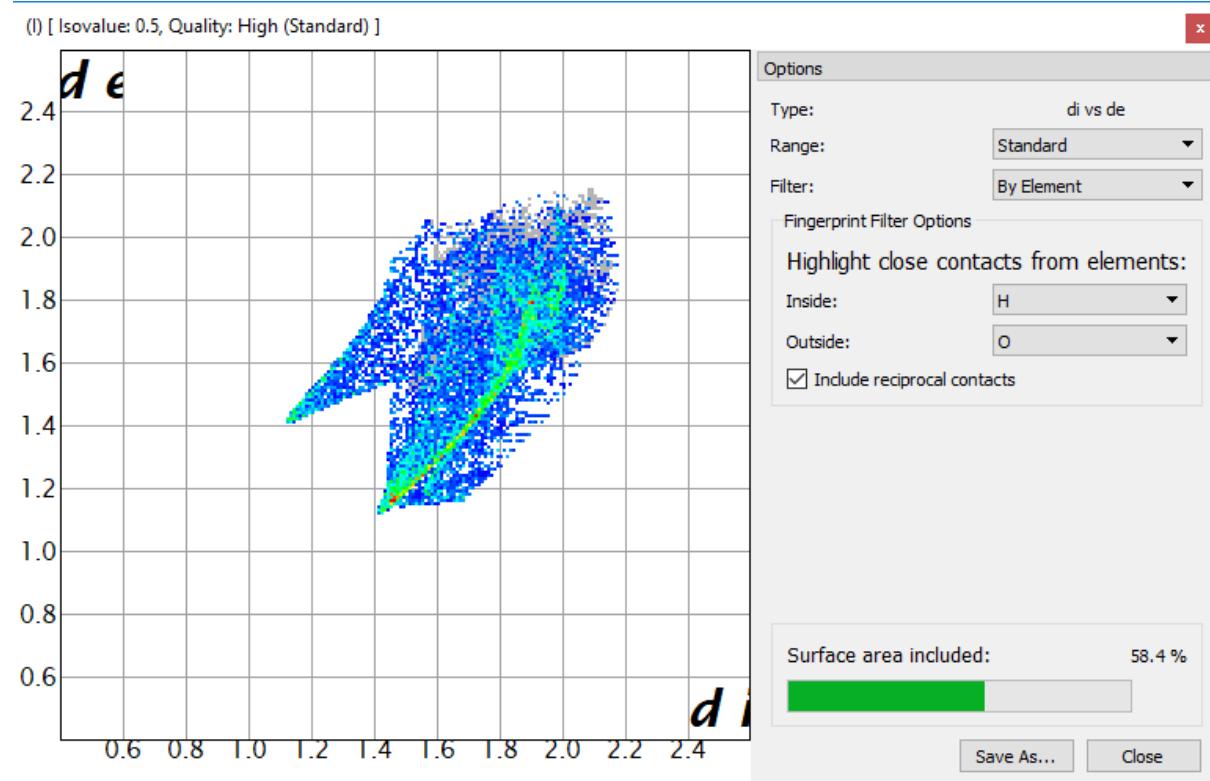
C-H: 3.9 %



C-O: 1.7 %

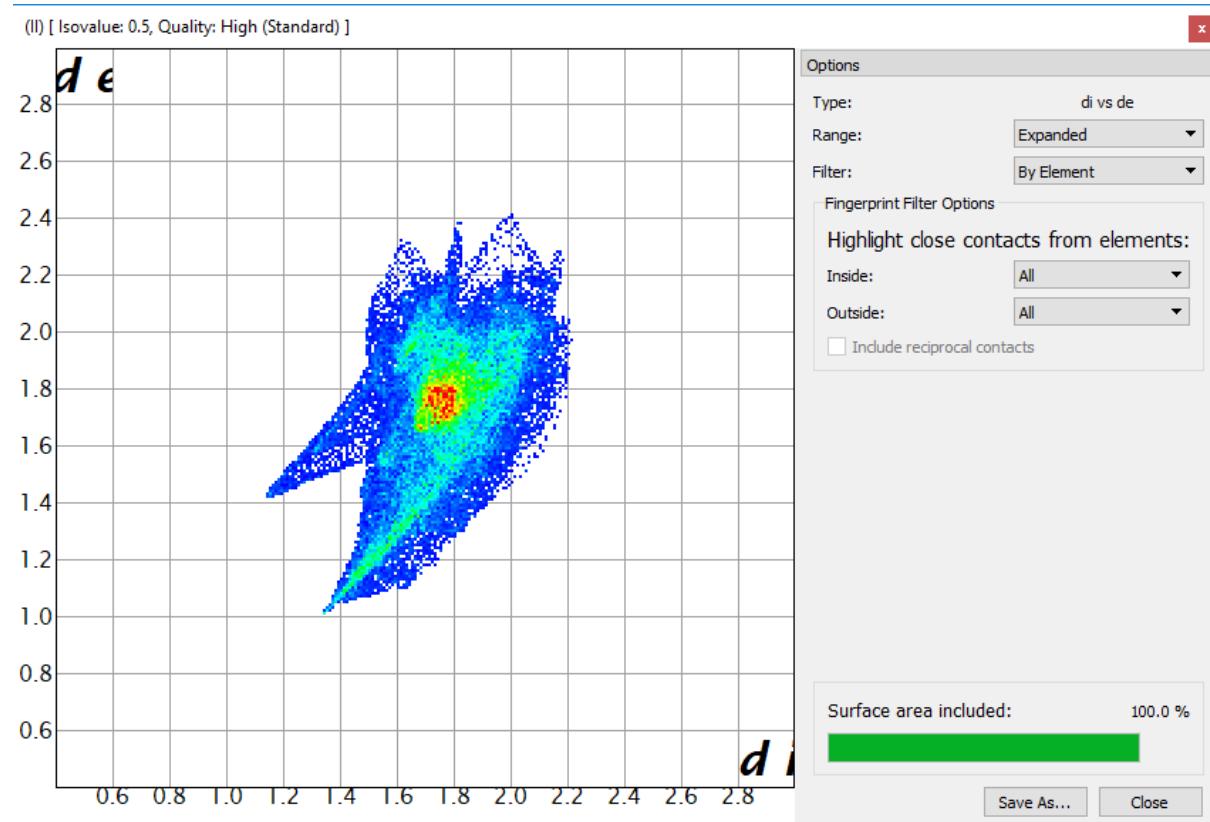


H-O: 58.4 %

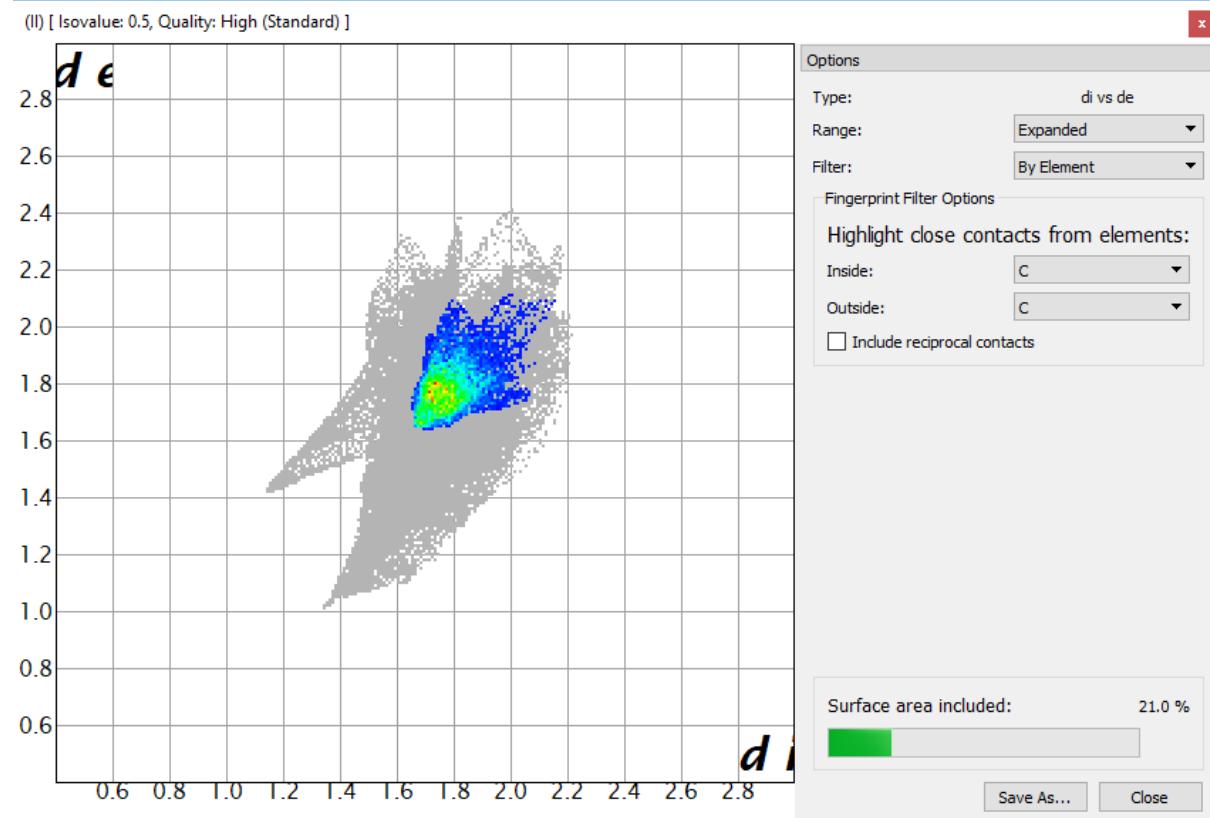


(II) pmda molecule 1 in ASU

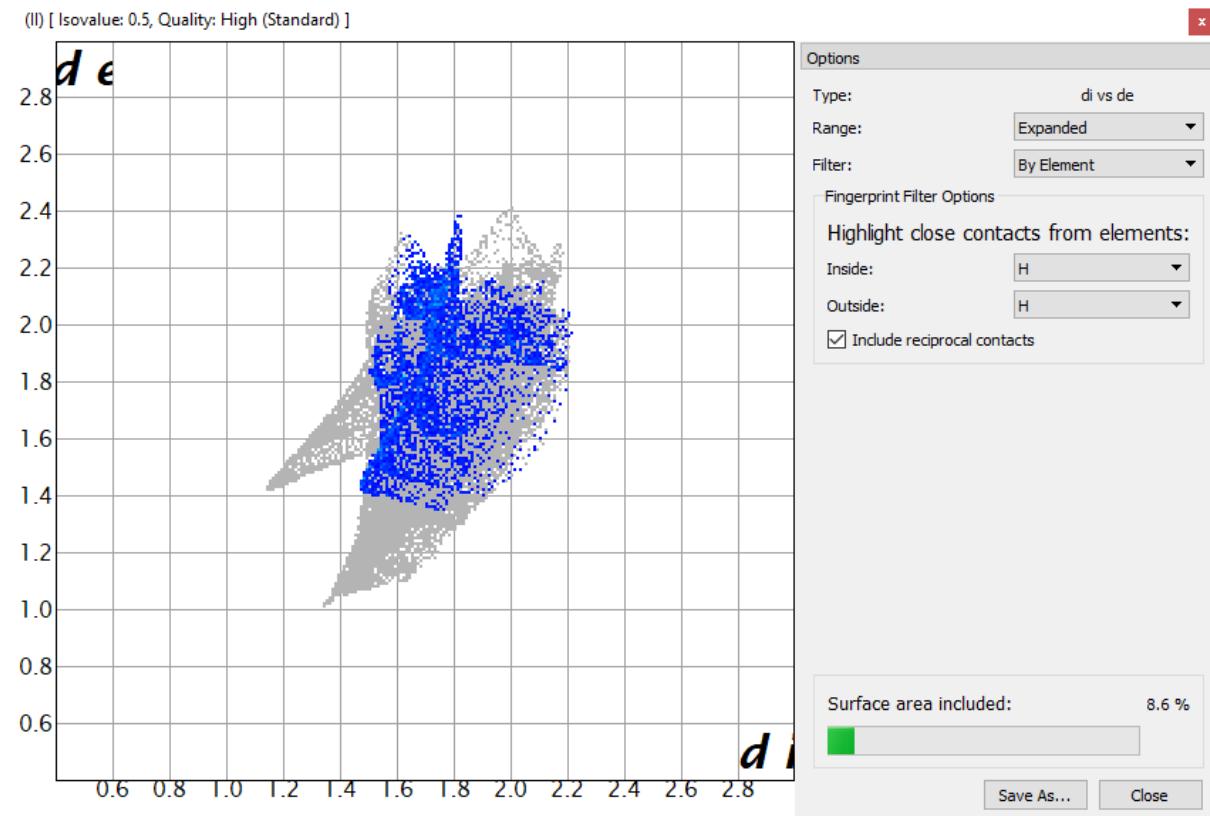
ALL: 100 %



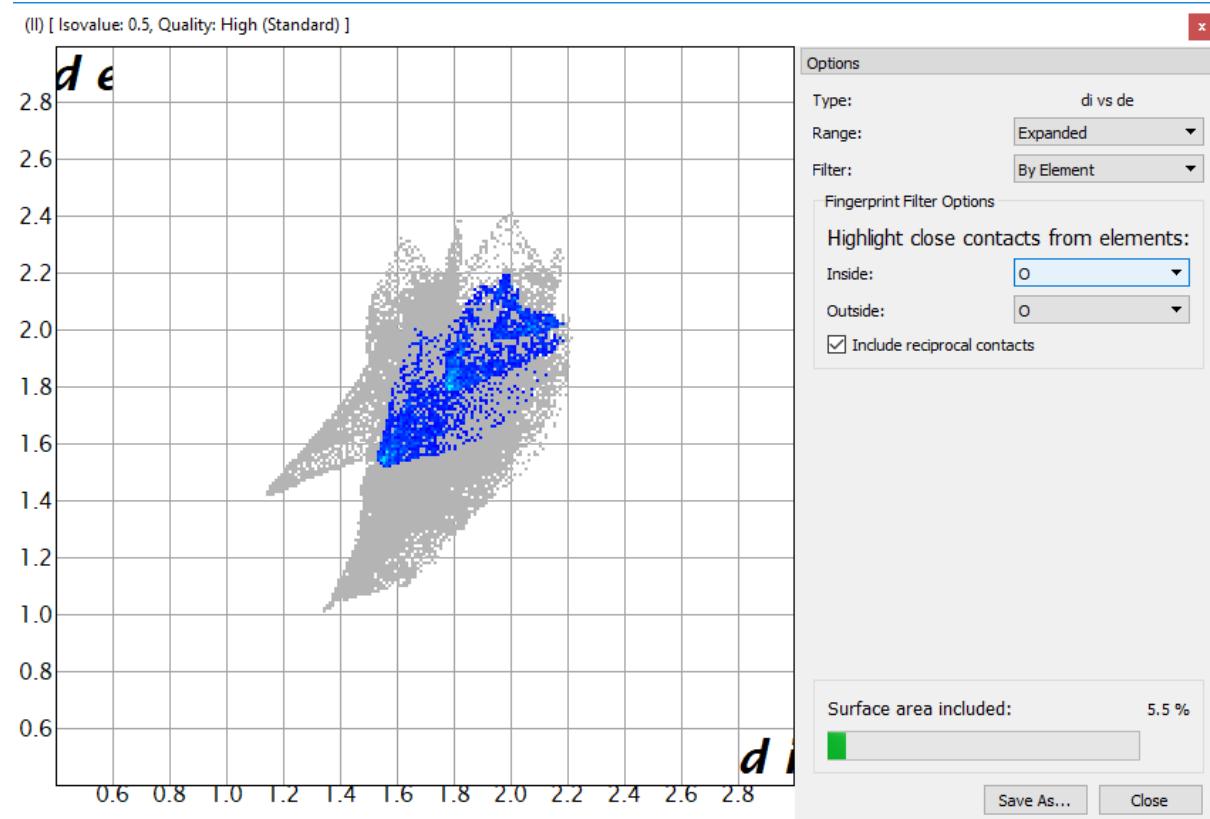
C-C: 21.0



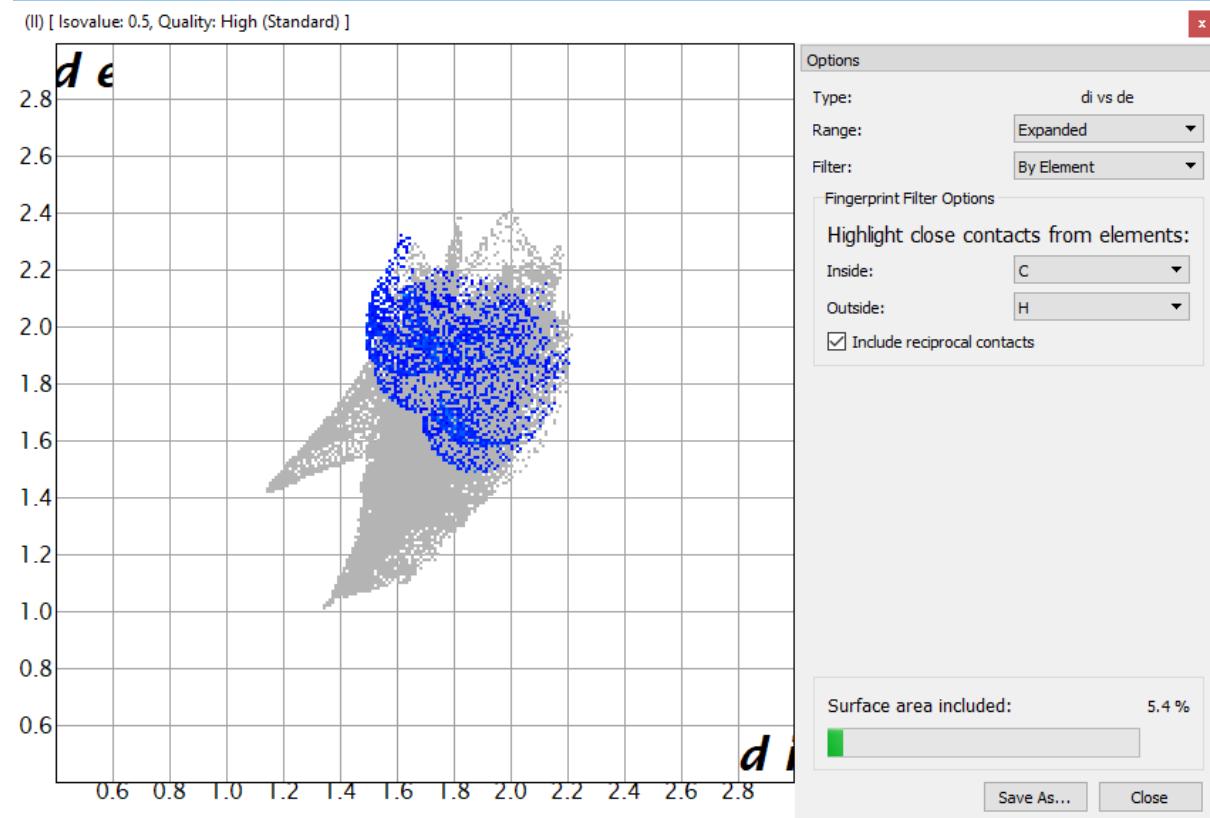
H-H: 8.6 %



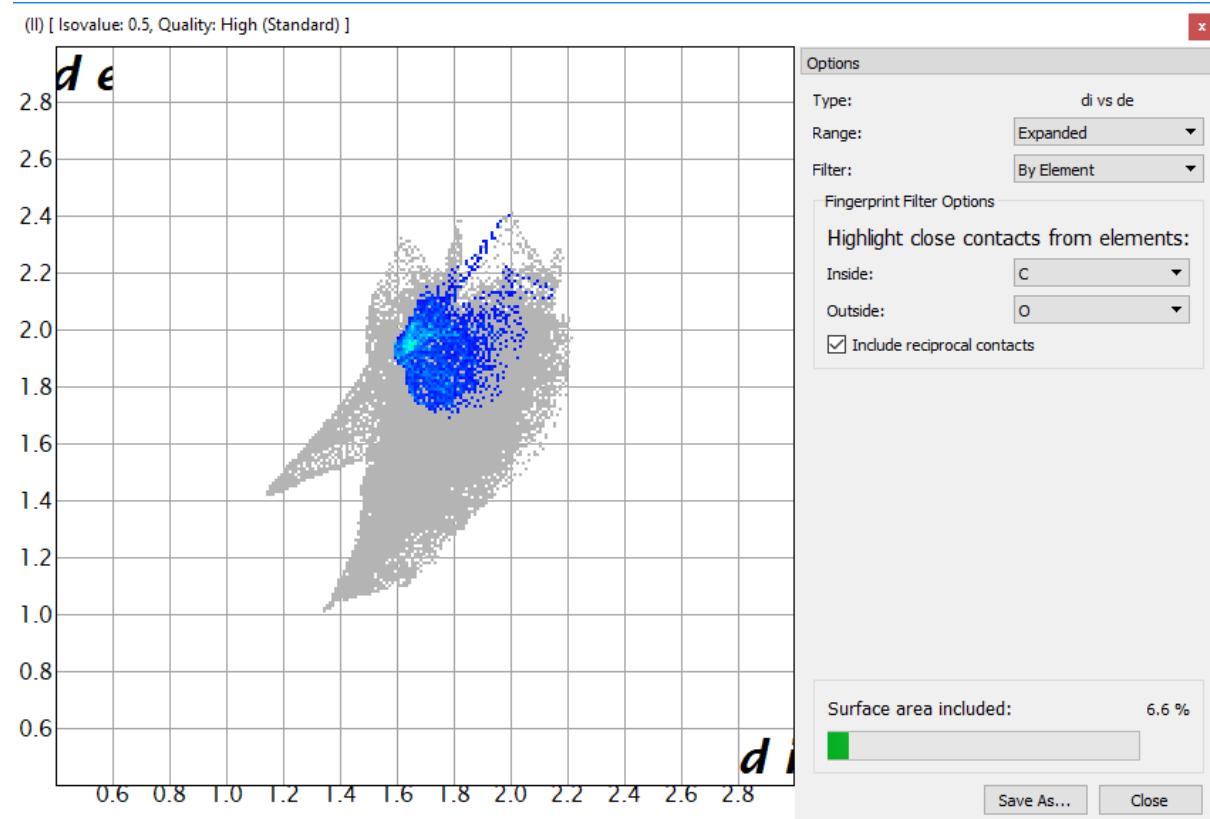
O-O: 5.5 %



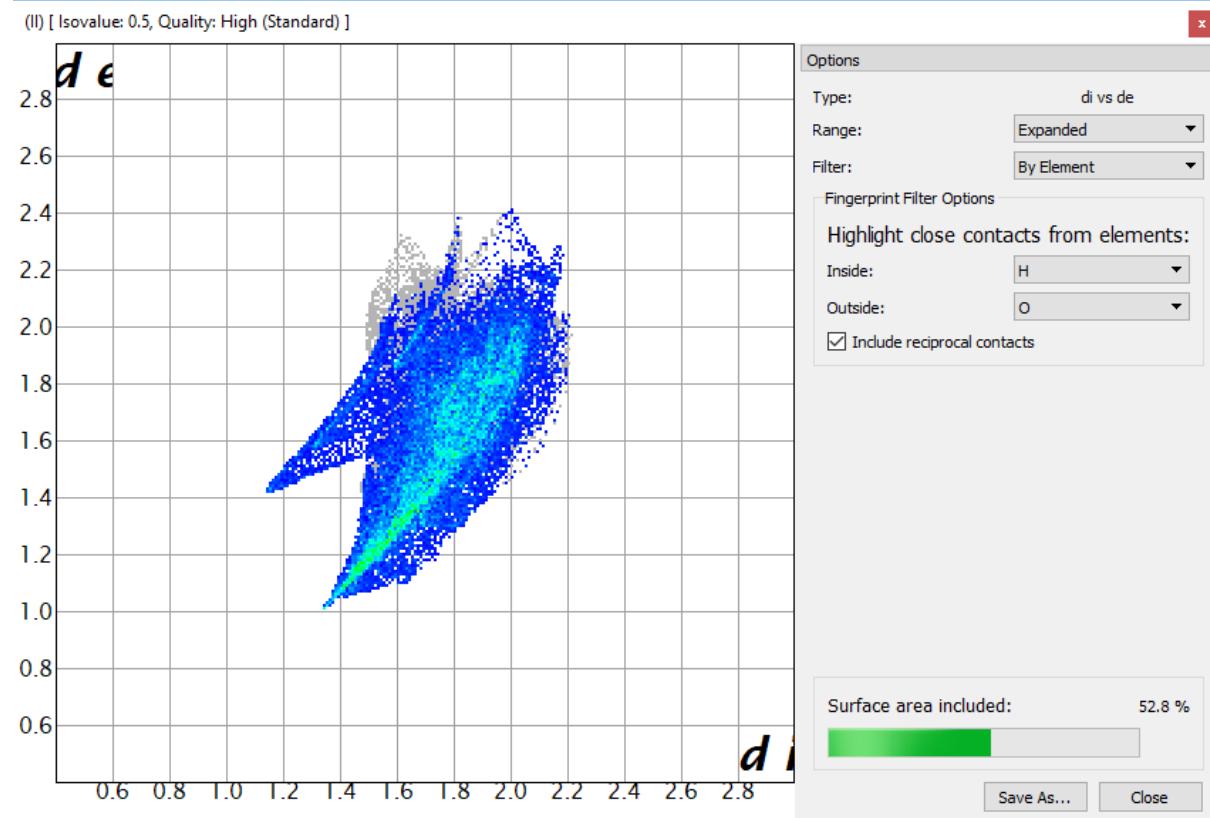
C-H: 5.4 %



C-O: 6.6 %

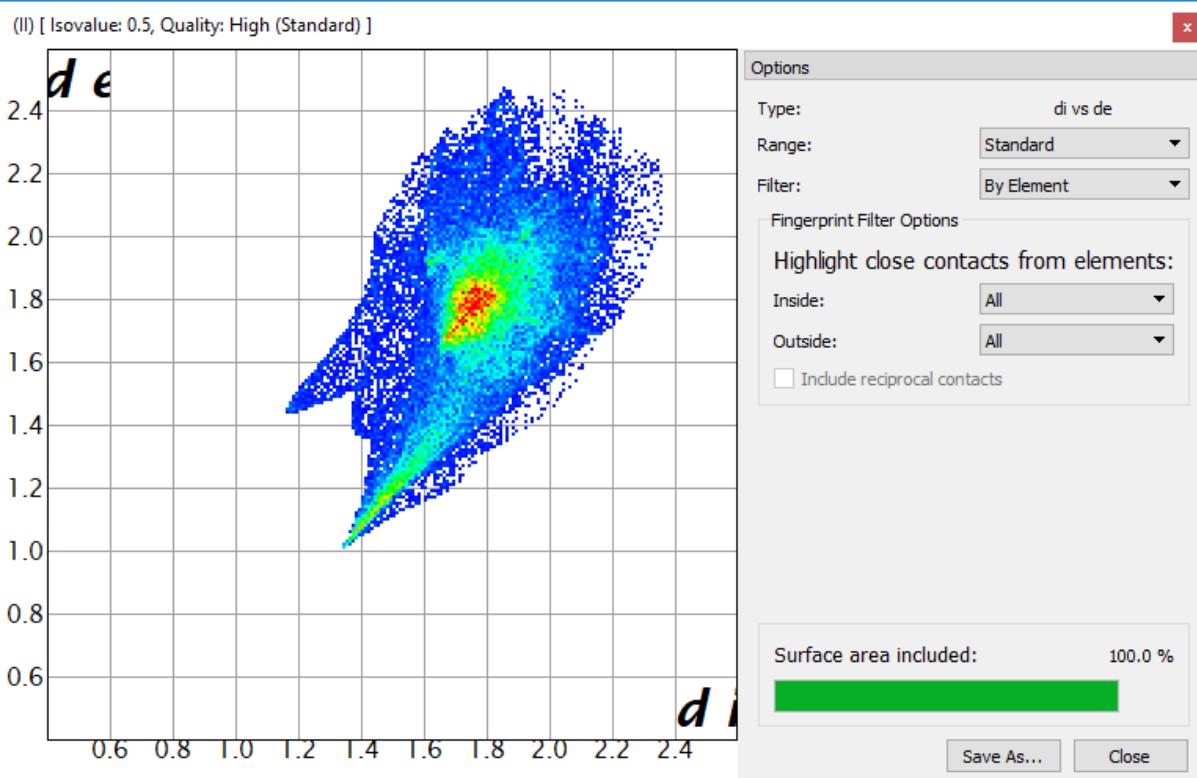


H-O: 52.8 %

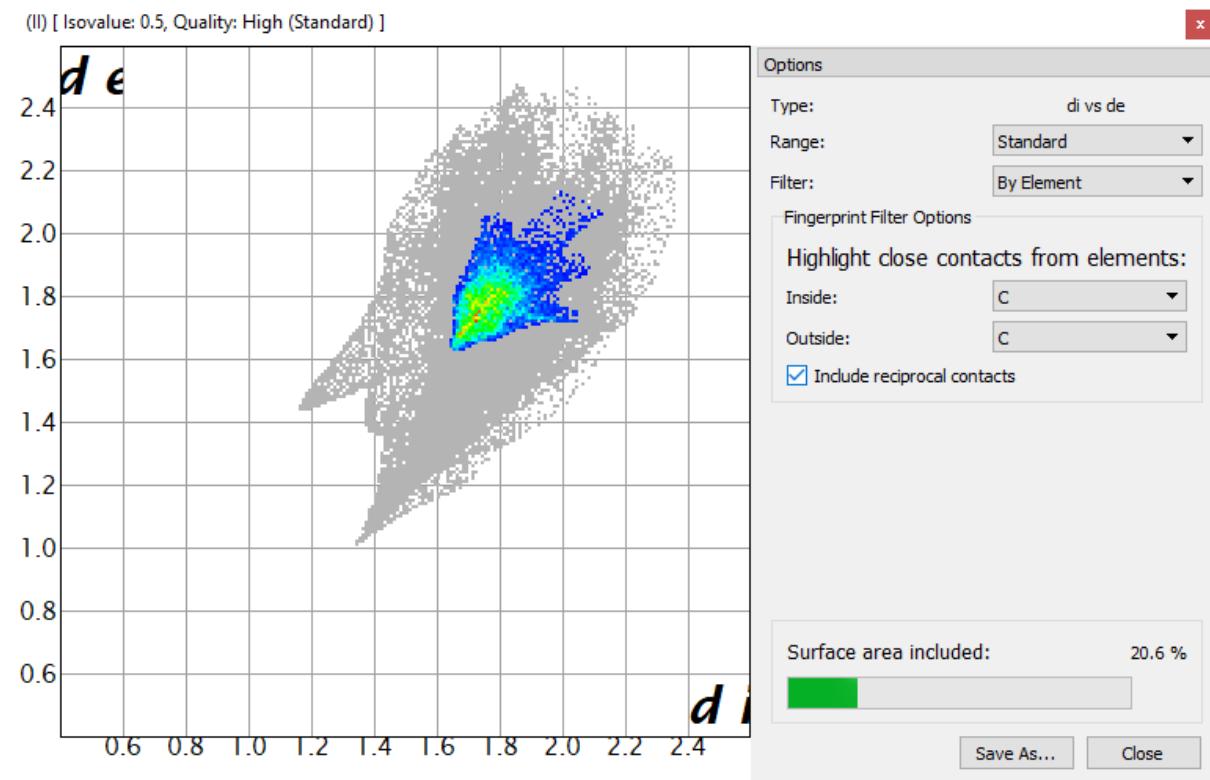


(II) pmda molecule 2 in ASU

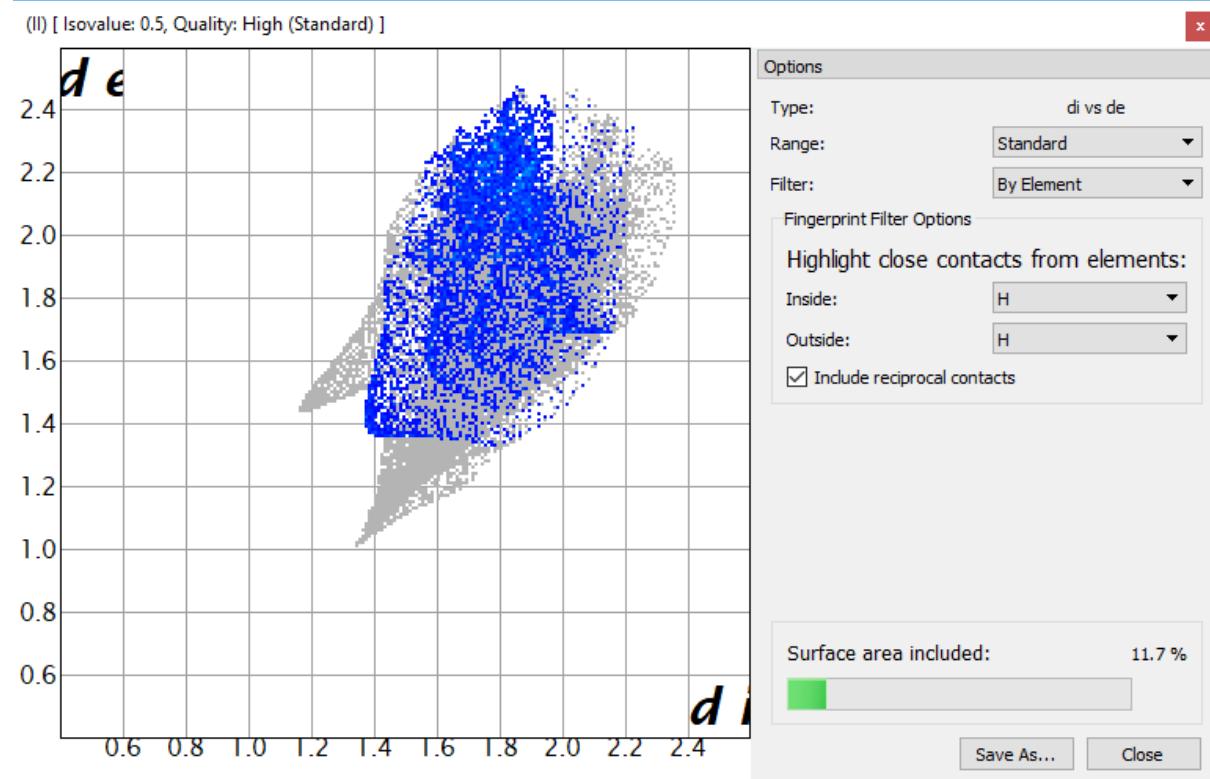
ALL: 100%



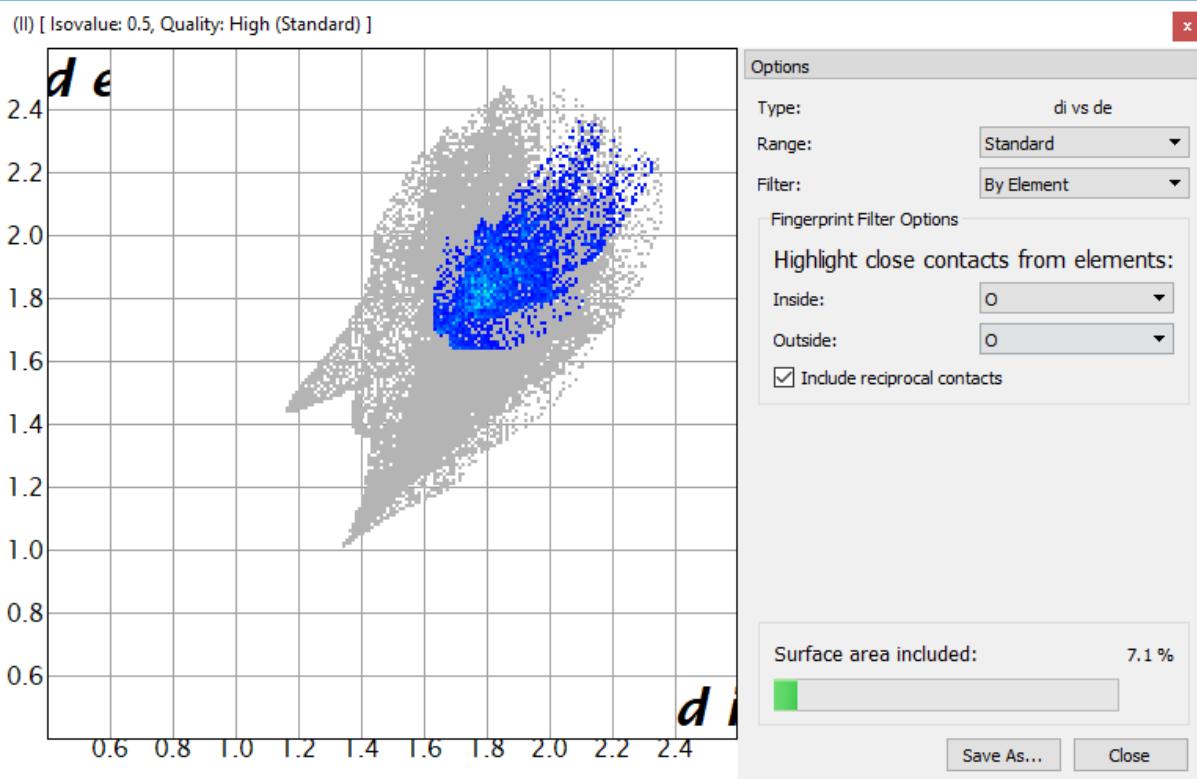
C-C: 20.6 %



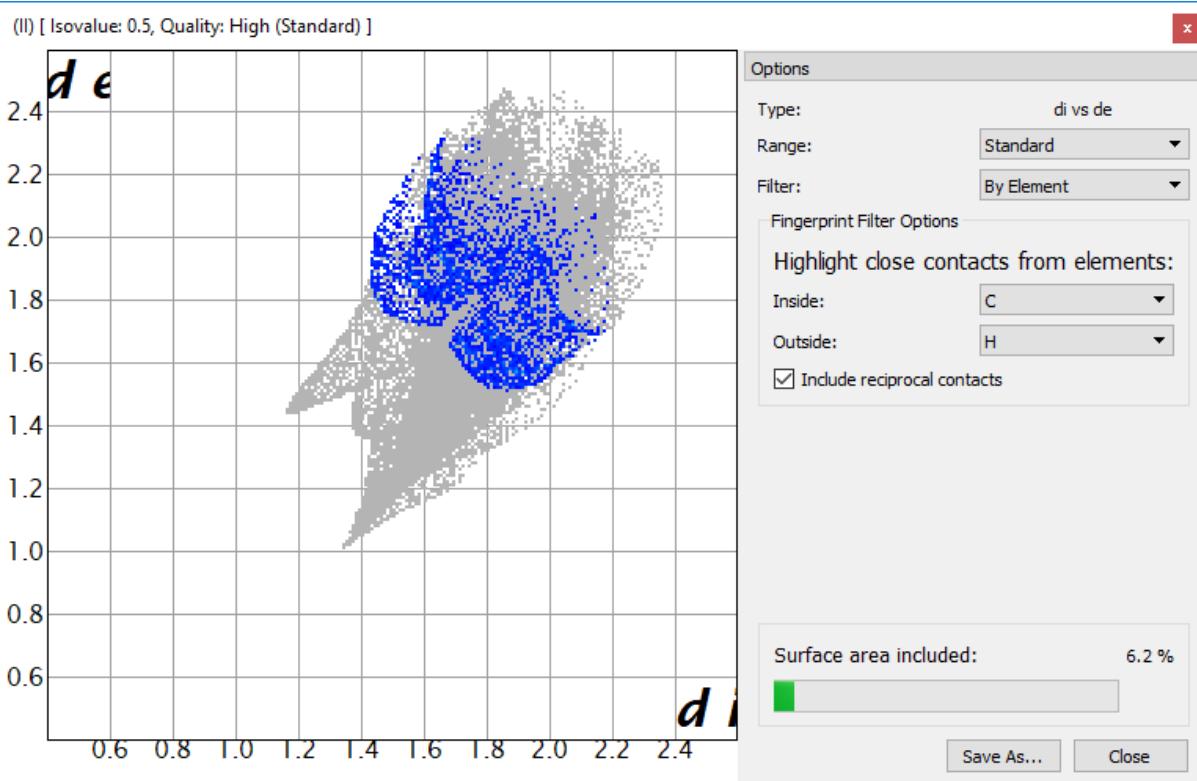
H-H: 11.7 %



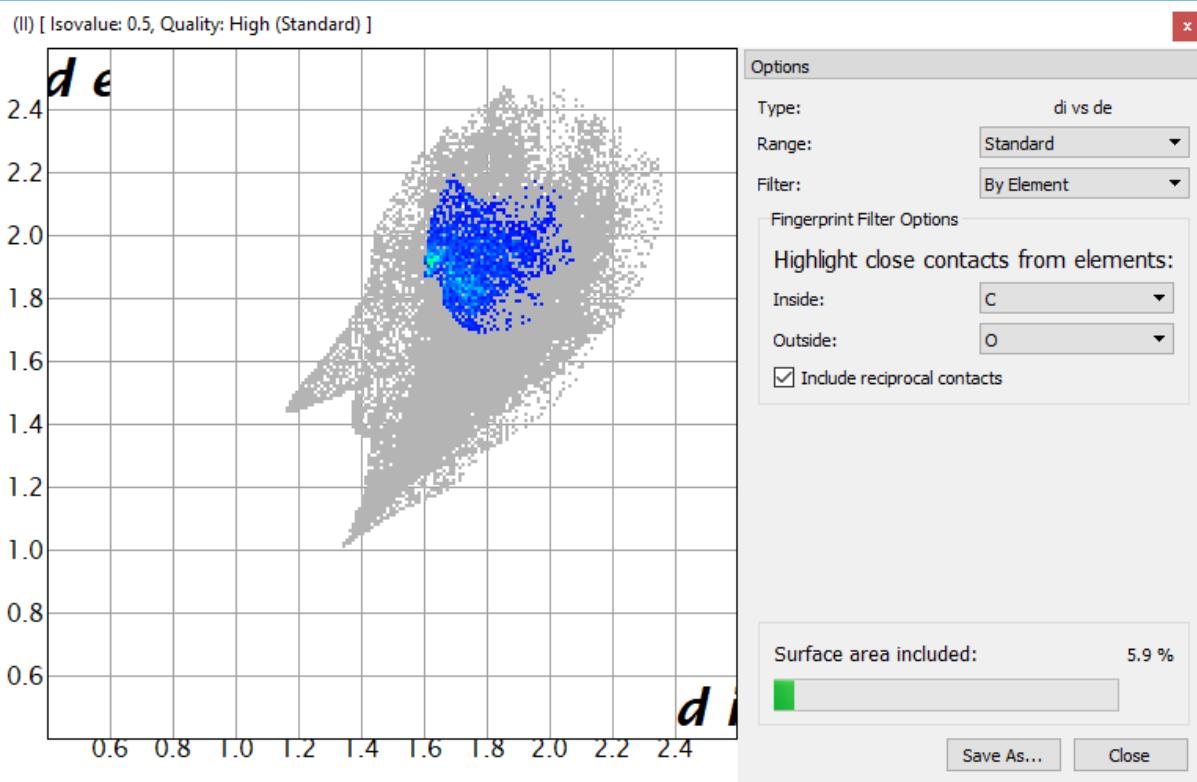
O-O: 7.1 %



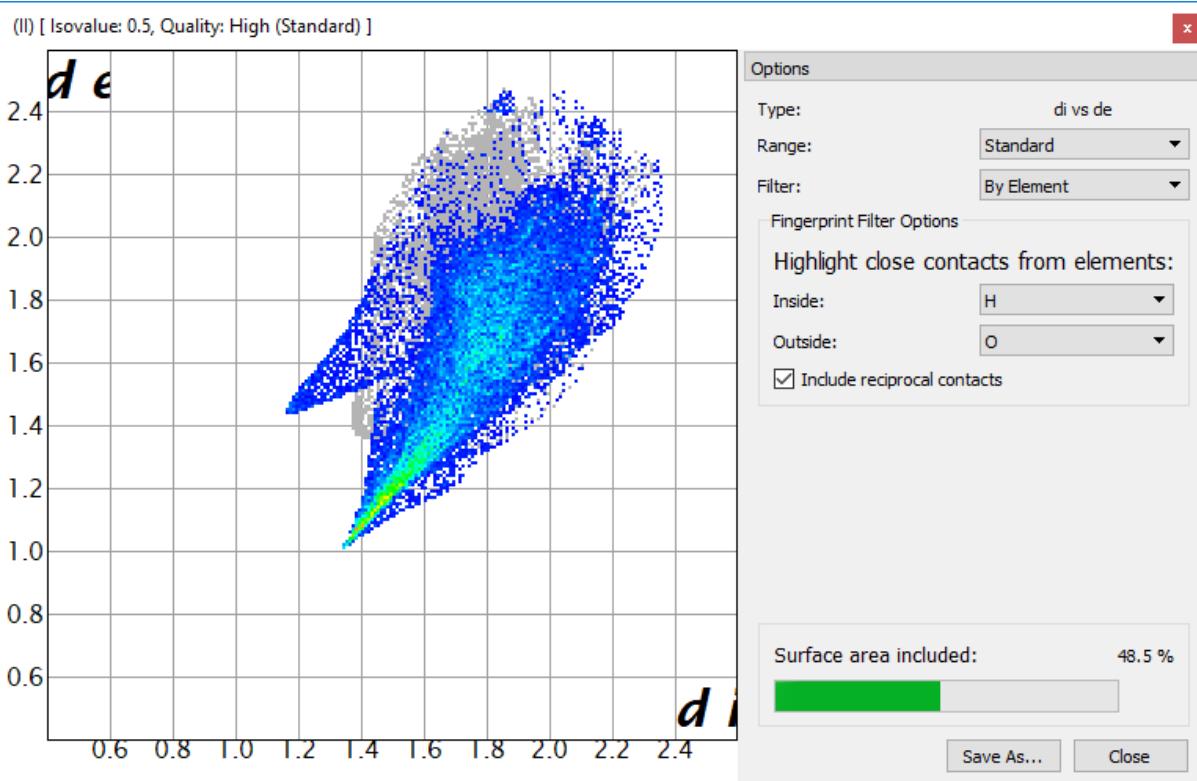
C-H: 6.2 %



C-O: 5.9 %

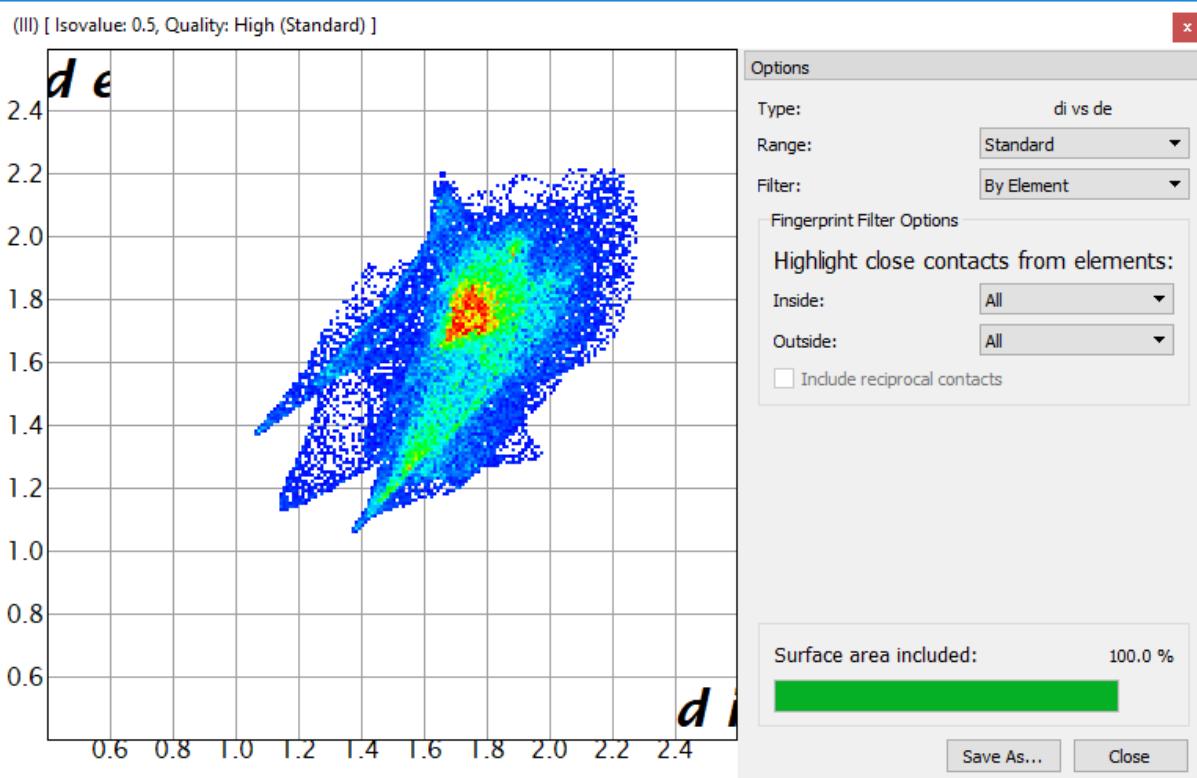


H-O: 48.5 %

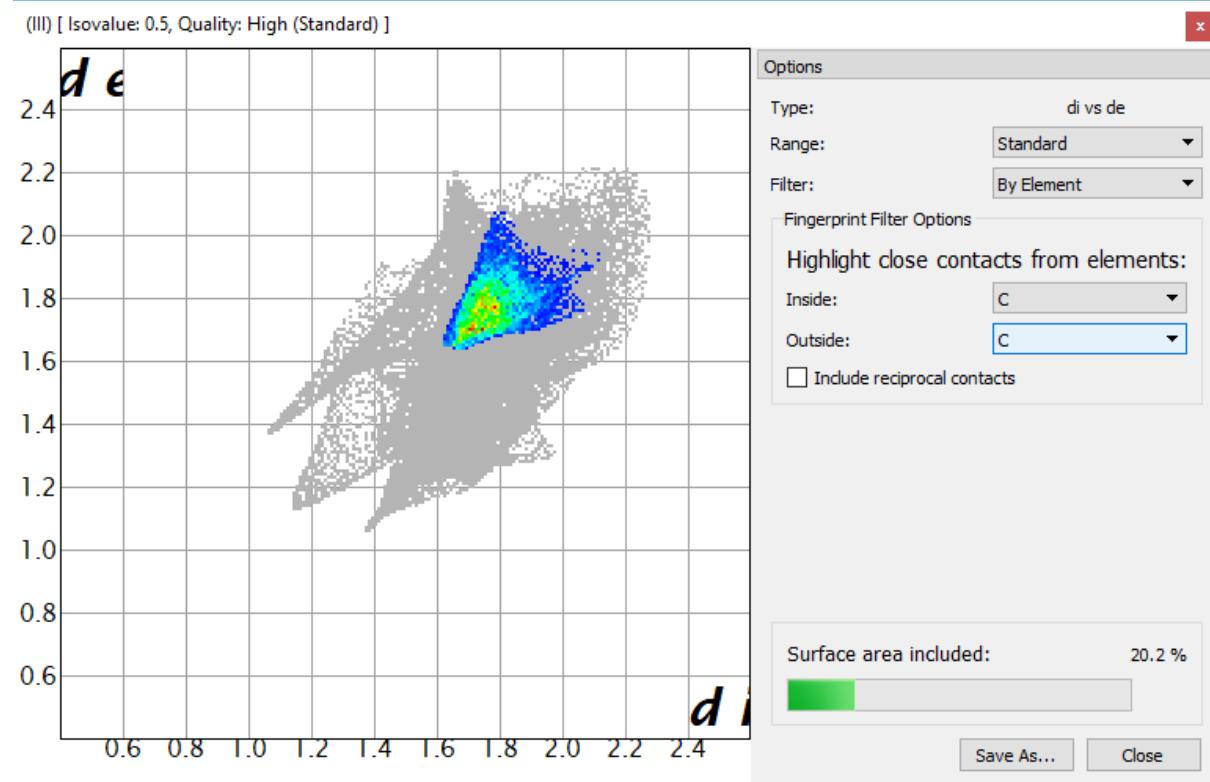


(III)

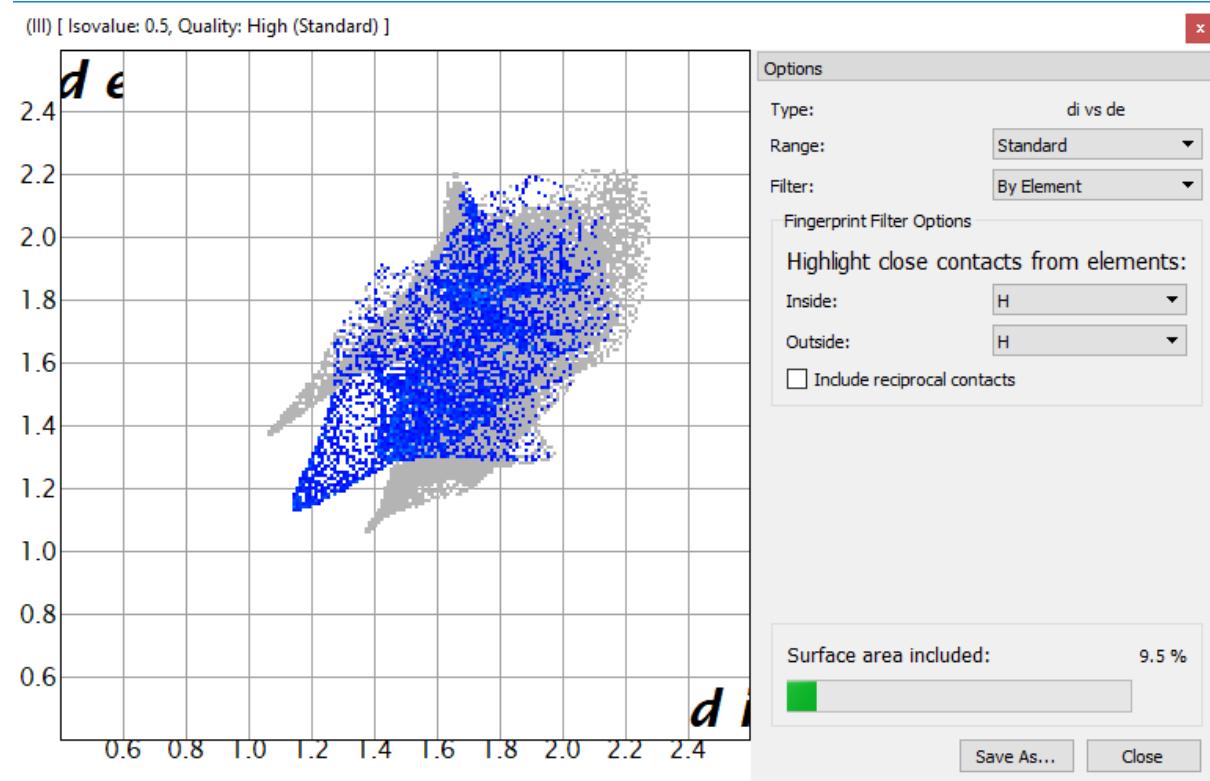
ALL: 100%



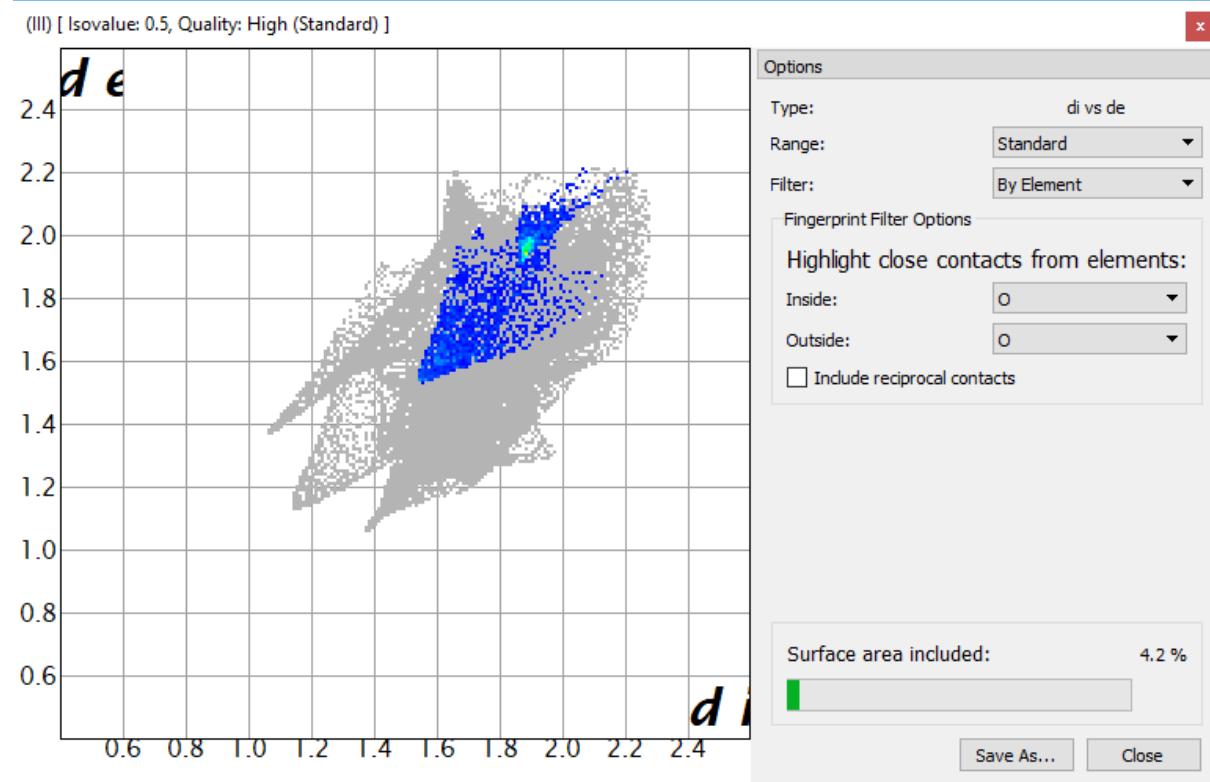
C-C: 20.2%



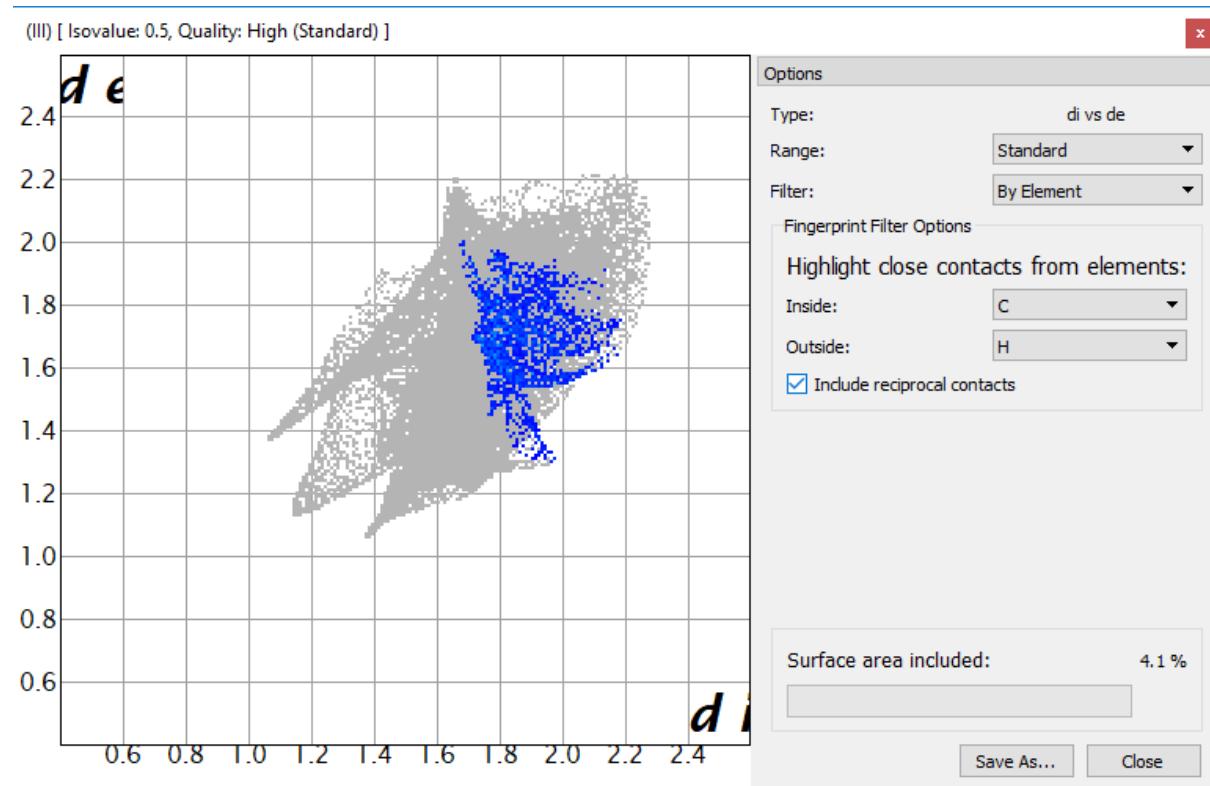
H-H: 9.5%



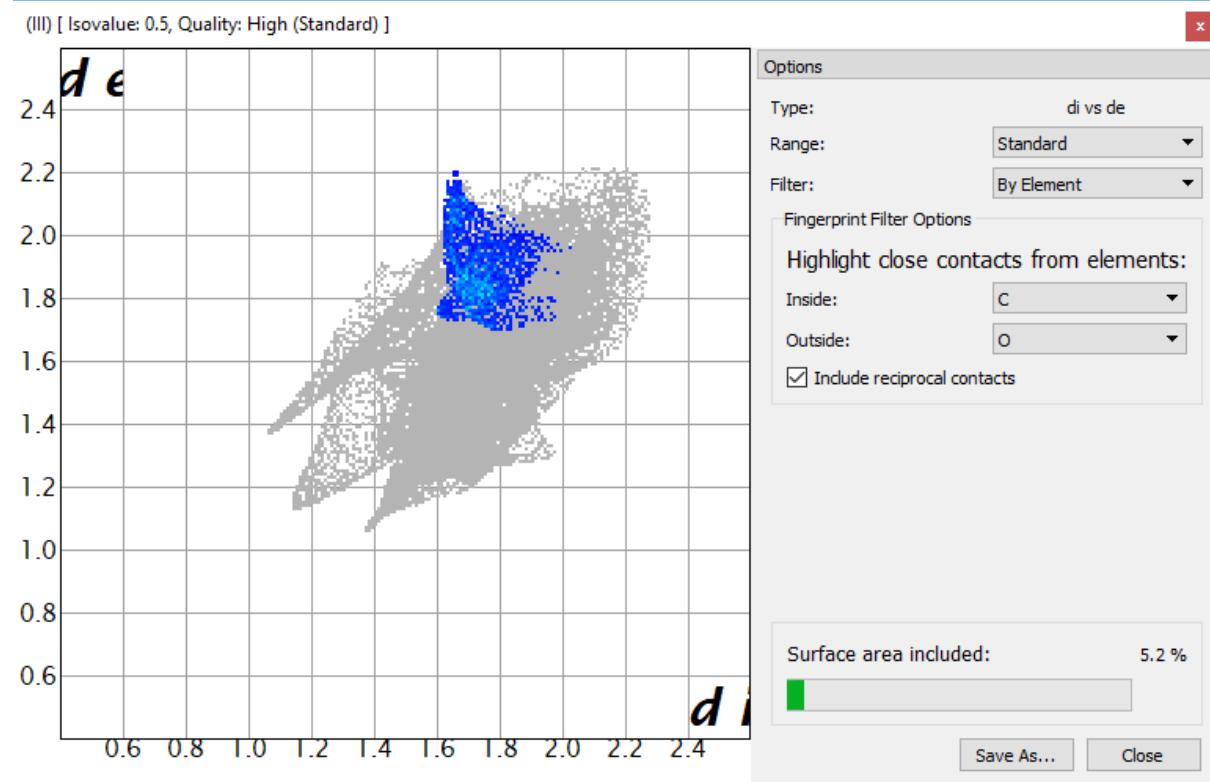
O-O: 4.2%



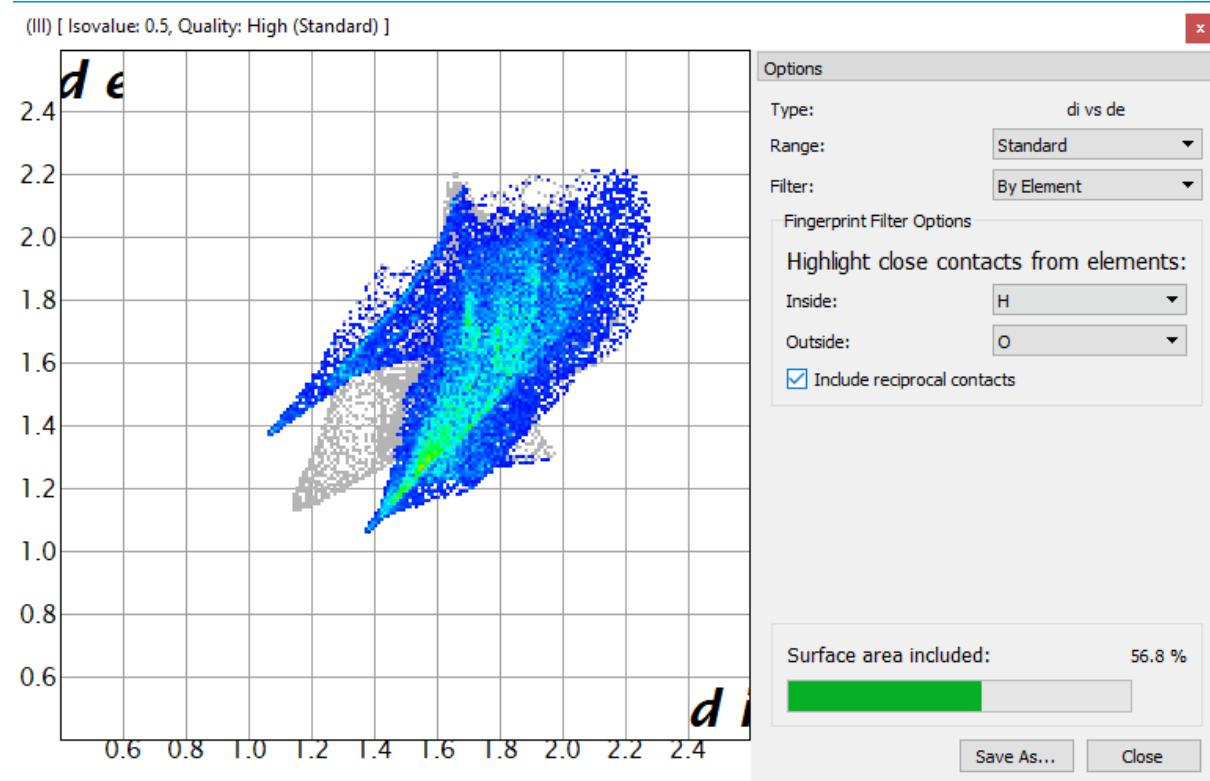
C-H: 4.1 %



C-O: 5.2 %

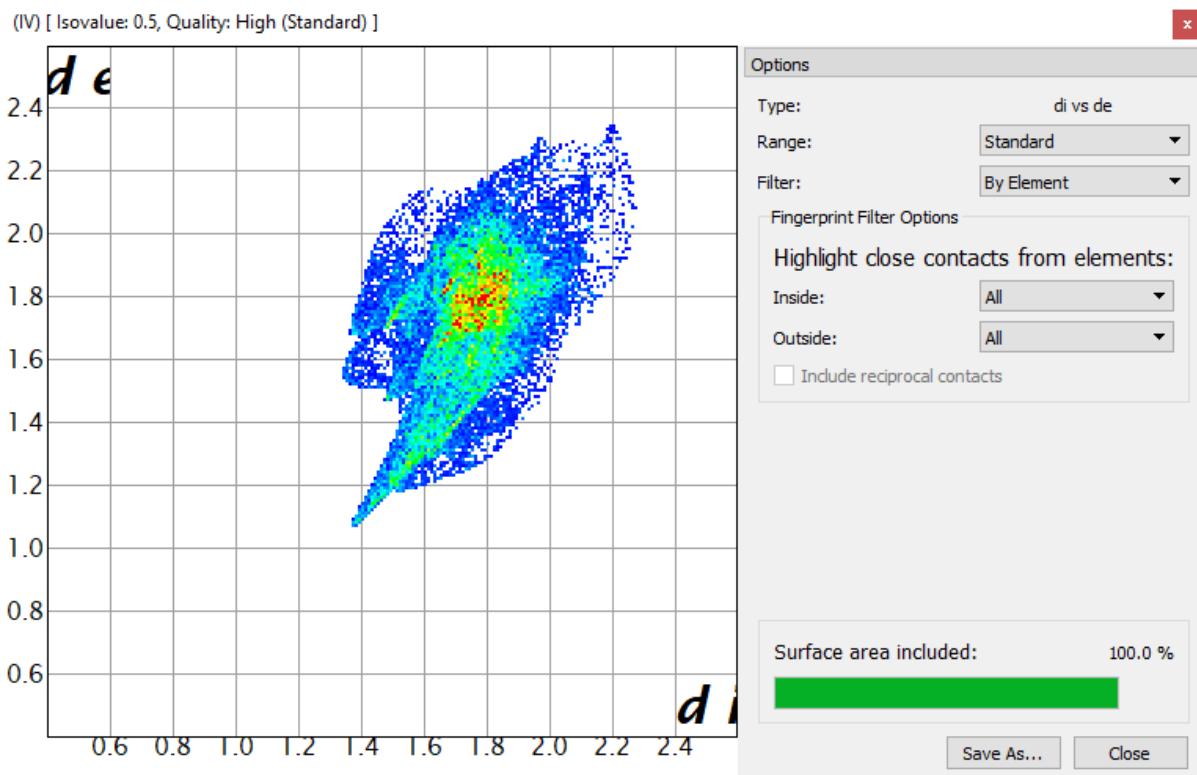


H-O: 56.8 %

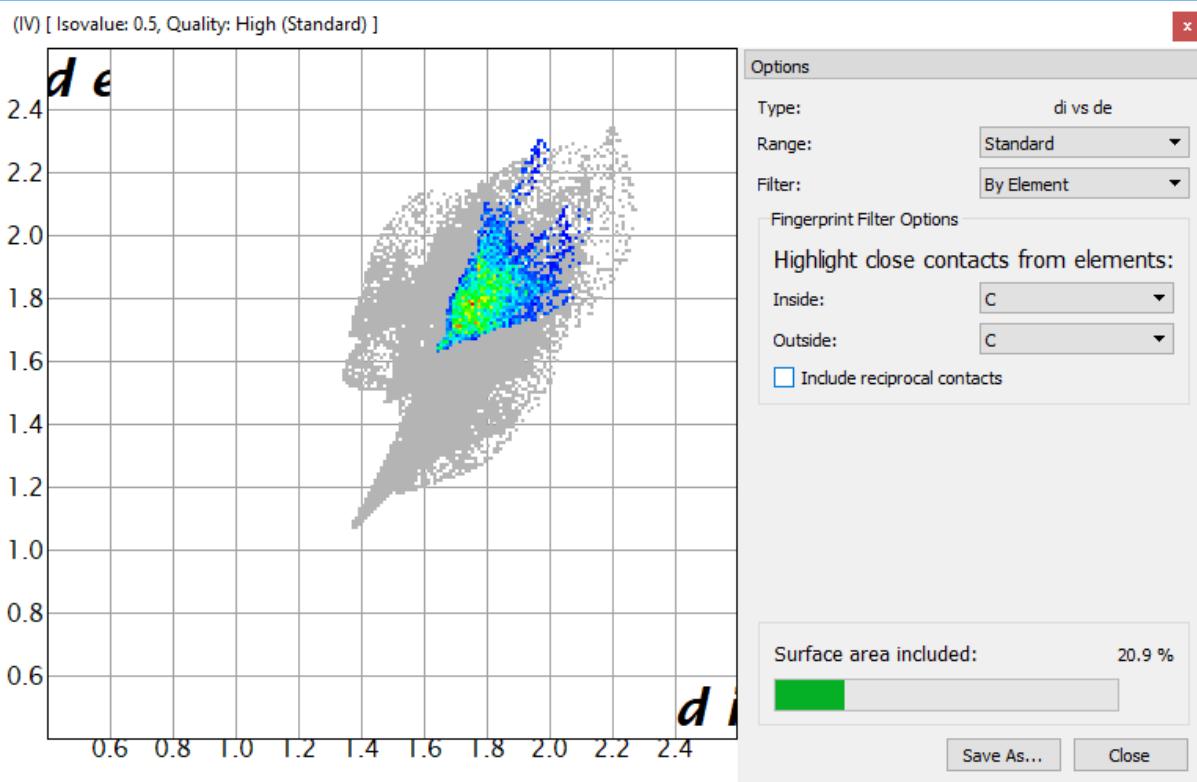


(IV)

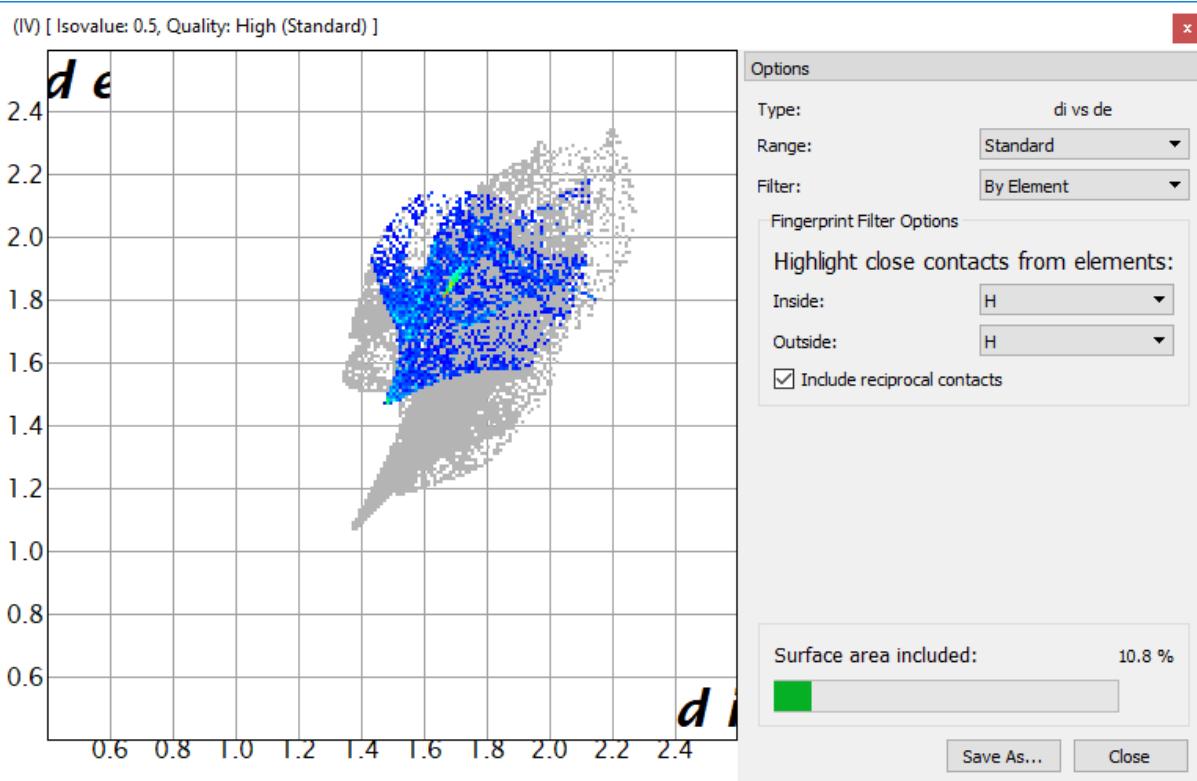
ALL 100%



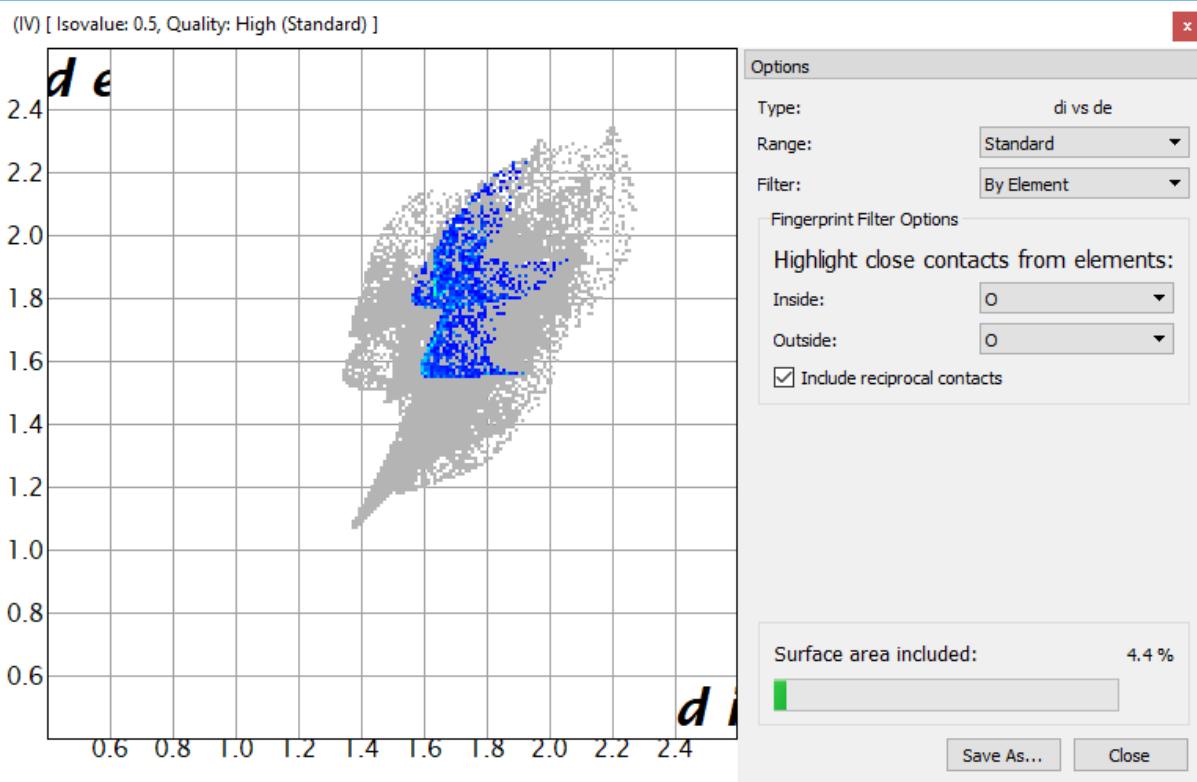
C-C: 20.9 %



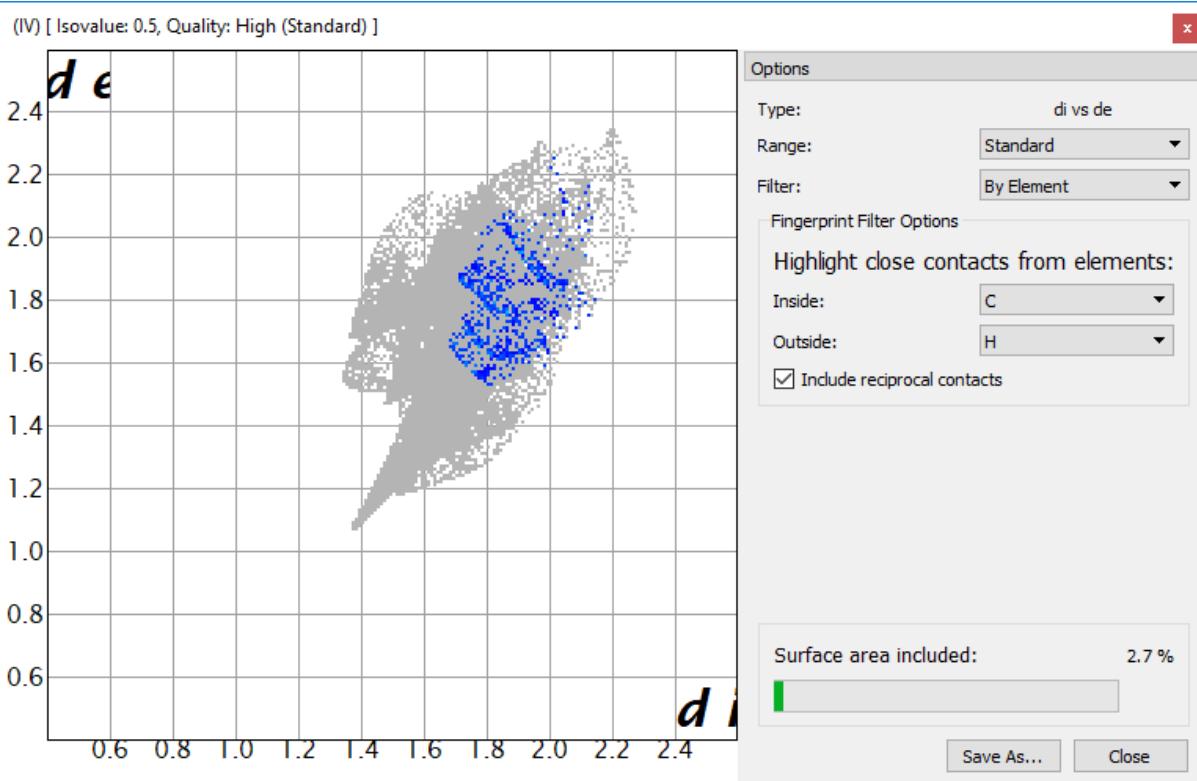
H-H: 10.8 %



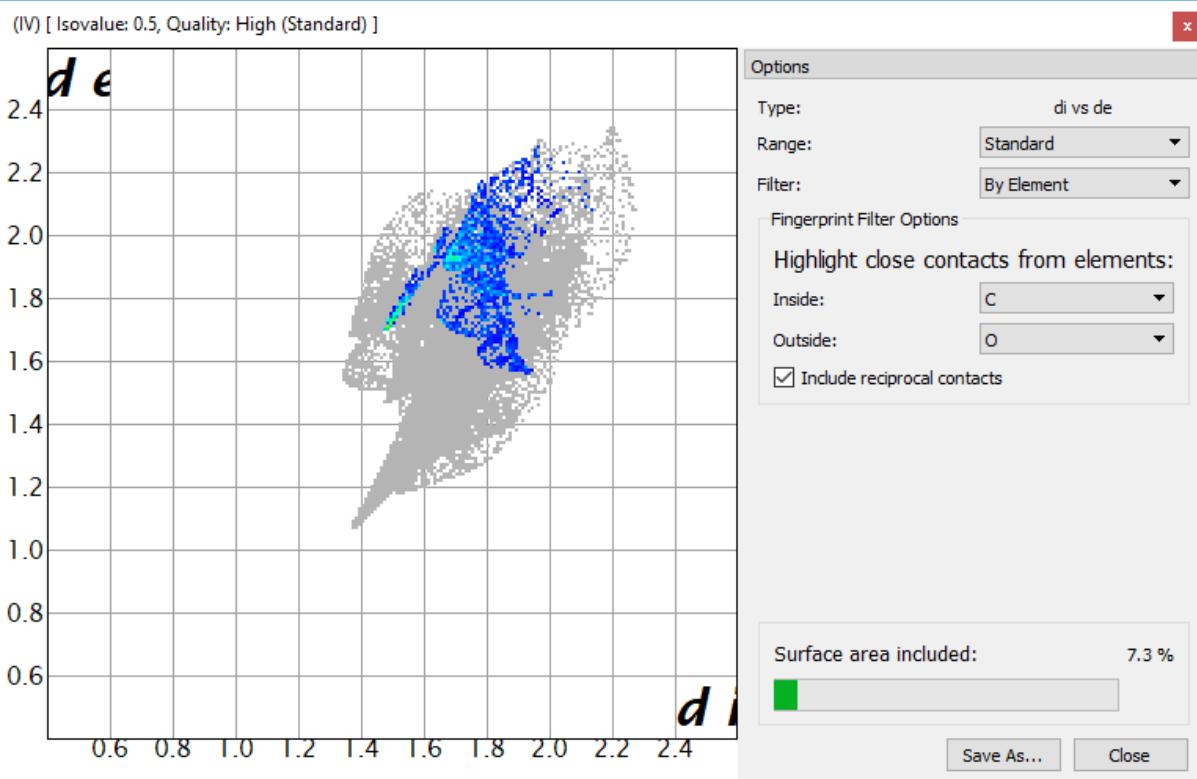
O-O: 4.4 %



C-H: 2.7 %



C-O: 7.3 %



O-H: 53.9 %

