

**IUCrJ**

**Volume 2 (2015)**

**Supporting information for article:**

**Likelihood of atom-atom contacts in crystal structures of halogenated organic compounds**

**Christian Jelsch, Sarra Soudani and Cherif Ben Nasr**

# **Supplementary Materials**

Likelihood of crystal contacts between chemical species  
for halogenated organic compounds.

Jelsch C., Soudani S. & Ben Nasr C.

List of compounds retrieved from the Cambridge Structural Database included in each family of molecules.

## **LIST of CHCl aliphatic compounds**

SEGWIK HCCYHE01 PCLCHX10 PEDGAI GOGXEF OCLOCT XOQLAR XILWEU  
PCCHLD TOCTCD ZAJLEB TEVQAN RIFWIM RIFWOS TUWBOC HEVNAX  
CADINC01 REZHIO FITVIN LESXOY YOCVUI RIQTOA GIQHIX RIQTUG

## **LIST of CHCl aromatic compounds**

PNCLBZ TCLBEN02 TCHLBZ ABUMIT DCLBEN01 MCBENZ YAFHUI TCNAPH  
DCLNAQ DUXRAP HCLBPH IRUYIE KASJIY POGNUU DAWRUO FUHDAN01  
GUQYOG DCLBIP SIFGIX DCLANT10 DMCPAY FIXWUE ZZZBLP01 CTCLST  
QQQFED02 LUXPUQ LIYPOZ FAHTEO FECZOE OVIRAN NEHZAD ELINUI

## **LIST of CHF aliphatic compounds**

AMECIE OCFCHX10 ADAREE BOMJIW DEZDUH DABLIB TELSEI TELSAE  
QEFDIO

## **LIST of CHF aromatic compounds**

CUWYUP FACJAU ZELDOJ PUGDEB PAVVAWA01 FACFOE FAGGEV FACFAQ  
AXUBUR01 AXUCEC01 CAXNUL DFNAPH10 FLNAPH BAWPUK FELLOY DEXWOU  
SERTOA DARXOK ATEVEB SETTOC AXIDER APUDEV

## **LIST of CHBr aliphatic compounds**

BROFRM05 BAVJUD GOPNEE FOXJUY IFOKOD IJUHAX FEHCOK EVEYAG  
BAHZEP HESCUD BATYUR BATWUP DATPAQ FUTXUO HADKEC BCYLON10  
BHPCHD10 COGTUN DAQTUK FEXDIW FITVEJ DEZLEZ IZAMUR

**LIST of CHBr aromatic compounds**

TETBBZ02 DEXXAG QOLLOS BRNPHL COXLOQ DAWSEZ FUBPUO HIQQON  
REBMES DEFBIA HOYWIB SECHOZ SECTEB QQQFDS02 GEQPOJ CARJEM  
DOTRUA MEGTOI DAHNEF FAHTIS IVUJIT PORRAQ KUSMAN JOGMUO  
FABSIK10 GAVBUB OKANOE APOWOS

**LIST of CHI aliphatic compounds**

HEHVEX DICHEP VADBUY GIHUTIA QIBMOE KANGUB DITCDC WAHRAY  
WAHREC XIFCIA IPCUND WAHLUM BOBLAG XUPMIE GISWAH LEDYIE TANRAB  
XEPPAJ IMTCOS

**LIST of CHI aromatic compounds**

REBBEG REKYAI TIGGUI ZZZPROO01 SOYGET POWNEV SAQZOY01 BOBGUV  
JEVMON NIFHAM XAMBAP ZZZSLE01 IVUHEN EFALUU KUZFAN IVUHAJ  
KEGXEA LITBIA MEBCOL WUMVOQ

**LIST of C H Cl O aliphatic compounds**

CLACET02 LIQVOW DISZIO PAMPEY CLSUCC CDCDOX PRCHLA CLCYHX  
GANKIP CEFZIX CUGNUO CUGPAW CUGPEA CUGPIE CUGPUQ CUGQAX  
CUGQEB CUGQIF CUGQOL HOYCOO HOYCUU POPFUV CLDTOL PRCHLA

**LIST of C H F O aliphatic compounds**

MEWZOF VEVSIZ IPUNEN MIJPUQ SINYUK SITFOR POMXEV BUYKOW  
ESIFIV PIBXUT OYAGEB BAPFEF BAPFIJ BAPFOP BAPFUV BAPGAC BAPGEG  
BAPGIK BAPGOQ

**LIST of C H Br O aliphatic compounds**

BRMACA CURLEG EQUTOA SEDGOZ SAZSES WOCHIF WANNEE PUZNAA  
QERVIS QERVOY WUQDOC WUQDUI YIVNEX JINYOV VAHZEJ BRDTOL

**LIST of C H N Cl aliphatic compounds**

VITRUL FELPIV ETEYAE CLTRZL BOTYIT DCPYZ AMCPYZ GAPPIY NIKSIK  
PUGWEU NUNKUC QEDCAF UKIWOB PIJBOO HCZCHP PECTUO QEGRUN  
XIXREC DCHLAN01 IJUTUD

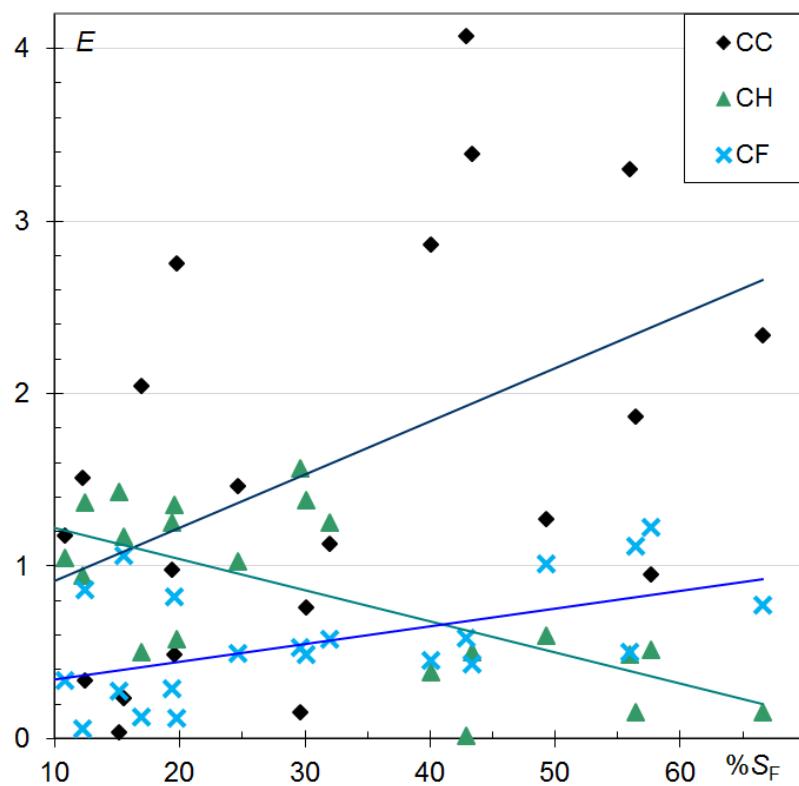
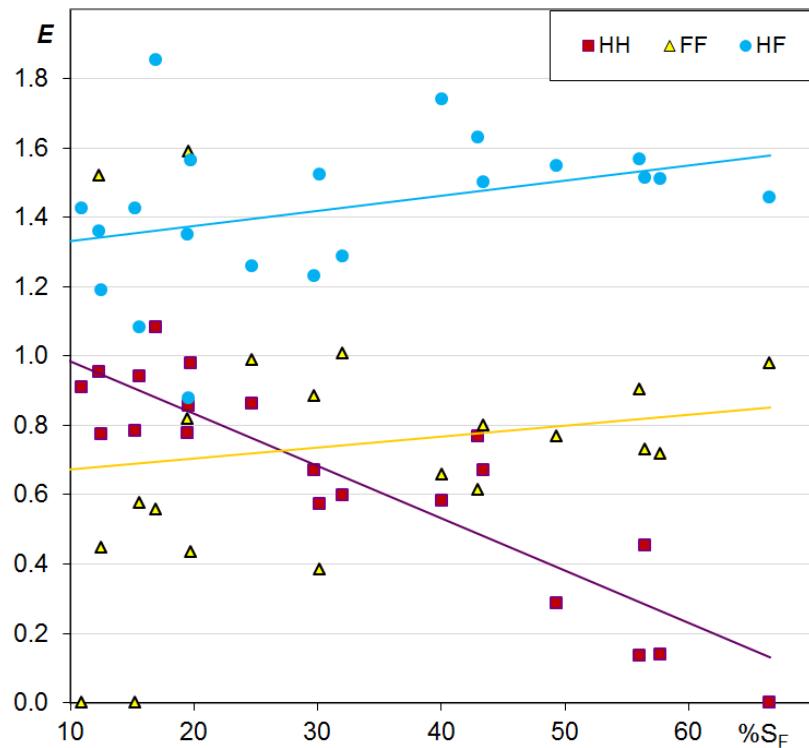
**LIST of C H Br Cl aliphatic compounds**

FEMLAK UROWEI VIOLAC DEKHAC VEQKOR SAFFIO YICLIF AFACIU MUKHUV  
WUGHAH HIJVIF IDOKOD

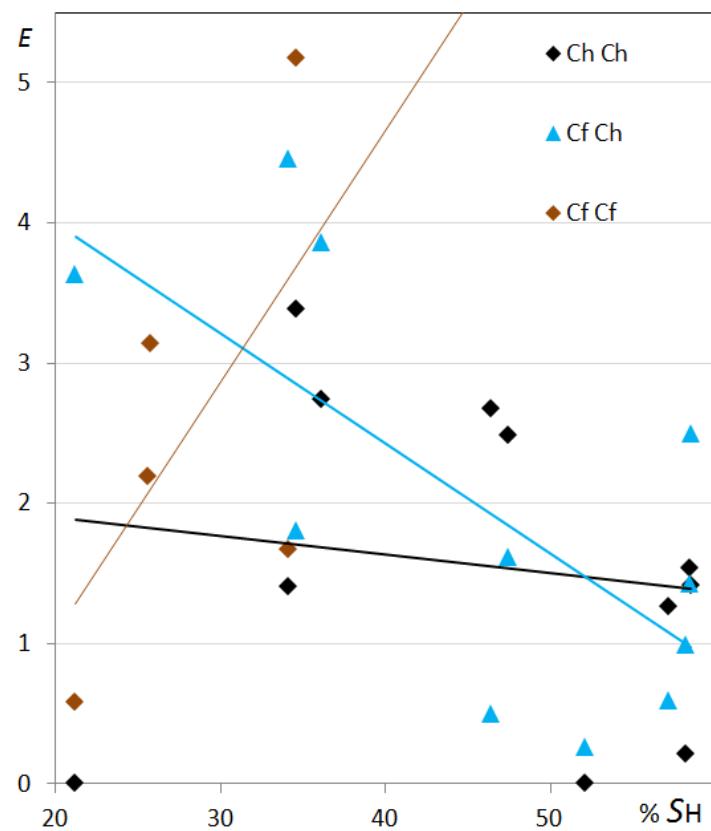
**LIST of C H F Cl aliphatic compounds**

FAVTAX XEZHAM XEZHEQ PICVUS KEQNAW JALLAK CLFBZD FPCLET  
GEFPAI

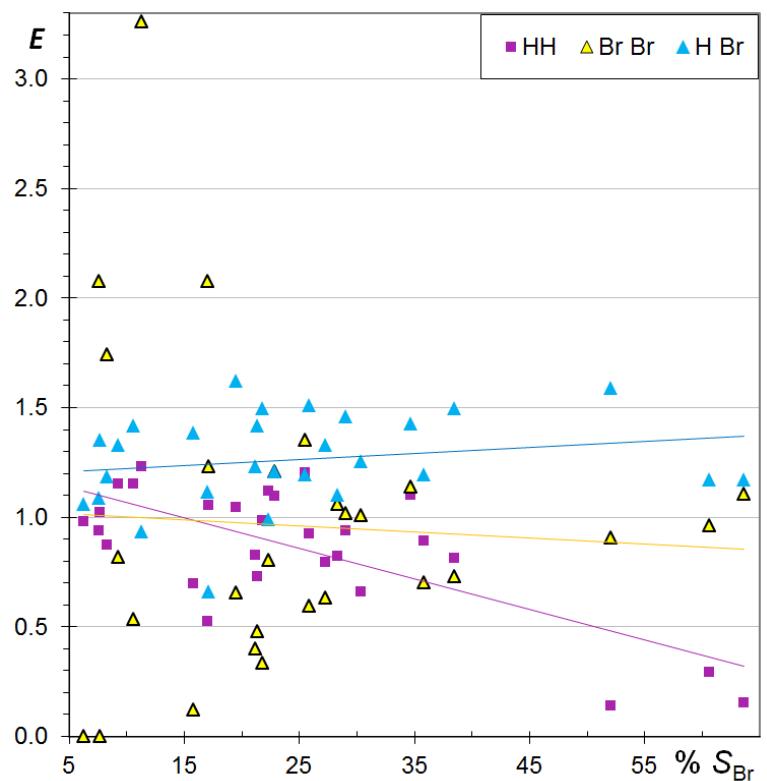
**Figure Sup1.** Enrichment ratios in CHF aromatic compounds as a function of fluorine proportion  $S_F$  on the molecular surface.



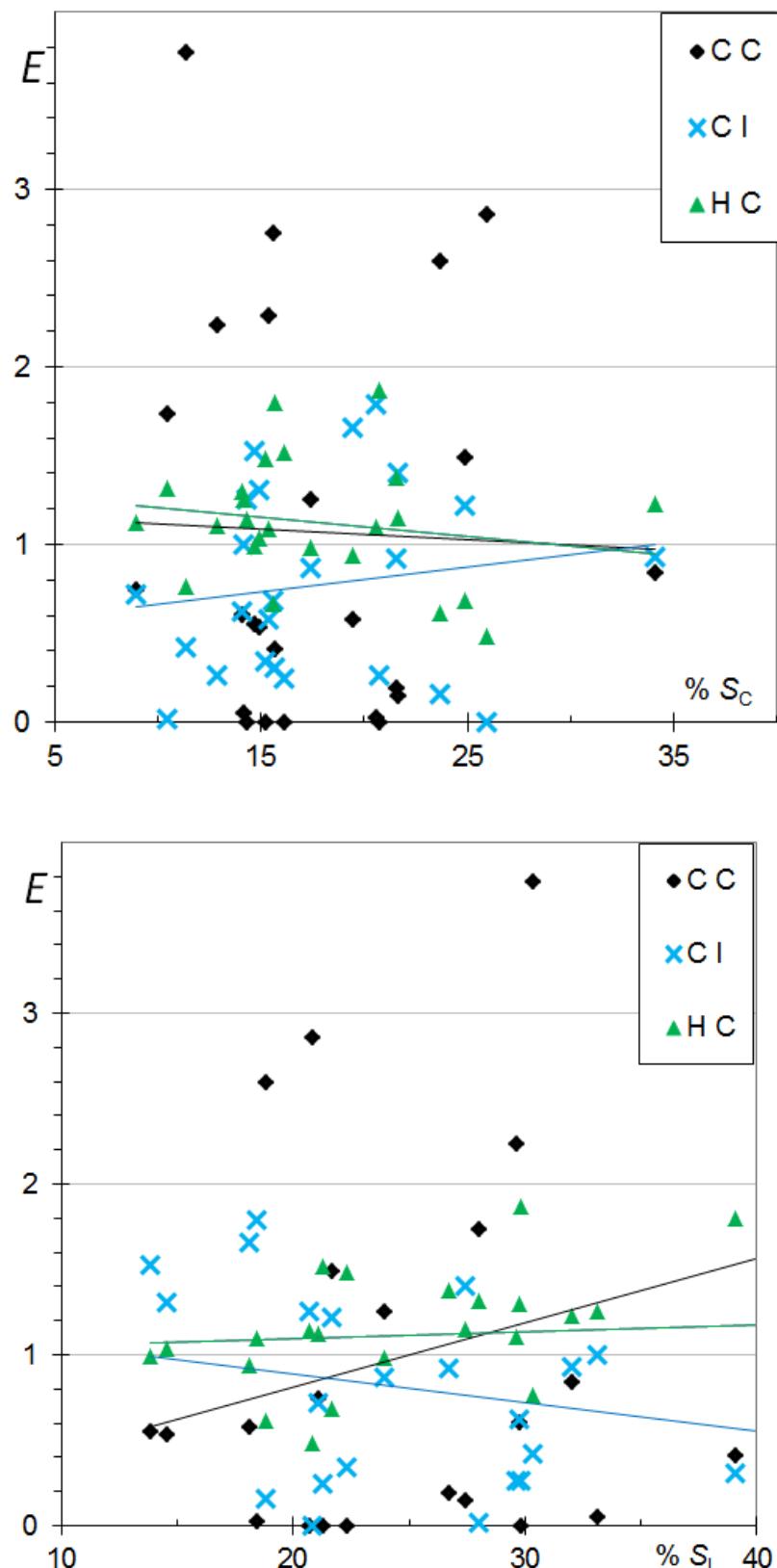
**Figure SUP2.** Enrichment ratios for the different C···C contacts in CHF aromatic compounds. Carbon atoms bound to F (Cf) or not (Ch) are differentiated.



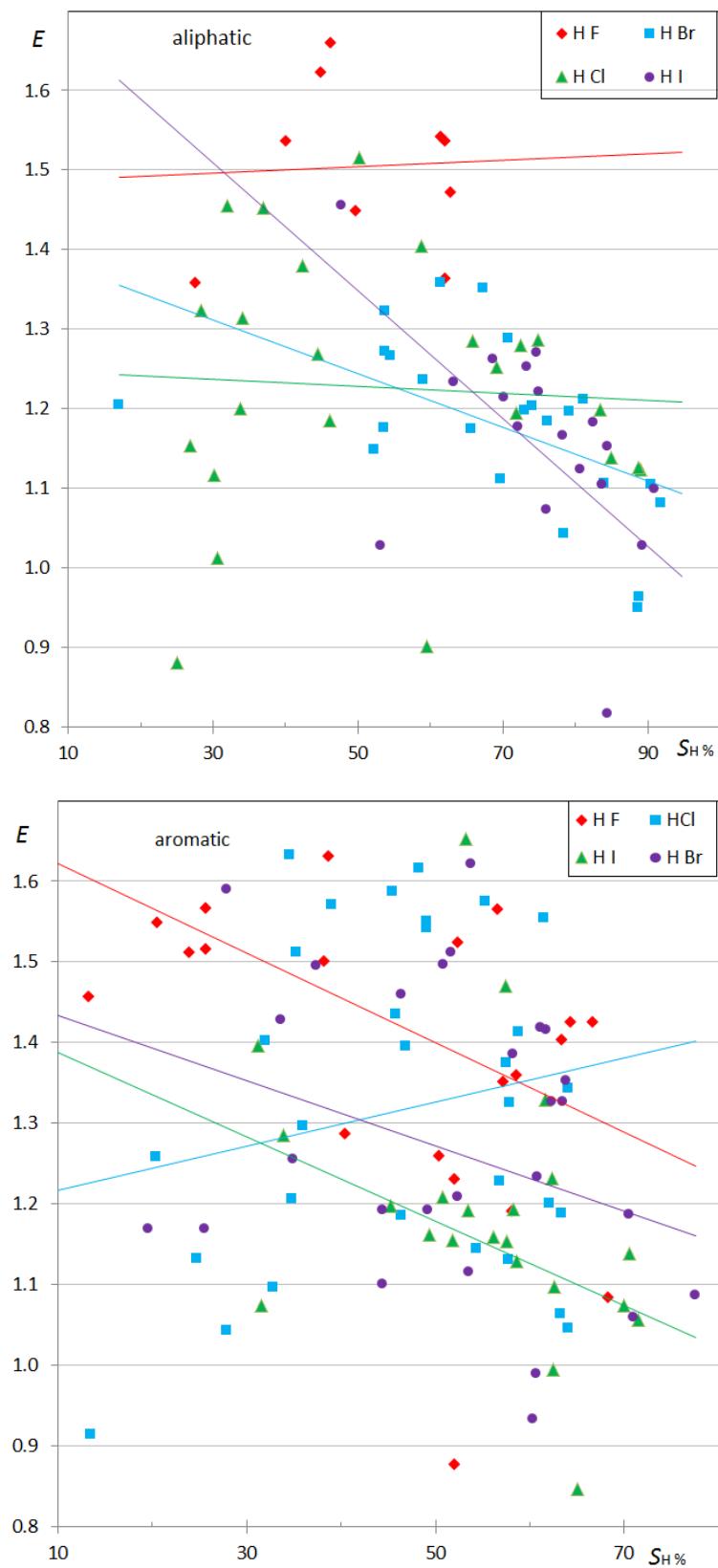
**Figure Sup3.** Alternative scatterplot of enrichment ratios in CHBr aromatic compounds as a function of bromine proportion  $S_{\text{Br}}$  on the molecular surface.



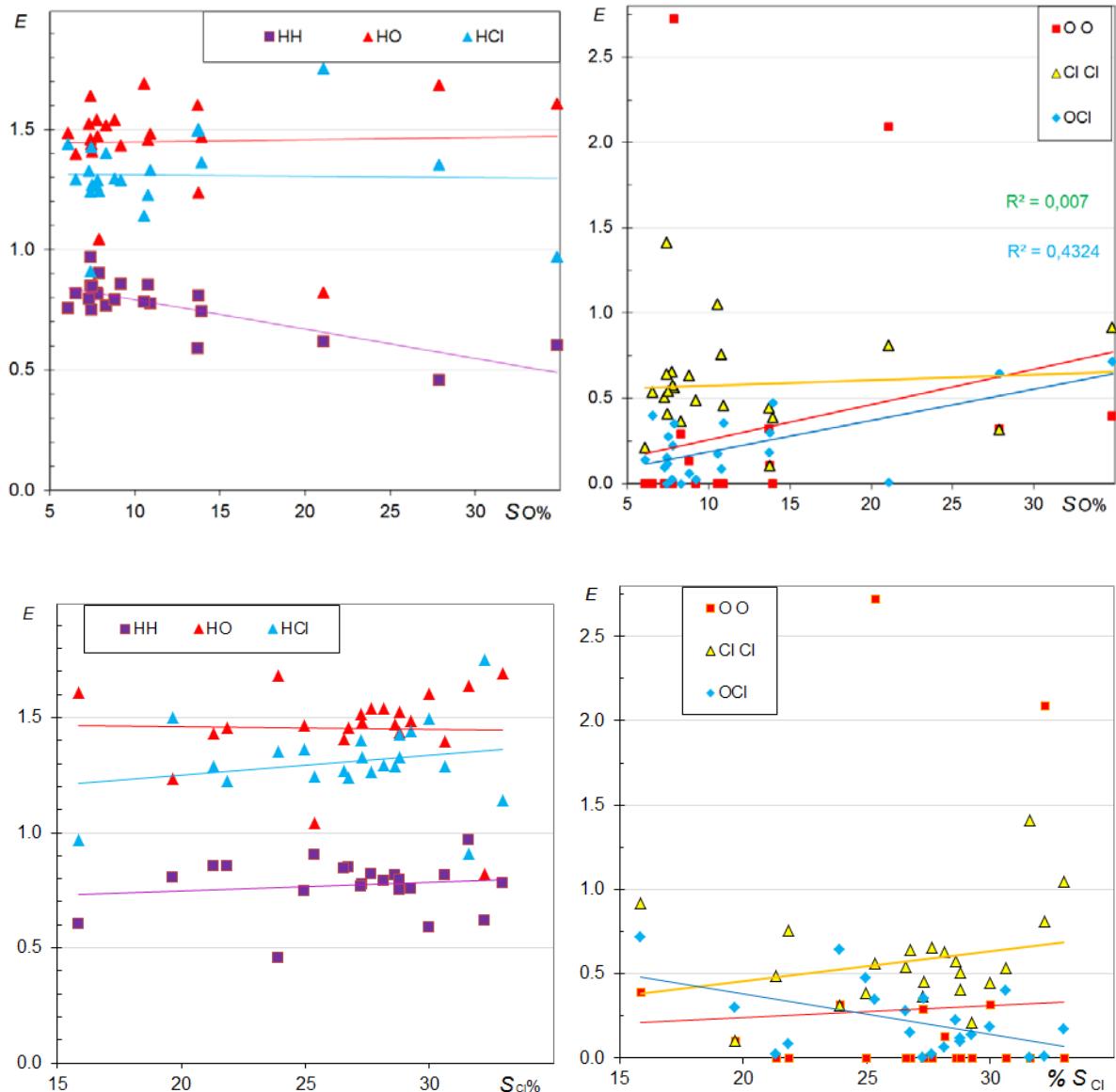
**Figure Sup4.** Alternative scatterplots of enrichment ratios in CH I aromatic compounds as a function of carbon and iodine proportion on the molecular surface.



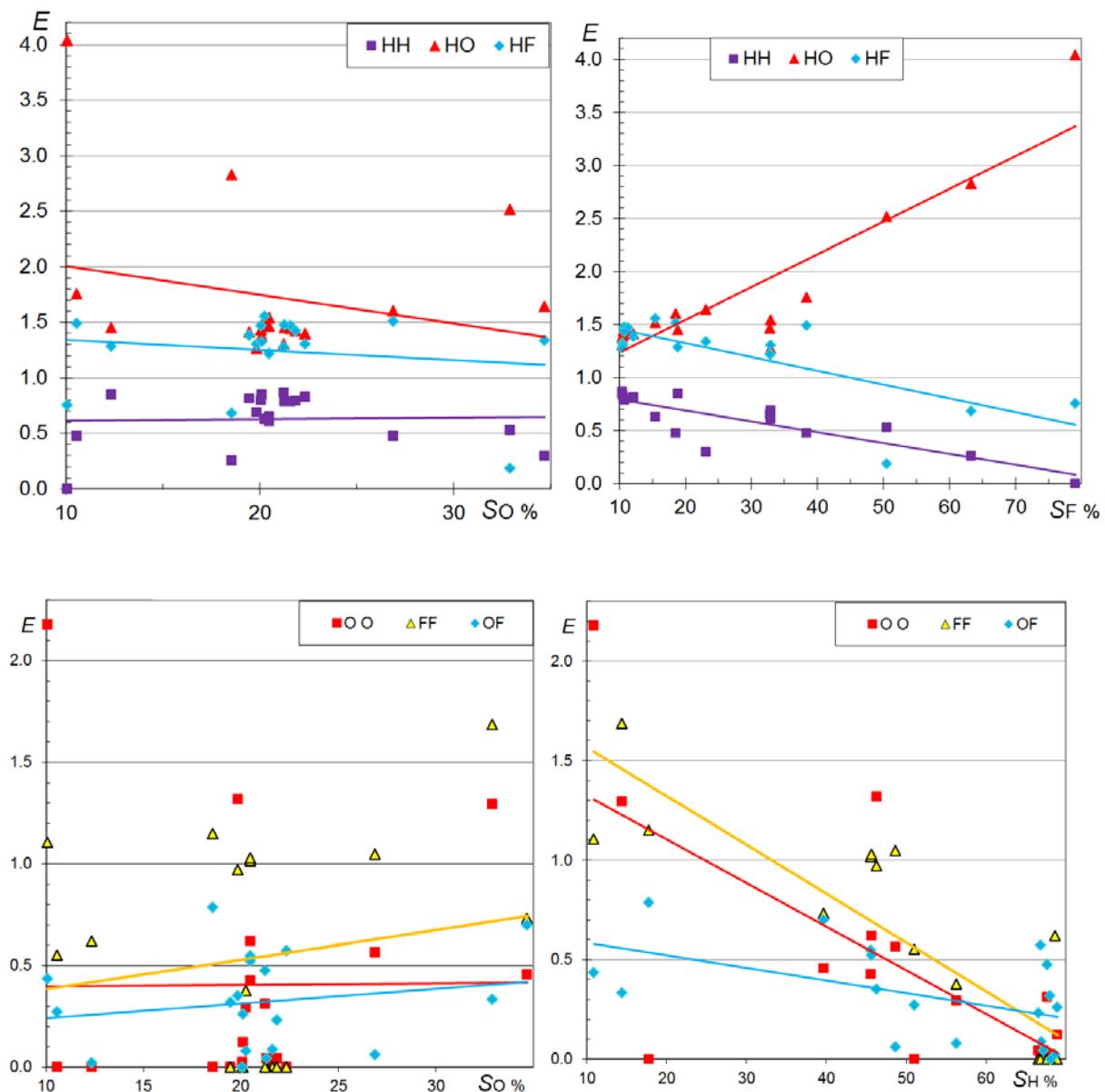
**Figure Sup5.** Comparison of hydrogen···halogen contact enrichment ratios in the different halogenated CHX compounds (aliphatic and aromatic).



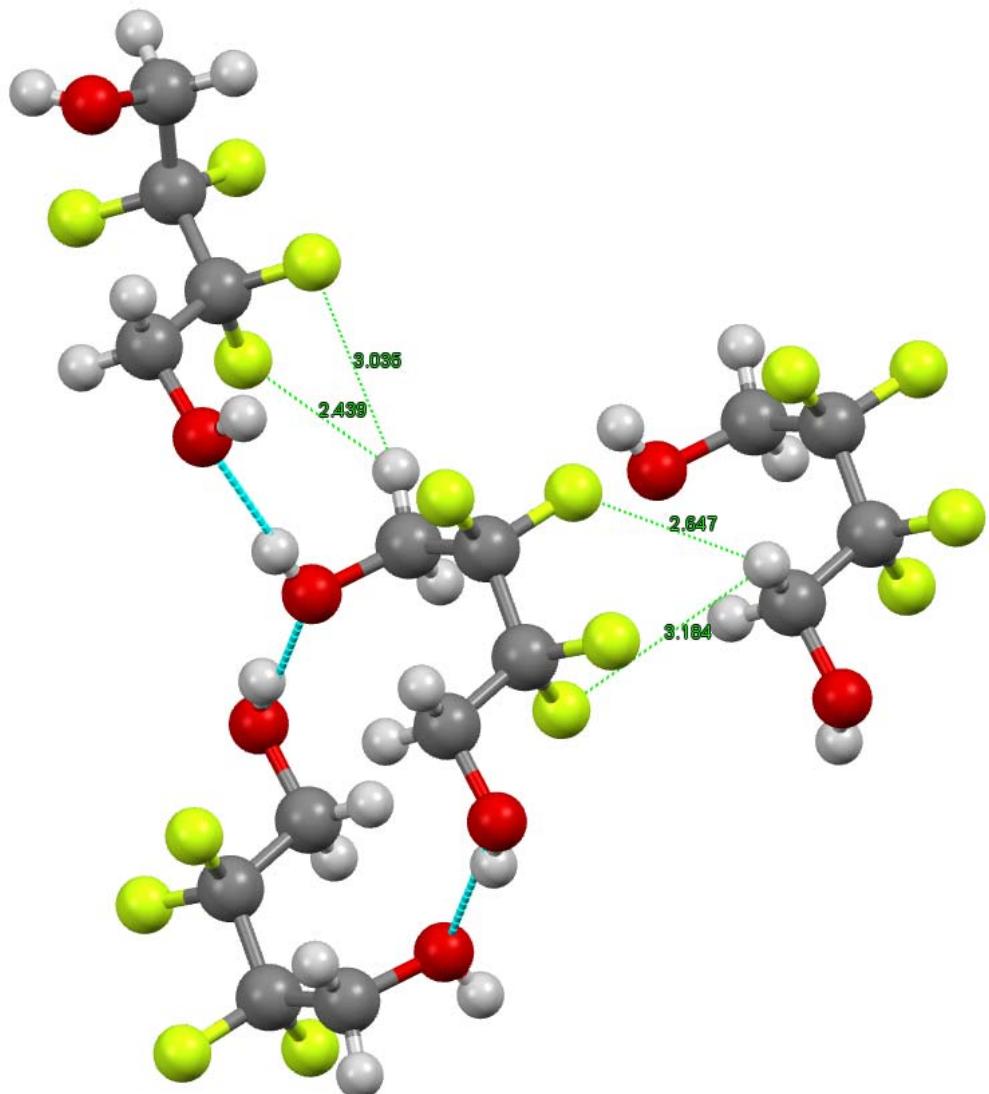
**Figure Sup6.** Scatterplots of enrichment ratios in C H O Cl aliphatic compounds as a function of oxygen and chlorine proportion on the molecular surface.



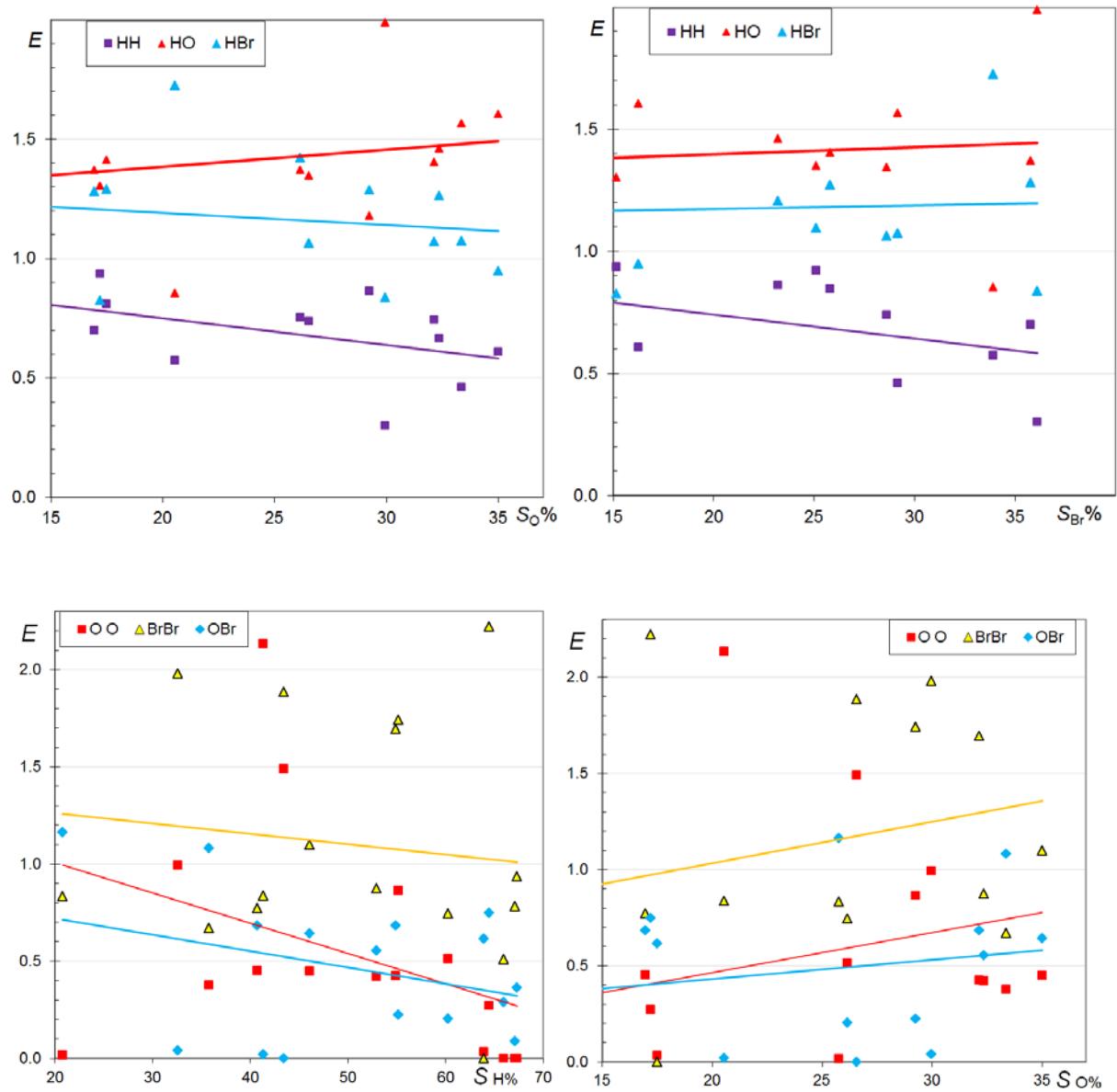
**Figure Sup7.** Scatterplots of enrichment ratios in C H O F aliphatic compounds as a function of oxygen and fluorine proportion on the molecular surface.



**Figure Sup8.** Preferential formation of O-H $\cdots$ O and C-H $\cdots$ F interactions in the crystal of compound 2,2,3,3-Tetrafluorobutane-1,4-diol (reference code POMXEV).



**Figure Sup9.** Alternative scatterplots of enrichment ratios in CHOB<sub>r</sub> aliphatic compounds as a function of different chemical proportions on the molecular surface.



**Figure Sup10.** Alternative scatterplots of enrichment ratios in CHNCl aliphatic compounds as a function of different chemical proportions on the molecular surface.

