

**Electronic Supplementary Information (ESI)**

**Crystallographic and computational investigation of intermolecular interactions involving organic fluorine with relevance to the hybridization of the carbon atom.**

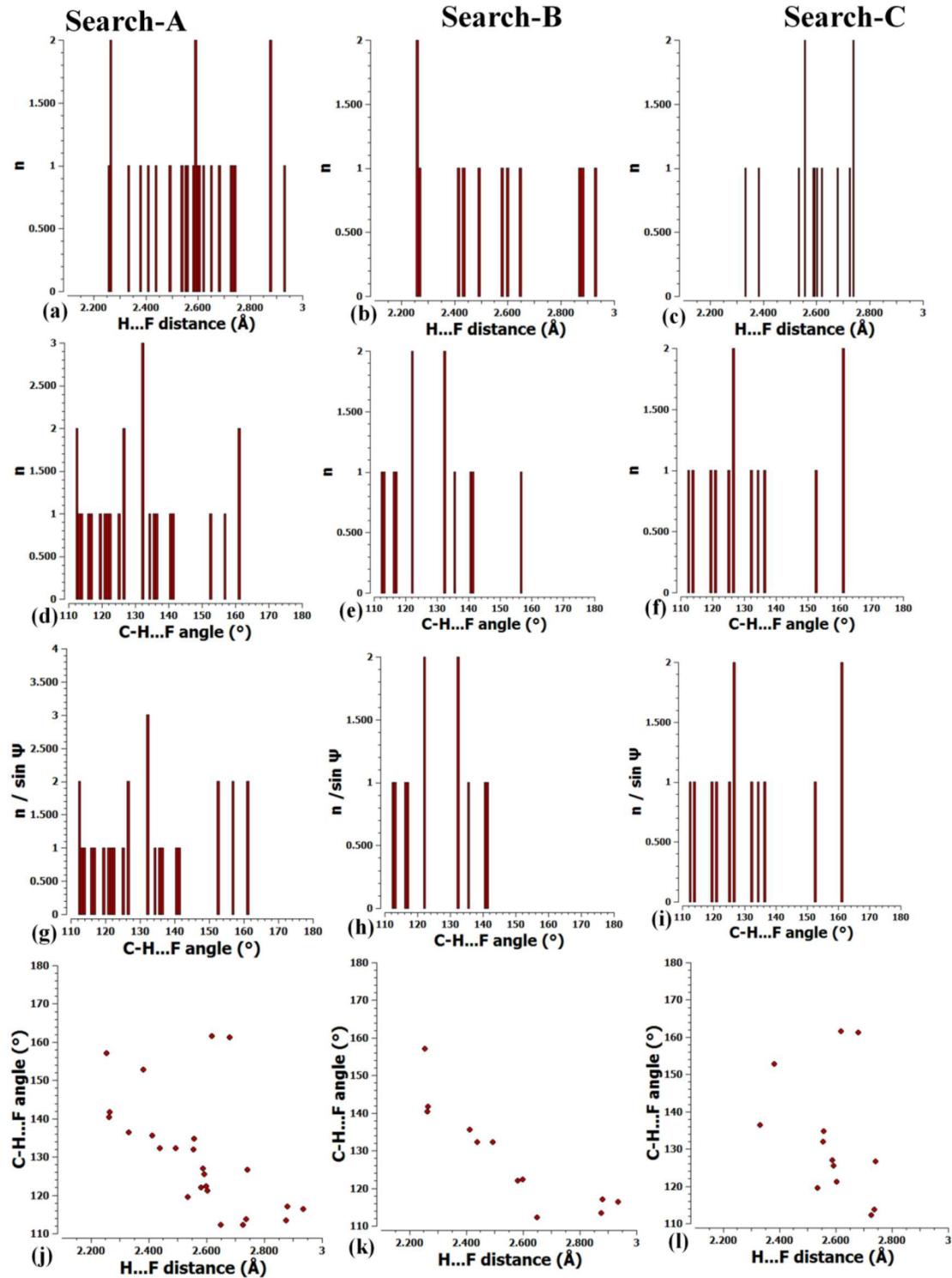
*Rahul Shukla<sup>a</sup> and Deepak Chopra\*<sup>a</sup>,*

*<sup>a</sup>Crystallography and Crystal Chemistry Laboratory,*

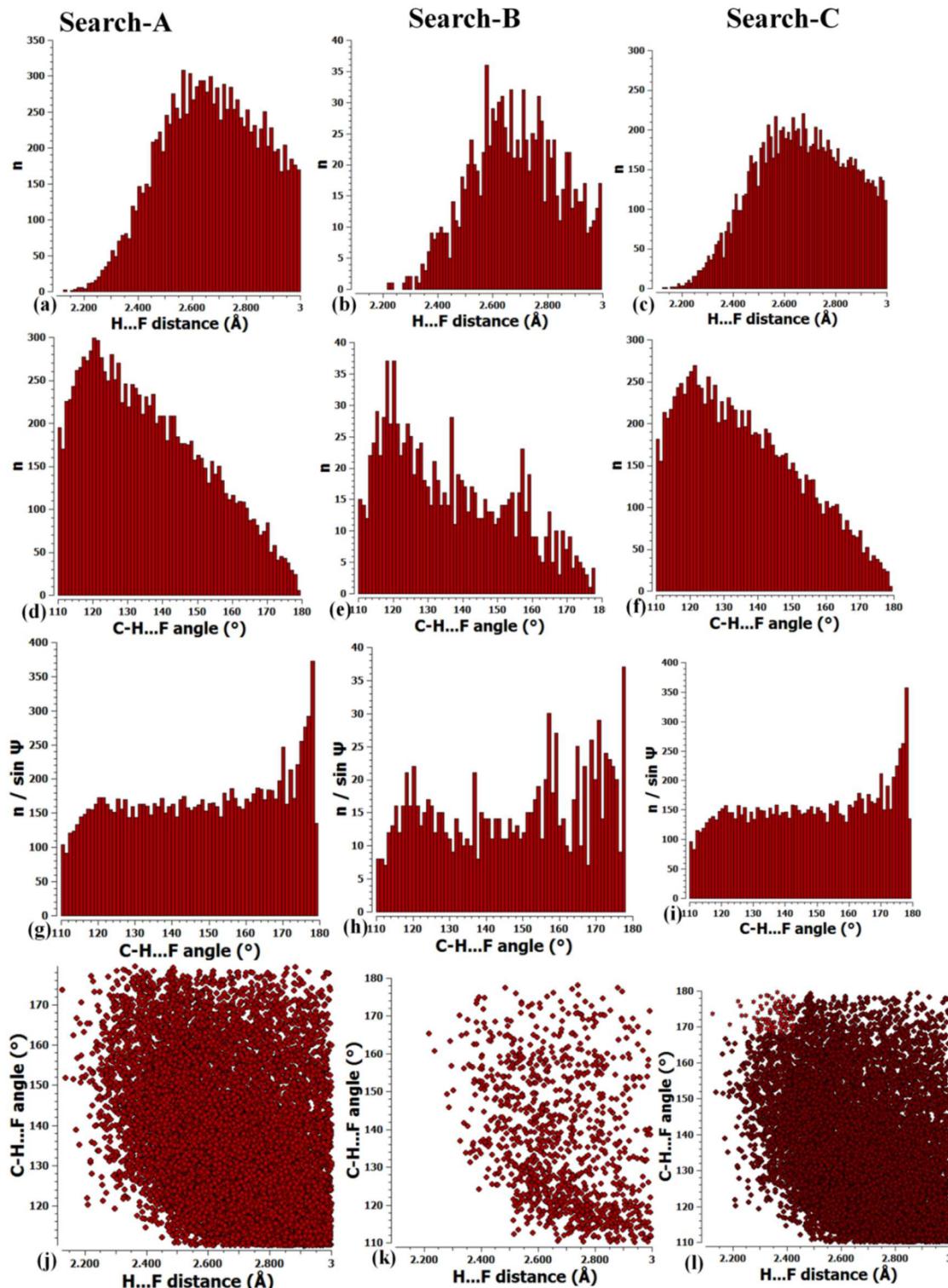
*Department of Chemistry, Indian Institute of Science Education and Research*

*Bhopal, Bhopal 462066, Madhya Pradesh, India.*

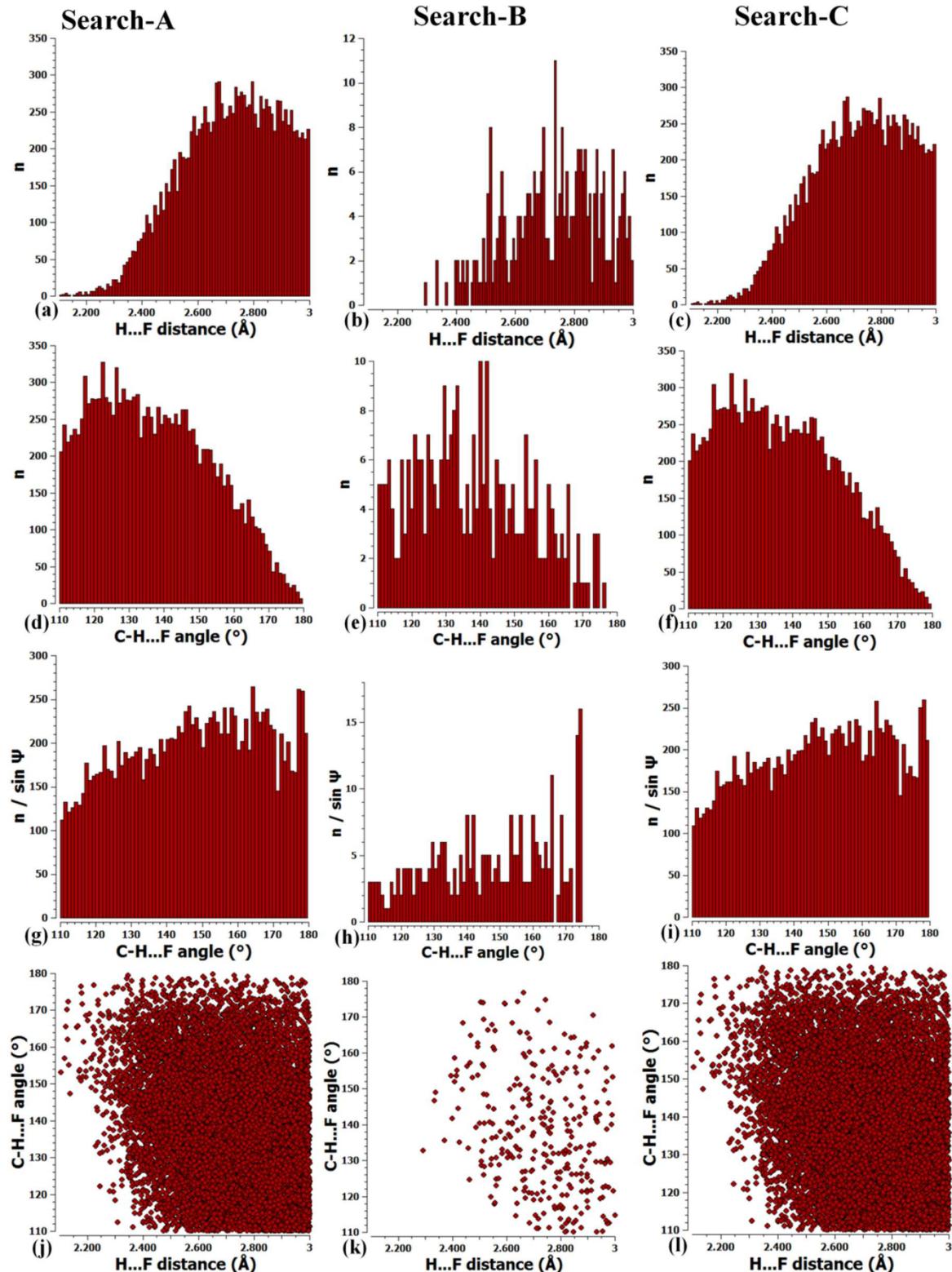
*Email: dchopra@iiserb.ac.in. Fax: 91-755-6692392.*



**Figure S1:** (a)-(c) H...F intermolecular distance distribution for **Subsection-2a**; (d)-(f) C-H...F angle distribution for Subsection-2a; (g)-(i) Cone corrected angle distribution for **Subsection-2a**; (j)-(l) Scatter plot between H...F distance and C-H...F angle for **Subsection-2a**.

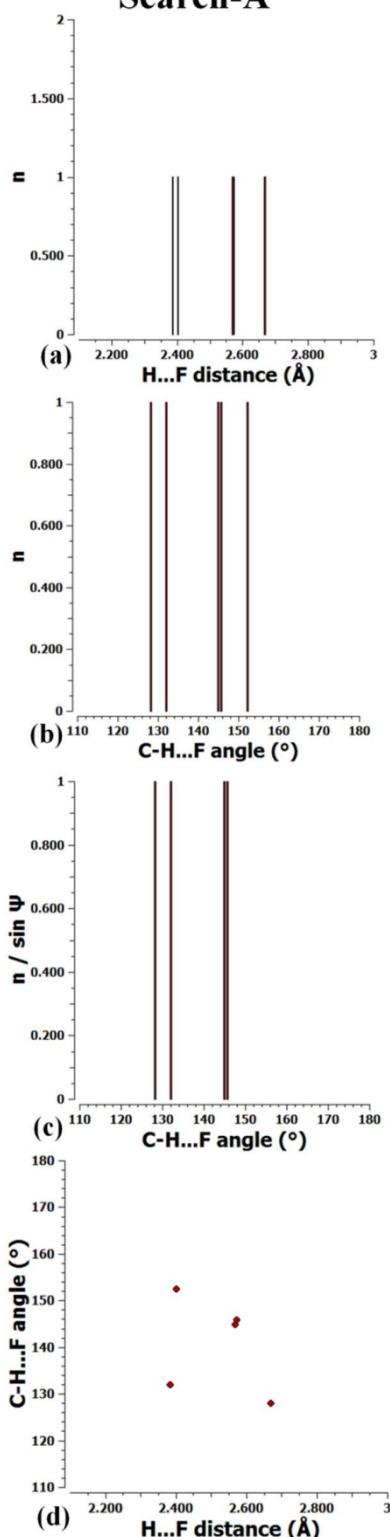


**Figure S2:** (a)-(c) H...F intermolecular distance distribution for **Subsection-2b**; (d)-(f) C-H...F angle distribution for Subsection-2b; (g)-(i) Cone corrected angle distribution for **Subsection-2b**; (j)-(l) Scatter plot between H...F distance and C-H...F angle for **Subsection-2b**.

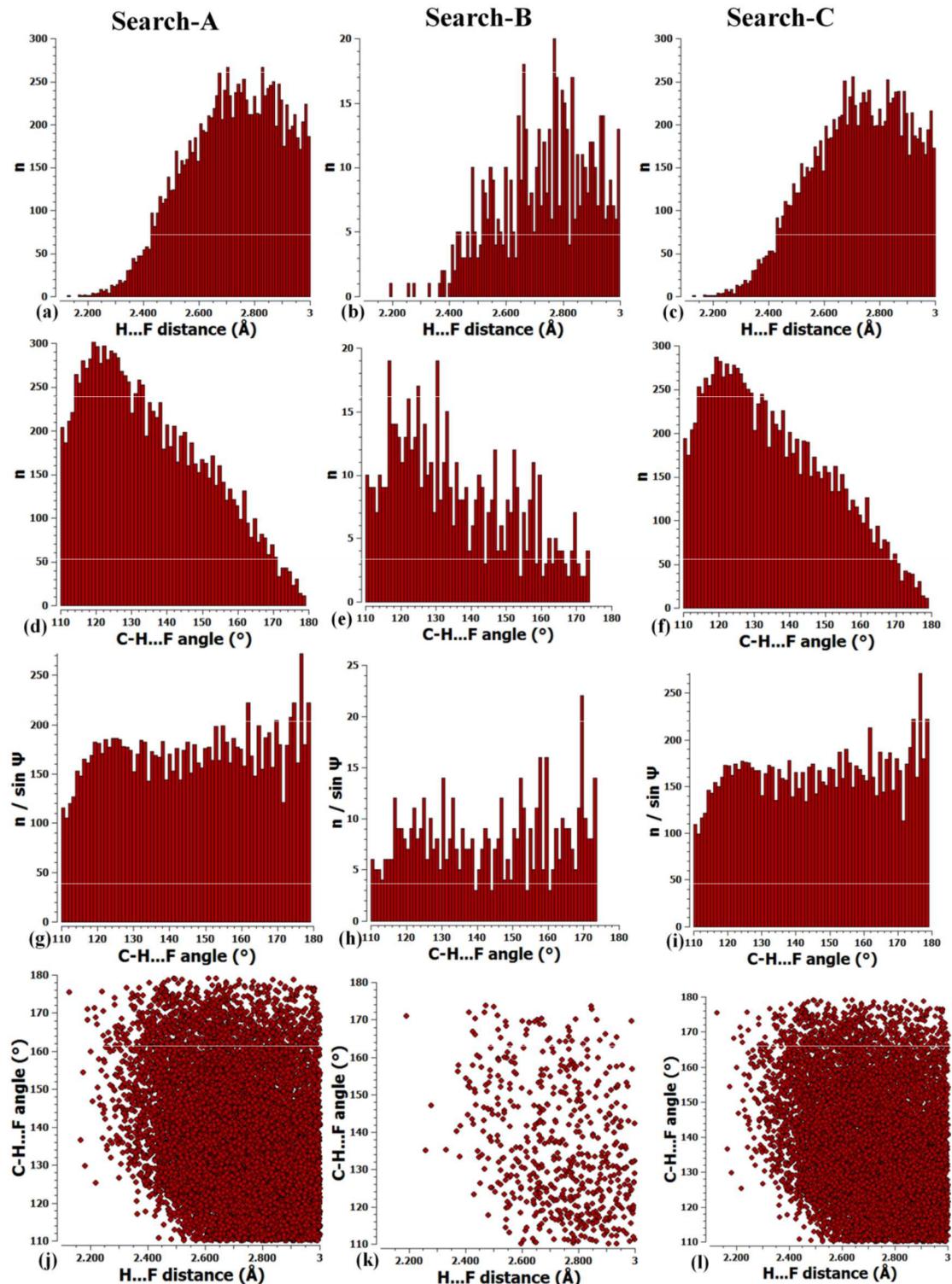


**Figure S3:** (a)-(c) H...F intermolecular distance distribution for **Subsection-2c**; (d)-(f) C-H...F angle distribution for **Subsection-2c**; (g)-(i) Cone corrected angle distribution for **Subsection-2c**; (j)-(l) Scatter plot between H...F distance and C-H...F angle for **Subsection-2c**.

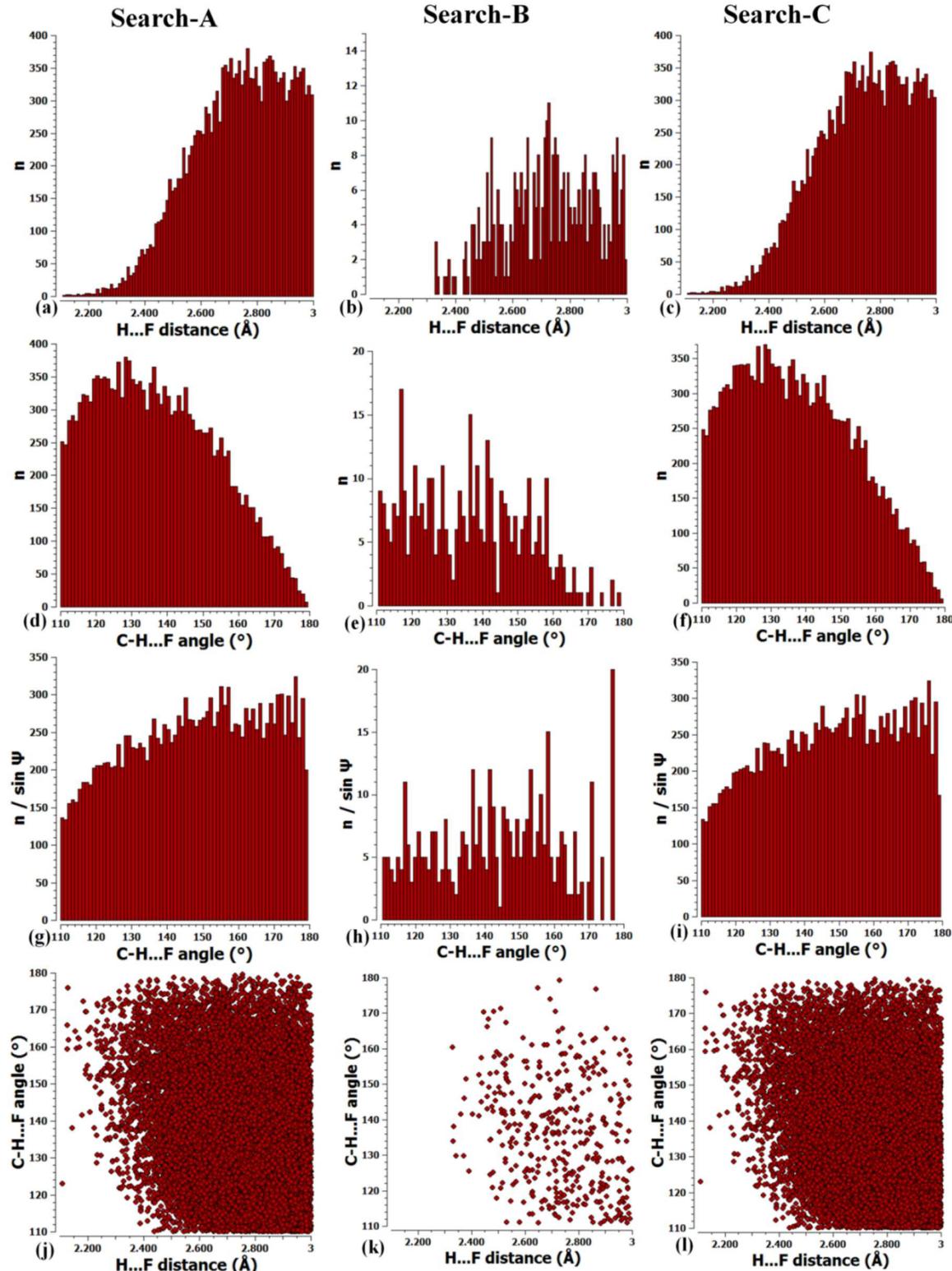
## Search-A



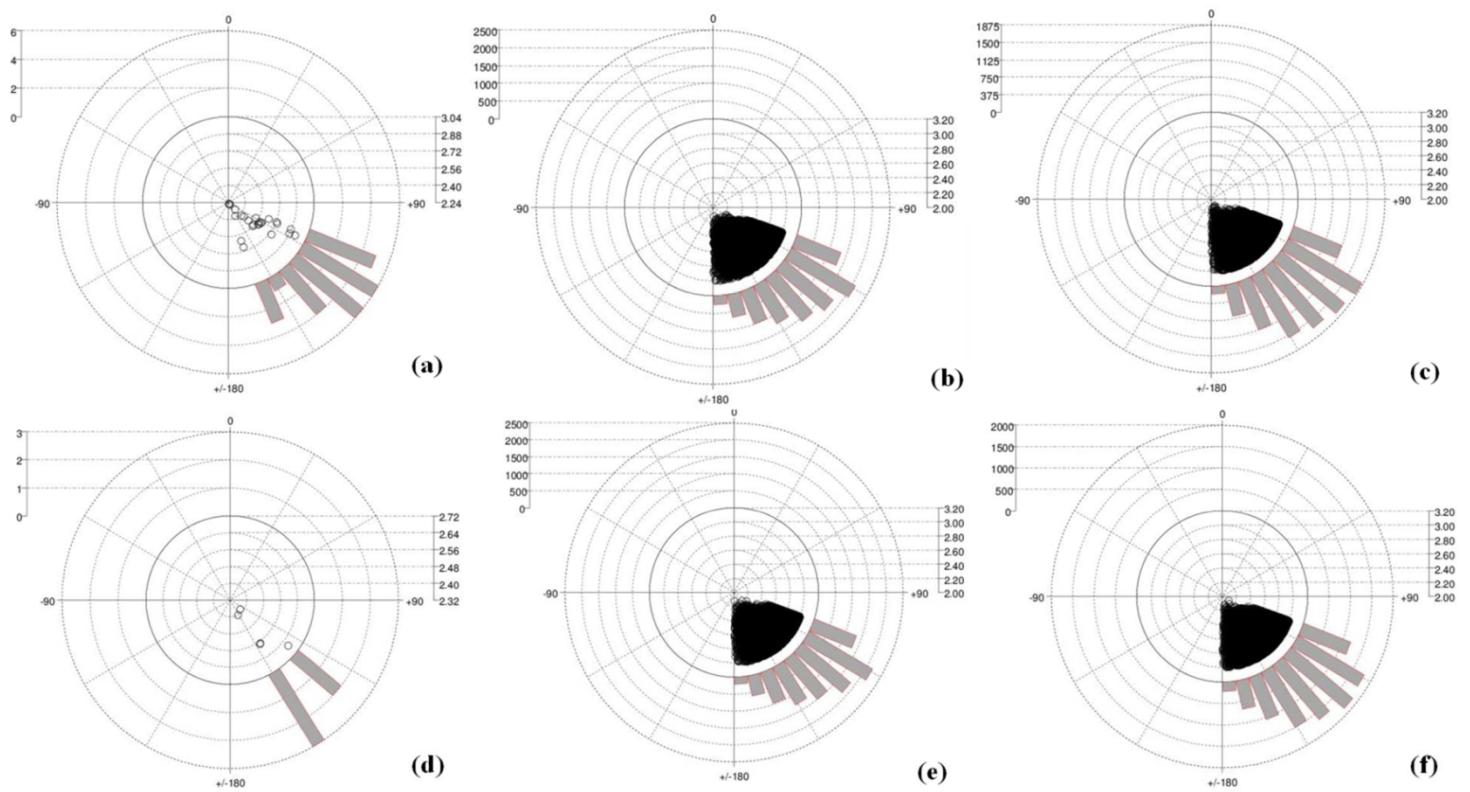
**Figure S4:** (a) H...F intermolecular distance distribution for **Subsection-3a**; (d) C-H...F angle distribution for Subsection-3a; (g) Cone corrected angle distribution for **Subsection-3a**; (j) Scatter plot between H...F distance and C-H...F angle for **Subsection-3a**.



**Figure S5:** (a)-(c) H...F intermolecular distance distribution for **Subsection-3b**; (d)-(f) C-H...F angle distribution for **Subsection-3b**; (g)-(i) Cone corrected angle distribution for **Subsection-3b**; (j)-(l) Scatter plot between H...F distance and C-H...F angle for **Subsection-3b**.

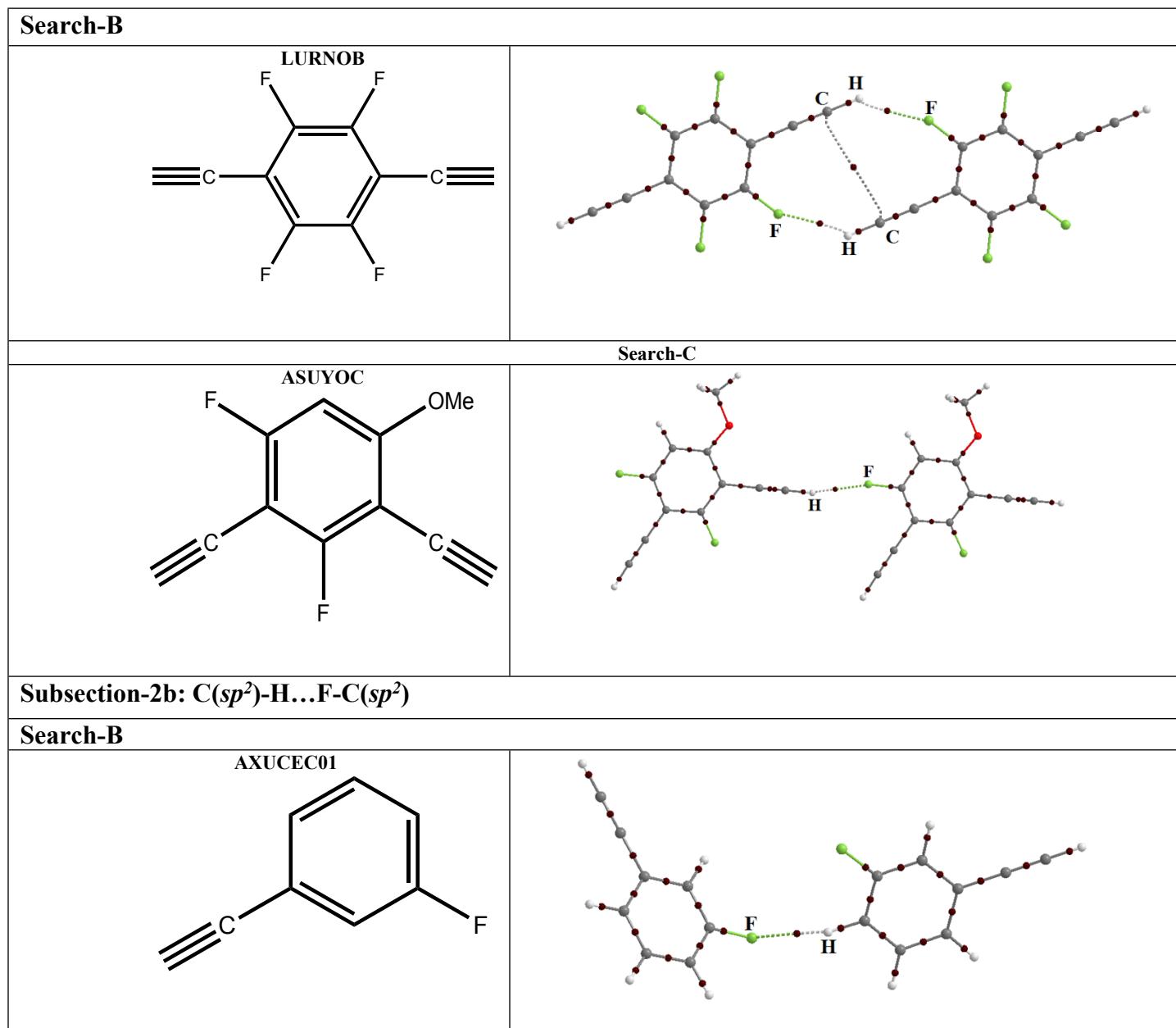


**Figure S6:** (a)-(c) H...F intermolecular distance distribution for **Subsection-3c**; (d)-(f) C-H...F angle distribution for **Subsection-3c**; (g)-(i) Cone corrected angle distribution for **Subsection-3c**; (j)-(l) Scatter plot between H...F distance and C-H...F angle for **Subsection-3c**.

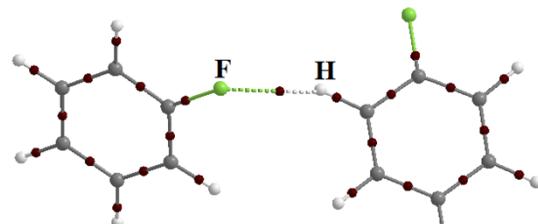
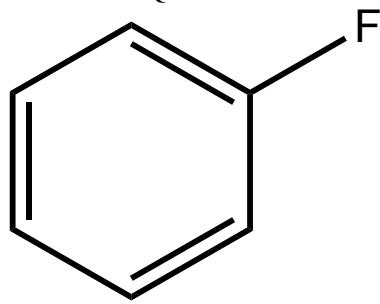


**Figure S7:** Polar scatterplots for (a) C(sp)-H...F-C(sp<sup>2</sup>) (b) ;C(sp<sup>2</sup>)-H...F-C(sp<sup>2</sup>) (c) C(sp<sup>3</sup>)-H...F-C(sp<sup>2</sup>) ;(d) C(sp)-H...F-C(sp<sup>3</sup>); (e) C(sp<sup>2</sup>)-H...F-C(sp<sup>3</sup>);(f) C(sp<sup>3</sup>)-H...F-C(sp<sup>3</sup>)

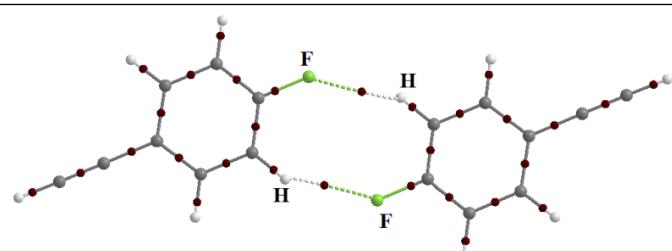
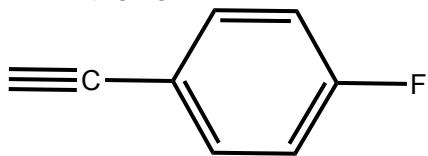
**Figure S8:** The selection of molecules for the study of C-H...F intermolecular interactions obtained from the CSD. Column 1 indicates REFCODE along with the molecule and Column 2 highlights the molecular graph depicting all the relevant intra- and intermolecular bond critical points (dotted lines) in the formation of molecular pairs at the crystal geometry obtained from different searches in different hybridization environment.



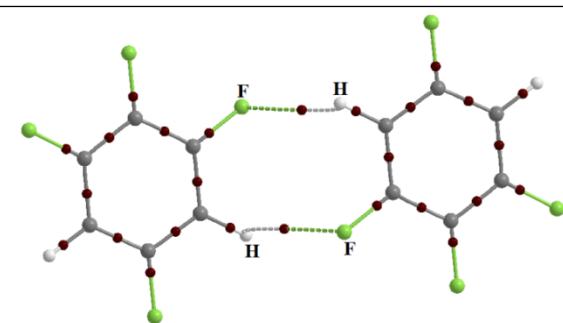
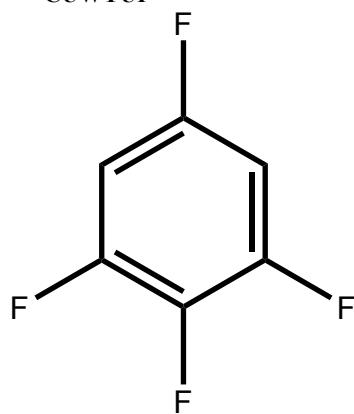
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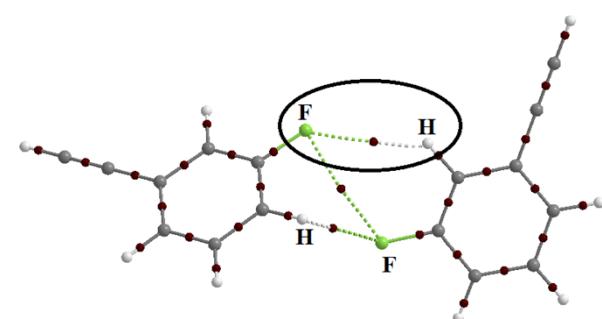
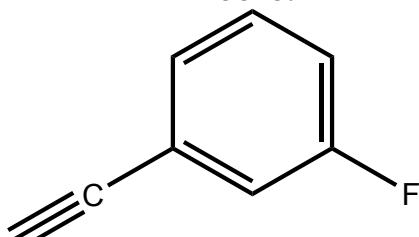
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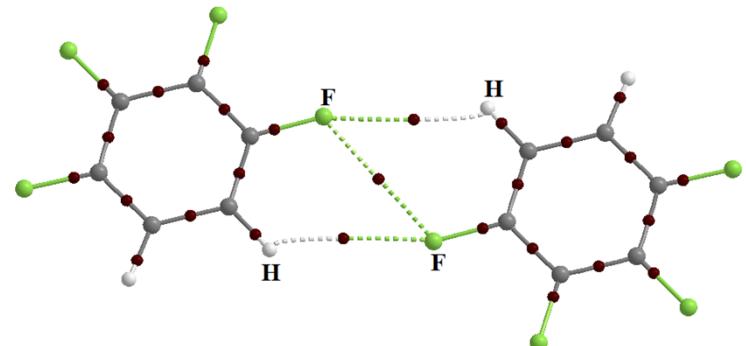
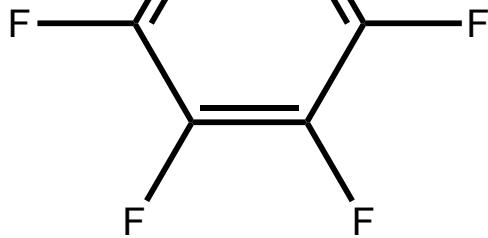
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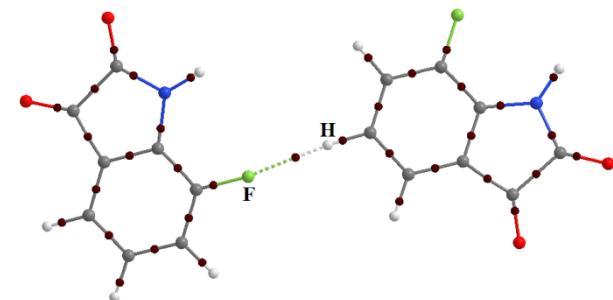
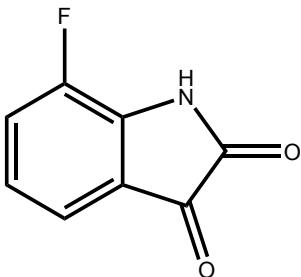


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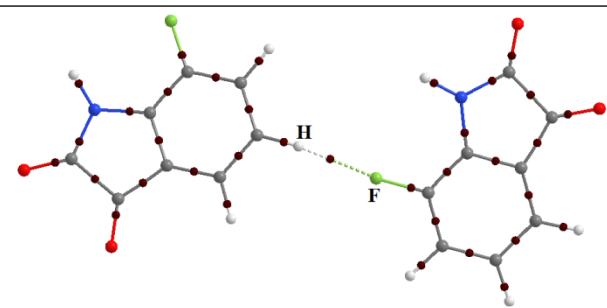
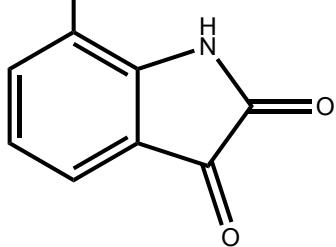


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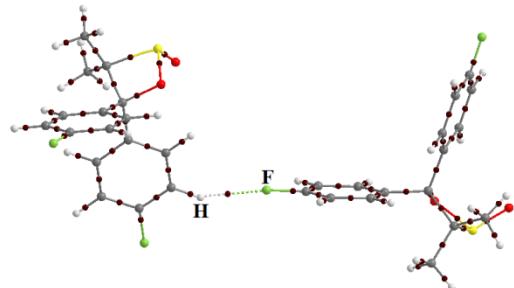
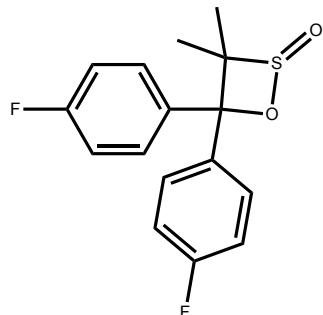
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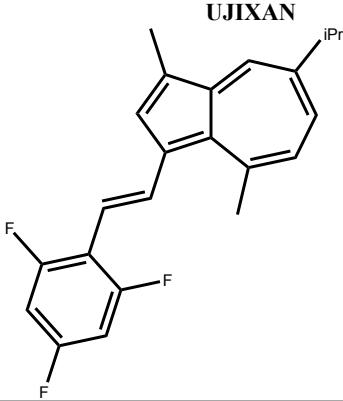
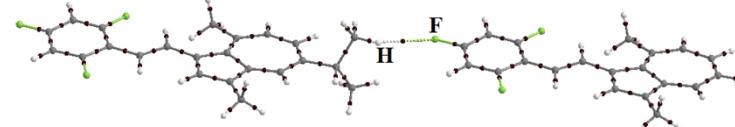
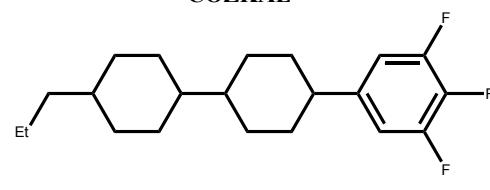
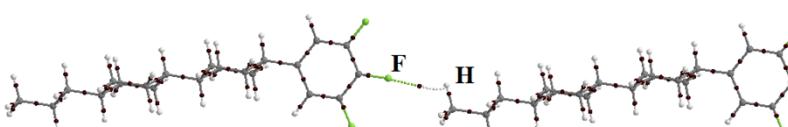
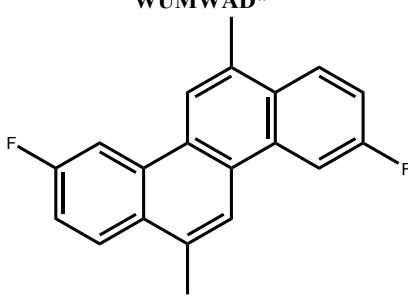
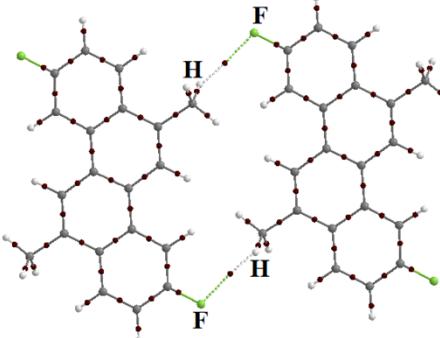
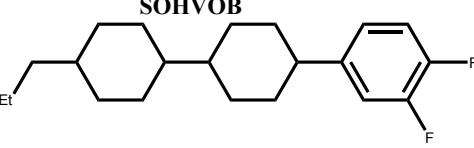
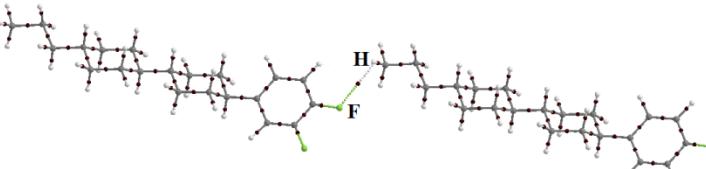
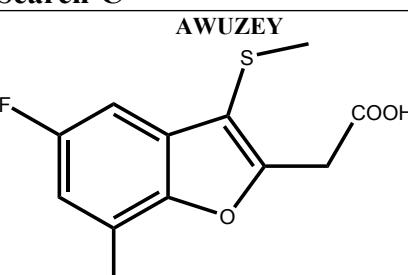
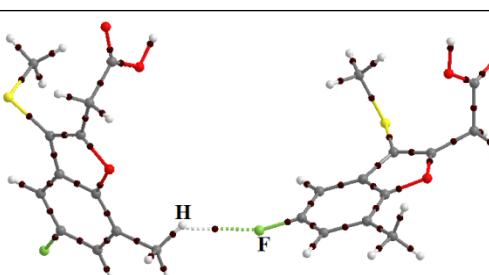
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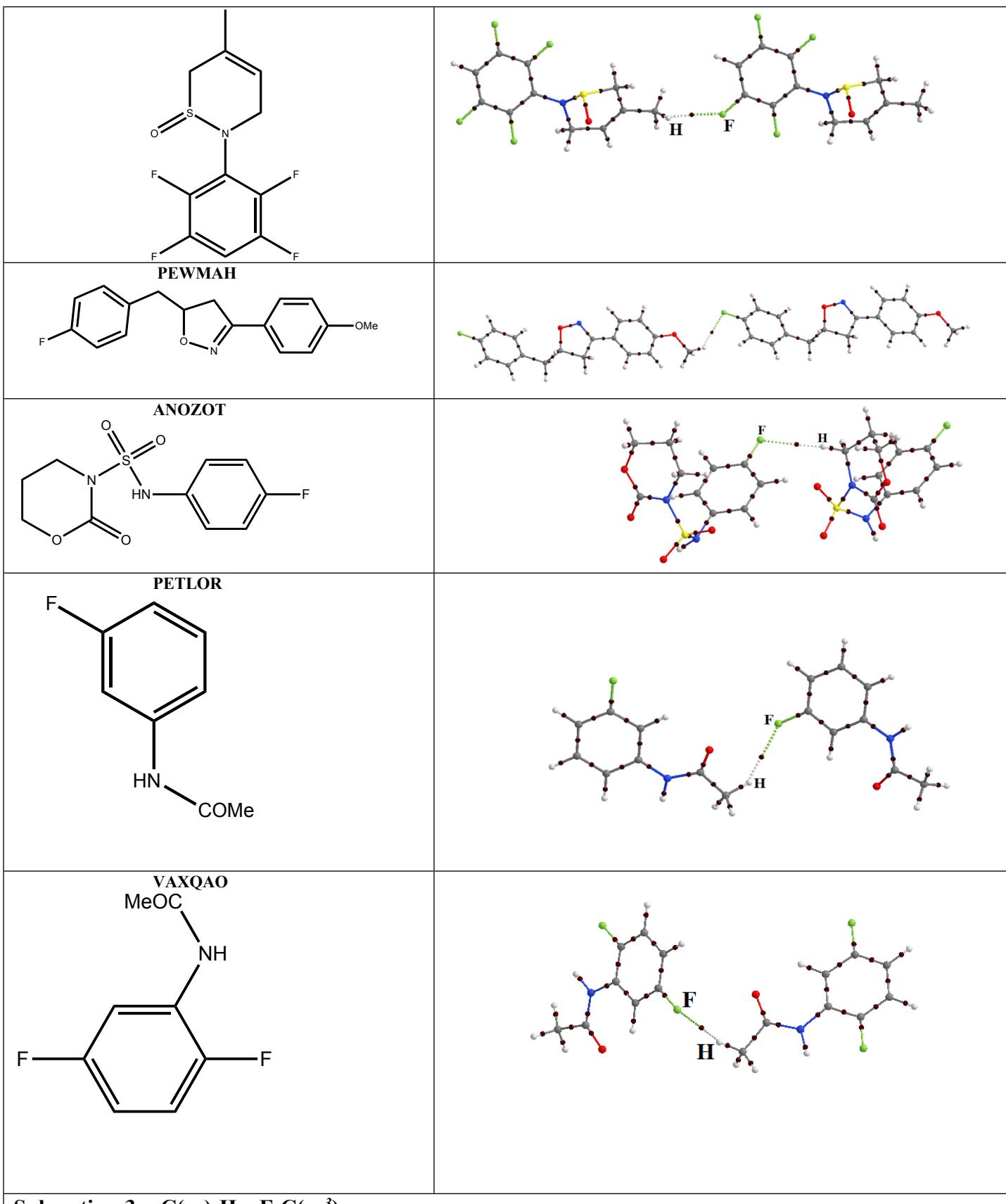


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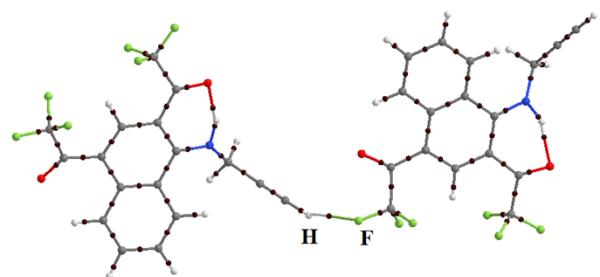
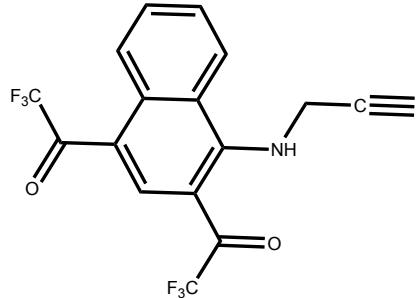
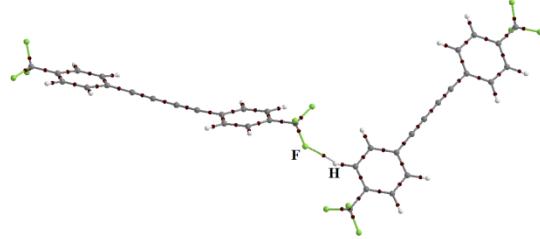
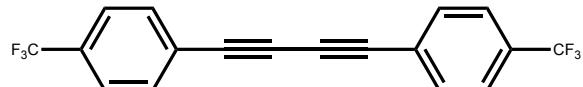
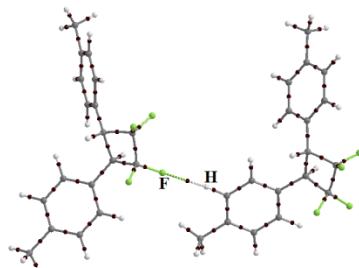
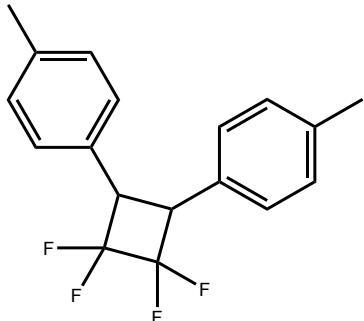
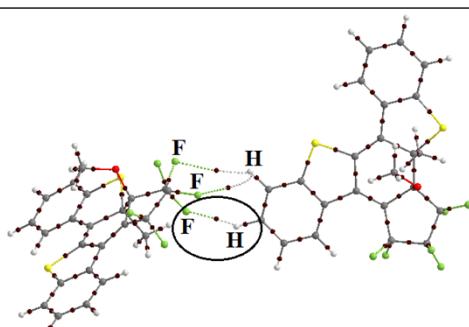
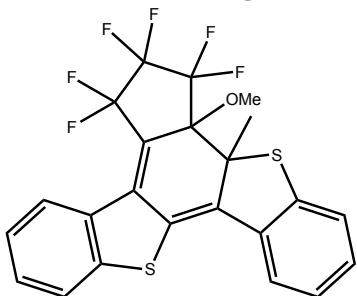


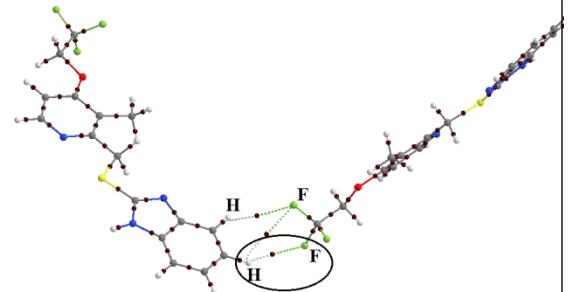
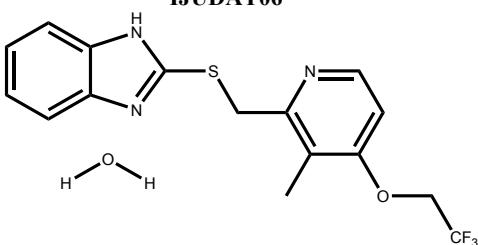
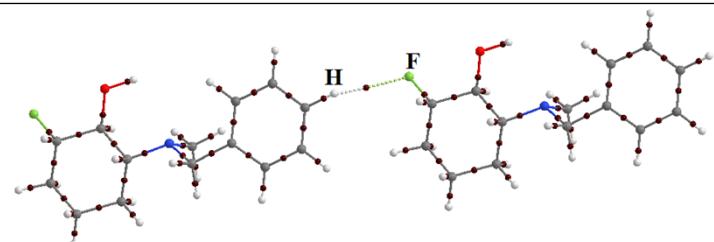
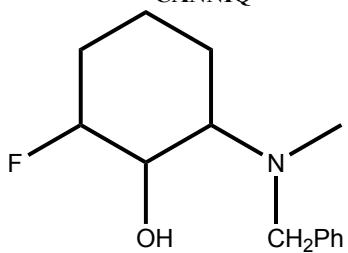
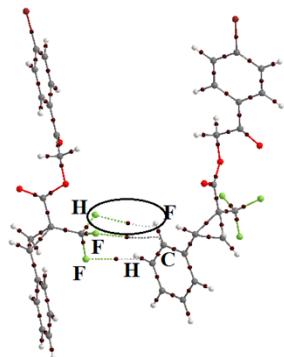
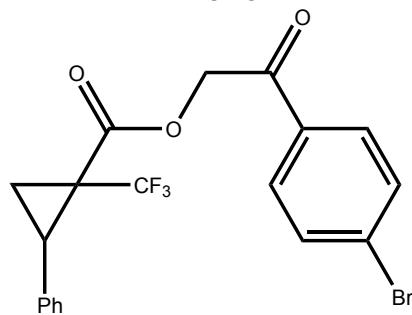
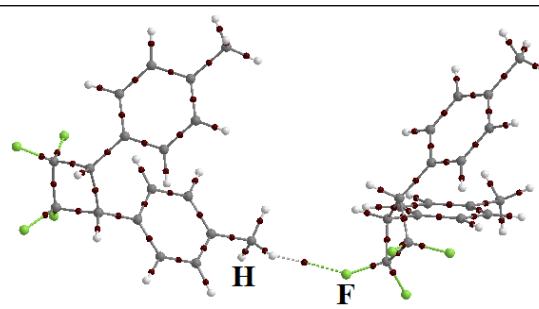
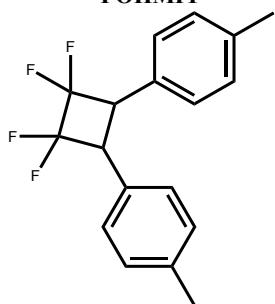
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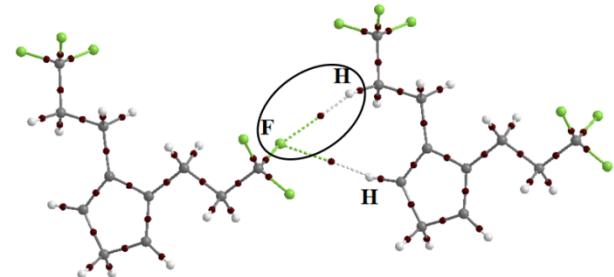
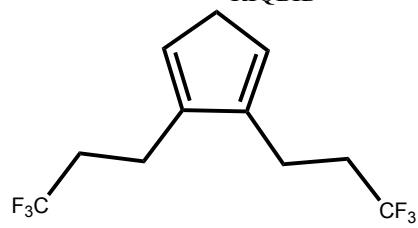
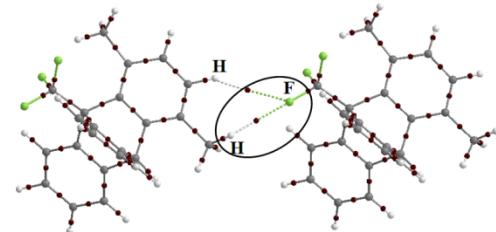
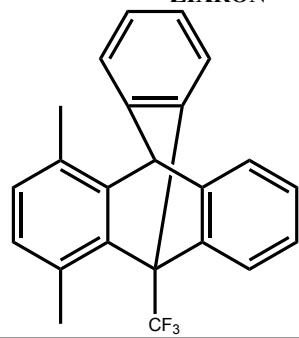
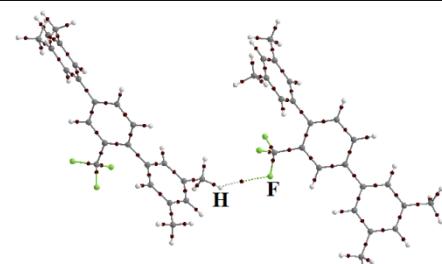
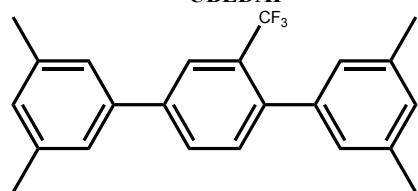
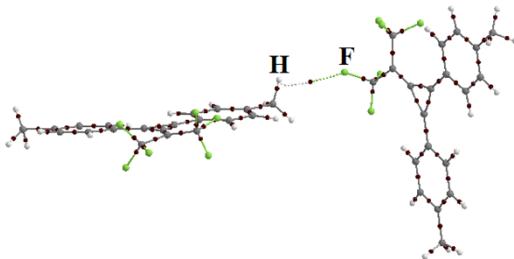
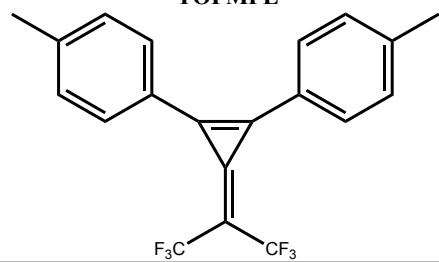
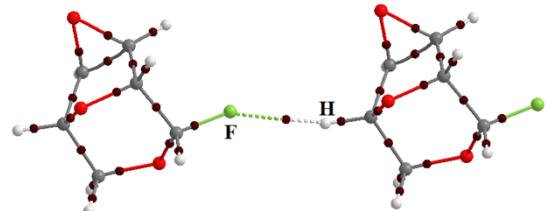
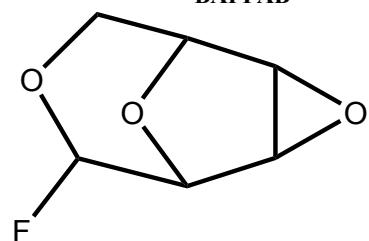
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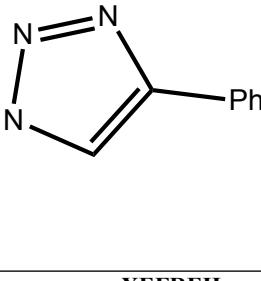
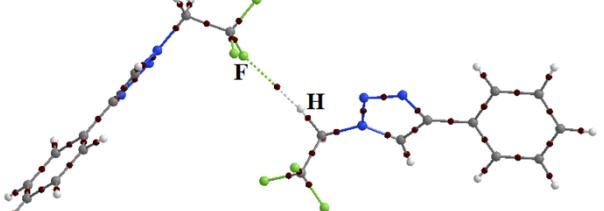
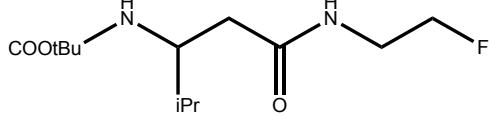
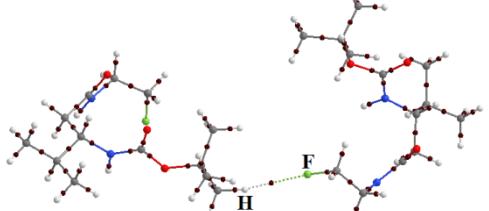
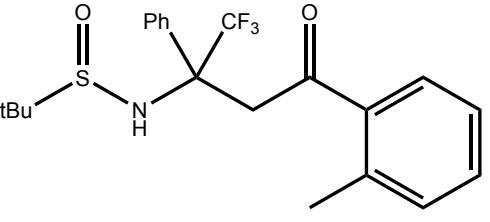
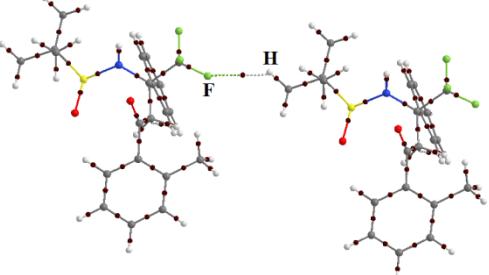
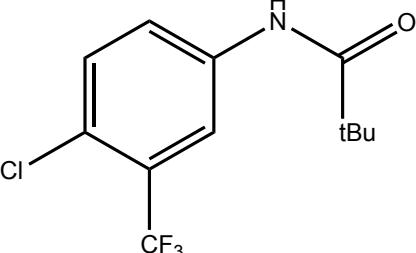
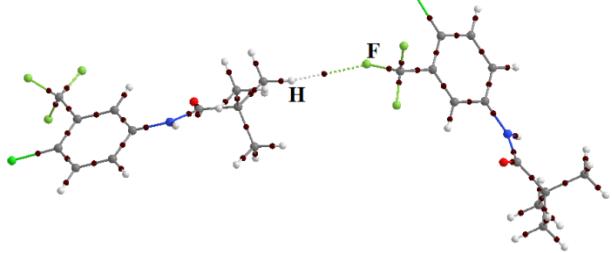
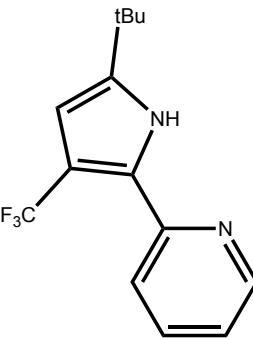
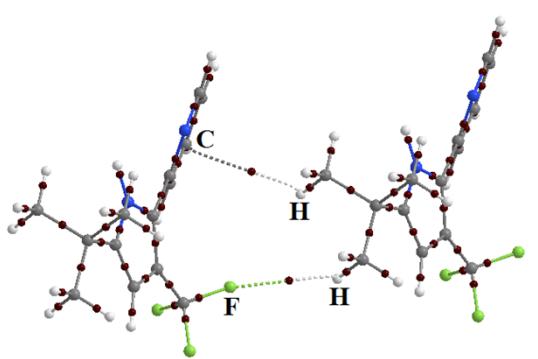


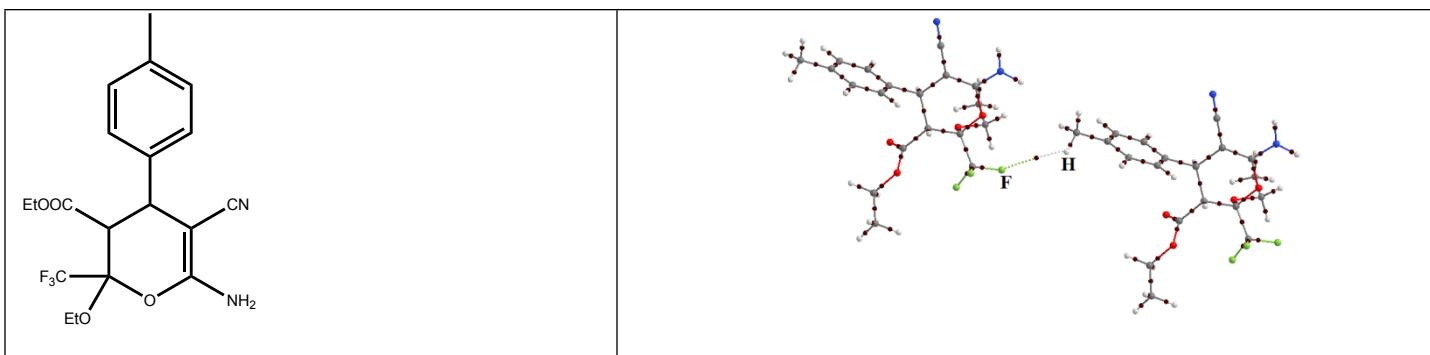
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**Search-C****AGAVOU****Subsection-3b: C(sp<sup>2</sup>)-H...F-C(sp<sup>3</sup>)****Search-B****FELLOY****FOHMEU****Search-C****BERGAH**

**IJUDAT06****CANNIQ****AZOKOP****Subsection-3c:  $\text{C}(sp^3)\text{-H}\dots\text{F-C}(sp^3)$** **Search-B****FOHMIY**

**RIQBID****ZIXRON****UBEDAI****TOFMFL****Search-C****BAPFAB**

<p><b>ACEJIC</b></p> 	
<p><b>XEFREH</b></p> 	
<p><b>GECLIL</b></p> 	
<p><b>LEGJIS</b></p> 	
<p><b>ABUDIM</b></p> 	
<p><b>DEFMUX</b></p>	



**Table S1: Bond precision values for molecules under investigation**

REFCODE	C-C Bond Precision ( $\text{\AA}$ )
LURNOB	0.0044
ASUYOC	0.0041
AXUCEC01	0.0061
FACFAQ	0.0020
NECMUD	0.0020
CUWYUP	0.0043
AXUCEC01	0.0061
ZELDOJ01	0.0019
NIZVAU02	0.0050
NIZVAU02	0.0050
BAJREJ	0.0016
LEGMOB	0.0061
VAYBUU	0.0021
ABABUC	0.0027
ACEWUB	0.0030
WESBEB	0.0017
UJIXAN	0.0043
COZKAE	0.0050
WUMWAD	0.0050
SOHVOB	0.0058
AWUZEY	0.0025
AMARUB	0.0031
PEWMAH	0.0022
ANOZOT	0.0028
PETLOR	0.0019
VAXQAO	0.0027
AGAVOU	0.0147
FELLOY	0.0026
FOHMEU	0.0028
BERGAH	0.0080
IJUDAT06	0.0042
CANNIQ	0.0041

AZOKOP	0.0050
FOHMIY	0.0100
RIQBID	0.0020
ZIXRON	0.0101
UBEDAI	0.0016
TOFMFL	0.0001
BAPFAB	0.0045
ACEJIC	0.0060
XEFRFH	0.0108
GECLIL	0.0021
LEGJIS	0.0050
ABUDIM	0.0033
DEFMUX	0.0054