

# Importance of intermolecular $-C\equiv C-H\cdots X-C$ ( $X = F, O, N$ ) and $-Y-H\cdots F-C$ ( $Y = O, N$ ) hydrogen bonds in crystal structures

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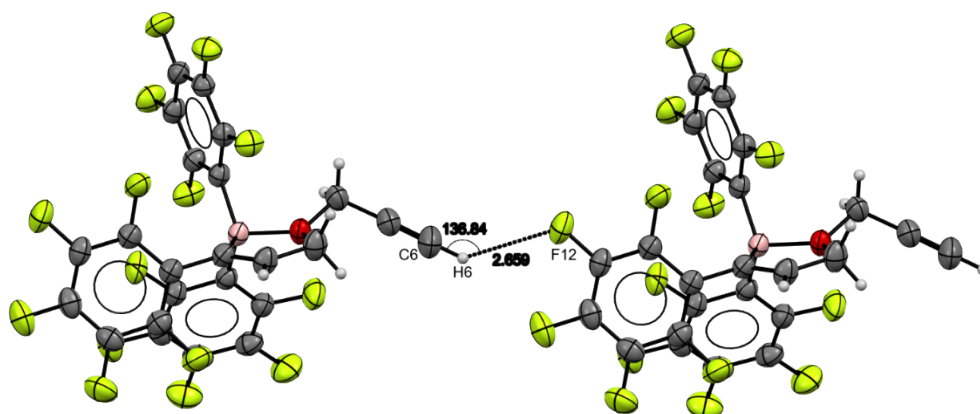
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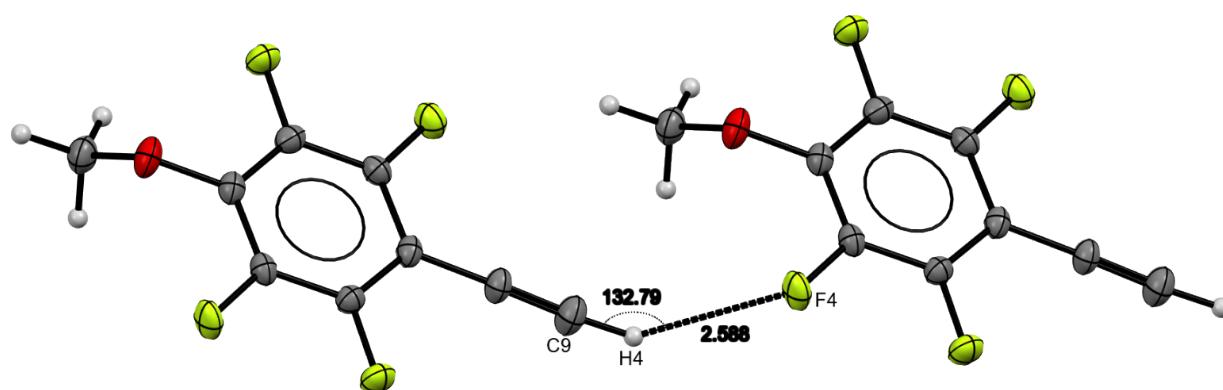
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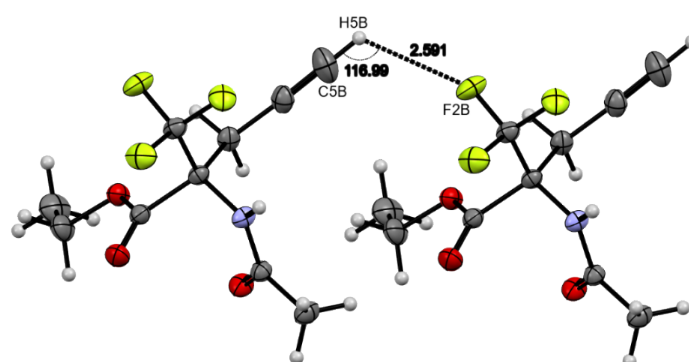
## 1. Representative Dimers



a) ASIKUJ

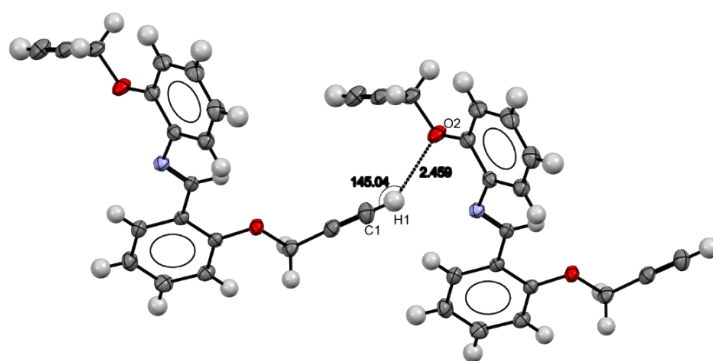


b) AYOHUR

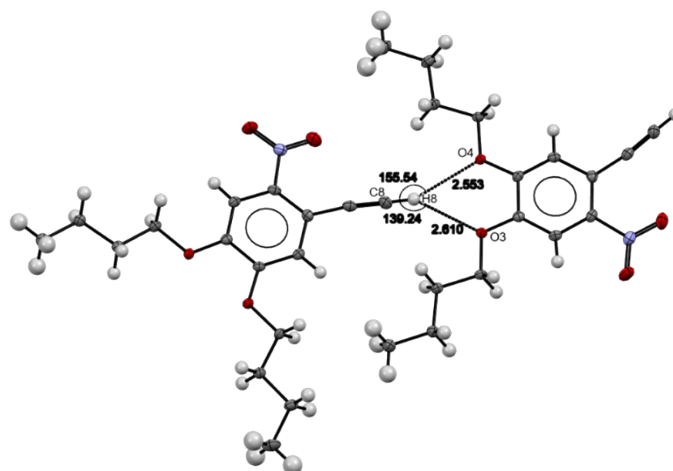


c) COJPIC

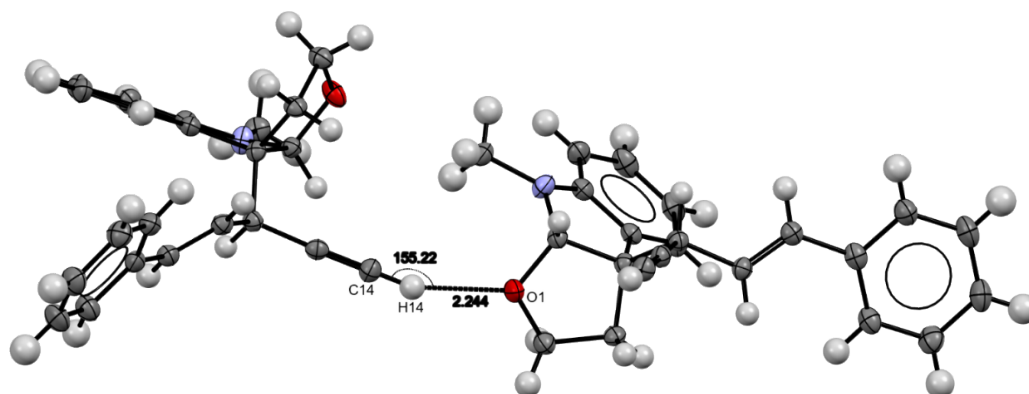
**Figure S1:** The above four structures are from the search1 results for the molecules a) ASIKUJ, b) AYOHUR, and c) COJPIC, having  $\text{C}\equiv\text{C}-\text{H}\cdots\text{F}-\text{C}$  interactions.



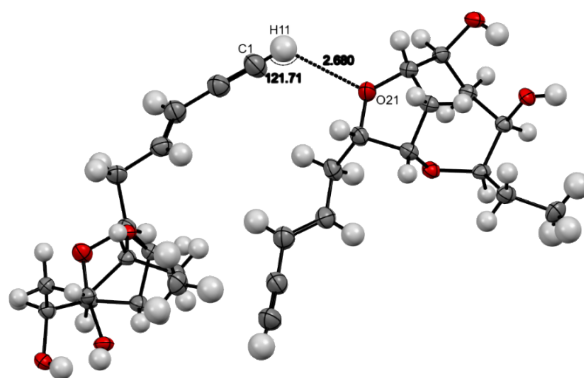
a) ACIXOC



b) ACOTIY

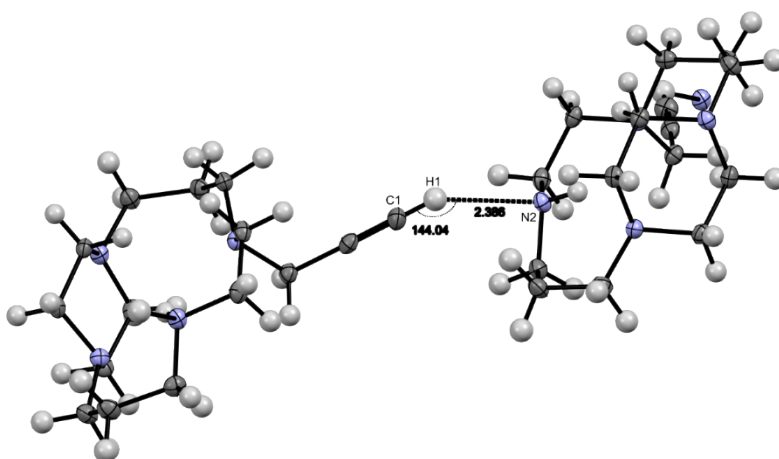


c) AHUHOc

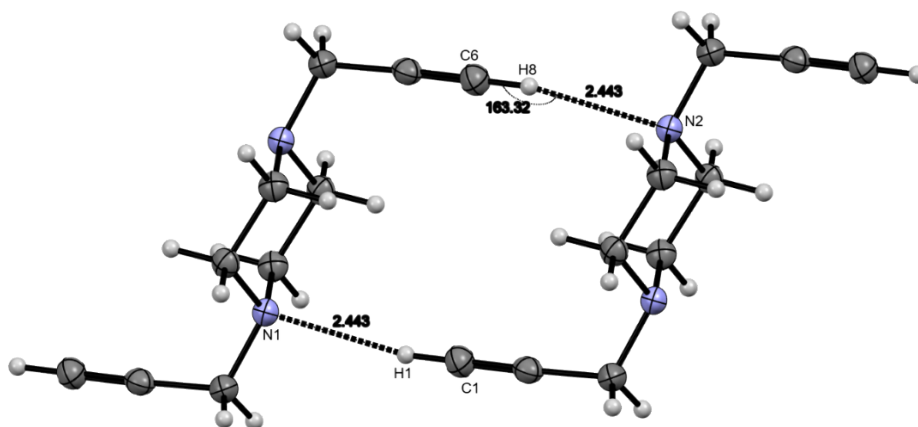


d) BAFXUF

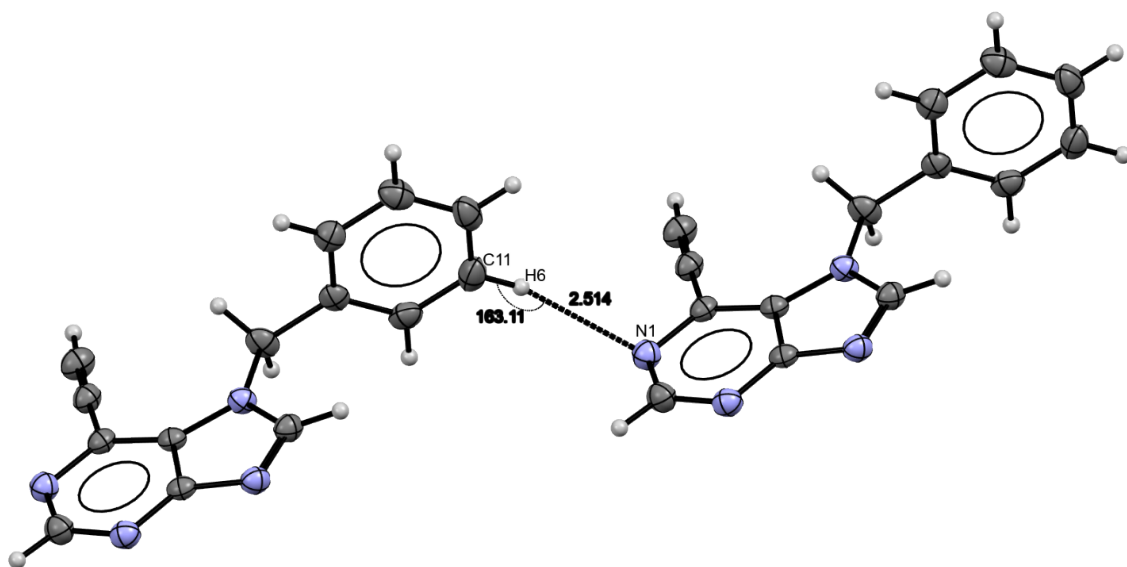
**Figure S2:** The above four structures are from the search8 results for the molecules with REFCODE a) ACIXOC, b) ACOTIY, c) AHUHOC, and d) BAFXUF, having  $\text{--C}\equiv\text{C--H}\cdots\text{O--C}$  interactions.



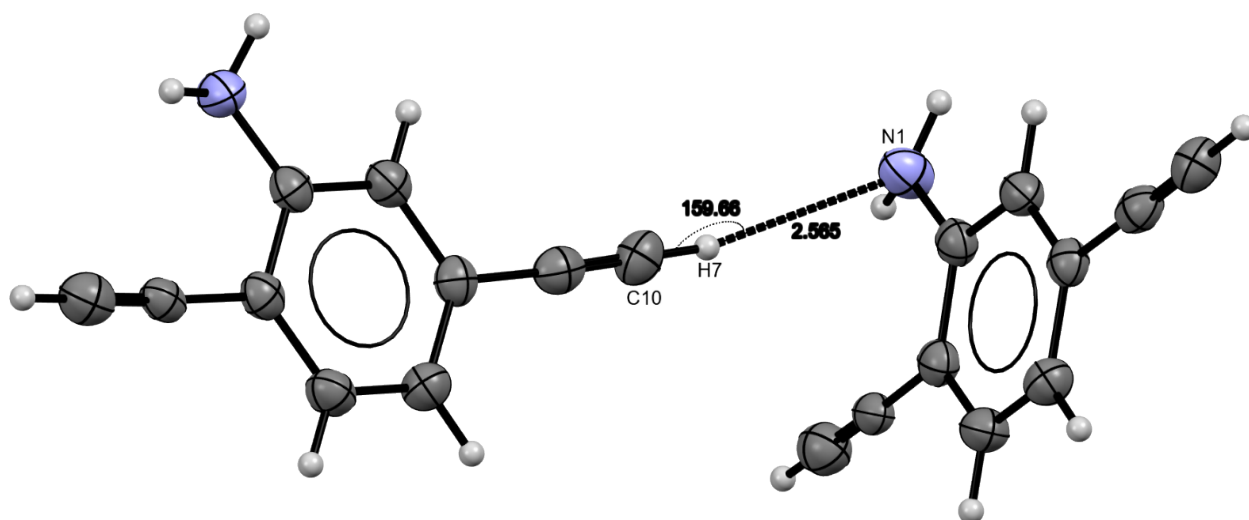
a) CUFFOB



b) HEKSAU

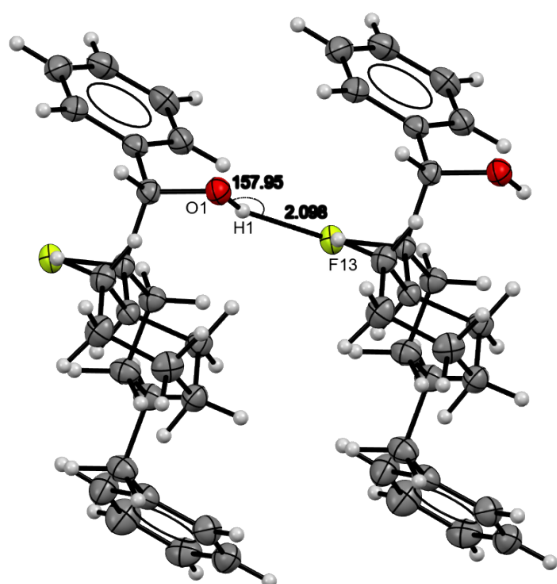


c) IZAQIK

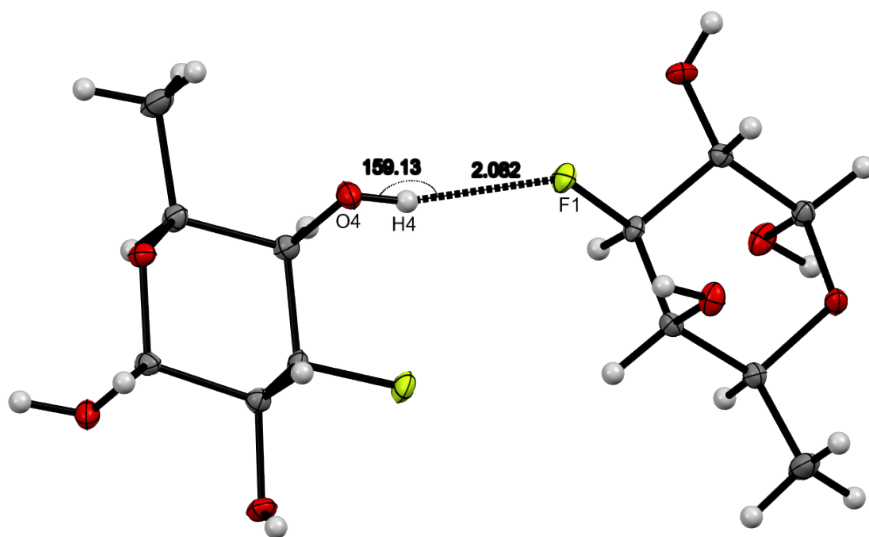


d) LURMOA

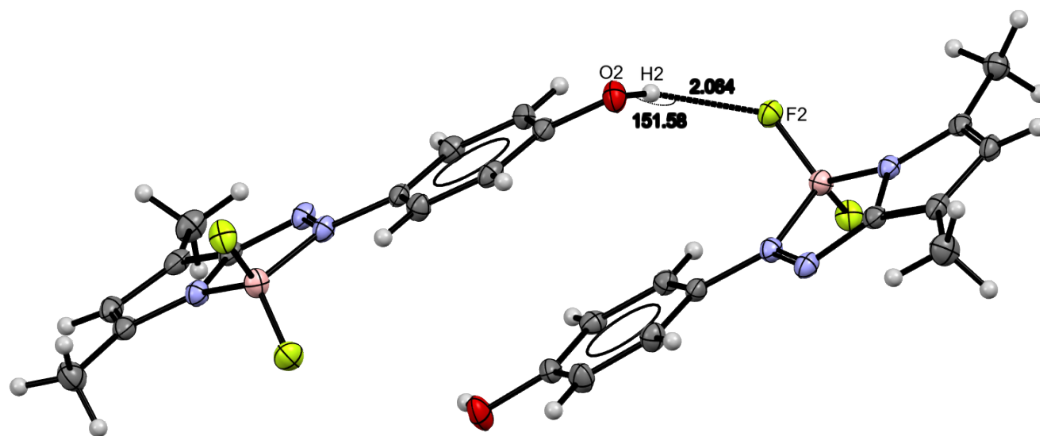
**Figure S3:** The above four structures are from the search9 results for the molecules with REFCODE a) CUFFOB, b) HEKSAU, c) IZAQIK, and d) LURMOA, having  $\text{--C}\equiv\text{C--H}\cdots\text{N--C}$  interactions (Search 9).



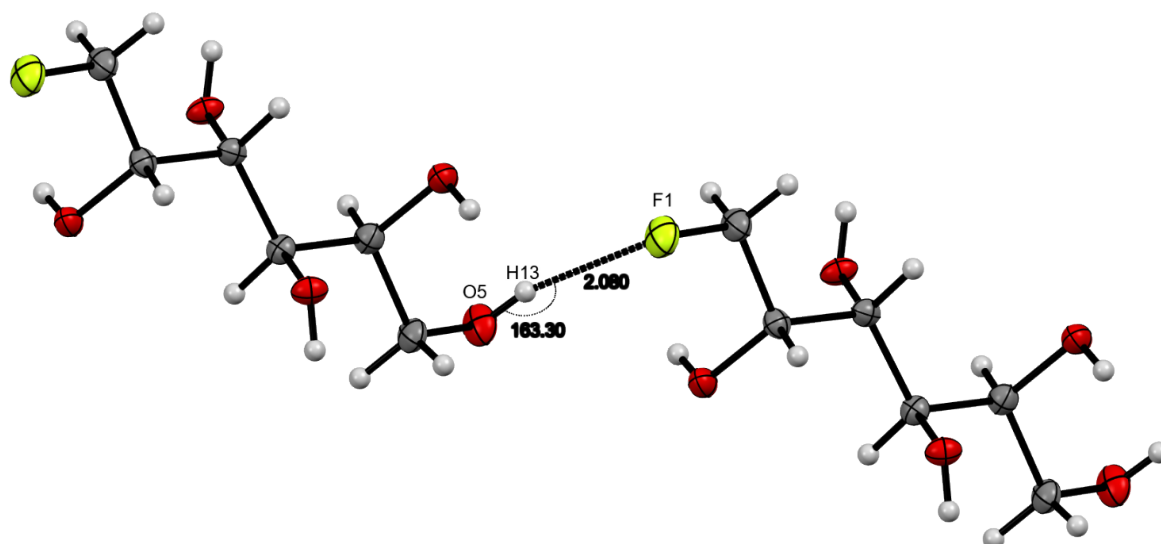
a) BUFQAX



b) CURKIM

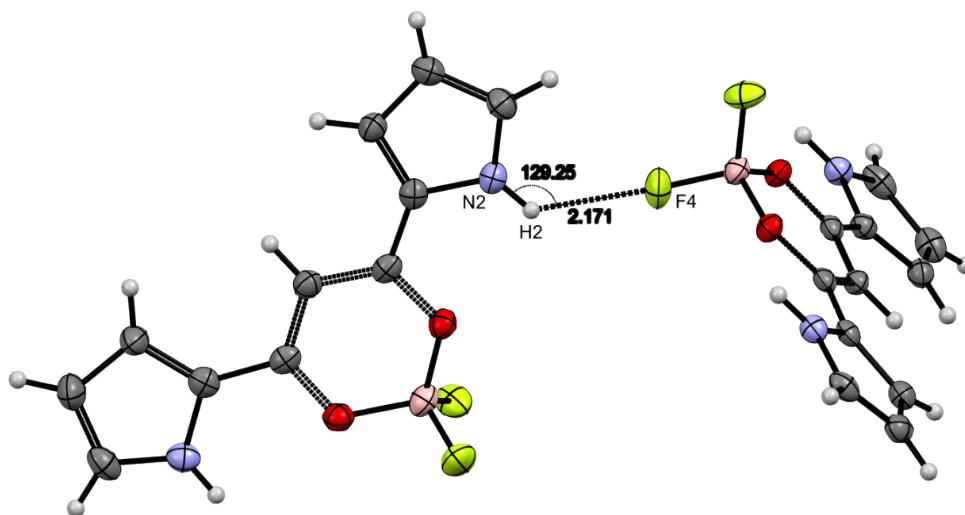


c) NIBVAY

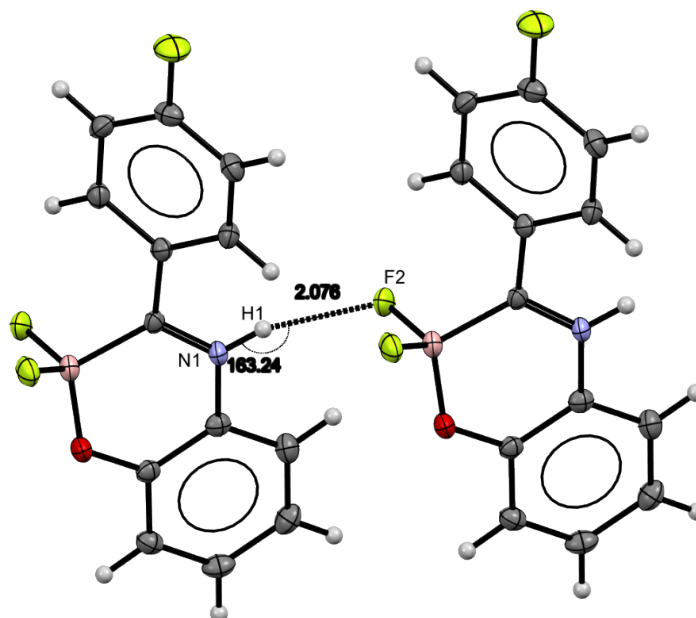


d) TUPBOW

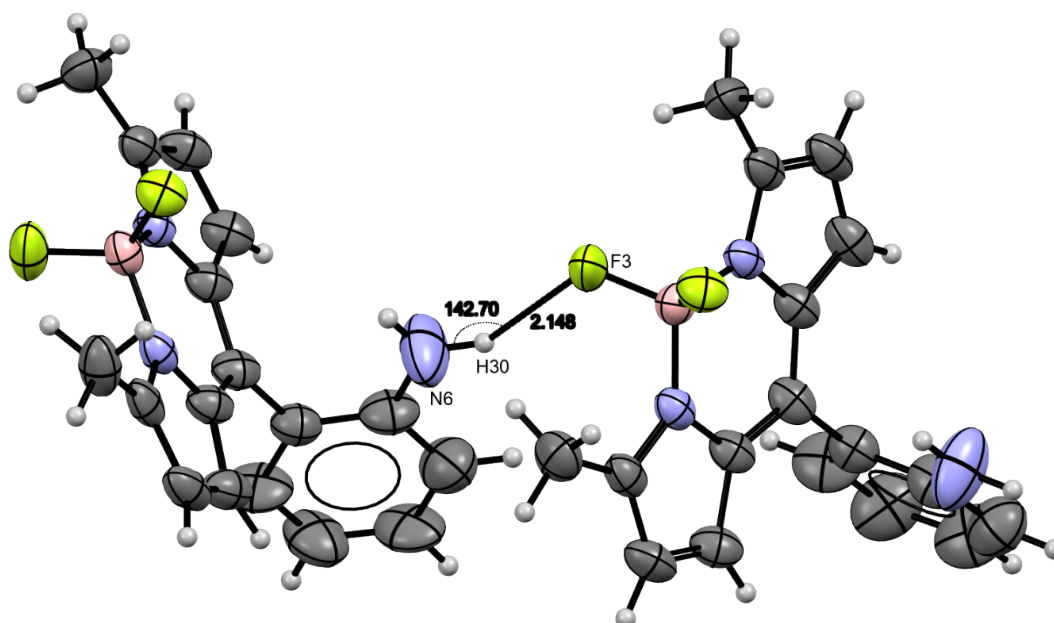
**Figure S4:** The above four structures are from the search10results for the molecules with REFCODE a) BUFQAX, b) CURKIM, c) NIBVAY, and d) TUPBOW, having  $\text{-O-H}\cdots\text{F-C}$  interactions (Search 10).



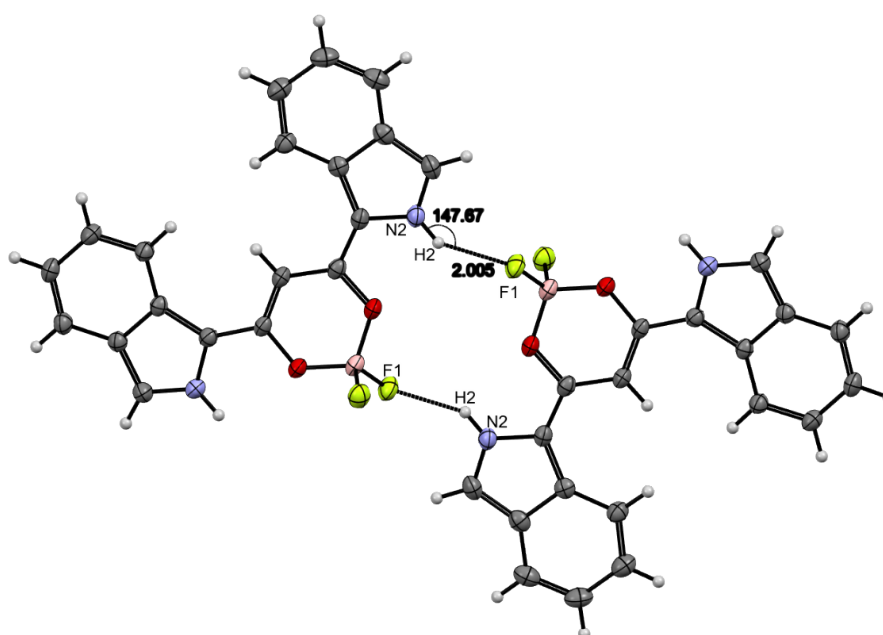
a) DATZAA



b) EBECOH



c) EGAGID



d) GADLUU

**Figure S5:** The above four structures are from the search11 results for molecules with REFCODE a) DATZAA, b) EBECOH, c) EGAGID, and d) GADLUU having  $\text{-N-H}\cdots\text{F-C}$  interactions (Search 11).

## ARTICLE

## 2. Topological Parameters

**Table S1-S5** provides a comprehensive list of dimers formed using  $\text{--C}\equiv\text{C--H}\cdots\text{X--C}$  (where X = F, N, O) and  $\text{Y--H}\cdots\text{F--C}$  (where Y = N, O) hydrogen bonds. Tables S1-S5 include the geometrical parameters (distance and angle), stabilization energy ( $\Delta E$ ), electron density ( $\rho$ ) and Laplacian of electron density ( $\nabla^2\rho$ ) at the bond critical point and the bond path ( $R_{ij}$ ) for all the molecules studied.

**Table S1:** Energies and Topological parameters corresponding to molecules having  $\text{--C}\equiv\text{C--H}\cdots\text{F--C}$  interactions (Search 1)

| S.no. | CSD REFCODE | $\Delta E$ (kcal/mol) | $\angle\text{C--H}\cdots\text{F}$ (°) | $d_{\text{H}\cdots\text{F}}$ (Å) | $\rho$ ( $\text{e}\text{\AA}^{-3}$ ) | $\nabla^2\rho$ ( $\text{e}\text{\AA}^{-5}$ ) | $R_{ij}$ (Å) |
|-------|-------------|-----------------------|---------------------------------------|----------------------------------|--------------------------------------|----------------------------------------------|--------------|
| 1     | AGAVOU      | -0.875                | 124.72                                | 2.612                            | 0.005                                | 0.002                                        | 2.596        |
| 2     | ASIKUJ      | -0.900                | 136.838                               | 2.659                            | 0.003                                | 0.001                                        | 2.781        |
| 3     | AYOHUR      | 0.236                 | 132.785                               | 2.588                            | 0.004                                | 0.001                                        | 2.711        |
| 4     | COJPIC      | -1.337                | 116.989                               | 2.591                            | 0.006                                | 0.002                                        | 2.672        |
| 5     | FEYSEK      | -0.045                | 156.010                               | 2.641                            | 0.002                                | 0.001                                        | 3.011        |
| 6     | FEYSIO      | 0.014                 | 154.536                               | 2.631                            | 0.003                                | 0.001                                        | 2.796        |
| 7     | FEYSUA      | 0.083                 | 149.224                               | 2.601                            | 0.002                                | 0.001                                        | 2.913        |
| 8     | FEYTAH      | 0.056                 | 150.189                               | 2.406                            | 0.007                                | 0.002                                        | 2.433        |
| 9     | FEYTEL      | -0.007                | 149.815                               | 2.476                            | 0.006                                | 0.002                                        | 2.503        |
| 10    | FEYTIP      | -0.339                | 158.442                               | 2.476                            | 0.006                                | 0.002                                        | 2.504        |
| 11    | FEYTOV      | -0.049                | 167.672                               | 2.363                            | 0.007                                | 0.002                                        | 2.391        |
| 12    | FITYAL01    | -0.318                | 164.463                               | 2.335                            | 0.008                                | 0.002                                        | 2.363        |
| 13    | FITYOZ      | -0.195                | 141.704                               | 2.527                            | 0.006                                | 0.002                                        | 2.554        |
| 14    | GEKGIP      | -0.440                | 158.687                               | 2.304                            | 0.009                                | 0.003                                        | 2.332        |
| 15    | GEKGOV01    | -0.411                | 155.806                               | 2.354                            | 0.008                                | 0.002                                        | 2.381        |
| 16    | KEQLAU      | 1.574                 | 153.865                               | 2.517                            | 0.006                                | 0.002                                        | 2.543        |
| 17    | LEBTAQ02    | -0.495                | 176.486                               | 2.281                            | 0.009                                | 0.003                                        | 2.309        |
| 18    | LEBTAQ03    | -0.450                | 161.623                               | 2.412                            | 0.007                                | 0.002                                        | 2.439        |
| 19    | LURNER      | -0.409                | 124.268                               | 2.647                            | 0.005                                | 0.002                                        | 2.697        |
| 20    | LURNOB      | -0.585                | 137.678                               | 2.507                            | 0.006                                | 0.002                                        | 2.542        |
| 21    | LURNOB01    | -0.568                | 134.332                               | 2.580                            | 0.005                                | 0.002                                        | 2.620        |
| 22    | LURNOB02    | -0.481                | 134.179                               | 2.520                            | 0.006                                | 0.002                                        | 2.558        |
| 23    | MIDXIH01    | -1.168                | 122.683                               | 2.624                            | 0.005                                | 0.002                                        | 2.683        |
| 24    | NECMUD01    | -0.220                | 143.868                               | 2.384                            | 0.008                                | 0.002                                        | 2.412        |
| 25    | OYONUO      | 0.061                 | 140.187                               | 2.386                            | 0.009                                | 0.003                                        | 2.412        |
| 26    | PACWUP      | 0.714                 | 153.057                               | 2.451                            | 0.006                                | 0.002                                        | 2.477        |
| 27    | PACXAW      | 0.714                 | 153.057                               | 2.451                            | 0.008                                | 0.002                                        | 2.367        |
| 28    | RADFUA      | -3.934                | 153.582                               | 2.340                            | 0.009                                | 0.003                                        | 2.429        |
| 29    | RADGAH      | -2.166                | 160.638                               | 2.368                            | 0.008                                | 0.002                                        | 2.397        |

**Table S2:** Energies and Topological Parameters corresponding to molecules having  $\text{--C}\equiv\text{C--H}\cdots\text{O--C}$  interactions (Search 8)

| S.no. | CSD REFCODE | $\Delta E$ (kcal/mol) | $\angle\text{C--H}\cdots\text{O}$ (°) | $d_{\text{H}\cdots\text{O}}$ (Å) | $\rho$ ( $\text{e}\text{\AA}^{-3}$ ) | $\nabla^2\rho$ ( $\text{e}\text{\AA}^{-5}$ ) | $R_{ij}$ (Å) |
|-------|-------------|-----------------------|---------------------------------------|----------------------------------|--------------------------------------|----------------------------------------------|--------------|
| 1     | ACIXOC      | -1.278                | 145.044                               | 2.459                            | 0.009                                | 0.002                                        | 2.486        |
| 2     | ACOTIY      | -0.227                | 139.241                               | 2.610                            | 0.007                                | 0.002                                        | 2.579        |
| 3     | AHUHOC      | -1.560                | 155.217                               | 2.244                            | 0.014                                | 0.003                                        | 2.270        |
| 4     | ANOQAX      | -2.694                | 167.553                               | 2.247                            | 0.016                                | 0.004                                        | 2.217        |
| 5     | BAFXUF      | 0.243                 | 121.711                               | 2.680                            | 0.012                                | 0.003                                        | 2.366        |
| 6     | CIZFAV      | 0.272                 | 132.227                               | 2.625                            | 0.005                                | 0.001                                        | 2.744        |
| 7     | DERRIC      | -0.154                | 141.138                               | 2.662                            | 0.008                                | 0.002                                        | 2.546        |
| 8     | DEQIF       | 0.232                 | 134.863                               | 2.697                            | 0.014                                | 0.004                                        | 2.329        |
| 9     | DOTTIQ      | -0.785                | 140.356                               | 2.415                            | 0.010                                | 0.002                                        | 2.443        |
| 10    | ETYXUR      | -0.636                | 115.943                               | 2.674                            | 0.007                                | 0.002                                        | 2.774        |
| 11    | FISSOS      | -0.575                | 106.154                               | 2.715                            | 0.012                                | 0.003                                        | 2.310        |
| 12    | GUSYUQ      | -0.119                | 166.028                               | 2.250                            | 0.012                                | 0.003                                        | 2.281        |
| 13    | HEZVEN      | -0.539                | 147.405                               | 2.409                            | 0.010                                | 0.002                                        | 2.441        |
| 14    | HIWSAH      | -1.200                | 165.002                               | 2.450                            | 0.009                                | 0.002                                        | 2.478        |
| 15    | ICUQUT      | -1.268                | 171.704                               | 2.231                            | 0.014                                | 0.003                                        | 2.260        |
| 16    | ICURUU      | -1.267                | 171.016                               | 2.257                            | 0.013                                | 0.003                                        | 2.287        |
| 17    | ICUTEG      | -0.018                | 166.177                               | 2.309                            | 0.013                                | 0.003                                        | 2.338        |
| 18    | KAFYEV      | 1.089                 | 165.060                               | 2.247                            | 0.015                                | 0.003                                        | 2.278        |
| 19    | LEHJOB      | -1.879                | 158.270                               | 2.336                            | 0.011                                | 0.003                                        | 2.359        |
| 20    | LEMKIB      | 0.398                 | 144.885                               | 2.312                            | 0.012                                | 0.003                                        | 2.804        |
| 21    | NEPXUC      | -1.051                | 161.453                               | 2.235                            | 0.015                                | 0.003                                        | 2.264        |
| 22    | ACEHEW      | -0.865                | 165.168                               | 2.346                            | 0.010                                | 0.002                                        | 2.376        |
| 23    | AMELUC      | -1.292                | 176.660                               | 2.318                            | 0.011                                | 0.003                                        | 2.346        |
| 24    | AYOHOL      | -2.046                | 168.548                               | 2.217                            | 0.015                                | 0.003                                        | 2.242        |
| 25    | AYOHOLO1    | -1.899                | 170.644                               | 2.246                            | 0.014                                | 0.003                                        | 2.273        |
| 26    | BAFPEF      | -4.438                | 160.379                               | 2.289                            | 0.011                                | 0.003                                        | 2.315        |
| 27    | CEKGAD      | 0.343                 | 162.620                               | 2.273                            | 0.011                                | 0.003                                        | 2.300        |
| 28    | CEKGAD      | 0.343                 | 162.620                               | 2.273                            | 0.010                                | 0.003                                        | 2.347        |
| 29    | CEYJAT      | -0.825                | 158.335                               | 2.654                            | 0.005                                | 0.001                                        | 2.682        |
| 30    | DADFEW      | -2.069                | 157.908                               | 2.393                            | 0.009                                | 0.002                                        | 2.423        |
| 31    | DAPXAX      | -7.882                | 162.130                               | 2.505                            | 0.006                                | 0.002                                        | 2.579        |
| 32    | DEMDUV      | -0.646                | 132.989                               | 2.460                            | 0.009                                | 0.002                                        | 2.490        |
| 33    | DEMDUV      | -0.646                | 162.641                               | 2.295                            | 0.012                                | 0.003                                        | 2.325        |
| 34    | DIJLAK      | -2.753                | 171.083                               | 2.188                            | 0.014                                | 0.003                                        | 2.215        |
| 35    | DIVDEV      | -1.455                | 166.875                               | 2.427                            | 0.008                                | 0.002                                        | 2.455        |
| 36    | DOXNAG      | -1.072                | 144.659                               | 2.451                            | 0.008                                | 0.002                                        | 2.478        |
| 37    | DURKEJ      | -1.083                | 146.705                               | 2.421                            | 0.010                                | 0.002                                        | 2.451        |

**Table S3:** Energies and Topological Parameters corresponding to molecules having  $\text{C}\equiv\text{C}\cdots\text{H}\cdots\text{N}\cdots\text{C}$  interactions (Search 9)

| S.no. | CSD REFCODE | $\Delta E$ (kcal/mol) | $\angle\text{C-H}\cdots\text{N}$ (°) | $d_{\text{H}\cdots\text{N}}$ (Å) | $\rho$ ( $\text{e}\text{\AA}^{-3}$ ) | $\nabla^2\rho$ ( $\text{e}\text{\AA}^{-5}$ ) | $R_{ij}$ (Å) |
|-------|-------------|-----------------------|--------------------------------------|----------------------------------|--------------------------------------|----------------------------------------------|--------------|
| 1     | CUFFOB      | -0.917                | 144.044                              | 2.386                            | 0.013                                | 0.003                                        | 2.417        |
| 2     | FEYSUZ      | 1.532                 | 112.639                              | 2.725                            | 0.007                                | 0.002                                        | 2.899        |
| 3     | FUCVOO      | -1.586                | 168.981                              | 2.507                            | 0.010                                | 0.002                                        | 2.538        |
| 4     | HEKSAU      | -1.093                | 163.323                              | 2.443                            | 0.012                                | 0.002                                        | 2.473        |
| 5     | IZAQIK      | -2.594                | 163.11                               | 2.514                            | 0.014                                | 0.003                                        | 2.753        |
| 6     | LURMOA      | 0.730                 | 159.663                              | 2.565                            | 0.008                                | 0.002                                        | 2.600        |
| 7     | OBUBUK      | 0.918                 | 145.018                              | 2.673                            | 0.007                                | 0.002                                        | 2.699        |
| 8     | UYIREB      | -0.217                | 139.424                              | 2.710                            | 0.006                                | 0.001                                        | 2.742        |
| 9     | XAZKAN      | -0.993                | 156.932                              | 2.326                            | 0.013                                | 0.003                                        | 2.358        |
| 10    | XOZFUP      | 1.200                 | 152.356                              | 2.504                            | 0.008                                | 0.002                                        | 2.630        |
| 11    | ZAZQOI      | -0.549                | 154.467                              | 2.498                            | 0.009                                | 0.002                                        | 2.533        |
| 12    | ZEMFUW      | -0.200                | 173.026                              | 2.307                            | 0.016                                | 0.003                                        | 2.338        |
| 13    | ACIYAP      | -0.526                | 159.725                              | 2.329                            | 0.015                                | 0.003                                        | 2.357        |
| 14    | ACIYIX      | -1.113                | 143.013                              | 2.504                            | 0.010                                | 0.002                                        | 2.538        |
| 15    | AQOSAD      | 0.279                 | 139.068                              | 2.723                            | 0.006                                | 0.001                                        | 2.758        |
| 16    | BOCHOT      | 0.083                 | 142.224                              | 2.625                            | 0.008                                | 0.002                                        | 2.656        |
| 17    | BOCHUZ      | -2.827                | 168.153                              | 2.324                            | 0.012                                | 0.003                                        | 2.363        |
| 18    | BOCIAH      | -3.847                | 177.917                              | 2.215                            | 0.015                                | 0.004                                        | 2.254        |
| 19    | DUCYUW      | -1.726                | 176.457                              | 2.543                            | 0.011                                | 0.002                                        | 2.463        |
| 20    | FEYSUZ      | 1.515                 | 112.639                              | 2.725                            | 0.007                                | 0.002                                        | 2.899        |
| 21    | HIMFES      | 2.172                 | 165.324                              | 2.349                            | 0.013                                | 0.003                                        | 2.379        |
| 22    | IZAQIK      | -2.610                | 171.439                              | 2.300                            | 0.014                                | 0.003                                        | 2.331        |
| 23    | JELTUP      | -2.434                | 156.989                              | 2.430                            | 0.011                                | 0.002                                        | 2.457        |
| 24    | OXIRUK      | -1.464                | 155.995                              | 2.584                            | 0.008                                | 0.002                                        | 2.611        |
| 25    | WEDWAE      | -1.081                | 137.787                              | 2.475                            | 0.010                                | 0.002                                        | 2.508        |
| 26    | XAZROH      | 0.018                 | 153.488                              | 2.652                            | 0.008                                | 0.002                                        | 2.681        |
| 27    | XOZFUP      | 1.200                 | 152.356                              | 2.504                            | 0.008                                | 0.002                                        | 2.630        |
| 28    | AFONUG01    | -3.746                | 153.767                              | 2.510                            | 0.008                                | 0.002                                        | 2.544        |

|    |        |        |         |       |       |       |       |
|----|--------|--------|---------|-------|-------|-------|-------|
| 29 | BIPFAJ | -2.161 | 158.981 | 2.361 | 0.011 | 0.003 | 2.388 |
| 30 | CAACTY | -3.022 | 178.421 | 2.350 | 0.011 | 0.003 | 2.378 |
| 31 | EFAVOA | -0.862 | 171.739 | 2.530 | 0.008 | 0.002 | 2.564 |
| 32 | EMUQOU | -0.408 | 172.608 | 2.376 | 0.011 | 0.003 | 2.409 |
| 33 | EMUREL | -3.478 | 165.096 | 2.451 | 0.009 | 0.002 | 2.482 |
| 34 | ESUQOZ | 0.293  | 141.686 | 2.524 | 0.008 | 0.002 | 2.556 |
| 35 | FADZOD | -2.573 | 155.233 | 2.405 | 0.010 | 0.002 | 2.435 |
| 36 | GURMUC | -1.273 | 166.156 | 2.631 | 0.006 | 0.001 | 2.668 |
| 37 | LUYLOI | -8.469 | 124.521 | 2.440 | 0.010 | 0.003 | 2.491 |
| 38 | NIFFIV | -1.652 | 137.784 | 2.685 | 0.006 | 0.002 | 2.720 |
| 39 | PUQSIG | -1.950 | 161.863 | 2.582 | 0.007 | 0.002 | 2.610 |
| 40 | QUNPOG | -0.402 | 147.060 | 2.432 | 0.010 | 0.002 | 2.462 |
| 41 | VASLEK | -1.844 | 167.602 | 2.442 | 0.009 | 0.002 | 2.475 |
| 42 | WIQQOE | -3.302 | 166.945 | 2.320 | 0.012 | 0.003 | 2.344 |
| 43 | WOWMIH | -1.519 | 156.120 | 2.469 | 0.009 | 0.002 | 2.502 |

**Table S4:** Energies and Topological Parameters corresponding to molecules having –O–H...F–C interactions (Search 10)

| S.no. | CSD REFCODE | $\Delta E$ (kcal/mol) | $\angle O-H \cdots F$ (°) | $d_{H \cdots F}$ (Å) | $\rho$ (eÅ <sup>-3</sup> ) | $\nabla^2\rho$ (eÅ <sup>-5</sup> ) | $R_{ij}$ (Å) |
|-------|-------------|-----------------------|---------------------------|----------------------|----------------------------|------------------------------------|--------------|
| 1     | BUFQAX      | 0.071                 | 157.954                   | 2.098                | 0.015                      | 0.004                              | 2.146        |
| 2     | CURKIM      | -2.919                | 159.129                   | 2.082                | 0.015                      | 0.004                              | 2.135        |
| 3     | KOVCAZ      | -0.789                | 152.655                   | 2.044                | 0.016                      | 0.004                              | 2.076        |
| 4     | LEWYER      | -3.139                | 142.738                   | 2.082                | 0.018                      | 0.005                              | 2.114        |
| 5     | LEWYER2     | 2.641                 | 150.331                   | 2.053                | 0.017                      | 0.004                              | 2.124        |
| 6     | TUPBOW      | -1.508                | 163.299                   | 2.080                | 0.016                      | 0.004                              | 2.128        |
| 7     | ZUCSOI      | -5.966                | 163.228                   | 2.071                | 0.017                      | 0.004                              | 2.119        |
| 8     | NUJQUE      | -4.536                | 173.516                   | 2.024                | 0.016                      | 0.004                              | 2.066        |
| 9     | NIBVAY      | -0.892                | 151.576                   | 2.064                | 0.016                      | 0.004                              | 2.114        |
| 10    | HIFMOC      | -1.247                | 129.474                   | 2.165                | 0.013                      | 0.004                              | 2.210        |
| 11    | LAWQUV01    | -4.491                | 151.591                   | 2.188                | 0.011                      | 0.004                              | 3.036        |
| 12    | MAVKUP      | -0.724                | 172.649                   | 2.194                | 0.011                      | 0.003                              | 2.595        |

|    |          |         |         |       |       |       |       |
|----|----------|---------|---------|-------|-------|-------|-------|
| 13 | MONGON   | -8.437  | 166.763 | 2.139 | 0.012 | 0.003 | 2.229 |
| 14 | TERRUG   | -8.128  | 163.585 | 2.131 | 0.014 | 0.004 | 2.181 |
| 15 | WEDSUW   | 0.397   | 160.300 | 2.143 | 0.013 | 0.004 | 2.201 |
| 16 | XEQBAZ   | 0.345   | 175.012 | 2.199 | 0.011 | 0.003 | 2.250 |
| 17 | CEHCUC   | -0.264  | 145.110 | 2.209 | 0.012 | 0.003 | 2.257 |
| 18 | CEVTIJ   | -3.125  | 144.884 | 2.291 | 0.009 | 0.003 | 2.336 |
| 19 | DIVGUN   | -12.068 | 133.001 | 2.264 | 0.009 | 0.003 | 2.308 |
| 20 | EDIHIL   | -8.983  | 127.385 | 2.232 | 0.011 | 0.003 | 2.275 |
| 21 | EYURUO   | 0.829   | 132.630 | 2.206 | 0.010 | 0.003 | 2.236 |
| 22 | HUVVIF   | -0.016  | 133.682 | 2.264 | 0.009 | 0.003 | 2.312 |
| 23 | LESJUP   | -1.198  | 147.181 | 2.293 | 0.026 | 0.007 | 1.952 |
| 24 | MATSEG   | -3.062  | 122.094 | 2.298 | 0.010 | 0.003 | 2.326 |
| 25 | ABENEB01 | 0.735   | 134.177 | 2.382 | 0.007 | 0.002 | 2.427 |
| 26 | BUQZIY   | -1.461  | 169.994 | 2.334 | 0.007 | 0.002 | 2.393 |
| 27 | CUQTUF   | -1.166  | 168.617 | 2.304 | 0.009 | 0.003 | 2.350 |
| 28 | FIYDUN   | -1.074  | 143.443 | 2.392 | 0.006 | 0.002 | 2.441 |
| 29 | HALNOZ   | -1.677  | 118.683 | 2.346 | 0.009 | 0.003 | 2.398 |
| 30 | KIGGAL   | -6.092  | 135.953 | 2.371 | 0.007 | 0.003 | 2.418 |
| 31 | LONGIH   | 0.449   | 141.434 | 2.378 | 0.007 | 0.002 | 2.440 |
| 32 | MECXUN   | 2.276   | 137.608 | 2.365 | 0.007 | 0.002 | 2.409 |
| 33 | LILZIT   | -1.275  | 135.279 | 2.404 | 0.007 | 0.002 | 2.447 |
| 34 | ABIHOL   | -0.105  | 98.085  | 2.586 | 0.009 | 0.003 | 2.587 |
| 35 | AXEGUH   | -0.287  | 101.320 | 2.567 | 0.005 | 0.002 | 2.646 |

**Table S5:** Energies and Topological Parameters corresponding to molecules having –N–H...F–C interactions (Search 11)

| S.no. | CSD REFCODE | $\Delta E$ (kcal/mol) | $\angle N-H \cdots F$ (°) | $d_{H \cdots F}$ (Å) | $\rho$ (eÅ <sup>-3</sup> ) | $\nabla^2 \rho$ (eÅ <sup>-5</sup> ) | $R_{ij}$ (Å) |
|-------|-------------|-----------------------|---------------------------|----------------------|----------------------------|-------------------------------------|--------------|
| 1     | AZITAH      | -2.517                | 155.881                   | 2.042                | 0.018                      | 0.005                               | 2.079        |
| 2     | AZITUB      | -8.376                | 137.770                   | 2.037                | 0.019                      | 0.005                               | 2.059        |
| 3     | CUQTIT      | -11.082               | 147.898                   | 2.092                | 0.016                      | 0.004                               | 2.129        |
| 4     | DABZAJ      | -14.879               | 157.651                   | 2.006                | 0.020                      | 0.005                               | 2.044        |

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|----|----------|---------|---------|-------|-------|-------|-------|
| 5  | DATZAA   | -12.745 | 129.25  | 2.171 | 0.018 | 0.005 | 2.082 |
| 6  | DATZAA02 | -7.173  | 154.732 | 2.067 | 0.017 | 0.004 | 2.105 |
| 7  | EBECOH   | -7.597  | 163.238 | 2.076 | 0.017 | 0.004 | 2.115 |
| 8  | EGAGID   | -1.911  | 142.70  | 2.148 | 0.015 | 0.004 | 2.136 |
| 9  | GADLUU   | -11.666 | 147.674 | 2.005 | 0.019 | 0.005 | 2.042 |
| 10 | BIPRIF   | -1.596  | 169.923 | 2.191 | 0.011 | 0.003 | 2.230 |
| 11 | FOHSIE   | -6.272  | 161.778 | 2.109 | 0.014 | 0.004 | 2.146 |
| 12 | GARYOP   | -7.692  | 161.478 | 2.112 | 0.015 | 0.004 | 2.150 |
| 13 | HAQZII   | -32.331 | 157.157 | 2.107 | 0.016 | 0.004 | 2.146 |
| 14 | HOTBUO   | -0.110  | 167.093 | 2.194 | 0.011 | 0.003 | 2.232 |
| 15 | HUPVUL   | -1.894  | 157.598 | 2.123 | 0.014 | 0.004 | 2.161 |
| 16 | JILCUF   | -3.628  | 143.240 | 2.112 | 0.015 | 0.004 | 2.148 |
| 17 | OBEPJ01  | -10.965 | 147.942 | 2.184 | 0.013 | 0.004 | 2.219 |
| 18 | CIFWIA   | -2.116  | 166.547 | 2.267 | 0.010 | 0.003 | 2.308 |
| 19 | CUQTUF   | -2.947  | 127.074 | 2.247 | 0.011 | 0.003 | 2.299 |
| 20 | EDAWAH   | 1.404   | 158.371 | 2.221 | 0.011 | 0.003 | 2.255 |
| 21 | EGAHAW   | -3.087  | 126.554 | 2.298 | 0.011 | 0.003 | 2.351 |
| 22 | EVIFEV   | -0.033  | 156.129 | 2.275 | 0.009 | 0.003 | 2.311 |
| 23 | HEPMIZ   | -6.267  | 121.924 | 2.267 | 0.011 | 0.003 | 2.331 |
| 24 | HIGWON   | -8.374  | 126.212 | 2.266 | 0.011 | 0.003 | 2.313 |
| 25 | LEFWIF   | -3.153  | 150.259 | 2.204 | 0.013 | 0.004 | 2.246 |
| 26 | MOCsAA   | -2.159  | 159.191 | 2.255 | 0.010 | 0.003 | 2.592 |
| 27 | AGETEP   | -0.471  | 170.049 | 2.329 | 0.009 | 0.003 | 2.364 |
| 28 | AMUDiy   | -1.364  | 163.369 | 2.364 | 0.008 | 0.002 | 2.403 |
| 29 | BORXUC   | -1.620  | 135.707 | 2.378 | 0.008 | 0.003 | 2.417 |
| 30 | COZTAP   | -0.588  | 164.364 | 2.372 | 0.008 | 0.002 | 2.404 |
| 31 | DEDZAQ   | -5.686  | 147.967 | 2.358 | 0.008 | 0.003 | 2.400 |
| 32 | EWAZEK   | -0.812  | 166.496 | 2.355 | 0.007 | 0.002 | 2.392 |
| 33 | EZONoy   | -0.777  | 126.393 | 2.388 | 0.008 | 0.003 | 2.438 |
| 34 | ACOKAI   | -10.082 | 173.973 | 2.448 | 0.005 | 0.002 | 2.484 |

|    |        |         |         |       |       |       |       |
|----|--------|---------|---------|-------|-------|-------|-------|
| 35 | AGETEP | -0.471  | 124.911 | 2.448 | 0.009 | 0.003 | 2.364 |
| 36 | AZOZEV | -0.976  | 138.372 | 2.404 | 0.008 | 0.002 | 2.448 |
| 37 | CINXEF | -0.106  | 136.474 | 2.445 | 0.007 | 0.002 | 2.484 |
| 38 | COZTAP | -1.443  | 140.420 | 2.426 | 0.008 | 0.002 | 2.453 |
| 39 | EGAGOJ | -3.420  | 156.056 | 2.440 | 0.005 | 0.002 | 2.625 |
| 40 | EWAZEK | 0.537   | 167.363 | 2.437 | 0.007 | 0.002 | 2.469 |
| 41 | GANBEF | -0.003  | 164.122 | 2.486 | 0.005 | 0.002 | 2.524 |
| 42 | ACOKAI | -10.082 | 135.542 | 2.593 | 0.006 | 0.002 | 2.484 |
| 43 | AYOPEK | -1.170  | 142.603 | 2.586 | 0.005 | 0.002 | 2.625 |
| 44 | CAFVAG | -0.392  | 135.559 | 2.574 | 0.005 | 0.002 | 2.608 |
| 45 | FABBAN | -0.131  | 129.159 | 2.562 | 0.006 | 0.002 | 2.681 |
| 46 | GADLOQ | -1.012  | 132.379 | 2.577 | 0.006 | 0.002 | 2.609 |
| 47 | GISVOU | -1.882  | 149.151 | 2.591 | 0.005 | 0.002 | 2.625 |
| 48 | AMADEZ | -0.024  | 122.357 | 2.678 | 0.005 | 0.001 | 2.870 |
| 49 | AMARUD | 0.061   | 132.028 | 2.676 | 0.004 | 0.001 | 2.730 |
| 50 | CIJGIL | -1.935  | 126.990 | 2.670 | 0.005 | 0.001 | 2.844 |
| 51 | CINWOO | 0.990   | 122.260 | 2.635 | 0.013 | 0.004 | 2.290 |
| 52 | CINXEF | 0.760   | 124.177 | 2.668 | 0.011 | 0.003 | 2.388 |
| 53 | DAFGUP | -0.063  | 172.070 | 2.661 | 0.004 | 0.001 | 2.701 |
| 54 | DAFMUV | -0.449  | 121.581 | 2.688 | 0.004 | 0.001 | 2.785 |

### 3. Energies at the Critical Point

**Table S6-S10** provides a comprehensive list of kinetic ( $G(r_{c,p})$ ), potential ( $V(r_{c,p})$ ), hydrogen bond energy ( $E_{HB}$ ) and total energy densities ( $E(r_{c,p})$ ) at the bond critical point for the dimers formed through the  $-C\equiv C-H\cdots X-C$  (where  $X = F, N, O$ ) and  $Y-H\cdots F-C$  (where  $Y = N, O$ ) hydrogen bonds.

Table S6 Topological Energy Densities corresponding to molecules having  $-C\equiv C-H\cdots F-C$  interactions (Searches 1-4)

| S.no. | CSD Ref Code | $G(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $V(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E_{HB}$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) |
|-------|--------------|----------------------------------------------------------|----------------------------------------------------------|----------------------------------------------------------|------------------------------------------------------|
| 1     | AGAVOU       | 0.019145                                                 | -0.02293                                                 | -0.00689                                                 | 0.011467                                             |
| 2     | ASIKUJ       | 0.010416                                                 | -0.01132                                                 | -0.00259                                                 | 0.005662                                             |
| 3     | AYOHUR       | 0.013946                                                 | -0.01616                                                 | -0.00447                                                 | 0.008079                                             |
| 4     | COJPIC       | 0.022481                                                 | -0.02735                                                 | -0.00851                                                 | 0.013676                                             |
| 5     | FEYSEK       | 0.005523                                                 | -0.00545                                                 | -0.00082                                                 | 0.002723                                             |
| 6     | FEYSIO       | 0.010773                                                 | -0.01178                                                 | -0.00275                                                 | 0.005889                                             |
| 7     | FEYSUA       | 0.007459                                                 | -0.0077                                                  | -0.00145                                                 | 0.00385                                              |
| 8     | FEYTAH       | 0.032865                                                 | -0.04212                                                 | -0.01457                                                 | 0.021059                                             |
| 9     | FEYTEL       | 0.025904                                                 | -0.03216                                                 | -0.01045                                                 | 0.016082                                             |
| 10    | FEYTIP       | 0.025849                                                 | -0.03222                                                 | -0.01055                                                 | 0.016108                                             |
| 11    | FEYTOV       | 0.032542                                                 | -0.04147                                                 | -0.01419                                                 | 0.020735                                             |
| 12    | FITYAL01     | 0.036641                                                 | -0.04744                                                 | -0.01672                                                 | 0.023719                                             |
| 13    | FITYOZ       | 0.023462                                                 | -0.0288                                                  | -0.00913                                                 | 0.014401                                             |
| 14    | GEKGIP       | 0.042805                                                 | -0.05657                                                 | -0.02068                                                 | 0.028284                                             |
| 15    | GEKGOV01     | 0.036768                                                 | -0.04777                                                 | -0.01695                                                 | 0.023885                                             |
| 16    | KEQLAU       | 0.024276                                                 | -0.02994                                                 | -0.00959                                                 | 0.014971                                             |
| 17    | LEBTAQ02     | 0.04359                                                  | -0.05763                                                 | -0.02108                                                 | 0.028813                                             |
| 18    | LEBTAQ03     | 0.027904                                                 | -0.03483                                                 | -0.01144                                                 | 0.017416                                             |
| 19    | LURNER       | 0.017804                                                 | -0.02094                                                 | -0.00601                                                 | 0.010468                                             |
| 20    | LURNOB       | 0.022656                                                 | -0.02734                                                 | -0.00835                                                 | 0.013671                                             |
| 21    | LURNOB01     | 0.018154                                                 | -0.02125                                                 | -0.00603                                                 | 0.010625                                             |
| 22    | LURNOB02     | 0.022184                                                 | -0.02673                                                 | -0.00813                                                 | 0.013364                                             |
| 23    | MIDXIH01     | 0.018336                                                 | -0.02149                                                 | -0.00612                                                 | 0.010743                                             |

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| S.no. | CSD Ref Code | $G(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $V(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E_{HB}$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) |
|-------|--------------|----------------------------------------------------------|----------------------------------------------------------|----------------------------------------------------------|------------------------------------------------------|
| 24    | NECMUD01     | 0.035277                                                 | -0.04542                                                 | -0.01585                                                 | 0.022711                                             |
| 25    | OYONUO       | 0.040046                                                 | -0.0526                                                  | -0.01903                                                 | 0.0263                                               |
| 26    | PACWUP       | 0.024346                                                 | -0.02963                                                 | -0.00922                                                 | 0.014814                                             |
| 27    | PACXAW       | 0.035277                                                 | -0.04505                                                 | -0.01547                                                 | 0.022524                                             |
| 28    | RADFUA       | 0.041384                                                 | -0.05423                                                 | -0.01954                                                 | 0.027116                                             |
| 29    | RADGAH       | 0.03569                                                  | -0.04633                                                 | -0.01642                                                 | 0.023167                                             |

**Table S7** Topological Energy Densities corresponding to molecules having  $\text{C}\equiv\text{C}\cdots\text{H}\cdots\text{O}\cdots\text{C}$  interactions (Search 8)

| S.no. | CSD Ref Code | $G(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $V(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E_{\text{HB}}$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) |
|-------|--------------|----------------------------------------------------------|----------------------------------------------------------|----------------------------------------------------------|-------------------------------------------------------------|
| 1     | ACIXOC       | 0.034548                                                 | -0.05618                                                 | -0.02163                                                 | 0.028088                                                    |
| 2     | ACOTIY       | 0.022919                                                 | -0.03551                                                 | -0.01259                                                 | 0.017753                                                    |
| 3     | AHUHOC       | 0.066517                                                 | -0.11449                                                 | -0.04797                                                 | 0.057243                                                    |
| 4     | ANOQAX       | 0.083287                                                 | -0.14356                                                 | -0.06027                                                 | 0.07178                                                     |
| 5     | BAFXUF       | 0.052498                                                 | -0.08929                                                 | -0.03679                                                 | 0.044645                                                    |
| 6     | CIZFAV       | 0.016055                                                 | -0.02404                                                 | -0.00798                                                 | 0.012018                                                    |
| 7     | DERRIC       | 0.027422                                                 | -0.04353                                                 | -0.01611                                                 | 0.021765                                                    |
| 8     | DEQIF        | 0.069625                                                 | -0.119                                                   | -0.04937                                                 | 0.059498                                                    |
| 9     | DOTTIQ       | 0.039011                                                 | -0.06416                                                 | -0.02515                                                 | 0.032078                                                    |
| 10    | ETXUR        | 0.024577                                                 | -0.03885                                                 | -0.01427                                                 | 0.019425                                                    |
| 11    | FISSOS       | 0.054773                                                 | -0.09282                                                 | -0.03804                                                 | 0.046408                                                    |
| 12    | GUSYUQ       | 0.056131                                                 | -0.09475                                                 | -0.03862                                                 | 0.047375                                                    |
| 13    | HEZVEN       | 0.039384                                                 | -0.06538                                                 | -0.026                                                   | 0.032692                                                    |
| 14    | HIWSAH       | 0.03653                                                  | -0.06027                                                 | -0.02374                                                 | 0.030134                                                    |
| 15    | ICUQUT       | 0.063555                                                 | -0.10876                                                 | -0.0452                                                  | 0.054378                                                    |
| 16    | ICURUU       | 0.057866                                                 | -0.09828                                                 | -0.04042                                                 | 0.049142                                                    |
| 17    | ICUTEG       | 0.056191                                                 | -0.0958                                                  | -0.03961                                                 | 0.047899                                                    |
| 18    | KAFYEV       | 0.07082                                                  | -0.1234                                                  | -0.05258                                                 | 0.061701                                                    |
| 19    | LEHJOB       | 0.047121                                                 | -0.07899                                                 | -0.03187                                                 | 0.039497                                                    |
| 20    | LEMKIB       | 0.055086                                                 | -0.09309                                                 | -0.03801                                                 | 0.046546                                                    |
| 21    | NEPXUC       | 0.074837                                                 | -0.13091                                                 | -0.05608                                                 | 0.065457                                                    |
| 22    | ACEHEW       | 0.040728                                                 | -0.06714                                                 | -0.02642                                                 | 0.033572                                                    |
| 23    | AMELUC       | 0.045255                                                 | -0.07553                                                 | -0.03028                                                 | 0.037767                                                    |
| 24    | AYOHOL       | 0.073929                                                 | -0.13001                                                 | -0.05608                                                 | 0.065006                                                    |
| 25    | AYOHOLO1     | 0.067257                                                 | -0.11714                                                 | -0.04988                                                 | 0.058568                                                    |
| 26    | BAFPEF       | 0.04433                                                  | -0.07281                                                 | -0.02848                                                 | 0.036403                                                    |
| 27    | CEKGAD       | 0.0475                                                   | -0.07837                                                 | -0.03087                                                 | 0.039183                                                    |
| 28    | CEKGAD       | 0.040878                                                 | -0.06673                                                 | -0.02586                                                 | 0.033367                                                    |
| 29    | CEYJAT       | 0.014225                                                 | -0.02074                                                 | -0.00651                                                 | 0.010369                                                    |
| 30    | DADFEW       | 0.033438                                                 | -0.05383                                                 | -0.02039                                                 | 0.026915                                                    |
| 31    | DAPXAX       | 0.021356                                                 | -0.03315                                                 | -0.0118                                                  | 0.016577                                                    |
| 32    | DEMDUV       | 0.03313                                                  | -0.05339                                                 | -0.02026                                                 | 0.026695                                                    |
| 33    | DEMDUV       | 0.049546                                                 | -0.08307                                                 | -0.03353                                                 | 0.041535                                                    |
| 34    | DIJLAK       | 0.068243                                                 | -0.11746                                                 | -0.04922                                                 | 0.058729                                                    |
| 35    | DIVDEV       | 0.029241                                                 | -0.0466                                                  | -0.01736                                                 | 0.023298                                                    |
| 36    | DOXNAG       | 0.029919                                                 | -0.04774                                                 | -0.01782                                                 | 0.02387                                                     |
| 37    | DURKEJ       | 0.037239                                                 | -0.06125                                                 | -0.02401                                                 | 0.030623                                                    |

**Table S8** Topological Energy Densities corresponding to molecules having  $\text{--C}\equiv\text{C--H}\cdots\text{N--C}$  interactions (Search 9)

| S.no. | CSD Ref Code | $G(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $V(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E_{HB}$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) |
|-------|--------------|----------------------------------------------------------|----------------------------------------------------------|----------------------------------------------------------|------------------------------------------------------|
| 1     | CUFFOB       | 0.060041                                                 | -0.10442                                                 | -0.04438                                                 | 0.052211                                             |
| 2     | FEYSUZ       | 0.025075                                                 | -0.04041                                                 | -0.01534                                                 | 0.020207                                             |
| 3     | FUCVOO       | 0.041502                                                 | -0.07067                                                 | -0.02917                                                 | 0.035336                                             |
| 4     | HEKSAU       | 0.053222                                                 | -0.0927                                                  | -0.03948                                                 | 0.046352                                             |
| 5     | IZAQIK       | 0.062617                                                 | -0.1084                                                  | -0.04578                                                 | 0.054199                                             |
| 6     | LURMOA       | 0.030474                                                 | -0.05037                                                 | -0.0199                                                  | 0.025185                                             |
| 7     | OBUBUK       | 0.022508                                                 | -0.03615                                                 | -0.01364                                                 | 0.018073                                             |
| 8     | UYIREB       | 0.01882                                                  | -0.02987                                                 | -0.01105                                                 | 0.014933                                             |
| 9     | XAZKAN       | 0.060786                                                 | -0.10479                                                 | -0.044                                                   | 0.052395                                             |
| 10    | XOZFUP       | 0.027149                                                 | -0.04395                                                 | -0.01681                                                 | 0.021977                                             |
| 11    | ZAZQOI       | 0.033772                                                 | -0.0559                                                  | -0.02213                                                 | 0.02795                                              |
| 12    | ZEMFUW       | 0.079502                                                 | -0.14114                                                 | -0.06164                                                 | 0.07057                                              |
| 13    | ACIYAP       | 0.068895                                                 | -0.12099                                                 | -0.05209                                                 | 0.060493                                             |
| 14    | ACIYIX       | 0.036928                                                 | -0.06181                                                 | -0.02489                                                 | 0.030907                                             |
| 15    | AQOSAD       | 0.019383                                                 | -0.03071                                                 | -0.01133                                                 | 0.015355                                             |
| 16    | BOCHOT       | 0.025708                                                 | -0.04166                                                 | -0.01595                                                 | 0.020829                                             |
| 17    | BOCHUZ       | 0.053379                                                 | -0.09033                                                 | -0.03695                                                 | 0.045166                                             |
| 18    | BOCJAH       | 0.07569                                                  | -0.13069                                                 | -0.055                                                   | 0.065347                                             |
| 19    | DUCYUW       | 0.045341                                                 | -0.0772                                                  | -0.03186                                                 | 0.038599                                             |
| 20    | FEYSUZ       | 0.025075                                                 | -0.04041                                                 | -0.01534                                                 | 0.020207                                             |
| 21    | HIMFES       | 0.060015                                                 | -0.10389                                                 | -0.04388                                                 | 0.051945                                             |
| 22    | IZAQIK       | 0.062617                                                 | -0.1084                                                  | -0.04578                                                 | 0.054199                                             |
| 23    | JELTUP       | 0.046996                                                 | -0.08027                                                 | -0.03327                                                 | 0.040133                                             |
| 24    | OXIRUK       | 0.026307                                                 | -0.04262                                                 | -0.01632                                                 | 0.021312                                             |
| 25    | WEDWAE       | 0.041602                                                 | -0.0695                                                  | -0.02789                                                 | 0.034748                                             |
| 26    | XAZROH       | 0.025681                                                 | -0.04211                                                 | -0.01643                                                 | 0.021057                                             |
| 27    | XOZFUP       | 0.027149                                                 | -0.04395                                                 | -0.01681                                                 | 0.021977                                             |
| 28    | AFONUG01     | 0.027532                                                 | -0.04438                                                 | -0.01684                                                 | 0.022188                                             |
| 29    | BIPFAJ       | 0.046935                                                 | -0.07878                                                 | -0.03184                                                 | 0.039388                                             |
| 30    | CAACTY       | 0.048243                                                 | -0.08112                                                 | -0.03288                                                 | 0.040562                                             |
| 31    | EFAVOA       | 0.026262                                                 | -0.04236                                                 | -0.0161                                                  | 0.021181                                             |
| 32    | EMUQOU       | 0.043448                                                 | -0.07242                                                 | -0.02897                                                 | 0.036211                                             |
| 33    | EMUREL       | 0.034797                                                 | -0.05725                                                 | -0.02246                                                 | 0.028627                                             |
| 34    | ESUQOZ       | 0.028792                                                 | -0.04637                                                 | -0.01758                                                 | 0.023186                                             |
| 35    | FADZOD       | 0.040941                                                 | -0.06807                                                 | -0.02713                                                 | 0.034035                                             |
| 36    | GURMUC       | 0.019372                                                 | -0.03035                                                 | -0.01098                                                 | 0.015175                                             |
| 37    | LUYLOI       | 0.041745                                                 | -0.06836                                                 | -0.02661                                                 | 0.034178                                             |
| 38    | NIFFIV       | 0.018621                                                 | -0.02832                                                 | -0.0097                                                  | 0.014158                                             |
| 39    | PUQSIG       | 0.022955                                                 | -0.03644                                                 | -0.01348                                                 | 0.01822                                              |
| 40    | QUNPOG       | 0.037435                                                 | -0.06176                                                 | -0.02432                                                 | 0.030878                                             |
| 41    | VASLEK       | 0.035592                                                 | -0.05862                                                 | -0.02303                                                 | 0.029311                                             |
| 42    | WIQQOE       | 0.053534                                                 | -0.09149                                                 | -0.03796                                                 | 0.045745                                             |

**Table S9** Topological Energy Densities corresponding to molecules having –O–H···F–C interactions (Search 10)

| S.no. | CSD Ref Code | $G(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $V(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E(r_{c,p})$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) | $E_{HB}$<br>(Kcal <sup>-1</sup> bohr <sup>-3</sup> ) |
|-------|--------------|----------------------------------------------------------|----------------------------------------------------------|----------------------------------------------------------|------------------------------------------------------|
| 1     | BUFAQX       | 0.073536                                                 | -0.12398                                                 | -0.05045                                                 | 0.061992                                             |
| S.No. | CSD Ref Code | $G(r_{c,p})$                                             | $V(r_{c,p})$                                             | $E(r_{c,p})$                                             | $E_{HB}$                                             |
| 3     | KOVCAZ       | 0.080354                                                 | -0.13683                                                 | -0.05648                                                 | 0.068417                                             |
| 4     | LEWYER       | 0.100674                                                 | -0.17323                                                 | -0.07255                                                 | 0.086613                                             |
| 5     | LEWYER2      | 0.087563                                                 | -0.15013                                                 | -0.06257                                                 | 0.075065                                             |
| 6     | TUPBOW       | 0.08117                                                  | -0.13846                                                 | -0.05729                                                 | 0.06923                                              |
| 7     | ZUCSOI       | 0.08726                                                  | -0.15009                                                 | -0.06283                                                 | 0.075043                                             |
| 8     | NUJQUE       | 0.087162                                                 | -0.14903                                                 | -0.06187                                                 | 0.074517                                             |
| 9     | NIBVAY       | 0.087419                                                 | -0.14936                                                 | -0.06194                                                 | 0.074678                                             |
| 10    | HIFMOC       | 0.06273                                                  | -0.10268                                                 | -0.03995                                                 | 0.051342                                             |
| 11    | LAWQUV01     | 0.048634                                                 | -0.07678                                                 | -0.02815                                                 | 0.03839                                              |
| 12    | MAVKUP       | 0.049104                                                 | -0.0787                                                  | -0.0296                                                  | 0.03935                                              |
| 13    | MONGON       | 0.056485                                                 | -0.0932                                                  | -0.03672                                                 | 0.046601                                             |
| 14    | TERRUG       | 0.066325                                                 | -0.11105                                                 | -0.04473                                                 | 0.055527                                             |
| 15    | WEDSUW       | 0.060726                                                 | -0.09958                                                 | -0.03886                                                 | 0.049792                                             |
| 16    | XEQBAZ       | 0.046946                                                 | -0.07549                                                 | -0.02854                                                 | 0.037744                                             |
| 17    | CEHCUQ       | 0.054735                                                 | -0.0894                                                  | -0.03466                                                 | 0.044698                                             |
| 18    | CEVTIJ       | 0.038998                                                 | -0.06174                                                 | -0.02274                                                 | 0.030868                                             |
| 19    | DIVGUN       | 0.03588                                                  | -0.05597                                                 | -0.02009                                                 | 0.027985                                             |
| 20    | EDIHIL       | 0.048745                                                 | -0.07736                                                 | -0.02861                                                 | 0.038678                                             |
| 21    | EYURUO       | 0.044949                                                 | -0.07117                                                 | -0.02622                                                 | 0.035585                                             |
| 22    | HUVVIF       | 0.038573                                                 | -0.05973                                                 | -0.02116                                                 | 0.029867                                             |
| 23    | LESJUP       | 0.176239                                                 | -0.3127                                                  | -0.13646                                                 | 0.156351                                             |
| 24    | MATSEG       | 0.041661                                                 | -0.06579                                                 | -0.02413                                                 | 0.032895                                             |
| 25    | ABENEBO1     | 0.025846                                                 | -0.03734                                                 | -0.0115                                                  | 0.018672                                             |
| 26    | BUQZIY       | 0.025405                                                 | -0.03701                                                 | -0.01161                                                 | 0.018506                                             |
| 27    | CUQTUF       | 0.035003                                                 | -0.05459                                                 | -0.01959                                                 | 0.027297                                             |
| 28    | FIYDUN       | 0.023609                                                 | -0.03394                                                 | -0.01034                                                 | 0.016972                                             |
| 29    | HALNOZ       | 0.034841                                                 | -0.05314                                                 | -0.0183                                                  | 0.02657                                              |
| 30    | KIGGAL       | 0.028634                                                 | -0.04221                                                 | -0.01357                                                 | 0.021104                                             |
| 31    | LONGIH       | 0.026871                                                 | -0.03997                                                 | -0.0131                                                  | 0.019986                                             |
| 32    | MECXUN       | 0.027726                                                 | -0.04111                                                 | -0.01338                                                 | 0.020555                                             |
| 33    | LILZIT       | 0.026792                                                 | -0.03936                                                 | -0.01257                                                 | 0.019679                                             |
| 34    | ABIHOL       | 0.03381                                                  | -0.0522                                                  | -0.01839                                                 | 0.026099                                             |
| 35    | AXEGUH       | 0.01566                                                  | -0.02161                                                 | -0.00595                                                 | 0.010806                                             |

**Table S10** Topological Energy Densities corresponding to molecules having –N–H···F–C interactions (Search 11)

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|    |          | (Kcal <sup>-1</sup> bohr <sup>3</sup> ) | (Kcal <sup>-1</sup> bohr <sup>3</sup> ) | (Kcal <sup>-1</sup> bohr <sup>3</sup> ) | (Kcal <sup>-1</sup> bohr <sup>3</sup> ) |
|----|----------|-----------------------------------------|-----------------------------------------|-----------------------------------------|-----------------------------------------|
| 1  | AZITAH   | 0.09943                                 | -0.17253                                | -0.0731                                 | 0.086263                                |
| 2  | AZITUB   | 0.107133                                | -0.18603                                | -0.0789                                 | 0.093014                                |
| 3  | CUQTIT   | 0.084831                                | -0.1452                                 | -0.06037                                | 0.072599                                |
| 4  | DABZAJ   | 0.118871                                | -0.20911                                | -0.09024                                | 0.104555                                |
| 5  | DATZAA   | 0.101166                                | -0.17439                                | -0.07323                                | 0.087196                                |
| 6  | DATZAA02 | 0.089355                                | -0.15351                                | -0.06416                                | 0.076756                                |
| 7  | EBECOH   | 0.091946                                | -0.15924                                | -0.06729                                | 0.07962                                 |
| 8  | EGAGID   | 0.074877                                | -0.12661                                | -0.05174                                | 0.063306                                |
| 9  | GADLUU   | 0.107856                                | -0.18612                                | -0.07826                                | 0.093058                                |
| 10 | BIPRIF   | 0.049397                                | -0.08015                                | -0.03075                                | 0.040073                                |
| 11 | FOHSIE   | 0.071972                                | -0.12139                                | -0.04942                                | 0.060697                                |
| 12 | GARYOP   | 0.075426                                | -0.12841                                | -0.05299                                | 0.064206                                |
| 13 | HAQZII   | 0.084639                                | -0.14563                                | -0.06099                                | 0.072814                                |
| 14 | HOTBUO   | 0.051375                                | -0.08381                                | -0.03243                                | 0.041903                                |
| 15 | HUPVUL   | 0.070494                                | -0.1186                                 | -0.0481                                 | 0.059299                                |
| 16 | JILCUF   | 0.07955                                 | -0.13522                                | -0.05567                                | 0.067608                                |
| 17 | OBEPJ01  | 0.062377                                | -0.10429                                | -0.04191                                | 0.052143                                |
| 18 | CIFWIA   | 0.039334                                | -0.06205                                | -0.02271                                | 0.031023                                |
| 19 | CUQTUF   | 0.047799                                | -0.07604                                | -0.02824                                | 0.038019                                |
| 20 | EDAWAH   | 0.046211                                | -0.07477                                | -0.02855                                | 0.037383                                |
| 21 | EGAHAW   | 0.049303                                | -0.07963                                | -0.03032                                | 0.039814                                |
| 22 | EVIFEV   | 0.03831                                 | -0.0604                                 | -0.02209                                | 0.0302                                  |
| 23 | HEPMIZ   | 0.046762                                | -0.07405                                | -0.02729                                | 0.037025                                |
| 24 | HIGWON   | 0.048444                                | -0.07754                                | -0.0291                                 | 0.038772                                |
| 25 | LEFWIF   | 0.058544                                | -0.0966                                 | -0.03805                                | 0.048299                                |
| 26 | MOCsAA   | 0.041831                                | -0.06693                                | -0.0251                                 | 0.033465                                |
| 27 | AGETEP   | 0.037334                                | -0.05898                                | -0.02165                                | 0.029492                                |
| 28 | AMUDIY   | 0.030805                                | -0.0476                                 | -0.0168                                 | 0.023801                                |
| 29 | BORXUC   | 0.03278                                 | -0.05039                                | -0.01761                                | 0.025195                                |
| 30 | COZTAP   | 0.02923                                 | -0.04517                                | -0.01594                                | 0.022586                                |
| 31 | DEDZAQ   | 0.029469                                | -0.04444                                | -0.01497                                | 0.022218                                |
| 32 | EWAZEK   | 0.025448                                | -0.03746                                | -0.01201                                | 0.018729                                |
| 33 | EZONoy   | 0.031647                                | -0.04845                                | -0.0168                                 | 0.024225                                |
| 34 | ACOKAI   | 0.016044                                | -0.02225                                | -0.00621                                | 0.011125                                |
| 35 | AGETEP   | 0.037334                                | -0.05898                                | -0.02165                                | 0.029492                                |
| 36 | AZOZEV   | 0.02864                                 | -0.04355                                | -0.0149                                 | 0.021773                                |
| 37 | CINXEF   | 0.023418                                | -0.03444                                | -0.01103                                | 0.017222                                |
| 38 | COZTAP   | 0.028458                                | -0.04393                                | -0.01547                                | 0.021966                                |
| 39 | EGAGOJ   | 0.016305                                | -0.02289                                | -0.00659                                | 0.011446                                |
| 40 | EWAZEK   | 0.024195                                | -0.0363                                 | -0.0121                                 | 0.01815                                 |
| 41 | GANBEF   | 0.018542                                | -0.02626                                | -0.00772                                | 0.013129                                |
| 42 | ACOKAI   | 0.022099                                | -0.03219                                | -0.01009                                | 0.016095                                |
| 43 | AYOPEK   | 0.015648                                | -0.02166                                | -0.00601                                | 0.010831                                |
| 44 | CAFVAG   | 0.016691                                | -0.02355                                | -0.00686                                | 0.011777                                |
| 45 | FABBAN   | 0.018061                                | -0.0261                                 | -0.00804                                | 0.01305                                 |

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|    |        |          |          |          |          |
|----|--------|----------|----------|----------|----------|
| 46 | GADLOQ | 0.018816 | -0.02673 | -0.00792 | 0.013367 |
| 47 | GISVOU | 0.014384 | -0.01951 | -0.00512 | 0.009754 |
| 48 | AMADEZ | 0.01448  | -0.02038 | -0.0059  | 0.010189 |
| 49 | AMARUD | 0.011851 | -0.0157  | -0.00385 | 0.007849 |
| 50 | CIJGIL | 0.015954 | -0.0233  | -0.00735 | 0.01165  |
| 51 | CINWOO | 0.059283 | -0.0976  | -0.03831 | 0.048799 |
| 52 | CINXEF | 0.048709 | -0.07819 | -0.02948 | 0.039095 |
| 53 | DAFGUP | 0.010692 | -0.01383 | -0.00314 | 0.006917 |
| 54 | DAFMUV | 0.012564 | -0.01679 | -0.00422 | 0.008393 |