# Supporting Information

## Structural and Energetic Aspects of Adamantane and Memantine Derivatives of Sulfonamide Molecular Crystals: Experimental and Theoretical Characterisation

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## S1. Correlation between $d_{norm}^{\min}(HB)$ and hydrogen bond energies

Besides comparing the crystal structures at a qualitative level, Hirshfeld surface analysis can be suitable for constructing quantitative relationships. Thus, the minimum value of $d_{norm}$ in the region of hydrogen bonding, obtained from Hirshfeld surface analysis, displays a linear correlation with the N···O distance in crystal (Figure 8SI). Similar nature of dependencies presented in Figure 8SI and Figure 3 allows to use $d_{norm}^{\min}(HB)$ as a descriptor for assessing the hydrogen bond energy obtained from Mayo equation and QTAIMC analysis with accuracy higher than 1 kJ·mol$^{-1}$ (Figure 9SI).

$$E(HB)_{QTAIMC}[kJ \cdot mol^{-1}] = -(2.4 \pm 1.5) - (47.2 \pm 3.0) \cdot d_{norm}^{\min}(HB) \quad \text{(S1)}$$

R = 0.9826; σ = 0.3 [kJ·mol$^{-1}$]; n = 11

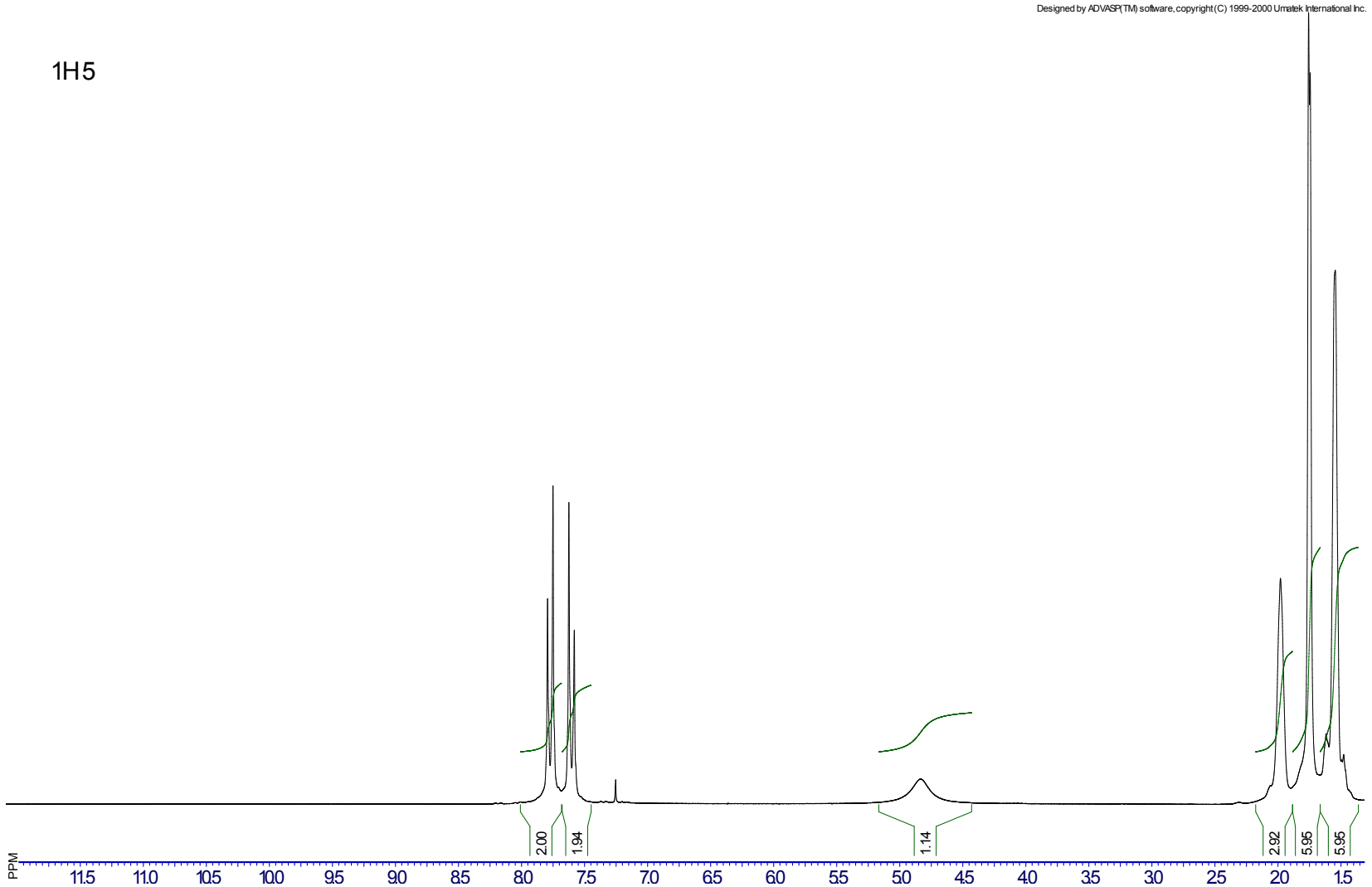
$$E(HB)_{Mayo}[kJ \cdot mol^{-1}] = -(4.3 \pm 1.2) - (37.8 \pm 2.3) \cdot d_{norm}^{\min}(HB) \quad \text{(S2)}$$

R = 0.9854; σ = 0.2 [kJ·mol$^{-1}$]; n = 10

The domain of applicability of the considered equations can be estimated using the parameters of compounds 6 and 11 excluded from the dependencies. As can be seen from Table 2 in the main text, the angles ∠ (N-H-O) in these compounds are equal to 146 ° and 130 ° respectively, which are anomalously low for hydrogen bonds of this type. Hence, the equations (S1) and (S2) can be considered suitable for estimating the hydrogen bond energies in crystals of adamantane derivatives of sulfonamides with ∠(N-H-O) ≥ 162°. Such correlations indicate the consistency of the results of the calculation approaches used.

## References

(S1) Perlovich, G. L.; Ryzhakov, A. M.; Tkachev, V. V.; Proshin, A. N. Adamantane derivatives of sulfonamide molecular crystals: structure, sublimation thermodynamic characteristics, molecular packing, and hydrogen bond networks. *CrystEngComm*, 2015, 17, 753-763.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1.14
2.92
5.95
5.95
PPM
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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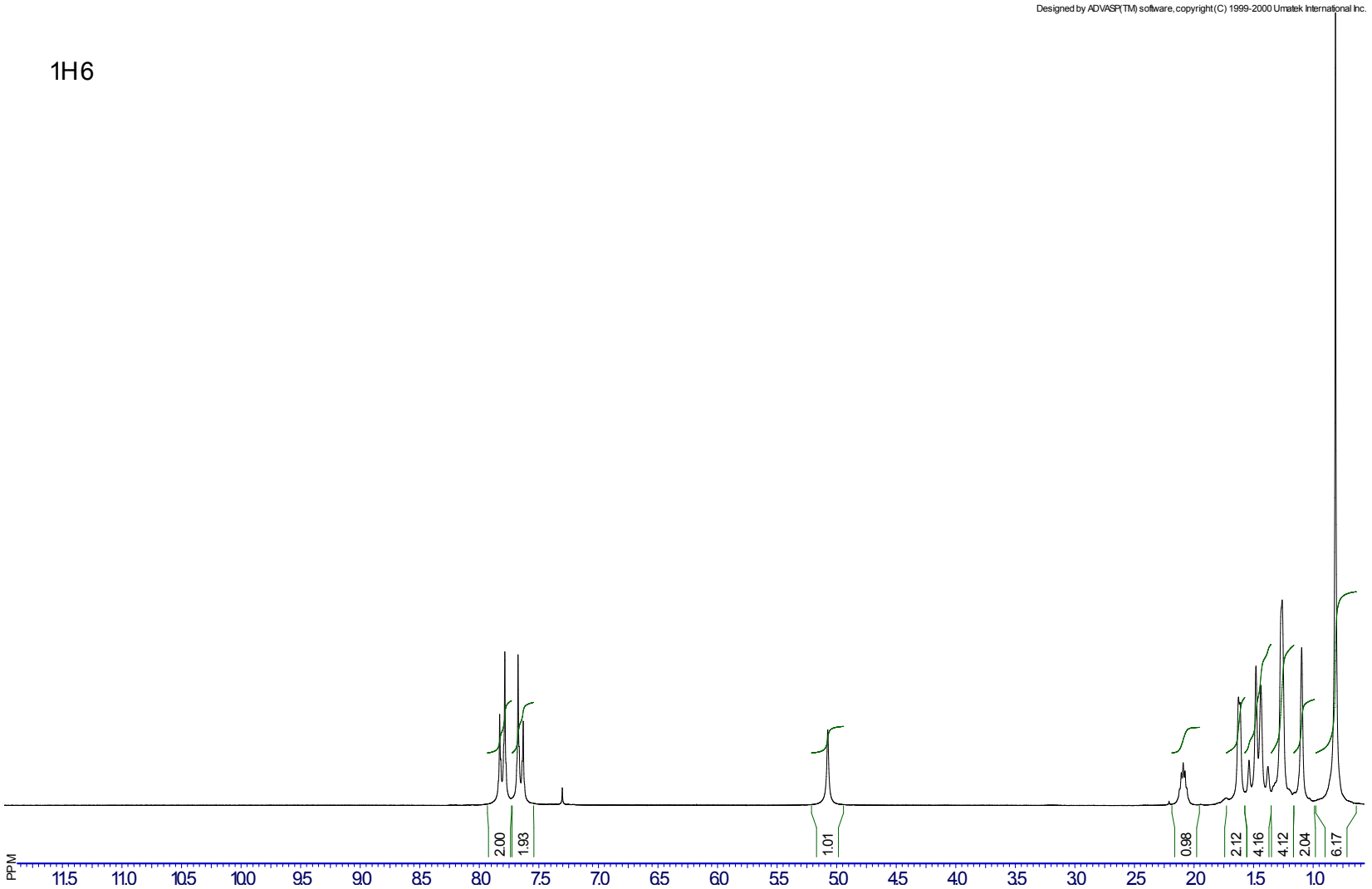
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2.04
6.17
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9.0
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7.0
6.5
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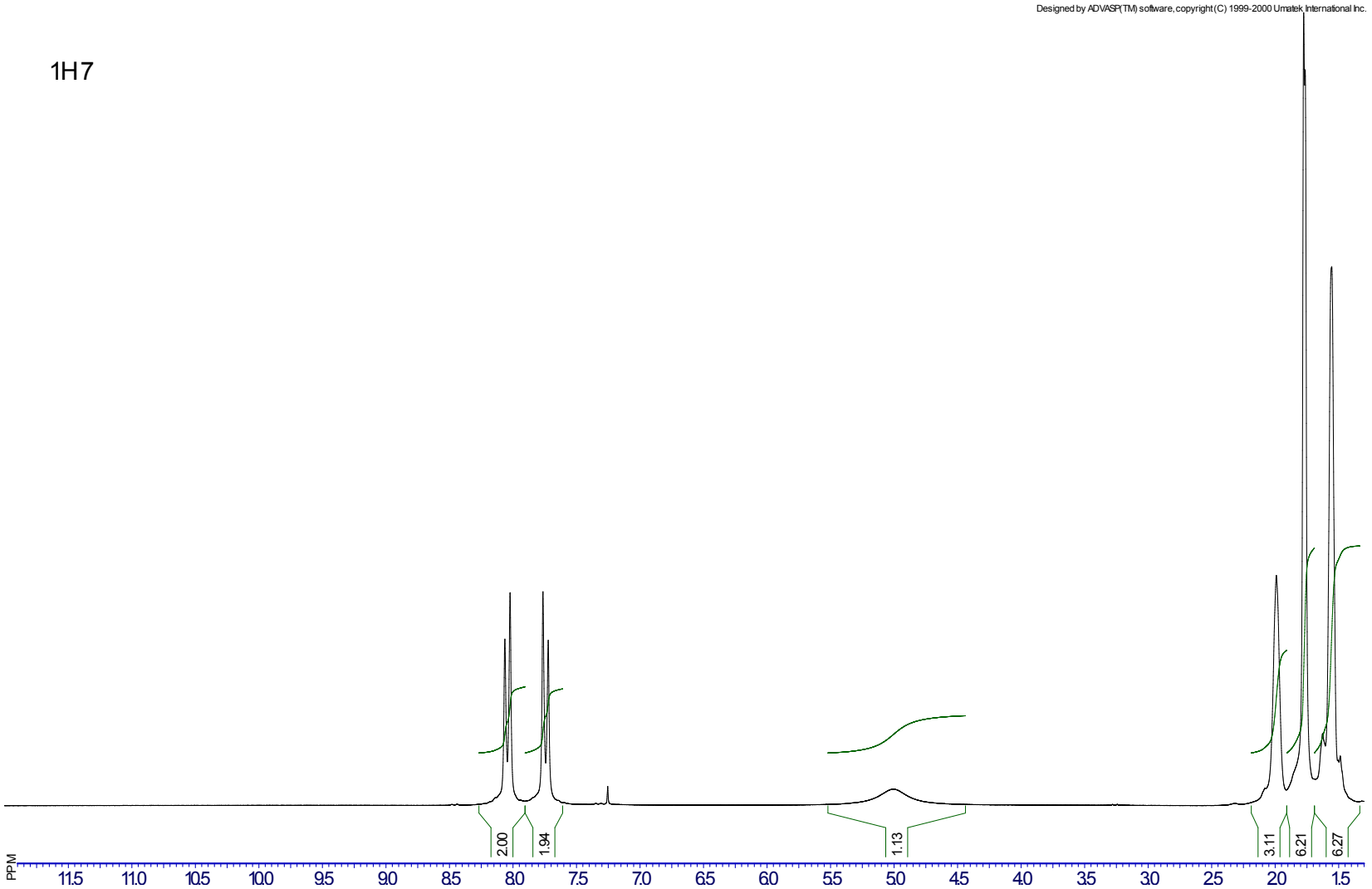
3.5
3.0
2.5
2.0
1.5
1.0

(b)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8.0
7.5
7.0
6.5
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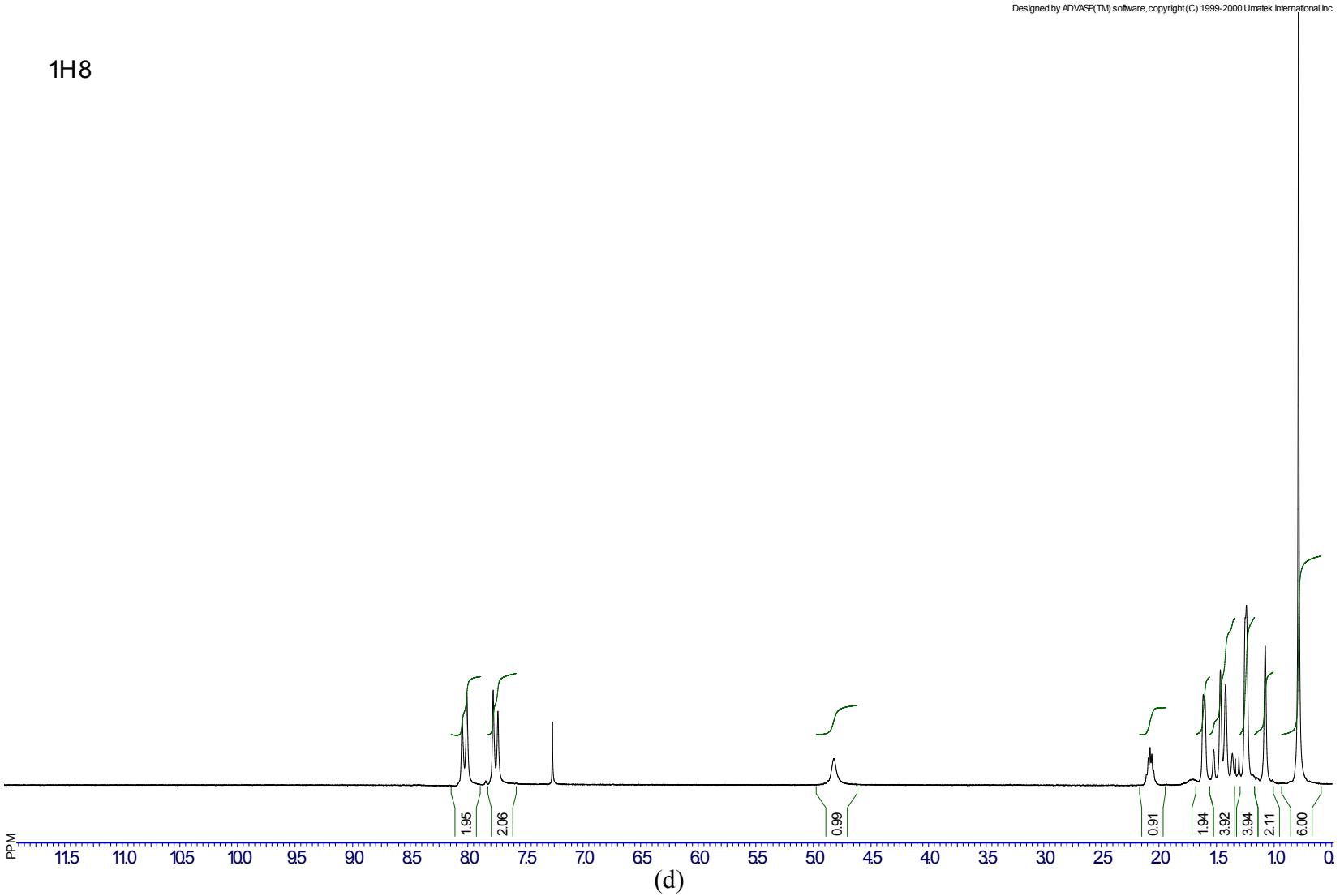
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5

(c)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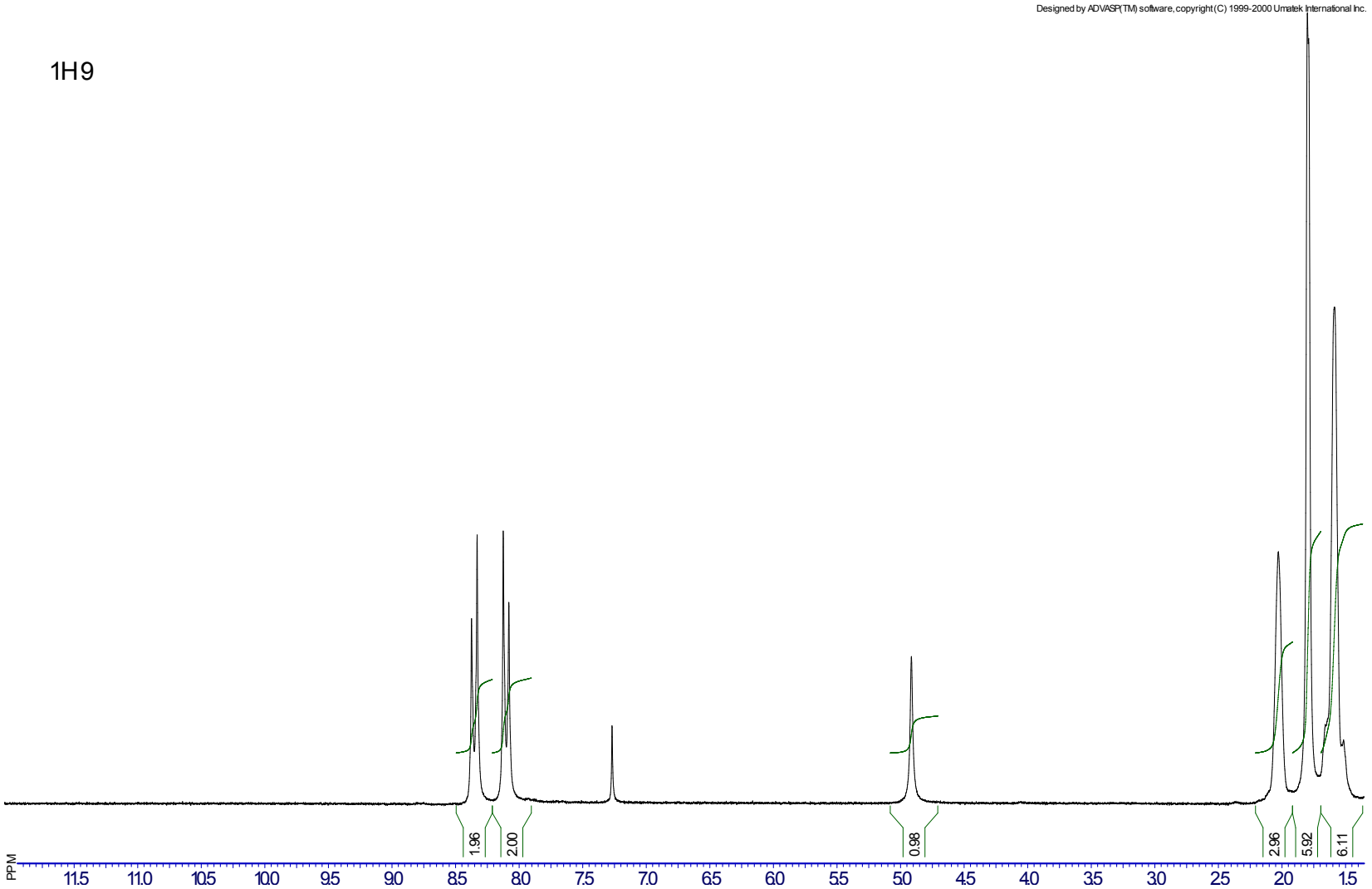
0.91
1.94
3.92
3.94
2.11
6.00
PPM
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.

(d)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1H9
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PPM
11.5
11.0
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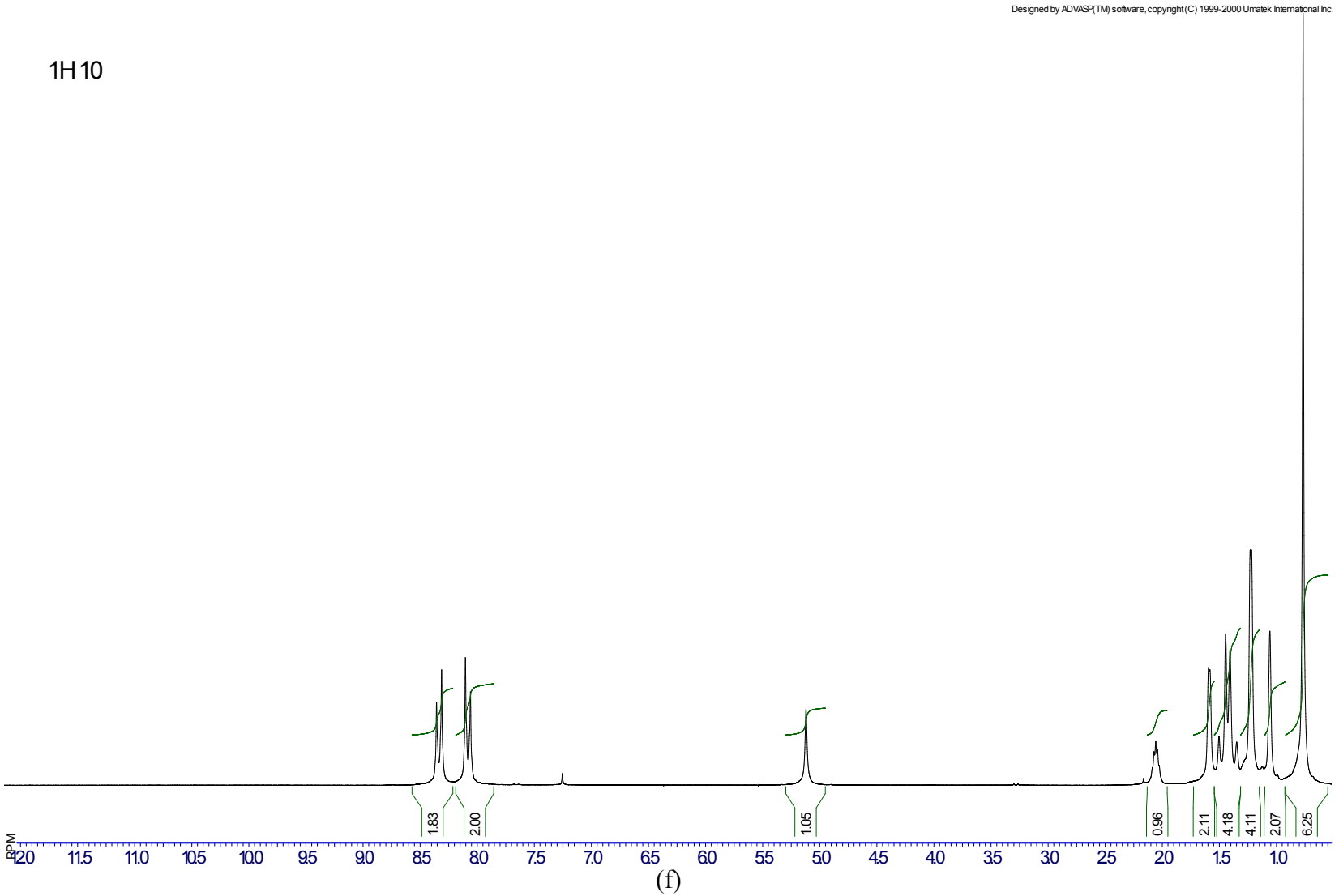
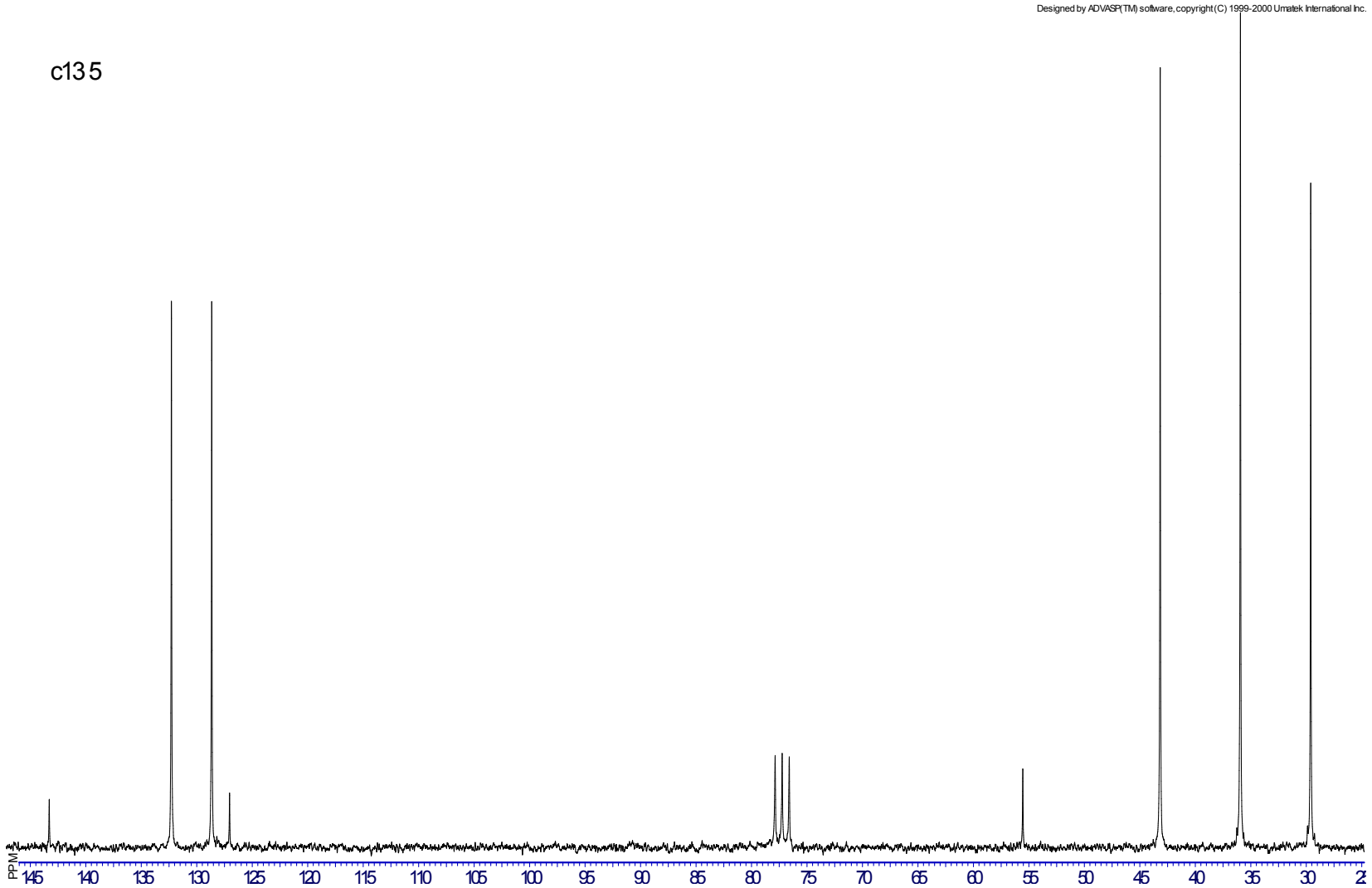
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5

(e)

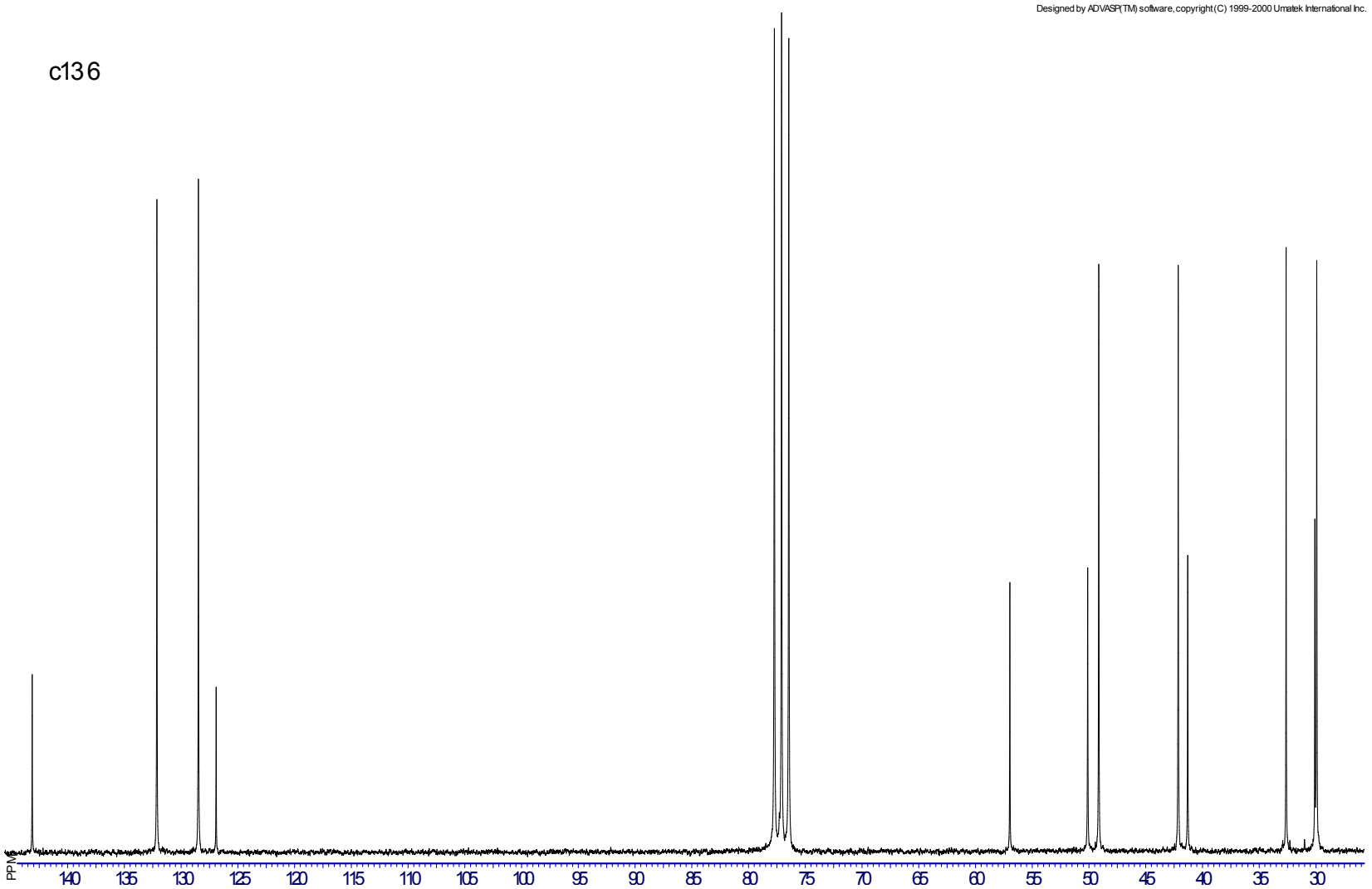



(f)

**Figure 1SI.** 1H NMR spectra for compounds **5** (a), **6** (b), **7** (c), **8** (d), **9** (e) and **10** (f).


Designed by ADVASP(TM) software, copyright (C) 1999-2000 Umatek International Inc.
c135
PPM
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 2

(a)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c136
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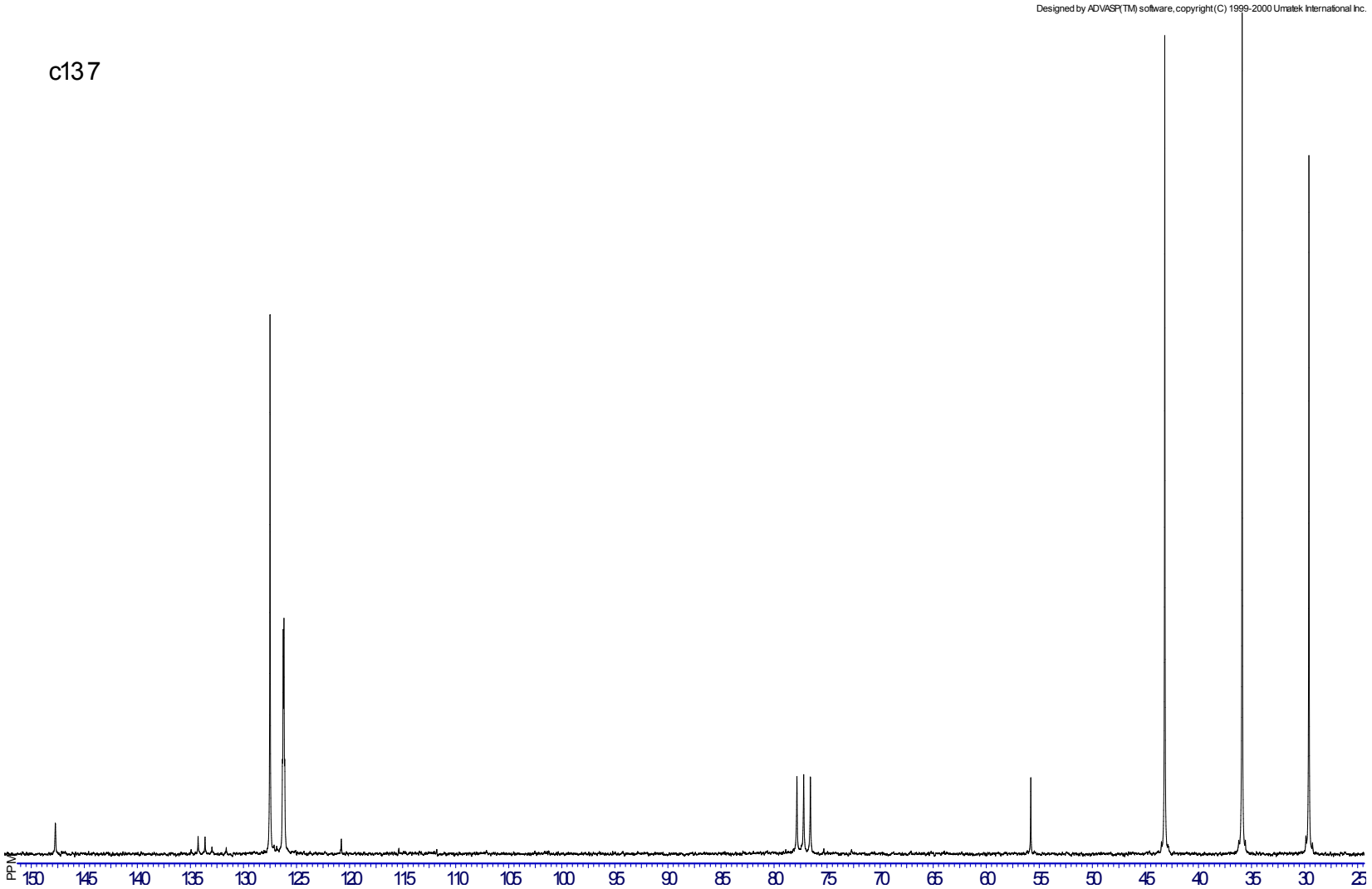
(b)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c137
PPM
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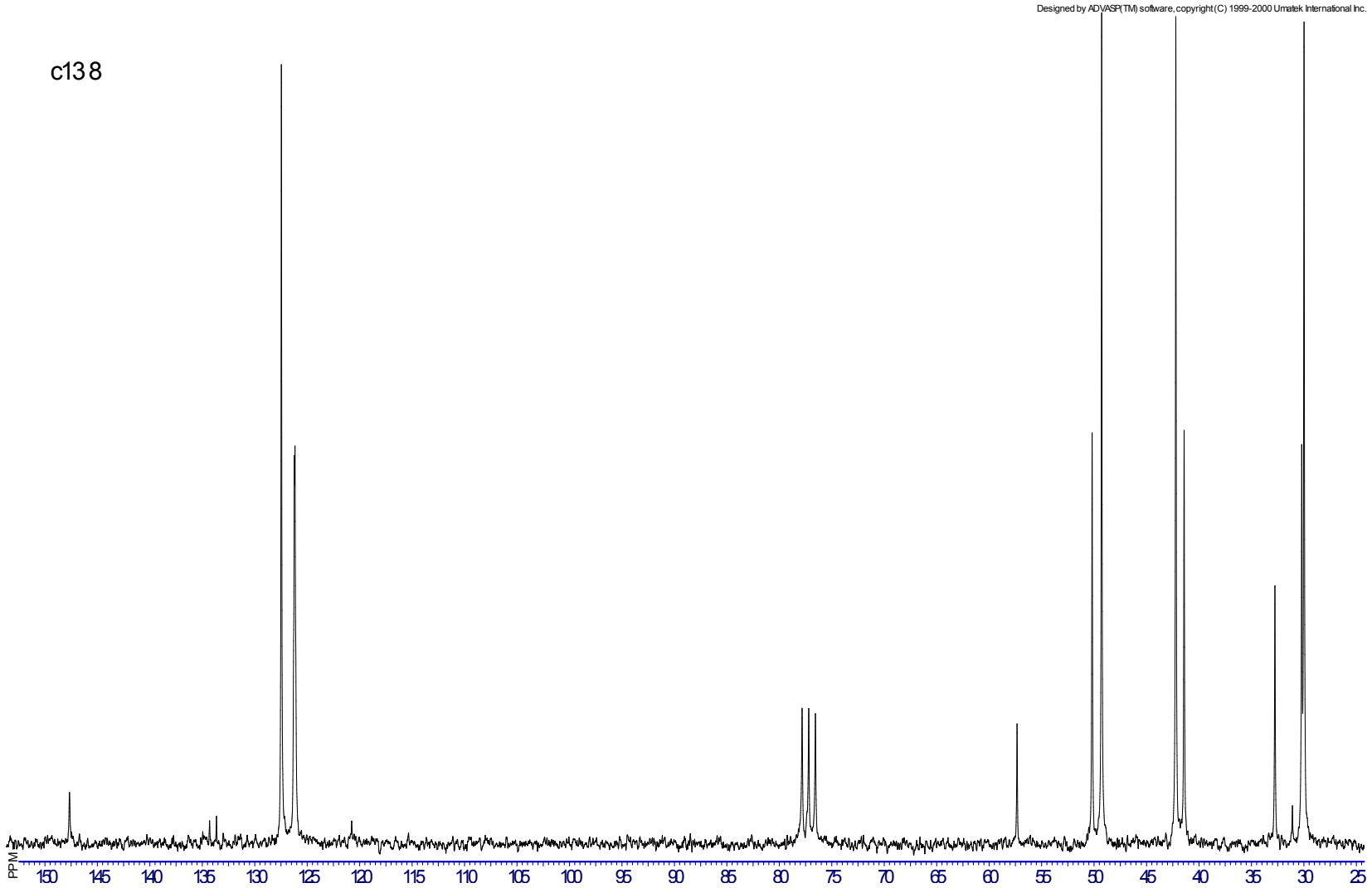
(c)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c138
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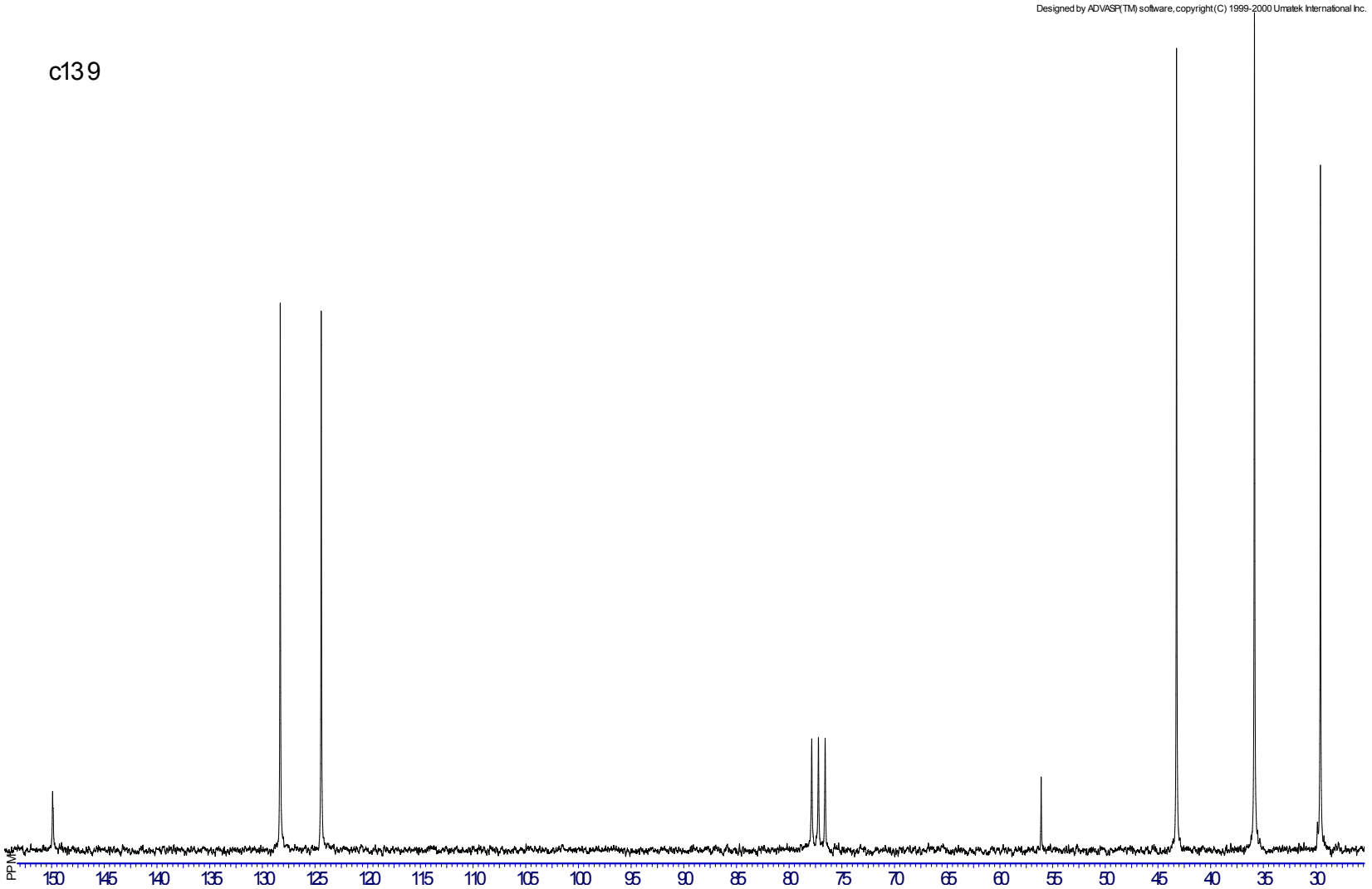
(d)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c139
PPM
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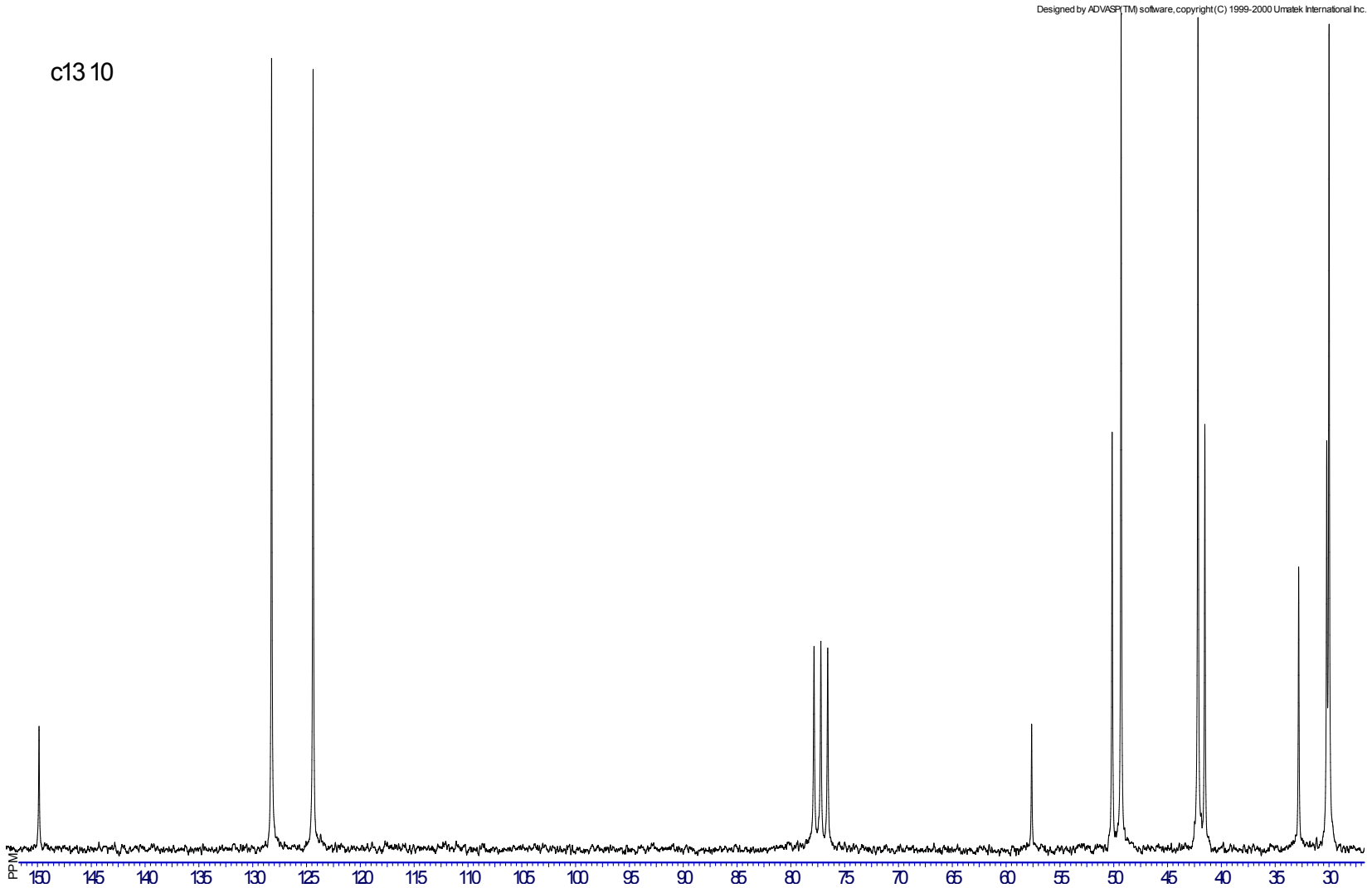
(e)




(f)

**Figure 2SI.** $^{13}C$ NMR spectra for compounds **5** (a), **6** (b), **7** (c), **8** (d), **9** (e) and **10** (f).

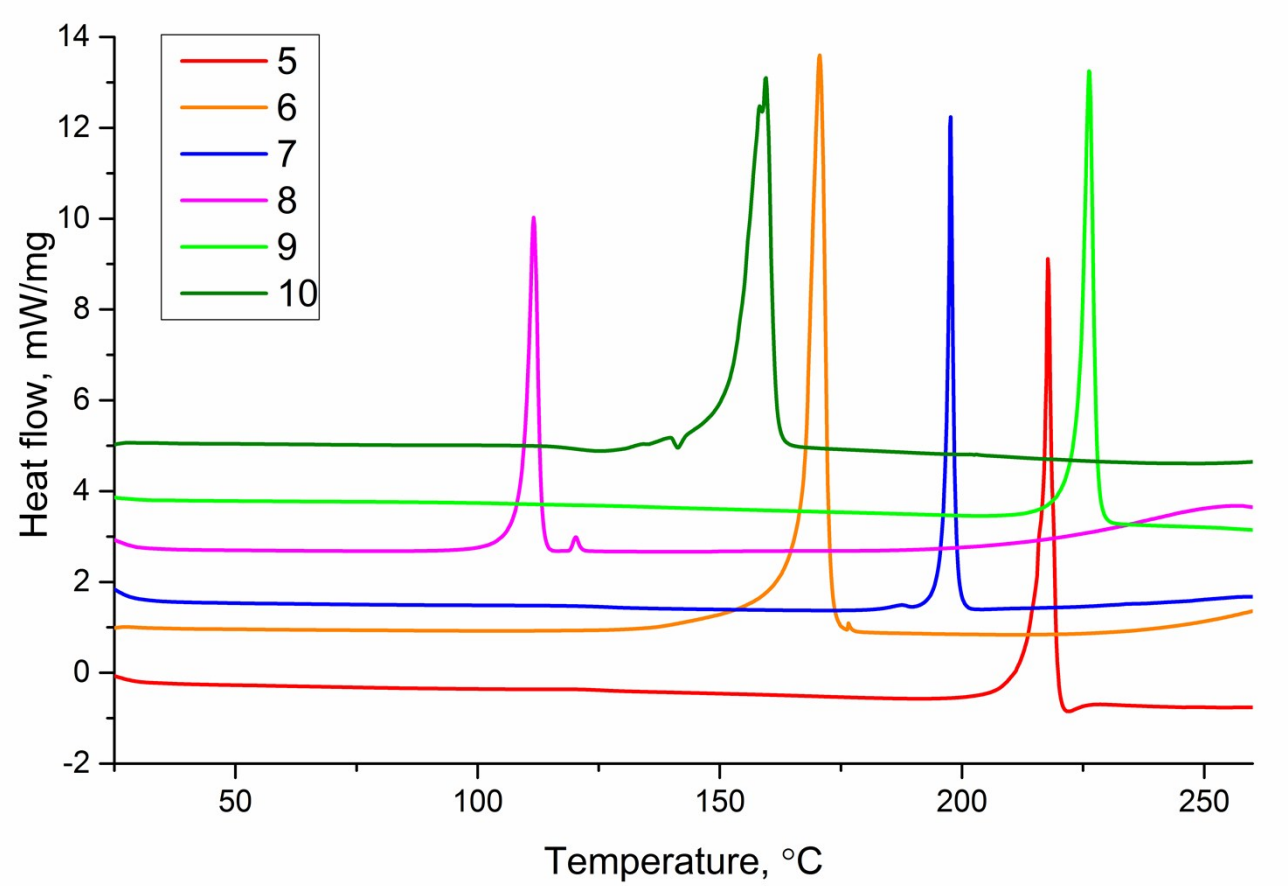



**Figure 3SI.** DSC curves of compounds **5-10** recorded at 10 K·min$^{-1}$.

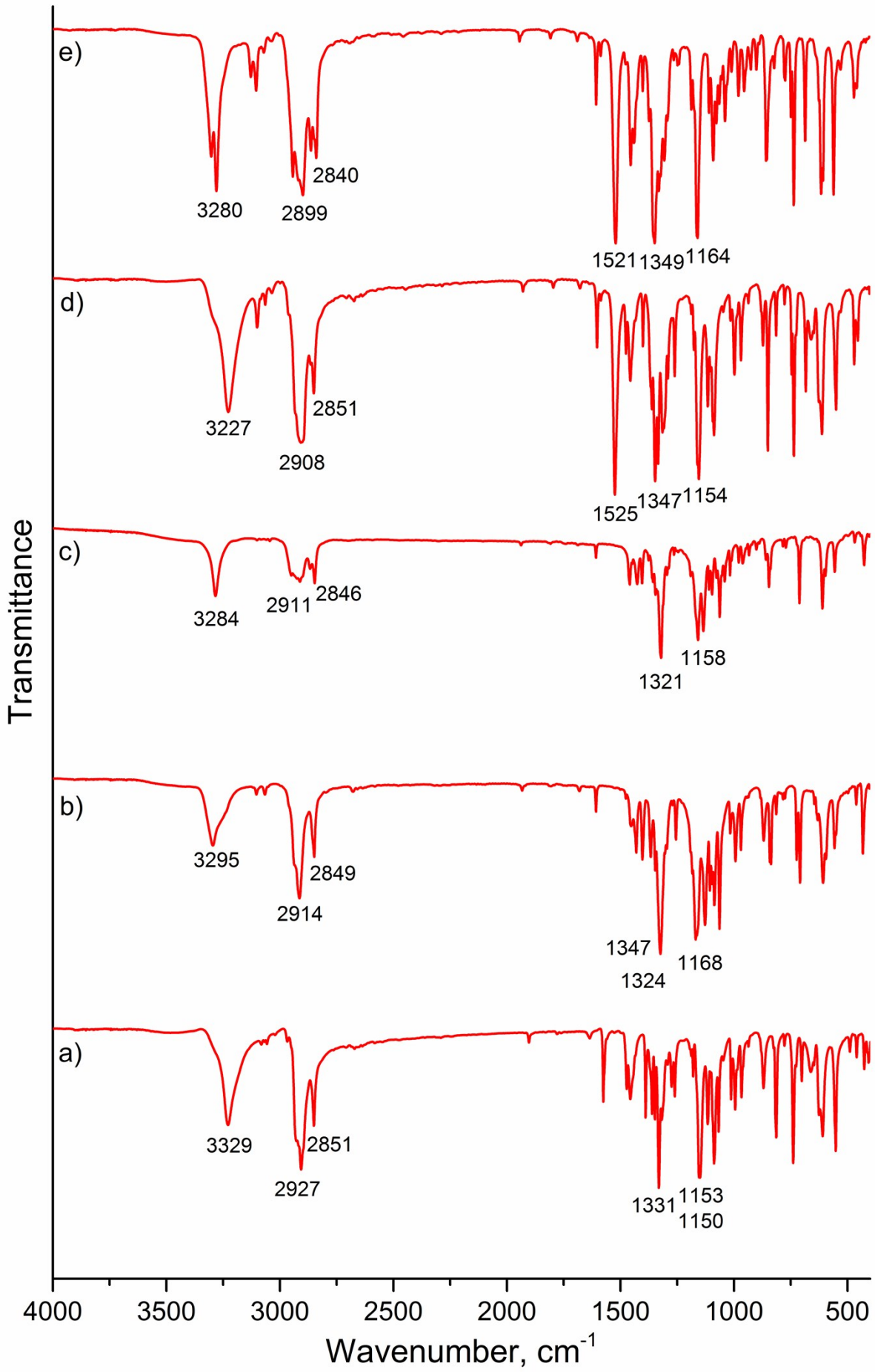
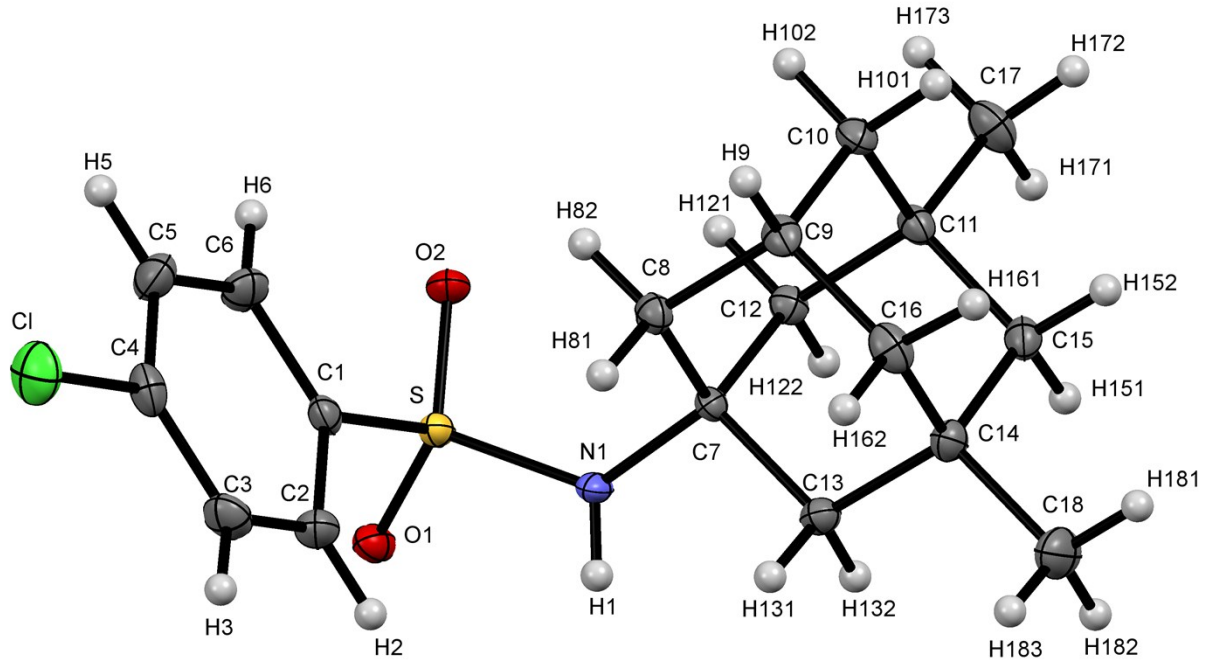
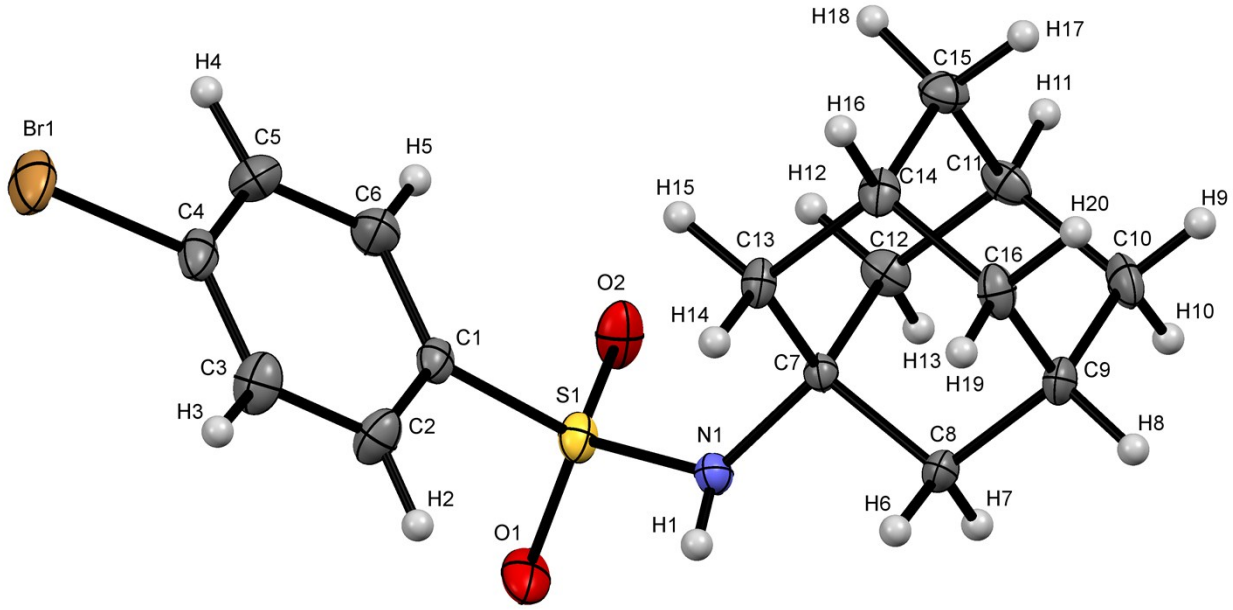



**Figure 4SI.** IR spectra for compounds **5** (a), **7** (b), **8** (c), **9** (d) and **10** (e)


H102
H173
H172
H101
C17
H171
C10
H9
H5
H6
H82
H121
C9
C11
C5
C6
O2
C8
H161
H152
C12
C16
Cl
C4
H81
C15
C1
S
H122
H151
H162
C14
N1
C7
C3
C2
C13
H181
C18
O1
H1
H131
H132
H3
H2
H183
H182

(a)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C15
H4
H11
H16
Br1
C5
H5
C14
C11
H12
H15
H20
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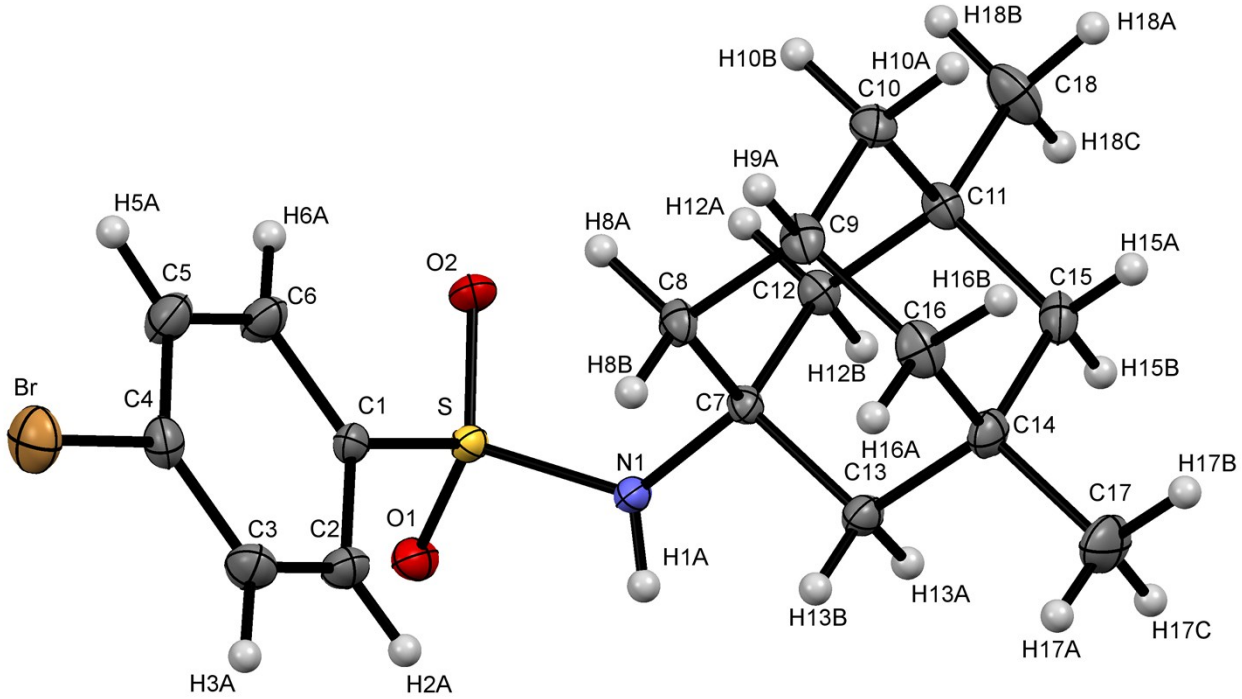
C6
C13
C12
C16
C10
O2
H14
H10
C1
H13
C7
C9
C3
H19
S1
H3
C2
N1
C8
H8
H2
H6
H7
O1
H1

(b)


H18B
H18A
H10B
H10A
C10
C18
H18C
H9A
C11
H5A
H6A
H12A
C9
H8A
H15A
C5
O2
C8
C12
H16B
C15
C6
C16
H8B
H12B
H15B
Br
C4
C1
S
C7
C14
H16A
N1
C13
H17B
C17
C3
C2
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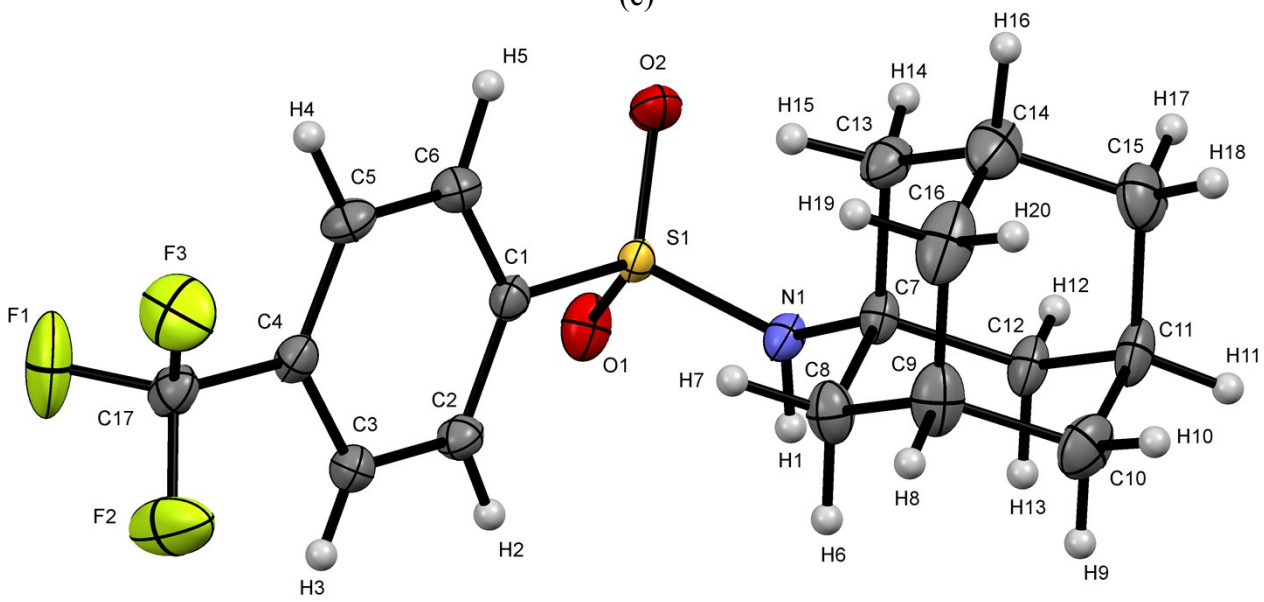
H17C
H17A
H3A
H2A

(c)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C14
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C6
C15
H18
C5
H19
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S1
F3
C1
C7
H12
F1
C4
N1
C12
C11
O1
H11
H7
C8
C9
C2
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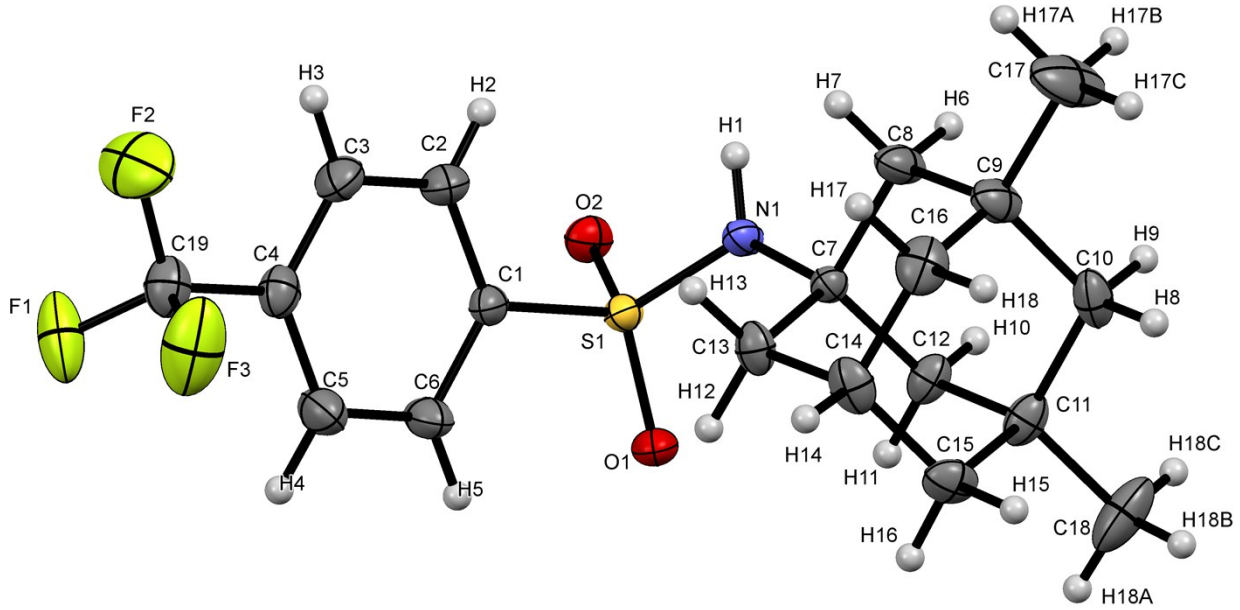
H1
C10
H8
H13
F2
H2
H6
H3
H9

(d)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H17C
H3
H2
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H6
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C3
C2
C8
C9
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C16
C19
C4
C1
C7
C10
H9
F1
H13
H18
H8
S1
C13
C14
C12
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F3
C5
C6
H12
C11
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H4
H5
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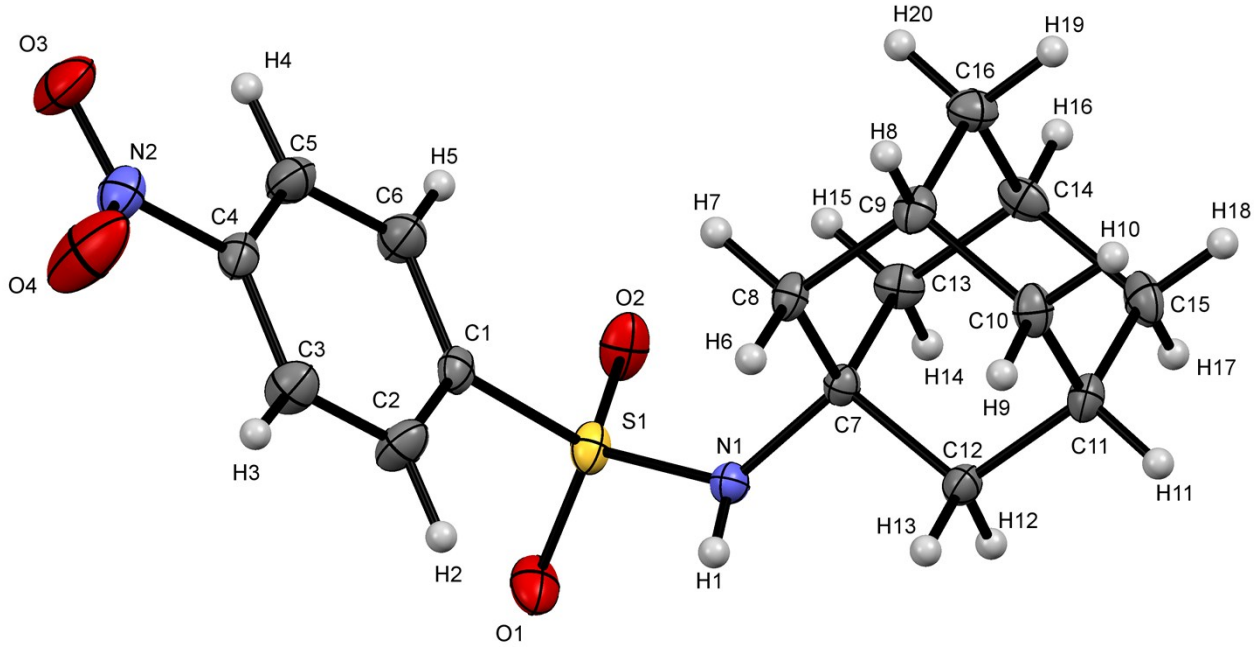
H18A

(e)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C3
H14
H17
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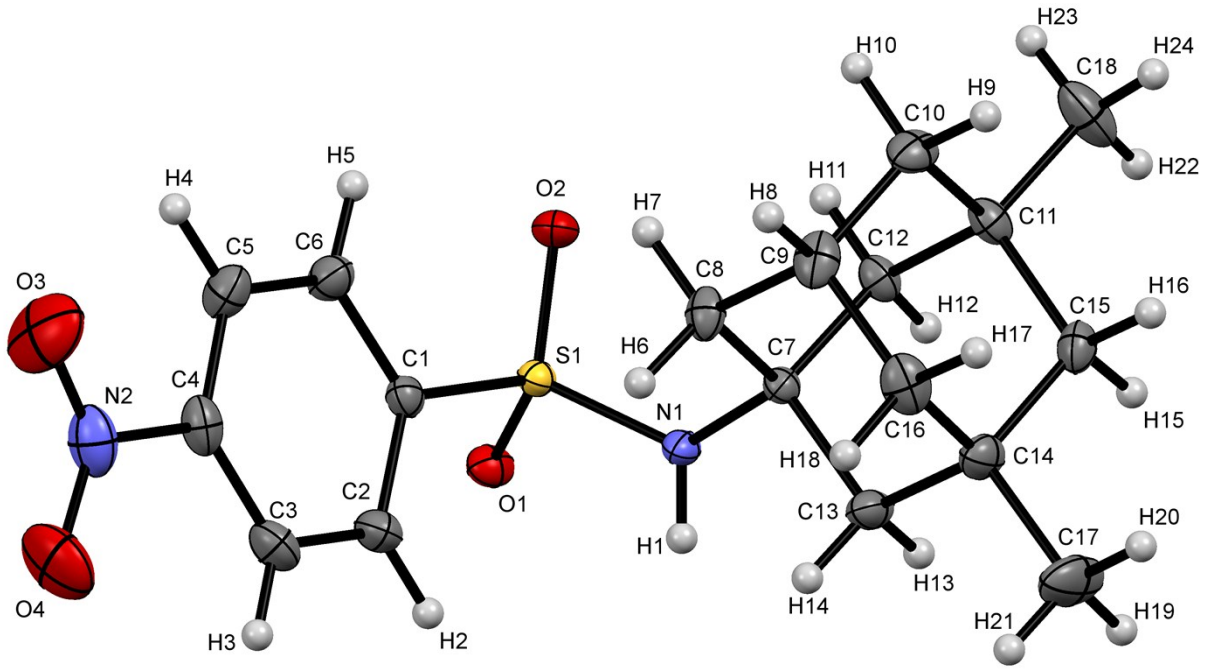
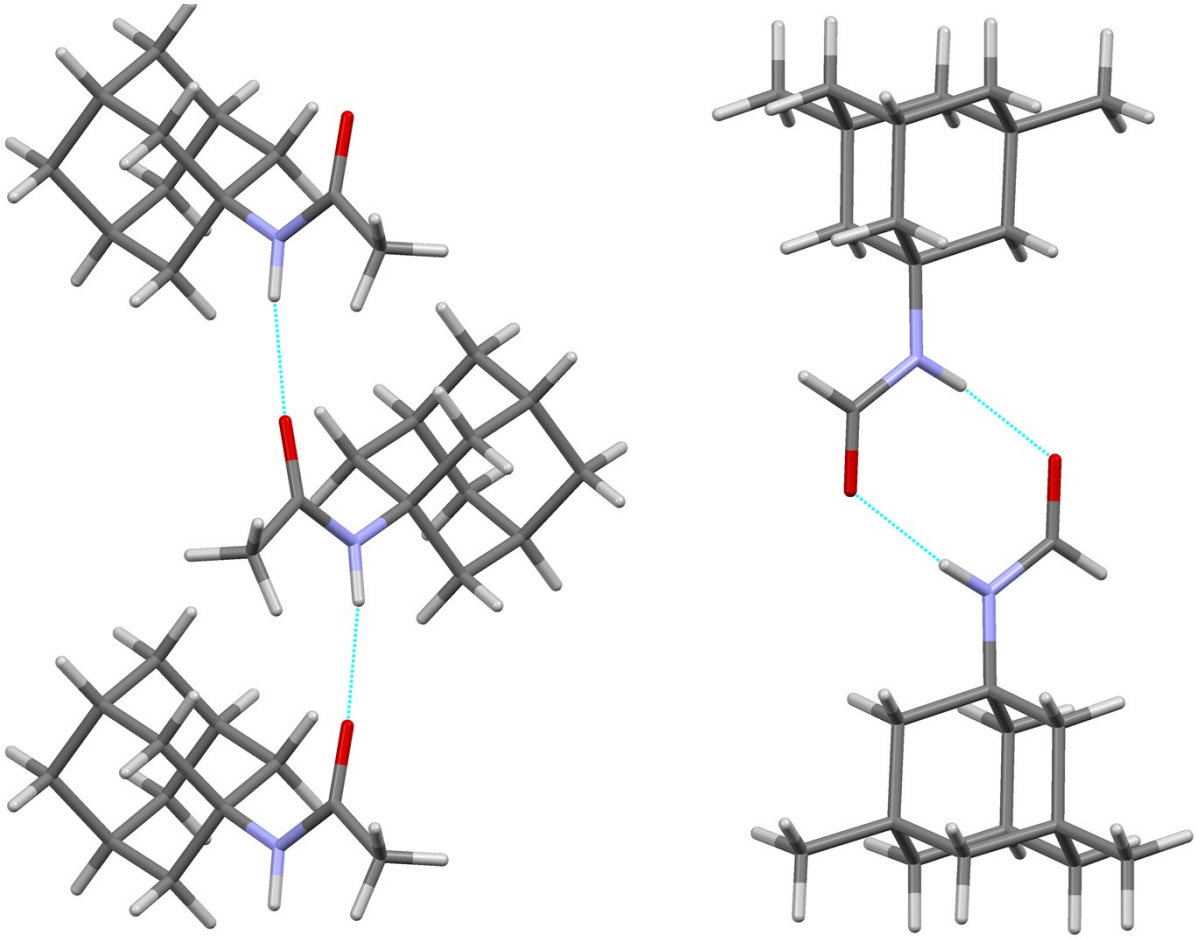
(f)



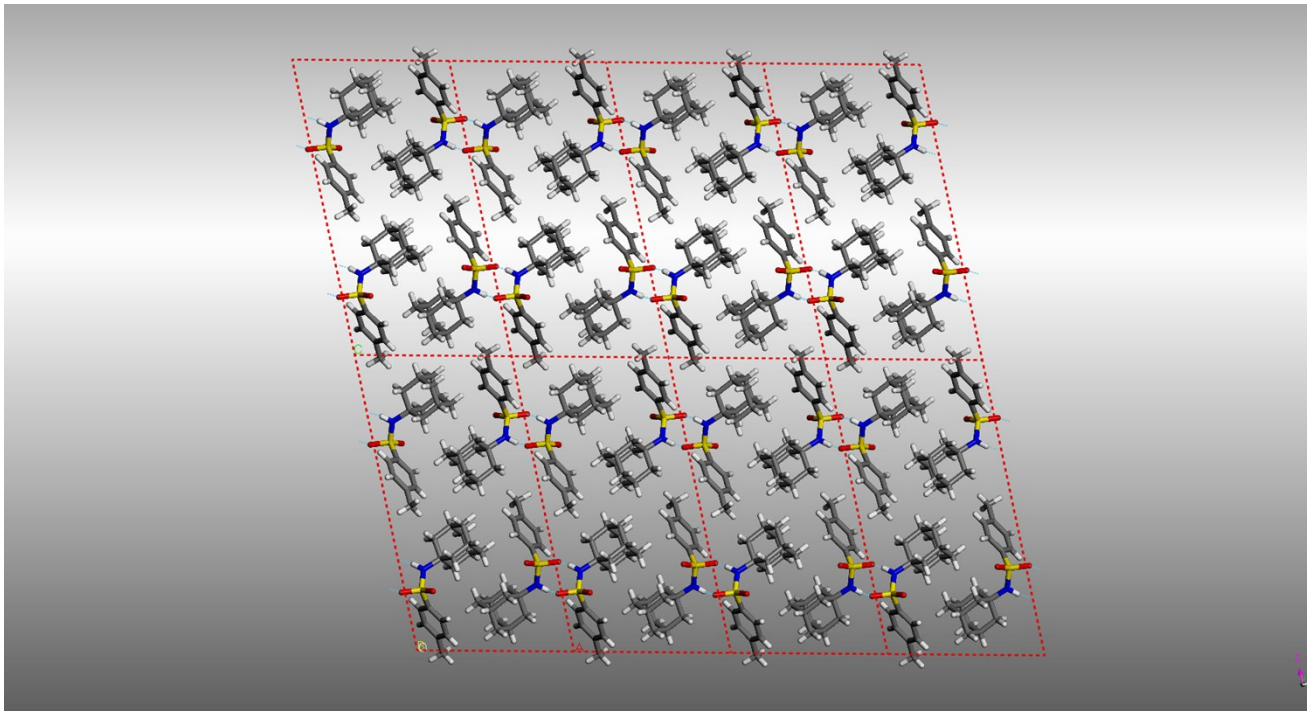

(g)

**Figure 5SI.** ORTEP diagrams for crystals of compounds **4** (a), **5** (b), **6** (c), **7** (d), **8** (e), **9** (f) and **10** (g) drawn at 50% probability level



(a) (b)

**Figure 6SI.** Patterns of hydrogen bonding in crystals of (a) N-adamantanyl-acetamide (refcode: ROLCOK01) and (b) N-(dimethyladamantanyl)-formamide (refcode: VICHAR).



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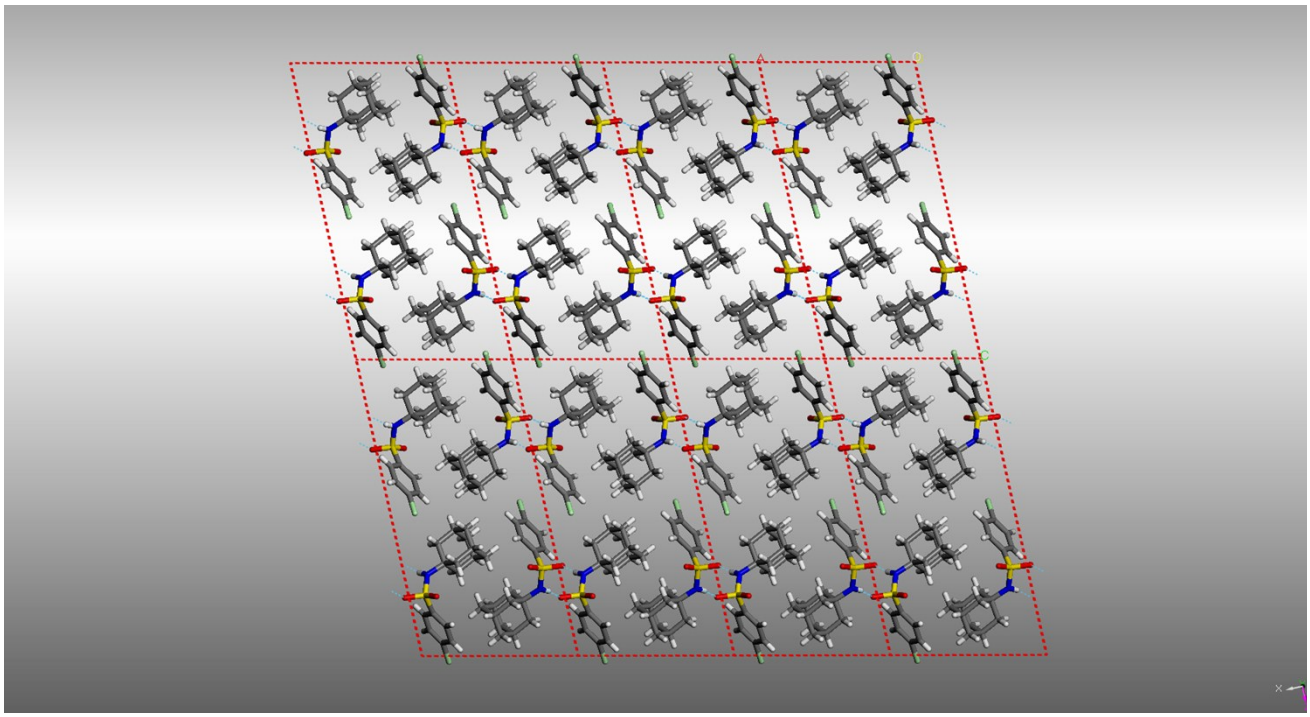
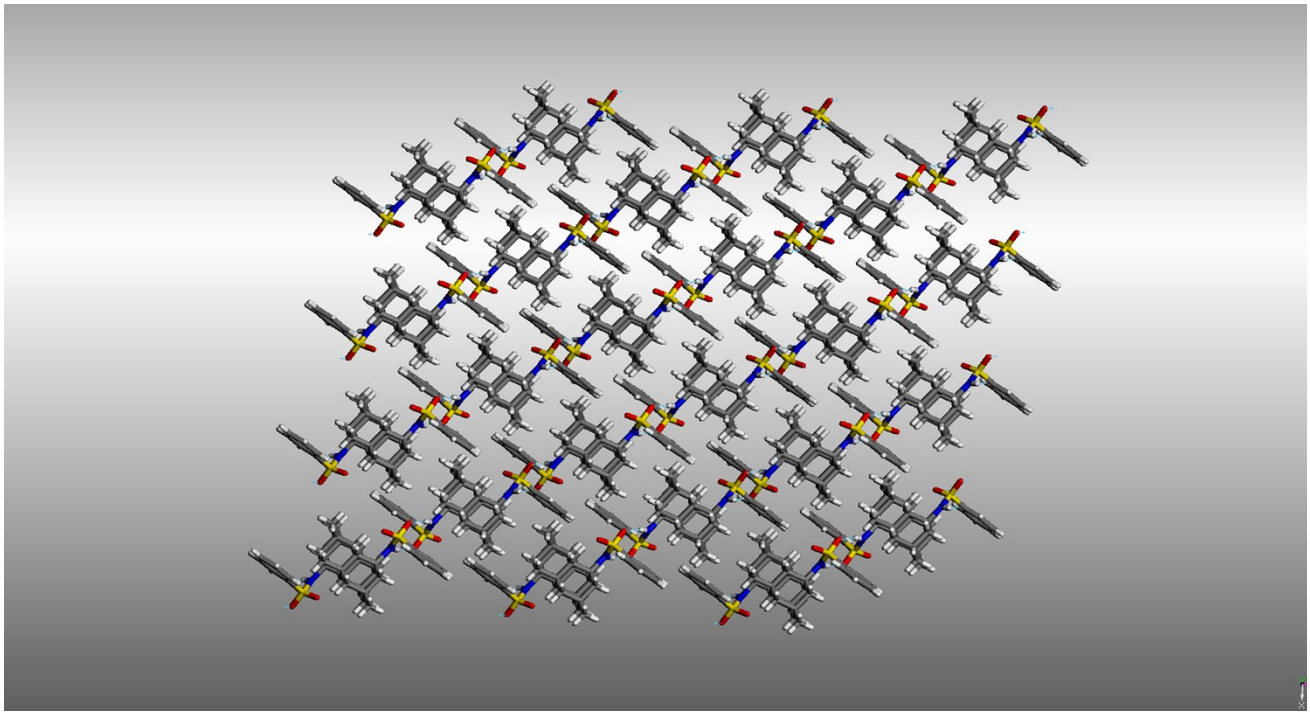


b

**Figure 7SI.** Molecular packing architectures of crystals **11** (a) and **3** (b).



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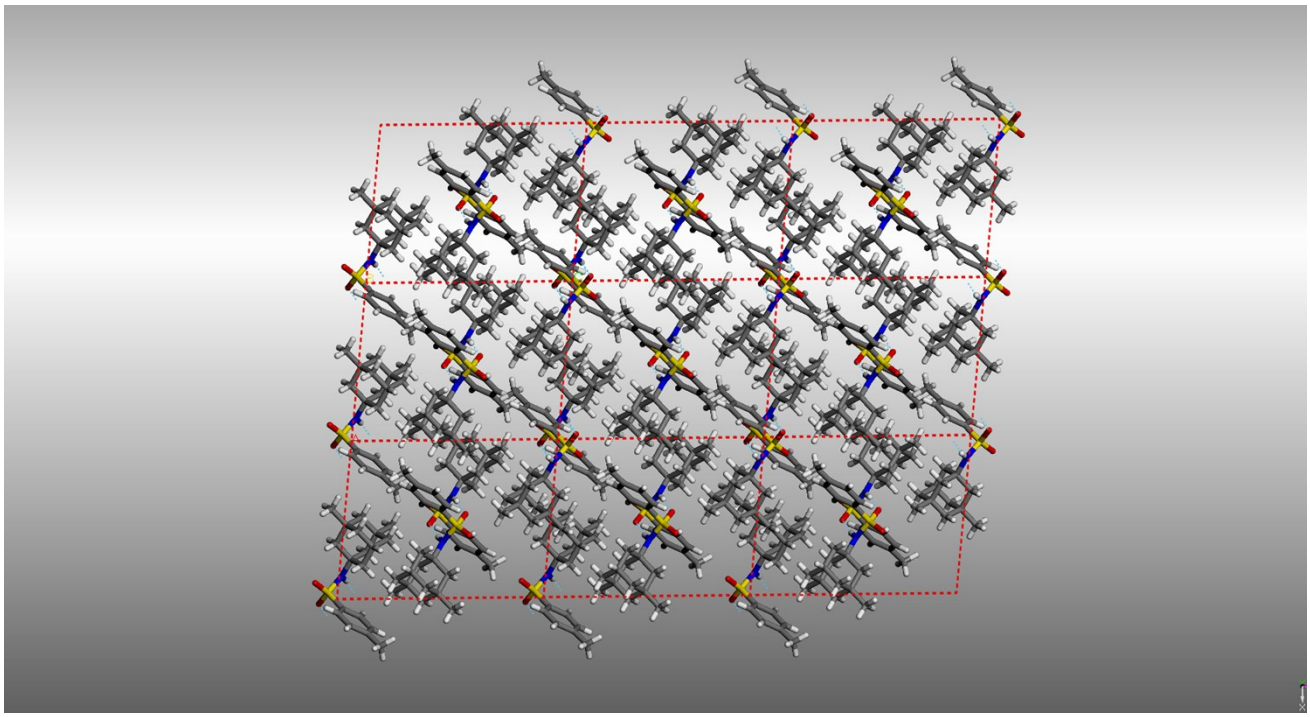
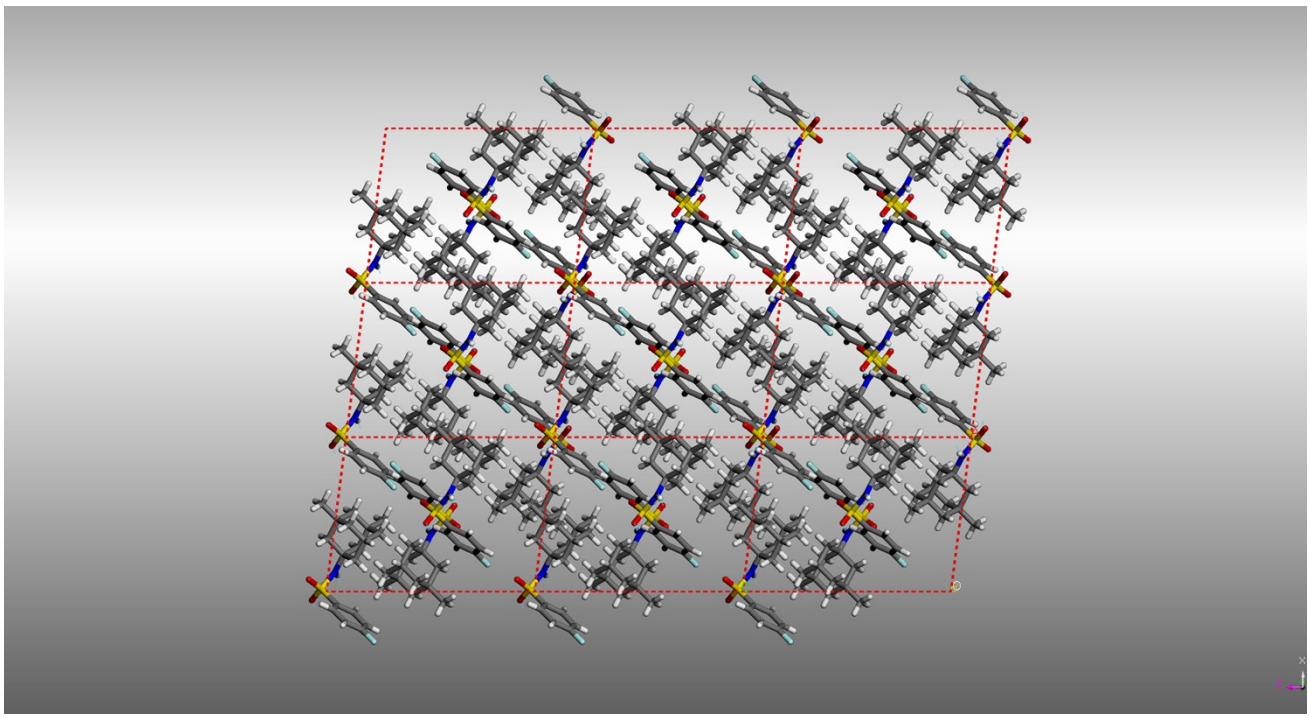


b



c

**Figure 8SI.** Molecular packing architectures of crystals **2** (a), **12** (b) and **14** (c).

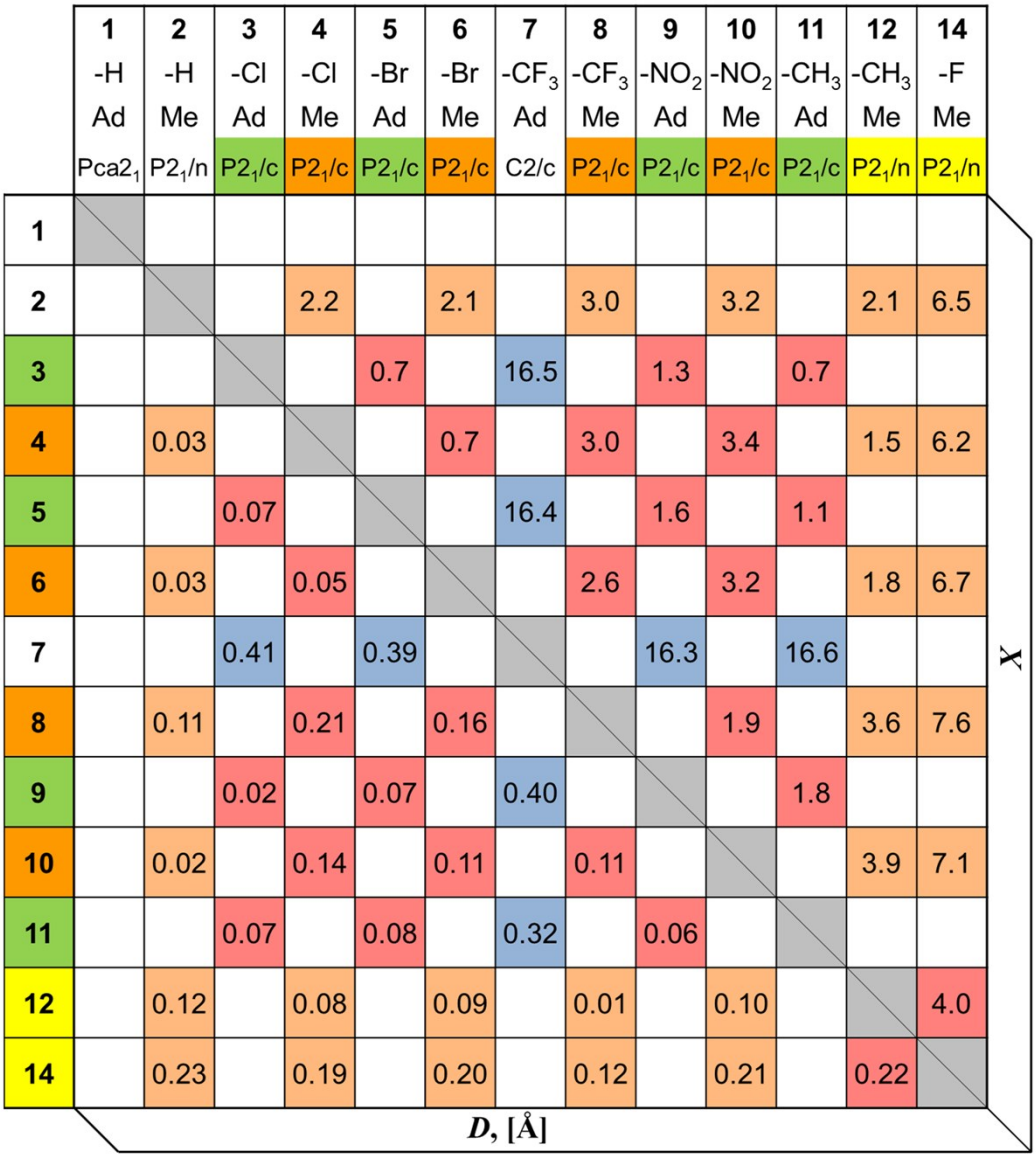
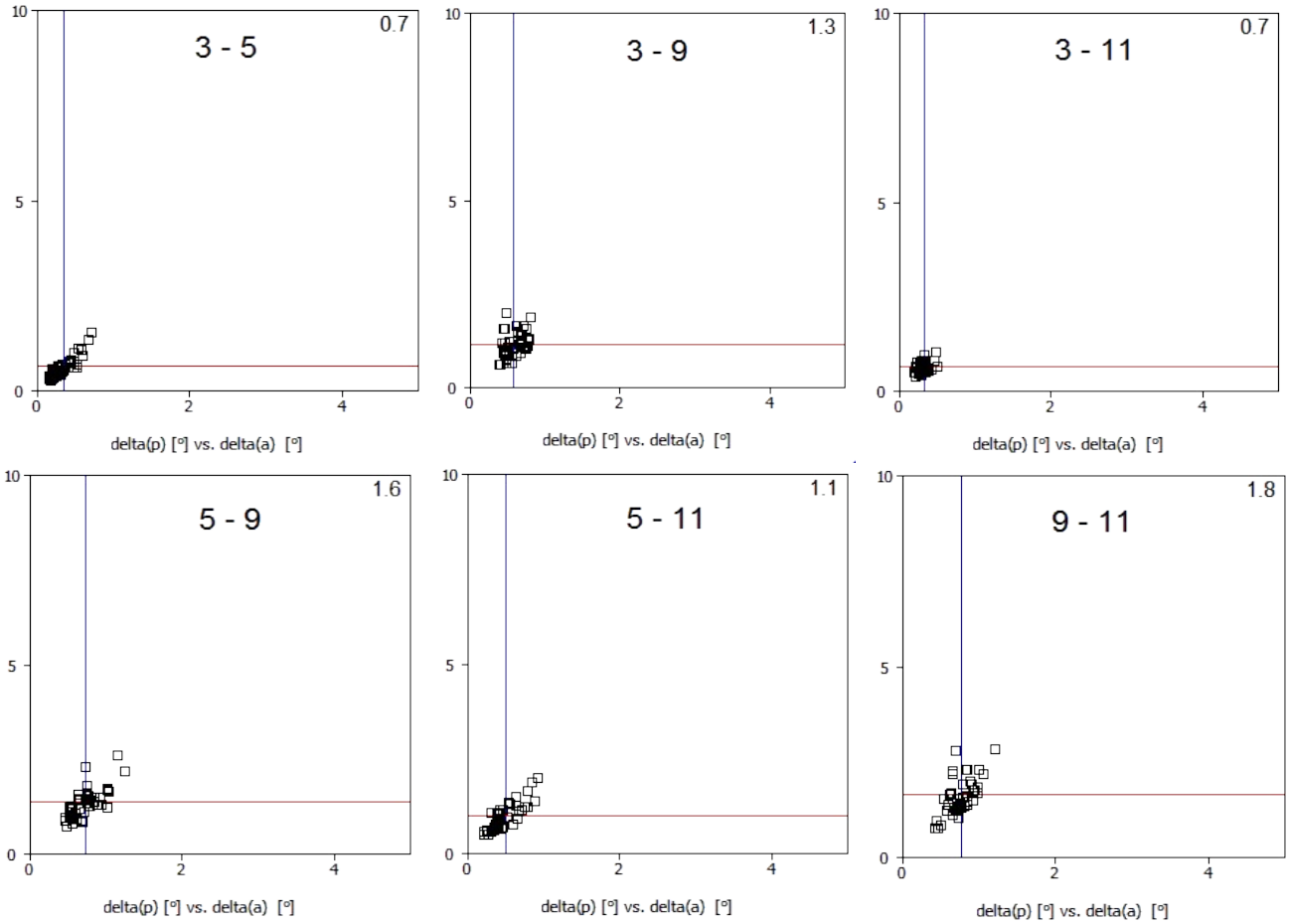
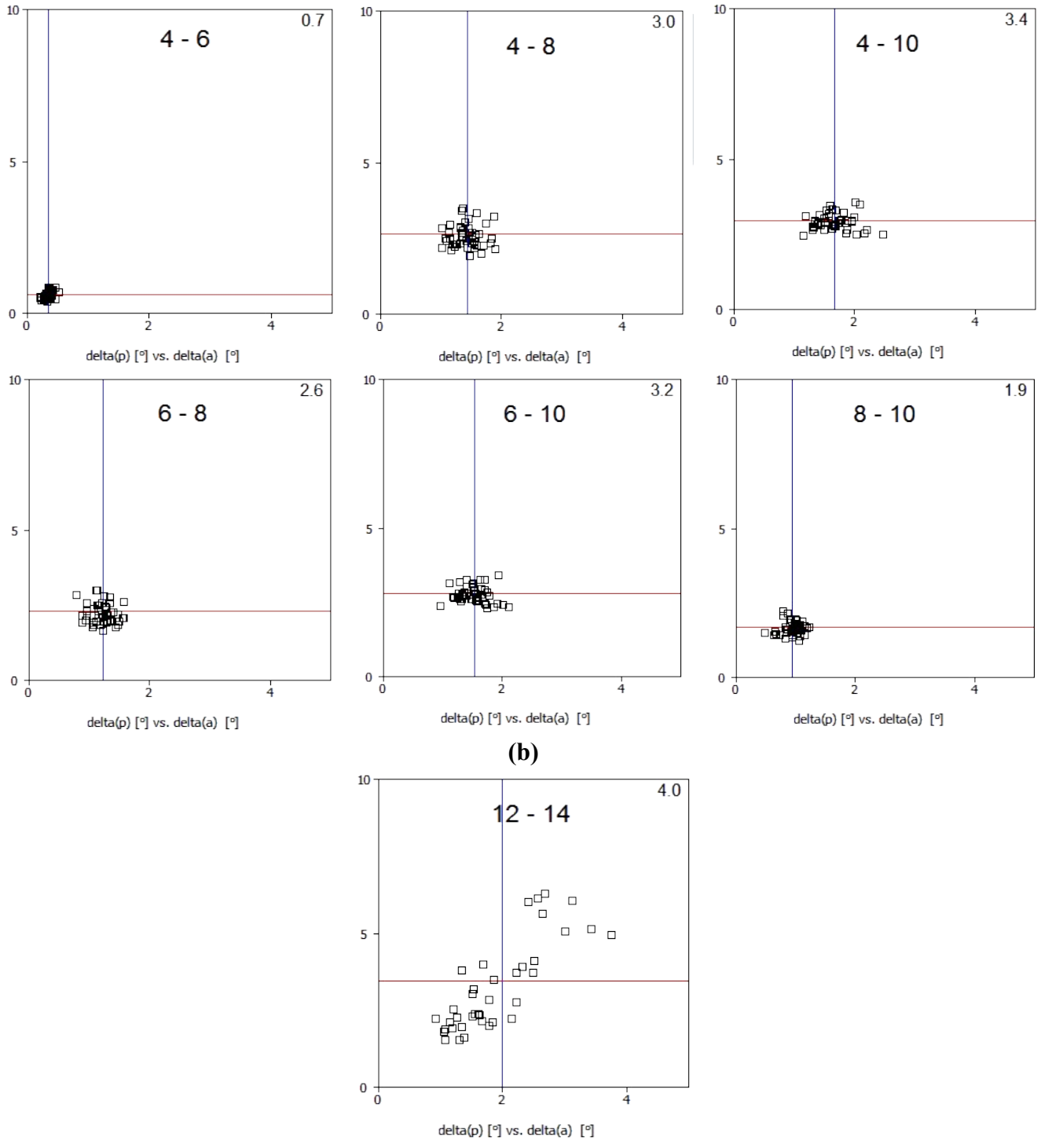



**Figure 9SI.** XPac map containing the dissimilarity indices X (upper right sector of the matrix) and stretch parameters D (bottom left sector) for 78 unique pairs of crystal structures of adamantane (Ad) and memantine (Me) derivatives with different substituents. The calculations were carried out for a cluster with n = 14 coordinating molecules on the basis of p = 20 non-H atomic positions in a molecule (see Scheme S1). Red, blue and brown boxes within the matrix correspond to identical 3D, 1D and 0D supramolecular constructs, respectively. Different families of 3D isostructural crystals are marked green, orange and yellow.




**(a)**




**(b)**

**(c)**

**Figure 10SI.** Selected XPac plots of $\delta_p$ against $\delta_a$ (in °) which indicate the degree of similarity in different crystal structure pairs of isostructural compounds within the group 1 (a), group 2 (b) and group 3 (c). The upper right corner of each plot displays the value of dissimilarity index X.

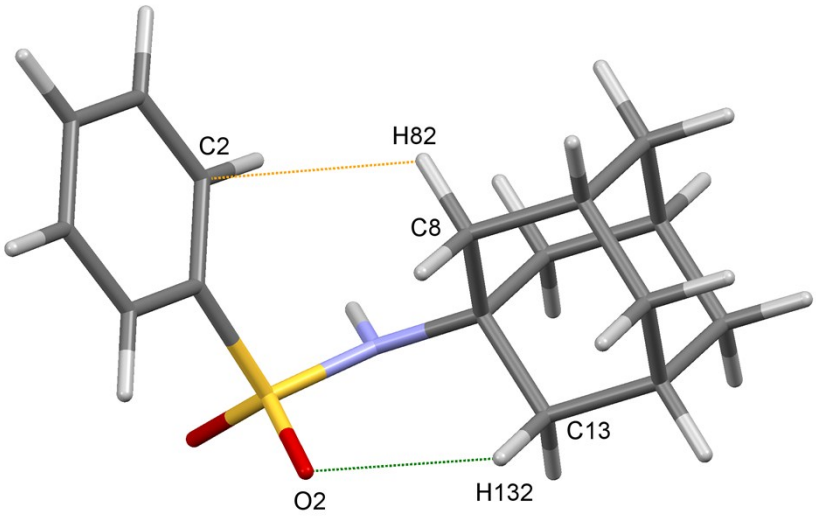



**Figure 11SI.** Intramolecular C-H···O (green) and C-H···π (orange) contacts in considered crystals detected by QTAIMC (exemplified by compound **1**).

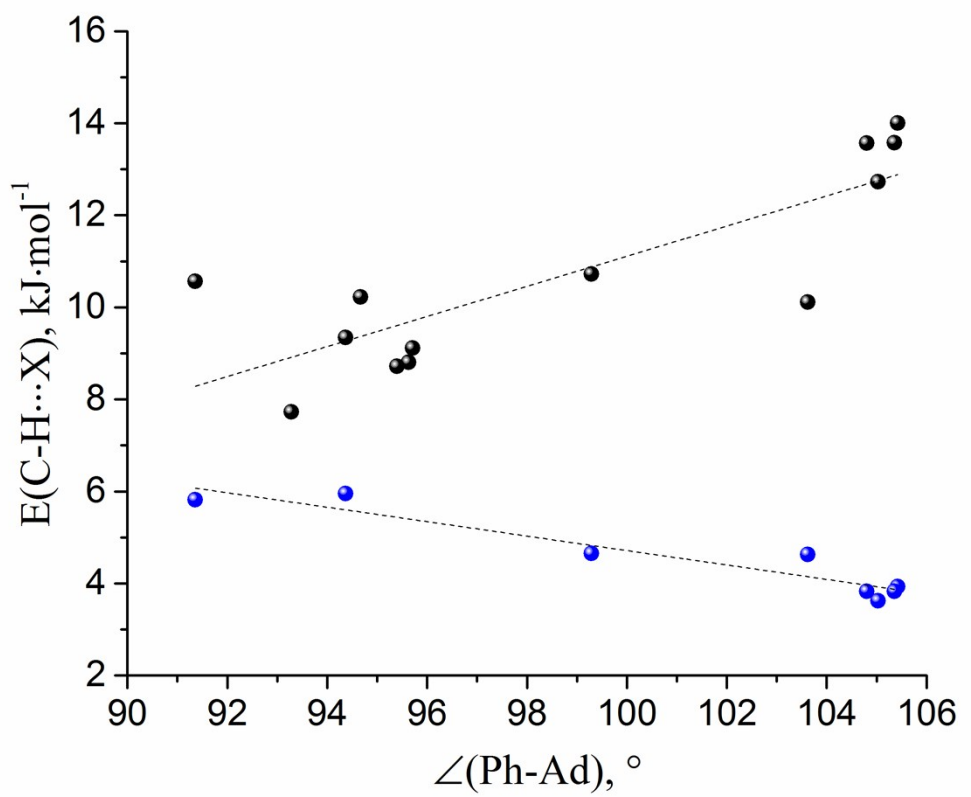



**Figure 12SI.** Energies of intramolecular C-H···O and C-H···π contacts in the considered crystals plotted against the angle between phenyl and adamantane fragments.

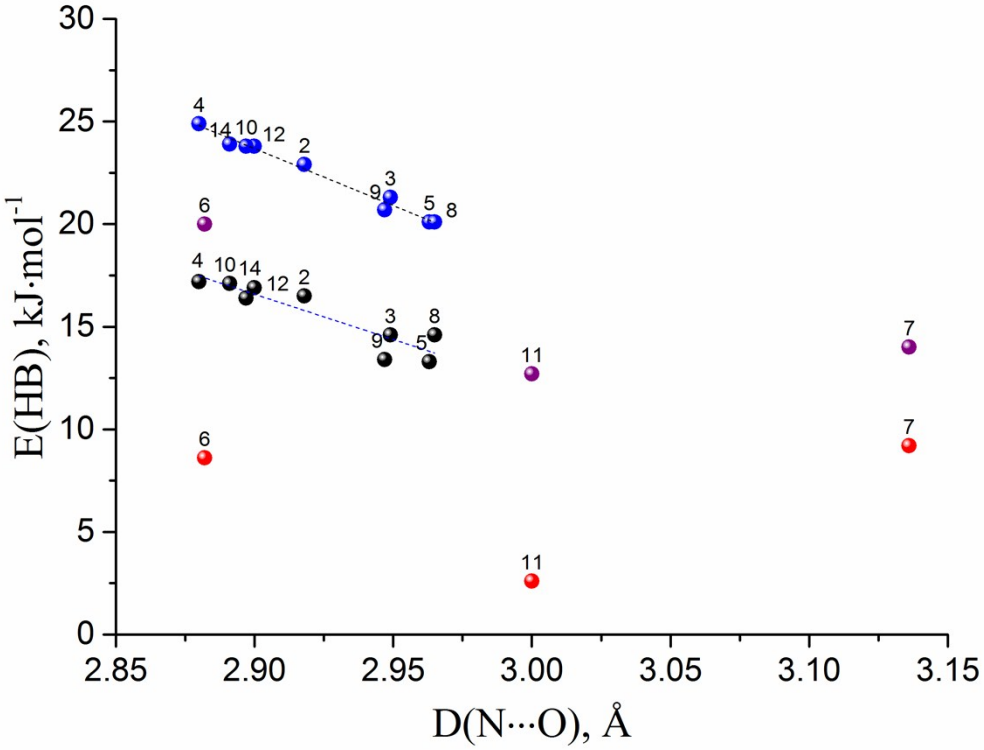



**Figure 13SI.** Correlation between the N···O distance within the hydrogen bond and the interaction energies evaluated using Mayo force field (black points) and QTAIMC (blue points). Compounds excluded from linear correlations are shown red and violet, respectively. The numbering of compounds corresponds to Figure 1.

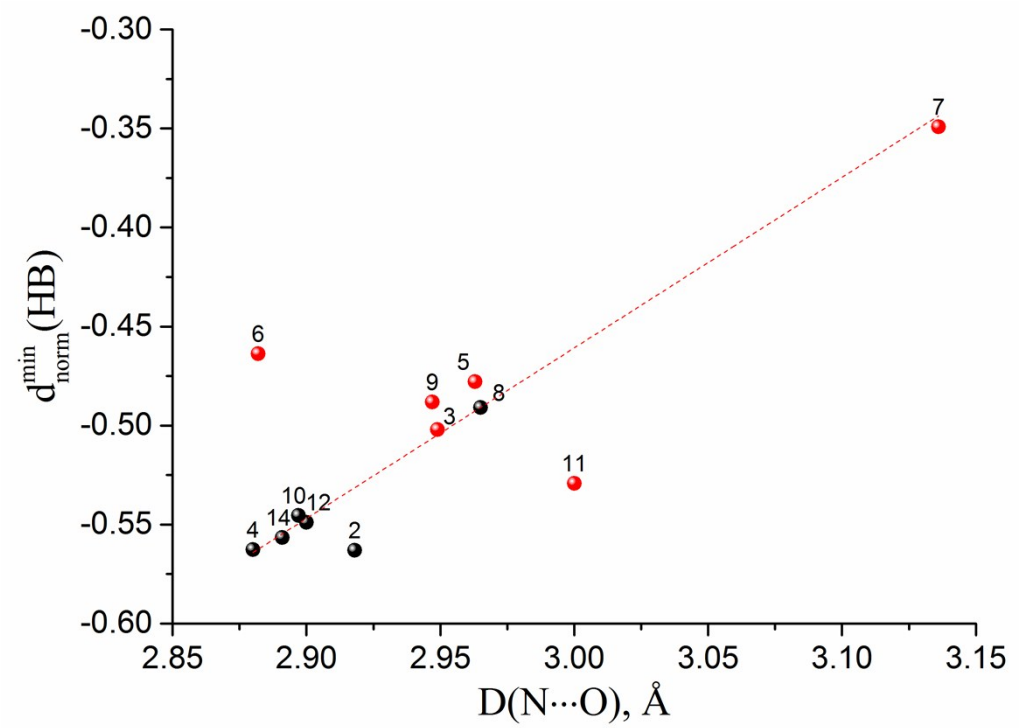



**Figure 14SI.** Correlation between the minimal normalised distance from the contact atoms involved into hydrogen bonding to the Hirshfeld surface $d_{norm}^{\min}(HB)$ and the interatomic distance D(N···O). The red points correspond to the compounds with C(4) hydrogen bonds topology, whereas the black points – with $R_2^2(8)$. The numbering of compounds corresponds to Figure 1.

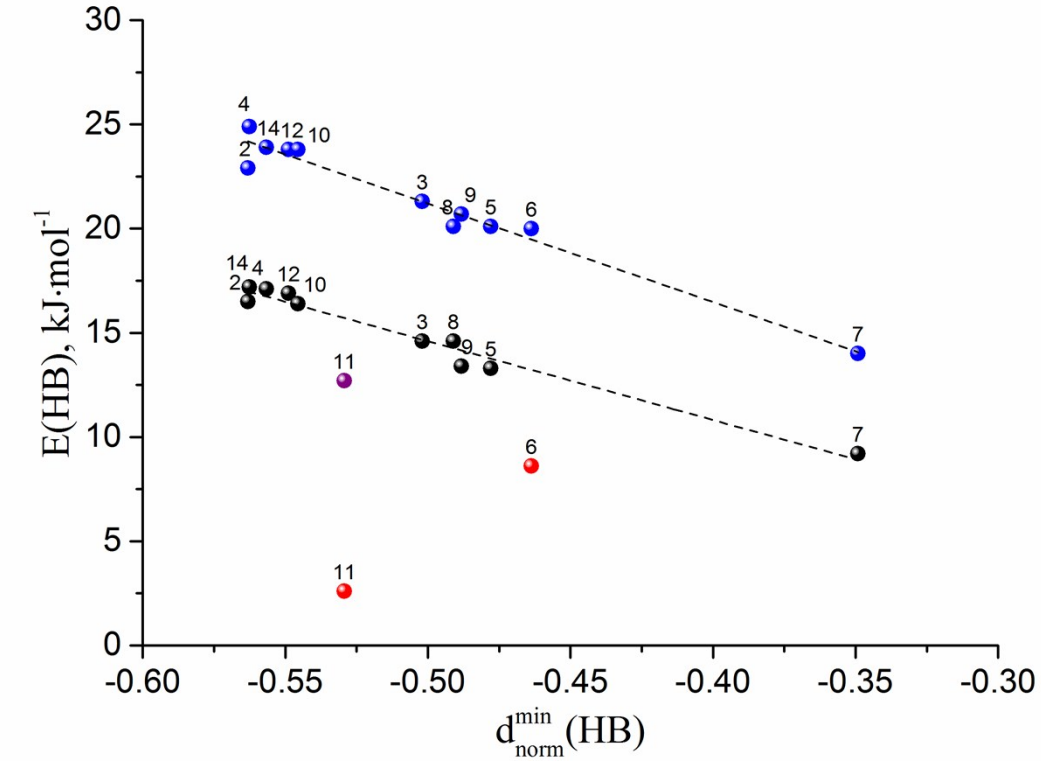
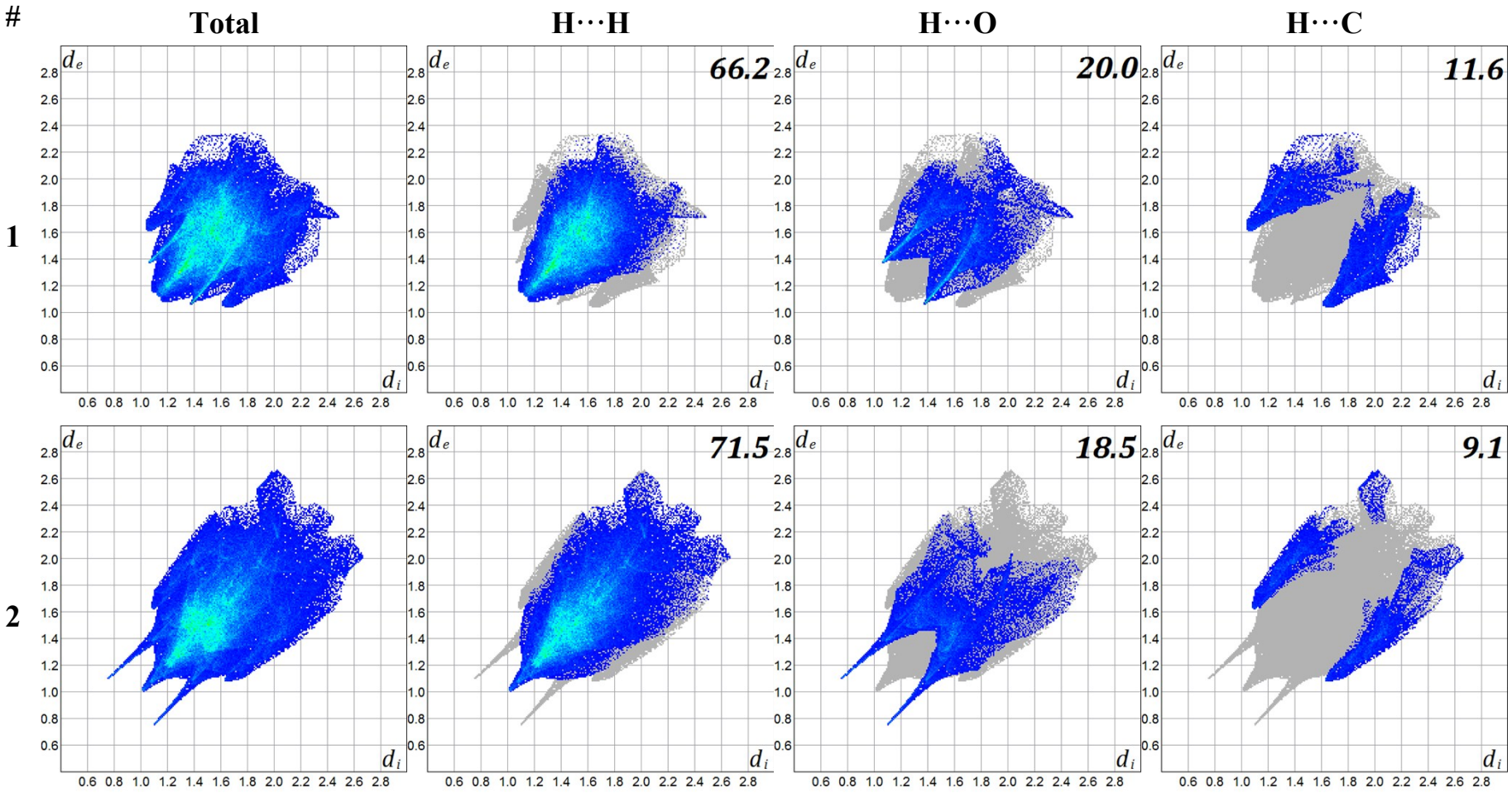
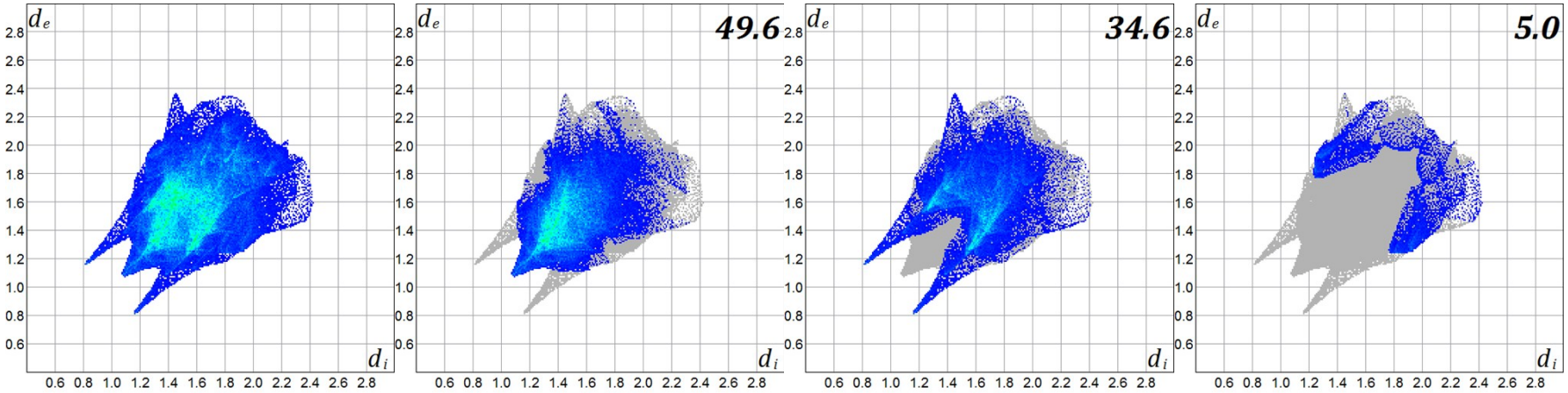


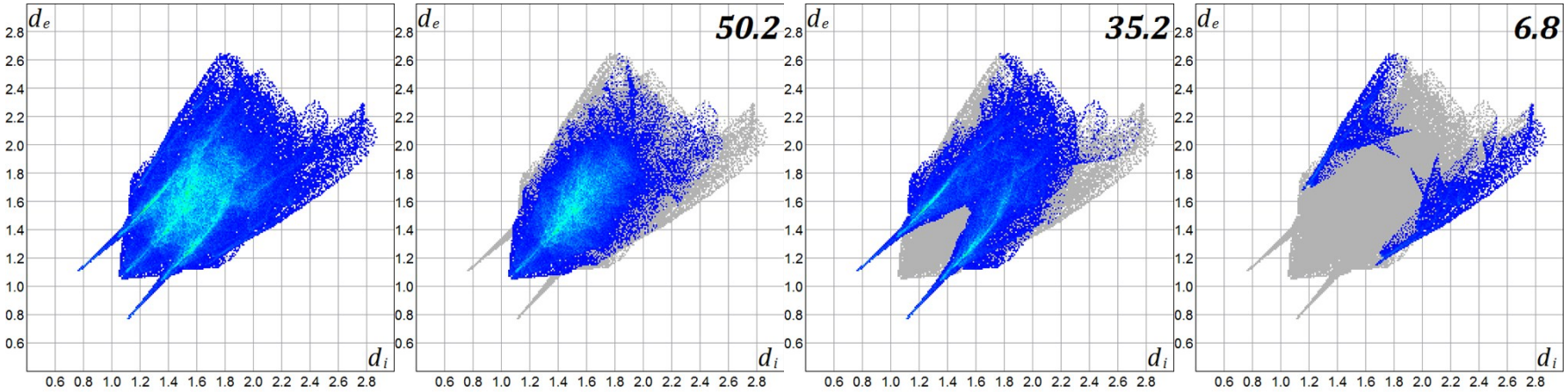

**Figure 15SI.** Correlation between the minimal normalised distance from the contact atoms involved into hydrogen bonding to the Hirshfeld surface $d_{norm}^{\min}(HB)$ and the energies of hydrogen bonds evaluated using Mayo force field (black points) and QTAIMC (blue points). Compounds 6 and 11 excluded from correlation equations are shown red and violet, respectively. The numbering of compounds corresponds to Figure 1.


#
Total
H···H
H···O
H···C
1
2
66.2
20.0
11.6
71.5
18.5
9.1
$d_e$
$d_i$
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

9


$d_e$
$d_i$
49.6
34.6
5.0
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

10


$d_e$
$d_i$
50.2
35.2
6.8
0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8

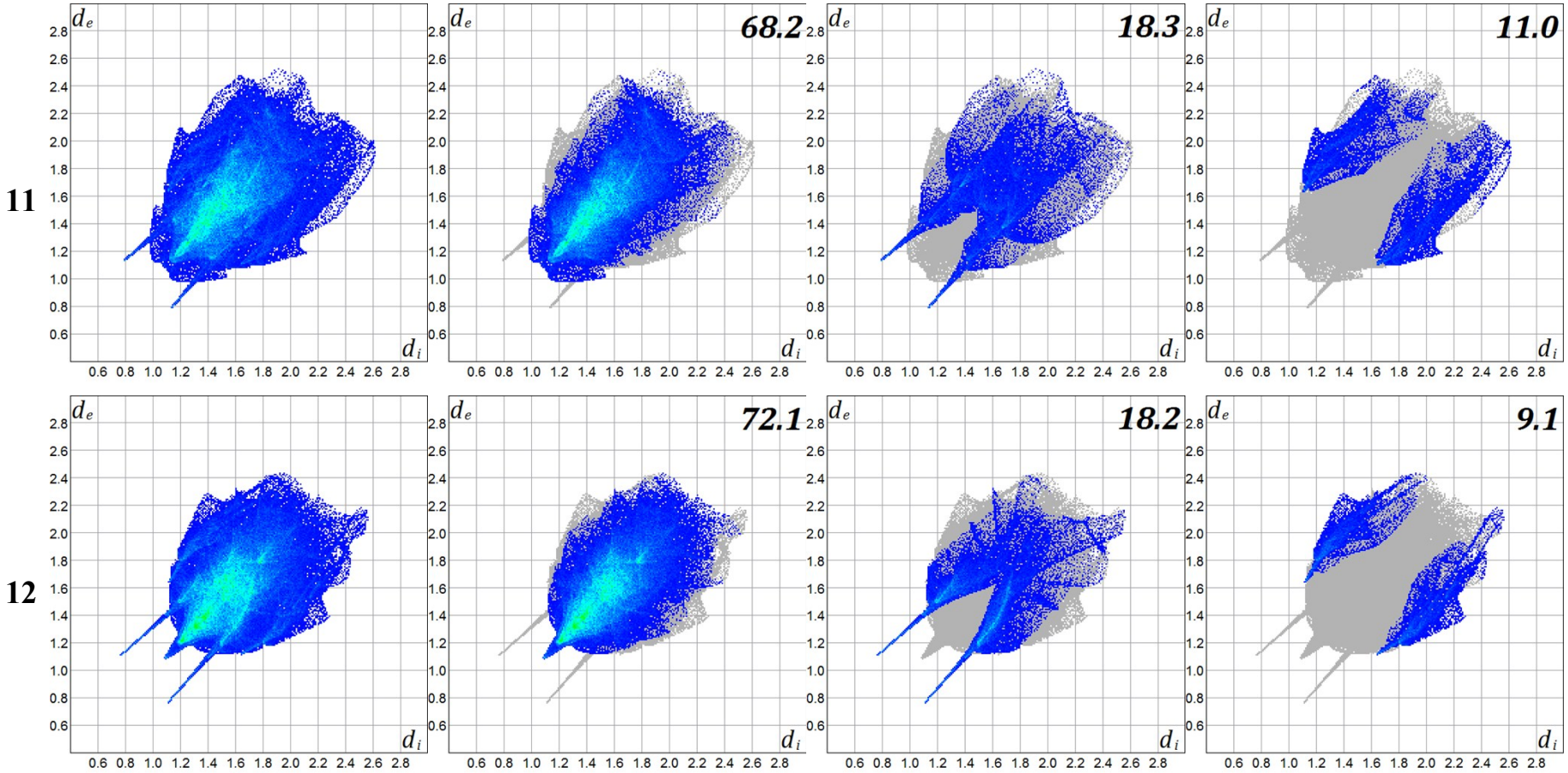
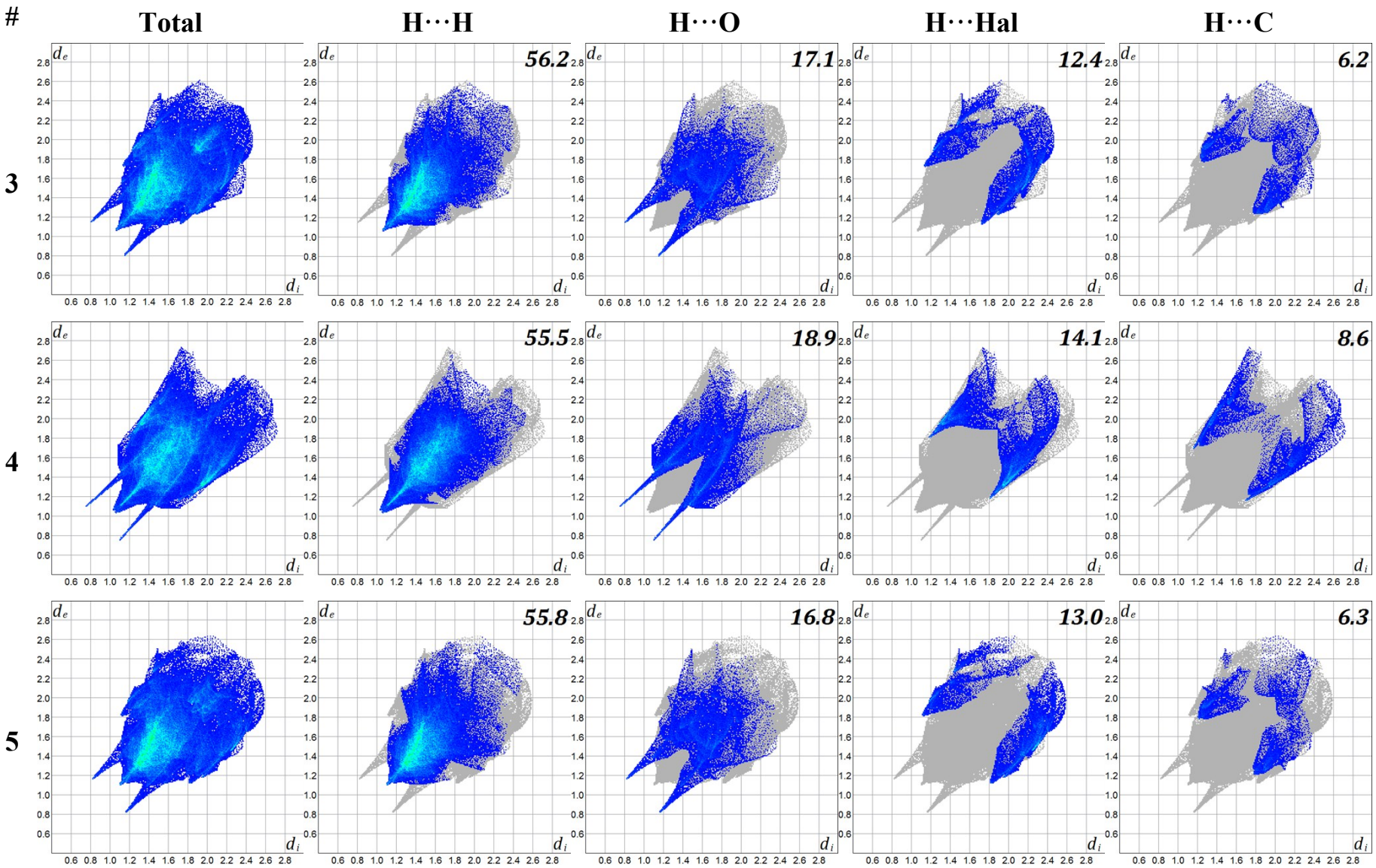
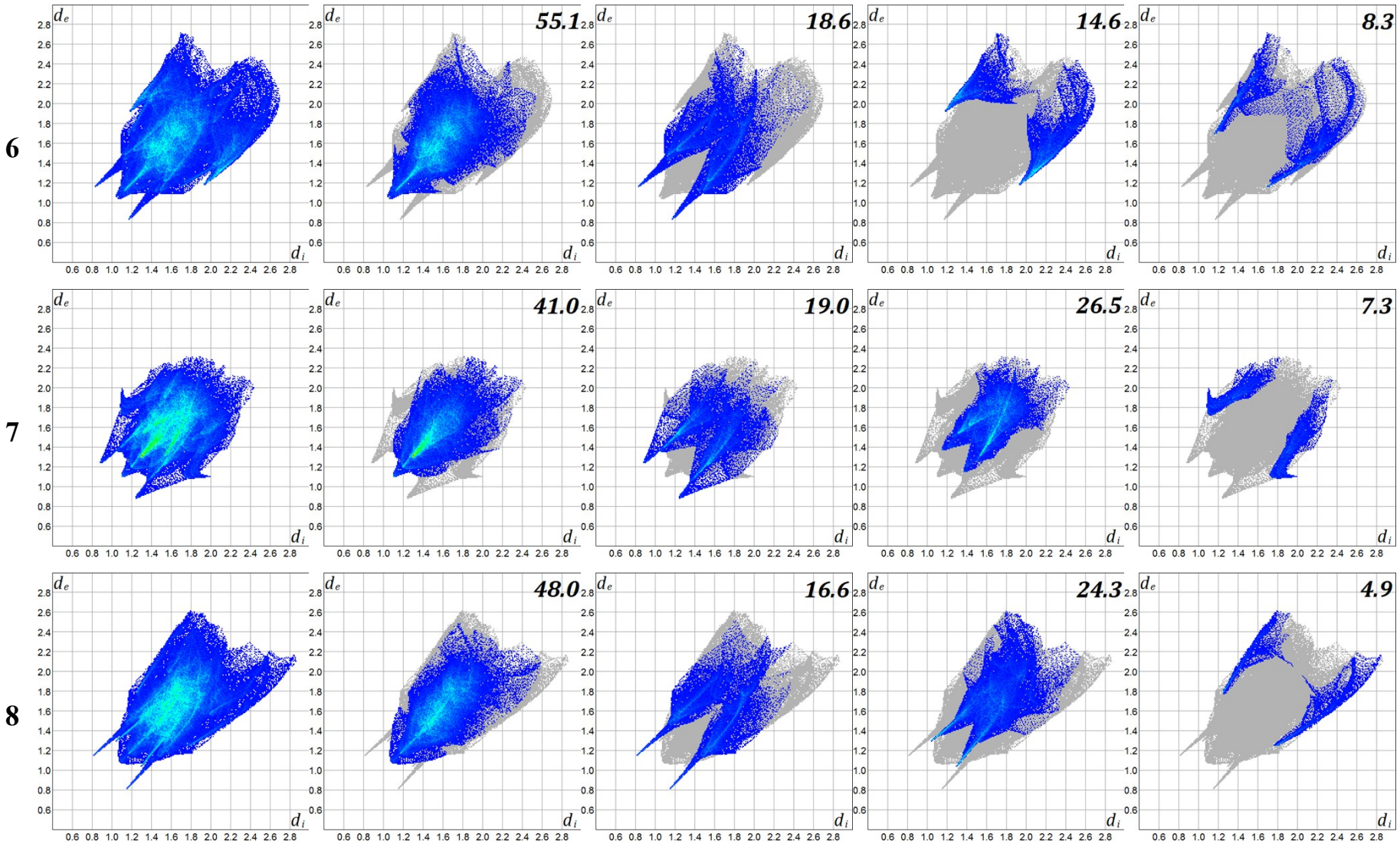



**Figure 16SI.** 2D fingerprint plots with decomposition to major contributions into the Hirshfeld surface of compounds with no halogen atoms in the structure. The numbers in the upper right corner denote the percentage of the particular interaction type.


#
Total
H···H
H···O
H···Hal
H···C
3
4
5
56.2
17.1
12.4
6.2
55.5
18.9
14.1
8.6
55.8
16.8
13.0
6.3
$d_e$
$d_i$


6
7
8
$d_e$
$d_i$
55.1
18.6
14.6
8.3
41.0
19.0
26.5
7.3
48.0
16.6
24.3
4.9

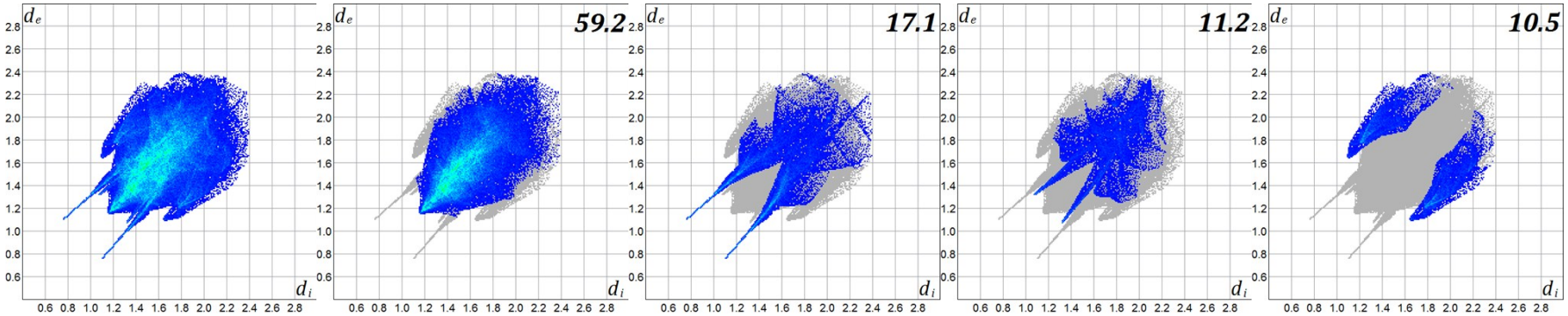
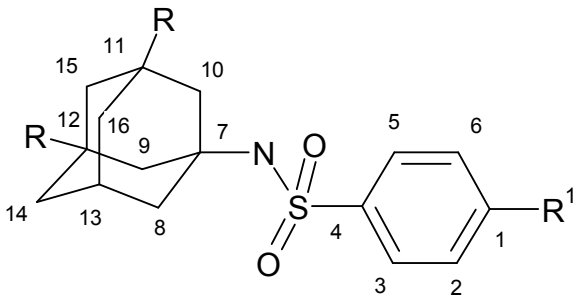
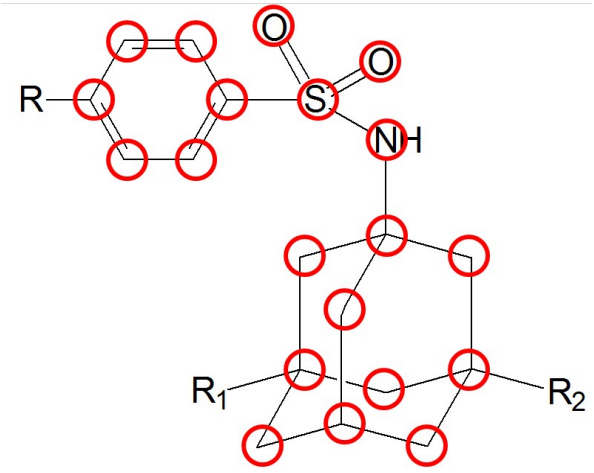



**Figure 17SI.** 2D fingerprint plots with decomposition to major contributions into the Hirshfeld surface of compounds containing the halogen atoms. The numbers in the upper right corner denote the percentage of the particular interaction type.




**Scheme 1SI.** Numeration of carbon atoms used in the description of the $^{13}C$ NMR spectra.




**Scheme 2SI.** Atoms chosen as common set of points for XPac analysis.

**Table 1SI.** Crystallographic data* for structurally relative compounds taken from CSD

| CSD refcode | Space group | a/ Å | b/ Å | c/ Å | α/ ° | β/ ° | γ/ ° | Z' | HB type** | Reference |
|---|---|---|---|---|---|---|---|---|---|---|
| Adamantane-substituted carboxamides | | | | | | | | | | |
| ADIQOV | $P2_1/c$ | 11.898(4) | 9.901(9) | 27.230(5) | 90 | 101.02(2) | 90 | 2 | chain | 1 |
| BUDVIG | C2/c | 32.257(7) | 9.4353(19) | 9.5328(19) | 90 | 101.69(3) | 90 | 1 | chain | 2 |
| EROTIP | Pbca | 9.3656(2) | 13.7515(3) | 18.7917(4) | 90 | 90 | 90 | 1 | chain | 3 |
| FISNEA | $P2_1/c$ | 6.832(2) | 22.995(4) | 10.200(3) | 90 | 102.06(2) | 90 | 1 | chain | 4 |
| FISNEA | $P2_1/c$ | 6.832(2) | 22.995(4) | 10.200(3) | 90 | 102.06(2) | 90 | 1 | chain | 4 |
| HALQER | P-1 | 6.433(3) | 6.769(3) | 17.241(12) | 85.67(5) | 84.39(5) | 63.00(5) | 1 | non-HB | 5 |
| HUGYAK | C2/m | 10.9958(10) | 6.8120(4) | 18.2231(16) | 90 | 94.155(11) | 90 | 0.5 | non-HB | 6 |
| KAJROD | C2/c | 27.6104(11) | 9.6240(4) | 9.0499(4) | 90 | 97.735(3) | 90 | 1 | chain | 7 |
| KAJROD01 | Iba2 | 9.862(2) | 28.095(5) | 8.664(3) | 90 | 90 | 90 | 1 | chain | 8 |
| KIZRUH | C c | 22.796(8) | 9.847(3) | 13.788(4) | 90 | 108.889(9) | 90 | 2 | chain | 9 |
| LEHYAZ | $P2_1/c$ | 13.070(2) | 8.9422(11) | 9.3904(11) | 90 | 109.819(8) | 90 | 1 | chain | 10 |
| LIPCAP | $P2_1/c$ | 15.818(4) | 8.225(2) | 10.423(2) | 90 | 108.897(18) | 90 | 1 | other | 11 |
| LOJXUE | $P2_1/n$ | 9.5310(19) | 10.785(2) | 34.013(7) | 90 | 91.11(3) | 90 | 2 | chain | 12 |
| PAKMOF | $P2_1/c$ | 9.2233(3) | 11.9184(3) | 13.3437(3) | 90 | 113.630(2) | 90 | 1 | chain | 13 |
| PUFJEG | Pccn | 30.708(7) | 9.7927(2) | 10.0203(6) | 90 | 90 | 90 | 1 | chain | 2 |
| RAPNII | $Pna2_1$ | 9.2558(12) | 13.0186(17) | 13.4684(18) | 90 | 90 | 90 | 1 | chain bif. | 14 |
| ROLCOK01 | C2/c | 24.312(5) | 9.464(2) | 9.454(3) | 90 | 90.06(2) | 90 | 1 | chain | 15 |
| SIVXUS | $P2_1/a$ | 8.72428(14) | 21.0562(3) | 14.1745(2) | 90 | 102.6122(17) | 90 | 1 | chain | 16 |
| TIHHID | $P2_1/c$ | 15.5349(5) | 8.4134(3) | 10.0678(3) | 90 | 94.753(2) | 90 | 1 | chain | 17 |
| USOFIT | C2/c | 27.3649(9 | 9.4960(3) | 10.0932(3) | 90 | 97.371(3) | 90 | 1 | chain | 18 |
| VASHOO | Pccn | 9.8846(2) | 27.5538(6) | 9.9296(2) | 90 | 90 | 90 | 2 | chain | 19 |
| VICHAR | P-1 | 6.8308(11) | 7.5584(11) | 12.480(2) | 104.658(18) | 96.18(2) | 102.556(19) | 1 | dimer | 20 |
| VUXCOI | Pbca | 13.173(3) | 13.173(3) | 25.804(5) | 90 | 90 | 90 | 2 | dimer | 21 |

**Table 1SI** (continuation)

| Adamantane derivatives of thiourea | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| CIXJEA | $P2_1/n$ | 21.627(5) | 7.7396(18) | 21.627(5) | 90 | 107.09 | 90 | 2 | dimer NHS | 22 |
| CIXKUR | $P2_1/n$ | 7.2067(7) | 17.2759(16) | 27.553(3) | 90 | 94.185(2) | 90 | 2 | dimer NHS | 22 |
| CIXLAY | $P2_1/c$ | 12.6285(10) | 9.8576(8) | 14.1746(11) | 90 | 107.507(2) | 90 | 1 | dimer NHS | 22 |
| EQIDAL | P-1 | 7.6584(7) | 10.2121(8) | 13.1295(11) | 108.228(6) | 97.789(7) | 92.502(7) | 1 | dimer NHO | 23 |
| EVOWIX | P-1 | 6.7936(2) | 10.3125(3) | 12.8879(4) | 103.973(2) | 92.063(2) | 94.913(3) | 1 | dimer NHS | 24 |
| EVOWOD | $P2_12_12_1$ | 6.4252(2) | 18.3151(6) | 29.3226(10) | 90 | 90 | 90 | 2 | dimer NHS | 24 |
| ILESOJ | Pbca | 12.0579(7) | 11.1213(5) | 21.9741(13) | 90 | 90 | 90 | 1 | dimer NHS | 25 |
| PAVBIZ | P-1 | 7.3985(9) | 10.4953(13) | 12.4094(15) | 65.554(2) | 79.372(2) | 89.766(2) | 1 | dimer NHO | 26 |
| PIBLAP | $P2_1/c$ | 14.4926(11) | 18.3737(12) | 6.6101(5) | 90 | 93.526(6) | 90 | 1 | dimer NHS | 27 |
| RIJNOP | P2/c | 14.0594(9) | 6.8628(6) | 17.7672(12) | 90 | 92.086(5) | 90 | 1 | dimer NHO | 27 |
| UXIBUA | Pbca | 17.2134(6) | 8.2251(2) | 22.5220(7) | 90 | 90 | 90 | 1 | chain bif. | 28 |

*Space group, metric parameters of the unit cell (angstroms and degrees), the number of molecules in asymmetric unit (Z') and pattern of hydrogen bonding (for notation, see below)

**chain – C(4) chain based on N-H···O bonds between amide groups; non-HB – structure with no intermolecular hydrogen bonds; other – substituents participate in hydrogen bonding; chain bif. – C(4) chains based on bifurcated hydrogen bonds formed by two N-H groups and a single O=C groups of (thio)urea moiety; dimer – centrosymmetric $R_2^2(8)$ dimer based on N-H···O bonds between amide groups; dimer NHS – centrosymmetric $R_2^2(8)$ dimer based on N-H···S bonds in thiourea derivatives; dimer NHO – combined $R_2^2(4)$ ring motif formed by two intermolecular N-H···O bonds and two intramolecular N-H···O bonds occurring in carbonylthioureas.

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**Table 2SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **1**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| C13-H132···O2[a] | 3.126 \| 2.395 | 122.88 | 0.013 | 0.043 | 0.010 | *11.1*** |
| C5-H5···O1[b] | 3.205 \| 2.492 | 122.20 | 0.010 | 0.035 | 0.008 | 8.7 |
| C3-H3···O2[c] | 3.360 \| 2.441 | 141.59 | 0.010 | 0.033 | 0.007 | 8.3 |
| C12-H121···O1[c] | 3.522 \| 2.434 | 171.13 | 0.010 | 0.032 | 0.007 | 8.2 |
| C6-H6···O1[b] | 3.224 \| 2.556 | 118.96 | 0.007 | 0.030 | 0.006 | 7.0 |
| C8-H82···C2[a] | 3.400 \| 2.473 | 118.19 | 0.007 | 0.027 | 0.005 | *5.8*** |
| H2···H5[d] | 2.245 | - | 0.007 | 0.027 | 0.005 | 5.8 |
| N1-H1···C6[d] | 3.669 \| 2.664 | 169.52 | 0.008 | 0.023 | 0.005 | 5.3 |
| H4···H11[e] | 2.246 | - | 0.007 | 0.024 | 0.005 | 5.2 |
| H132···H101[f] | 2.295 | - | 0.006 | 0.023 | 0.004 | 5.0 |
| H14···H101[f] | 2.376 | - | 0.006 | 0.021 | 0.004 | 4.5 |
| H131···H162[d] | 2.269 | - | 0.006 | 0.020 | 0.004 | 4.5 |
| C12-H122···O2[d] | 3.671 \| 2.776 | 138.49 | 0.005 | 0.019 | 0.004 | 4.4 |
| H11···H161[g] | 2.368 | - | 0.006 | 0.020 | 0.004 | 4.3 |
| C10-H102···C1[c] | 3.969 \| 2.903 | 164.10 | 0.006 | 0.018 | 0.004 | 4.0 |
| H151···H9[h] | 2.487 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| C4···O1[i] | 3.448 | - | 0.004 | 0.015 | 0.003 | 3.4 |
| C8-H82···C6[j] | 3.819 \| 2.951 | 136.39 | 0.005 | 0.015 | 0.003 | 3.2 |
| C9-H9···C5[c] | 3.731 \| 2.955 | 128.00 | 0.005 | 0.014 | 0.003 | 3.1 |
| H6···H121[i] | 2.533 | - | 0.004 | 0.015 | 0.003 | 3.1 |
| C15-H152···O2[j] | 3.969 \| 2.930 | 157.87 | 0.004 | 0.014 | 0.003 | 3.0 |
| H132···H152[f] | 2.591 | - | 0.004 | 0.013 | 0.002 | 2.6 |
| H4···H14[k] | 2.518 | - | 0.004 | 0.012 | 0.002 | 2.5 |
| H161···H3[l] | 2.564 | - | 0.003 | 0.012 | 0.002 | 2.5 |
| C8-H81···N1[i] | 4.054 \| 3.154 | 139.79 | 0.003 | 0.010 | 0.002 | 2.3 |
| C6-H6···C3[m] | 4.162 \| 3.104 | 165.14 | 0.003 | 0.010 | 0.002 | 2.1 |
| H81···H122[i] | 2.655 | - | 0.003 | 0.009 | 0.002 | 1.9 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **108.4** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) x,y,z; b) 2-x,1-y,-1/2+z; c) -1/2+x,1-y,z; d) 1.5-x,y,1/2+z; e) 1-x,1-y,-1/2+z; f) 1/2+x,-y,z; g) 1-x,-y,1/2+z; h) 1-x,-y,-1/2+z; i) 1.5-x,y,-1/2+z; j) -1/2+x,-y,z; k) 1.5-x,1+y,-1/2+z; l) x,1+y,z; m) 1/2+x,1-y,z.

**Table 3SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **2**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.887 \| 1.864 | 174.62 | 0.030 | 0.092 | 0.023 | 25.8 |
| C12-H12B···O2[b] | 3.206 \| 2.494 | 121.47 | 0.011 | 0.036 | 0.008 | *9.1*** |
| C2-H2···O1[a] | 3.481 \| 2.463 | 155.51 | 0.010 | 0.032 | 0.007 | 8.3 |
| H13A···H10A[c] | 2.026 | - | 0.010 | 0.033 | 0.007 | 7.9 |
| C3-H3···O2[d] | 3.347 \| 2.491 | 135.02 | 0.008 | 0.030 | 0.007 | 7.4 |
| C18-H18C···O1[e] | 3.239 \| 2.756 | 106.31 | 0.007 | 0.027 | 0.005 | 6.2 |
| C8-H8A···C1[b] | 3.235 \| 2.797 | 103.58 | 0.008 | 0.028 | 0.005 | *6.1*** |
| H16A···H13B[f] | 2.149 | - | 0.008 | 0.026 | 0.005 | 5.9 |
| H17A···H13A[c] | 2.287 | - | 0.007 | 0.025 | 0.005 | 5.3 |
| C14-H14···C3[f] | 3.636 \| 2.731 | 139.69 | 0.007 | 0.024 | 0.005 | 5.2 |
| C15-H15A···O2[c] | 3.317 \| 2.757 | 111.28 | 0.006 | 0.023 | 0.005 | 5.2 |
| C18-H18C···O2[e] | 3.754 \| 2.718 | 157.55 | 0.006 | 0.021 | 0.004 | 5.1 |
| C10-H10B···C3[d] | 3.788 \| 2.728 | 162.46 | 0.007 | 0.022 | 0.004 | 4.9 |
| C16-H16B···O1[e] | 3.343 \| 2.861 | 106.57 | 0.005 | 0.021 | 0.004 | 4.8 |
| H6A···H15A[c] | 2.297 | - | 0.006 | 0.022 | 0.004 | 4.7 |
| H8B···H16A[f] | 2.386 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| H18B···H17A[d] | 2.421 | - | 0.005 | 0.016 | 0.003 | 3.5 |
| H15B···H8A[c] | 2.385 | - | 0.005 | 0.016 | 0.003 | 3.4 |
| H13B···H18Bf | 2.421 | - | 0.005 | 0.016 | 0.003 | 3.3 |
| C4-H4···O2[d] | 3.573 \| 2.986 | 114.28 | 0.004 | 0.015 | 0.003 | 3.3 |
| H2···H16B[f] | 2.525 | - | 0.004 | 0.015 | 0.003 | 3.1 |
| H17B···H6A[c] | 2.601 | - | 0.004 | 0.014 | 0.003 | 3.0 |
| H4···H12A[d] | 2.527 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| H15B···H10A[c] | 2.542 | - | 0.004 | 0.013 | 0.002 | 2.7 |
| C17-H17B···C6[g] | 4.122 \| 3.026 | 176.28 | 0.004 | 0.012 | 0.002 | 2.7 |
| H17C··· H5[h] | 2.772 | - | 0.003 | 0.012 | 0.002 | 2.5 |
| H14···H12B[c] | 2.590 | - | 0.003 | 0.011 | 0.002 | 2.3 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **133.1** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) 1-x,1-y,1-z; b) x,y,z; c) 1.5-x,1/2+y,1/2-z; d) 1/2+x,1/2-y,1/2+z; e) 1+x,y,z; f) 2-x,1-y,1-z; g) 1/2+x,1/2-y,-1/2+z; h) 1.5-x,-1/2+y,1/2-z.

**Table 4SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **3**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.949 \| 1.952 | 166.94 | 0.025 | 0.073 | 0.019 | 21.3 |
| C13-H132···O2[b] | 2.926 \| 2.347 | 111.37 | 0.015 | 0.054 | 0.012 | *13.6*** |
| C12-H122···O1[a] | 3.343 \| 2.456 | 137.73 | 0.010 | 0.034 | 0.008 | 8.6 |
| H11···H102[c] | 2.127 | - | 0.009 | 0.029 | 0.006 | 6.7 |
| H101···H131[d] | 2.214 | - | 0.007 | 0.025 | 0.005 | 5.6 |
| C3···O2[d] | 3.187 | - | 0.006 | 0.024 | 0.005 | 5.5 |
| C2-H2···N1[b] | 3.736 \| 2.790 | 160.96 | 0.008 | 0.022 | 0.005 | 5.5 |
| C12-H122···Cl1[e] | 3.624 \| 2.866 | 126.77 | 0.006 | 0.023 | 0.004 | 4.9 |
| H6···H162[f] | 2.235 | - | 0.006 | 0.022 | 0.004 | 4.7 |
| H161···H81[f] | 2.442 | - | 0.006 | 0.022 | 0.004 | 4.7 |
| H161···H9[f] | 2.383 | - | 0.005 | 0.019 | 0.004 | 4.2 |
| C16-H162···O2[g] | 3.417 \| 2.866 | 111.40 | 0.005 | 0.018 | 0.004 | 4.2 |
| H101···H14[d] | 2.557 | - | 0.005 | 0.018 | 0.003 | 3.9 |
| C8-H81···C1[b] | 3.549 \| 2.952 | 114.85 | 0.005 | 0.017 | 0.003 | *3.8*** |
| H9···H132[g] | 2.418 | - | 0.005 | 0.017 | 0.003 | 3.7 |
| H161···H132[g] | 2.436 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| C11-H11···Cl1[e] | 3.740 \| 3.092 | 118.73 | 0.005 | 0.016 | 0.003 | 3.5 |
| C15-H151···Cl1[f] | 4.175 \| 3.120 | 163.53 | 0.004 | 0.014 | 0.003 | 3.0 |
| H101···H152[d] | 2.567 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| H11···H5[h] | 2.561 | - | 0.004 | 0.013 | 0.003 | 2.9 |
| H9···H14[d] | 2.570 | - | 0.004 | 0.013 | 0.003 | 2.8 |
| H152···H5[h] | 2.509 | - | 0.004 | 0.013 | 0.003 | 2.8 |
| C14-H14···C5[f] | 3.817 \| 3.034 | 129.22 | 0.004 | 0.013 | 0.002 | 2.8 |
| H121···H5[h] | 2.529 | - | 0.004 | 0.013 | 0.002 | 2.8 |
| H152···H152[i] | 2.707 | - | 0.004 | 0.013 | 0.002 | 2.8 |
| Cl1···C2[j] | 3.752 | - | 0.004 | 0.012 | 0.002 | 2.7 |
| H82···H131[d] | 2.564 | - | 0.004 | 0.013 | 0.002 | 2.7 |
| C16-H162···C4[f] | 3.961 \| 3.065 | 139.89 | 0.004 | 0.012 | 0.002 | 2.6 |
| H102···H6[f] | 2.626 | - | 0.003 | 0.012 | 0.002 | 2.5 |
| H151···H11[c] | 2.648 | - | 0.003 | 0.012 | 0.002 | 2.5 |
| C4···C4[j] | 3.689 | - | 0.003 | 0.010 | 0.002 | 2.3 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **133.1** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, Cl, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) -x,-1/2+y,1/2-z; b) x,y,z; c) 1-x,1-y,1-z; d) x,-1+y,z; e) x,1/2-y,1/2+z; f) 1-x,1/2+y,1/2-z; g) 1-x,-1/2+y,1/2-z; h) x,1.5-y,1/2+z; i) 1-x,2-y,1-z; j) -x,1-y,-z.

**Table 5SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **4**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.881 \| 2.077 | 171.23 | 0.028 | 0.090 | 0.022 | 24.9 |
| C12-H121···O2[b] | 3.201 \| 2.556 | 121.20 | 0.010 | 0.035 | 0.008 | *8.8*** |
| C15-H152···O2[c] | 3.543 \| 2.628 | 156.72 | 0.008 | 0.028 | 0.006 | 7.2 |
| C5-H5···O1[d] | 3.428 \| 2.703 | 133.64 | 0.008 | 0.028 | 0.006 | 6.7 |
| H161···H151[e] | 2.288 | - | 0.009 | 0.029 | 0.006 | 6.6 |
| C17-H171···O2[f] | 3.634 \| 2.736 | 158.32 | 0.008 | 0.026 | 0.006 | 6.4 |
| H152···H6[c] | 2.363 | - | 0.008 | 0.028 | 0.006 | 6.3 |
| C5-H5···O2[d] | 3.710 \| 2.767 | 171.86 | 0.007 | 0.024 | 0.005 | 5.8 |
| H82···H9[g] | 2.429 | - | 0.006 | 0.022 | 0.004 | 4.8 |
| H9···H9[g] | 2.530 | - | 0.006 | 0.022 | 0.004 | 4.8 |
| H181···H121[c] | 2.432 | - | 0.006 | 0.022 | 0.004 | 4.7 |
| H9···H102[g] | 2.483 | - | 0.006 | 0.021 | 0.004 | 4.5 |
| C18-H181···O2[c] | 3.700 \| 2.862 | 148.13 | 0.005 | 0.019 | 0.004 | 4.3 |
| C2-H2···O1[a] | 3.792 \| 2.942 | 152.08 | 0.005 | 0.018 | 0.004 | 4.0 |
| C8-H81···Cl[h] | 4.038 \| 3.117 | 154.88 | 0.005 | 0.017 | 0.003 | 3.6 |
| C10-H101···C5[g] | 3.963 \| 2.990 | 174.05 | 0.005 | 0.015 | 0.003 | 3.3 |
| C18-H183···C3[i] | 3.661 \| 3.027 | 123.38 | 0.005 | 0.015 | 0.003 | 3.2 |
| H162···H182[e] | 2.598 | - | 0.004 | 0.015 | 0.003 | 3.1 |
| H2···H173[j] | 2.674 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| C16-H162···Cl[h] | 4.098 \| 3.199 | 150.51 | 0.004 | 0.014 | 0.003 | 2.9 |
| H3···H173[j] | 2.712 | - | 0.004 | 0.013 | 0.002 | 2.7 |
| C3···Cl[h] | 3.776 | - | 0.004 | 0.011 | 0.002 | 2.5 |
| C3···C3[h] | 3.645 | - | 0.003 | 0.011 | 0.002 | 2.5 |
| C18-H182···Cl[i] | 4.021 \| 3.311 | 128.88 | 0.003 | 0.011 | 0.002 | 2.4 |
| H172···H6[c] | 2.811 | - | 0.003 | 0.011 | 0.002 | 2.3 |
| C17-H172···Cl[g] | 4.304 \| 3.336 | 163.30 | 0.003 | 0.010 | 0.002 | 2.2 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **124.5** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, Cl, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) -x,-y,-z; b) x,y,z; c) 1-x,-1/2+y,1/2-z; d) x,1/2-y,1/2+z; e) x,-1/2-y,-1/2+z; f) 1-x,-y,-z; g) 1-x,-y,1-z; h) -x,-y,1-z; i) -x,-1/2+y,1/2-z; j) -1+x,y,z.

**Table 6SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **5**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.963 \| 2.160 | 163.09 | 0.024 | 0.069 | 0.018 | 20.1 |
| C12-H12···O2[b] | 2.927 \| 2.382 | 113.63 | 0.015 | 0.053 | 0.012 | *13.6*** |
| C8-H6···O1[a] | 3.378 \| 2.568 | 141.47 | 0.009 | 0.032 | 0.007 | 8.2 |
| C3···O2[c] | 3.168 | - | 0.007 | 0.025 | 0.005 | 5.8 |
| H8···H20[d] | 2.323 | - | 0.007 | 0.025 | 0.005 | 5.6 |
| C2-H2···N1[a] | 3.728 \| 2.822 | 161.21 | 0.008 | 0.022 | 0.005 | 5.5 |
| H15···H18[e] | 2.469 | - | 0.006 | 0.023 | 0.004 | 4.9 |
| C8-H6···Br1[f] | 3.658 \| 3.008 | 125.83 | 0.007 | 0.021 | 0.004 | 4.9 |
| H19···H13[c] | 2.517 | - | 0.006 | 0.022 | 0.004 | 4.8 |
| C2-H2···O1[a] | 3.736 \| 2.901 | 148.00 | 0.005 | 0.020 | 0.004 | 4.7 |
| H17···H5[e] | 2.513 | - | 0.006 | 0.020 | 0.004 | 4.3 |
| C9-H8···Br1[f] | 3.777 \| 3.140 | 122.65 | 0.006 | 0.018 | 0.004 | 4.1 |
| C15-H17···O2[e] | 3.416 \| 2.956 | 110.06 | 0.004 | 0.017 | 0.003 | 3.9 |
| C13-H15···C1[b] | 3.542 \| 2.979 | 115.79 | 0.005 | 0.017 | 0.003 | *3.8*** |
| H19···H11[c] | 2.630 | - | 0.005 | 0.018 | 0.003 | 3.8 |
| C10-H9···Br1[g] | 4.202 \| 3.263 | 167.27 | 0.006 | 0.016 | 0.003 | 3.7 |
| H16···H18[e] | 2.579 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| H18···H12[e] | 2.561 | - | 0.005 | 0.017 | 0.003 | 3.5 |
| H12···H16[e] | 2.555 | - | 0.005 | 0.016 | 0.003 | 3.5 |
| C2···Br1[h] | 3.772 | - | 0.005 | 0.013 | 0.003 | 3.2 |
| H10···H10[i] | 2.712 | - | 0.004 | 0.014 | 0.003 | 3.1 |
| C15-H17···C4[g] | 3.927 \| 3.092 | 144.33 | 0.004 | 0.014 | 0.003 | 3.0 |
| H8···H4[j] | 2.673 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| H19···H10[c] | 2.726 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| H16···H11[c] | 2.649 | - | 0.004 | 0.013 | 0.002 | 2.8 |
| C11-H11···C5[g] | 3.813 \| 3.096 | 128.71 | 0.004 | 0.012 | 0.002 | 2.7 |
| H7···H4[j] | 2.719 | - | 0.004 | 0.013 | 0.002 | 2.7 |
| H20···H5[e] | 2.729 | - | 0.003 | 0.012 | 0.002 | 2.6 |
| H14···H13[c] | 2.807 | - | 0.003 | 0.012 | 0.002 | 2.5 |
| O1···Br1[h] | 3.845 | - | 0.003 | 0.011 | 0.002 | 2.4 |
| C4···C4[h] | 3.704 | - | 0.003 | 0.011 | 0.002 | 2.3 |
| H10···H4[j] | 2.776 | - | 0.003 | 0.011 | 0.002 | 2.3 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **130.4** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, Br, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) 1-x,1/2+y,1/2-z; b) x,y,z; c) x,1+y,z; d) -x,1-y,-z; e) -x,1/2+y,1/2-z; f) x,1.5-y,-1/2+z; g) -x,-1/2+y,1/2-z; h) 1-x,1-y,1-z; i) -x,-y,-z; j) x,1/2-y,-1/2+z.

**Table 7SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **6**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1A···O1[a] | 2.882 \| 2.000 | 143.79 | 0.023 | 0.071 | 0.018 | 20.1 |
| C12-H12A···O2[b] | 3.192 \| 2.490 | 124.11 | 0.011 | 0.037 | 0.008 | *9.3*** |
| C15-H15A···O2[c] | 3.570 \| 2.552 | 155.20 | 0.008 | 0.027 | 0.006 | 6.7 |
| H6A···H15A[c] | 2.105 | - | 0.008 | 0.028 | 0.006 | 6.5 |
| C18-H18C···O2[d] | 3.634 \| 2.613 | 125.22 | 0.008 | 0.025 | 0.006 | 6.2 |
| C5-H5A···O2[e] | 3.675 \| 2.591 | 173.58 | 0.007 | 0.025 | 0.005 | 6.2 |
| H9A···H9A[f] | 2.345 | - | 0.007 | 0.028 | 0.005 | 6.1 |
| C5-H5A···O1[e] | 3.464 \| 2.664 | 129.84 | 0.007 | 0.025 | 0.005 | 6.0 |
| C1···C8[b] | 3.272 | - | 0.007 | 0.027 | 0.005 | *6.0*** |
| H15B···H16B[g] | 2.182 | - | 0.008 | 0.026 | 0.005 | 6.0 |
| O1···O1[a] | 3.288 | - | 0.006 | 0.023 | 0.005 | 5.7 |
| H8A···H9A[f] | 2.246 | - | 0.007 | 0.025 | 0.005 | 5.6 |
| H17B ···H12A[d] | 2.241 | - | 0.006 | 0.021 | 0.004 | 4.6 |
| C2-H2A···O1 | 3.743 \| 2.745 | 152.28 | 0.005 | 0.019 | 0.004 | 4.5 |
| H9A···H10B | 2.375 | - | 0.006 | 0.020 | 0.004 | 4.4 |
| C17-H17B···O2[c] | 3.707 \| 2.743 | 147.33 | 0.005 | 0.019 | 0.004 | 4.4 |
| C8-H8B···Br[h] | 4.128 \| 3.115 | 155.00 | 0.006 | 0.016 | 0.003 | 3.6 |
| C10-H10A···C5[f] | 3.939 \| 2.856 | 172.74 | 0.005 | 0.016 | 0.003 | 3.5 |
| C17-H17A···C3[i] | 3.719 \| 2.940 | 128.70 | 0.005 | 0.015 | 0.003 | 3.2 |
| C16-H16A···Br[h] | 4.170 \| 3.171 | 152.78 | 0.005 | 0.014 | 0.003 | 3.2 |
| H18B···H3A[j] | 2.572 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| H17C···H16A[g] | 2.521 | - | 0.004 | 0.013 | 0.002 | 2.8 |
| C18-H18A···Br[f] | 4.307 \| 3.260 | 161.74 | 0.005 | 0.012 | 0.002 | 2.8 |
| C3···Br[h] | 3.861 | - | 0.004 | 0.011 | 0.002 | 2.7 |
| C17-H17C···Br[i] | 4.098 \| 3.359 | 126.26 | 0.004 | 0.012 | 0.002 | 2.6 |
| H18B···H2A[j] | 2.690 | - | 0.003 | 0.012 | 0.002 | 2.6 |
| C6··· Br[k] | 3.653 | - | 0.004 | 0.010 | 0.002 | 2.4 |
| O1···Br[k] | 3.909 | - | 0.003 | 0.011 | 0.002 | 2.4 |
| C13-H13A···Br[i] | 4.145 \| 3.392 | 127.38 | 0.004 | 0.011 | 0.002 | 2.4 |
| H18C···H12B[d] | 2.838 | - | 0.003 | 0.010 | 0.002 | 2.2 |
| C13-H13B···Br[h] | 4.274 \| 3.306 | 148.69 | 0.003 | 0.010 | 0.002 | 2.2 |
| H17C···H10B[c] | 2.777 | - | 0.003 | 0.009 | 0.002 | 1.9 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **136.3** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, Br, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) 2-x,1-y,1-z; b) x,y,z; c) 1-x,-1/2+y,1/2-z; d) 1-x,1-y,1-z; e) x,1.5-y,-1/2+z; f) 1-x,1-y,-z; g) x,1/2-y,1/2+z; h) 2-x,1-y,-z; i) 2-x,-1/2+y,1/2-z; j) -1+x,y,z; k) x,1.5-y,1/2+z.

**Table 8SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **7**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O2[a] | 3.136 \| 2.144 | 163.54 | 0.017 | 0.049 | 0.013 | 14.3 |
| C13···O2[b] | 2.985 | - | 0.011 | 0.041 | 0.009 | *9.9*** |
| C3-H3···O2[c] | 3.167 \| 2.443 | 112.53 | 0.010 | 0.036 | 0.008 | 9.0 |
| F1···F1[d] | 2.803 | - | 0.005 | 0.034 | 0.007 | 8.2 |
| C13-H14···O1[e] | 3.518 \| 2.502 | 153.95 | 0.008 | 0.028 | 0.006 | 7.1 |
| C6-H5···F2[f] | 3.329 \| 2.553 | 127.76 | 0.006 | 0.028 | 0.006 | 6.4 |
| C8-H6···O1[a] | 3.647 \| 2.614 | 156.71 | 0.007 | 0.024 | 0.005 | 5.9 |
| C13-H15···F3[g] | 3.311 \| 2.625 | 119.93 | 0.006 | 0.026 | 0.005 | 5.8 |
| C2-H2···N1[a] | 3.770 \| 2.688 | 175.33 | 0.007 | 0.022 | 0.005 | 5.4 |
| C2-H2···O2[c] | 3.290 \| 2.717 | 123.20 | 0.005 | 0.023 | 0.005 | 5.1 |
| C8-H7···C1[b] | 3.495 \| 2.779 | 122.64 | 0.007 | 0.022 | 0.004 | *5.1*** |
| H3···H5[c] | 2.230 | - | 0.006 | 0.022 | 0.004 | 4.7 |
| C15-H18···C1[h] | 3.838 \| 2.854 | 149.25 | 0.006 | 0.021 | 0.004 | 4.7 |
| C11-H11···O1[h] | 3.718 \| 2.757 | 146.04 | 0.006 | 0.020 | 0.004 | 4.6 |
| C12-H12···O1[e] | 3.722 \| 2.774 | 144.67 | 0.005 | 0.019 | 0.004 | 4.4 |
| H9···H13[i] | 2.410 | - | 0.005 | 0.020 | 0.004 | 4.2 |
| H2···H12[e] | 2.420 | - | 0.005 | 0.019 | 0.004 | 4.0 |
| C14-H16···F1[g] | 3.762 \| 2.771 | 150.09 | 0.004 | 0.018 | 0.003 | 3.9 |
| C14-H16···F3[g] | 3.539 \| 2.872 | 119.23 | 0.003 | 0.018 | 0.003 | 3.7 |
| C3···F3[j] | 3.321 | - | 0.004 | 0.017 | 0.003 | 3.6 |
| H3···H10[k] | 2.401 | - | 0.005 | 0.016 | 0.003 | 3.3 |
| C9-H8···F1[l] | 3.824 \| 2.878 | 144.37 | 0.003 | 0.015 | 0.003 | 3.1 |
| C9-H8···F1[j] | 3.767 \| 2.865 | 141.64 | 0.003 | 0.014 | 0.003 | 2.9 |
| C5···F2[j] | 3.461 | - | 0.003 | 0.013 | 0.002 | 2.8 |
| C8-H7···F3[j] | 3.679 \| 2.938 | 124.99 | 0.003 | 0.014 | 0.002 | 2.8 |
| H19···H20[m] | 2.567 | - | 0.004 | 0.013 | 0.002 | 2.8 |
| H9···H11[i] | 2.586 | - | 0.004 | 0.013 | 0.002 | 2.7 |
| N1···O1[e] | 3.691 | - | 0.003 | 0.012 | 0.002 | 2.7 |
| C12-H13···O1[a] | 4.043 \| 3.142 | 139.82 | 0.003 | 0.011 | 0.002 | 2.3 |
| H17···H9[c] | 2.586 | - | 0.003 | 0.011 | 0.002 | 2.2 |
| H16···H8[c] | 2.588 | - | 0.003 | 0.010 | 0.002 | 2.2 |
| C10-H10···C6[h] | 4.120 \| 3.125 | | 0.003 | 0.010 | 0.002 | 2.2 |
| H6···H14[c] | 2.608 | - | 0.003 | 0.010 | 0.002 | 2.1 |
| H19···H4[g] | 2.604 | - | 0.003 | 0.010 | 0.002 | 2.0 |
| H11···H17[n] | 2.680 | - | 0.003 | 0.009 | 0.002 | 1.9 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **142.8** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C, F and A= O, N, C, F, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) 1.5-x,1/2+y,1.5-z; b) x,y,z; c) x,1+y,z; d) 1-x,y,1/2-z; e) 1.5-x,-1/2+y,1.5-z; f) x,-1+y,z; g) 1-x,-y,1-z; h) x,-y,1/2+z; i) 1.5-x,1/2-y,2-z; j) 1-x,1-y,1-z; k) x,1-y,-1/2+z; l) x,1-y,1/2+z; m) 1-x,y,1.5-z; n) 1.5-x,-1/2-y,2-z.

**Table 9SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **8**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O2[a] | 2.965 \| 1.966 | 167.44 | 0.023 | 0.072 | 0.018 | 20.1 |
| C18-H18B···F3[b] | 3.391 \| 2.335 | 163.00 | 0.009 | 0.038 | 0.009 | 9.6 |
| C13-H13···F2[c] | 3.428 \| 2.365 | 164.86 | 0.009 | 0.036 | 0.008 | 9.1 |
| C12-H11···O1[d] | 3.218 \| 2.527 | 120.38 | 0.010 | 0.035 | 0.008 | *8.7*** |
| H14···H14[b] | 2.174 | - | 0.009 | 0.035 | 0.007 | 7.8 |
| C8-H6···F1[e] | 3.251 \| 2.503 | 124.92 | 0.007 | 0.032 | 0.007 | 7.6 |
| C18-H18C···O1[f] | 3.615 \| 2.620 | 151.59 | 0.008 | 0.025 | 0.005 | 6.2 |
| O2···O2[a] | 3.235 | - | 0.006 | 0.024 | 0.005 | 6.1 |
| C2-H2···O2[a] | 3.620 \| 2.611 | 153.74 | 0.007 | 0.024 | 0.005 | 6.0 |
| O2···F1[g] | 3.092 | - | 0.005 | 0.025 | 0.005 | 5.9 |
| H8···H5[h] | 2.167 | - | 0.007 | 0.024 | 0.005 | 5.5 |
| C10-H8···O1[h] | 3.689 \| 2.681 | 153.71 | 0.006 | 0.021 | 0.005 | 5.1 |
| H12···H14[b] | 2.371 | - | 0.006 | 0.021 | 0.004 | 4.6 |
| C5-H4···O1[i] | 3.821 \| 2.735 | 175.42 | 0.006 | 0.019 | 0.004 | 4.5 |
| C17-H17C···O1[h] | 3.746 \| 2.756 | 151.05 | 0.005 | 0.018 | 0.004 | 4.2 |
| C5-H4···O2[i] | 3.647 \| 2.832 | 131.64 | 0.005 | 0.018 | 0.004 | 4.1 |
| H9···H18[j] | 2.353 | - | 0.006 | 0.019 | 0.004 | 4.0 |
| C3-H3···F3[c] | 3.366 \| 2.865 | 108.06 | 0.004 | 0.019 | 0.003 | 3.9 |
| H11···H17C[h] | 2.328 | - | 0.005 | 0.018 | 0.003 | 3.8 |
| C17-H17B···F2[e] | 3.687 \| 2.811 | 137.37 | 0.004 | 0.018 | 0.003 | 3.7 |
| H18A···H3[k] | 2.532 | - | 0.004 | 0.015 | 0.003 | 3.1 |
| C16-H17···F2[c] | 3.815 \| 2.911 | 140.54 | 0.003 | 0.014 | 0.003 | 2.9 |
| H10···H18A[f] | 2.587 | - | 0.004 | 0.013 | 0.003 | 2.8 |
| C17-H17A···C3[e] | 3.825 \| 3.035 | 129.83 | 0.004 | 0.012 | 0.002 | 2.7 |
| H11···H18C[f] | 2.645 | - | 0.003 | 0.012 | 0.002 | 2.6 |
| C15-H15···C5[b] | 4.114 \| 3.045 | 167.20 | 0.004 | 0.011 | 0.002 | 2.3 |
| H16···H17B[h] | 2.748 | - | 0.003 | 0.010 | 0.002 | 2.1 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **140.1** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C, F and A= O, N, C, F, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) 1-x,1-y,1-z; b) -x,1-y,-z; c) 1-x,1-y,-z; d) x,y,z; e) 1-x,1/2+y,1/2-z; f) -x,1-y,1-z; g) x,1/2-y,1/2+z; h) -x,1/2+y,1/2-z; i) x,1/2-y,-1/2+z; j) x,1.5-y,1/2+z; k) -1+x,y,z.

**Table 10SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **9**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.947 \| 1.970 | 160.65 | 0.024 | 0.071 | 0.018 | 20.7 |
| C13-H15···O2[b] | 2.949 \| 2.379 | 110.90 | 0.014 | 0.050 | 0.011 | *12.7*** |
| C12-H13···O1[a] | 3.363 \| 2.465 | 138.93 | 0.010 | 0.033 | 0.007 | 8.3 |
| H10···H11[c] | 2.158 | - | 0.008 | 0.028 | 0.006 | 6.4 |
| C2-H2···N1[a] | 3.765 \| 2.708 | 163.50 | 0.007 | 0.021 | 0.005 | 5.2 |
| C3···O2[d] | 3.228 | - | 0.006 | 0.022 | 0.004 | 5.0 |
| H19···H5[e] | 2.209 | - | 0.006 | 0.023 | 0.004 | 5.0 |
| H9···H14[d] | 2.284 | - | 0.006 | 0.023 | 0.004 | 4.9 |
| C12-H13···O3[f] | 3.584 \| 2.746 | 133.46 | 0.006 | 0.021 | 0.004 | 4.9 |
| C16-H20···C8[g] | 3.763 \| 2.791 | 148.63 | 0.006 | 0.023 | 0.004 | 4.9 |
| O4···O4[h] | 3.174 | - | 0.004 | 0.019 | 0.004 | 4.7 |
| C15-H17···O3[i] | 3.774 \| 2.764 | 154.21 | 0.005 | 0.018 | 0.004 | 4.1 |
| H8···H20[e] | 2.402 | - | 0.005 | 0.019 | 0.004 | 4.1 |
| C10-H9···O3[f] | 3.651 \| 2.794 | 135.47 | 0.005 | 0.018 | 0.004 | 4.1 |
| C12-H13···O4[f] | 3.485 \| 2.905 | 113.52 | 0.004 | 0.018 | 0.004 | 4.0 |
| C15-H18···O3[g] | 3.861 \| 2.824 | 159.22 | 0.005 | 0.017 | 0.003 | 3.9 |
| C6···O4[j] | 3.351 | - | 0.004 | 0.017 | 0.003 | 3.8 |
| H9···H16[d] | 2.558 | - | 0.005 | 0.018 | 0.003 | 3.8 |
| C16-H19···O2[e] | 3.470 \| 2.904 | 112.48 | 0.004 | 0.017 | 0.003 | 3.8 |
| C12-H12···O3[i] | 3.803 \| 2.862 | 148.45 | 0.004 | 0.016 | 0.003 | 3.7 |
| H8···H15[e] | 2.436 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| C8-H7···C1[b] | 3.570 \| 2.986 | 114.01 | 0.005 | 0.016 | 0.003 | *3.6*** |
| H20···H15[e] | 2.429 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| C3-H3···O4[h] | 3.791 \| 2.808 | 150.13 | 0.004 | 0.015 | 0.003 | 3.3 |
| H11···H18[c] | 2.516 | - | 0.004 | 0.014 | 0.003 | 3.1 |
| H9···H17[d] | 2.569 | - | 0.004 | 0.013 | 0.003 | 2.8 |
| C14-H16···C5[g] | 3.809 \| 3.019 | 129.76 | 0.004 | 0.013 | 0.002 | 2.8 |
| H8···H16[d] | 2.587 | - | 0.004 | 0.013 | 0.002 | 2.8 |
| C2···O3[k] | 3.496 | - | 0.003 | 0.012 | 0.002 | 2.7 |
| C11-H11···O4[f] | 3.782 \| 3.068 | 123.70 | 0.003 | 0.012 | 0.002 | 2.7 |
| H10···H5[e] | 2.600 | - | 0.004 | 0.013 | 0.002 | 2.7 |
| C16-H19···C4[g] | 3.937 \| 3.052 | 138.82 | 0.004 | 0.012 | 0.002 | 2.7 |
| H17···H17[l] | 2.736 | - | 0.004 | 0.012 | 0.002 | 2.5 |
| H6···H14[d] | 2.606 | - | 0.003 | 0.012 | 0.002 | 2.4 |
| C4···C4[k] | 3.656 | - | 0.004 | 0.010 | 0.002 | 2.4 |
| H12···H4[i] | 2.597 | - | 0.003 | 0.011 | 0.002 | 2.4 |
| H17···H4[i] | 2.602 | - | 0.003 | 0.011 | 0.002 | 2.3 |
| H7···H8[e] | 2.657 | - | 0.003 | 0.010 | 0.002 | 2.0 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **152.3** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) -x,1/2+y,1/2-z; b) x,y,z; c) 1-x,1-y,1-z; d) x,1+y,z; e) 1-x,1/2+y,1/2-z; f) x,1.5-y,1/2+z; g) 1-x,-1/2+y,1/2-z; h) -x,2-y,-z; i) x,1/2-y,1/2+z; j) x,-1+y,z; k) -x,1-y,-z; l) 1-x,-y,1-z.

**Table 11SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **10**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.897 \| 1.896 | 168.31 | 0.027 | 0.086 | 0.021 | 23.8 |
| C8-H6···O4[b] | 3.434 \| 2.407 | 156.55 | 0.010 | 0.033 | 0.008 | 8.6 |
| C15-H16···O2[c] | 3.479 \| 2.440 | 159.17 | 0.010 | 0.032 | 0.007 | 8.4 |
| C12-H11···O2[d] | 3.267 \| 2.592 | 119.34 | 0.009 | 0.032 | 0.007 | *7.7*** |
| H8···H8[e] | 2.183 | - | 0.009 | 0.033 | 0.007 | 7.4 |
| C8-H7···O2[d] | 3.340 \| 2.691 | 117.77 | 0.008 | 0.031 | 0.006 | *7.2*** |
| C17-H19···O4[f] | 3.526 \| 2.599 | 142.46 | 0.007 | 0.025 | 0.005 | 6.1 |
| H16···H5[c] | 2.148 | - | 0.007 | 0.026 | 0.005 | 5.9 |
| C18-H22···O2[g] | 3.612 \| 2.648 | 147.19 | 0.007 | 0.024 | 0.005 | 5.9 |
| C2-H2···O1[a] | 3.639 \| 2.637 | 152.66 | 0.007 | 0.023 | 0.005 | 5.7 |
| H15···H17[h] | 2.250 | - | 0.007 | 0.024 | 0.005 | 5.3 |
| C5-H4···O2[i] | 3.750 \| 2.665 | 174.70 | 0.006 | 0.021 | 0.005 | 5.1 |
| H20···H11[c] | 2.219 | - | 0.006 | 0.022 | 0.004 | 4.9 |
| H7···H8[e] | 2.334 | - | 0.006 | 0.022 | 0.004 | 4.8 |
| C5-H4···O1[i] | 3.545 \| 2.785 | 126.78 | 0.005 | 0.020 | 0.004 | 4.6 |
| C6···O3[j] | 3.195 | - | 0.005 | 0.019 | 0.004 | 4.4 |
| C17-H20···O2[c] | 3.700 \| 2.757 | 144.76 | 0.005 | 0.019 | 0.004 | 4.3 |
| C18-H24···O3[e] | 3.814 \| 2.733 | 171.51 | 0.005 | 0.018 | 0.004 | 4.2 |
| C3···O4[b] | 3.367 | - | 0.004 | 0.016 | 0.003 | 3.6 |
| C16-H18···O4[b] | 3.748 \| 2.862 | 138.53 | 0.004 | 0.016 | 0.003 | 3.6 |
| C10-H9···C5e | 3.920 \| 2.860 | 164.37 | 0.005 | 0.016 | 0.003 | 3.5 |
| O1···O3[j] | 3.431 | - | 0.003 | 0.015 | 0.003 | 3.3 |
| C17-H21···C3[f] | 3.677 \| 2.946 | 124.72 | 0.005 | 0.015 | 0.003 | 3.2 |
| H23···H3[k] | 2.608 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| H19···H10[c] | 2.604 | - | 0.004 | 0.013 | 0.002 | 2.7 |
| H23···H12[g] | 2.600 | - | 0.004 | 0.012 | 0.002 | 2.5 |
| H23···H2[k] | 2.698 | - | 0.003 | 0.012 | 0.002 | 2.4 |
| H24···H5[c] | 2.650 | - | 0.003 | 0.011 | 0.002 | 2.3 |
| H11···H22[g] | 2.705 | - | 0.003 | 0.011 | 0.002 | 2.2 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **141.7** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) -x,-y,-z; b) -x,-y,1-z; c) 1-x,-1/2+y,1/2-z; d) x,y,z; e) 1-x,-y,1-z; f) -x,-1/2+y,1/2-z; g) 1-x,-y,-z; h) x,-1/2-y,1/2+z; i) x,1/2-y,1/2+z; j) x,1/2-y,-1/2+z; k) 1+x,y,z.

**Table 12SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **11**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.924 \| 1.905 | 170.59 | 0.027 | 0.082 | 0.020 | 23.1 |
| C3-H3B···O2[b] | 3.041 \| 2.314 | 122.25 | 0.015 | 0.050 | 0.012 | *13.2*** |
| H8A···H3A[c] | 2.129 | - | 0.011 | 0.040 | 0.008 | 9.1 |
| C12-H12A···O1[a] | 3.474 \| 2.489 | 150.33 | 0.010 | 0.032 | 0.007 | 8.2 |
| H8A···H7A[c] | 2.163 | - | 0.010 | 0.036 | 0.007 | 8.1 |
| C4-H4A···O1[a] | 3.362 \| 2.550 | 130.03 | 0.008 | 0.029 | 0.006 | 7.0 |
| C12-H12A···N1[a] | 3.595 \| 2.624 | 148.99 | 0.009 | 0.025 | 0.006 | 6.4 |
| H8B ···H16A[d] | 2.254 | - | 0.007 | 0.025 | 0.005 | 5.5 |
| H9B···H9B[e] | 2.422 | - | 0.007 | 0.025 | 0.005 | 5.4 |
| H9A···H5A[f] | 2.240 | - | 0.007 | 0.024 | 0.005 | 5.4 |
| C13···O2[c] | 3.228 | - | 0.006 | 0.021 | 0.004 | 5.0 |
| C2-H2B···C11[b] | 3.389 \| 2.864 | 109.34 | 0.007 | 0.022 | 0.004 | *4.9*** |
| C10-H10B···O2[d] | 3.285 \| 2.804 | 106.34 | 0.005 | 0.021 | 0.004 | 4.9 |
| C10-H10A···C2[g] | 3.857 \| 2.784 | 165.86 | 0.006 | 0.022 | 0.004 | 4.8 |
| C10-H10B···C14[g] | 3.651 \| 2.741 | 140.16 | 0.007 | 0.022 | 0.004 | 4.8 |
| C17-H1A···C13[h] | 3.734 \| 2.800 | 142.89 | 0.007 | 0.021 | 0.004 | 4.7 |
| C7-H7A···C15[g] | 3.599 \| 2.784 | 131.10 | 0.007 | 0.021 | 0.004 | 4.6 |
| H9B···H15A[i] | 2.267 | - | 0.006 | 0.021 | 0.004 | 4.6 |
| H9A···H1C[g] | 2.312 | - | 0.006 | 0.019 | 0.004 | 4.2 |
| C6-H6A···O2[d] | 3.588 \| 2.895 | 121.18 | 0.004 | 0.018 | 0.003 | 3.9 |
| H10B···H16A[d] | 2.363 | - | 0.005 | 0.018 | 0.003 | 3.8 |
| H6A···H2B[d] | 2.340 | - | 0.005 | 0.018 | 0.003 | 3.8 |
| H6A···H10A[g] | 2.443 | - | 0.005 | 0.018 | 0.003 | 3.8 |
| H8B···H5A[f] | 2.437 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| H1B···H16A[c] | 2.535 | - | 0.004 | 0.014 | 0.003 | 3.0 |
| C13-H13A···O1[c] | 3.840 \| 3.014 | 133.78 | 0.004 | 0.013 | 0.003 | 2.9 |
| H6A···H3B[d] | 2.584 | - | 0.003 | 0.012 | 0.002 | 2.5 |
| H4B···H15A[i] | 2.589 | - | 0.003 | 0.012 | 0.002 | 2.4 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **145.4** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, angle ∠(D-H-A), electron density in bond CP $\rho_{b,}$ Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) -x,1/2+y,1/2-z; b) x,y,z; c) x,1+y,z; d) 1-x,1/2+y,1/2-z; e) 1-x,-y,1-z; f) 1-x,1-y,1-z; g) 1-x,-1/2+y,1/2-z; h) -x,1-y,-z; i) x,1/2-y,1/2+z.

**Table 13SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **12**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.900 \| 1.892 | 171.28 | 0.027 | 0.086 | 0.021 | 23.8 |
| C12-H12B···O2[b] | 3.134 \| 2.431 | 120.97 | 0.012 | 0.041 | 0.009 | *10.6*** |
| C3-H3···O2[c] | 3.504 \| 2.513 | 150.86 | 0.008 | 0.028 | 0.006 | 7.0 |
| C19-H27···O1[c] | 3.465 \| 2.647 | 131.41 | 0.007 | 0.026 | 0.006 | 6.3 |
| C16-H16A···O2[d] | 3.584 \| 2.662 | 142.03 | 0.007 | 0.024 | 0.005 | 5.9 |
| C8-H8B···C1[b] | 3.270 \| 2.847 | 103.07 | 0.007 | 0.026 | 0.005 | *5.8*** |
| C5-H5···O2[e] | 3.524 \| 2.698 | 133.28 | 0.006 | 0.023 | 0.005 | 5.3 |
| H5···H8B[e] | 2.190 | - | 0.007 | 0.024 | 0.005 | 5.3 |
| C18-H15···O2[d] | 3.609 \| 2.705 | 140.14 | 0.006 | 0.021 | 0.004 | 5.0 |
| C16-H16A···O1[d] | 3.579 \| 2.780 | 130.04 | 0.006 | 0.021 | 0.004 | 5.0 |
| C2-H2···C19[f] | 3.631 \| 2.794 | 133.56 | 0.006 | 0.021 | 0.004 | 4.5 |
| C15-H15A···C3[d] | 3.873 \| 2.785 | 176.86 | 0.006 | 0.018 | 0.004 | 4.1 |
| C6-H6···C5[e] | 3.617 \| 2.899 | 123.61 | 0.005 | 0.018 | 0.003 | 3.9 |
| H16···H9[h] | 2.385 | - | 0.005 | 0.017 | 0.003 | 3.7 |
| H26···H3[i] | 2.413 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| H10B···H27[g] | 2.484 | - | 0.005 | 0.016 | 0.003 | 3.5 |
| H6···H16[h] | 2.466 | - | 0.005 | 0.016 | 0.003 | 3.3 |
| H16A···H27[g] | 2.392 | - | 0.004 | 0.016 | 0.003 | 3.2 |
| H25···H22[j] | 2.413 | - | 0.005 | 0.015 | 0.003 | 3.2 |
| C2-H2···O1[a] | 3.905 \| 2.918 | 150.93 | 0.004 | 0.015 | 0.003 | 3.2 |
| H22···H12A[j] | 2.431 | - | 0.005 | 0.015 | 0.003 | 3.1 |
| H15B···H13B[j] | 2.438 | - | 0.005 | 0.015 | 0.003 | 3.1 |
| H15B···H15B[j] | 2.459 | - | 0.005 | 0.015 | 0.003 | 3.1 |
| C17-H24···C5[f] | 4.084 \| 3.022 | 165.04 | 0.005 | 0.013 | 0.003 | 3.0 |
| H15···H21[h] | 2.618 | - | 0.004 | 0.014 | 0.003 | 3.0 |
| C18-H15···C4[f] | 3.753 \| 3.124 | 117.48 | 0.004 | 0.012 | 0.002 | 2.6 |
| H13A···H9[h] | 2.569 | - | 0.004 | 0.011 | 0.002 | 2.3 |
| H15B···H12A[j] | 2.631 | - | 0.003 | 0.010 | 0.002 | 2.2 |
| H10A···H5[e] | 2.650 | - | 0.003 | 0.010 | 0.002 | 2.2 |
| H25···H13B[j] | 2.636 | - | 0.003 | 0.010 | 0.002 | 2.1 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **126.6** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) 1-x,1-y,1-z; b) x,y,z; c) -1/2+x,1/2-y,-1/2+z; d) 1/2+x,1/2-y,-1/2+z; e) 1-x,-y,1-z; f) 1/2-x,1/2+y,1/2-z; g) 1+x,y,z; h) 1.5-x,1/2+y,1/2-z; i) 1/2-x,-1/2+y,1/2-z; j) 2-x,1-y,1-z.

**Table 14SI.** Metric parameters and electron-density features at the bond critical points of non-covalent interactions* in compound **14**.

| Interaction | D(D···A)/ Å \| D(H···A)/ Å | ∠(D-H-A)/ ° | $\rho_b$/ a.u. | $\nabla^2\rho_b$/ a.u. | $G_b$/ a.u. | $E_{int}$/ kJ·mol$^{-1}$ |
|---|---|---|---|---|---|---|
| N1-H1···O1[a] | 2.891 \| 1.883 | 171.60 | 0.027 | 0.088 | 0.021 | 23.9 |
| C12-H121···O2[b] | 3.159 \| 2.452 | 121.39 | 0.012 | 0.040 | 0.009 | *10.2*** |
| C3-H3···O2[c] | 3.361 \| 2.358 | 152.35 | 0.011 | 0.036 | 0.009 | 9.7 |
| C2-H2···F[d] | 3.377 \| 2.417 | 146.30 | 0.008 | 0.032 | 0.007 | 7.9 |
| C5-H5···O2[e] | 3.338 \| 2.555 | 128.10 | 0.008 | 0.028 | 0.006 | 6.8 |
| C18-H182···O2[f] | 3.537 \| 2.726 | 130.98 | 0.005 | 0.021 | 0.004 | 4.8 |
| C15-H152···C3[g] | 3.840 \| 2.775 | 165.83 | 0.007 | 0.020 | 0.004 | 4.6 |
| C16-H161···O2[f] | 3.602 \| 2.827 | 129.63 | 0.005 | 0.019 | 0.004 | 4.3 |
| H6···H6[e] | 2.464 | - | 0.005 | 0.021 | 0.004 | 4.3 |
| H3···H121[c] | 2.334 | - | 0.005 | 0.020 | 0.004 | 4.2 |
| H181···H9[h] | 2.395 | - | 0.005 | 0.018 | 0.003 | 3.8 |
| C16-H161···O1[f] | 3.597 \| 2.939 | 119.15 | 0.004 | 0.016 | 0.003 | 3.6 |
| H151···H151[i] | 2.380 | - | 0.005 | 0.017 | 0.003 | 3.6 |
| H183···H172[i] | 2.365 | - | 0.005 | 0.017 | 0.003 | 3.5 |
| H5···H121[e] | 2.400 | - | 0.004 | 0.015 | 0.003 | 3.2 |
| H132···H9[h] | 2.447 | - | 0.004 | 0.014 | 0.003 | 3.0 |
| H102···H102[j] | 2.716 | - | 0.004 | 0.014 | 0.003 | 2.9 |
| C18-H182···C5[h] | 3.766 \| 3.040 | 124.56 | 0.004 | 0.013 | 0.002 | 2.8 |
| C10-H101···C4[g] | 4.024 \| 3.002 | 156.48 | 0.004 | 0.012 | 0.002 | 2.7 |
| C17-H173···C6[g] | 4.100 \| 3.015 | 174.44 | 0.004 | 0.012 | 0.002 | 2.6 |
| C16-H162···C17[c] | 4.129 \| 3.060 | 167.21 | 0.004 | 0.012 | 0.002 | 2.6 |
| H183···H123[i] | 2.532 | - | 0.004 | 0.012 | 0.002 | 2.5 |
| H151···H131[i] | 2.557 | - | 0.004 | 0.012 | 0.002 | 2.4 |
| H5···H82[e] | 2.637 | - | 0.003 | 0.011 | 0.002 | 2.2 |
| H5···H102[e] | 2.661 | - | 0.003 | 0.010 | 0.002 | 2.1 |
| H151···H123[i] | 2.727 | - | 0.003 | 0.009 | 0.002 | 1.8 |
| | | | | | $E_{latt}$/ kJ·mol$^{-1}$ | **115.9** |

*Distance between the donor and acceptor atoms D(D···A) and between the hydrogen and acceptor atom D(H···A), where D= O, N, C and A= O, N, C, angle ∠(D-H-A), electron density in bond CP $\rho_b$, Laplacian of electron density in bond CP $\nabla^2\rho_b$, local kinetic energy in bond CP $G_b$, energy of intermolecular interaction $E_{int}$ obtained using eq. (3). All solid-state calculations are performed in B3LYP-D2/6-31G(d,p) approximation.

**Intramolecular contacts do not count in $E_{latt}$ evaluation.

Symmetry codes: a) 1-x,-y,1-z; b) x,y,z; c) -1/2+x,1/2-y,-1/2+z; d) 1/2-x,-1/2+y,1/2-z; e) 1-x,1-y,1-z; f) 1/2+x,1/2-y,-1/2+z; g) 1+x,y,z; h) 1.5-x,-1/2+y,1/2-z; i) 2-x,-y,1-z; j) 2-x,1-y,1-z.