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—— Supplementary Material ——

Experimental and Theoretical Study of Intramolecular O···O Interaction in Structurally Rigid β-Keto Carboxylic Esters

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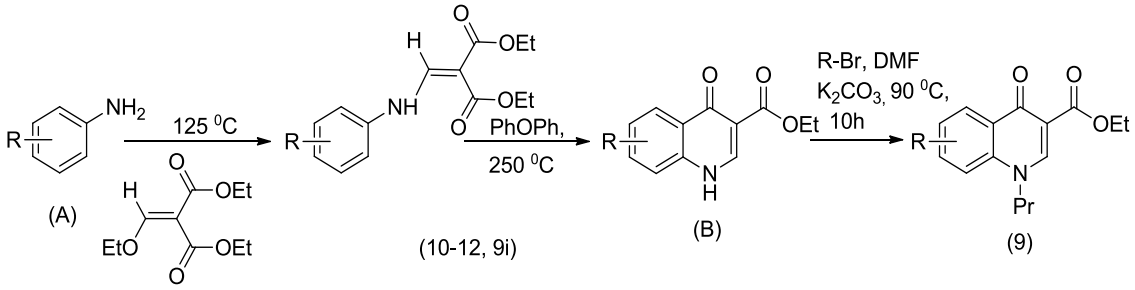
Material and Methods

All solvents and reagents were obtained commercially and used as received. ^{1}H NMR and ^{13}C NMR data were collected on JEOL GS-400 model FT-NMR spectrometer and processed with its Delta software. The compounds were purified by column chromatography using 100-200 mess size silica. The chemical shifts in spectra were measured in parts per million (ppm) on the delta (δ) scale relative to the resonance of the solvent peak ($CDCl_3$ signal as reference, ^{1}H = 7.24 ppm, ^{13}C = 77.0 ppm). FT-IR spectra was recorded neat and in KBr pellets in the range of 400–4000 cm^{-1} at room temperature using a Perkin Elmer 400 FT-IR spectrometer. The crystals were subjected to X-ray diffraction studies and data was collected in an Oxford Diffraction Xcalibur CCD diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) at 298 (2) K. The structure was solved by direct method using SHELXL-97 and refined by full matrix least-squares method on F2 (SHELXL-97). All calculations were carried out using the WinGX package of the crystallographic program and PLATON. Program ORTEP-3 and Mercury were used to generate molecular graphics.

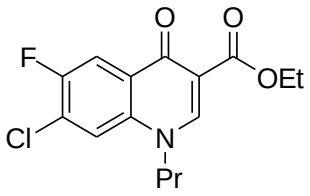
Experimental Procedure



General Procedure

A mixture of substituted anilines (1 equiv) and diethyl ethoxymethylenemalonate (1.5 equiv) were refluxed for one hour at 125 °C. The reaction mixture was cooled to room temperature and the ethanol formed during this reaction was removed under pressure to yield (90%) compound **10**-**12** and **9i**. Compound **9i** was then cyclized to compound B by refluxing in diphenylether at 250 °C. Compound **9** was obtained on subsequent reaction of compound B (1 equiv) with K_2CO_3 (5 equiv) and propyl bromide (5 equiv) at 90 °C in dry DMF for 15 h. The reaction mixture was concentrated under reduced pressure and standard workup procedure was followed using chloroform. After washing the organic layer with saturated solution of $NaHCO_3$ and brine, Na_2SO_4 was added. The solvent was removed in vaccuo and purification on SiO_2 by column chromatography gave 60% yield of compound **9**.

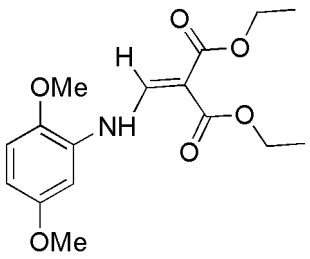
Compound 9: Ethyl 7-chloro-6-fluoro-4oxo-1-propyl-1, 4-dihydroquinoline-3-carboxylate



Mp: 167.2 °C, ^{1}HNMR (400MHz, $CDCl_3$): 8.45 (s, 1H, ArH), 8.26 (d, 1H, ArH), 7.51 (d, 1H, ArH), 4.41 (q, 2H, OCH_2CH_3), 4.14 (t, 2H, NCH2), 1.95 (q, 2H, NCH_2CH_2), 1.43 (t, 3H, $OCH_2CH_2CH_3$), 1.07 (t, 3H, $NCH_2CH_2CH_3$). ^{13}C NMR (100MHz, $CDCl_3$): 10.4, 13.9, 21.3, 55.2, 60.3, 109.9, 113.2, 118.1, 126.3, 128.7,

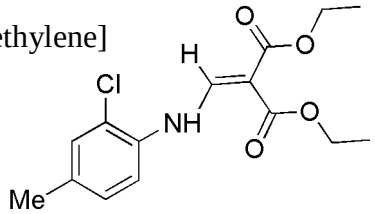
135.1, 148.9, 153.1, 164.4, 172.2. IR: 3045, 1727, 1690 cm^{-1}.

Compound 10: 2-[(2, 5-Dimethoxy-phenylamino)-methylene] -malonic acid diethyl ester



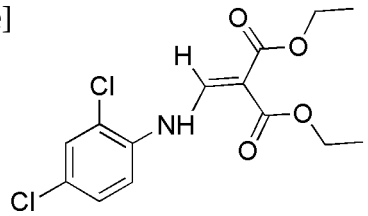
Mp: 82.54 °C. ^{1}HNMR (400MHz, $CDCl_3$): 11.09 (d, 1H, NH), 8.51 (d, 1H) 6.86 (d, 1H), 6.62 (d, 1H), 4.35 (q, 2H), 4.28 (q, 2H), 3.89 (s, 3H), 3.80 (s, 3H), 1.40 (t, 3H), 1.35 (t, 3H). ^{13}C NMR (100MHz, $CDCl_3$):168.3, 165.9, 154.21, 150.0, 143.2, 129.3, 112.0, 108.2, 101.4, 93.9, 60.2, 56.3, 55.8, 14.4. IR: 1733, 1637, 1603, 1516.

Compound 11: 2-[(2-Chloro-4-methyl-phenylamino)-methylene] -malonic acid diethylester



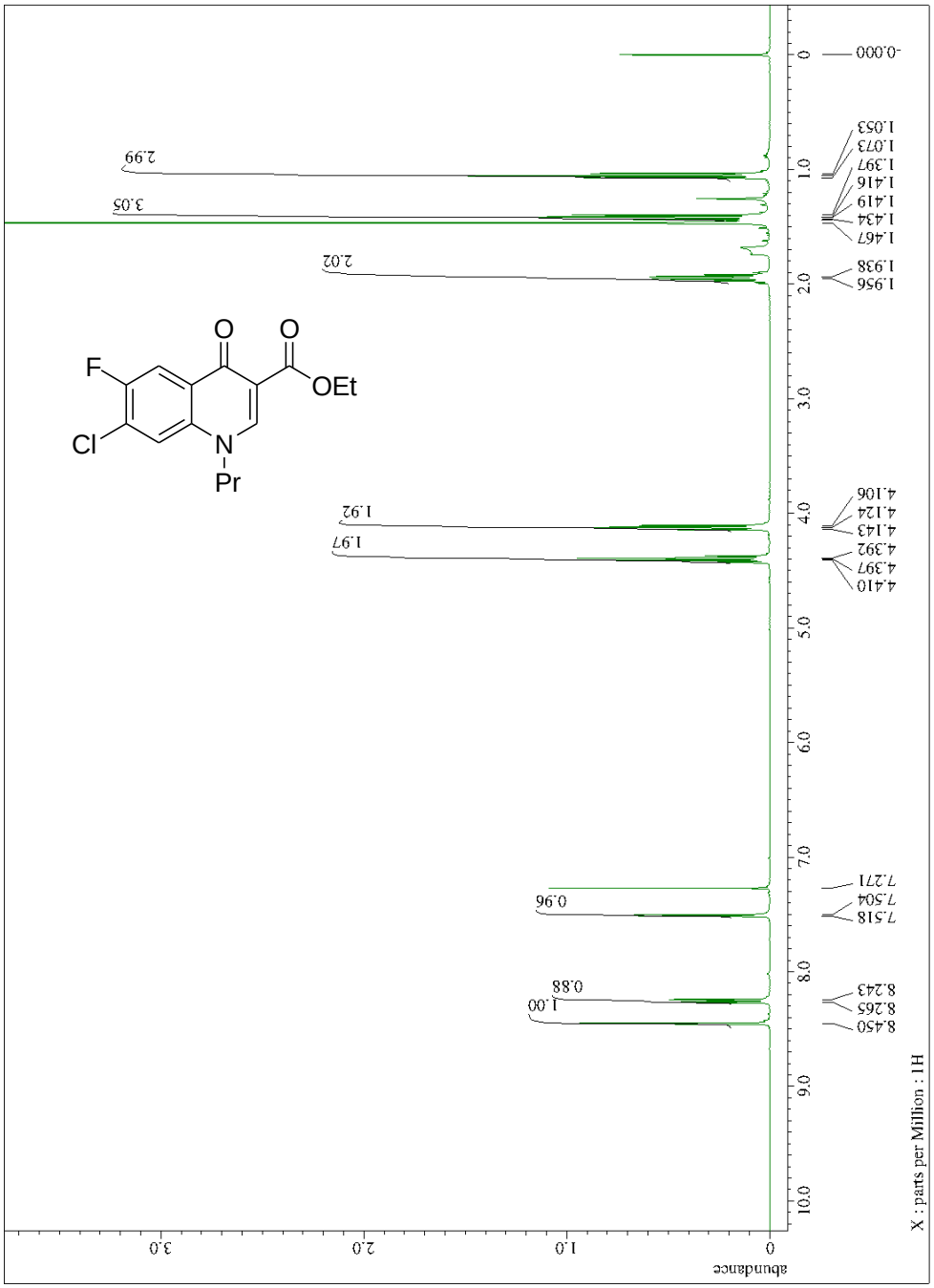
Mp: 102.2 °C, ^{1}HNMR (400MHz, $CDCl_3$): 11.28 (d, 1H), 8.51 (d, 1H), 7.27 (d, 1H), 7.21 (s, 1H), 7.11 (d, 1H), 4.37 (q, 2H), 4.28 (q, 2H), 2.32 (s, 3H), 1.40 (t, 3H), 1.35 (t, 3H). ^{13}C NMR (100MHz, $CDCl_3$): 168.4, 165.7, 150.6, 135.2, 133.8, 130.4, 128.7, 123.3, 115.5, 94.7, 60.5, 60.2, 20.5, 14.3. IR: 1685, 1606, 1423.

Compound 12: 2-[(2,4-Dichloro-phenylamino)-methylene] -malonic acid diethyl ester

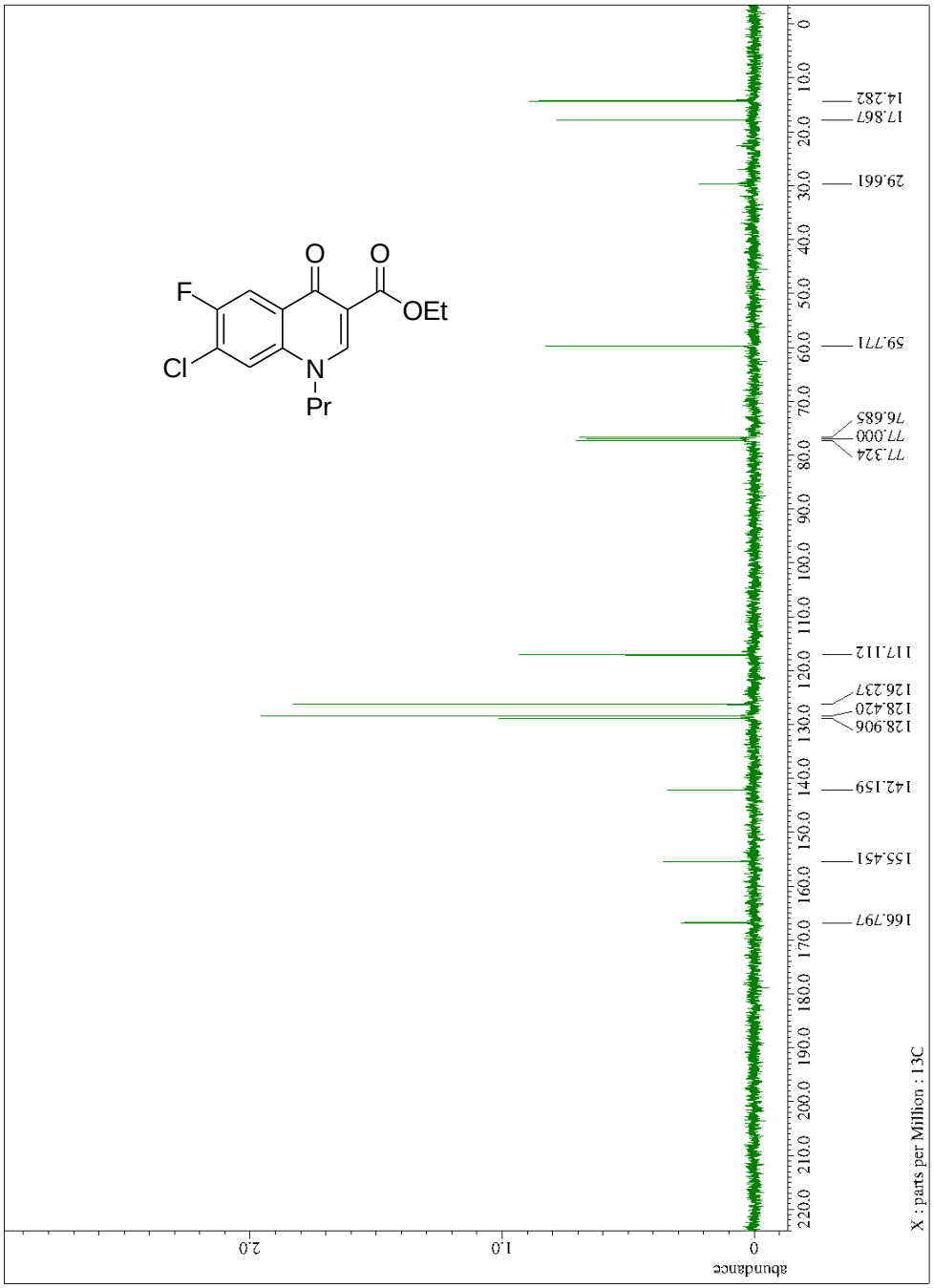


Mp: 114.9 °C.,^{1}HNMR (400MHz, $CDCl_3$): 11.32 **(**d, 1H), 8.47 (d, 1H), 7.45 (s, 1H), 7.31 (m, 1H), 7.27 (t, 1H), 4.37 (q, 2H), 4.27 (q, 2H), 1.40 (t, 3H), 1.34 (t, 3H).^{13}CNMR (100MHz, $CDCl_3$): 168.3, 165.4, 149.9, 135.2, 129.9, 129.5, 128.2, 124.1, 116.2, 96.11, 60.7, 60.4, 14.3. IR: 1711, 1629, 1591.

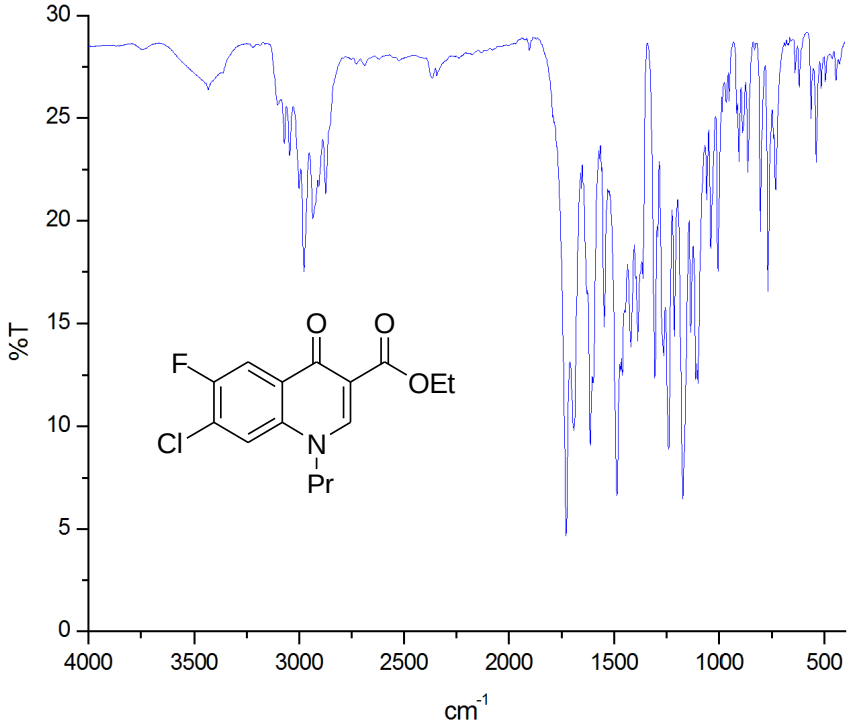
^{1}H NMR (400MHz, $CDCl_3$) of compound 9



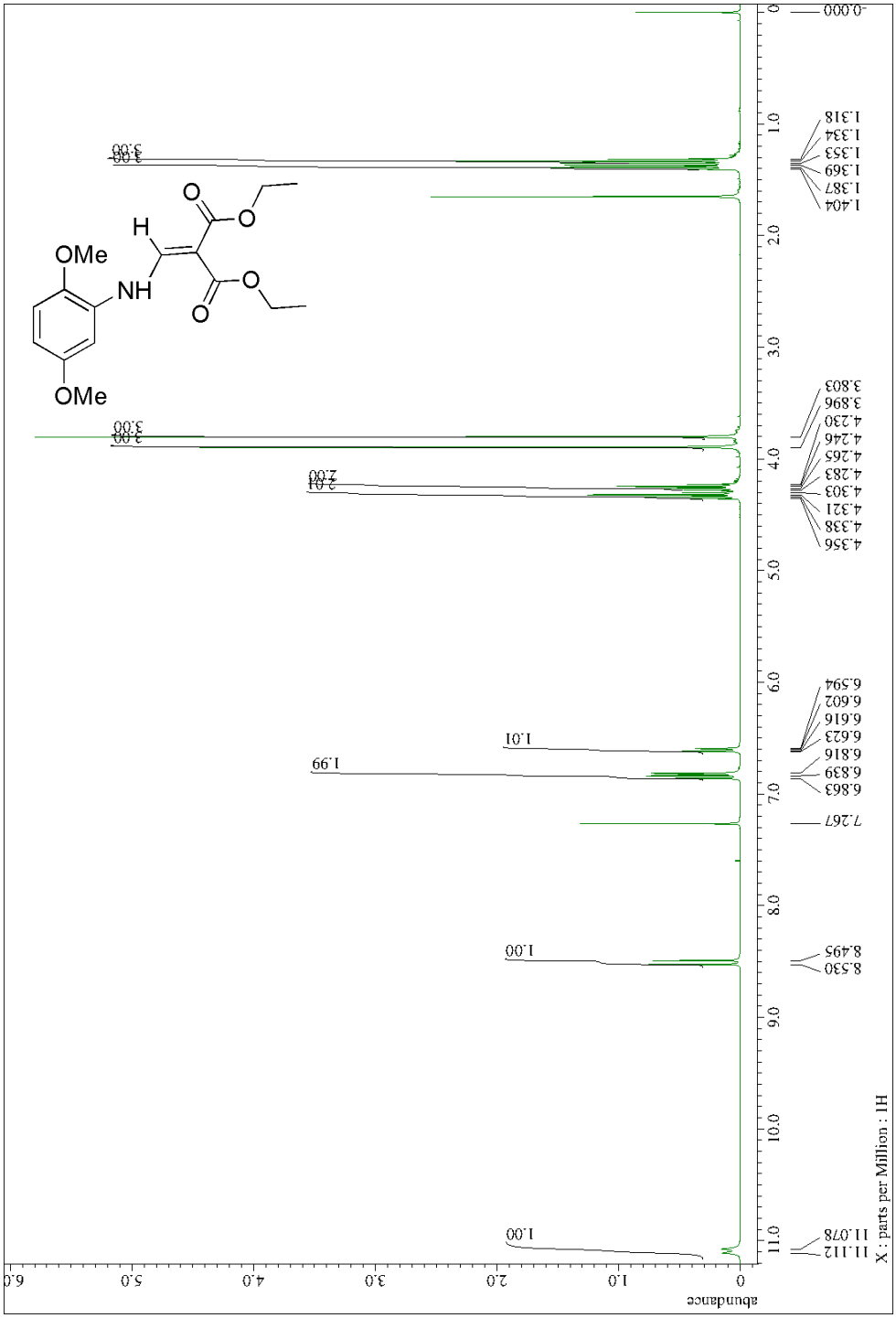
^{13} C NMR (100MHz, $CDCl_3$) of compound 9



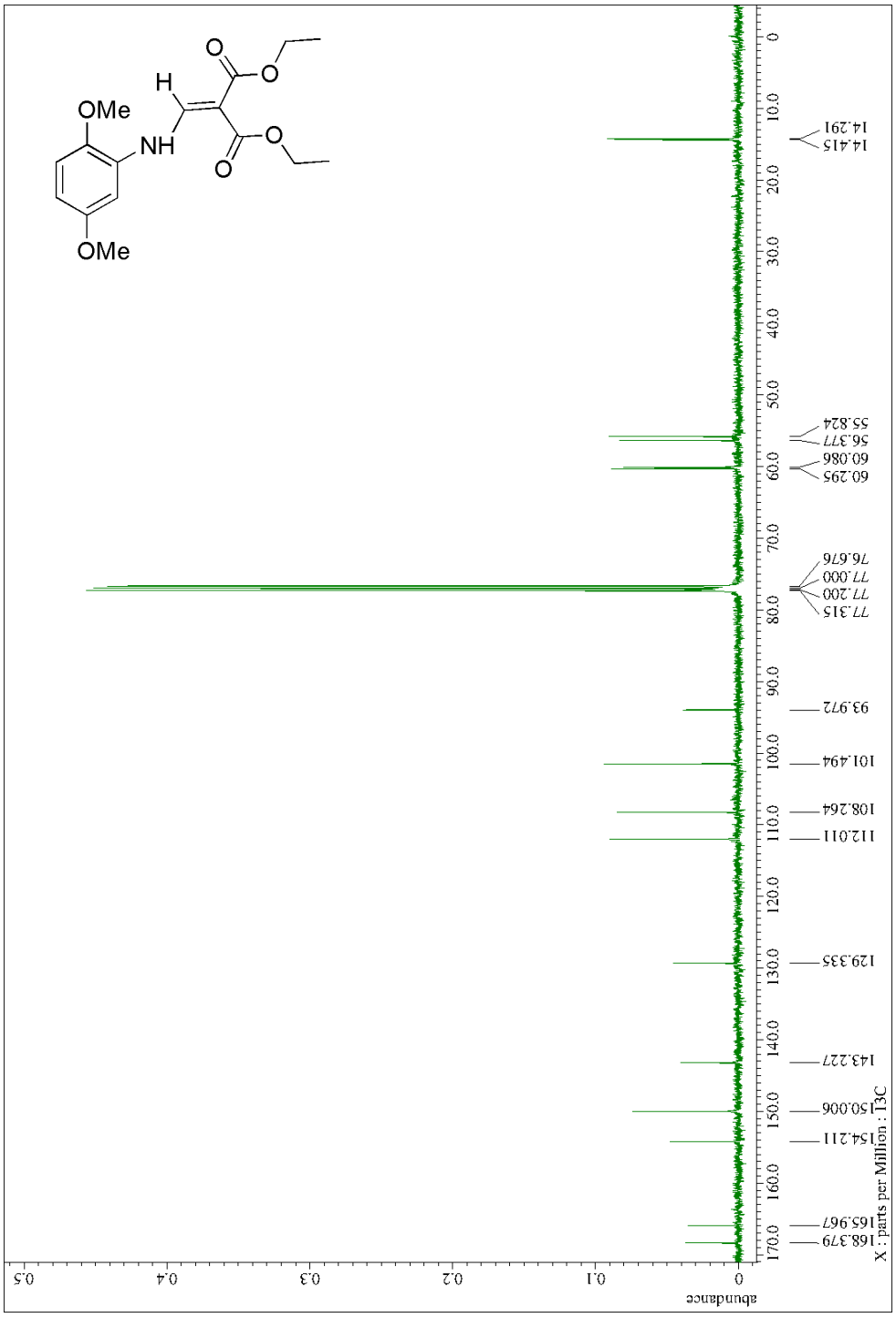
IR spectrum of compound 9



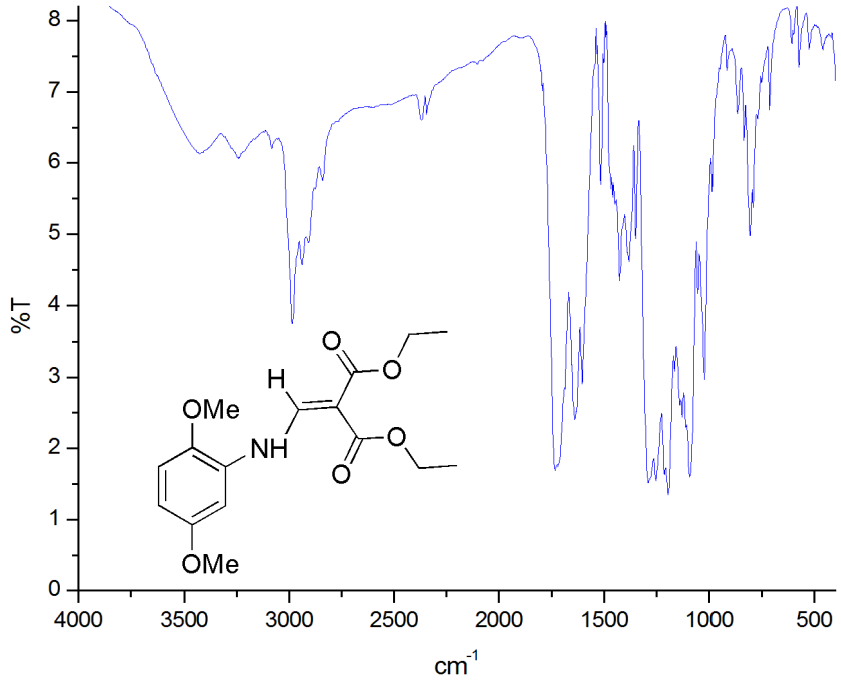
^{1}HNMR (400MHz, $CDCl_3$) of compound 10



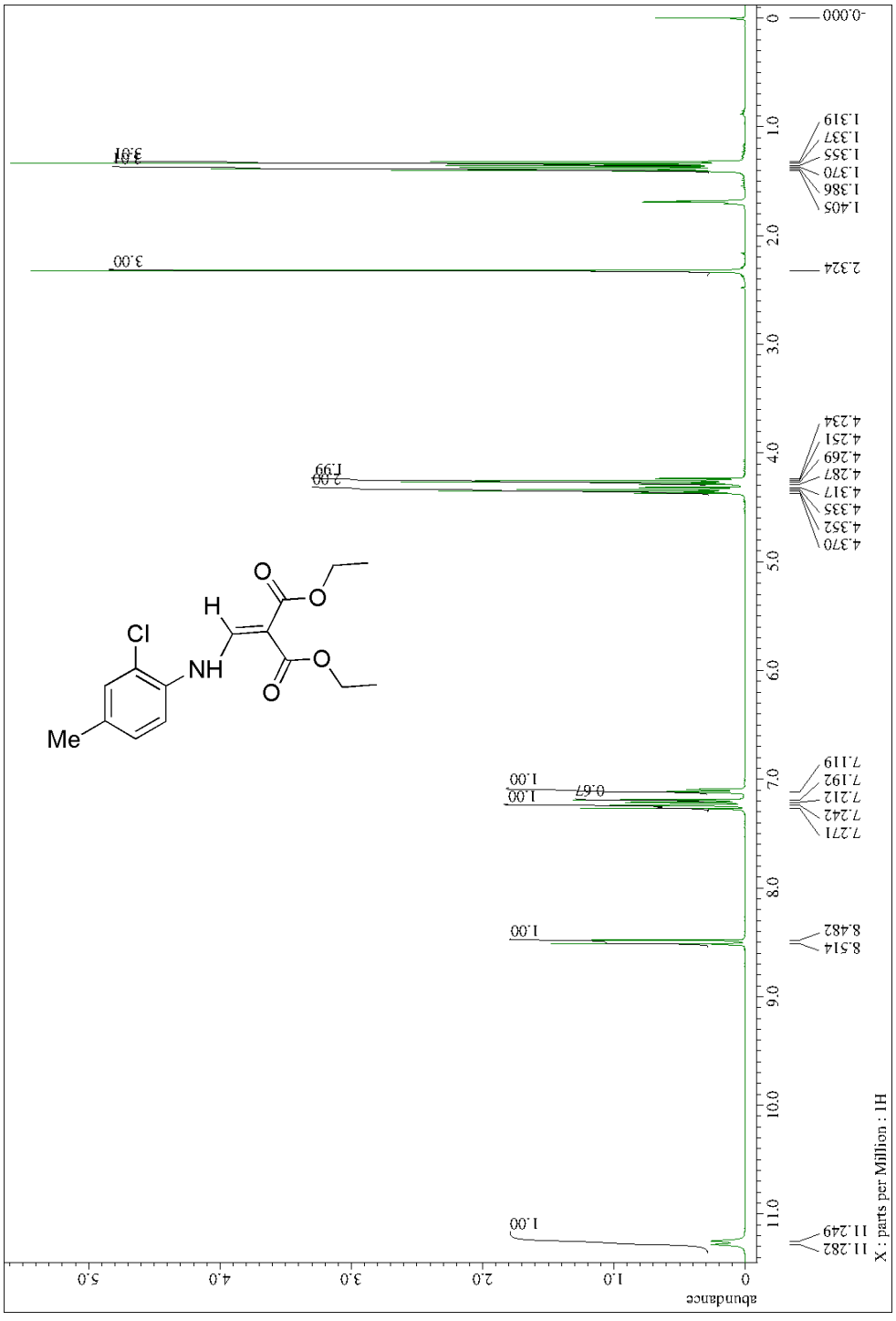
^{13}C NMR (100MHz, $CDCl_3$) of compound 10



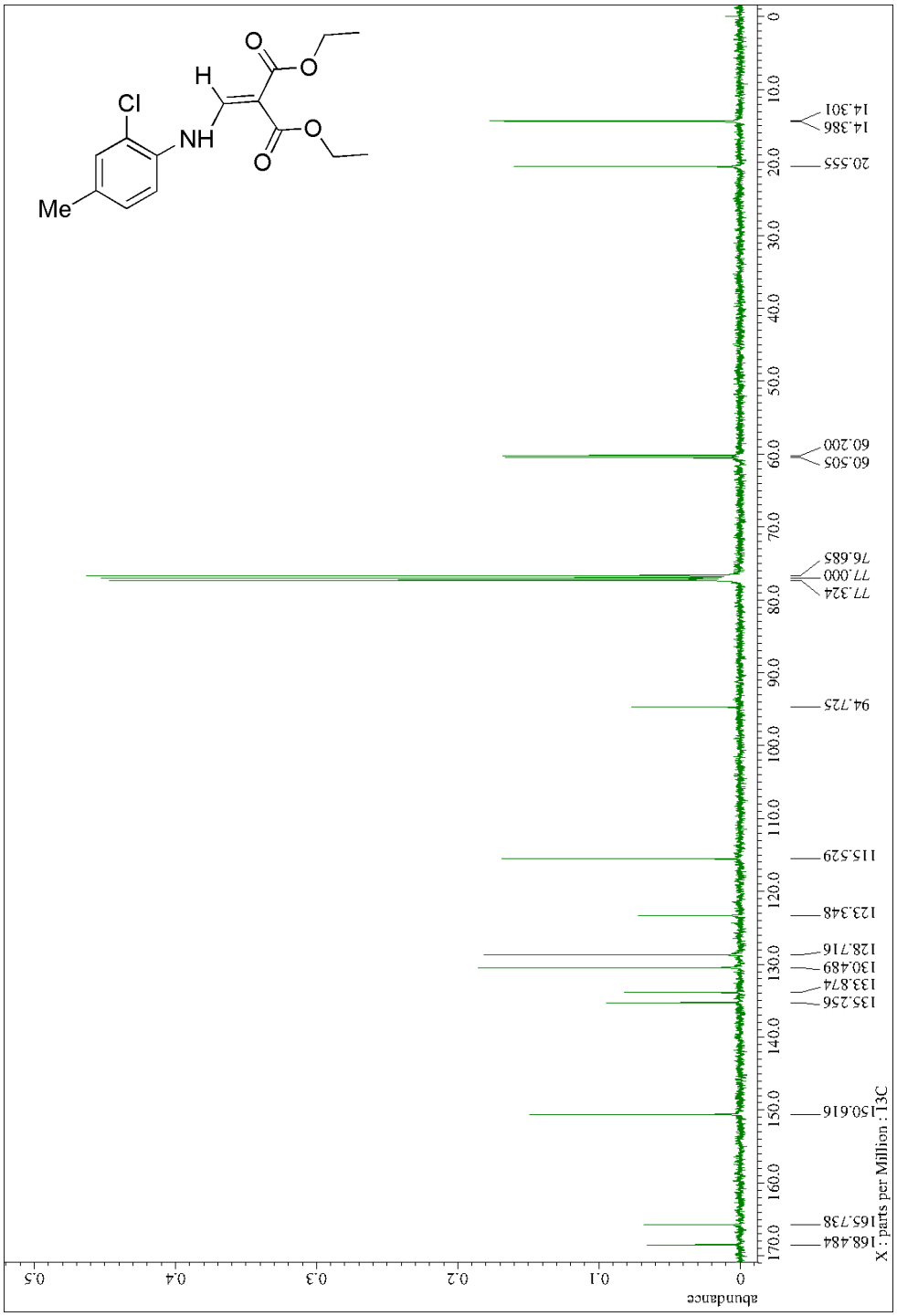
IR Spectrum of compound 10



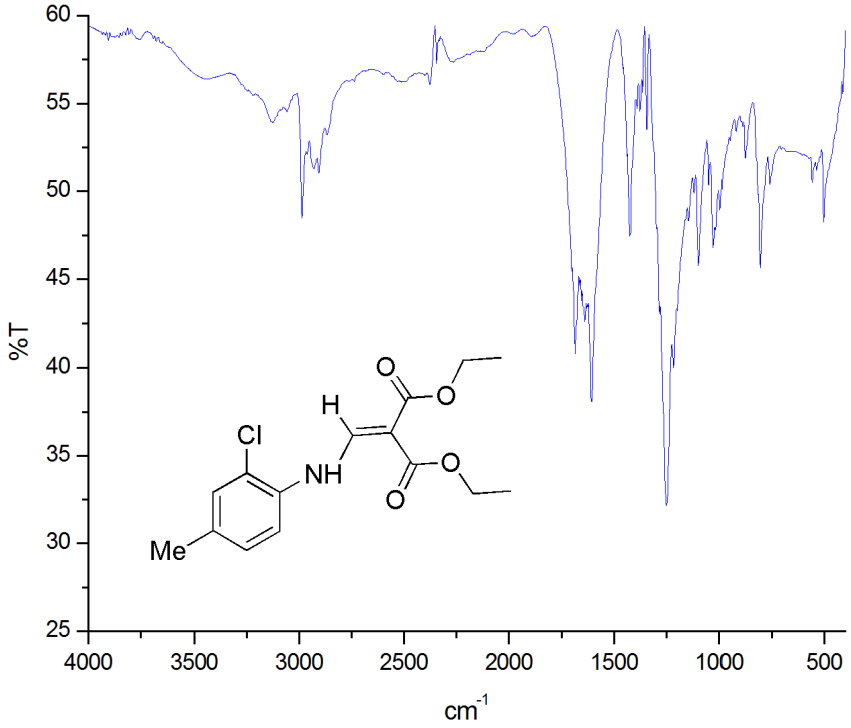
^{1}H NMR (400MHz, $CDCl_3$) of compound 11



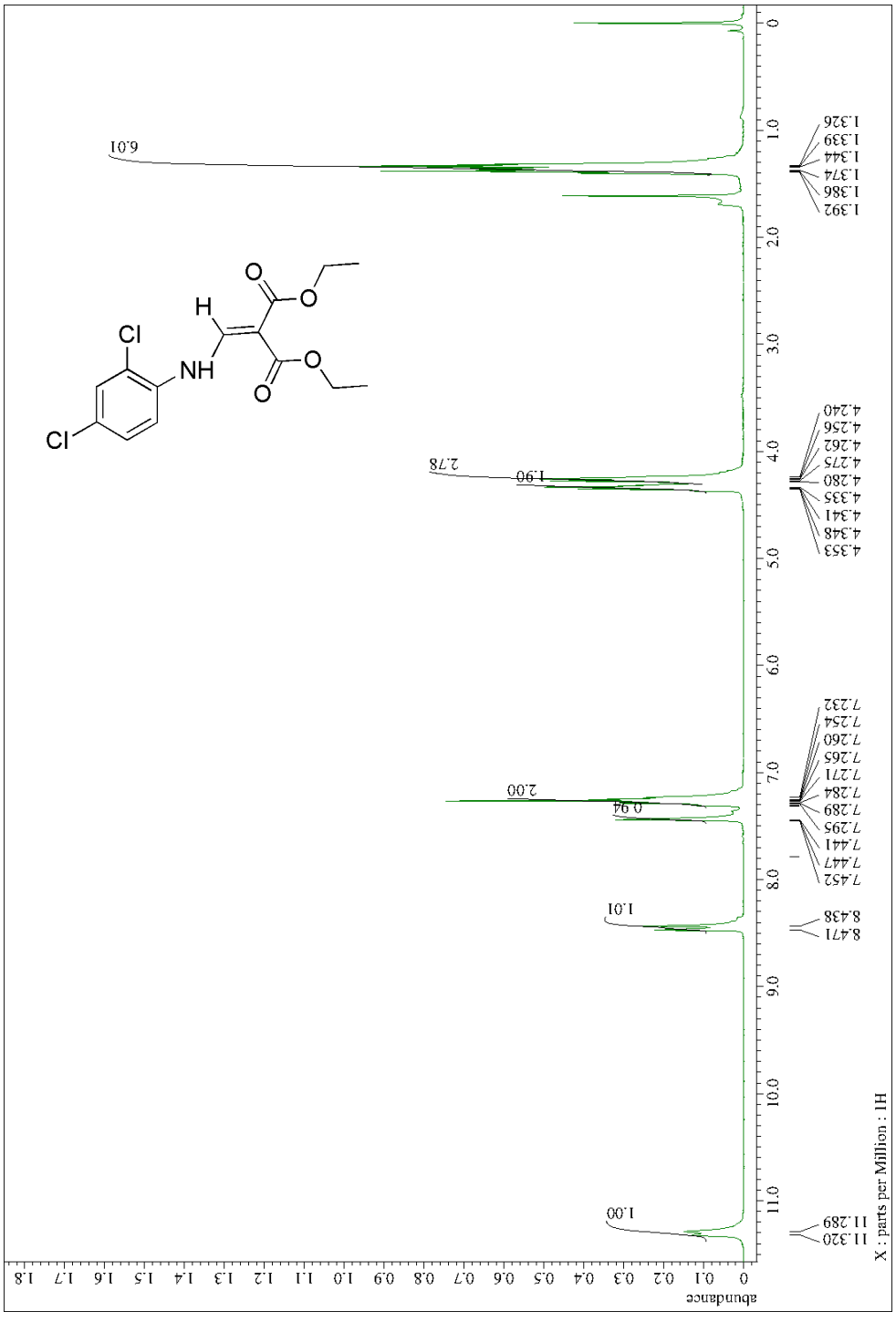
^{13}C NMR (100MHz, $CDCl_3$) of compound 11



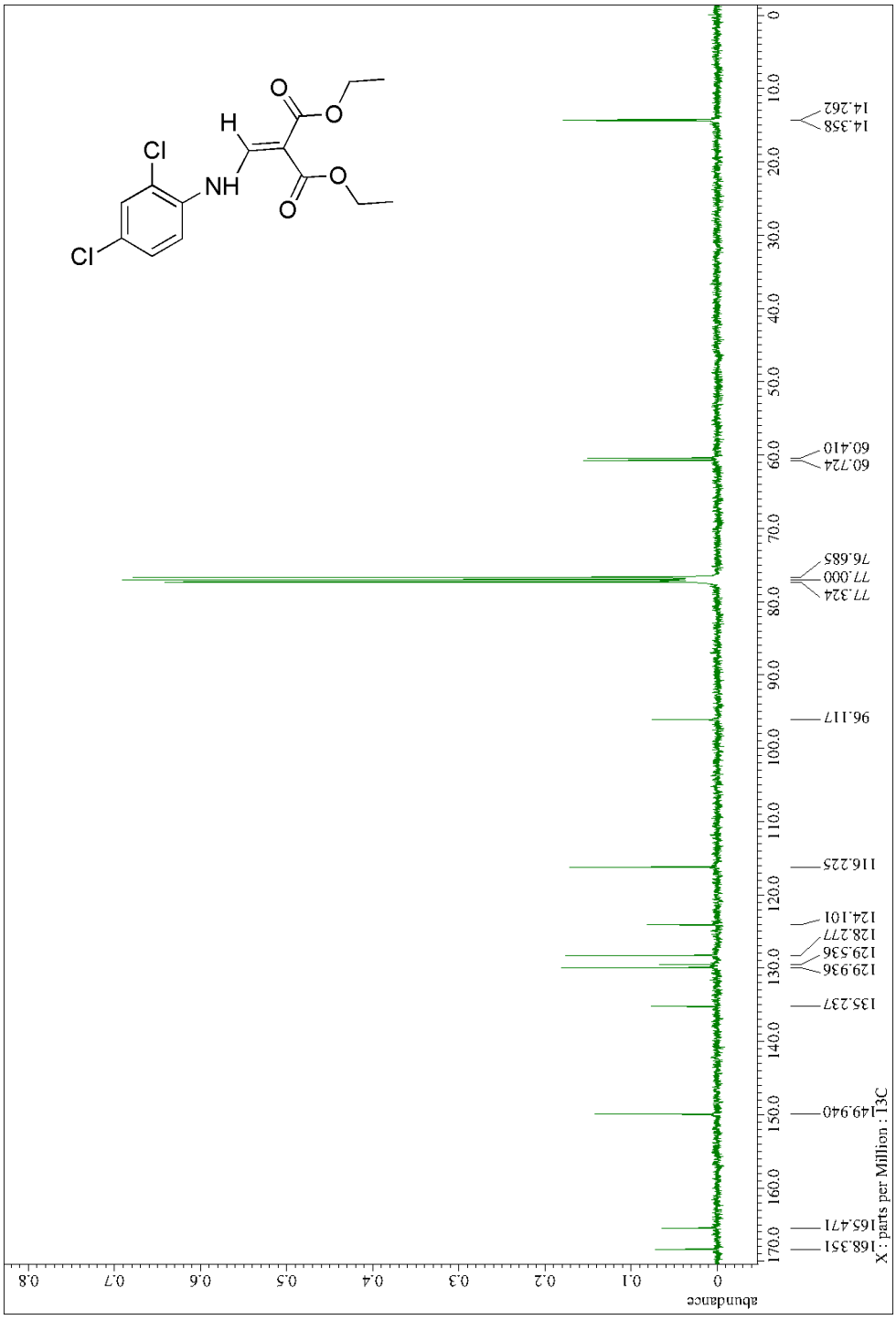
IR spectrum of compound 11



^{1}H NMR (400MHz, $CDCl_3$) of compound 12



^{13}C NMR (100MHz, $CDCl_3$) of compound 12



IR spectrum of compound 12

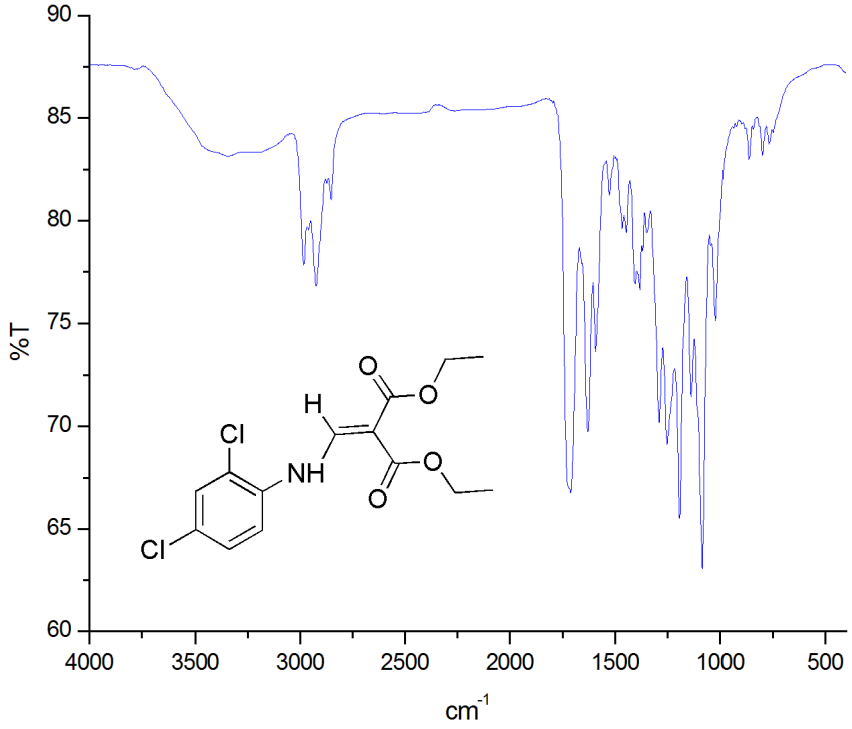


Table S1. Crystal data and Refinement details of compounds **9-12**.

CIF Details	**9**	**10**	**11**	**12**
CCDC no.	**915054**	**920032**	**920439**	**916682**
Empirical formula	$C_{15}H_{15}ClFNO_3$	$C_{16}H_{21}NO_6$	$C_{15}H_{18}ClNO_4$	C14 H15 Cl2 N O4
Formula weight	311.73	323.34	311.75	332.17
Temperature	293(2)	293(2)	293(2)	293(2)
Wavelength	0.71073	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
Space group	P 21/n	P 21/n	P 21 21 21	P 21/n
Hall group	-P 2yn	-P 2ybc	P 2ac 2ab	-P 2ybc
Unit cell dimensions	a = 10.3931(6) Å b = 11.4141(7) Å C = 12.5948(8) Å α = 90^0 β = 100.798^0 (6)	a = 4.5426(5) Å b = 16.585(2) Å c = 22.273(3) Å α = 90° β = 92.979^0 (12)	a = 6.2728(6) Å b = 9.4396(11) Å c = 26.241(4) Å α = 90° β = 90°	a =14.5383 (9) Å a = 6.1794 (4) Å c = 17.9542 (14) Å α = 90° β = 101.022^0 (7)

	γ = 90^0	γ = 90°	γ = 90°	γ = 90°
Volume	1467.64(15) Å^3	1675.8(4) Å^3	1553.8(3) Å^3	1582.13 (19) Å^3
Z	4	4	4	4
Density	1.411 g/cm^3	1.282 g/cm^3	1.333 g/cm^3	1.395 g/cm^3
Absorption coefficient	0.280 mm^{-1}	0.098 mm^{-1}	0.260 mm^{-1}	0.424 mm^{-1}
F(000)	648	688	656	688
Theta range for data collection	3.28 - 29.161	3.66 - 26.00	3.09 - 29.03	3.27 - 28.92
Index ranges	-12 < h <12	-5 ≤ h ≤ 5	-7≤ h ≤7	-18≤ h ≤18
	-14 < h< 14	-20 ≤ k ≤ 20	-11≤ h ≤11	-7≤ h ≤7
	-15 ≤ h ≤ 15	-27 ≤ l ≤ 27	-32≤ h ≤32	-22≤ h ≤22
Reflections collected	12618	13399	6111	12132
Completeness to theta	99.8%	99.8%	100%	100%
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	0.946 and 0.927	0.976 and 0.973	0.937 and 0.925	0.919 and 0.903
Refinement	Full-matrix	Full-matrix	Full-matrix	Full-matrix

method	least-squares on F2	least-squares on F2	least-squares on F2	least-squares on F2
Goodness-of-fit on F2	1.087	1.129	1.023	0.824
Final R indices [I>2sigma(I)]	R1 = 0.0418, wR2 = 0.1128	R1 = 0.0757, wR2 = 0.1848	R1 = 0.0508 , wR2 = 0.1163	R1 = 0.0563, wR2 = 0.2059

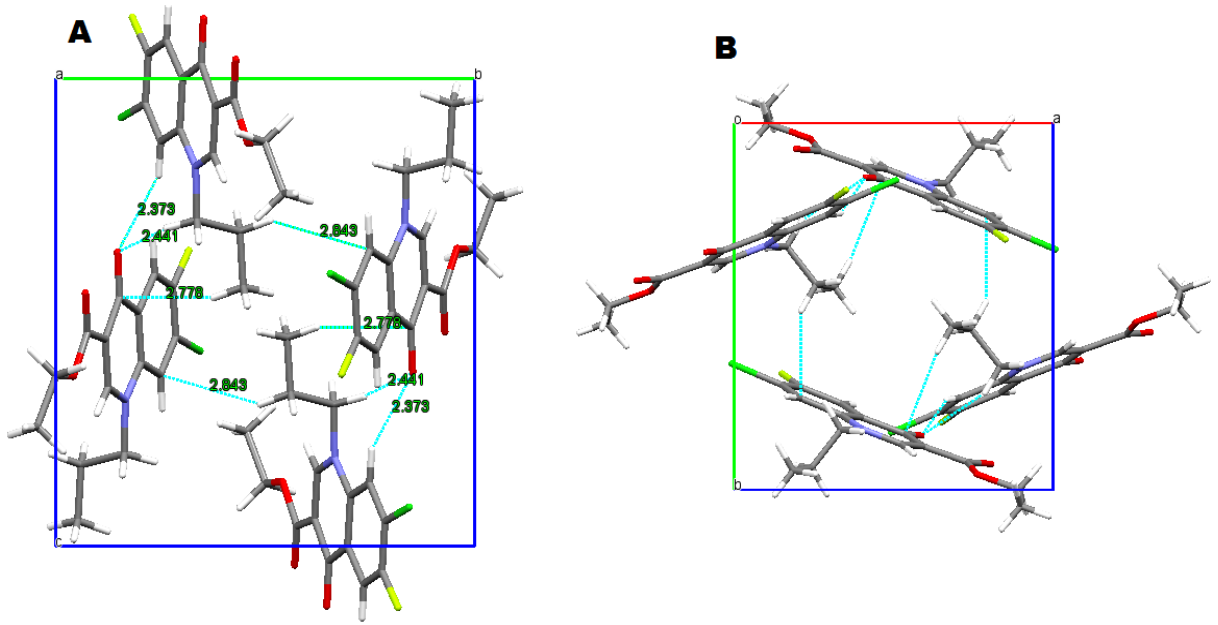


Figure. S1 C-H···π and hydrogen bonding interactions in the crystal lattice of **9**. (a) along A axis; (b) along C axis.

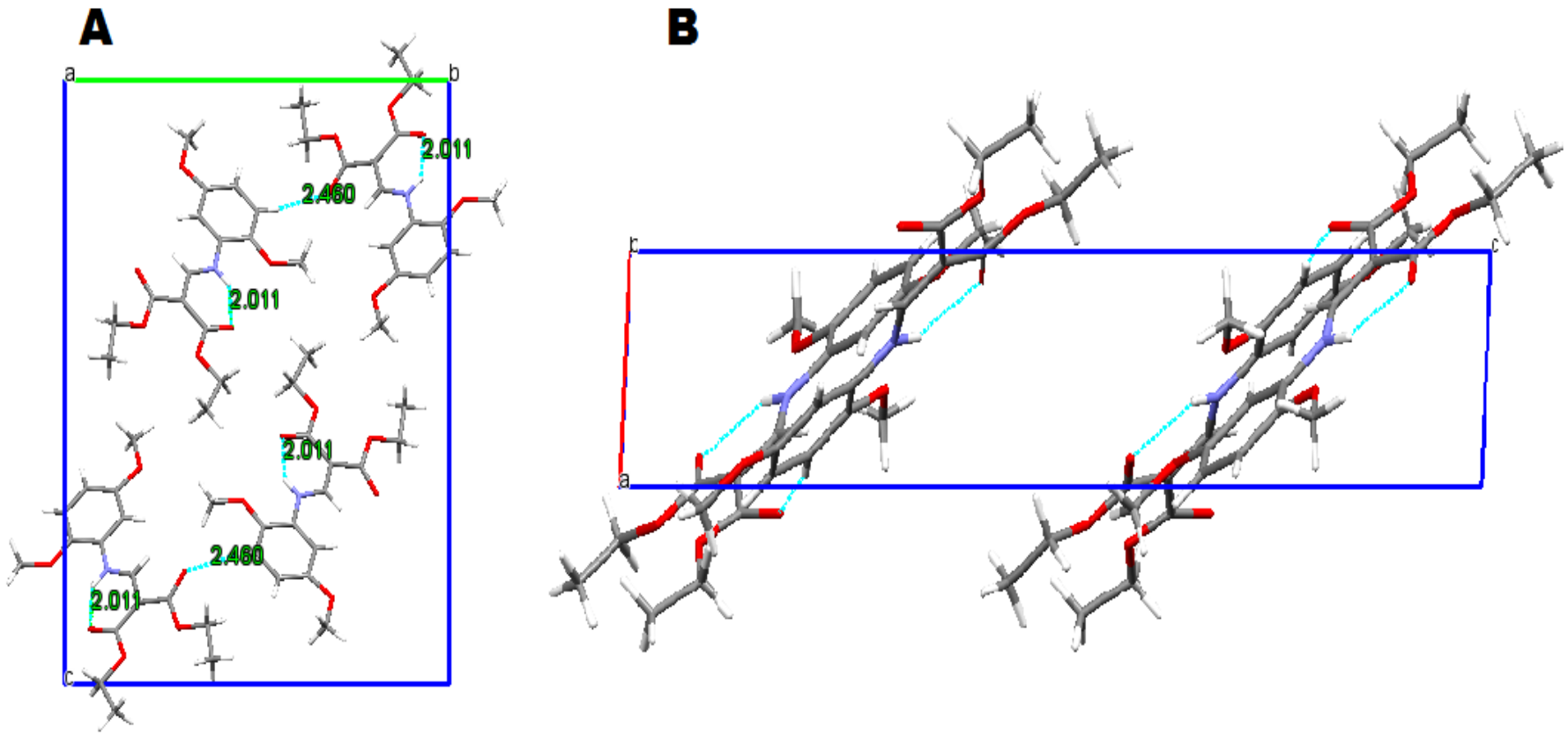


Figure. S2 Hydrogen bonding interactions in the crystal lattice of **10**. (a) along A axis; (b) along B axis.

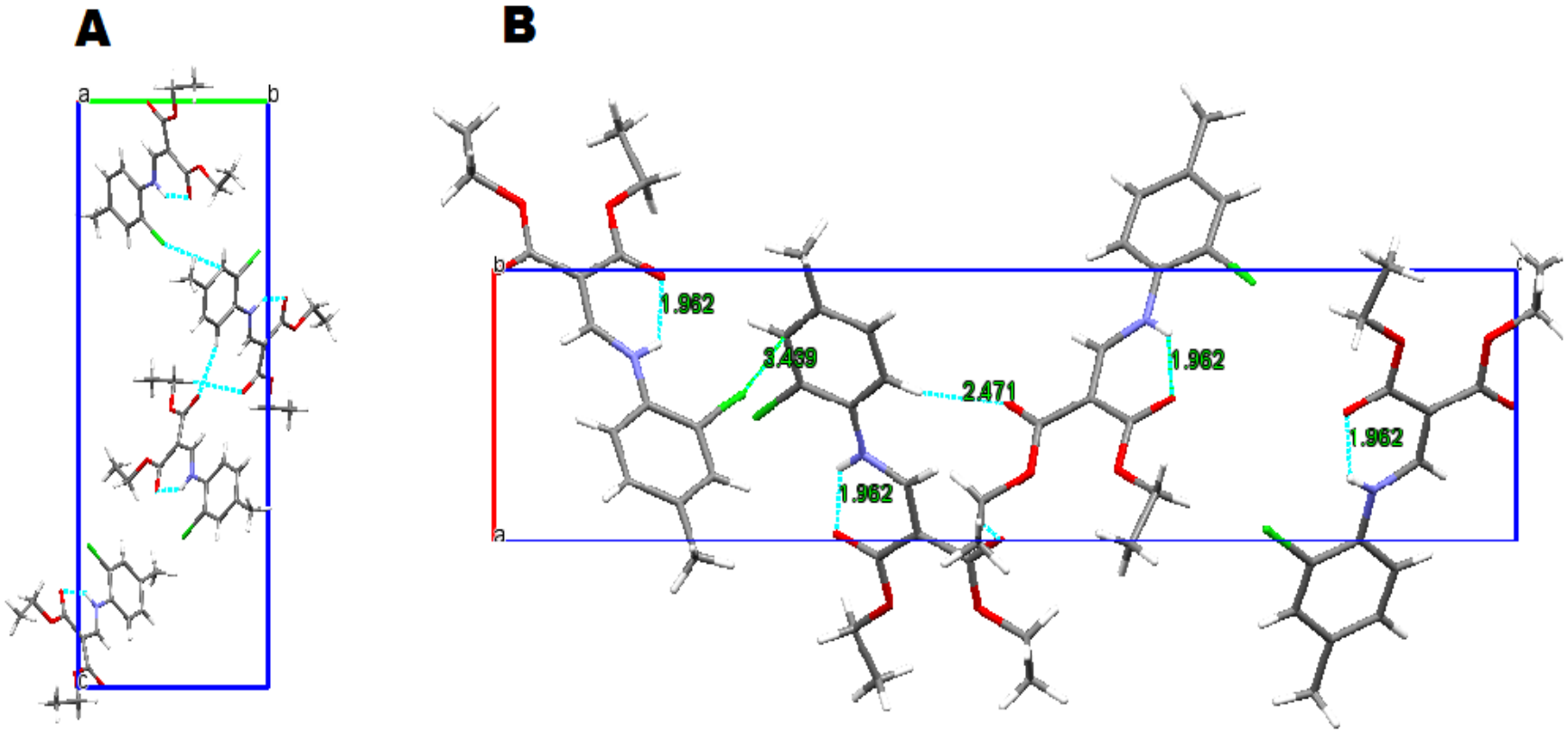


Figure. S3 C-H···π and hydrogen bonding interactions in the crystal lattice of **11**. (a) along A axis; (b) along B axis.

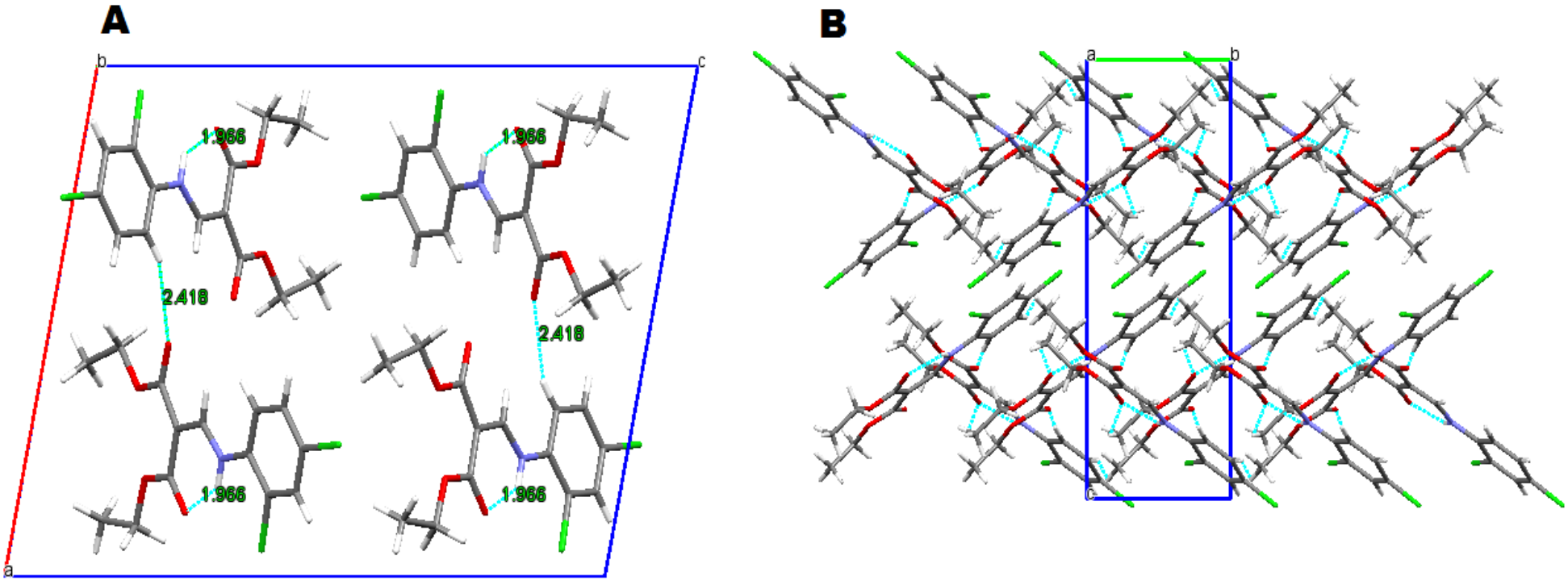


Figure. S4 Hydrogen bonding interactions in the crystal lattice of **12**. (a) along B axis; (b) along A axis.

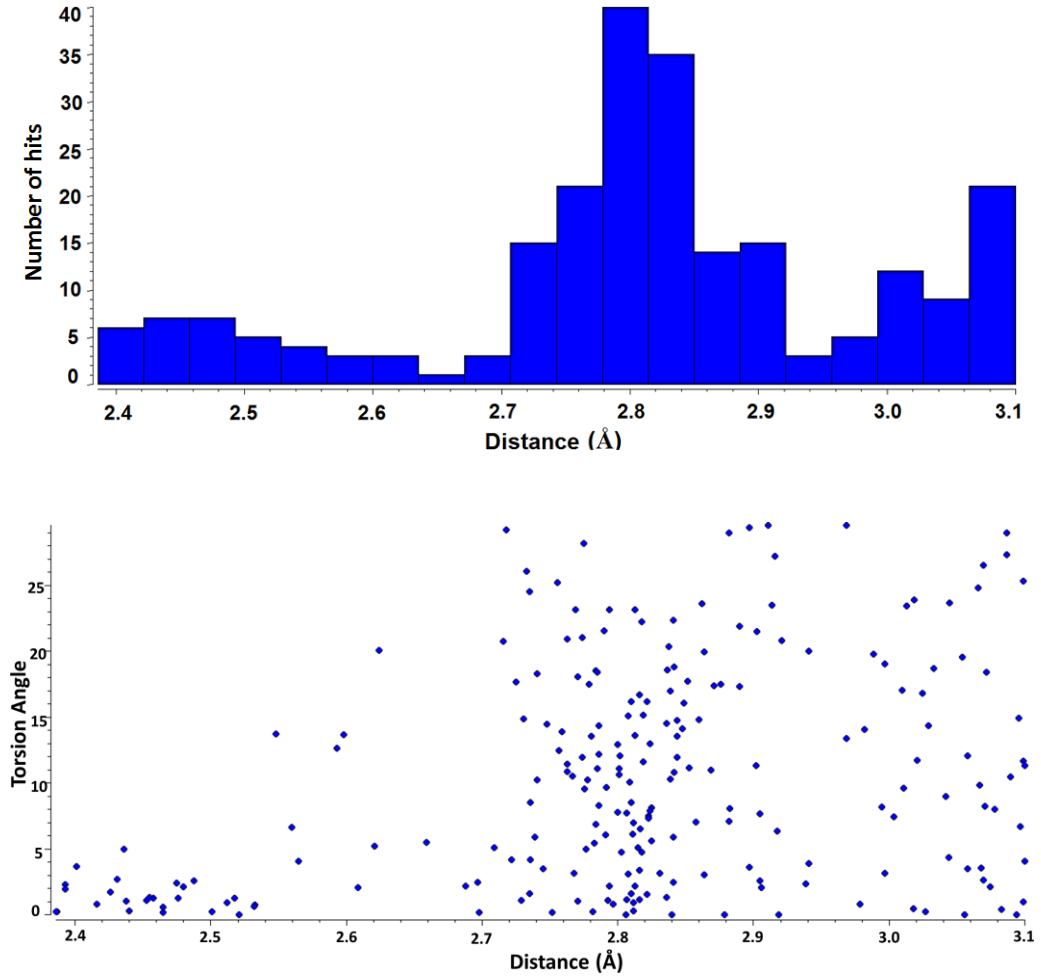
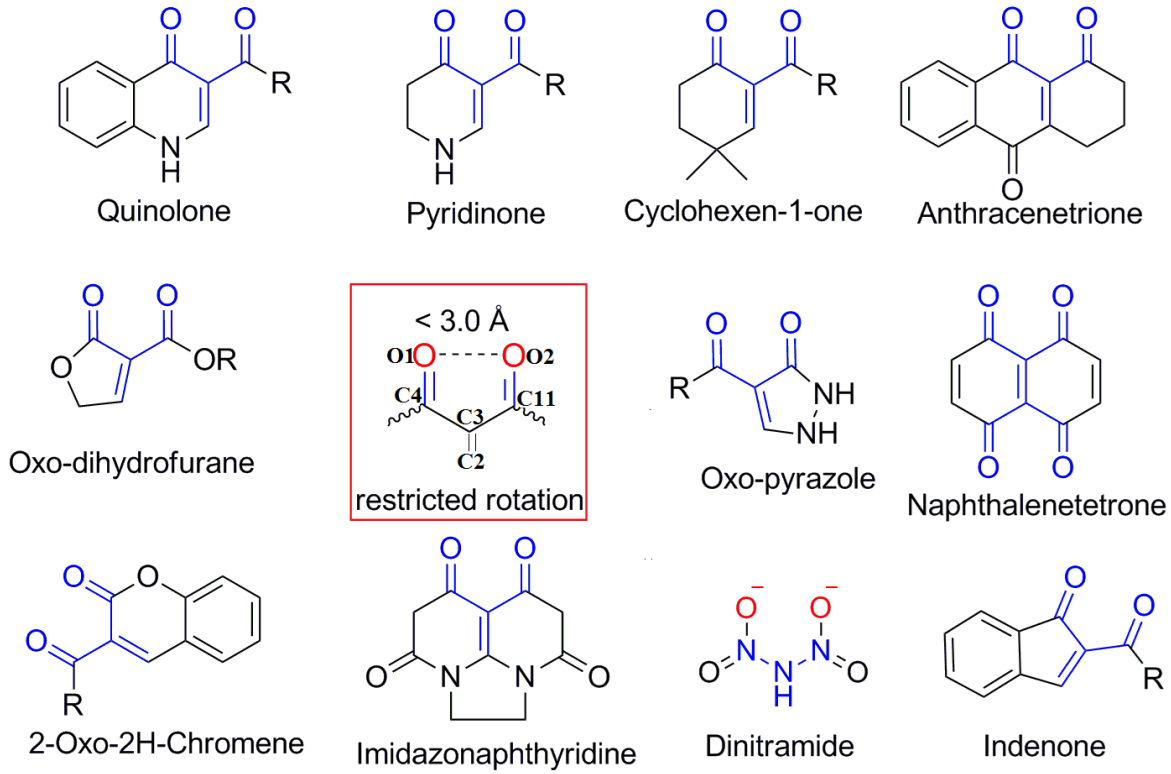
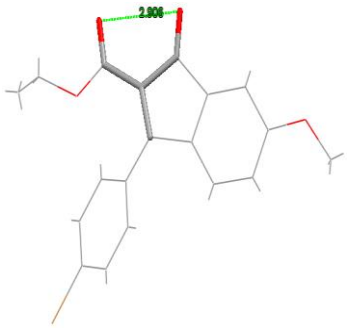


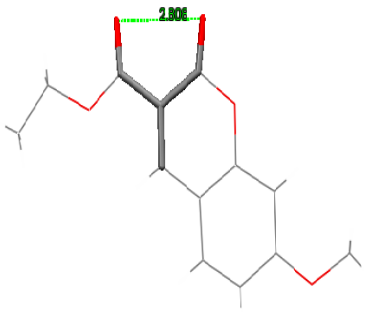
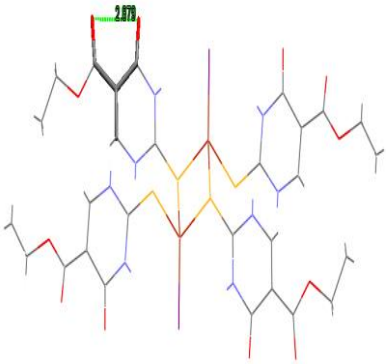
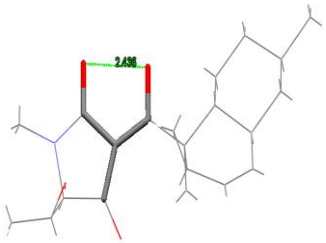
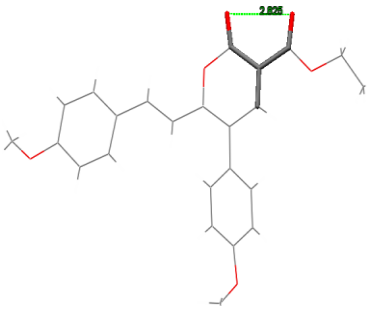
Figure. S5 Cambridge Structural Database search result for O···O short contact distance and torsional angle.

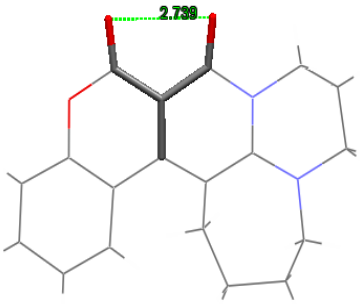
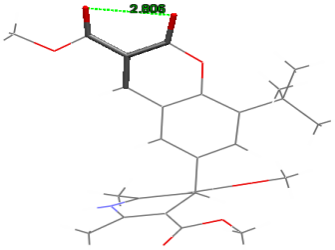
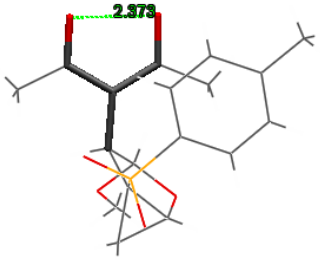
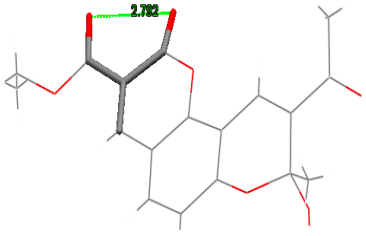
Table S2. Literature search results for short O···O contact.

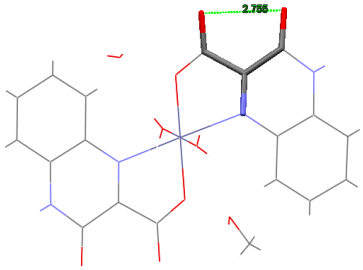
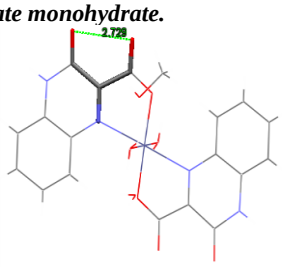
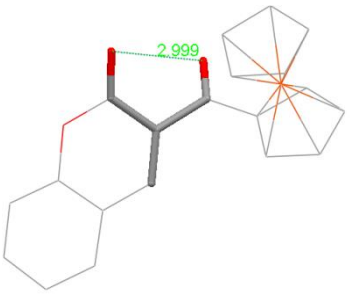
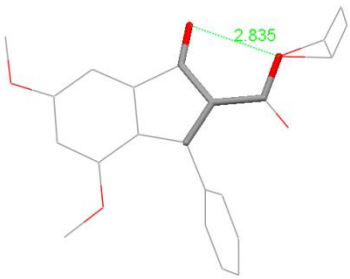


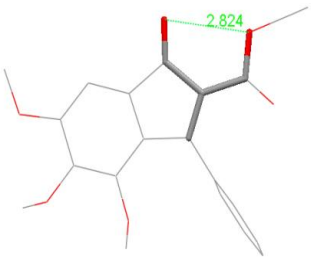
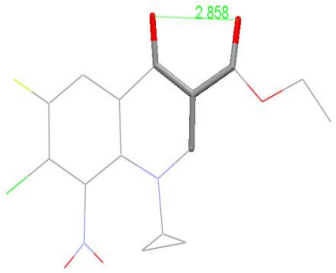
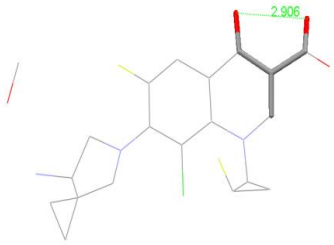
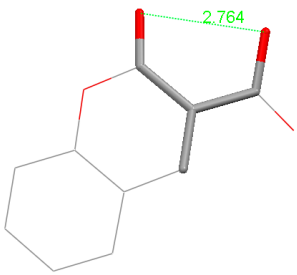
*χ_1 = O1-C4-C3-C2, χ_2 = O2-C11-C3-C2, χ_3 = O1-C4-C3-C2, χ_4 = O2-C11-C3-C2.

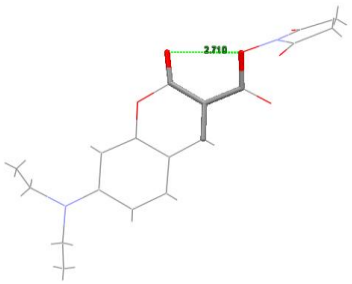
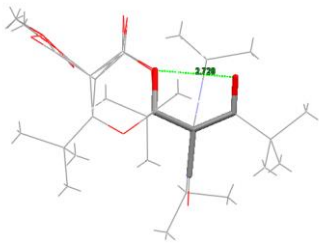
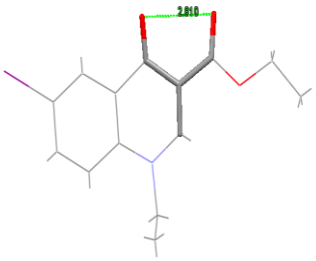
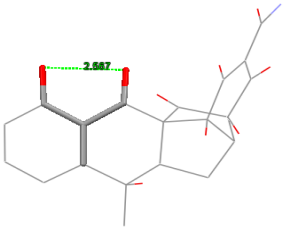
Sl. No	Distance	Torsional angle (χ_1, χ_2, χ_3, χ_4)*	Structure	Details	Reference
1	2.906	-0.15 2.72 -177.65 -179.35	 ***Ethyl-3-(4-bromophenyl)-6-methoxy -1-oxo-1H-indene-2-carboxylate.***	***Space Group:*** *P-1* ***Cell parameter: a*** *8.835*(0), α 109.56 ***b*** *8.881*(0), β 92.68 ***c*** *11.329*(0), γ 93.70 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.543	A.Cappelli et al. (2014) *J. Mater. Chem. C*, **2,** 7897.

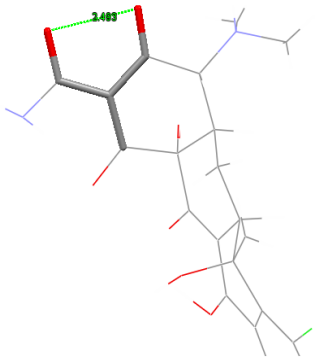
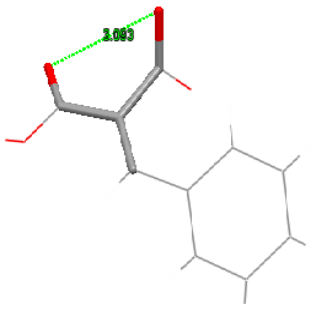
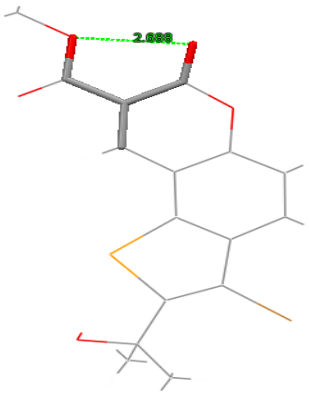
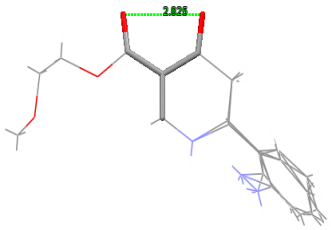
2	2.808	-0.13 3.92 175.82 179.61	 ***Ethyl-7-methoxy-2-oxo-2H-chromene-3-carboxylate.***	***Space Group: C2/c Cell parameter: a*** *25.884*(4), α 90.00 ***b*** *6.837*(1), β 104.88 ***c*** *13.816*(2), γ 90.00 ***Temperature(K):*** 296 ***Density(g/cm^3):*** 1.396	Limei Song,et al. (2014) *Chin. J. Struct. Chem. 33,* 57.
3	2.879	-9.07 1.08 170.09 -178.09	 ***bis(μ_2-Ethyl4-oxo-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate)-bis(ethyl-4-oxo-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate)-bis(iodo)-di-copper.***	***Space Group: P-1 Cell parameter: a*** *7.853*(2), α 64.21 ***b*** *11.272*(1), β 85.40 ***c*** *12.403*(2), γ 83.02 ***Temperature(K):*** *100* ***Density(g/cm^3):*** 1.997	I. Papazoglou et al. (2014) *Eur. J. Med. Chem. **78,** 383.*
4	2.436	0.80 4.77 179.23 -173.09	 ***5-(1-Hydroxyethyl)-1-methyl-3-((1,2,6-trimethyl-1,2,4a,5,6,7,8,8aoctahydronaphthalen-1-yl)carbonyl)pyrrolidine-2,4-dione.***	***Space Group: P21 Cell parameter: a*** *7.700*(0), α 90.00 ***b*** *8.154*(0), β 91.41 ***c*** *16.002*(1), γ 90.00 ***Temperature(K):*** *173* ***Density(g/cm^3):*** 1.194	Lili Kong et al. (2014) *Org. Biomol. Chem. **12,** 7591.*
5	2.825	-6.42 -0.48 177.09 176.09	 ***Ethyl-(4-methoxyphenyl)-6-(2-(4-methoxyphenyl)vinyl)-2-oxo-2H-pyran-3-carboxylate***	***Space Group: P-1 Cell parameter: a*** ***9****.352*(0), α 99.90 ***b*** *10.615*(0), β 109.55 ***c*** *11.229*(0), γ 90.84 ***Temperature(K):*** *293* ***Density(g/cm^3):*** 1.308	G. Sathishkannan et al. (2014) *Adv. Synth. Catal. **356,** 729.*

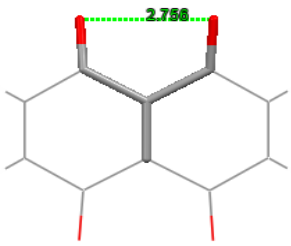
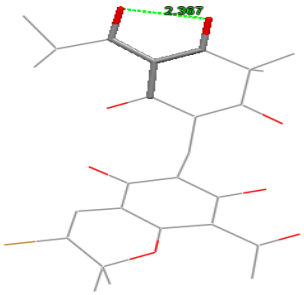
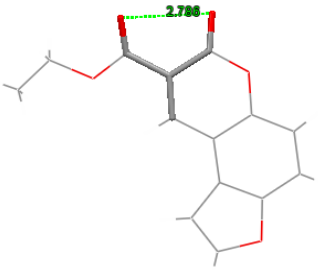
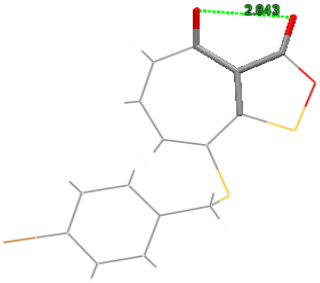
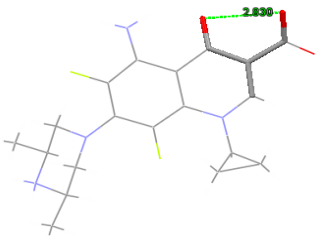
6	2.739	-1.01 8.25 -173.22 -179.43	 ***9,10,11,12,13,14-hexahydro-6H,7H,8H-5-oxa-7a,10a-diazacyclohepta[1,2,3-no]tetraphene-6,7-dione***	***Space Group: Pbca Cell parameter: a*** *14.939(1).*, α 90.00 ***b*** *9.916(1)*, β 90.00 ***c*** *19.963(2)*, γ 90.00 ***Temperature(K):*** *296* ***Density(g/cm^3):*** 1.448	Y. M. Poronik etal. (2014) *Chem.Commun.* ***50,*** *5688.*
7	2.806	-0-00 0.00 180.00 -180.00	 ***Dimethyl4-(8-t-butyl-3-(methoxycarbonyl)-2-oxo-2H-chromen-6-yl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate.***	***Space Group: Pnma Cell parameter: a*** *18.388*(6), α 90.00 ***b*** *12.020*(4), β 90.00 ***c*** *12.141*(0), γ 90.00 ***Temperature(K):*** *294* ***Density(g/cm^3):*** 1.197	K. V. Sashidhara et al. (2013) *J. Med. Chem.* **56,** 109.
8	2.373	-2.51 1.54 176.91 -177.92	 ***3-(3-Methoxy-5-((4-methylphenyl)sulfonyl)-2-oxabicyclo[3.1.0]hex-4-yl)pentane-2,4-dione.***	**Space Group**: **P21 Cell parameter**: **a** 9.994(0), α 90.00 **b** 12.399(1), β 108.16 **c** 15.468(1), γ 90.00 **Temperature(K)**: 293 **Density(g/cm^3)**: 1.336.	*C. Manna et al. (2013) Eur. J. Org. Chem.* ***6084.***
9	2.792	-7.98 -4.00 175.67 172.35	 ***Ethyl-9-acetyl-8-hydroxy-8-methyl-2-oxo-2H,8H-pyrano[2,3-f]chromene-3-carboxylate.***	***Space Group: Cc Cell parameter: a*** *8.320*(10), α 90.00 ***b*** *28.090*(30), β 115.89 ***c*** *7.621*(9), γ 90.00 ***Temperature(K):*** *296* ***Density(g/cm^3):*** 1.427	Lingliang Long et al.(2013) *Org. Biomol. Chem.* ***11,*** *8214.*

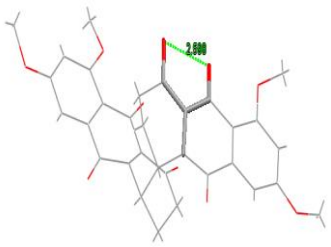
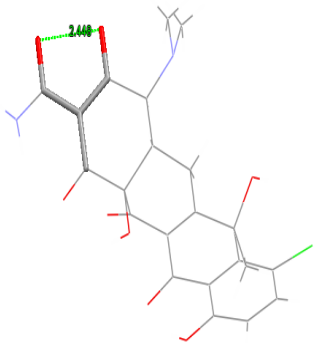
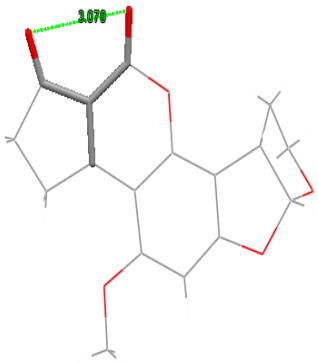
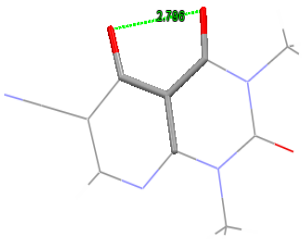
10	2.755	-9.67 5.87 166.34 178.48	***Diaqua-bis(3-oxo-3,4-dihydroquinoxaline-2-carboxylato)-zinc*** 	***Space Group:*** ***P21*** ***Cell parameter:*** ***a*** *7.054*(0), α 90.00 ***b*** *16.181*(1), β 101.09 ***c*** *9.485*(0), γ 90.00 ***Temperature(K):*** *293* ***Density(g/cm^3):*** 1.656.	Bo Xiao et al. *(2013)* *Inorg. Chim. Acta.* ***407,*** *274.*
11	2.729	-2.53 4.97 178.32 -175.84	***Diaqua-bis(3-oxo-3,4-dihydroquinoxaline-2-carboxylato)-zincmethanolsolvate monohydrate.*** 	***Space Group:*** *P21* ***Cell parameter:*** ***a*** ***7.***054(0), α 90.00 ***b*** *16.181*(1), β 101.09 ***c*** *9.485*(0), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.656	Du-Liang He et al. (*2013)* *New Cryst. Struct.* ***2013,*** ***228,*** *323.*
12.	2.999	-9.61 -52.33 173.00 124.97	 ***2-Oxo-2H-chromene-3-carbonyl)ferrocene.***	***Space Group:*** Pbca ***Cell parameter:*** ***a*** 12.377(5), α 90.00 ***b*** 10.686(5), β 90.00 ***c*** 23.309(5), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.543	R. K. Verma et al. (2012) *RSC Advances* 2012 , **2,** 2413
13.	2.835	-2.74 6.72 177.75 179.22	 ***Ethyl-4,6-dimethoxy-1-oxo-3-phenyl-1H-indene-2-carboxylate.***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 12.466(4), α 90.00 ***b*** 19.438(6), β 98.53 ***c*** 7.173(3), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.307.	A. Cappelli, et al. (2012) *J. Mater .Chem,* **22,** 9611.

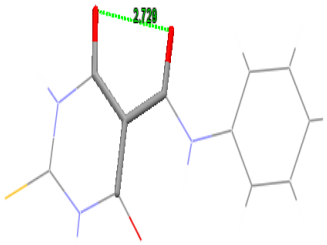
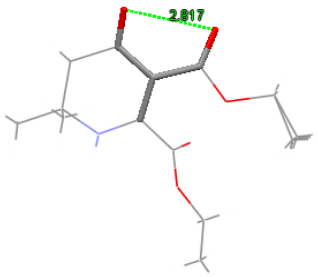
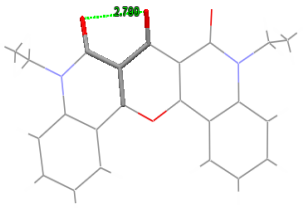
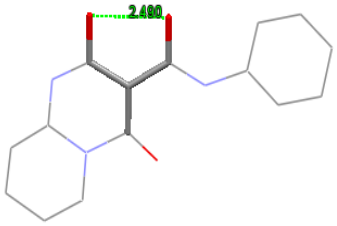
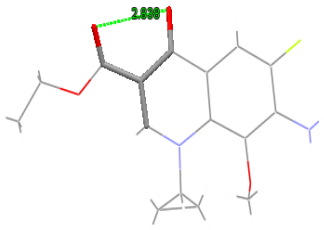
14.	2.824	0.63 3.27 178.67 175.93	 ***Ethyl-4,5,6-trimethoxy-1-oxo-3-phenyl-1H-indene-2-carboxylate.***	***Space Group:*** C2/c ***Cell parameter: a*** 15.777(0), α 90.00 ***b*** 11.500(0), β 90.79 ***c*** 20.411(0), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.322	A.Cappelli, et al. (2012) *J. Mater. Chem.* **22,** 9611.
15.	2.858	4.69 -13.44 -172.37 163.62	 ***Ethyl-7-chloro-1-cyclopropyl-6-fluoro-8-nitro-4-oxo-1,4-dihydroquinoline-3-carboxylate.***	***Space Group:*** P-1 ***Cell parameter: a*** 8.234(1), α 85.60(3) ***b*** 9.152(1), β 81.20(3) ***c*** 0.736(2), γ 74.13(3) ***Temperature(K):*** 291 ***Density(g/cm3):*** 1.533	R.A.Al-Qawasmeh, et al. (2012) *Acta Crystallogr. Sect. E: Struct. Rep. Online* **68,** o 2533.
16.	2.906	-2.21 -33.80 -175.53 139.64	 ***7-[(7S)-7-Azaniumyl-5-azaspiro[2.4]hept-5-yl]-8-chloro-6-fluoro-1-[(1S,2R)-2-fluorocyclopropyl]-4-oxo-1,4-dihydroquinoline-3-carboxylate methanolSolvate.***	***Space Group:*** P21 ***Cell parameter: a*** 8.745(0), α 90.00 ***b*** 8.297(0), β 104.47(0) ***c*** 14.064(0), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.485	Wen-jie Xu, et al. (2012) *Acta Crystallogr. Sect.E. Struct. Rep. Online.***68,** o2794.
17.	2.764	0.63 15.24 -167.56 -167.52	 ***2-Oxo-2H-chromene-3-carboxylic acid.***	***Space Group:*** P21/c ***Cell parameter: a*** 3.910(0), α 90.00 ***b*** 20.264(0), β 91.35(0) ***c*** 15.309(0), γ 90.00 ***Temperature (K) :*** 180 ***Density (g/cm3):*** 1.469	Dongpeng Yan, et al. (2012) *Cryst. Eng. Comm.* **14,** 5121.

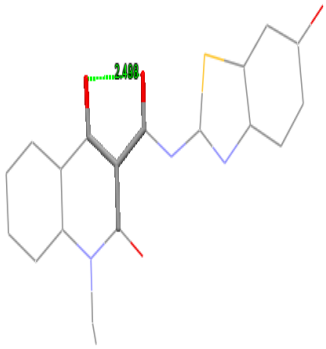
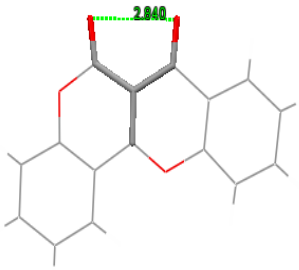
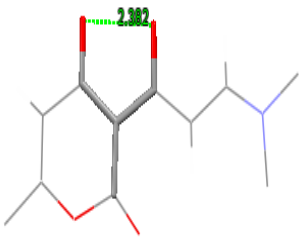
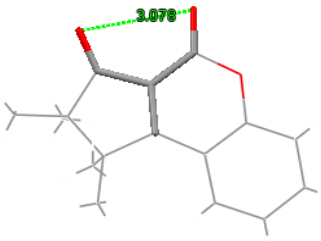
18.	2.710	3.48 10.57 -179.00 -167.05	 ***Succinimidyl-7-(diethylamino)-2-oxo-2H-chromene-3-carboxylate.***	***Space Group:*** C2/c ***Cell parameter:*** ***a*** 19.601(3), α 90.00 ***b*** 9.317(1), β 93.43 ***c*** 22.807(3), γ 90.00 ***Temperature (K):*** 150 ***Density (g/cm3):*** 1.526.	G. R .Bardajee, et al. (2006) *Acta. Crystallogr. Sect.E: Struct. Rep. Online.* **62,** o 3079.
19.	2.728	61.21 -41.30 -154.21 177.08	 ***(R,R)-2-(1-Isopropyl-4-(isopropylimino)-2-oxo-3-pivaloylazetidin-3-yl)-2, 6-di-tert-butyl-5-methoxycarbonyl-1, 3-dioxin-4(2H)-one.***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 9.885(3), α 90.00 ***b*** 16.338(5), β90.00 ***c*** 17.537(5), γ 90.00 ***Temperature (K):*** 90 ***Density (g/cm3):*** 1.221.	B. C. Wallfisch, et al. (2002) *J. Chem. Soc. Perkin Trans.**1*** ,599.
20.	2.810	-4.24 -6.15 178.94 170.72	 ***Ethyl-1-ethyl-6-iodo-4-oxo-1,4-dihydroquinoline-3-carboxylate***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 10.817(0), α 90.00 ***b*** 8.059(0), β 91.33 ***c*** 15.842(0), γ 90.00	J. Bauer, et al. (2009) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.*.**65,** o512.
21.	2.567	4.78 -14.32 -177.90 168.39	 ***4-Deamino-4-hydroxy-4,11a-anhydrotetracycline***	***Space Group:*** P21 ***Cell parameter:*** ***a*** 7.579(1), α 90.00 ***b*** 13.534(1), β 96.91 ***c*** 10.744(1), γ 90.00	D. H. R. Barton, et al. (1977) *Chem. Commun.* 790.

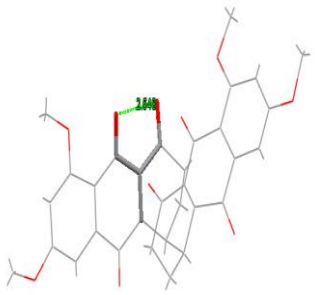
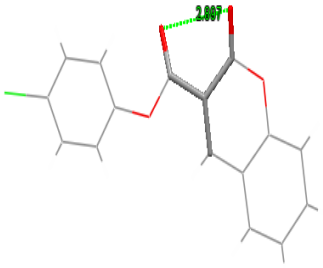
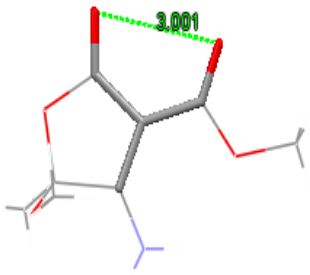
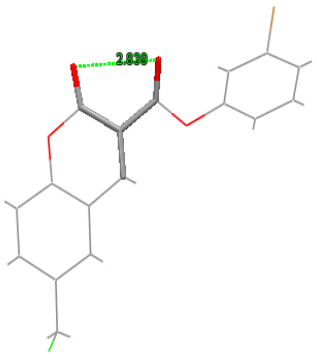
22.	2.493	9.73 -9.98 -169.35 169.11	 ***Aureomycin hydrochloride***	***Space Group:*** P212121 ***Cell parameter: a*** 11.200, α 90.00 ***b*** 12.890, β 90.00 ***c*** 15.470, γ 90.00	R. R .Boggs, et al. (1978) *J. Cryst. Mol. Struct.* **8,** 35.
23.	3.093	10.83 70.90 -165.70 -112.82	 ***Ammonium hydrogen benzylidenepropanedioate.***	***Space Group:*** P21/c ***Cell parameter: a*** 16.616(2), α 90.00 ***b*** 5.488(0), β 95.20 ***c*** 11.381(2), γ 90.00	C. N. O' Callaghan, et al. (1998) *J. Chem. Res.* **732,** 3224.
24.	2.688	-3.51 10.31 177.70 -170.34	 ***Methyl-3-bromo-2-(2-hydroxypropan-2-yl)-7-oxo-7H-selenolo[2,3-f]chromene-8-carboxylate.***	***Space Group:*** P-1 ***Cell parameter: a*** 7.783(0), α 92.00(0) ***b*** 8.707(0), β 105.09(0) ***c*** 12.560(0), γ 109.23(0)	P. Arsenyan, *et al. SSSR (Russ.) Chem. Heterocycl. Compd.*296.
25.	2.825	10.19 -4.59 -177.05 -177.45	 ***2-Methoxyethyl-6-(2-aminophenyl)-4-oxo-1,4,5,6-tetrahydropyridine-3-Carboxylate.***	***Space Group:*** P21/c ***Cell parameter: a*** 14.154(3), α 90.00 ***b*** 9.409(1), β 114.41 ***c*** 12.276(3), γ 90.00	V. Karapetyan, et al. (2011) *Helv. Chim .Acta.* **94,** 2045.

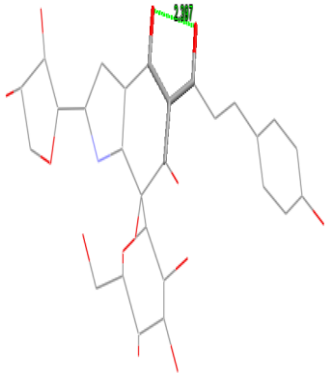
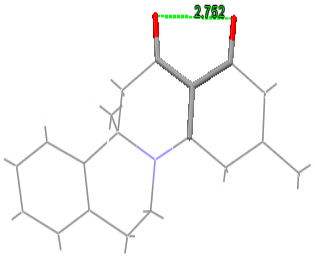
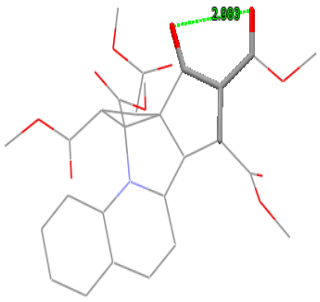
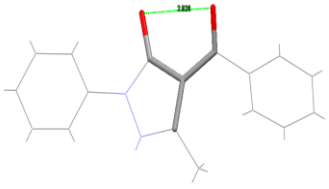
26.	2.756	14.83 14.97 -165.53 -164.66	 ***Naphthalene-1,4,5,8-tetrone.***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 6.510(4), α 90.00 ***b*** 13.220(5), β 110.00(50) ***c*** 4.855(4), γ 90.00	F. H. Herbstein, M .Kapon, et al. (1982) *Acta Crystallogr. Sect.B: Struct. Crystallogr. Cryst. Chem.*, **38,** 3123
27.	2.367	7.08 -7.79 -177.47 176.49	 ***Bromovliginosin B***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 10.438(12), α 103.62(5) ***b*** 10.792(14), β 99.18(5) ***c*** 13.367(17), γ 102.73(5)	W. L. Parker, et al. (1968) *J .Am. Chem. Soc.* **90,** 4723.
28.	2.786	-14.05 -3.70 167.56 174.71	 ***3-Carbethoxy-furo(3,2-f)coumarin***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 16.952(10), α 90.00 ***b*** 16.160(10), β 92.80(10) ***c*** 4.330(3), γ 90.00	G. Bravic, et al (1978) *Cryst. Struct. Commun.***7,** 633.
29.	2.843	-16.33 -4.77 160.37 178.06	 ***Thiotropocin-p-bromobenzyl-thioether.***	***Space Group:*** C2/c ***Cell parameter:*** ***a*** 15.664(3), α 90.00 ***b*** 14.557(2), β 102.61 ***c*** 12.983(3), γ 90.00	S. Tsubotani, et al. (1984) *Tetrahedron Lett.* **25,** 419.
30.	2.830	6.92 29.38 -169.78 -153.87	 ***5-Amino-1-cyclopropyl-7-((3R,5S)-3,5-dimethylpiperazin-1-yl)-6,8-difluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 11.850(3), α 90.00 ***b*** 10.913(4), β 107.76(1) ***c*** 17.506(2), γ 90.00	A. Sivalakshmidevi, et al. (2000) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **56,** e115.

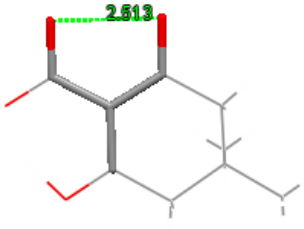
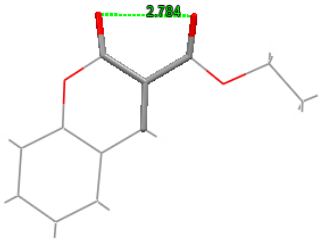
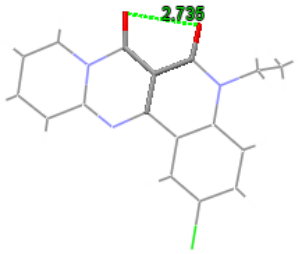
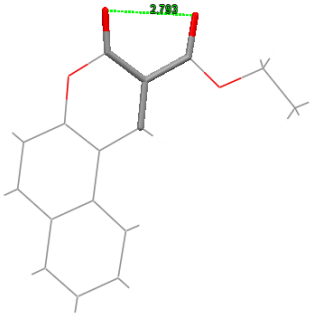
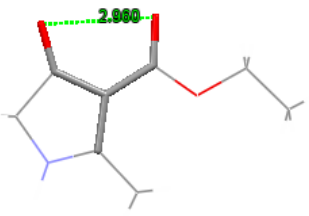
31.	2.589	-8.09 -7.87 176.75 167.17	 ***5,5',7,7'-tetramethoxy-2,2',3,3'-tetrahydro-1,1'-bianthracene-4,4',9,9',10,10'(1H,1'H)-hexone***	***Space Group:*** C2/c ***Cell parameter:*** ***a*** 9.370(1), α 90.00 ***b*** 20.283(4), β 108.28(3) ***c*** 14.007(3), γ 90.00	K. C. Nicolaou, et al. (2005) *Angew. Chem., Int. Ed.***44,** 5846.
32.	2.448	1.81 -3.56 178.28 -179.28	 ***5a,11a-Dehydro-7-chlorotetracycline***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 16.942(2), α 90.00 ***b*** 11.618(1), β 90.00 ***c*** 10.606(1), γ 90.00	R. Prewo, et al. (1980) J. *Am. Chem. Soc.* **102,** 7015.
33.	3.070	2.00 1.26 -179.13 -177.48	 ***Aflatoxin B2***	**Space Group:** P212121 **Cell parameter:** **a** 6.927(2) α 90.00 **b** 10.146(2), β 90.00 **c** 20.171(2), γ 90.00	T. C. van Soest, et al. (1970) *Acta Crystallogr. Sect.B: Struct. Crystallogr. Cryst. Chem.***26,** 1956.
34.	2.796	0.34 1.51 -177.76 177.59	 ***6-cyano-1,3-dimethyl-2,4,5-trioxo-1,3,4,5-tetrahydro-2H-pyrido[2,3-d]pyrimidin-8-ide***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 8.152(0), α 69.61(0) ***b*** 9.298(0), β 70.74(0) ***c*** 9.730(0), γ 79.45(0)	J. Quiroga, (2010) *Acta. Crystallogr. Sect.C: Cryst.Struct. Commun.* ,**66,** o 39.

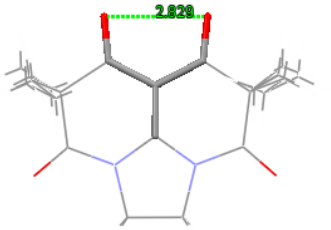
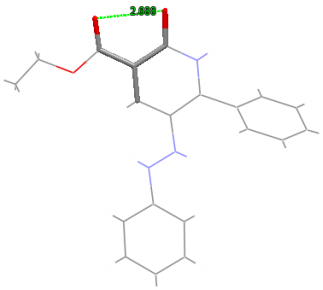
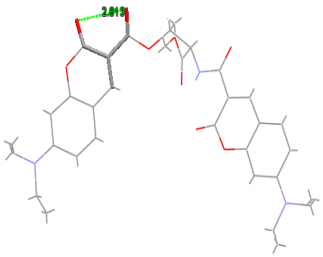
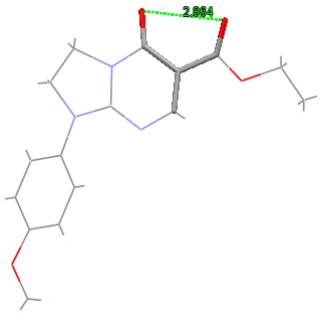
35.	2.729	3.06 2.70 -176.02 -178.25	 ***1,2,3,4-tetrahydro-6-hydroxy-4-oxo-N-phenyl-2-thio-5-pyrimidinecarboxamide***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 11.765(3), α 90.00 ***b*** 12.788(3), β 90.00 ***c*** 15.011(3), γ 90.00.	A. D. Brewer, et al. (1987) *Acta Crystallogr. Sect. C: Cryst.Struct. Commun.***43,** 144.
36.	2.817	-2.31 -16.77 177.05 163.88	 ***Diethyl-6,6-dimethyl-4-oxo-1,4,5,6-tetrahydropyridine-2,3-dicarboxylate***	***Space Group:*** C2/c ***Cell parameter:*** ***a*** 16.784(1), α 90.00 ***b*** 16.711(1), β 114.78(0) ***c*** 13.025(1), γ 90.00	P. V. Novikov, et. al. (2004) *Mendeleev Commun.* 310.
37.	2.790	9.75 15.90 -171.73 -162.51	 ***5,9-Diethyl-6,7,8-trioxodiquinolino(3,4-b;3',4'-e)-4H-pyran***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 12.555(3), α 110.43 ***b*** 12.617(3), β 95.82 ***c*** 13.630(3), γ 114.32	I. V. Ukrainets, et. al. (2000) *Khim. Get. Soedin. SSSR (Russ.) Chem. Heterocycl.Compd.*,516.
38.	2.490	0.06 0.88 -178.90 178.05	 ***2-Hydroxy-N-phenyl-4-oxo-4H-pyrido(1,2-a)pyrimidine-3-carboxamide***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 5.843(1) α 90.00 ***b*** 25.648(5), β 96.94(1) ***c*** 20.372(2), γ 90.00	R. Bossio, et. al. (1993) *J.Heterocycl.Chem.* ,**30,**33
39.	2.838	-17.68 -7.00 164.10 171.32	 ***Ethyl-7-amino-1-cyclopropyl-6-fluoro-8-methoxy-4-oxo-1,4-dihydroquinoline-3-carboxylate***	***Space Group:*** P21/n ***Cell:*** ***a*** 10.096(4), α 90.00 ***b*** 14.699(5), β 94.26(4) ***c*** 11.028(6), γ 90.00	Jia Pan, Li Yang, et al. (2008) *Acta Crystallogr. Sect.E: Struct. Rep. Online.***64,** o 527.

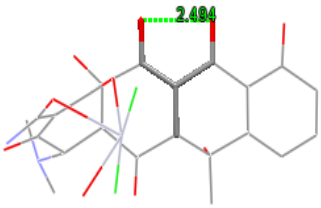
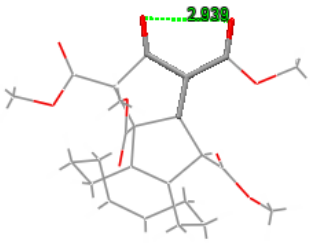
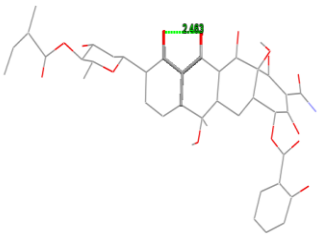
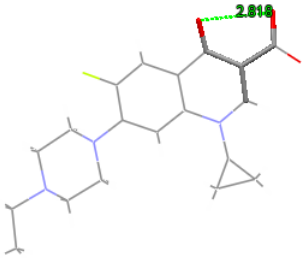
40.	2.498	1.48 -0.22 -179.39 -179.35	 ***N-(6-Hydroxybenzothiazol-2-yl)-1-ethyl-4-hydroxy-2-oxo-1,2-dihydroquinolinyl-3-carboxamide***	***Space Group:*** P21/c ***Cell:*** ***a*** 7.948(3), α 90.00 ***b*** 7.766(3), β 90.47(3) ***c*** 26.830(10), γ 90.00	R. I. Zubatyuk, (2004) *Zh. Strukt. Khim. (Russ.) J.Struct.Chem.* **45,** 365.
41.	2.840	-0.00 0.00 180 -180	 ***6H,7H-(1)Benzopyrano(4,3-b)(1)benzopyran-6,7-dione***	***Space Group:*** Pnam ***Cell:*** ***a*** 22.630(9), α 90.00 ***b*** 7.892(1), β 90.00 ***c*** 6.484(1), γ 90.00	E. R. Di Paolo, et al. (1989) *Helv. Chim. Acta.* **72,** 1455.
42.	2.382	0.00 -0.00 180 180	 ***4-Hydroxy-6-methyl-3-(3-dimethylaminoacryloyl)-2H-pyran-2-one***	***Space Group:*** Pnma ***Cell parameter:*** ***a*** 12.652(1), α 90.00 ***b*** 6.775(1), β 90.00 ***c*** 12.907(1), γ 90.00	O. Carugo, (1990) *Polyhedron.* **9,** 2061.
43.	3.078	-11.10 1.17 169.27 -179.25	 ***1,1,2,2-Tetramethyl-1,2-dihydro-1H,4H-cyclo-penta(c)benzopyran-3,4-dione***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 8.663(1), α 90.00 ***b*** 7.135(1), β 101.59(1) ***c*** 20.999(2) γ 90.00	D.Schwebel,et al. (1999) *Helv. Chim. Acta.* **82,** 177.

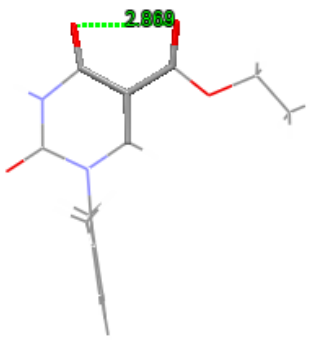
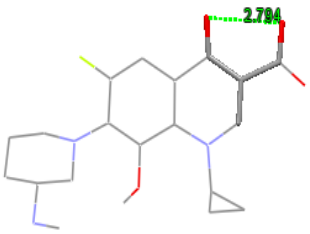
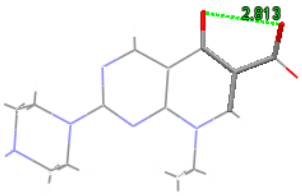
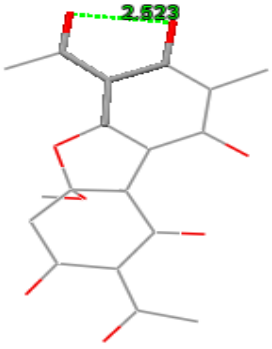
44.	2.548	-1.50 -14.09 175.86 168.57	 ***Di-isopropyl,3-dithiol-2-ylidenemalonate***	***Space Group:*** P21/a ***Cell parameter:*** ***a*** 22.425(3), α 90.00 ***b*** 8.273(2), β 96.66(1) ***c*** 15.713(3), γ 90.00	D. R. Vega, et al. (1989) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **45,** 1612.
45.	2.897	28.82 7.84 -146.27 -177.08	 ***4-Chlorophenyl-2-oxo-2H-chromene-3-carboxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 15.759(0), α 90.00 ***b*** 7.069(0), β 113.04(0) ***c*** 12.717(0), γ 90.00	Xiao-Qiang Guo, et al. (2012) *Acta Crystallogr.,Sect. E:Struct.Rep.Online* ,**68,** o574
46.	3.001	0.73 3.28 -179.92 -175.93	 ***Methyl-4-amino-5-methoxy-5-methyl-2-oxo-2,5-dihydrofuran-3-carboxylate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 9.516(1), α 94.40(10) ***b***7.245(1), β 98.40(10) ***c*** 6.915(1) γ 81.20(10)	A. C. Veronese, et al. (1994) *J. Chem. Soc., Perkin Trans. **1*** ,1779.
47.	2.839	0.24 21.00 179.79 -158.56	 ***3-Bromophenyl-6-(chloromethyl)-2-oxo-2H-1-benzopyran-3-carboxylate***	***Space Group:*** P21 ***Cell parameter:*** ***a*** 6.248(1), α 90.00 ***b*** 7.618(1), β 94.87 ***c*** 15.975(2), γ 90.00	L. Pochet, et al. (2000) *Bioorg .Med. Chem.* **8,** 1489.

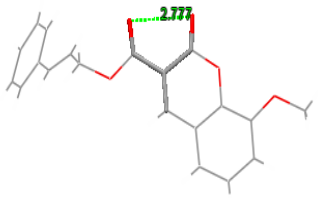
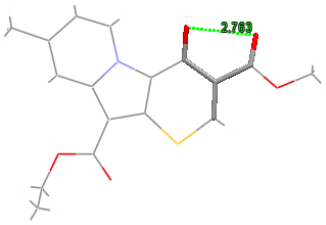
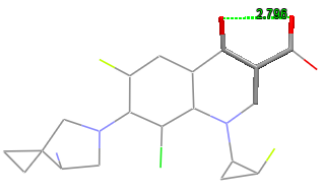
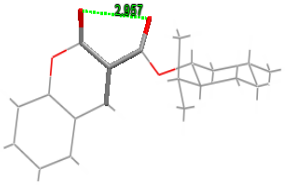
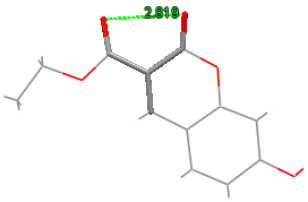
48.	2.397	-10.82 7.07 171.21 -175.02	 ***Cartormin***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 11.979(3), α 90.00 ***b*** 29.256(3), β 90.00 ***c*** 7.761(2), γ 90.00	Hong-Bin Yin, et al. (2000) *Tetrahedron Lett.* **41,** 1955.
49.	2.752	-2.40 2.46 177.15 -177.09	 ***(9R,16R:9S,16S)-9,16-Dimethyl-8-aza-D-homogona-12,17a-dione***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 13.292(2), α 90.00 ***b*** 8.404(1), β 97.17(1) ***c*** 13.986(2), γ 90.00	O. V. Gulyakevich, et al. (1999) *Mendeleev Commun.* 119.
50.	2.983	-7.72 5.94 174.28 -176.47	 ***Pentamethyl-11,11a-dihydro-9-oxo-9H,10H-cyclobuta(4,5)cyclopenta(3,4)pyrrolo(1,2-a)quinoline-7,8,10,11,11a-pentacarboxylate***	***Space Group:*** P1121/b ***Cell parameter:*** ***a*** 10.410(10), α 90.00 ***b*** 14.310(10), β 91.91(5) ***c*** 16.890(20), γ 90.00	P. J. Abbott, et al. (1976) *Acta Crystallogr ,Sect. B: Struct. Crystallogr. Cryst. Chem.* **32,** 1927.
51.	2.826	5.94 20.39 178.29 -149.38	 ***4-benzoyl-3-methyl-1-phenyl-2H-pyrazoline-5-one***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 18.100(4), α 90.00 ***b*** 13.158(3), β 116.44(3) ***c*** 19.277(4), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.614	A.L.Litvinov,et al. (2001) *Synth.Met.* ,**121,** 1119

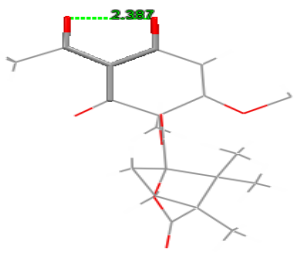
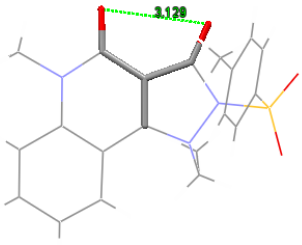
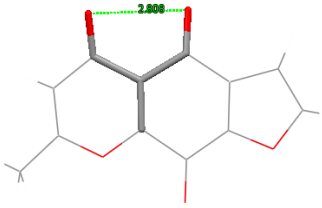
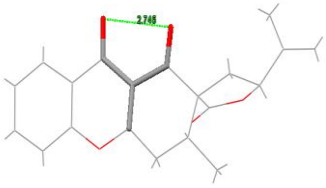
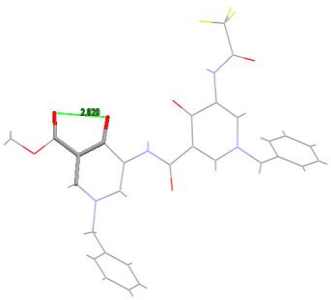
52.	2.513	4.24 -5.39 178.99 179.89	 ***4,4-Dimethyl-2-hydroxy-6-oxo-cyclo hexene-1-carboxylic acid***	***Space Group:*** Cmc21 ***Cell parameter:*** ***a*** 10.474(5), α 90.00 ***b*** 66.240(30), β 90.00 ***c*** 6.662(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.323	L. L. Duncan, et al. (2002) *Acta Crystallogr. Sect.B: Struct.Sci.* ,**58,** 502.
53.	2.784	11.05 11.05 -169.49 -167.70	 ***Ethyl-2-oxo-2H-1-benzopyran-3-car boxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 7.935(0), α 90.00 ***b*** 15.774(0), β 108.22(0) ***c*** 8.758(0), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.392	E.V.Garcia-Baez, et al. (2003) *Cryst. Growth Des.* **3,** 35.
54.	2.735	2.07 -0.05 179.31 -177.23	 ***2-Chloro-5-ethyl-5H-5,7a,12-triazab enzo(a)anthracene-6,7-dione***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 8.730(2), α 90.00 ***b*** 15.672(5), β 111.05(2) ***c*** 11.484(4), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.476	I.V.Ukrainets, et al. (2005) *Khim.Get.Soedin., SSSR(Russ.)Chem .Heterocycl.Comp d)* , 1060.
55.	2.793	0.08 0.63 -178.99 -179.71	 ***Ethyl-5,6-benzocoumarin-3-carboxyl ate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 8.649(0), α 90.00 ***b*** 7.774(0), β 92.05(0) ***c*** 29.196(1), γ 90.00 ***Temperature(K):*** 273 ***Density(g/cm3):*** 1.417	Yi-Feng Sun, et al. (2008) *Jiegou Huaxue(Chin.J.Str uct.Chem.),* **27,** 1526.
56.	2.960	0.91 -5.93 -176.94 171.44	 ***Ethyl-2-methyl-4-oxo-4,5-dihydro-1 H-pyrrole-3-carboxylate***	***Space Group:*** Pbcn ***Cell parameter:*** ***a*** 12.152(5), α 90.00 ***b*** 7.851(4), β 90.00 ***c*** 17.523(5), γ 90.00 ***Temperature(K):*** 220 ***Density(g/cm3):*** 1.344	S.Parsons, et al. (2004) *Private Communication.*

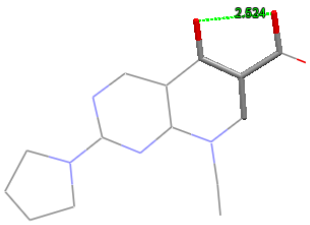
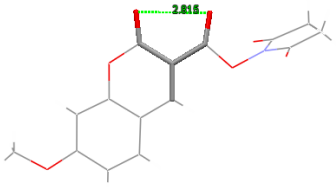
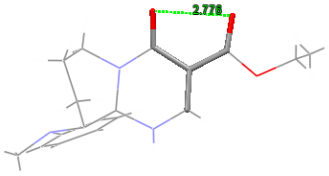
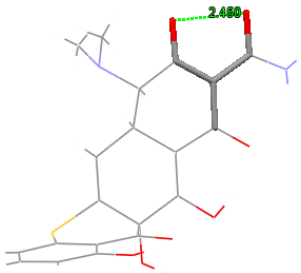
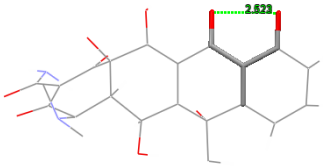
57.	2.829	1.31 -1.87 -178.57 178.00	 ***5,5,8,8-Tetrapropyl-1,2-dihydroimidazo(1,2,3-ij)(1,8)naphthyridine-4,6,7,9(5H,8H)-tetraone***	***Space Group:*** P21/c ***Cell parameter: a*** 10.815(9), α 90.00 ***b*** 21.724(18), β 104.10(1) ***c*** 11.663(10), γ 90.00 ***Temperature(K):*** 273 ***Density(g/cm3):*** 1.151	Guozhong Ye, et al. (2008) *J.Org.Chem.* **73,** 5170.
58.	2.688	4.14 -1.56 -177.30 179.83	 ***Ethyl-2-oxo-6-phenyl-5-(2-phenylhydrazino)-1,2-dihydropyridine-3-carboxylate***	***Space Group:*** P21/c ***Cell parameter: a*** 14.809(0), α 90.00 ***b*** 12.443(0), β 117.30 ***c*** 22.057(0), γ 90.00 ***Temperature(K):*** 298 ***Density(g/cm3):*** 1.285	S.M.Al-Mousawi, et al. (2011) *Tetrahedron Lett.* **52,** 202.
59.	2.813	9.23 7.75 -170.13 -172.91	 ***(2S,3R)-N,O-bis(7-Diethylaminocoumarin-3-carbonyl)threonine methyl ester***	***Space Group:*** P21 ***Cell parameter: a*** 9.017(0), α 90.00 ***b*** 14.023(0), β 100.21 ***c*** 14.643(0), γ 90.00 ***Temperature(K):*** 150 ***Density(g/cm3):*** 1.283	Lee-Chiang Lo, et al. (2001) *Chirality.* **13,** 266.
60.	2.864	6.26 18.24 -176.74 -158.67	 ***Ethyl-1-(4-methoxyphenyl)-5(1H)-oxo-2,3-dihydroimidazo(1,2-a)pyrimidine-6-carboxylate***	***Space Group:*** P21/c ***Cell parameter: a*** 6.962(1), α 90.00 ***b*** 29.693(6), β 107.89(3) ***c*** 7.514(2), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.417	D. Matosiuk, et al. (2003) *J. Heterocycl. Chem.* **40,** 93.

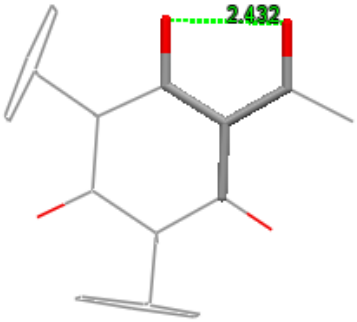
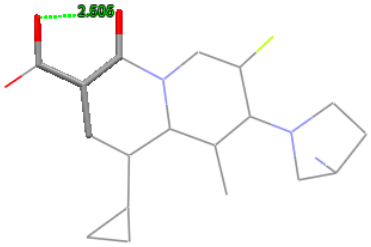
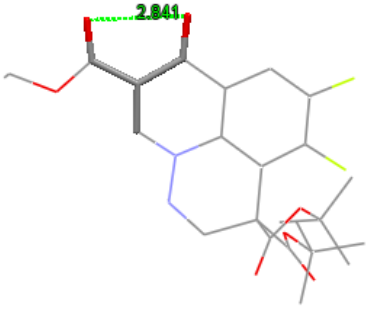
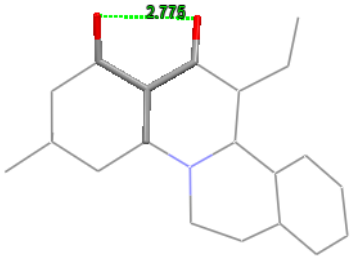
61.	2.494	2.21 -8.39 -175.84 169.79	 ***Oxytetracycline mercury(ii) chloride***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 11.377(1), α 90.00 ***b*** 17.277(2), β 90.00 ***c*** 12.731(2) γ 90.00 ***Temperature(K):*** 123 ***Density(g/cm3):*** 2.038	K. H. Jogun, et al (1976) *J. Am. Chem. Soc.* **98,** 6018.
62.	2.939	-7.39 10.00 174.64 -172.45	 ***Tetramethyl(3R,3aR,12S)-2,3a,4,5,6, 9,10,11-octahydro-2-oxocyclodeca(a) pentalene-1,3,3a,12(3H)-tetracarbox ylate***	***Space Group:*** Pbca ***Cell parameter:*** ***a*** 9.186(2), α 90.00 ***b*** 28.360(3), β 90.00 ***c*** 17.483(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.343	L. A. Paquette, (1992) *J. Org. Chem.* **57,** 3512.
63.	2.463	11.77 -19.62 178.72 174.22	 ***3,10,12-Trihydroxy-6,12a-dimethoxy -6-methyl-1,11-dioxo-4-salicyloyloxy -9-(1,2,6-trideoxy-4-angeloyloxy-C-g lycosyl)naphthacene-2-carboxamide***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 18.137(9), α 90.00 ***b*** 24.355(12), β 90.00 ***c*** 9.269(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.349	M. Hatsu, et al. (1992) *J. Antibiot.***45,** 325.
64.	2.818	-0.91 -23.41 179.32 156.37	 ***1-cyclopropyl-7-(4-ethylpiperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinol ine-3-carboxylate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 9.791(2), α 69.12(1) ***b*** 9.858(1), β 75.74(1) ***c*** 12.274(2), γ 89.54(1) ***Temperature(K):*** 298 ***Density(g/cm3):*** 1.307	Hong-Xiang Sun, et al. (2004) *Acta Crystallogr. Sect.E: Struct. Rep. Online*. **60,** o 1694.

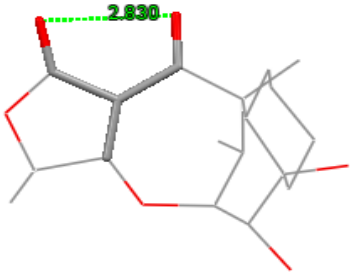
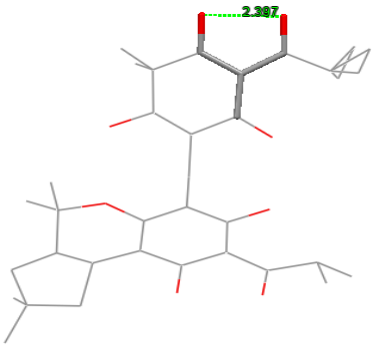
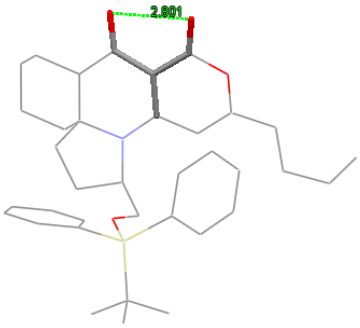
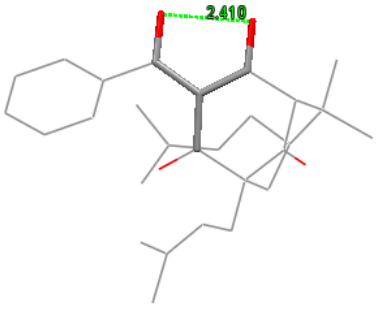
65.	2.869	5.71 8.38 -177.54 -168.88	 ***Ethyl1-(2,6-dimethylphenyl)-2,4-dio xo-1,2,3,4-tetrahydropyrimidine-5-ca rboxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 11.445(0), α 90.00 ***b*** 12.764(0), β 114.51(0) ***c*** 11.105(0), γ 90.00 ***Temperature(K):*** 273 ***Density(g/cm3):*** 1.297	M. E. Light, et al (2005) *Private Communication.*
66.	2.794	-3.26 1.28 173.36 -175.42	 ***(rac)-1-Cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7-(3'-methyla minopiperidin-1'-yl)-4-oxoquinol ine-3-carboxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 11.448(1), α 90.00 ***b*** 15.902(1), β 90.88(1) ***c*** 10.888(1), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.366	Y. Nawata, et al. (1993) *Anal. Sci.* **9,** 565.
67.	2.813	6.96 19.82 -172.04 -161.16	 ***8-Ethyl-5,8-dihydro-5-oxo-2-(1-piper azinyl)-pyrido(2,3-d)pyrimidine-6-ca rboxylic acid***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 8.584(1), α 94.87(1) ***b*** 12.571(1), β 113.93(1) ***c*** 8.519(1), γ 88.61(1) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.418	I. Fonseca, et al (1986) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **42,** 1618.
68.	2.523	-0.78 -0.17 178.60 -179.62	 ***(-)-Pseudoplacodiolic acid***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 9.281(3) , α90.00 ***b*** 18.357(6), β 90.00 ***c*** 10.500(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.397	S. Huneck, et al. (1981) *Tetrahedron Lett.* **22,** 351.

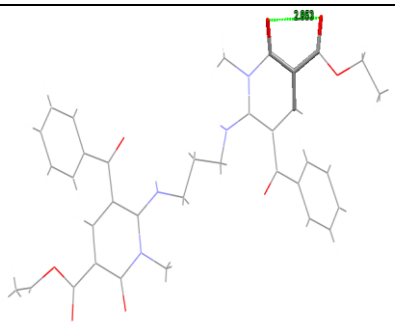
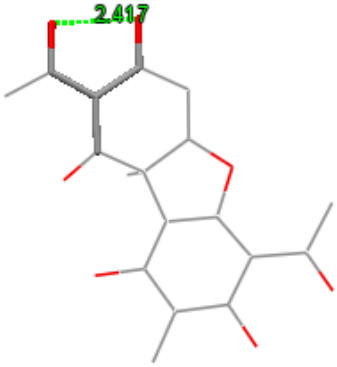
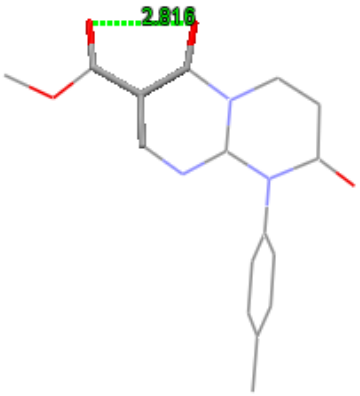
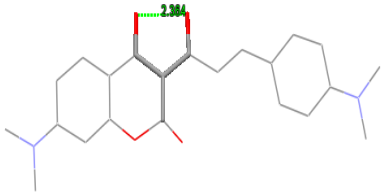
69.	2.777	-4.95 -1.13 172.94 -179.08	 ***Cinnamyl-8-methoxy-2-oxo-2H-chromene-3-carboxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 19.226(4), α 90.00 ***b*** 9.548(1), β 90.97(3) ***c*** 9.005(1), γ 90.00 ***Temperature(K):*** 296 ***Density(g/cm3):*** 1.352	Cui-Lian Xu, (2009) *Acta Crystallogr, Sect.E: Struct. Rep. Online.* **65,** o 2817.
70.	2.763	-7.53 -17.95 173.88 160.72	 ***10-Ethyl-3-methyl-8-methyl-4-oxo-4 H-thiino(2,3-b)indolizine-3,10-dicarboxylate***	***Space Group:*** P21/a ***Cell parameter:*** ***a*** 8.812(2), α 90.00 ***b*** 18.792(2), β 111.45(1) ***c*** 10.146(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.467	A. Kakehi, (2000) *Heterocycles.* **52,** 215.
71.	2.796	-4.41 -14.62 173.32 167.63	 ***(-)-7-((7S)-7-Amino-5-azaspiro(2.4)hept-5-yl)-8-chloro-6-fluoro-1-((1R,2S)-2-fluorocyclopropyl)-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 13.749(4), α 90.00 ***b*** 20.990(5), β 90.00 ***c*** 13.609(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.478	T. Suzuki, et al. (2000) *Anal. Sci.* **16,** 343.
72.	2.957	-6.56 -44.85 175.41 133.13	 ***2-Isopropyl-5-methylcyclohexyl-2-oxo-2H-chromene-3-carboxylate***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 11.080(2), α 90.00 ***b*** 12.408(3), β 90.00 ***c*** 13.532(3), γ 90.00 ***Temperature(K):*** 291 ***Density(g/cm3):*** 1.173	Cui-Lian Xu, et al. (2009) *Acta Crystallogr ,Sect. E: Struct. Rep. Online.* **65,** o2431.
73.	2.819	15.98 2.72 -162.87 -178.41	 ***Ethyl-7-hydroxy-2-oxo-2H-chromene-3-carboxylate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 6.718(1), α 104.06(0) ***b*** 7.264(1), β 95.51(0) ***c*** 12.618(3), γ 99.39(0) ***Temperature(K):*** 298 ***Density(g/cm3):*** 1.436	A. Galdamez, et al. (2011) *J. Chil. Chem .Soc.* **56,** 546.

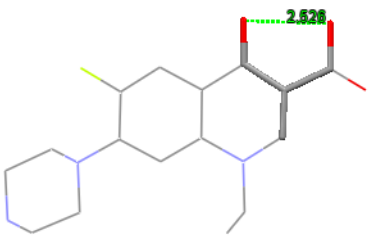
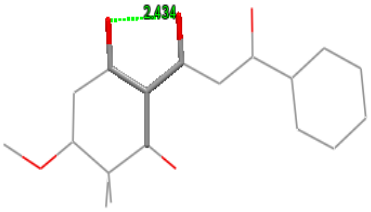
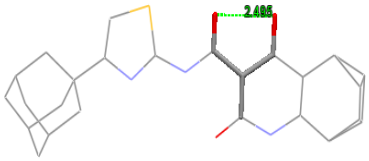
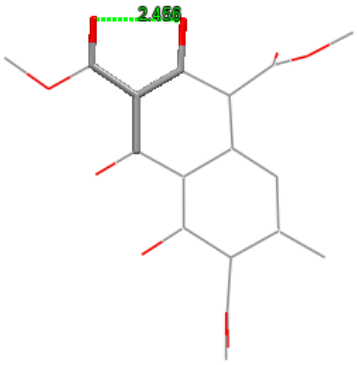
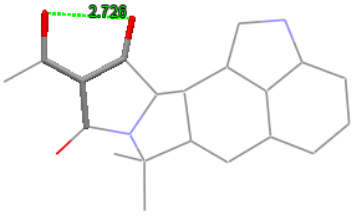
74.	2.387	0.99 -0.72 -179.36 179.63	 ***4-O-((1S)-(-)-Camphanoyl)-2-acetyl-3-hydroxy-4-methyl-5-methoxycyclohexadienone***	***Space Group:*** P21 ***Cell parameter:*** ***a*** 11.881(4), α 90.00 ***b*** 7.377(2), β 113.86(2) ***c*** 12.310(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.321	S. Sato, et al. (1996) *Chem. Lett.*833.
75.	3.129	-0.18 7.40 -177.63 -174.85	 ***1-Ethyl-5-methyl-2-(p-tosyl)-1,2-dihydro-5H-pyrazolo(4,3-c)quinolin-3,4-dione***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 7.527(2), α 80.35(3) ***b*** 9.596(3), β 83.91(2) ***c*** 13.758(4), γ 79.20(2) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.376	I. V. Ukrainets, et al. (2009) *Khim. Get. Soedin. SSSR (Russ.) Chem.Heterocycl. Compd.* 59.
76.	2.808	-8.11 -9.88 170.61 171.41	 ***2-Dehydro-2-methyl-5,8-dioxo-5,8-dihydrofuro(3,2-g)chromen-4-one***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 7.552(3), α 90.00 ***b*** 8.172(1), β 99.29(2) ***c*** 15.624(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.607	A. Yakoubi, et al. (1997) *Acta Crystallogr. Sect.C: Cryst.Struct.Commun.* **53,** 1949.
77.	2.745	-7.72 11.59 174.01 -170.11	 ***5-Isopropenyl-3'-methyl-4,4a',5,9a'-tetrahydro-1'H,3'H-spiro(furan-3,2'-xanthene)-1',2,9'(4'H)-trione***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 6.683(0), α 105.93(0) ***b*** 9.040(0), β 92.70(0) ***c*** 14.350(1), γ 101.49(0) ***Temperature(K):*** 223 ***Density(g/cm3):*** 1.384	J. W. Bode, et al. (2003) *Org. Lett.* **5,** 395.
78.	2.820	-1.35 0.24 179.72 179.16	 ***Methyl-1-benzyl-5-(((1-benzyl-4-oxo-5-((trifluoroacetyl)amino)-1,4-dihydropyridin-3-yl)carbonyl)amino)-4-oxo-1,4-dihydropyridine-3-carboxylate***	***Space Group:*** P21 ***Cell parameter:*** ***a*** 4.742, α 90.00 ***b*** 25.691, β 90.00 ***c*** 12.212, γ 90.00 ***Temperature(K):*** 173 ***Density(g/cm3):*** 1.470	Changliang Ren, et al. (2011) *J .Am. Chem. Soc.* **133,** 13930.

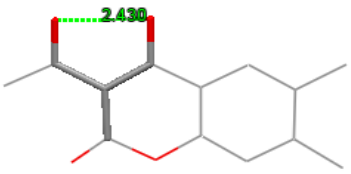
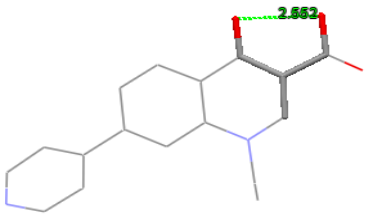
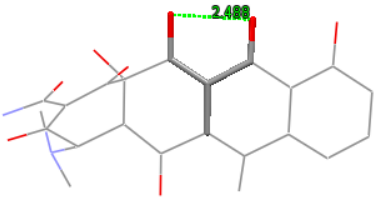
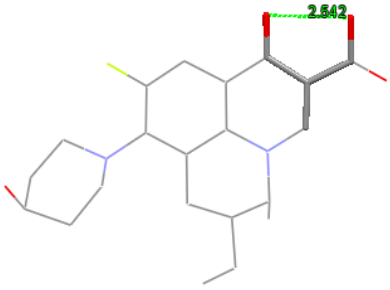
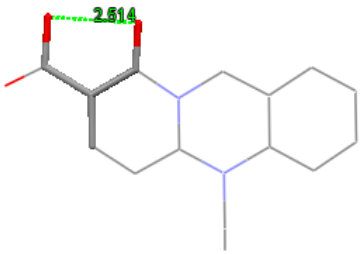
79.	2.524	0.98 -0.35 -178.15 178.79	 ***8-Ethyl-5,8-dihydro-5-oxo-2-(1-pyrrolidinyl)pyrido(2,3-d)pyrimidine-6-carboxylic acid***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 7.123(1), α 103.33(1) ***b*** 10.149(1), β 109.79(2) ***c*** 10.223(2), γ 92.43(2) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.427	H. Song, et al. (1998) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **54,** 1915.
80.	2.815	2.57 -9.10 -178.13 171.62	 ***Succinimidyl-7-methoxy-2-oxo-2H-chromene-3-carboxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 8.416(0), α 90.00 ***b*** 19.430(1), β 94.48(0 ***c*** 8.552(0), γ 90.00 ***Temperature(K):*** 150 ***Density(g/cm3):*** 1.511	G.R.Bardajee,et al. (2007) *Acta Crystallogr.,Sect. E:Struct.Rep.Online* ,**63,**o1513
81.	2.776	-6.01 -5.63 168.07 -179.59	 ***Ethyl-8aR-9-methyl-4-oxo-6,7,8,8a-tetrahydro-1H,9H-pyrimido(1',2':1,2)pyrido(3,2-b)indole-3-carboxylate.***	***Space Group:*** P21/c ***Cell parameterl:*** ***a*** 12.843(6), α 90.00 ***b*** 10.935(4), β 114.98(3) ***c*** 12.860(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.328	I. Hermecz, et al. (1991) *J. Heterocycl. Chem.* **28,** 1405.
82.	2.450	6.92 -2.98 -175.96 179.91	 ***11a-Hydroxy-12a-dehydroxy-6-thiatetracycline***	***Space Group:*** P21/c ***Cell:*** ***a*** 12.049(1), α 90.00 ***b*** 10.698(1), β 93.46(1) ***c*** 17.240(2), γ 90.00 ***Temperature(K):*** 120 ***Density(g/cm3):*** 1.469	R. Prewo, et al. (1980) *J. Am .Chem. Soc.* **102,** 7021.
83.	2.523	9.76 0.22 -161.06 171.08	 ***Oxytetracyclinehydrochloride***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 11.190, α 90.00 ***b*** 12.490, β 90.00 ***c*** 15.680, γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.505	H. Cid-Dresdner, et al. (1965) *Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem.* **121,** 170.

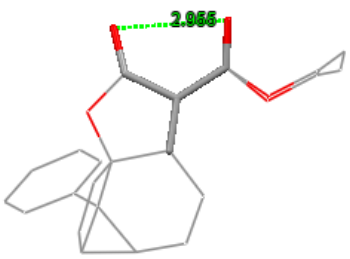
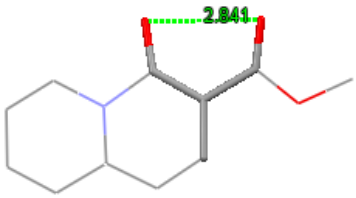
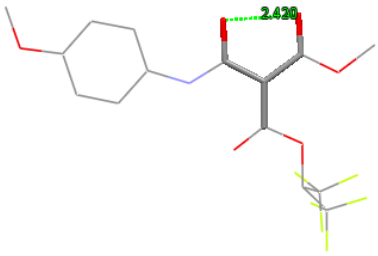
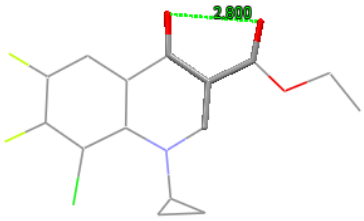
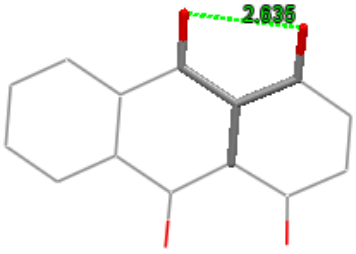
84.	2.432	2.85 -0.91 -176.55 178.46	 ***rac-4-Acetyl-2,6-dibenzyl-5-hydroxy-2,6-dimethyl-4-cyclohexen-1,3-dione***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 10.561(3, α 98.74(0) ***b*** 13.317(5), β 98.87(0) ***c*** 7.596(2), γ 108.14(0) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.276	R. Stomberg, et al. (1996) *Z. Kristallogr.* **211,** 491.
85.	2.505	-2.04 -2.21 179.60 176.17	 ***8-(3-Ammonio-1-pyrrolidinyl)-1-cyclopropyl-7-fluoro-9-methyl-4-oxo-4Hquinolizine-3-carboxylic acid***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 10.319(2), α 90.00 ***b*** 29.785(8), β 90.00 ***c*** 6.778(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.364	Qun Li, et al. (1996) *J. Med. Chem.* **39,** 3070.
86.	2.841	9.23 -6.17 -171.84 174.92	 ***Ethyl3,3-bis(t-butoxycarbonyl)-4,5-difluoro-1-methyl-7-oxo-2,3-dihydro-1H,7H-pyrido(3,2,1-ij)cinnoline-8-carboxylate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 10.788(1), α104.67(0) ***b*** 14.720(7), β 95.50(0) ***c*** 8.531(0), γ 97.93(0) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.313	D. Barrett, et al. (1996) *Bull. Chem. Soc. Jpn.* **69,** 1371.
87.	2.775	-16.67 -16.91 163.81 162.60	 ***16,16-Dimethyl-11-vinyl-8-aza-D-gomogone-1,3,5(10),9(11),13-pentaene-12,17a-dione***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 8.857(3), α 93.89(2) ***b*** 9.821(3), β 100.92(3) ***c*** 12.547(3), γ 112.91(2) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.088	O. V. Gulyakevich, et al.(1996) *Khim. Get. Soedin SSSR(Russ.) Chem. Heterocycl. Compd.* 965.

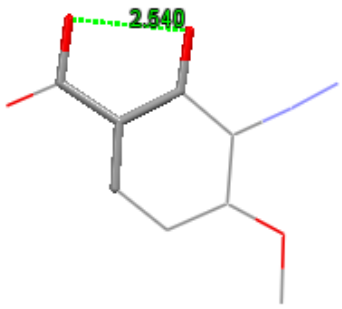
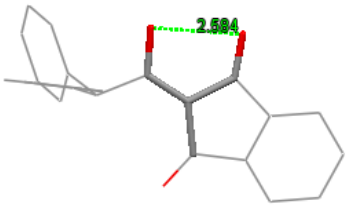
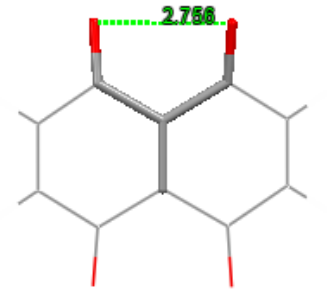
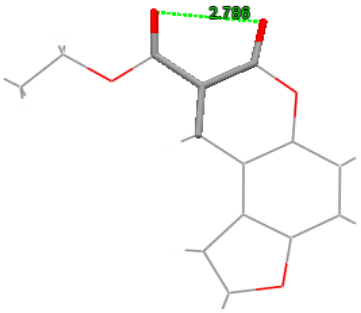
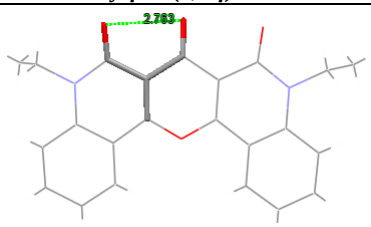
88.	2.830	-4.67 -10.48 177.67 166.52	 ***Dihydrotetrodecamycin***	***Space Group:*** P61 ***Cell parameter:*** ***a*** 16.788(2), α 90.00 ***b*** 16.788(2), β 90.00 ***c*** 11.742(2), γ 120.00 ***R-Factor (%):*** 6.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.176	T. Tsuchida, et al (1995) *J.Antibiot.* **48,** 1110.
89.	2.397	-3.56 1.34 176.81 -179.05	 ***Hyperbrasilol A***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 5.989(0), α 90.00 ***b*** 21.209(1), β 90.00 ***c*** 25.613(1), γ 90.00 ***Temperature(K):*** 173 ***Density(g/cm3):*** 1.194	H. Stoeckli-Evans, et al. (2007) *Private Communication.*
90.	2.801	0.28 13.90 -173.02 -172.84	 ***11-n-butyl-1-(((t-butyl(diphenyl)silyl) oxy)methyl)-2,3,5,6,7,7a-hexahydro-1H,9H-pyran[4,3-b]pyrrolo[2,1-j]quinoline-8,9(4H)-dione***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 8.302(0), α 90.00 ***b*** 14.633(1), β 90.00 ***c*** 26.376(2), γ 90.00 ***Temperature(K):*** 173 ***Density(g/cm3):*** 1.210	J. J. Swidorski, et al. (2006) *Org. Lett.* **8,** 777.
91.	2.410	6.94 -1.94 -164.02 169.45	 ***rel-(1R,5R,7R)-3-Benzoyl-4-hydroxy-6,6-dimethyl-1,7-bis(3-methylbut-2-enyl)bicyclo(3.3.1)non-3-ene-2,9-dione***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 8.998(0), α 90.00 ***b*** 14.459(0), β 90.00 ***c*** 18.432(0), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.204	F. T. Martins, et al. (2008) *Helv. Chim. Acta.* **91,** 1313.

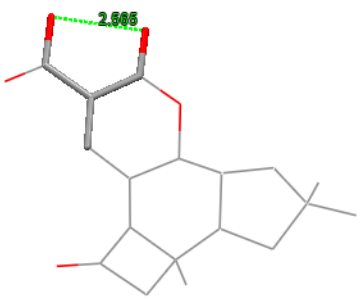
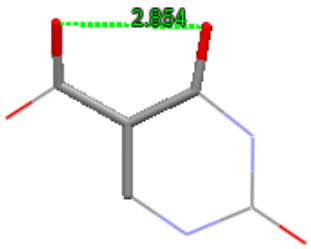
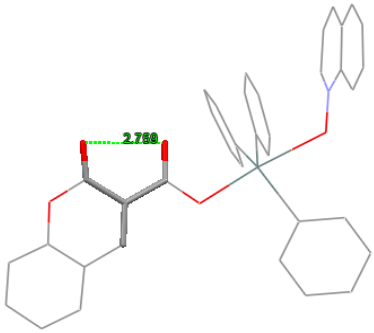
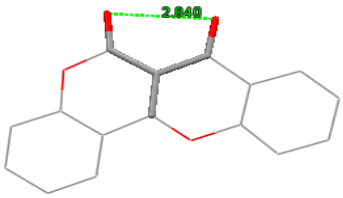
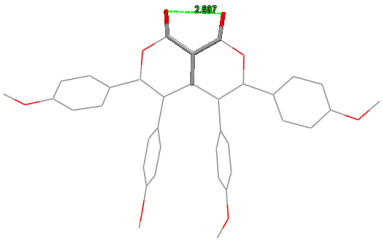
92.	2.853	1.34 -15.32 -179.37 165.39	 ***Diethyl-6,6'-(propane-1,3-diyldiimino)bis(5-benzoyl-1-methyl-2-oxo-1,2-dihydropyridine-3-carboxylate)***	***Space Group:*** Pc ***Cell parameter:*** ***a*** 12.210(0), α 90.00 ***b*** 11.414(0), β 108.73(0) ***c*** 12.072(0), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.335	V. N. Britsun, et al. (2009) *Zh. Org. Khim. (Russ.) Russ. J. Org. Chem.* **45,** 1837.
93.	2.417	3.99 -5.35 -179.91 178.51	 ***Usnic acid***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 19.014(4), α 90.00 ***b*** 20.294(5), β 90.00 ***c*** 8.012(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.479	U. Behrens, et al. (1976) *Cryst. Struct. Commun.* **5,** 51.
94.	2.816	0.08 4.20 -178.89 -176.79	 ***Methyl-1-(4-methylphenyl)-2,6-dioxo-1,6-dihydro-2H-pyrimido[1,2-a]pyrimidine-7-carboxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 14.129(0), α 90.00 ***b*** 6.496(0), β 96.81(0) ***c*** 15.032(1), γ 90.00 ***Temperature(K):*** 170 ***Density(g/cm3):*** 1.509	S. Grosjean, et al. (2010) *Tetrahedron.* **6,** 9912.
95.	2.364	-3.99 3.94 177.00 -177.08	 ***7-(Dimethylamino)-3-(3-(4-(dimethylamino)phenyl)acryloyl)-4-hydroxy-2Hchromen-2-one***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 5.734(5), α 90.00 ***b*** 8.583(8), β 90.00 ***c*** 38.350(30), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.332	Jiun-Han Lin, et al. (2012) *Tetrahedron. Lett.* **53,** 778.

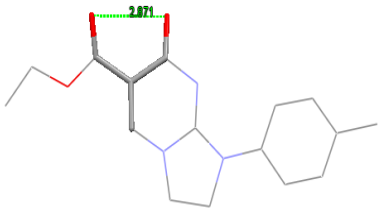
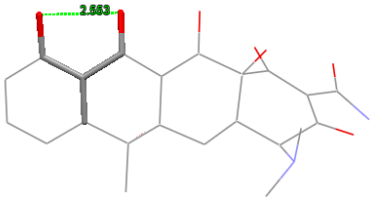
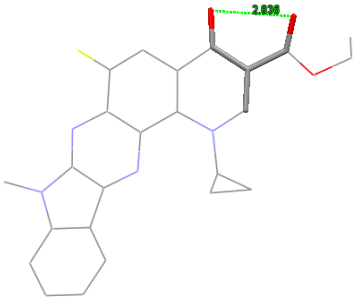
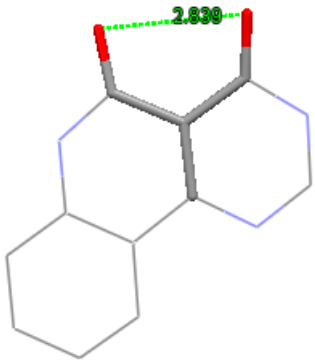
96.	2.526	-2.42 0.53 178.55 179.58	 ***Norfloxacin***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 4.324(1), α 78.51(1) ***b*** 9.635(1), β 87.12(1) ***c*** 18.089(1), γ 80.57(1) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.456	S. Basavoju, et al. (2006) *Cryst. Growth. Des.* **6,** 2699.
97.	2.434	2.07 -3.04 -177.43 176.43	 ***1,2-Dihydro-5-hydroxy-6-(γ-hydroxy -α-oxo-cinnamyl)-2,2-dimethyl-3-me thoxy-1-oxo-benzene.***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 9.976(3), α 91.85(2) ***b*** 10.246(2), β 91.58(2) ***c*** 8.061(2), γ 110.18(2) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.352	M. Nishizawa, et al. (1991) *Tetrahedron. Lett* **32,** 211.
98.	2.495	3.52 -4.53 -179.93 178.81	 ***N-(4-(1-Adamantyl)-1,3-thiazol-2-yl) -4-hydroxy-2-oxo-1,2,5,6,7,8-hexahy droquinoline-3-carboxamide***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 6.498(1), α 71.92(2) ***b*** 15.476(4), β 89.58(2) ***c*** 22.411(6), γ 88.24(2) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.302	I. V. Ukrainets, et al. (2006) *Khim. Get. Soedin. SSSR (Russ.) Chem.Heterocycl. Compd.*,874.
99.	2.456	-7.56 1.04 174.78 178.82	 ***2,5-dihydroxy-1,3,6,-tris(methoxycar bonyl)-7-methyl-4-oxo-1,4,6,7,8,8ah exahydronaphthalene***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 6.839(1), α 90.00 ***b*** 13.943(3), β 97.94(3) ***c*** 18.082(4), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.433	J. K. F. Geirsson, et al. (2001) *Synlett.* 664.
100.	2.726	2.92 -2.66 -172.83 173.73	 ***α–Cyclopiazonic acid***	***Space Group:*** P43212 ***Cell parameter:*** ***a*** 10.406(1), α 90.00 ***b*** 10.406(1), β 90.00 ***c*** 61.549(14), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.341	P. H. van Rooyen, et al (1992) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **48,** 551.

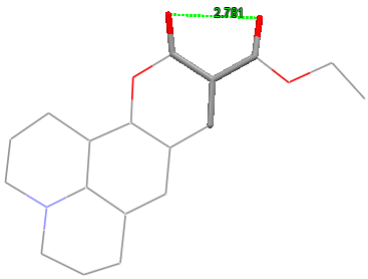
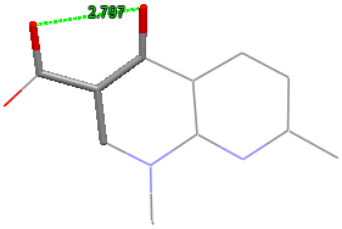
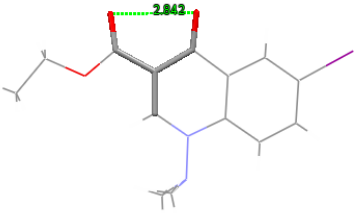
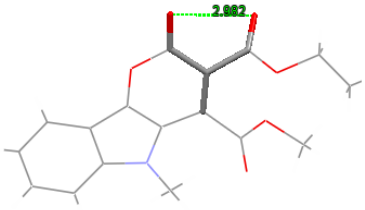
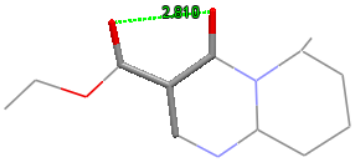
101.	2.430	-0.22 -1.47 -179.98 178.31	 ***3-(1-Hydroxyethylidene)-6,7-dimethyl-2H-chromene-2,4(3H)-dione***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 3.949(0), α 90.00 ***b*** 12.136(1), β 90.56(0) ***c*** 22.101(2), γ 90.00 ***Temperature(K):*** 100 ***Density(g/cm3):*** 1.456	M. Asad, et al. (2010) *Acta Crystallogr. Sect.E: Struct. Rep. Online*. **66,** o 3129.
102.	2.552	-2.44 0.49 177.32 -179.28	 ***1-Ethyl-1,4-dihydro-4-oxo-7-(4-pyridyl)quinoline-3-carboxylic acid***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 8.153, α 73.57 ***b*** 8.960, β 82.87 ***c*** 10.443, γ 74.41 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.389	R. E. Marsh, et al. (2005) *Acta Crystallogr. Sect.B: Struct. Sci.* **61,** 359.
103.	2.488	0.77 -6.48 -176.08 170.53	 ***4-Dimethylamino-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12apentahydroxy-6-methylene-1,11-dioxo-2-naphthacenecarboxamide Hydrobromide***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 9.580(1), α 90.00 ***b*** 12.147(2), β 90.00 ***c*** 18.735(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.594	M. A. A. F. de C. T. Carrondo, et al. (1994) *Struct. Chem.* **5,** 73.
104	2.542	-0.14 5.34 177.80 -172.64	 ***6-Ethyl-9-fluoro-6,7-dihydro-8-(4-hydroxy-1-piperidino)-5-methyl-1-oxo-1H,5H-benzo(i,j)quinolizine-2-carboxylic acid***	***Space Group:*** Pna21 ***Cell parameter:*** ***a*** 15.387(2), α 90.00 ***b*** 7.705(2), β 90.00 ***c*** 16.013(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.359	K. Hashimoto, et al. (1995) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **51,** 519.
105.	2.514	3.17 0.81 -179.38 -176.67	 ***5-Ethyl-8-carboxy-9-oxo-11-methylpyrido(2,1-b)quinazoline***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 9.775(1), α 90.00 ***b*** 15.868(1), β 113.50(1) ***c*** 9.799(1), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.355	Rajnikant, et al. (2000) *Kristallografiya (Russ.) Crystallogr. Rep.* **45,** 669.

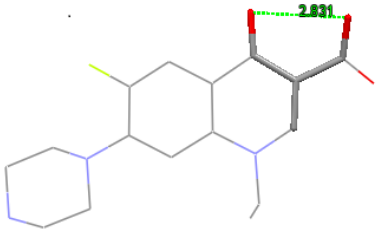
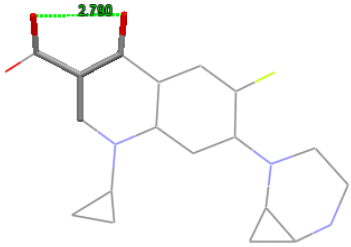
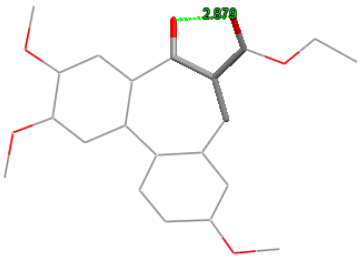
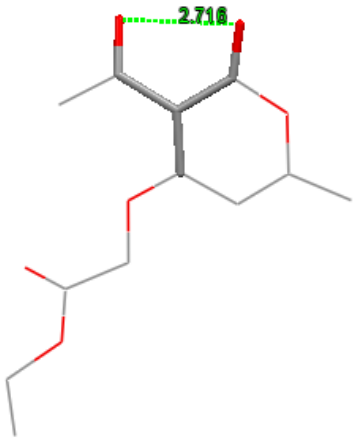
106.	2.955	2.32 14.26 -178.02 -165.32	 ***Ethyl-3-oxo-9-phenyl-2-oxatetracyclo(7.3.0.01,5.08,10)dodeca-4,6,11-triene-4-carboxylate***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 7.409(0), α 90.00 ***b*** 10.581(0), β 90.49(0) ***c*** 20.234(0), γ 90.00 ***Temperature(K):*** 213 ***Density(g/cm3):*** 1.342	V. Nair, et al. (2000) *J. Chem. Soc. Perkin Trans.* ***1*** , 3795.
107.	2.841	1.90 5.46 -178.26 -174.38	 ***3-(Methoxycarbonyl)-4H-quinolizone monohydrate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 6.905(2), α 70.63(2) ***b*** 7.789(2), β 75.80(2) ***c*** 10.458(2), γ 74.48(2) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.459	G. R. Newkome, et al. (1988) *Heterocycles.* **27,** 385.
108.	2.420	3.88 -6.78 -176.34 173.45	 ***1,1,1,3,3,3-Hexafluoroisopropyl(E)-2-(methoxycarbonyl)-3-hydroxy-3-(pmethoxyphenylamino)prop-2-enoate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 14.934(6), α 90.00 ***b*** 7.403(4), β 96.23(3) ***c*** 16.014(4), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.575	Yi Xiong Lei, et al. (2001) *J .Org. Chem.* **66,** 8379.
109.	2.800	1.27 8.25 177.62 -168.07	 ***Ethyl8-chloro-1-cyclopropyl-6,7-difluoro-4-oxo-1,4-dihydroquinoline-3-Carboxylate***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 11.336(2), α 90.00 ***b*** 7.744(1), β 95.40(3) ***c*** 16.157(3), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.542	Hong-shun Sun, et al. (2011) *Acta Crystallogr. Sect.E: Struct. Rep Online* , **67,** o 2974.
110.	2.635	7.37 -1.61 -175.62 -178.66	 ***1,4,9,10-anthracenetetronide***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 11.022(5), α 90.00 ***b*** 13.924(3), β 110.99(2) ***c*** 12.365(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.659	H. Asahi, et al (1994) *Chem. Mater.* **6,** 1875.

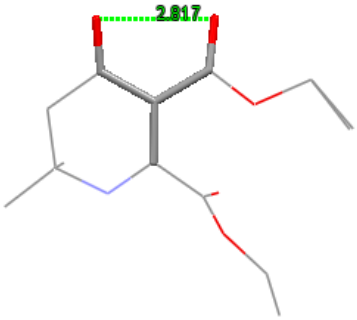
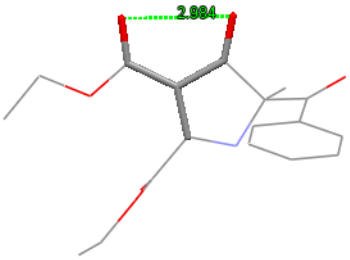
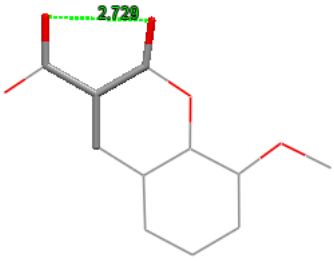
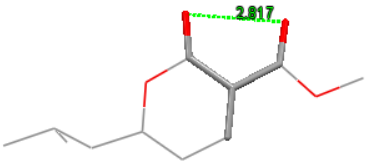
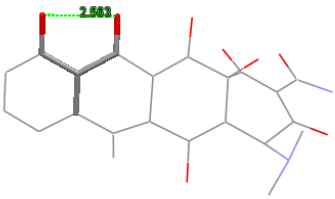
111.	2.540	-0.00 -0.00 180.00 180.00	 ***6-Diazo-5-methoxycyclohexa-2,4-die none-2-carboxylic acid***	***Space Group:*** P21 ***Cell parameter:*** ***a*** 7.746(2), α 90.00 ***b*** 5.919(2), β 98.98(2) ***c*** 9.111(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.563	J. N. Mc Guire, et al. (1995) *J .Antibiot.* **48,** 516.
112.	2.584	-1.59 0.81 -179.87 179.44	 ***2-(1-Hydroxy-2,2-diphenylethylidene)-1H-indene-1,3(2H)-dione***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 10.459(2), α 90.00 ***b*** 12.354(2), β 96.67(3) ***c*** 13.290(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.326	K. K. Palkina, et al. (2006) *Zh .Neorg. Khim. (Russ.) Russ.J.Inorg.Che m.* **51,** 1852.
113.	2.756	14.83 14.97 -165.53 -164.66	 ***Naphthalene-1,4,5,8-tetrone***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 6.510(4), α 90.00 ***b*** 13.220(5), β 110.00(50) ***c*** 4.855(4), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.591	F. H. Herbstein, et al. (1982) *Acta Crystallogr. Sect.B: Struct. Crystallogr. Cryst. Chem.* **38,** 3123.
114.	2.786	-14.05 -3.70 167.56 174.71	 ***3-Carbethoxy-furo(3,2-f)coumarin***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 16.952(10), α 90.00 ***b*** 16.160(10), β 92.80(10) ***c*** 4.330(3), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.447	G. Bravic, et al. (1978) *Cryst. Struct. Commun.* **7,** 633.
115.	2.763	-6.32 -7.32 175.64 170.69	 ***5,9-Diethyl-6,7,8-trioxodiquinolino(3,4-b;3',4'-e)-4H-pyran***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 12.555(3), α 110.43 ***b*** 12.617(3), β 95.82 ***c*** 13.630(3), γ 114.32 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.453	I. V. Ukrainets, et al. (2000) *Khim. Get. Soedin. SSSR (Russ.) Chem.Heterocycl. Compd.* 516.

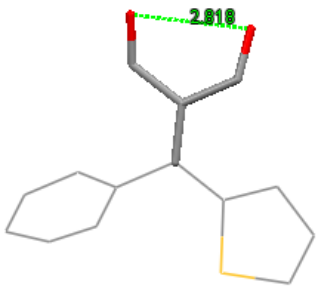
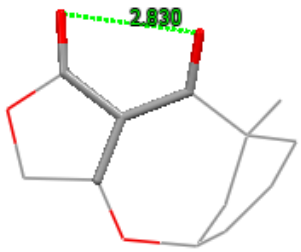
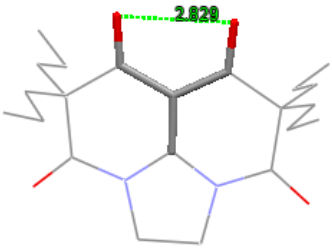
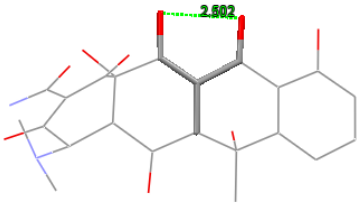
116.	2.565	2.03 2.59 179.26 -174.26	 ***Lentinellic acid***	***Space Group:*** P212121 ***Cellparameter: a*** 6.506(1), α 90.00 ***b*** 10.807(3), β 90.00 ***c*** 22.706(5), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.316	A. Stark, (1988) *Z. Naturforsch. C: J. Biosci.* **43,** 177.
117.	2.854	-12.19 -2.16 166.66 178.97	 ***2,4-dioxo-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate dihydrate***	***Space Group:*** Pbnb ***Cell parameter: a*** 7.486(0), α 90.00 ***b*** 12.798(0), β 90.00 ***c*** 26.457(1), γ 90.00 ***Temperature(K):*** 298 ***Density(g/cm3):*** 1.589	G. Portalone, et al. (2009) *J. Chem. Cryst.* **39,** 193.
118.	2.759	-2.78 -10.52 176.96 169.75	 ***(Coumarin-3-carboxylato)-quinoline -N-oxide-triphenyl-tin***	***Space Group:*** P-1 ***Cell parameter: a*** 10.410(0), α 111.75(0) ***b*** 1.520(1), β 95.76(0) ***c*** 13.725(2), γ 98.70(0) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.526	Seik Weng, et al. (1999) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **55,** 523.
119.	2.840	0.00 -0.00 180.00 -180.00	 ***6H,7H-(1)Benzopyrano(4,3-b)(1)benzopyran-6,7-dione***	***Space Group:*** Pnam ***Cell parameter: a*** 22.630(9), α 90.00 ***b*** 7.892(1), β 90.00 ***c*** 6.484(1), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.516	E. R. Di Paolo, et al. (1989) *Helv. Chim. Acta.* **72,** 1455.
120.	2.697	-5.57 2.49 175.43 -178.49	 ***3,4,5,6-tetrakis(4-Methoxyphenyl)pyrano(3,4-c)pyran-1,8-dione***	***Space Group:*** P-1 ***Cell parameter: a*** 13.355(0), α 100.45(1) ***b*** 14.968(2), β 93.70(0) ***c*** 16.467(2), γ 115.15(1) ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.351	F. V. Singh, et al. (2007) *Tetrahedron. Lett.* **48,** 8998.

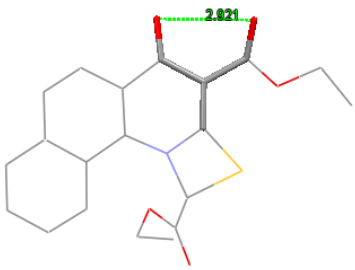
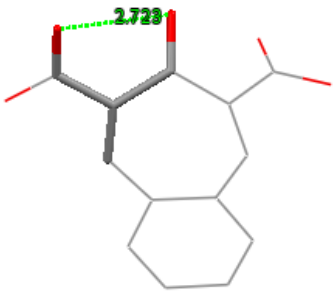
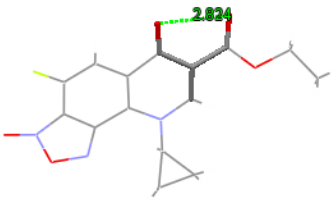
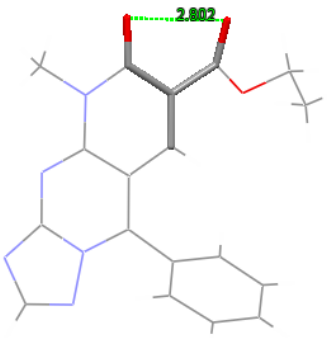
121.	2.871	-14.46 -6.77 163.39 175.37	 ***Ethyl-1-(4-methylphenyl)-7(1H)-oxo-2,3-dihyroimidazo(1,2-a)pyrimidine-6-Carboxylate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 6.880(1), α 101.08(3) ***b*** 7.417(1), β 95.77(3) ***c*** 5.056(3), γ 104.60(3) ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.380	D.Matosiuk, (2003) *J.Heterocycl.Chem.* ,**40,**93
122.	2.553	-0.53 -13.33 179.60 166.54	 ***Tetracycline***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 12.084(5), α 90.00 ***b*** 21.580(10), β 90.00 ***c*** 9.561(5), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.472	M. R. Caira, et al. (1977) *Acta Crystallogr. Sect.B: Struct. Crystallogr. Cryst. Chem.* **33,** 1171.
123.	2.836	4.95 12.80 -178.26 -164.00	 ***Ethyl-1-cyclopropyl-6-fluoro-8-methyl-4-oxo-4,8-dihydro-1H-indolo(2,3-b)pyrido(2,3-f)quinoxaline-3-carboxylate***	***Space Group:*** I2/a ***Cell parameter:*** ***a*** 20.473(1), α 90.00 ***b*** 9.044(0), β 99.83(0) ***c*** 21.311(1), γ 90.00 ***Temperature(K):*** 203 ***Density(g/cm3):*** 1.471	E. S. Abu-Sheaib, et al. (2008) *Monatsh.Chem.* **139,** 1061.
124.	2.839	7.24 5.38 -174.25 -173.13	 ***Pyrimido-(5,4-c)quinoline-4,5(3H,6H)-dione***	***Space Group:*** Pn21a ***Cell parameter:*** ***a*** 6.835(0) , α 90.00 ***b*** 12.827(1), β 90.00 ***c*** 12.332(2), γ 90.00 ***Temperature(K):*** 298 ***Density(g/cm3):*** 1.593	S. Parsons, (2004) *Private Communication.*

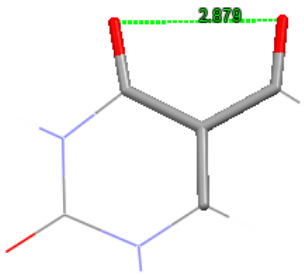
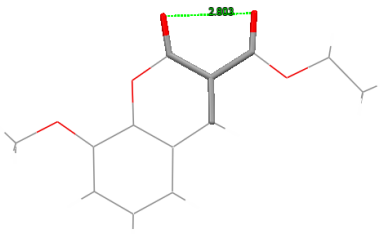
125.	2.781	-3.56 -13.08 178.31 165.01	 ***Ethyl-2,3,6,7-tetrahydro-11-oxo-1H, 5H,11H-(1)benzopyrano(6,7,8-ij)quinolizine-10-carboxylate***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 8.532(1), α 90.00 ***b*** 14.946(1), β 95.24(1) ***c*** 12.022(1), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.363	Boon-Chuan Yip, Hoong-Kun Fun, et al. (1995) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **51,** 956.
126.	2.797	2.33 0.77 -179.84 -176.95	 ***Nalidixate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 10.558(3), α 110.16(5) ***b*** 11.351(5), β 99.73(3) ***c*** 14.803(10), γ 110.77(2) ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.767	Sung Sil Lee, (1995) *Inorg. Chim. Acta.* **239,** 133.
127.	2.842	6.10 7.08 -174.24 -172.58	 ***Ethyl-1-(dimethylamino)-6-iodo-4-oxo-1,4-dihydroquinoline-3-Carboxylate.***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 10.844(0), α 90.00 ***b*** 9.966(0) β 108.44(0) ***c*** 14.448(0), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.732	J. Bauer, et al. (2009) *Acta Crystallogr. ect.C: Cryst. Struct. Commun.* **65,** o 512.
128.	2.982	-2.92 -55.54 -179.45 120.95	 ***7,8-Benzo-3-ethoxycarbonyl-2-methoxycarbonyl-9-methyl-9-aza-5-oxabicyclo(4.3.0)nona-1(6),2-dien-4-one***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 10.906(1), α 90.00 ***b*** 7.498(1), β 96.54(1) ***c*** 19.200(1), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.402	A. J. Frew, (1980) *J. Chem. Soc. Perkin Trans. 1* , 1251.
129.	2.810	-2.04 0.08 179.97 178.13	 ***3-(Ethoxycarbonyl)-4-oxo-6-methyl-6,7,8,9-tetrahydrohomopyrimidazole.***	***Space Group:*** A2/a ***Cell parameter:*** ***a*** 10.040(10), α 90.00 ***b*** 16.730(10), β 90.10(50) ***c*** 14.660(20), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.275	K. Sasvari, et al. (1973) *Acta Crystallogr. Sect.B: Struct. Crystallogr. Cryst. Chem.* **29,** 1245.

130.	2.831	-0.08 18.91 -178.23 -162.92	 ***1-Ethyl-6-fluoro-4-oxo-7-(piperazin-4-ium-1-yl)-1,4-dihydro-3-Quinoline carboxylate***	***Space Group:*** P21/c ***Cell parameter: a*** 17.534(1), α 90.00 ***b*** 8.994(0), β 90.41(0) ***c*** 19.919(1), γ 90.00 ***Temperature(K):*** 100 ***Density(g/cm3):*** 1.446	S. Roy, et al (2008) *Cryst. Growth Des.* **8,** 4343.
131.	2.790	-15.15 -0.54 163.46 -179.11	 ***(+-)-7-(2,5-Diazabicyclo[4.1.0]heptan-2-yl)-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid***	***Space Group:*** P-1 ***Cell parameter: a*** 7.308(1), α 111.14(3) ***b*** 10.658(2), β 96.04(3) ***c*** 13.416(3), γ 99.91(3) ***Temperature(K):*** 200 ***Density(g/cm3):*** 1.336	R. R. R. Taylor, et al. (2010) *Tetrahedron.* **66,** 3370.
132.	2.879	41.46 21.11 -137.00 -160.34	 ***Ethyl-2,3,9-trimethoxy-5-oxo-5H-dibenzo[a,c][7]annulene-6-carboxylate***	***Space Group:*** P-1 ***Cell parameter: a*** 7.755(0), α 105.36(0) ***b*** 9.871(0), β 92.52(0) ***c*** 12.140(0), γ 100.28(0) ***Temperature(K):*** 123 ***Density(g/cm3):*** 1.394	K. Hackeloer, et al. (2011) *Eur. J. Org. Chem.* 6314.
133.	2.716	26.10 -2.17 -153.27 177.24	 ***Ethyl-2-(3-acetyl-6-methyl-2-oxo-2H-pyran-4-yloxy)acetate***	***Space Group:*** P-1 ***Cell parameter: a*** 7.826(1), α 77.37(0) ***b*** 8.272(1), β 77.76(0) ***c*** 10.084(1), γ 88.86(0) ***Temperature(K):*** 298 ***Density(g/cm3):*** 1.357	M. Rabnawaz, Et al. (2010) *Acta Crystallogr. Sect.E: Struct. Rep. Online.* **66,** o 397.

134.	2.817	-2.31 -16.77 177.05 163.88	 ***Diethyl-6,6-dimethyl-4-oxo-1,4,5,6-tetrahydropyridine-2,3-dicarboxylate***	***Space Group:*** C2/c ***Cell parameter:*** ***a*** 16.784(1), α 90.00 ***b*** 16.711(1), β 114.78(0) ***c*** 13.025(1), γ 90.00 ***Temperature(K):*** 120 ***Density(g/cm3):*** 1.235	P. V. Novikov, et al. (2004) *Mendeleev Commun.* 310.
135.	2.984	-1.13 3.10 -179.82 -177.97	 ***Diethyl-5-benzoyl-5-methyl-4-oxo-4,5-dihydro-1H-pyrrole-2,3-dicarboxylate***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 8.597(0), α 90.00 ***b*** 11.880(1), β 92.99(0) ***c*** 17.422(1), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.291	G. Guerrini, et al. (2010) *Eur. J. Org. Chem.* 3919.
136.	2.729	2.82 -1.76 -177.22 178.28	 ***8-Methoxy-2-oxo-2H-chromene-3-carboxylic acid***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 5.152(0), α 90.00 ***b*** 19.922(2), β 100.47(0) ***c*** 9.458(1), γ 90.00 ***Temperature(K):*** 296 ***Density(g/cm3):*** 1.532	Xiaochuan Li, et al. (2010) *Z. Kristallogr. New Cryst. Struct.* **225,** 65.
137.	2.917	-2.57 -5.59 -179.49 171.21	 ***Methyl-6-isobutyl-2-oxo-2H-pyran-3-carboxylate***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 9.026(0), α 102.16(0) ***b*** 11.223(1), β 107.43(0) ***c*** 11.744(1), γ 90.06(0) ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.262	Lei Wu, et al. (2011) *Eur. J. Org. Chem.*1099.
138.	2.563	-2.17 -8.06 -177.57 167.30	 ***6-Methylene-5-oxytetracycline***	***Space Group:*** P212121 ***Cell parameter:*** ***a*** 9.472(1), α 90.00 ***b*** 11.921(3), β 90.00 ***c*** 18.945(4), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.487	A. E. Koziol, et al. (1992) *J. Crystallogr. Spectrosc. Res.* **22,** 493.

139.	2.818	-8.66 -18.47 170.90 161.97	 ***Phenyl-2-(thienyl)methylenemalonaldehyde***	***Space Group:*** C2/c ***Cell parameter:*** ***a*** 16.670(20), α 90.00 ***b*** 9.310(10), β 107.80(1) ***c*** 15.880(20), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.372	T. A. Pakkanen, et al. (1987) *Collect. Czech. Chem. Commun.* **52,** 714.
140.	2.830	1.35 15.36 -179.30 -163.79	 ***(1RS,9RS)-9-Methyl-2,5-dioxatricyclo(7.3.1.03,7)trideca-3(7),11-diene-6,8-dione***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 6.537(4), α 90.00 ***b*** 8.520(3), β 95.02(5) ***c*** 18.460(8), γ 90.00 ***Temperature(K):*** 293 ***Density(g/cm3):*** 1.428	F. F. Paintner, et al. (2002) *Synlett.* 1308.
141.	2.829	-1.87 1.31 178.00 -178.57	 ***5,5,8,8-Tetrapropyl-1,2-dihydroimidazo(1,2,3-ij)(1,8)naphthyridine-4,6,7,9(5H,8H)-tetraone***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 10.815(9), α 90.00 ***b*** 21.724(18), β 104.10(1) ***c*** 11.663(10), γ 90.00 ***Temperature(K):*** 273 ***Density(g/cm3):*** 1.151	Guozhong Ye,et al. (2008) *J. Org. Chem.* **73,** 5170.
142.	2.502	8.89 -7.59 -174.82 175.95	 ***Oxytetracycline hydrobromide***	***Space Group:*** C2 ***Cell parameter:*** ***a*** 21.326(4), α 90.00 ***b*** 12.265(2), β 117.00(10) ***c*** 11.213(1), γ 90.00 ***Temperature(K):*** 123 ***Density(g/cm3):*** 1.468	K. H. Jogun, et al. (1976) *Cryst. Struct. Commun.* **5,** 381.

143.	2.921	7.45 17.96 -174.98 -159.55	 ***Diethyl-4-oxo-4H-benzo[h][1,3]thiazeto[3,2-a]quinoline-1,3-dicarboxylate***	***Space Group:*** P21/c ***Cell parameter:*** ***a*** 11.676(2), α 90.00 ***b*** 9.941(1), β 101.91(0) ***c*** 15.266(3), γ 90.00 ***Temperature(K):*** 153 ***Density(g/cm3):*** 1.469	A. Ahmed, et al. (2012) *Heterocycles.* **85,** 123.
144.	2.723	-12.14 -33.23 171.69 142.54	 ***7-Oxo-7H-benzocycloheptene-6,8-dicarboxylic acid***	***Space Group:*** P21/n ***Cell parameter:*** ***a*** 7.191(7), α 90.00 ***b*** 9.912(5) β 95.53(5) ***c*** 14.430(9), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.584	H. W. Thompson, et al. (1996) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **52,** 2372.
145.	2.824	1.06 -16.88 -176.24 160.45	 ***Ethyl-9-cyclopropyl-4-fluoro-6-oxo-6,9-dihydro(1,2,5)oxadiazolo(3,4-h)-quinoline-7-carboxylate 3-oxide***	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 6.907(1), α 81.49(0) ***b*** 9.566(1), β 86.66(0) ***c*** 11.072(1), γ 79.37(0) ***Temperature(K):*** 203 ***Density(g/cm3):*** 1.557	Y. M. Al-Hiari, et al. (2006) *Heterocycles.* **68,** 1163.
146.	2.802	-3.94 18.85 176.44 -161.52	 ***Ethyl-9-methyl-6-oxo-5-phenyl-5,6-dihydropyrido(2,3-d)(1,2,4)triazolo(1,5-a)pyrimidine-7-carboxylate***	***Space Group:*** Pbca ***Cell parameter:*** ***a*** 10.155(0), α 90.00 ***b*** 16.904(1), β 90.00 ***c*** 19.354(2), γ 90.00 ***Temperature(K):*** 295 ***Density(g/cm3):*** 1.397	V. N. Britsun, et al. (2008) *Khim. Get. Soedin.,SSSR (Russ.) Chem.Heterocycl. Compd.* 1660.

147.	2.879	0.00 -0.00 -180.00 180.00	 ***2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carbaldehyde***	***Space Group:*** Cmc21 ***Cell parameter:*** ***a*** 6.284(0), α 90.00 ***b*** 6.705(0), β 90.00 ***c*** 12.830(0), γ 90.00 ***Temperature(K):*** 298 ***Density(g/cm3):*** 1.721	G. Portalone, et al. (2007) *Acta Crystallogr. Sect.C: Cryst. Struct. Commun.* **63,** o 650.
148.	2.803	-5.00 -0.90 175.98 178.11	 ***Ethyl-8-methoxy-2-oxo-2H-chromene-3-carboxylate*.**	***Space Group:*** P-1 ***Cell parameter:*** ***a*** 9.598(1), α 71.30(3) ***b*** 10.686(2), β 70.43(3) ***c*** 10.693(2), γ 88.99(3) ***Temperature(K):*** 291 ***Density(g/cm3):*** 1.359	Yi-feng Sun,et al. (2008) *Yingxiang Kexue Yu Guang Huaxue (Chin.) Imiaging Science and Photochemistry.* **26,** 393.

Computational Details

Geometry optimization of all the compounds studied here are carried out at the DFT level using Gaussian09 quantum chemistry package.[1] We employed M06-2X functional in association with 6-311+g(d,p) basis set for all the calculations since it is proved to perform superior for main group thermochemistry and non-covalent interactions.[2-4] Optimized geometries show good agreement with crystal structures, Table S3. The true minimum nature of the optimized structures were verified by analyzing the vibrational frequencies. The topological features of the optimized geometries were analyzed using Bader's "Quantum Theory of Atoms in Molecules" (QTAIM) implemented in AIMALL package.[5-6] The wavefunction files required for QTAIM analysis were generated from M06-2X/6-311+g(d,p) calculations. The intramolecular charge transfer interaction between the interacting oxygens are probed using NBO-6 program package.[7]

Table S3. Selected geometric parameters from the crystal structure are given. DFT-optimized values are given in the bracket. [a]χ is the torsion angles between O_1-C_4-C_{11}-O_2

	compounds	Geometric parameters			
		$O_1\cdots O_2$ (Å)	O_1-C_4-C_3 (°)	C_3-C_{11}-O_2 (°)	$\chi^{[a]}$ (°)
M06-2X/6-311+g(d,p)	**9**	2.847 (2.842)	126.01 (125.88)	125.91 (125.96)	-4.84 (-6.81)
	10	2.580 (2.622)	115.68 (115.63)	115.81 (114.43)	7.26 (18.66)
	11	2.516 (2.627)	115.83 (115.62)	113.71 (114.28)	-1.71 (-20.07)
	12	2.539 (2.629)	115.44 (115.59)	114.51 (114.25)	2.32 (20.193)
wB97XD/6-311+g(d,p)	**9**	2.847 (2.857)	126.01 (126.15)	125.91 (125.99)	-4.84 (1.39)
	10	2.580 (2.617)	115.68 (115.54)	115.81 (114.38)	7.26 (17.96)
	11	2.516 (2.628)	115.83 (115.49)	113.71 (114.13)	-1.71 (-21.38)
	12	2.539 (2.636)	115.44 (115.36)	114.51 (114.00)	2.32 (23.70)
CAM-B3LYP /6-311+g(d,p)	**9**	2.847 (2.850)	126.01 (126.14)	125.91 (125.90)	-4.84 (-5.29)
	10	2.580 (2.623)	115.68 (116.14)	115.81 (114.90)	7.26 (12.59)
	11	2.516 (2.635)	115.83 (116.13)	113.71 (114.74)	-1.71 (16.57)
	12	2.539 (2.638)	115.44 (116.07)	114.51 (114.67)	2.32 (17.59)

Optimized structures

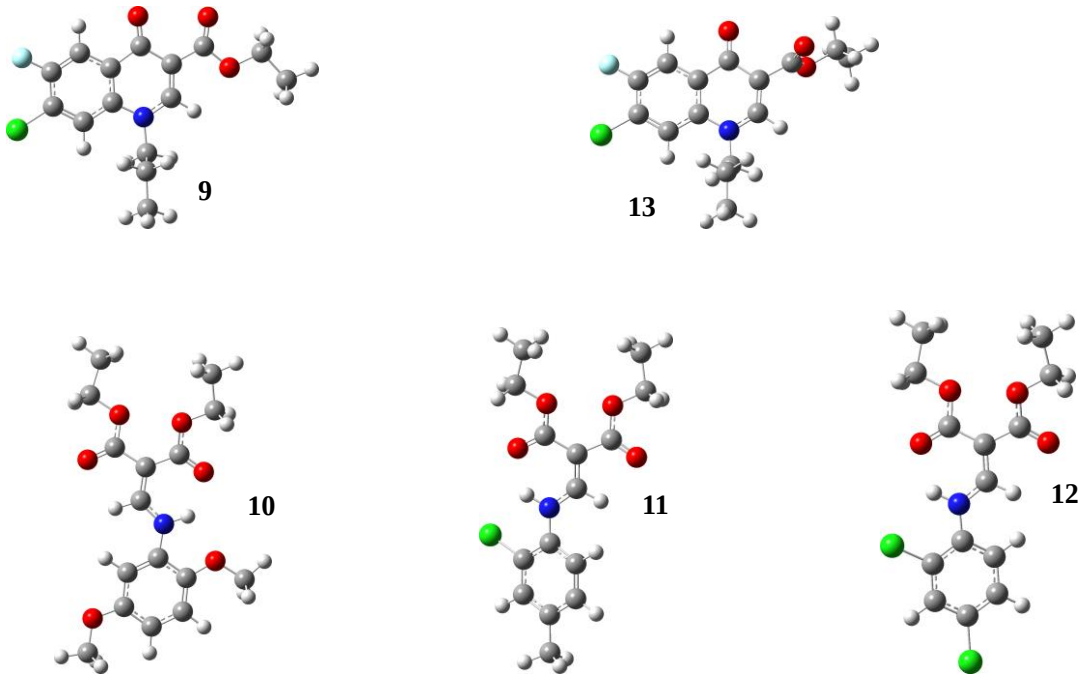


Figure S6. Chemical Structure of compounds **9 -13** optimized at M06-2x/6-311+g(d,p) level of theory

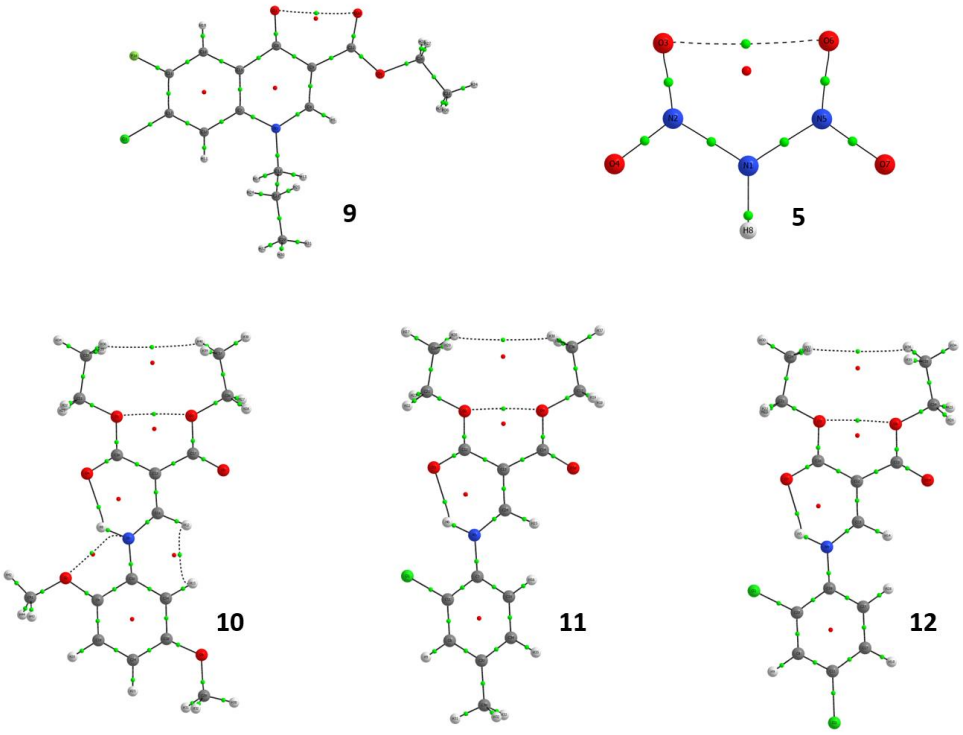


Figure S7. QTAIM topological map of compounds **5** and **9** - **13**.

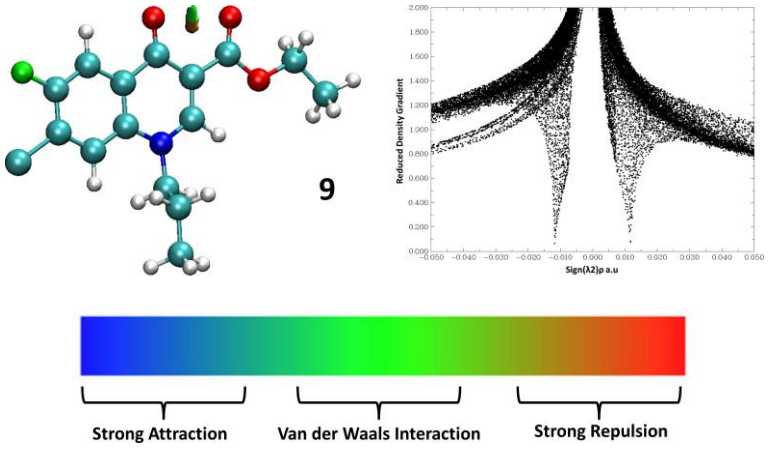


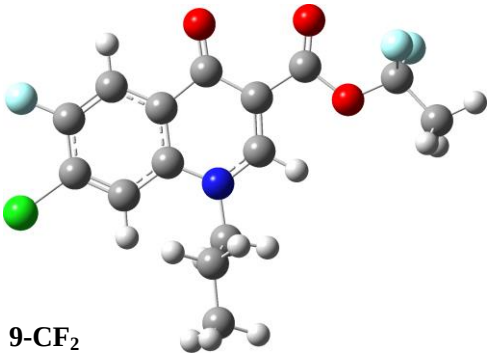
Figure S8. NCI-plot of compound **9** showing the nature O---O interaction as van der Waals type.

Table S4. Various negative hyperconjugative stabilizations of compound **9** in comparison with reference compound **13**. Large fluctuations in the interactions are shown in bold numbers. Results obtained from NBO-6 calculations at M06-2x/6-311+g(d,p) level of theory.

Molecule	LP O_x ⟶ BD* orbital			
9	LP O_1	→	BD* C_3- C_4	25.78
	LP O_1	→	BD* C_4- C_5	26.80
	LP O_2	→	BD* C_{11}- O_3	**43.18**
	LP O_2	→	BD* C_{11}- C_3	24.10
	LP (1)O_3	→	BD* C_{11}-O_2	7.35
	LP (2)O_3	→	BD* C_{11}-O_2	**51.17**
	LP (2)O_3	→	BD* C_{26}- H_{27}	5.86
	LP(2) O_3	→	BD* C_{26}- H_{28}	6.08
	Total			**190.32 kcal/mol**
13	LP O_1	→	BD*C_3- C_4	25.43
	LP O_1	→	BD*C_4- C_5	25.74
	LP O_2	→	BD* C_{11}- O_3	**39.65**
	LP O_2	→	BD* C_{11}- C_3	23.52
	LP (1)O_3	→	BD* C_{11}-O_2	8.33
	LP (2)O_3	→	BD* C_{11}-O_2	**58.00**
	LP (2)O_3	→	BD* C_{26}- H_{27}	5.66
	LP (2)O_3	→	BD* C_{26}- H_{28}	5.88
	Total			**192.21 kcal/mol**

Table S5. Major components of negative hyperconjugation calculated at three different DFT functionals (M06-2X, CAM-B3LYP, and wB97XD) in conjunction with three different basis sets (6-311+g(d,p), Aug-cc-pVTZ, and Def2-TZVP). All values are in kcal/mol.

Functional/Basis set		**Compound-9**		**Compound-13**	
		$LPO_2 \rightarrow BD^*\ C_{11}\text{-}O_3$	**$LP(2)O_3 \rightarrow BD^*C_{11}\text{-}O_2$**	**$LPO_2 \rightarrow BD^*\ C_{11}\text{-}O_3$**	**$LP(2)O_3 \rightarrow BD^*C_{11}\text{-}O_2$**
M06-2X	6-311+g(d,p)	43.18	51.17	39.65	58.00
	Aug-cc-pVTZ	43.04	53.13	40.34	55.67
	Def2-TZVP	44.36	53.51	41.71	61.40
CAM-B3LYP	6-311+g(d,p)	43.16	55.15	39.88	60.46
	Aug-cc-pVTZ	43.72	57.15	40.37	62.67
	Def2-TZVP	44.37	55.56	41.58	63.69
wB97XD	6-311+g(d,p)	46.82	60.02	42.63	66.24
	Aug-cc-pVTZ	46.27	59.72	43.16	62.08
	Def2-TZVP	47.58	60.23	44.51	69.47



9-CF_2

Figure S9. Compounds obtained from **9** replacing CH_2 group of C2H5COO- arm with CF_2 group. Extra internal stabilizations leads to only 2.62˚ dihedral angle flip in **9**-CF_2.

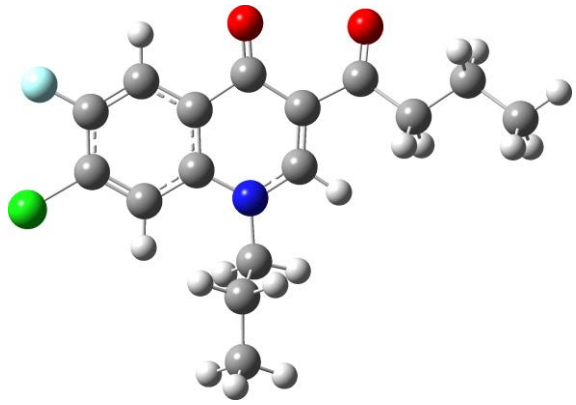


Figure S10. Compound obtained from **9** by replacing O_3 with CH_2 group. Lack of internal stabilizations lead to 20.80˚ dihedral angle flip at the O_1-C_4-C_{11}-O_2 contact.

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Optimized coordinates of the compounds studied

All the geometries are optimized at M06-2X/6-311+g(d,p) level of theory.

Compound-9

Electronic energy + ZPE = -1420.714538 a.u
Number of imaginary frequencies = 0

Cl	4.970405000	0.323784000	-0.233797000
O	-0.821856000	-2.925233000	0.376267000
N	-0.118075000	1.040843000	-0.359180000
C	-1.376030000	0.556006000	-0.268797000
H	-2.161208000	1.290436000	-0.397052000
O	-3.948865000	-0.046018000	-0.070768000
C	0.967302000	0.176828000	-0.201178000
C	-0.651912000	-1.747008000	0.146009000
C	-1.706249000	-0.748895000	-0.043819000
C	2.288028000	0.644865000	-0.284592000
H	2.517758000	1.686299000	-0.457999000
C	0.084946000	2.480367000	-0.543121000
H	-0.835186000	2.882324000	-0.970562000
H	0.866006000	2.632338000	-1.292022000
C	0.727523000	-1.183928000	0.039020000
F	4.122259000	-2.426451000	0.241044000
C	3.338162000	-0.238504000	-0.135660000
C	1.804166000	-2.060698000	0.187401000
H	1.603135000	-3.109428000	0.372465000
O	-3.564848000	-2.249760000	0.065356000
C	3.090510000	-1.593066000	0.099654000
C	-3.138282000	-1.133312000	-0.005865000
C	0.415793000	3.206205000	0.759007000
H	1.270950000	2.726552000	1.242490000
H	-0.431197000	3.096529000	1.442507000
C	-5.355455000	-0.326707000	-0.059515000
H	-5.594216000	-0.892969000	0.843002000
H	-5.596603000	-0.955315000	-0.919544000
C	0.710190000	4.681561000	0.504202000
H	0.918735000	5.205499000	1.437343000
H	-0.138409000	5.176492000	0.025154000
H	1.579236000	4.801757000	-0.147891000
C	-6.079630000	0.999798000	-0.105375000
H	-7.158194000	0.833598000	-0.097054000
H	-5.823215000	1.549697000	-1.012487000
H	-5.818105000	1.611035000	0.759992000

Compound-10

Electronic energy + ZPE = -1127.946539 a.u
Number of imaginary frequencies = 0

O	3.375121000	1.110874000	-0.296397000
O	-2.281713000	2.515400000	0.332909000
O	3.605632000	-1.439260000	0.266727000
O	1.356096000	2.013423000	-0.017309000
O	1.796869000	-2.699451000	-0.077911000
O	-4.622465000	-2.417164000	-0.327756000
N	-0.778456000	0.419743000	0.001832000
H	-0.457340000	1.386654000	0.031946000
C	-2.969508000	1.349538000	0.183164000
C	-2.163625000	0.205141000	0.001240000
C	0.162096000	-0.527409000	0.006631000
H	-0.178375000	-1.556329000	0.032202000
C	1.523946000	-0.342825000	-0.012357000
C	-2.758445000	-1.030898000	-0.173370000
H	-2.180384000	-1.929849000	-0.341662000
C	2.060567000	1.019782000	-0.093176000
C	2.299274000	-1.603268000	0.040403000
C	-4.151516000	-1.153500000	-0.151387000
C	-4.344445000	1.220415000	0.195871000
H	-4.974293000	2.088543000	0.335680000
C	3.903914000	2.440215000	-0.393296000
H	3.669607000	2.982015000	0.525645000
H	3.411456000	2.958188000	-1.219202000
C	-4.947631000	-0.032826000	0.031829000
H	-6.025979000	-0.100616000	0.047260000
C	4.384721000	-2.641318000	0.320659000
H	4.255162000	-3.187699000	-0.616075000
H	4.008971000	-3.273147000	1.128594000
C	-6.021380000	-2.599766000	-0.303856000
H	-6.189445000	-3.665018000	-0.445205000
H	-6.507284000	-2.044550000	-1.112777000
H	-6.443628000	-2.288474000	0.657138000
C	5.394151000	2.306681000	-0.611128000
H	5.847134000	3.296353000	-0.695153000
H	5.599323000	1.751773000	-1.527753000
H	5.858025000	1.780035000	0.224099000
C	5.821491000	-2.225114000	0.542916000
H	6.463155000	-3.107479000	0.580226000
H	5.922368000	-1.681169000	1.483277000
H	6.161152000	-1.579952000	-0.268677000
C	-3.029095000	3.701424000	0.498801000
H	-2.301734000	4.503895000	0.595700000
H	-3.644343000	3.653367000	1.402766000
H	-3.667751000	3.887043000	-0.370614000

Compound-11

Electronic energy + ZPE = -1397.876382 a.u
Number of imaginary frequencies = 0

Cl	2.890366000	2.312667000	0.861344000
O	-3.035229000	1.221145000	-0.381443000
O	-0.948418000	1.952047000	-0.098656000
O	-3.485276000	-1.272888000	0.308708000
N	1.035428000	0.189912000	-0.074019000
H	0.781813000	1.177035000	-0.040285000
C	2.389668000	-0.167929000	-0.132448000
C	4.717272000	0.422719000	0.227112000
H	5.438781000	1.161511000	0.555949000
O	-1.801347000	-2.702695000	-0.010185000
C	3.368334000	0.741813000	0.276615000
C	-1.737872000	1.023159000	-0.159932000
C	-1.321539000	-0.378847000	-0.038642000
C	-2.204077000	-1.563294000	0.072367000
C	2.816059000	-1.407417000	-0.615451000
H	2.088774000	-2.115166000	-0.993471000
C	-4.369087000	-2.395693000	0.430241000
H	-4.040608000	-3.016013000	1.267174000
H	-4.301977000	-2.998748000	-0.477752000
C	5.138217000	-0.824117000	-0.226614000
C	-3.451005000	2.589097000	-0.507811000
H	-2.917465000	3.045817000	-1.344226000
H	-3.171131000	3.127991000	0.399790000
C	0.017597000	-0.677599000	-0.028149000
H	0.277525000	-1.728770000	0.035182000
C	-4.947328000	2.574686000	-0.723388000
H	-5.318723000	3.596364000	-0.820810000
H	-5.449816000	2.099091000	0.120078000
H	-5.198973000	2.024880000	-1.631457000
C	6.599144000	-1.189084000	-0.245541000
H	7.228490000	-0.298428000	-0.250528000
H	6.842438000	-1.784926000	-1.126913000
H	6.860845000	-1.779283000	0.636875000
C	4.163703000	-1.728891000	-0.649137000
H	4.464950000	-2.698548000	-1.030090000
C	-5.759282000	-1.840185000	0.643596000
H	-6.475429000	-2.657488000	0.746141000
H	-6.056503000	-1.219787000	-0.203199000
H	-5.793864000	-1.231650000	1.548512000

Compound-12

Electronic energy + ZPE = -1818.205433 a.u
Number of imaginary frequencies = 0

Cl	2.480469000	2.466458000	-0.825997000
Cl	6.513486000	-0.958837000	0.192333000
O	-3.383831000	1.175757000	0.378096000
N	0.710835000	0.256560000	0.057780000
H	0.425343000	1.235111000	0.025205000
O	-3.766188000	-1.335954000	-0.299532000
O	-1.317952000	1.961953000	0.091047000
C	4.376197000	0.635923000	-0.258569000
H	5.082667000	1.394145000	-0.568931000
C	-2.083122000	1.013343000	0.156759000
C	4.808726000	-0.612595000	0.162136000
C	-1.628242000	-0.378824000	0.039969000
C	-0.283970000	-0.641672000	0.022047000
H	0.002660000	-1.685735000	-0.040355000
C	-2.479289000	-1.589419000	-0.060190000
C	2.073064000	-0.056523000	0.102101000
C	3.899912000	-1.580460000	0.565892000
H	4.251696000	-2.543713000	0.911105000
O	-2.043143000	-2.715107000	0.033756000
C	3.016081000	0.902390000	-0.287533000
C	-3.837690000	2.532806000	0.501912000
H	-3.573610000	3.076171000	-0.407685000
H	-3.314994000	3.005288000	1.336283000
C	-4.620449000	-2.483760000	-0.409697000
H	-4.536059000	-3.074904000	0.504603000
H	-4.275044000	-3.103052000	-1.240487000
C	2.543521000	-1.294946000	0.545625000
H	1.844976000	-2.040384000	0.903416000
C	-5.332464000	2.478198000	0.720105000
H	-5.729959000	3.489913000	0.818347000
H	-5.567982000	1.922532000	1.628896000
H	-5.824450000	1.990179000	-0.122403000
C	-6.024927000	-1.967963000	-0.627463000
H	-6.718937000	-2.805536000	-0.717373000
H	-6.077656000	-1.372757000	-1.540280000
H	-6.336899000	-1.344911000	0.211987000

Compound-13

Electronic energy + ZPE = -1420.710179 a.u
Number of imaginary frequencies = 1 (-35.46)

Cl	4.947360000	-0.344623000	0.200337000
O	-1.382710000	-2.510617000	-0.007725000
N	0.129482000	1.246091000	-0.602484000
C	-1.205079000	0.986425000	-0.686208000
H	-1.821605000	1.849372000	-0.912780000
O	-3.909677000	-0.110029000	0.401467000
C	1.009548000	0.210506000	-0.307581000
C	-0.935645000	-1.393696000	-0.199513000
C	-1.756453000	-0.237303000	-0.521173000
C	2.393629000	0.437754000	-0.204498000
H	2.823216000	1.420830000	-0.333106000
C	0.598615000	2.626547000	-0.735818000
H	-0.166088000	3.174085000	-1.289951000
H	1.495037000	2.635782000	-1.360701000
C	0.512381000	-1.090332000	-0.113800000
F	3.583355000	-2.896813000	0.536080000
C	3.242940000	-0.611904000	0.075180000
C	1.391323000	-2.139505000	0.171448000
H	0.987796000	-3.134928000	0.315879000
O	-3.734294000	-0.872320000	-1.698813000
C	2.737101000	-1.902287000	0.262909000
C	-3.227561000	-0.448947000	-0.698492000
C	0.853512000	3.303555000	0.609278000
H	1.541010000	2.695297000	1.203313000
H	-0.088773000	3.339877000	1.163882000
C	-5.327068000	-0.356183000	0.354252000
H	-5.484762000	-1.412679000	0.128951000
H	-5.757100000	0.229195000	-0.461618000
C	1.417106000	4.708699000	0.419779000
H	1.571942000	5.200494000	1.380602000
H	0.737927000	5.330665000	-0.168869000
H	2.378566000	4.679903000	-0.099471000
C	-5.894793000	0.032784000	1.699615000
H	-6.971811000	-0.143090000	1.711173000
H	-5.713577000	1.088927000	1.904826000
H	-5.437347000	-0.559426000	2.493093000

Compound-9 with O_3 replaced by CH_2 group

Electronic energy + ZPE = -1384.755019 a.u
Number of imaginary frequencies = 0

Cl	5.039481000	0.191696000	-0.137702000
O	-0.878547000	-2.831806000	0.397035000
N	-0.015562000	1.081700000	-0.424645000
C	-1.293991000	0.634636000	-0.373736000
H	-2.033842000	1.408048000	-0.544167000
C	1.033899000	0.184571000	-0.223801000
C	-0.659882000	-1.674310000	0.111021000
C	-1.681997000	-0.653551000	-0.153663000
C	2.372725000	0.605063000	-0.273906000
H	2.644805000	1.634967000	-0.455252000
C	0.240872000	2.510438000	-0.619861000
H	-0.650493000	2.938111000	-1.082558000
H	1.049256000	2.627223000	-1.345758000
C	0.740383000	-1.163332000	0.029481000
F	4.082019000	-2.520658000	0.348371000
C	3.386320000	-0.312137000	-0.081672000
C	1.780988000	-2.074655000	0.222033000
H	1.538388000	-3.112358000	0.419323000
O	-3.493817000	-2.145300000	-0.371902000
C	3.084763000	-1.653935000	0.164562000
C	-3.132491000	-1.008460000	-0.202664000
C	0.555093000	3.244770000	0.681666000
H	1.379718000	2.745217000	1.196977000
H	-0.314958000	3.172180000	1.341011000
C	-5.577900000	-0.413451000	0.113620000
H	-5.619176000	-1.086762000	0.973309000
H	-5.823264000	-1.023820000	-0.757753000
C	0.903657000	4.706408000	0.415881000
H	1.100303000	5.237216000	1.347717000
H	0.086116000	5.220622000	-0.095959000
H	1.795661000	4.789508000	-0.210471000
C	-6.588073000	0.718912000	0.275850000
H	-7.601205000	0.329522000	0.389737000
H	-6.581775000	1.380779000	-0.594764000
H	-6.362712000	1.325505000	1.157339000
C	-4.155696000	0.113590000	-0.033090000
H	-3.880543000	0.723184000	0.835194000
H	-4.099786000	0.775547000	-0.907203000

Compound-9-CF_2

Electronic energy + ZPE = -1619.232419 a.u
Number of imaginary frequencies = 0

Cl	5.489872000	0.160250000	-0.224038000
O	-0.436482000	-2.842540000	0.348789000
N	0.435913000	1.093938000	-0.356084000
C	-0.839916000	0.667412000	-0.258087000
H	-1.590253000	1.437770000	-0.380227000
O	-3.437019000	0.192367000	-0.094440000
C	1.485269000	0.182904000	-0.201855000
C	-0.213017000	-1.670671000	0.137582000
C	-1.224876000	-0.623667000	-0.030426000
C	2.824198000	0.594992000	-0.280621000
H	3.099259000	1.626794000	-0.445317000
C	0.700857000	2.524022000	-0.542501000
H	-0.198050000	2.962337000	-0.979362000
H	1.492994000	2.639401000	-1.285833000
C	1.187862000	-1.167435000	0.029108000
F	4.524288000	-2.556334000	0.220110000
C	3.835918000	-0.333692000	-0.137191000
C	2.225057000	-2.091476000	0.169804000
H	1.979855000	-3.132091000	0.347329000
O	-3.136713000	-2.040532000	0.179472000
C	3.530231000	-1.678557000	0.085529000
C	-2.659392000	-0.964973000	0.037350000
C	1.051227000	3.239215000	0.760057000
H	1.883296000	2.727817000	1.251346000
H	0.195708000	3.165666000	1.437914000
C	-4.816183000	0.075338000	-0.063556000
C	1.405318000	4.701120000	0.503000000
H	1.623217000	5.220194000	1.436639000
H	0.581721000	5.226335000	0.012572000
H	2.285734000	4.785104000	-0.139347000
C	-5.438924000	1.434492000	-0.222220000
H	-6.522163000	1.323243000	-0.199299000
H	-5.132600000	1.862061000	-1.175693000
H	-5.117192000	2.076190000	0.596623000
F	-5.230328000	-0.748431000	-1.051990000
F	-5.205160000	-0.485360000	1.102711000