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Supplementary Material

Structural and spectroscopic study and intermolecular chalcogen bonding interactions in 1,3-dicarbonyl compounds.

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Table S1. Crystal data and structure refinement results for **I**.

Empirical formula	$C_{19}H_{13}ClO_3$
Formula weight	324.74
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2_1/c
Unit cell dimensions	a = 11.213(1) Å b = 7.9744(9) Å c = 17.775(1) Å b = 106.759(9)°.
Volume	1521.9(3) $Å^3$
Z	4
Density (calculated)	1.417 Mg/m^3
Absorption coefficient	0.263 mm^{-1}
F(000)	672
Crystal size	0.708 x 0.306 x 0.200 mm^3
ϑ-range for data collection	3.457 to 25.250°
Index ranges	-13 ≤ h ≤ 13, -7 ≤ k ≤ 9, -21 ≤ l ≤ 14
Reflections collected	4349
Independent reflections	2505 [R(int) = 0.0275]

Observed reflections [I>2σ(I)]	1658
Completeness to ϑ = 25.000°	90.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2505 / 0 / 261
Goodness-of-fit on F^2	1.042
Final R indices [I>2σ(I)]	R1 = 0.0504, wR2 = 0.1254
R indices (all data)	R1 = 0.0807, wR2 = 0.1533
Extinction coefficient	0.015(2)
Largest diff. peak and hole	0.249 and -0.387 e.$Å^{-3}$

[a] $R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2=[\Sigma w(|F_o|^2-|F_c|^2)^2/\Sigma w(|F_o|^2)^2]^{1/2}$

Table S2. Crystal data and structure refinement results for **II**.

Empirical formula	$C_{20}H_{15}ClO_3$
Formula weight	338.77
Temperature	297(2) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	P 2_1/c
Unit cell dimensions	a = 3.8968(2) Å b = 13.416(1) Å c = 30.169(2) Å b= 87.761(5)°
Volume	1576.0(2) $Å^3$
Z	4
Density (calculated)	1.428 Mg/m^3
Absorption coefficient	2.274 mm^{-1}
F(000)	704
Crystal size	0.493 x 0.197 x 0.033 mm^3
ϑ-range for data collection	3.606 to 72.255°.
Index ranges	-4 ≤ h ≤ 2, -16 ≤ k ≤ 16, -36 ≤ l ≤ 37
Reflections collected	11069
Independent reflections	3077 [R(int) = 0.0473]
Observed reflections [I>2σ(I)]	2026
Completeness to ϑ = 67.684°	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3077 / 0 / 220
Goodness-of-fit on F^2	1.056
Final R indices [I>2σ(I)]]	R1 = 0.0584, wR2 = 0.1584
R indices (all data)	R1 = 0.0888, wR2 = 0.1861
Largest diff. peak and hole	0.348 and -0.225 e.$Å^{-3}$

Table S3. Bond lengths [Å] and angles [°] in **I**.

Cl-C(5)	1.739(3)	C(3)-C(2)-C(1)	119.8(3)
O(1)-C(2)	1.348(4)	C(4)-C(3)-C(2)	120.6(3)
O(2)-C(7)	1.254(3)	C(3)-C(4)-C(5)	120.3(3)
O(3)-C(9)	1.322(3)	C(6)-C(5)-C(4)	119.6(3)
C(1)-C(6)	1.390(4)	C(6)-C(5)-Cl	119.6(2)
C(1)-C(2)	1.408(4)	C(4)-C(5)-Cl	120.8(3)
C(1)-C(7)	1.481(4)	C(5)-C(6)-C(1)	121.5(3)
C(2)-C(3)	1.392(5)	O(2)-C(7)-C(8)	119.8(3)
C(3)-C(4)	1.362(5)	O(2)-C(7)-C(1)	119.3(2)
C(4)-C(5)	1.387(4)	C(8)-C(7)-C(1)	120.9(3)
C(5)-C(6)	1.374(4)	C(9)-C(8)-C(7)	122.0(3)
C(7)-C(8)	1.438(4)	O(3)-C(9)-C(8)	122.7(2)
C(8)-C(9)	1.359(4)	O(3)-C(9)-C(10)	115.4(2)
C(9)-C(10)	1.476(3)	C(8)-C(9)-C(10)	121.9(3)
C(10)-C(11)	1.360(4)	C(11)-C(10)-C(19)	120.1(3)
C(10)-C(19)	1.435(4)	C(11)-C(10)-C(9)	118.4(3)
C(11)-C(12)	1.412(5)	C(19)-C(10)-C(9)	121.5(2)
C(12)-C(13)	1.349(6)	C(10)-C(11)-C(12)	120.8(4)
C(13)-C(14)	1.400(5)	C(13)-C(12)-C(11)	120.2(4)
C(14)-C(19)	1.424(3)	C(12)-C(13)-C(14)	121.6(3)
C(14)-C(15)	1.423(5)	C(13)-C(14)-C(19)	119.1(3)
C(15)-C(16)	1.348(5)	C(13)-C(14)-C(15)	122.0(3)
C(16)-C(17)	1.388(5)	C(19)-C(14)-C(15)	118.9(3)
C(17)-C(18)	1.365(4)	C(16)-C(15)-C(14)	121.8(3)
C(18)-C(19)	1.406(4)	C(15)-C(16)-C(17)	119.1(4)
		C(18)-C(17)-C(16)	121.5(4)
C(6)-C(1)-C(2)	118.0(3)	C(17)-C(18)-C(19)	121.4(3)
C(6)-C(1)-C(7)	121.6(2)	C(18)-C(19)-C(14)	117.3(3)
C(2)-C(1)-C(7)	120.4(3)	C(18)-C(19)-C(10)	124.4(2)
O(1)-C(2)-C(3)	116.8(3)	C(14)-C(19)-C(10)	118.3(3)
O(1)-C(2)-C(1)	123.4(3)		

Table S4. Bond lengths [Å] and angles[°] in **II**.

Cl-C(5)	1.737(3)	C(3)-C(2)-C(1)	120.0(3)
O(1)-C(2)	1.349(4)	C(4)-C(3-C(2)	122.3(3)
O(2)-C(7)	1.276(3)	C(3)-C(4)-C(5)	117.1(3)
O(3)-C(9)	1.323(3)	C(3)-C(4)-C(20)	120.9(3)
C(1)-C(6)	1.396(4)	C(5)-C(4)-C(20)	122.1(3)
C(1)-C(2)	1.408(4)	C(6)-C(5)-C(4)	122.0(3)
C(1)-C(7)	1.471(4)	C(6)-C(5)Cl	118.8(2)
C(2)-C(3)	1.401(4)	C(4)-C(5)-Cl	119.2(2)
C(3)-C(4)	1.371(5)	C(5)-C(6)-C(1)	120.9(3)
C(4)-C(5)	1.403(4)	O(2)-C(7)-C(8)	119.0(3)
C(4)-C(20)	1.502(4)	O(2)-C(7)-C(1)	118.5(2)
C(5)-C(6)	1.379(4)	C(8)-C(7)-C(1)	122.4(2)
C(7)-C(8)	1.432(4)	C(9)-C(8-C(7)	120.9(3)
C(8)-C(9)	1.376(4)	O(3)-C(9)-C(8)	121.6(3)
C(9)-C(10)	1.480(4)	O(3)-C(9)-C(10)	115.2(2)
C(10)-C(11)	1.368(4)	C(8)-C(9)-C(10)	123.2(2)
C(10)-C(19)	1.438(4)	C(11)-C(10)-C(19)	120.2(3)
C(11)-C(12)	1.404(4)	C(11)-C(10)-C(9)	118.8(3)
C(12)-C(13)	1.360(5)	C(19)-C(10)-C(9)	121.0(2)
C(13)-C(14)	1.414(4)	C(10)-C(11)-C(12)	121.3(3)
C(14)-C(15)	1.428(4)	C(13)-C(12)-C(11)	120.3(3)
C(14)-C(19)	1.426(4)	C(12)-C(13)-C(14)	120.6(3)
C(15)-C(16)	1.343(5)	C(15)-C(14)-C(13)	121.3(3)
C(16)-C(17)	1.409(5)	C(15)-C(14)-C(19)	118.7(3)
C(17)-C(18)	1.366(4)	C(13)-C(14)-C(19)	120.1(3)
C(18)-C(19)	1.416(4)	C(16)-C(15)-C(14)	121.4(3)
C(6)-C(1)-C(2)	117.7(3)	C(18)-C(17)-C(16)	120.7(3)
C(6)-C(1)-C(7)	122.2(2)	C(17)-C(18)-C(19)	120.9(3)
C(2)-C(1)-C(7)	120.1(3)	C(14)-C(19)-C(18)	118.2(3)
O(1)-C(2)-C(3)	116.9(3)	C(14)-C(19)-C(10)	117.5(3)
O(1)-C(2)-C(1)	123.0(3)	C(18)-C(19)-C(10)	124.2(3)

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **I**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Cl	1959(1)	1078(1)	5035(1)	96(1)
O(1)	5056(2)	6778(4)	6500(1)	94(1)
O(2)	4537(2)	8145(3)	5123(1)	74(1)
O(3)	3951(2)	9640(3)	3798(1)	72(1)
C(1)	3677(2)	5533(4)	5322(1)	55(1)
C(2)	4311(3)	5520(5)	6131(2)	69(1)
C(3)	4198(3)	4145(6)	6588(2)	77(1)
C(4)	3485(3)	2804(6)	6260(2)	74(1)
C(5)	2861(3)	2790(4)	5463(2)	65(1)
C(6)	2954(3)	4147(4)	5007(2)	58(1)
C(7)	3788(2)	6989(4)	4829(2)	54(1)
C(8)	3053(2)	7089(4)	4021(2)	55(1)
C(9)	3160(2)	8390(4)	3551(1)	52(1)
C(10)	2404(2)	8490(4)	2722(1)	53(1)
C(11)	2312(3)	7099(5)	2265(2)	71(1)
C(12)	1574(4)	7110(6)	1474(2)	93(1)
C(13)	943(4)	8505(6)	1161(2)	85(1)
C(14)	998(3)	9971(5)	1603(1)	62(1)
C(15)	312(3)	11435(6)	1284(2)	77(1)
C(16)	351(3)	12834(6)	1716(2)	80(1)
C(17)	1074(3)	12843(5)	2495(2)	71(1)
C(18)	1754(3)	11474(4)	2829(2)	58(1)
C(19)	1750(2)	9992(4)	2400(1)	50(1)

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **II**.

Atom	x	y	z	U(eq)
Cl	1945(3)	9259(1)	-483(1)	88(1)
O(1)	3434(8)	5556(2)	510(1)	79(1)
O(2)	6285(7)	6549(2)	1113(1)	63(1)
O(3)	8370(7)	7439(2)	1770(1)	60(1)
C(1)	4089(7)	7352(2)	487(1)	45(1)
C(2)	3127(8)	6437(2)	300(1)	54(1)
C(3)	1729(8)	6415(3)	-121(1)	59(1)
C(4)	1354(8)	7259(3)	-371(1)	56(1)
C(5)	2330(8)	8165(2)	-181(1)	54(1)
C(6)	3673(8)	8213(2)	235(1)	49(1)
C(7)	5583(7)	7375(2)	927(1)	46(1)
C(8)	6204(7)	8286(2)	1157(1)	44(1)
C(9)	7503(7)	8279(2)	1575(1)	44(1)
C(10)	8082(7)	9195(2)	1835(1)	44(1)
C(11)	9595(7)	9997(2)	1626(1)	50(1)
C(12)	10354(8)	10869(2)	1859(1)	57(1)
C(13)	9561(8)	10938(2)	2301(1)	56(1)
C(14)	7920(7)	10139(2)	2530(1)	48(1)
C(15)	7014(8)	10206(3)	2992(1)	58(1)
C(16)	5405(9)	9455(3)	3209(1)	64(1)
C(17)	4594(8)	8574(3)	2981(1)	59(1)
C(18)	5405(7)	8475(2)	2539(1)	50(1)
C(19)	7145(6)	9243(2)	2300(1)	44(1)
C(20)	-79(10)	7205(3)	-825(1)	77(1)

Table S7. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **I**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ hk\ a^*b^*U^{12}]$.

Atom	U11	U22	U33	U23	U13	U12
Cl	151(1)	62(1)	88(1)	9(1)	55(1)	-10(1)
O(1)	82(2)	121(3)	65(1)	12(2)	1(1)	-21(2)
O(2)	66(1)	69(2)	72(1)	4(1)	-2(1)	-8(1)
O(3)	67(1)	61(2)	74(1)	9(1)	0(1)	-16(1)
C(1)	48(1)	62(2)	56(2)	6(1)	16(1)	14(1)
C(2)	48(2)	94(3)	62(2)	9(2)	12(1)	11(2)
C(3)	57(2)	111(3)	61(2)	21(2)	16(2)	7(2)
C(4)	65(2)	89(3)	78(2)	33(2)	35(2)	19(2)
C(5)	72(2)	63(2)	68(2)	13(2)	34(1)	15(2)
C(6)	68(2)	54(2)	57(2)	7(1)	24(1)	13(2)
C(7)	47(1)	51(2)	63(2)	1(1)	13(1)	5(1)
C(8)	50(1)	53(2)	58(2)	-2(1)	12(1)	-3(1)
C(9)	51(1)	45(2)	58(1)	-1(1)	14(1)	-1(1)
C(10)	61(2)	51(2)	52(1)	-7(1)	24(1)	-9(1)
C(11)	97(2)	56(2)	67(2)	-10(2)	34(2)	-12(2)
C(12)	142(3)	77(3)	70(2)	-32(2)	48(2)	-34(3)
C(13)	105(3)	105(4)	45(2)	-8(2)	20(2)	-27(2)
C(14)	63(2)	85(3)	41(1)	2(2)	19(1)	-21(2)
C(15)	59(2)	118(4)	51(2)	28(2)	12(2)	-7(2)
C(16)	66(2)	97(4)	81(2)	27(2)	27(2)	11(2)
C(17)	71(2)	70(3)	75(2)	9(2)	27(2)	10(2)
C(18)	63(2)	60(2)	51(2)	-1(1)	18(1)	-1(2)
C(19)	49(1)	60(2)	44(1)	2(1)	19(1)	-9(1)

Table S8. Anisotropic displacement parameters ($Å^2$ x 10^3) for **II**.

Atom	U11	U22	U33	U23	U13	U12
Cl	125(1)	80(1)	62(1)	20(1)	-40(1)	-19(1)
O(1)	127(2)	48(1)	63(2)	-5(1)	-17(2)	-9(1)
O(2)	97(2)	46(1)	45(1)	-1(1)	-10(1)	6(1)
O(3)	89(2)	49(1)	44(1)	0(1)	-17(1)	13(1)
C(1)	51(1)	46(2)	38(1)	-5(1)	2(1)	-2(1)
C(2)	66(2)	49(2)	46(2)	-6(1)	2(1)	-4(1)
C(3)	66(2)	61(2)	48(2)	-18(1)	1(1)	-12(2)
C(4)	53(2)	74(2)	40(2)	-11(1)	0(1)	-10(1)
C(5)	57(2)	64(2)	40(2)	3(1)	-7(1)	-8(1)
C(6)	59(2)	49(2)	40(2)	-4(1)	-7(1)	-8(1)
C(7)	54(2)	46(2)	38(1)	-2(1)	2(1)	1(1)
C(8)	54(2)	45(2)	35(1)	0(1)	-6(1)	4(1)
C(9)	49(1)	46(2)	38(1)	-1(1)	-2(1)	5(1)
C(10)	44(1)	47(2)	40(2)	-3(1)	-12(1)	4(1)
C(11)	54(2)	56(2)	41(2)	3(1)	-9(1)	3(1)
C(12)	58(2)	50(2)	63(2)	8(1)	-13(2)	-5(1)
C(13)	58(2)	50(2)	59(2)	-7(1)	-15(1)	2(1)
C(14)	44(1)	52(2)	49(2)	-7(1)	-12(1)	5(1)
C(15)	60(2)	66(2)	50(2)	-20(2)	-12(1)	5(2)
C(16)	66(2)	85(2)	40(2)	-9(2)	0(1)	2(2)
C(17)	60(2)	72(2)	45(2)	3(1)	0(1)	-2(2)
C(18)	50(2)	55(2)	47(2)	-3(1)	-6(1)	0(1)
C(19)	40(1)	51(2)	41(2)	-3(1)	-9(1)	6(1)
C(20)	78(2)	110(3)	44(2)	-16(2)	-13(2)	-15(2)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **I**.

Atom	x	y	z	U(eq)
H(O1)	5080(40)	7500(60)	6150(20)	117(16)
H(O3)	4390(30)	9460(60)	4350(20)	133(15)
H(3)	4660(30)	4340(50)	7144(19)	91(10)
H(4)	3380(30)	1940(50)	6550(20)	100(12)
H(6)	2490(20)	4120(40)	4483(16)	65(8)
H(8)	2430(20)	6160(30)	3787(13)	50(6)
H(11)	2760(20)	6130(40)	2499(15)	60(8)
H(12)	1620(30)	6090(50)	1245(18)	86(11)
H(13)	370(30)	8500(50)	622(19)	90(10)
H(15)	-160(30)	11360(50)	800(20)	98(12)
H(16)	-150(40)	13900(60)	1460(20)	117(13)
H(17)	1150(30)	13880(50)	2820(20)	92(11)
H(18)	2190(20)	11530(40)	3357(17)	77(9)

Table S10. Hydrogen coordinates (x10^4) and isotropic displacement parameters (Å^2 x 10^3) for **II**.

Atom	x	y	z	U(eq)
H(1)	4422	5641	742	119
H(3)	7867	6965	1614	90
H(3A)	1032	5807	-235	70
H(6)	4311	8827	348	59
H(8)	5722	8892	1023	53
H(11)	10130	9963	1323	60
H(12)	11405	11403	1711	68
H(13)	10102	11515	2454	67
H(15)	7549	10782	3146	70
H(16)	4826	9517	3510	77
H(17)	3494	8055	3134	71
H(18)	4806	7894	2392	60
H(20A)	1652	7404	-1043	116
H(20B)	-2020	7643	-840	116
H(20C)	-786	6534	-884	116

Table S11. Torsion angles [°] for **I.**

C(6)-C(1)-C(2)-O(1)	178.9(3)	O(3)-C(9)-C(10)-C(19)	-49.1(3)
C(7)-C(1)-C(2)-O(1)	-1.1(4)	C(8)-C(9)-C(10)-C(19)	131.6(3)
C(6)-C(1)-C(2)-C(3)	-0.1(4)	C(19)-C(10)-C(11)-C(12)	-0.2(4)
C(7)-C(1)-C(2)-C(3)	179.9(3)	C(9)-C(10)-C(11)-C(12)	178.2(3)
O(1)-C(2)-C(3)-C(4)	-178.6(3)	C(10)-C(11)-C(12)-C(13)	-0.3(5)
C(1)-C(2)-C(3)-C(4)	0.4(5)	C(11)-C(12)-C(13)-C(14)	0.0(6)
C(2)-C(3)-C(4)-C(5)	0.0(5)	C(12)-C(13)-C(14)-C(19)	0.7(5)
C(3)-C(4)-C(5)-C(6)	-0.8(4)	C(12)-C(13)-C(14)-C(15)	-178.4(3)
C(3)-C(4)-C(5)-Cl	179.4(3)	C(13)-C(14)-C(15)-C(16)	178.8(3)
C(4)-C(5)-C(6)-C(1)	1.1(4)	C(19)-C(14)-C(15)-C(16)	-0.3(4)
Cl-C(5)-C(6)-C(1)	-179.1(2)	C(14)-C(15)-C(16)-C(17)	-0.4(5)
C(2)-C(1)-C(6)-C(5)	-0.6(4)	C(15)-C(16)-C(17)-C(18)	0.7(5)
C(7)-C(1)-C(6)-C(5)	179.4(2)	C(16)-C(17)-C(18)-C(19)	-0.2(5)
C(6)-C(1)-C(7)-O(2)	-173.7(2)	C(17)-C(18)-C(19)-C(14)	-0.6(4)
C(2)-C(1)-C(7)-O(2)	6.3(4)	C(17)-C(18)-C(19)-C(10)	-177.6(3)
C(6)-C(1)-C(7)-C(8)	6.1(4)	C(13)-C(14)-C(19)-C(18)	-178.4(3)
C(2)-C(1)-C(7)-C(8)	-173.9(2)	C(15)-C(14)-C(19)-C(18)	0.8(3)
O(2)-C(7)-C(8)-C(9)	1.5(4)	C(13)-C(14)-C(19)-C(10)	-1.1(4)
C(1)-C(7)-C(8)-C(9)	-178.3(3)	C(15)-C(14)-C(19)-C(10)	178.0(2)
C(7)-C(8)-C(9)-O(3)	0.8(4)	C(11)-C(10)-C(19)-C(18)	178.0(3)
C(7)-C(8)-C(9)-C(10)	-180.0(2)	C(9)-C(10)-C(19)-C(18)	-0.4(4)
O(3)-C(9)-C(10)-C(11)	132.4(3)	C(11)-C(10)-C(19)-C(14)	0.9(4)
C(8)-C(9)-C(10)-C(11)	-46.8(4)	C(9)-C(10)-C(19)-C(14)	-177.5(2)

Table S12. Torsion bond angles [°] for **II**.

C(6)-C(1)-C(2)-O(1)	179.5(3)	C(8)-C(9)-C(10)-C(11)	-44.4(4)
C(7)-C(1)-C(2)-O(1)	1.5(5)	O(3)-C(9)-C(10)-C(19)	-44.1(4)
C(6)-C(1)-C(2)-C(3)	-1.5(4)	C(8)-C(9)-C(10)-C(19)	136.8(3)
C(7)-C(1)-C(2)-C(3)	-179.5(3)	C(19)-C(10)-C(11)-C(12)	1.8(4)
O(1)-C(2)-C(3)-C(4)	-178.7(3)	C(9)-C(10)-C(11)-C(12)	-177.0(3)
C(1)-C(2)-C(3)-C(4)	2.3(5)	C(10)-C(11)-C(12)-C(13)	-0.7(4)
C(2)-C(3)-C(4)-C(5)	-2.1(5)	C(11)-C(12)-C(13)-C(14)	-0.9(4)
C(2)-C(3)-C(4)-C(20)	178.6(3)	C(12)-C(13)-C(14)-C(15)	-178.8(3)
C(3)-C(4)-C(5)-C(6)	1.3(5)	C(12)-C(13)-C(14)-C(19)	1.3(4)
C(20)-C(4)-C(5)-C(6)	-179.4(3)	C(13)-C(14)-C(15)-C(16)	178.9(3)
C(3)-C(4)-C(5)-Cl	179.5(2)	C(19)-C(14)-C(15)-C(16)	-1.3(4)
C(20)-C(4)-C(5)-Cl	-1.2(5)	C(14)-C(15)-C(16)-C(17)	0.4(5)
C(4)-C(5)-C(6)-C(1)	-0.6(5)	C(15)-C(16)-C(17)-C(18)	-0.4(5)
Cl-C(5)-C(6)-C(1)	-178.9(2)	C(16)-C(17)-C(18)-C(19)	1.4(5)
C(2)-C(1)-C(6)-C(5)	0.7(4)	C(15)-C(14)-C(19)-C(18)	2.1(4)
C(7)-C(1)-C(6)-C(5)	178.7(3)	C(13)-C(14)-C(19)-C(18)	-178.1(2)
C(6)-C(1)-C(7)-O(2)	-171.2(3)	C(15)-C(14)-C(19)-C(10)	179.9(2)
C(2)-C(1)-C(7)-O(2)	6.7(4)	C(13)-C(14)-C(19)-C(10)	-0.2(4)
C(6)-C(1)-C(7)-C(8)	10.2(4)	C(17)-C(18)-C(19)-C(14)	-2.2(4)
C(2)-C(1)-C(7)-C(8)	-171.9(3)	C(17)-C(18)-C(19)-C(10)	-179.9(3)
O(2)-C(7)-C(8)-C(9)	-0.7(4)	C(11)-C(10)-C(19)-C(14)	-1.3(4)
C(1)-C(7)-C(8)-C(9)	177.9(3)	C(9)-C(10)-C(19)-C(14)	177.4(2)
C(7)-C(8)-C(9)-O(3)	3.1(4)	C(11)-C(10)-C(19)-C(18)	176.4(3)
C(7)-C(8)-C(9)-C(10)	-177.8(3)	C(9)-C(10)-C(19)-C(18)	-4.9(4)
O(3)-C(9)-C(10)-C(11)	134.7(3)		

Table S13. Intra and intermolecular hydrogen bond distances and angles in **I**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
O(1)-H(1) ···O(2)	0.86(5)	1.82(4)	2.588(3)	148(4)
O(1)-H(1) ···O(3^{i})	0.86(5)	2.51(5)	3.165(4)	133(4)
O(3)-H(3) ···O(2)	0.98(4)	1.70(4)	2.551(3)	144(4)
O(3)-H(3) ···O(2^{i})	0.98(4)	2.31(4)	2.793(3)	110(4)

Symmetry transformations used to generate equivalent atoms: (i) -x+1, -y+2, -z+1.

Table S14. Intra and intermolecular hydrogen bond distances and angles in **II**.

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
O(1)-H(1) ···O(2)	0.82	1.82	2.544(3)	146
O(3)-H(3) ···O(2)	0.82	1.75	2.479(3)	148

Table S15: Experimental and calculated[a] ^{1}H NMR chemical shifts (in ppm) of **I** and **II**.

	I		**II**	
	Exp.	Calc.	Exp.	Calc.
HO-enol	15.57	15.30	15.54	15.26
HO-phenol	12.10	12.90	11.99	12.85
HO-phenol (diketo)[b]	11.86	12.61	11.80	12.56
H3	6.98	7.21	6.91	7.16
H6	7.64	7.94	7.63	7.86
H4	7.41	7.65	-	-
H2'	7.8	8.12	7.80	8.08
H3'	7.63 – 7.53	8.57	7.62 – 7.55	7.89
H4'	8.01	8.57	8.01	8.56
H5'	7.93	8.40	7.93	8.41
H6'	7.63 – 7.53	7.98	7.62 – 7.55	7.98
H7'	7.63 – 7.53	8.02	7.62 – 7.55	8.02
H8'	8.43	9.01	8.43	9.02
$HC_{methine}$	6.61	6.80	6.59	6.74
CH_2 (diketo)[c]	4.73	4.73	4.72	4.70
CH_3	-	-	2.38	2.40

[a] Isotropic shielding calculated by the GIAO method using the corresponding TMS shielding, determined at the same level of theory (B3LYP/6-311++g (d,p) from the optimized geometries)

[b] Integrates for approximately 0.05 H

[c] Integrates for approximately 0.1 H

Table S16: Experimental and calculated[a] ^{13}C NMR chemical shifts (in ppm) of **I** and **II**.

	I		**II**	
	Exp.	Calc.	Exp.	Calc.
C=O	194.5	201.59	194.5	201.23
HO-C_{enol}	181.8	192.29	181.2	191.79
C1	119.6	125.63	117.9	123.94
C2	161.2	171.95	161.4	171.66
C3	120.5	126.78	120.3	127.05
C4	135.8	143.93	145.2	155.99
C5	124	139.63	124.8	140
C6	128.8	135.04	128.8	135.31
C1'	132.5	140.97	132.7	141.07
C2'	127.6	133.37	127.6	136
C3'	125	131.07	125.1	130.88
C4'	132.2	140.80	132.1	140.68
C4'a	133.9	143.26	134	143.50
C5'	127.9	136.62	128.4	136.60
C6'	126.7	133.32	126.7	133.37
C7'	127.6	136	134.61	127.6
C8'	125.4	133.47	125.5	133.54
C8'a	130.2	138.89	130.3	138.97
$C_{methine}$	97.7	101.84	97.6	101.67
CH_2 (diketo)	52.5	59.26	-	59.28
CH_3	-	-	20.9	24.17

[a] Isotropic shielding calculated by the GIAO method using the corresponding TMS shielding, determined at the same level of theory (B3LYP/6-311++g (d,p) from the optimized geometries)

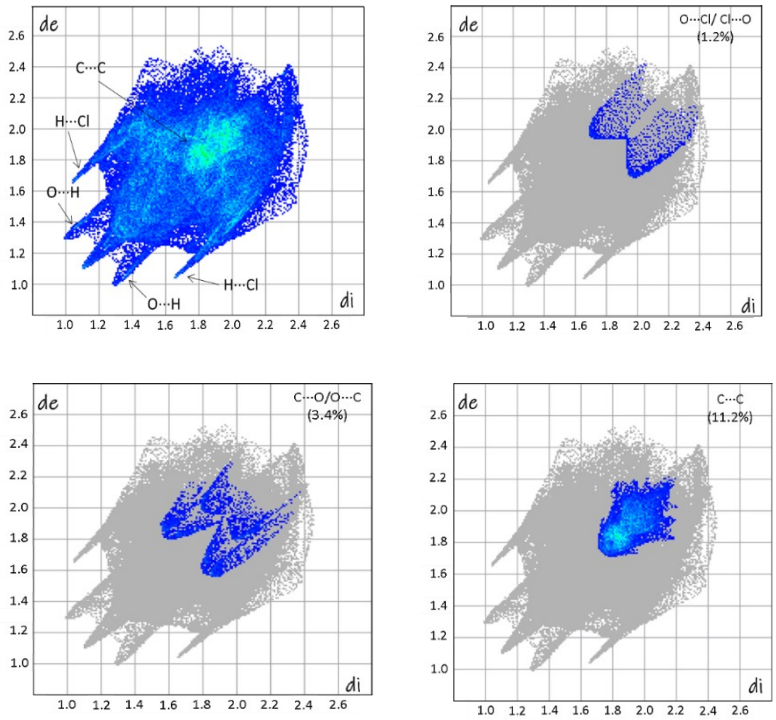


Figure S1. 2D decomposition plot of the contacts different from X···H (X = H, O, C and Cl) surface of **I**.

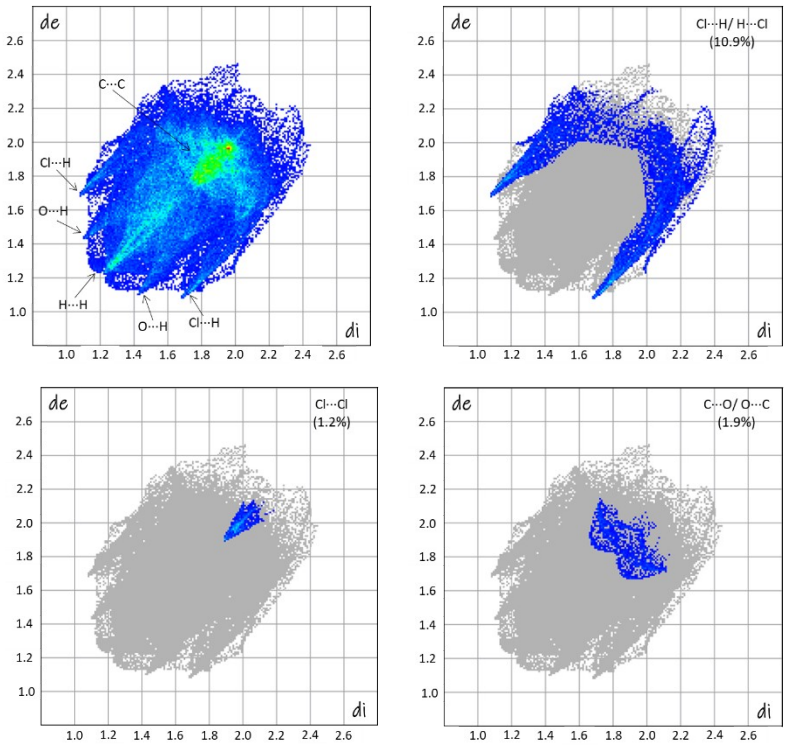
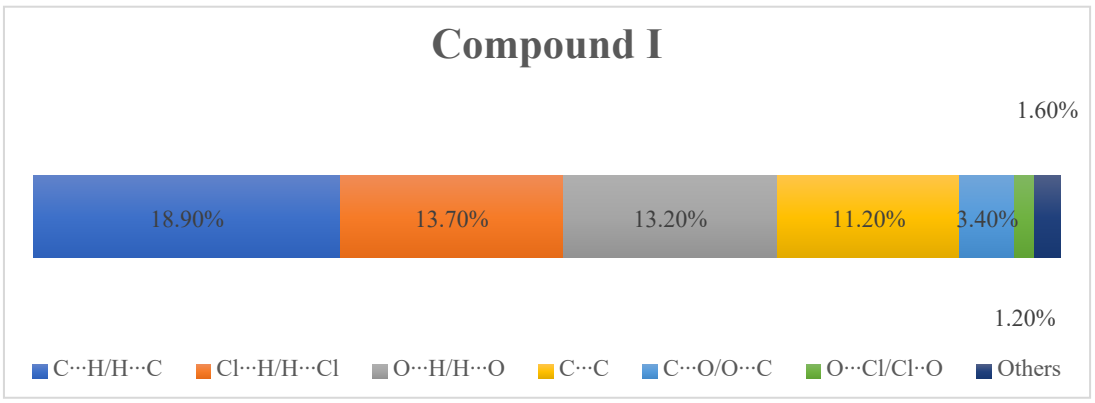


Figure S2. 2D decomposition plot of the Cl-H, C-O and Cl-Cl contacts surface of **II**.



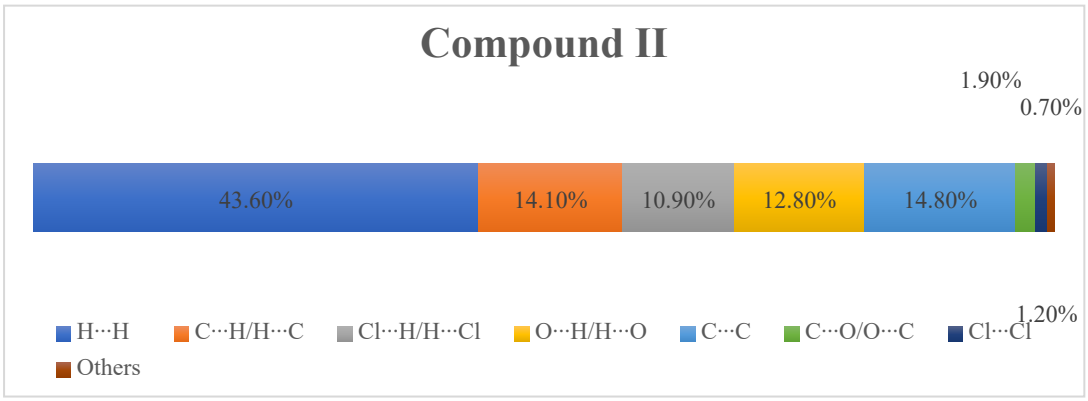


Figure S3. Percentual distribution of the intermolecular interactions of the Hirshfeld surface for **I** and **II**.

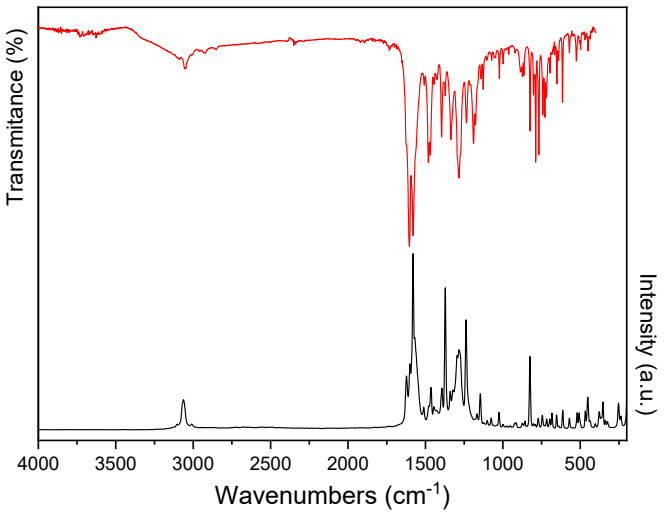


Figure S4. Infrared spectrum (upper trace, KBr pellets) and Raman spectrum (solid, lower trace) of **I**.

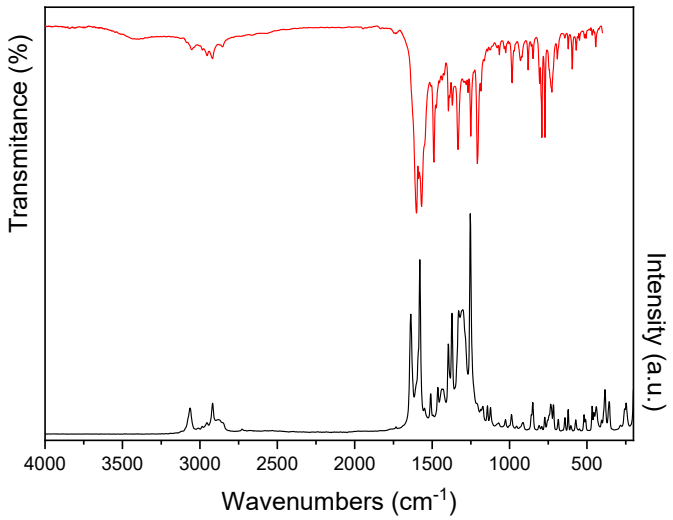


Figure S5. Infrared spectrum (upper trace, KBr pellets) and Raman spectrum (solid, lower trace) of **II**.

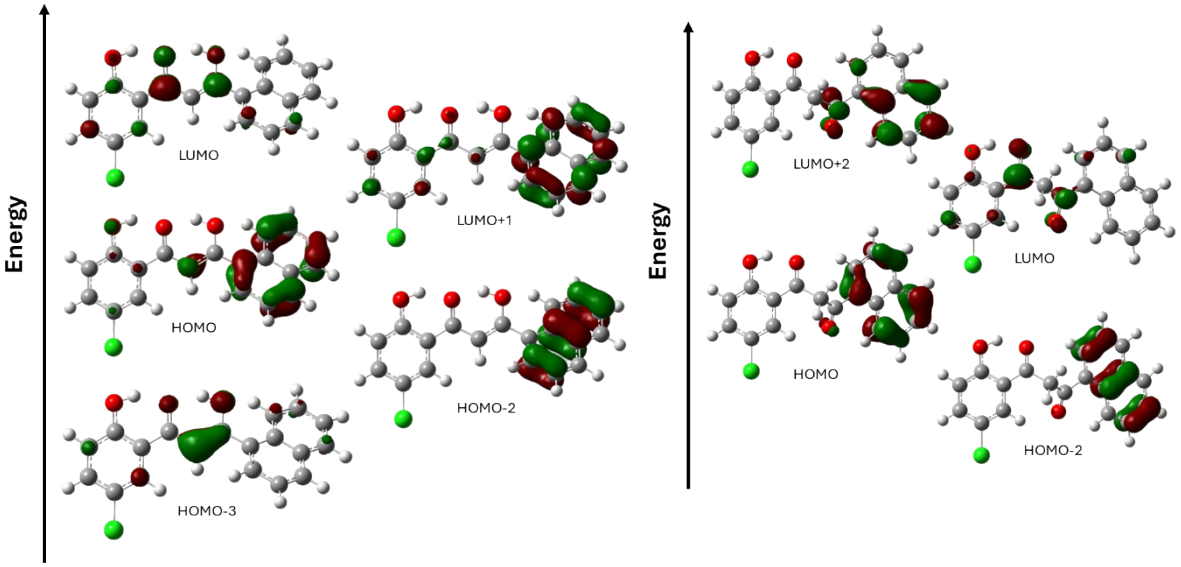


Figure S6. Electronic transitions (solvent: CH_3CN) of **I**, to the left transitions from the keto-enol tautomer and to the right from diketo tautomer.

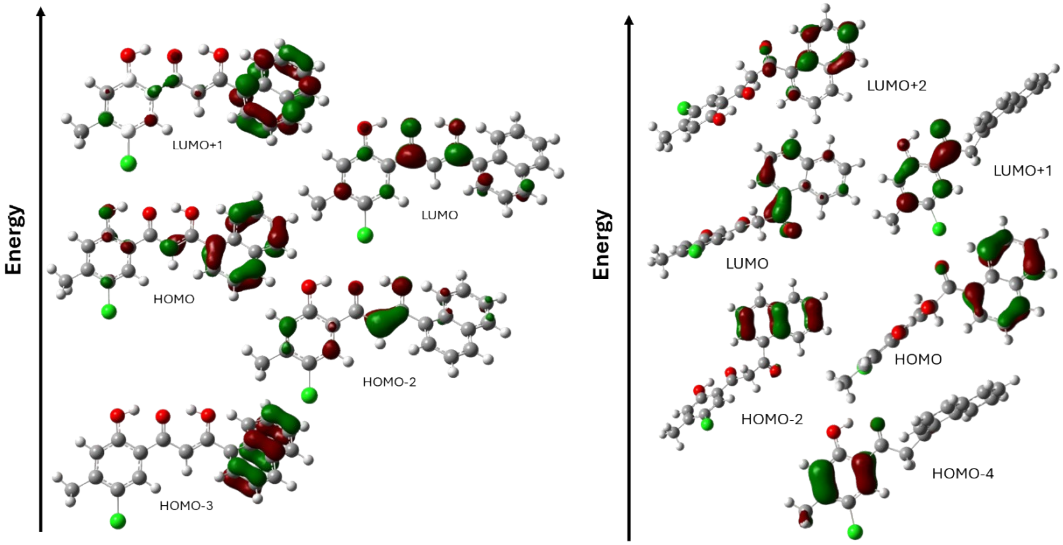


Figure S7. Electronic transitions (solvent: CH_3CN) of **II**, to the left transitions from the Keto-enol tautomer and to the right from diketo tautomer.

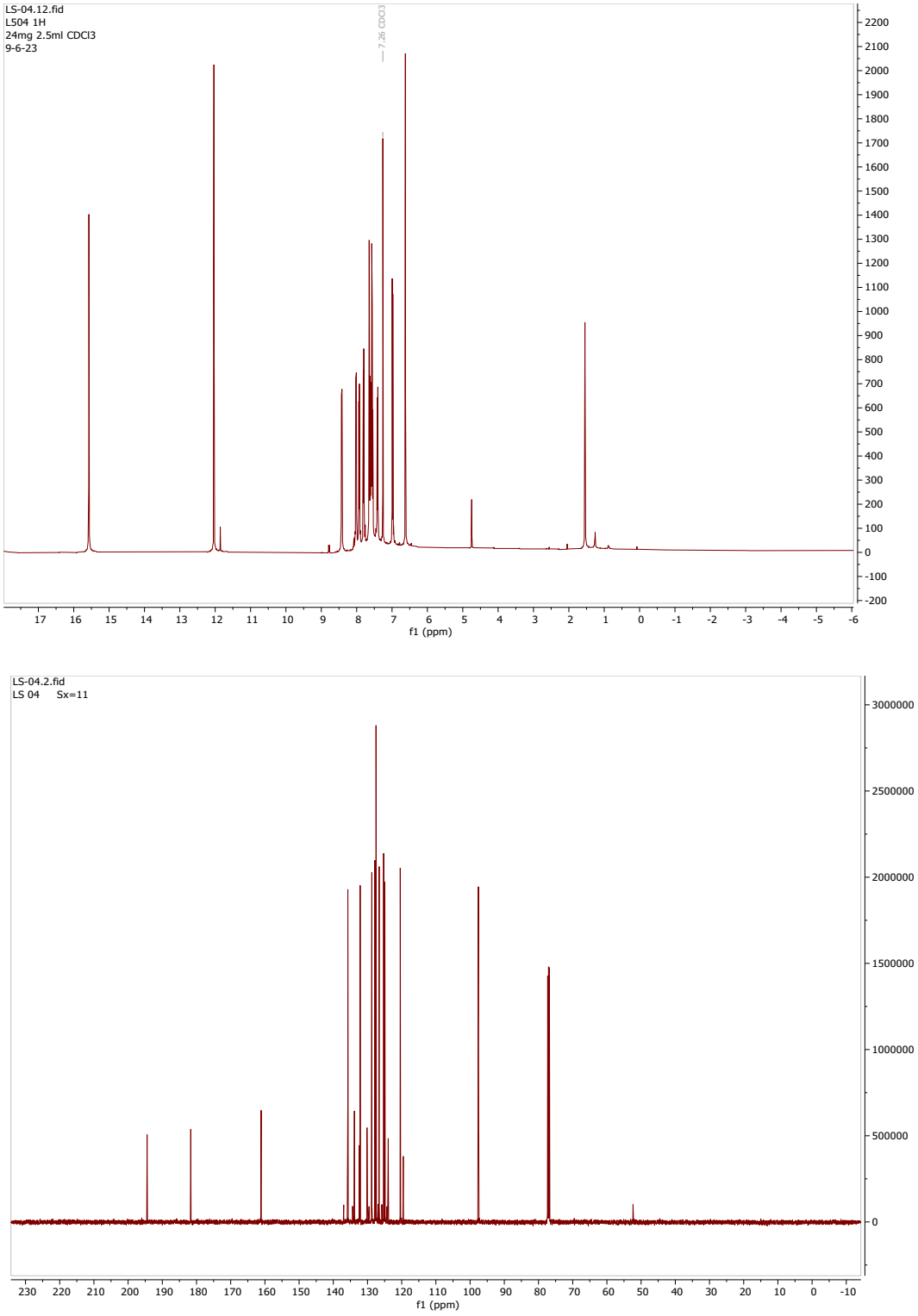


Figure S8. ^{1}H and ^{13}C NMR spectra of **I**.

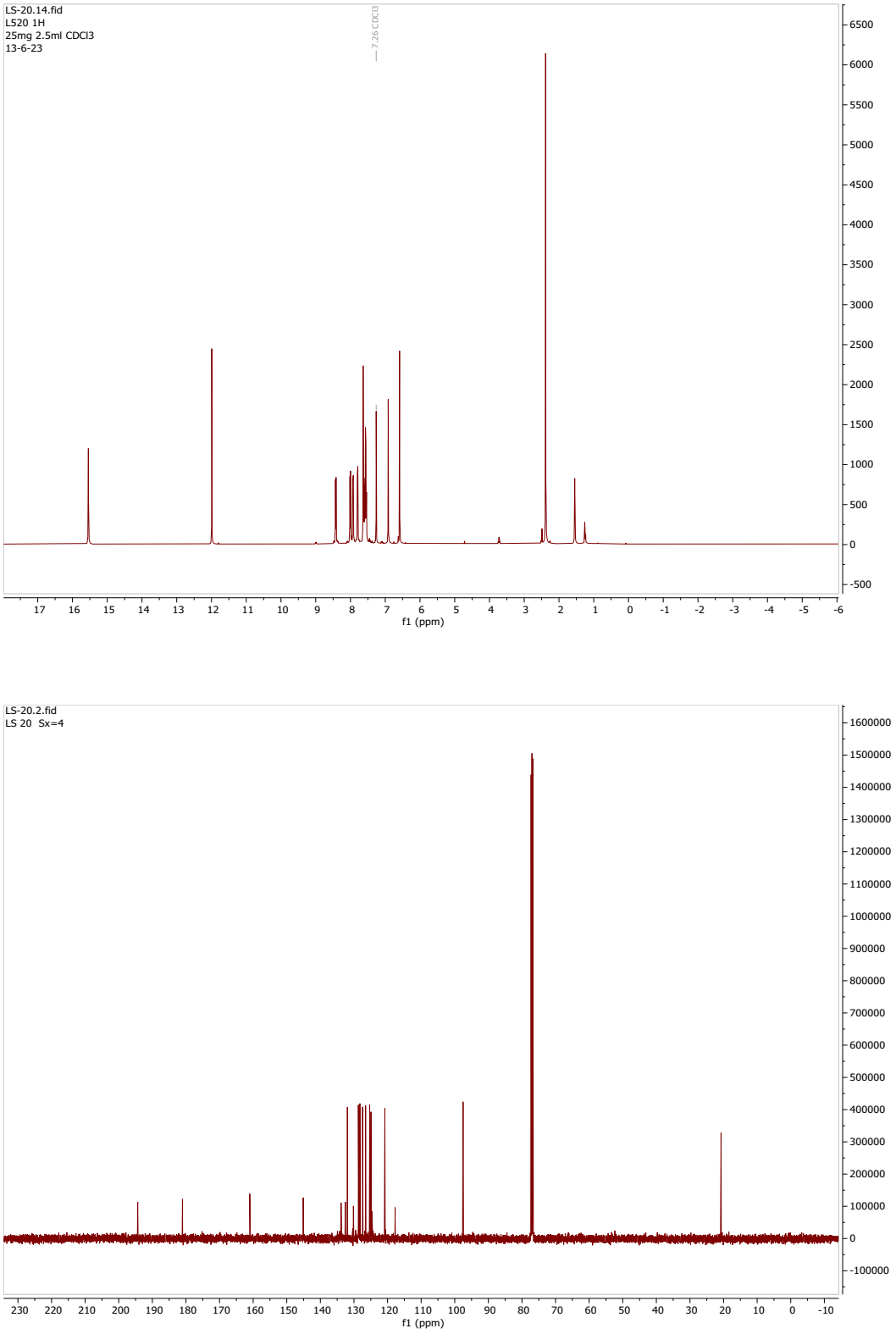
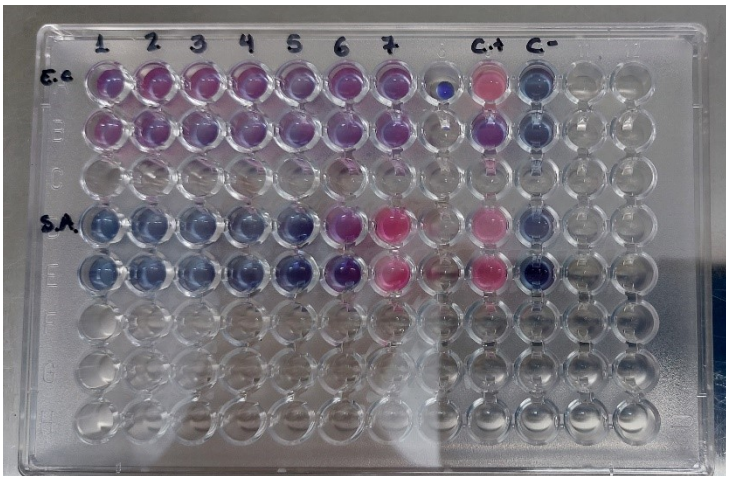


Figure S9. ^{1}H and ^{13}C NMR spectra of **II**.

Compound I



Compound II

Figure S10. Colour change of the resazurin, with the lowest compound concentration remaining blue indicating the MIC 3.125 µg/mL for **I** and 6.250 µg/mL for **II** just for *S. aureus*.

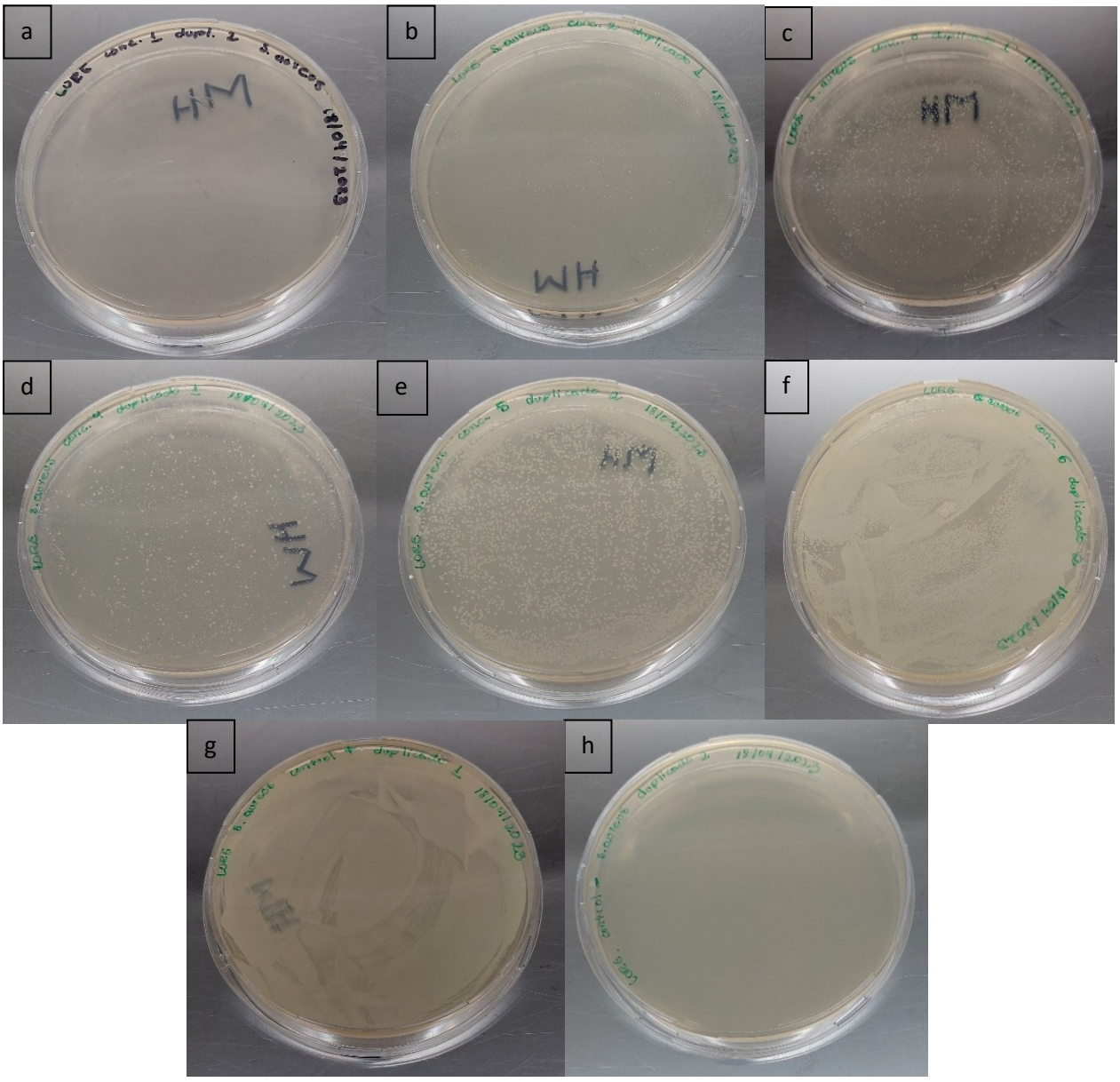


Figure S11. MBC test compound **I** for *S. aureus*. Concentration: a) 100 µg/mL; b) 50 µg/mL; c) 25 µg/mL; d) 12.5 µg/mL; e) 6.25 µg/mL; f) 3.125 µg/mL; f) 1.5625 µg/mL; g) Positive Control (*S. aureus*); h) Negative Control. MBC concentration 100 µg/mL.