Supplementary Table 1| Primers used in this study.

Primers	Sequence (5'→3')	Description
XbaI-*ras1*-UF	AAAAATCTAGAAATGGCTGATCGCCGACTGCGACT	deletion and complementation of *ras1*
EcoRI-*ras1*-DR	AAAAAGAATTCGGTAGACACCGATGAAACCACACATG	deletion and complementation of *ras1*
ras1-UR	CATGGTCGTCAGCTCGCCATCTTCAAATGCCGATTTTC ATGTGTATGCCC	deletion of *ras1*
ras1-DF	GGGCATACACATGAAAATCGGCATTTGAAGATGGCGA GCTGACGACCATG	deletion of *ras1*
Xbal-*ras2*-UF	AAAAATCTAGAGCCTGGGCCTGGAAGACATGAGCT	deletion and complementation of *ras2*
EcoRI-*ras2*-DR	AAAAAGAATTCTCATGCTGGGTGTAGAACAGCGGC	deletion and complementation of *ras2*
ras2-UR	GCGCACCCAGGGTTCATTGCGCCCGTCGCTCATGGTCG TCAGCTCGCC	deletion of *ras2*
ras2 DF	GGCGAGCTGACGACCATGAGCGACGGGCGCAATGAAC CCTGGGTGCGC	deletion of *ras2*
XbaI-*ras3*-UF	AAAAATCTAGAGATGCGCGTTTCTGCTTCAGCGAG	deletion and complementation of *ras3*
EcoRI-*ras3*-DR	AAAAAGAATTCCCGATCACCAGGTCGAAGTCTTCC	deletion and complementation of *ras3*
ras3-DF	GAAAAGGATTTTGCCATGTGTGGTCTGACCAGCCTGTG CCTGCTGCAG	deletion of *ras3*
ras3-UR	CTGCAGCAGGCACAGGCTGGTCAGACCACACATGGCA AAATCCTTTTC	deletion of *ras3*
Xbal-*ras4*-UF	AAAAATCTAGAAACTCCATGTACCTGTGGGCCAAG	deletion and complementation of *ras4*
EcoRI-*ras4*-DR	AAAAAGAATTCGGCACGGGTGGCGTTGCAGATGAA	deletion and complementation of *ras4*
ras4-DF	CTCAATGGCTTGGCCTGCGCCCTGAGTGCCATGACCTC GTCGCGGATC	deletion of *ras4*
ras4-UR	GATCCGCGACGAGGTCATGGCACTCAGGGCGCAGGCC AAGCCATTGAG	deletion of *ras4*
ras5-DF	GCCATGACCGACGCATACCGCCAGCGGCGGCACCCAC GAAATCATGCT	deletion of *ras5*
ras5-UR	AGCATGATTTCGTGGGTGCCGCCGCTGGCGGTATGCGT CGGTCATGGC	deletion of *ras5*
Xbal-*ras5*-UF	AAAAATCTAGACGACCGCCCGTACCGCTACTGGTT	deletion and complementation of *ras5*
EcoRI-*ras5*-DR	AAAAAGAATTCCTCGCGCTTGAGCCTGAACTTGCT	deletion and complementation of *ras5*
XbaI-*ras6*-UF	AAAAATCTAGAACCTGGAGCTTGTGGACGTGCCAG	deletion and complementation of *ras6*

EcoRI-*ras6*-DR	AAAAAGAATTCTCGACGTAGGTGAAGGTGACGCCG	deletion and complementation of *ras6*
ras6-DF	AGGATCACACCATGAGCACCATCAGAGTGGTAAGGGC GTAATCACCCA	deletion of *ras6*
ras6-UR	TGGGTGATTACGCCCTTACCACTCTGATGGTGCTCATG GTGTGATCCT	deletion of *ras6*
pEx18-seqF	GGATGTGCTGCAAGGCGATTAAGTTGG	amplification of deletion mutant construct pEx18
pEx18-seqR	GTGAGCGCAACGCAATTAATGTGAGTTA	amplification of deletion mutant construct pEx18

Supplementary Table 2| Number of base pairs used in BGC9 gene deletion.

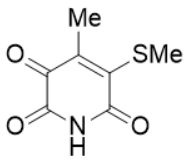
Gene	Gene (bp)	Upstream (bp)	Downstream (bp)	Fusion UD (bp)	Deletion (bp)
ras1	1188	714	910	1624	1156
ras2	783	542	552	1094	505
ras3	1944	491	529	1020	1854
ras4	1125	558	546	1104	998
ras5	1077	529	493	1022	1004
ras6	438	519	583	1102	415

Supplementary Data 1| The fire blight field trials conducted over two years at various locations and involving different apple cultivars are meticulously detailed as follows:

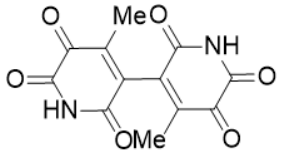
1. In 2022, from May 16 to June 16, the Northwest Michigan Horticultural Research Center near Traverse City, MI (44°88’ 19.96" N, −85°67’ 52.51" W), hosted trials on 5-year-old ‘Buckeye Gala’ apple trees. The daily temperature here ranged from 46°F to 79°F, with humidity levels varying between 51% and 94%. **2.** In 2022, from May 6 to May 24, at Lockwood Farm, part of the Connecticut Agricultural Experiment Station in Hamden (41.406 N, 72.906 W), 40-year-old ‘Spartan’ apple trees were the subjects of the trials. The daily temperature averaged between 54°F and 74°F, with humidity levels fluctuating from 25% to 92%. **3.** In 2023, from May 8 to May 24, 19-year-old ‘Idared’ apple trees at Cornell AgriTech in Geneva, NY (42.864744, -77.025179), were tested. Daily temperatures during this period ranged from 54°F to 71°F, with humidity averages moving between 54% and 83%. **4.** In 2023, from April 21 to May 18, at Lockwood Farm, Connecticut Agricultural Experiment Station in Hamden, CT, trials involved 33-year-old ‘Early Macoun’ apple trees. The observed daily temperatures averaged from 51°F to 73°F, while humidity ranged from 42% to 95%. **5.** In 2023, additional trials were conducted in California from 30 March to 5 May on 25-year-old ‘Bartlett’ pear trees located in Live Oak, CA. The daily temperatures averaged from 46°F to 70°F, and the humidity ranged from 47% to 84%.

Supplementary Data 2| Physicochemical properties of RejuAgro A and B.

Structures of RejuAgro A and B

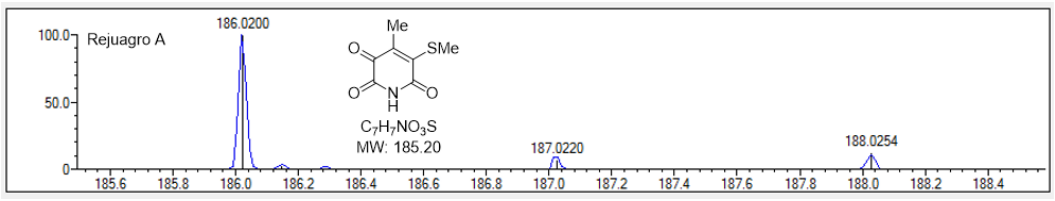


$C_7H_7NO_3S$
MW: 185.20
RejuAgro A

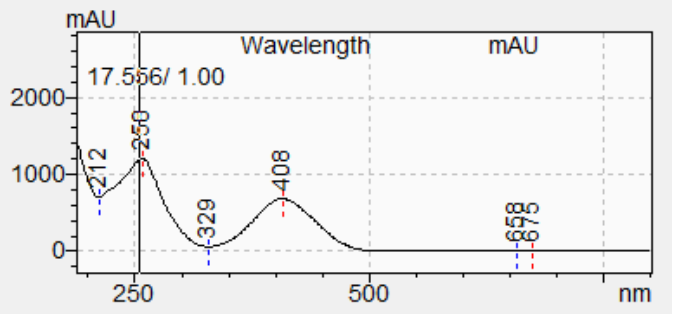


$C_{12}H_8N_2O_6$
MW: 276.20
RejuAgro B

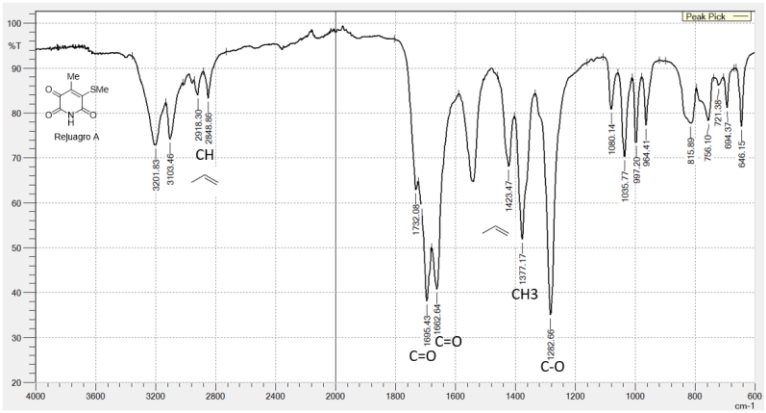
HR-MS of RejuAgro A



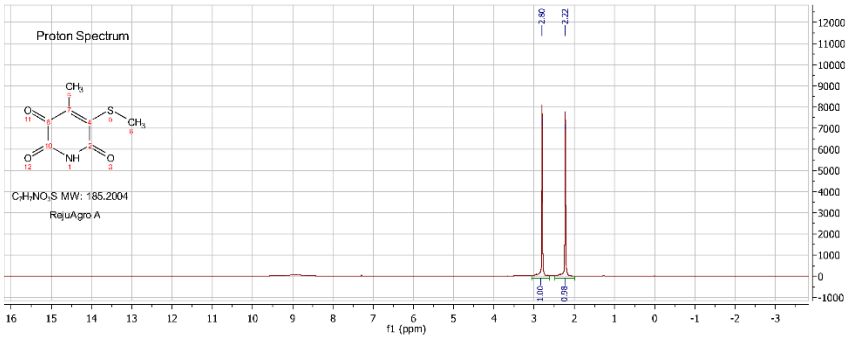
UV spectrum of RejuAgro A



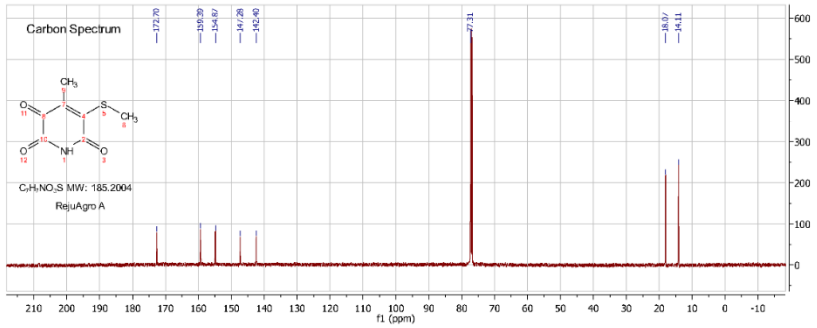
IR spectrum of RejuAgro A



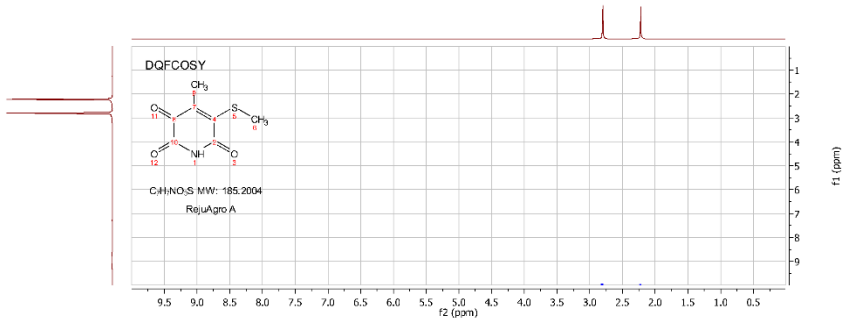
Proton spectrum of RejuAgro A in $CDCl_3$



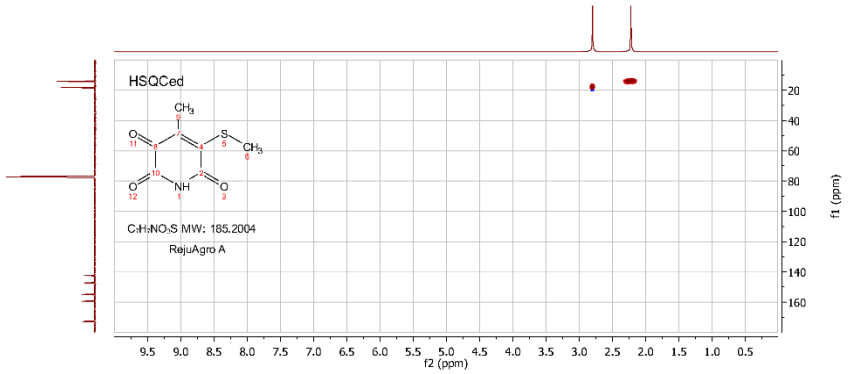
Carbon spectrum of RejuAgro A in $CDCl_3$



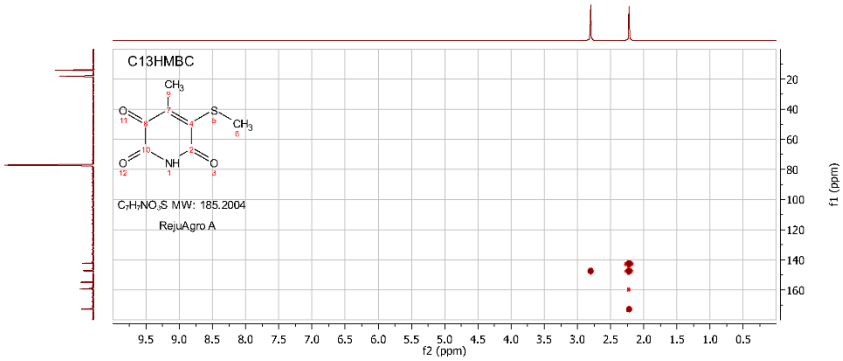
COSY spectrum of RejuAgro A in $CDCl_3$



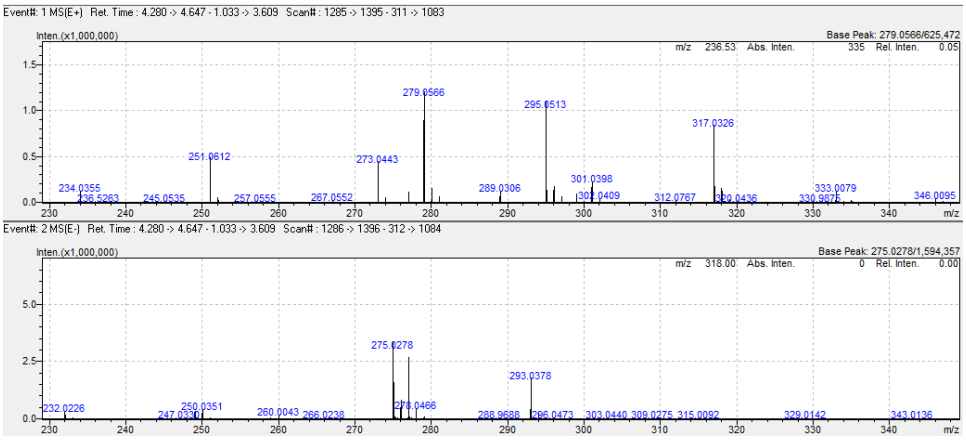
HSQC spectrum of RejuAgro A in $CDCl_3$



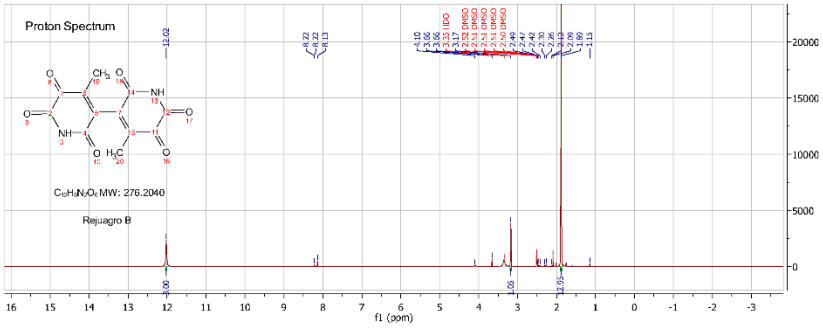
HMBC spectrum of RejuAgro A in $CDCl_3$



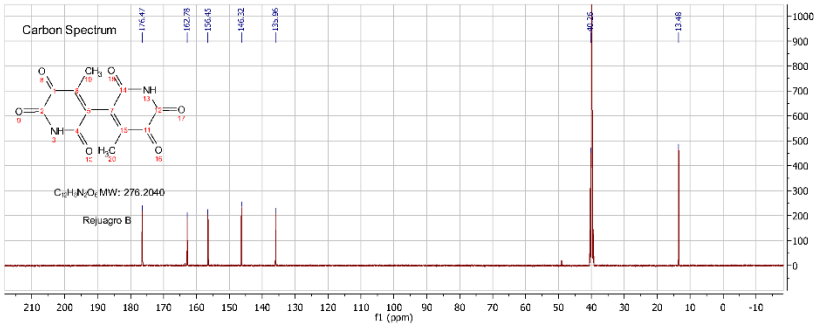
HR-MS of RejuAgro B in positive (up panel) and negative mode (down panel)



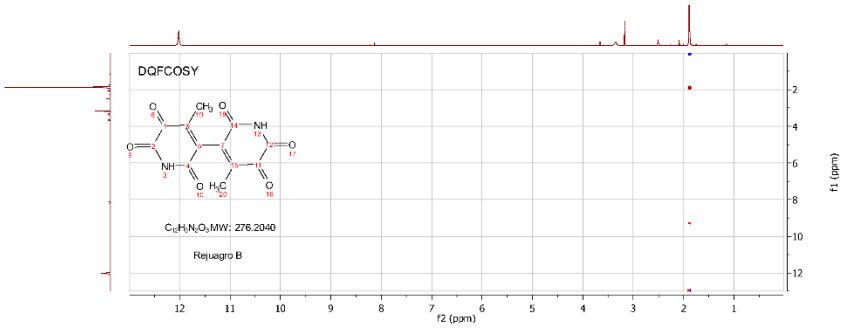
Proton spectrum of RejuAgro B in DMSO-d6



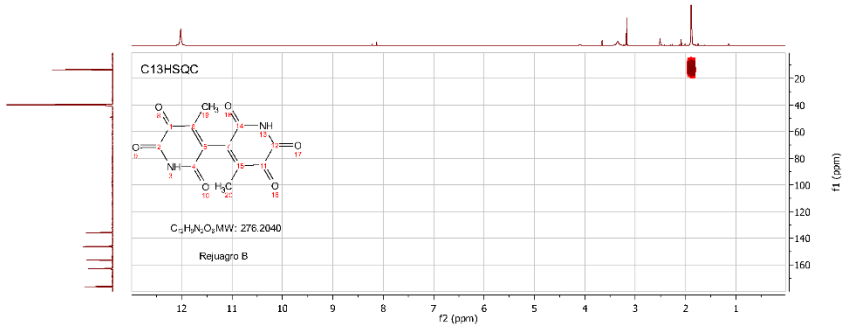
Carbon spectrum of RejuAgro B in DMSO-d6



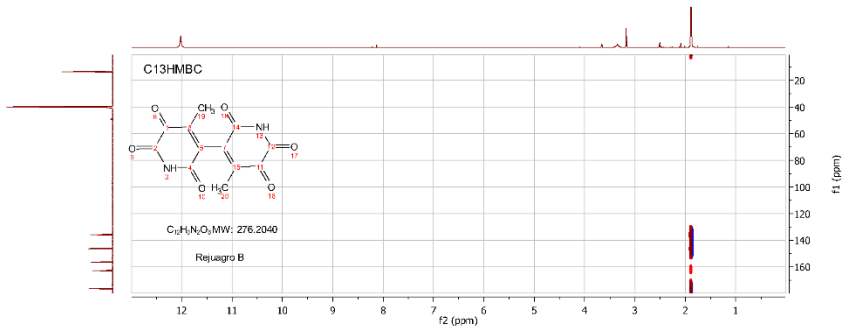
DQF-COSY spectrum of RejuAgro B in DMSO-d6



HSQC_ed spectrum of RejuAgro B in DMSO-d6

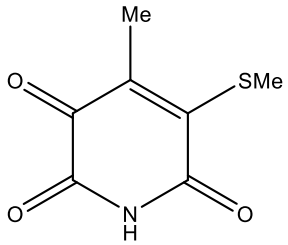


HMBC spectrum of RejuAgro B in DMSO-d6



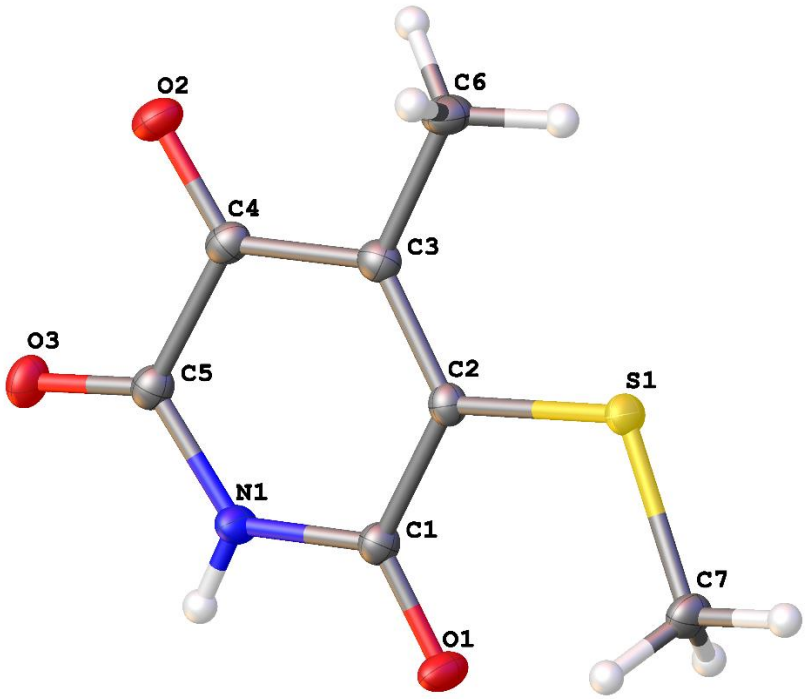
Supplementary Data 3| Crystal structures of RejuAgro A and B.

The crystal structure data of RejuAgro A



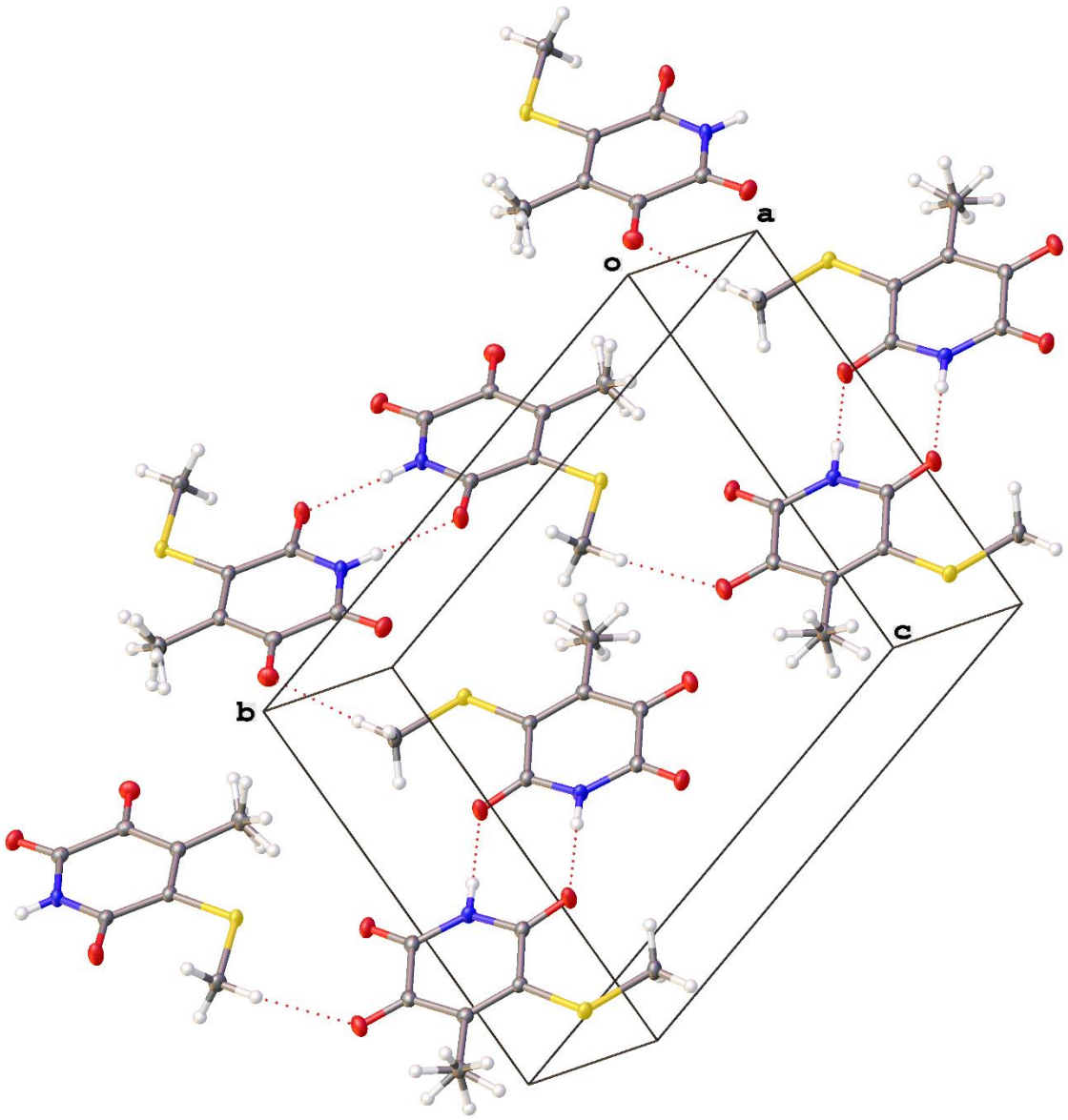
Experimental features:

Orange tablets. The dataset was collected at 100K with an Oxford SuperNova diffractometer using Cu(Kα) radiation.



Structure description:

The molecule has a planar structure – with S-Me group rotated only by 8.7° relative to the heterocycle. There is a notable break of π-conjugation in the molecule at C4-C5 bond (1.531 Å) – apparently, because of some orbital reasons. The Me-group connected to sp^2 carbon atom is rotationally disordered over 2 positions.



Crystal packing:

The molecules in crystal form centrosymmetric H-bonded dimers through N-H…O interactions. Further, these dimers form 2-dimensional layers along [-3 0 1] plane via weaker C-H…O interactions.

Crystal data and structure refinement for RejuAgro A.

Identification code	RejuAgro A
Empirical formula	$C_7H_7NO_3S$
Formula weight	185.20
Temperature/K	100.05(10)
Crystal system	Monoclinic
Space group	$P2_1/n$
a/Å	5.30391(6)
b/Å	13.97822(13)
c/Å	10.74471(13)
α/°	90
β/°	101.5883(12)
γ/°	90
Volume/Å^3	780.367(15)
Z	4
ρ_{calc}g/cm^3	1.576
μ/mm^{-1}	3.429
F(000)	384.0
Crystal size/mm^3	0.874 × 0.274 × 0.118
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.522 to 140.8
Index ranges	$-6 \leq h \leq 6$, $-17 \leq k \leq 17$, $-13 \leq l \leq 12$
Reflections collected	13936
Independent reflections	1496 [R_{int} = 0.0220, R_{sigma} = 0.0083]
Data/restraints/parameters	1496/0/117
Goodness-of-fit on F^2	1.067

Final R indexes [I>=2σ (I)] $R_1 = 0.0253$, $wR_2 = 0.0700$

Final R indexes [all data] $R_1 = 0.0254$, $wR_2 = 0.0702$

Largest diff. peak/hole / e $Å^{-3}$ 0.33/-0.29

Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for RejuAgro A. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*Y*	*z*	U(eq)
S1	6015.2(6)	2181.9(2)	7360.1(3)	14.21(13)
O1	2838.4(18)	479.2(7)	5956.1(10)	21.0(2)
O2	-1864.8(19)	3816.9(7)	4920.5(10)	20.3(2)
O3	-4128.5(19)	2125.4(7)	3998.6(10)	19.1(2)
N1	-625(2)	1317.3(8)	5012.2(11)	14.8(2)
C1	1795(2)	1257.7(9)	5770.8(12)	14.1(3)
C2	3003(2)	2163.2(9)	6326.8(12)	12.9(3)
C3	1866(3)	3025.4(10)	6015.7(12)	14.5(3)
C4	-699(3)	3073.5(10)	5196.4(12)	14.7(3)
C5	-2010(3)	2140.2(9)	4672.1(13)	14.9(3)
C6	3049(3)	3965.2(10)	6489.7(14)	19.0(3)
C7	7080(3)	978.0(10)	7802.9(13)	17.9(3)

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for RejuAgro A. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	12.06(19)	13.72(19)	14.8(2)	-0.65(11)	-2.16(13)	-1.00(10)
O1	18.6(5)	11.9(5)	27.2(5)	-1.4(4)	-7.8(4)	1.5(4)
O2	20.2(5)	15.0(5)	24.3(5)	2.8(4)	1.0(4)	4.3(4)

O3	13.9(5)	22.2(5)	18.4(5)	0.8(4)	-3.7(4)	2.2(4)
N1	13.8(6)	11.8(5)	16.4(6)	-1.3(4)	-2.8(4)	-1.4(4)
C1	13.7(6)	14.9(7)	12.8(6)	1.0(5)	0.3(5)	0.2(5)
C2	11.8(6)	15.1(7)	11.3(6)	-0.5(5)	1.1(5)	-0.6(5)
C3	15.4(6)	14.5(6)	13.4(6)	-0.4(5)	2.6(5)	-0.6(5)
C4	16.1(6)	14.9(6)	13.4(6)	1.7(5)	3.3(5)	2.3(5)
C5	14.9(6)	16.3(7)	13.1(6)	1.4(5)	1.9(5)	1.3(5)
C6	20.7(7)	12.3(6)	21.9(7)	-0.9(5)	-0.8(5)	0.7(5)
C7	15.9(6)	16.6(6)	18.3(7)	2.0(5)	-3.1(5)	2.0(5)

Bond Lengths for RejuAgro A.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C2	1.7529(13)	N1	C5	1.3742(17)
S1	C7	1.8082(14)	C1	C2	1.4886(17)
O1	C1	1.2190(16)	C2	C3	1.3593(18)
O2	C4	1.2150(17)	C3	C4	1.4658(18)
O3	C5	1.2083(18)	C3	C6	1.5002(18)
N1	C1	1.3778(17)	C4	C5	1.5314(18)

Bond Angles for RejuAgro A.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	S1	C7	110.46(6)	C2	C3	C6	123.92(12)
C5	N1	C1	126.34(12)	C4	C3	C6	116.00(12)
O1	C1	N1	119.28(12)	O2	C4	C3	123.44(12)
O1	C1	C2	123.28(12)	O2	C4	C5	117.88(12)
N1	C1	C2	117.44(11)	C3	C4	C5	118.68(11)

C1	C2	S1	122.08(9)	O3	C5	N1	121.87(12)
C3	C2	S1	116.47(10)	O3	C5	C4	122.26(12)
C3	C2	C1	121.41(12)	N1	C5	C4	115.87(12)
C2	C3	C4	120.06(12)				

Hydrogen Bonds for RejuAgro A.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O1[1]	0.845(18)	2.032(19)	2.8768(15)	178.8(17)
C7	H7C	O2[2]	0.98	2.58	3.5549(16)	175.3

[1]-X,-Y,1-Z; [2]3/2+X,1/2-Y,1/2+Z

Torsion Angles for RejuAgro A.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C2	C3	C4	-177.63(9)	C1	C2	C3	C6	-176.67(12)
S1	C2	C3	C6	0.76(18)	C2	C3	C4	O2	177.16(13)
O1	C1	C2	S1	-2.63(19)	C2	C3	C4	C5	-1.90(19)
O1	C1	C2	C3	174.66(13)	C3	C4	C5	O3	179.49(12)
O2	C4	C5	O3	0.4(2)	C3	C4	C5	N1	-0.66(18)
O2	C4	C5	N1	-179.77(11)	C5	N1	C1	O1	-177.26(13)
N1	C1	C2	S1	177.32(9)	C5	N1	C1	C2	2.78(19)
N1	C1	C2	C3	-5.39(19)	C6	C3	C4	O2	-1.36(19)
C1	N1	C5	O3	179.92(13)	C6	C3	C4	C5	179.58(11)
C1	N1	C5	C4	0.07(19)	C7	S1	C2	C1	-8.68(13)
C1	C2	C3	C4	4.9(2)	C7	S1	C2	C3	173.90(10)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for RejuAgro A.

Atom	*X*	*y*	*z*	U(eq)
H1	-1260(30)	789(13)	4721(17)	20(4)
H6A	2408.52	4468.05	5871.25	23
H6B	4925.78	3921.96	6602.43	23
H6C	2587.06	4119.49	7305.04	23
H6D	4205.71	3871.61	7314.56	23
H6E	1688.46	4417.71	6583.38	23
H6F	4027.18	4220.17	5880.78	23
H7A	7306.25	625.34	7044.62	27
H7B	5790.31	654.5	8190.27	27
H7C	8721.96	1001.76	8413.78	27

Atomic Occupancy for RejuAgro A.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
H6A	0.485(15)	H6B	0.515(15)	H6C	0.515(15)
H6D	0.485(15)	H6E	0.515(15)	H6F	0.485(15)

Experimental

Single crystals of $C_7H_7NO_3S$ RejuAgro A were grown by slow evaporation in chloroform. A suitable crystal was selected and loaded on a SuperNova, Dual, Cu at home/near, Atlas diffractometer. The crystal was kept at 100.05(10) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimization.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of RejuAgro A

Crystal Data for $C_7H_7NO_3S$ (*M* =185.20 g/mol): monoclinic, space group $P2_1/n$ (no. 14), *a* = 5.30391(6) Å, *b* = 13.97822(13) Å, *c* = 10.74471(13) Å, *β* = 101.5883(12)°, *V* =

780.367(15) $Å^3$, Z = 4, T = 100.05(10) K, μ(CuKα) = 3.429 mm^{-1}, *Dcalc* = 1.576 g/cm^3, 13936 reflections measured (10.522° ≤ 2Θ ≤ 140.8°), 1496 unique (R_{int} = 0.0220, R_{sigma} = 0.0083) which were used in all calculations. The final R_1 was 0.0253 (I > 2σ(I)) and wR_2 was 0.0702 (all data).

Refinement model description

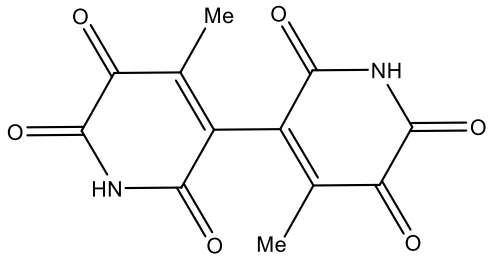
Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H,H,H,H,H,H) groups
 At 1.5 times of:
  All C(H,H,H) groups
2. Others
 Sof(H6A)=Sof(H6D)=Sof(H6F)=1-FVAR(1)
 Sof(H6B)=Sof(H6C)=Sof(H6E)=FVAR(1)
3.a Disordered Me refined as rotating group:
 C6(H6A,H6B,H6C,H6D,H6E,H6F)
3.b Idealised Me refined as rotating group:
 C7(H7A,H7B,H7C)

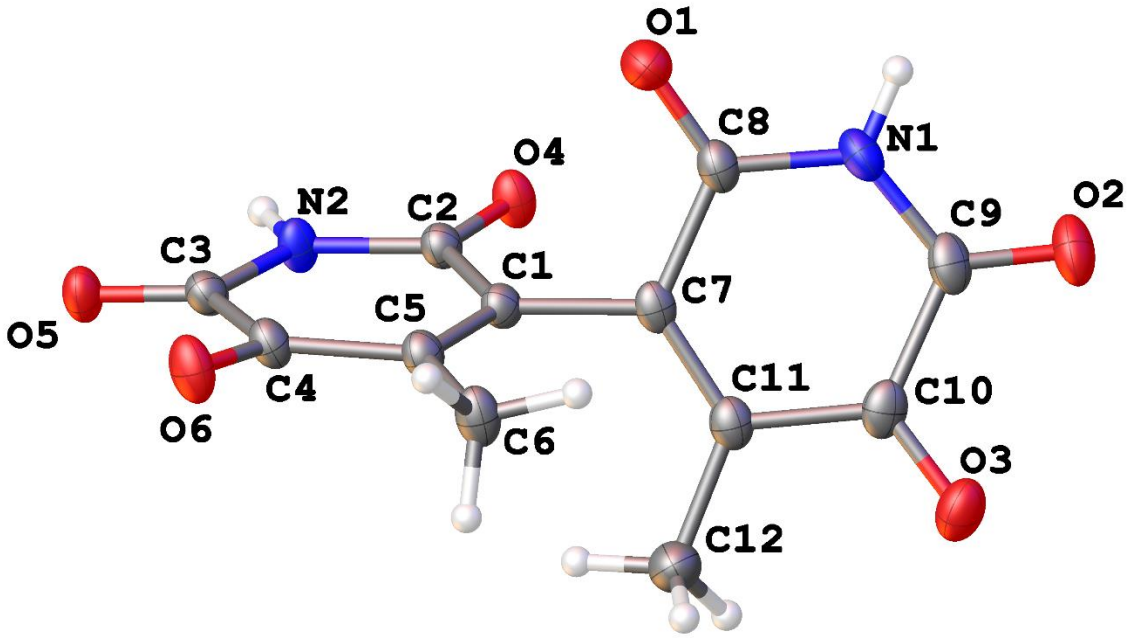
This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys.

The crystal structure data of RejuAgro B



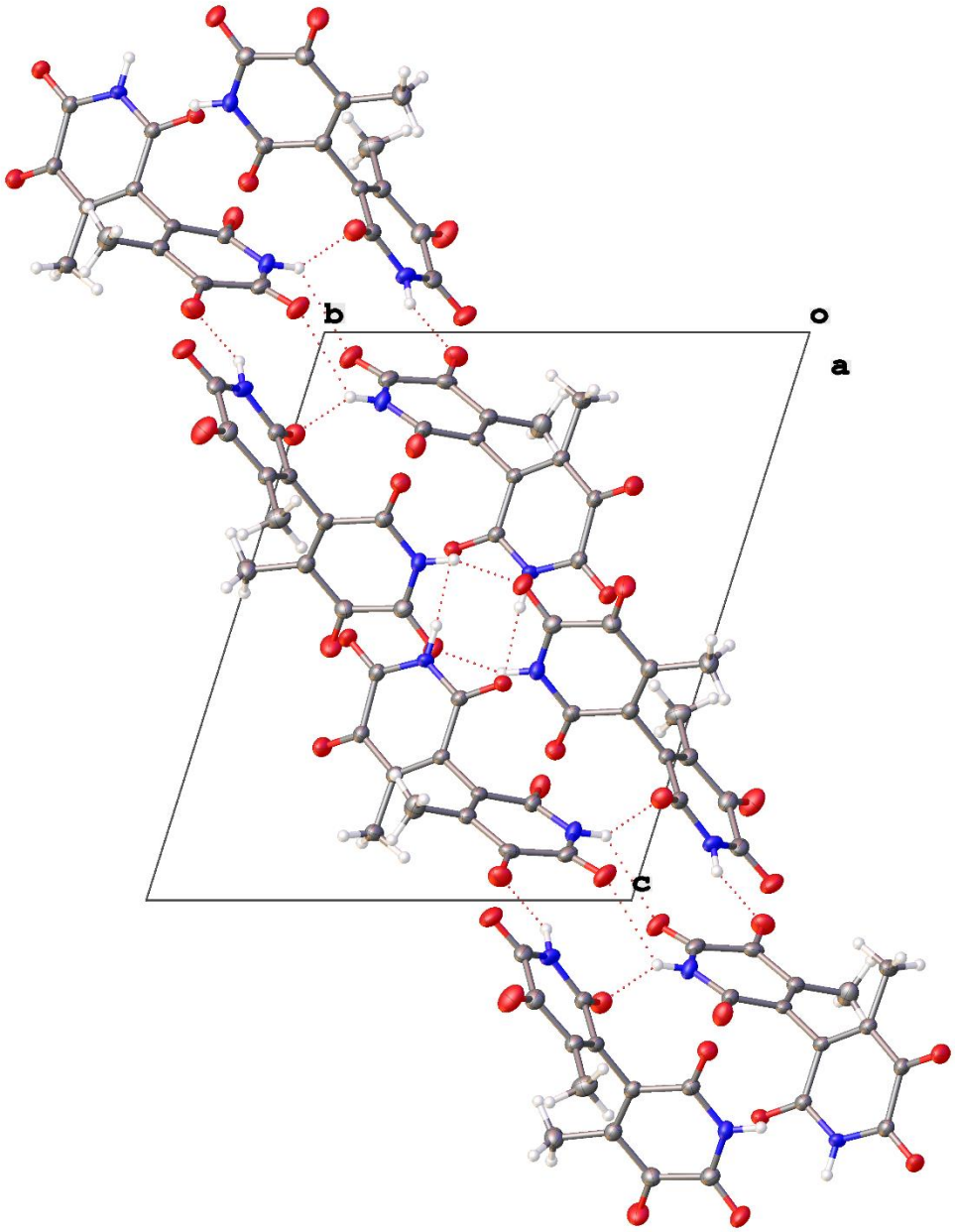
Experimental features:

Orange pyramids. The dataset was collected at 100K with an Oxford SuperNova diffractometer using Cu(Kα) radiation.



Structure description:

The structure contains two symmetrically independent molecules. Each molecule has a twisted structure – with dihedral angle between mean planes of the linked heterocycles of 70. 3 and 80.6°. There is a notable break of π-conjugation in each heterocycle at $C(sp^2)$-$C(sp^2)$ bond between two adjacent carbonyl groups (the bond lengths are in the 1.534-1.539 Å range) – apparently, because of some orbital reasons.



Crystal packing:

The molecules in crystal form centrosymmetric H-bonded dimers through N-H…O interactions. These dimers are linked in stacks along x direction by other N-H…O interactions, Finally, the stacks are linked by third kind of N-H…O interactions into layers along [011].

Crystal data and structure refinement for RejuAgro B.

Identification code	RejuAgro B
Empirical formula	$C_{12}H_8N_2O_6$
Formula weight	276.20
Temperature/K	100.05(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.0528(3)
b/Å	11.7911(5)
c/Å	14.6888(6)
α/°	72.249(4)
β/°	79.265(3)
γ/°	86.633(3)
Volume/Å^3	1143.02(8)
Z	4
ρ_{calc}g/cm^3	1.605
μ/mm^{-1}	1.139
F(000)	568.0
Crystal size/mm^3	0.3 × 0.22 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.872 to 141.144
Index ranges	-8 ≤ h ≤ 8, -12 ≤ k ≤ 14, -17 ≤ l ≤ 17
Reflections collected	15292
Independent reflections	4304 [R_{int} = 0.0258, R_{sigma} = 0.0234]
Data/restraints/parameters	4304/0/365
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0419, wR_2 = 0.1043
Final R indexes [all data]	R_1 = 0.0517, wR_2 = 0.1124
Largest diff. peak/hole / e Å^{-3}	0.31/-0.25

Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for RejuAgro B. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	2961(2)	7383.5(12)	2001.1(11)	31.9(3)
O2	-1826(2)	9293.7(13)	432.4(11)	35.5(4)
O3	-3044(2)	7134.9(13)	421.6(10)	34.1(3)
O4	182(2)	5943.5(11)	3820.2(9)	24.6(3)
O5	3410(2)	2456.2(11)	4624.7(9)	27.0(3)
O6	4494(2)	2636.3(12)	2701.7(10)	31.2(3)
N1	593(2)	8361.8(14)	1206.5(12)	25.6(4)

N2	1809(2)	4204.9(13)	4225.8(11)	22.5(3)
C1	1436(3)	5154.4(16)	2526.1(12)	19.3(4)
C2	1083(3)	5152.6(16)	3557.2(13)	20.0(4)
C3	2860(3)	3281.2(16)	4009.9(13)	21.6(4)
C4	3360(3)	3353.0(16)	2929.1(13)	22.3(4)
C5	2479(3)	4308.1(16)	2217.5(13)	21.0(4)
C6	2868(3)	4264.1(17)	1193.1(13)	27.0(4)
C7	537(3)	6175.3(16)	1875.4(12)	19.6(4)
C8	1477(3)	7336.7(16)	1708.5(13)	22.7(4)
C9	-1015(3)	8384.0(17)	814.7(13)	25.8(4)
C10	-1777(3)	7166.6(18)	869.1(13)	24.7(4)
C11	-992(3)	6069.0(16)	1488.2(13)	22.5(4)
C12	-2025(3)	4934.9(19)	1648.0(16)	33.7(5)
O1A	3249(2)	2542.2(12)	7353.0(10)	29.1(3)
O2A	6867(2)	4284.9(12)	4433.3(10)	33.3(3)
O3A	8705(2)	2165.5(13)	4475.5(11)	36.7(4)
O4A	7213(2)	37.3(12)	8198.9(10)	30.6(3)
O5A	2666(2)	-2784.5(13)	9706.4(10)	36.6(4)
O6A	580(2)	-1850.3(14)	8272.4(12)	42.8(4)
N1A	5218(2)	3432.4(14)	5950.6(11)	24.6(4)
N2A	4869(2)	-1309.3(14)	9003.5(11)	26.3(4)
C1A	4443(3)	197.8(16)	7467.5(13)	21.3(4)
C2A	5632(3)	-339.4(16)	8237.7(13)	23.9(4)
C3A	3220(3)	-1884.4(17)	9063.4(14)	27.5(4)
C4A	2026(3)	-1349.2(18)	8259.8(15)	27.9(4)
C5A	2747(3)	-250.9(17)	7474.9(14)	24.8(4)
C6A	1500(3)	238(2)	6728.1(15)	33.8(5)
C7A	5314(3)	1250.6(16)	6665.8(13)	20.2(4)
C8A	4511(3)	2434.0(16)	6711.8(13)	21.9(4)
C9A	6479(3)	3408.2(17)	5139.6(14)	25.0(4)
C10A	7408(3)	2197.3(17)	5129.5(14)	25.4(4)
C11A	6631(3)	1122.0(16)	5922.8(13)	23.0(4)
C12A	7343(3)	-57.7(18)	5817.8(15)	30.6(5)

Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for RejuAgro B. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	33.5(8)	24.6(7)	37.9(8)	-5.9(6)	-12.5(6)	-2.0(6)
O2	38.2(8)	25.5(8)	32.6(8)	3.8(6)	-4.8(6)	7.4(6)
O3	39.2(8)	37.3(8)	28.2(7)	-9.7(6)	-15.1(6)	8.0(7)

O4	34.1(7)	21.0(7)	17.2(6)	-5.5(5)	-3.2(5)	6.3(6)
O5	40.0(8)	19.7(7)	21.1(7)	-3.3(5)	-11.5(6)	5.2(6)
O6	41.1(8)	23.2(7)	25.3(7)	-5.6(6)	-2.6(6)	10.7(6)
N1	30.1(9)	15.4(8)	28.0(9)	-2.9(6)	-3.1(7)	0.5(6)
N2	34.8(9)	19.1(8)	12.8(7)	-4.1(6)	-5.5(6)	5.0(7)
C1	23.4(9)	17.5(9)	15.2(8)	-2.4(7)	-3.1(7)	-1.0(7)
C2	23.7(9)	17.6(9)	17.2(9)	-3.0(7)	-3.7(7)	-0.5(7)
C3	26.6(10)	17.2(9)	20.6(9)	-4.0(7)	-5.6(7)	-1.3(7)
C4	28.7(10)	16.2(9)	19.8(9)	-3.5(7)	-2.9(7)	1.3(7)
C5	24.8(9)	18.4(9)	17.6(9)	-2.8(7)	-3.0(7)	0.1(7)
C6	37.7(11)	23.1(10)	19.0(9)	-6.5(8)	-4.0(8)	7.2(8)
C7	25.6(9)	18.4(9)	12.8(8)	-4.1(7)	-0.3(7)	3.2(7)
C8	28.1(10)	18.4(9)	19.3(9)	-3.6(7)	-2.9(7)	2.8(7)
C9	30.7(10)	23.1(10)	17.2(9)	-0.2(8)	0.7(7)	4.0(8)
C10	28.7(10)	29.8(10)	14.7(9)	-6.4(8)	-3.6(7)	5.9(8)
C11	27.1(10)	21.4(9)	17.4(9)	-5.2(7)	-2.1(7)	3.4(8)
C12	36.9(12)	28.6(11)	37.8(12)	-7.7(9)	-15.5(9)	-1.4(9)
O1A	32.5(8)	26.5(7)	25.4(7)	-7.3(6)	-0.5(6)	6.2(6)
O2A	40.9(8)	21.2(7)	29.3(8)	0.0(6)	2.0(6)	-1.0(6)
O3A	39.6(9)	29.7(8)	33.2(8)	-7.5(6)	9.6(7)	-1.9(6)
O4A	32.5(8)	28.8(8)	30.1(8)	-5.3(6)	-10.7(6)	0.1(6)
O5A	46.2(9)	28.2(8)	25.3(8)	2.1(6)	1.6(6)	-0.1(7)
O6A	36.0(9)	34.1(9)	49.6(10)	1.6(7)	-7.1(7)	-7.7(7)
N1A	31.8(9)	16.0(8)	24.2(8)	-5.0(6)	-2.8(7)	2.3(6)
N2A	34.6(9)	22.7(8)	17.8(8)	-1.0(6)	-6.1(7)	6.9(7)
C1A	27.1(10)	17.8(9)	16.7(9)	-4.0(7)	-1.4(7)	4.1(7)
C2A	30.6(10)	19.3(9)	20.4(9)	-4.8(7)	-3.9(8)	4.6(8)
C3A	32.7(11)	23.7(10)	21.9(10)	-6.4(8)	3.9(8)	3.7(8)
C4A	27.6(10)	25.1(10)	27.8(10)	-6.4(8)	0.4(8)	1.3(8)
C5A	28.8(10)	22.0(10)	21.0(9)	-4.6(8)	-1.3(8)	0.6(8)
C6A	30.4(11)	39.5(12)	28.2(11)	-3.0(9)	-7.5(8)	-5.5(9)
C7A	22.8(9)	18.2(9)	19.1(9)	-2.7(7)	-7.0(7)	0.0(7)
C8A	25.6(9)	20.7(9)	18.5(9)	-3.5(7)	-6.1(7)	1.4(7)
C9A	26.2(10)	24.4(10)	22.8(10)	-4.9(8)	-3.2(8)	-2.2(8)
C10A	26.5(10)	24.8(10)	23.7(10)	-7.3(8)	-0.9(8)	-2.1(8)
C11A	25.5(9)	20.3(9)	22.7(9)	-5.1(7)	-5.4(7)	-0.1(7)
C12A	33.3(11)	25.6(10)	30.4(11)	-9.9(9)	3.0(8)	-0.3(8)

Bond Lengths for RejuAgro B.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

O1	C8	1.213(2)	O1A	C8A	1.202(2)
O2	C9	1.214(2)	O2A	C9A	1.222(2)
O3	C10	1.212(2)	O3A	C10A	1.205(2)
O4	C2	1.217(2)	O4A	C2A	1.209(2)
O5	C3	1.210(2)	O5A	C3A	1.213(2)
O6	C4	1.208(2)	O6A	C4A	1.203(3)
N1	C8	1.390(2)	N1A	C8A	1.394(2)
N1	C9	1.360(3)	N1A	C9A	1.354(2)
N2	C2	1.388(2)	N2A	C2A	1.388(2)
N2	C3	1.366(2)	N2A	C3A	1.356(3)
C1	C2	1.488(2)	C1A	C2A	1.496(3)
C1	C5	1.344(3)	C1A	C5A	1.333(3)
C1	C7	1.483(2)	C1A	C7A	1.495(2)
C3	C4	1.538(3)	C3A	C4A	1.534(3)
C4	C5	1.480(3)	C4A	C5A	1.488(3)
C5	C6	1.495(3)	C5A	C6A	1.491(3)
C7	C8	1.489(3)	C7A	C8A	1.491(3)
C7	C11	1.338(3)	C7A	C11A	1.335(3)
C9	C10	1.537(3)	C9A	C10A	1.539(3)
C10	C11	1.481(3)	C10A	C11A	1.486(3)
C11	C12	1.494(3)	C11A	C12A	1.493(3)

Bond Angles for RejuAgro B.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	N1	C8	125.07(16)	C9A	N1A	C8A	125.23(16)
C3	N2	C2	125.15(15)	C3A	N2A	C2A	125.18(17)
C5	C1	C2	122.84(16)	C5A	C1A	C2A	122.52(17)
C5	C1	C7	123.43(16)	C5A	C1A	C7A	121.91(17)
C7	C1	C2	113.73(15)	C7A	C1A	C2A	115.53(16)
O4	C2	N2	120.22(16)	O4A	C2A	N2A	120.41(17)
O4	C2	C1	122.04(16)	O4A	C2A	C1A	122.03(17)
N2	C2	C1	117.74(15)	N2A	C2A	C1A	117.55(17)
O5	C3	N2	122.60(17)	O5A	C3A	N2A	123.6(2)
O5	C3	C4	121.02(17)	O5A	C3A	C4A	119.50(19)
N2	C3	C4	116.37(15)	N2A	C3A	C4A	116.89(17)
O6	C4	C3	117.92(16)	O6A	C4A	C3A	118.93(18)
O6	C4	C5	123.19(17)	O6A	C4A	C5A	122.62(19)
C5	C4	C3	118.87(16)	C5A	C4A	C3A	118.42(17)
C1	C5	C4	118.55(16)	C1A	C5A	C4A	119.10(18)
C1	C5	C6	125.01(17)	C1A	C5A	C6A	125.12(18)

C4	C5	C6	116.43(16)	C4A	C5A	C6A	115.74(17)
C1	C7	C8	113.48(16)	C8A	C7A	C1A	115.80(16)
C11	C7	C1	123.39(16)	C11A	C7A	C1A	121.49(17)
C11	C7	C8	123.12(17)	C11A	C7A	C8A	122.54(16)
O1	C8	N1	121.37(17)	O1A	C8A	N1A	120.00(17)
O1	C8	C7	121.04(17)	O1A	C8A	C7A	122.46(17)
N1	C8	C7	117.59(17)	N1A	C8A	C7A	117.48(16)
O2	C9	N1	123.67(19)	O2A	C9A	N1A	123.12(18)
O2	C9	C10	120.36(19)	O2A	C9A	C10A	120.17(17)
N1	C9	C10	115.97(16)	N1A	C9A	C10A	116.70(16)
O3	C10	C9	118.81(17)	O3A	C10A	C9A	118.60(17)
O3	C10	C11	121.85(19)	O3A	C10A	C11A	123.38(18)
C11	C10	C9	119.32(17)	C11A	C10A	C9A	118.00(16)
C7	C11	C10	117.85(17)	C7A	C11A	C10A	119.31(17)
C7	C11	C12	125.55(17)	C7A	C11A	C12A	123.69(17)
C10	C11	C12	116.58(17)	C10A	C11A	C12A	116.97(17)

Hydrogen Bonds for RejuAgro B.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O2[1]	0.88	2.51	3.104(2)	125.1
N1	H1	O4A[2]	0.88	2.17	2.928(2)	143.6
N2	H2	O4[3]	0.88	2.09	2.909(2)	154.7
N1A	H1A	O2A[2]	0.88	2.14	2.940(2)	150.8
N2A	H2A	O3[4]	0.88	2.08	2.892(2)	153.8

[1]-X,2-Y,-Z; [2]1-X,1-Y,1-Z; [3]-X,1-Y,1-Z; [4]1+X,-1+Y,1+Z

Torsion Angles for RejuAgro B.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O2	C9	C10	O3	9.1(3)	O2A	C9A	C10A	O3A	10.0(3)
O2	C9	C10	C11	-169.03(18)	O2A	C9A	C10A	C11A	-169.05(18)
O3	C10	C11	C7	173.21(18)	O3A	C10A	C11A	C7A	173.9(2)
O3	C10	C11	C12	-8.5(3)	O3A	C10A	C11A	C12A	-8.1(3)
O5	C3	C4	O6	-8.1(3)	O5A	C3A	C4A	O6A	-1.6(3)
O5	C3	C4	C5	173.42(17)	O5A	C3A	C4A	C5A	-179.46(18)
O6	C4	C5	C1	-171.34(18)	O6A	C4A	C5A	C1A	-174.5(2)
O6	C4	C5	C6	7.3(3)	O6A	C4A	C5A	C6A	3.5(3)
N1	C9	C10	O3	-170.34(17)	N1A	C9A	C10A	O3A	-171.13(19)
N1	C9	C10	C11	11.5(2)	N1A	C9A	C10A	C11A	9.8(3)

N2	C3	C4	O6	170.50(17)	N2A	C3A	C4A	O6A	178.04(19)
N2	C3	C4	C5	-7.9(2)	N2A	C3A	C4A	C5A	0.2(3)
C1	C7	C8	O1	7.7(3)	C1A	C7A	C8A	O1A	0.3(3)
C1	C7	C8	N1	-172.31(16)	C1A	C7A	C8A	N1A	-176.82(16)
C1	C7	C11	C10	178.53(16)	C1A	C7A	C11A	C10A	178.16(17)
C1	C7	C11	C12	0.4(3)	C1A	C7A	C11A	C12A	0.3(3)
C2	N2	C3	O5	-177.67(18)	C2A	N2A	C3A	O5A	174.19(19)
C2	N2	C3	C4	3.7(3)	C2A	N2A	C3A	C4A	-5.5(3)
C2	C1	C5	C4	-1.8(3)	C2A	C1A	C5A	C4A	-1.9(3)
C2	C1	C5	C6	179.67(17)	C2A	C1A	C5A	C6A	-179.68(19)
C2	C1	C7	C8	70.3(2)	C2A	C1A	C7A	C8A	-103.24(19)
C2	C1	C7	C11	-108.6(2)	C2A	C1A	C7A	C11A	81.3(2)
C3	N2	C2	O4	-179.02(17)	C3A	N2A	C2A	O4A	-172.19(18)
C3	N2	C2	C1	1.4(3)	C3A	N2A	C2A	C1A	6.9(3)
C3	C4	C5	C1	7.0(3)	C3A	C4A	C5A	C1A	3.3(3)
C3	C4	C5	C6	-174.34(16)	C3A	C4A	C5A	C6A	-178.77(18)
C5	C1	C2	O4	177.87(18)	C5A	C1A	C2A	O4A	176.18(19)
C5	C1	C2	N2	-2.6(3)	C5A	C1A	C2A	N2A	-2.9(3)
C5	C1	C7	C8	-109.5(2)	C5A	C1A	C7A	C8A	78.8(2)
C5	C1	C7	C11	71.6(3)	C5A	C1A	C7A	C11A	-96.6(2)
C7	C1	C2	O4	-2.0(3)	C7A	C1A	C2A	O4A	-1.8(3)
C7	C1	C2	N2	177.59(16)	C7A	C1A	C2A	N2A	179.16(16)
C7	C1	C5	C4	178.00(16)	C7A	C1A	C5A	C4A	175.89(17)
C7	C1	C5	C6	-0.5(3)	C7A	C1A	C5A	C6A	-1.9(3)
C8	N1	C9	O2	175.24(18)	C8A	N1A	C9A	O2A	169.92(19)
C8	N1	C9	C10	-5.4(3)	C8A	N1A	C9A	C10A	-8.9(3)
C8	C7	C11	C10	-0.3(3)	C8A	C7A	C11A	C10A	3.0(3)
C8	C7	C11	C12	-178.45(18)	C8A	C7A	C11A	C12A	-174.84(18)
C9	N1	C8	O1	176.67(18)	C9A	N1A	C8A	O1A	-172.43(18)
C9	N1	C8	C7	-3.3(3)	C9A	N1A	C8A	C7A	4.8(3)
C9	C10	C11	C7	-8.7(3)	C9A	C10A	C11A	C7A	-7.1(3)
C9	C10	C11	C12	169.60(17)	C9A	C10A	C11A	C12A	170.89(17)
C11	C7	C8	O1	-173.40(18)	C11A	C7A	C8A	O1A	175.71(19)
C11	C7	C8	N1	6.6(3)	C11A	C7A	C8A	N1A	-1.4(3)

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for RejuAgro B.

Atom	*x*	*y*	*z*	U(eq)
H1	1115.22	9049.78	1137.02	31
H2	1572.72	4198.81	4837.04	27

H6A	4232.36	4076.12	1013.7	40
H6B	2564.31	5038.79	758.38	40
H6C	2062.97	3648.38	1135.45	40
H12A	-1685.96	4670.99	1066.64	51
H12B	-3421.18	5067.41	1777.57	51
H12C	-1645.33	4322.49	2204.55	51
H1A	4812.5	4134.48	6001.06	30
H2A	5506.16	-1572.03	9488.94	32
H6AC	1266.79	-381.27	6443.7	51
H6AA	2147.29	916.19	6217.2	51
H6AB	266.47	500.23	7032.58	51
H12D	6459.43	-365.46	5507.86	46
H12E	7403.89	-616.99	6460.59	46
H12F	8633.15	35.4	5415.92	46

Experimental

Single crystals of $C_{12}H_8N_2O_6$ **[RejuAgro B]** were **grown by slow evaporation in chloroform.** A suitable crystal was selected and **mounted** on a **SuperNova, Dual, Cu at home/near, Atlas** diffractometer. The crystal was kept at 100.05(10) K during data collection. Using Olex2 [1], the structure was solved with the XS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [RejuAgro B]

Crystal Data for $C_{12}H_8N_2O_6$ (M =276.20 g/mol): triclinic, space group P-1 (no. 2), a = 7.0528(3) Å, b = 11.7911(5) Å, c = 14.6888(6) Å, α = 72.249(4)°, β = 79.265(3)°, γ = 86.633(3)°, V = 1143.02(8) Å^3, Z = 4, T = 100.05(10) K, μ(CuKα) = 1.139 mm^{-1}, $Dcalc$ = 1.605 g/cm^3, 15292 reflections measured (7.872° ≤ 2Θ ≤ 141.144°), 4304 unique (R_{int} = 0.0258, R_{sigma} = 0.0234) which were used in all calculations. The final R_1 was 0.0419 (I > 2σ(I)) and wR_2 was 0.1124 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:
1. Fixed Uiso
At 1.2 times of:
All N(H) groups
At 1.5 times of:
All C(H,H,H) groups
2.a Aromatic/amide H refined with riding coordinates:
N1(H1), N2(H2), N1A(H1A), N2A(H2A)

2.b Idealised Me refined as rotating group:
C6(H6A,H6B,H6C), C12(H12A,H12B,H12C), C6A(H6AC,H6AA,H6AB), C12A(H12D,H12E,H12F)

This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys.