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Betti reaction of 2-naphthol, furfural, and acetamide: an unexpected case of secondary carbo-Piancatelli rearrangement

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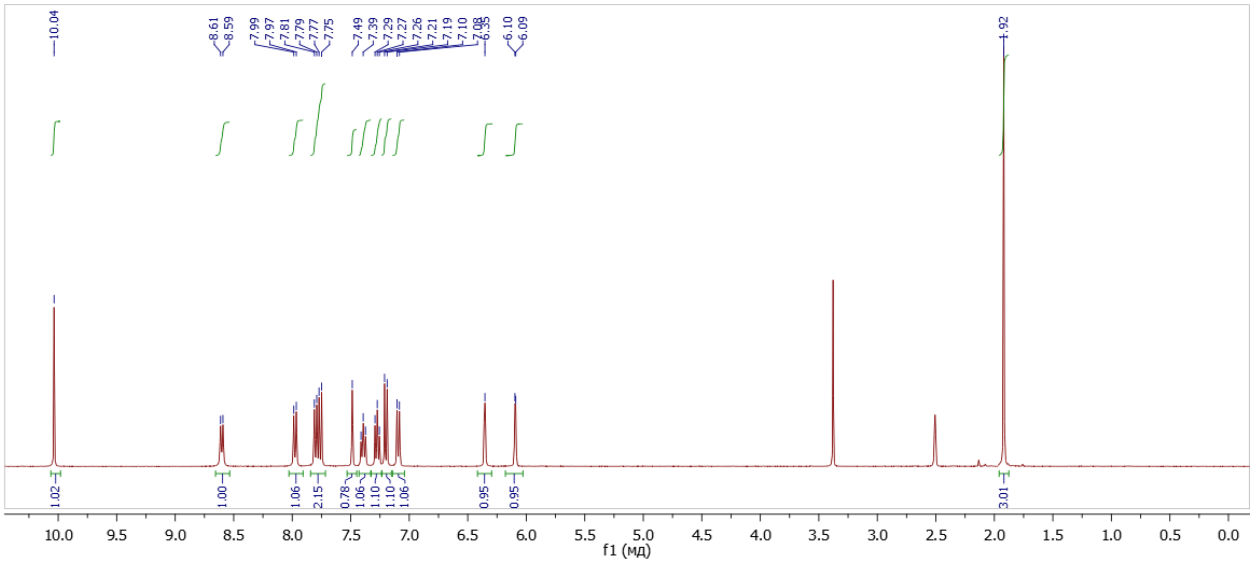
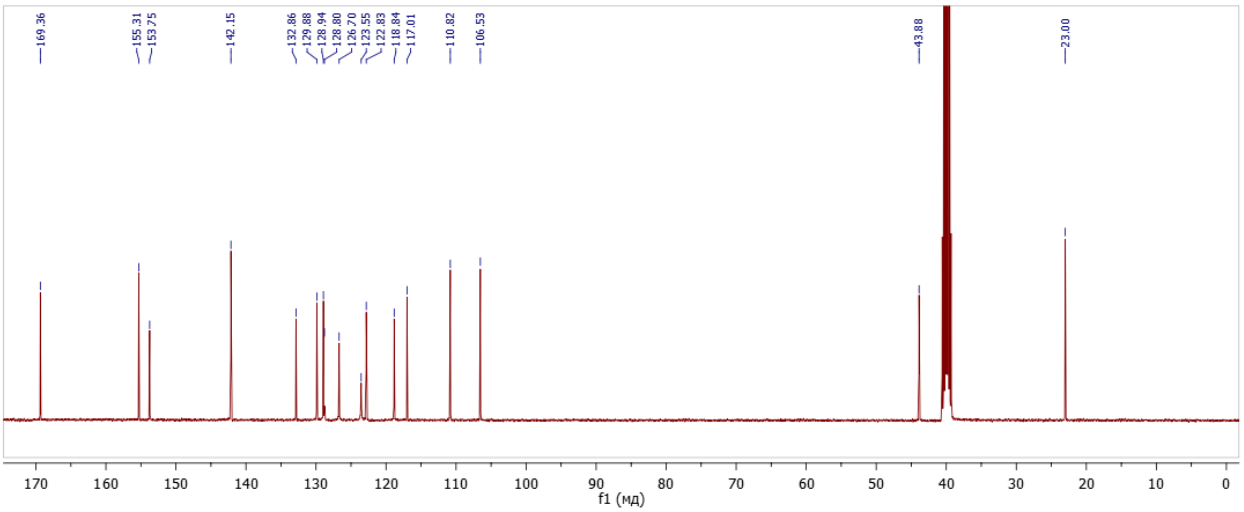
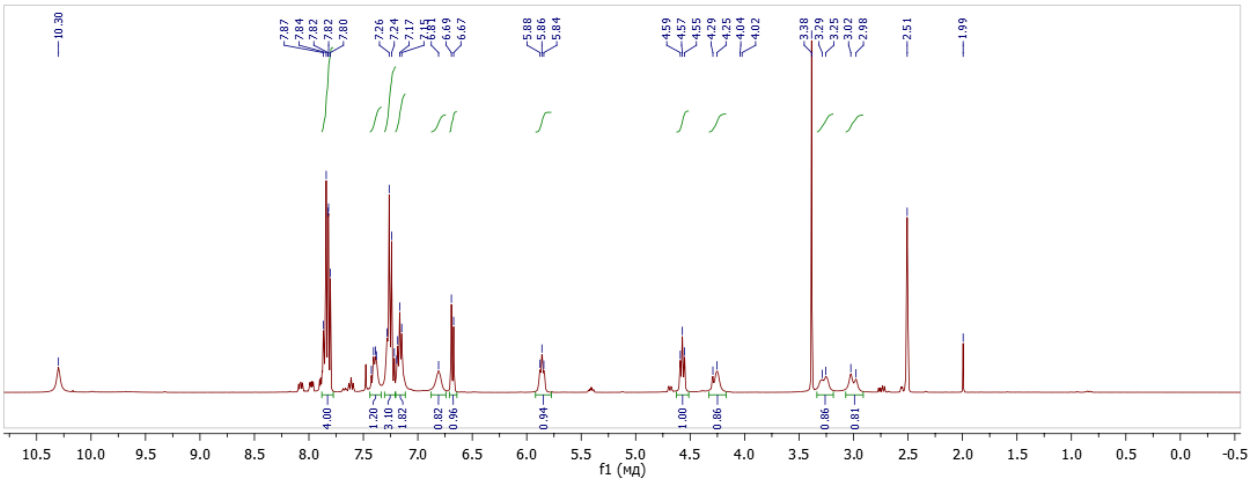
SUPPLEMENTARY INFORMATION

N-[furan-2-yl(2-hydroxynaphthalen-1-yl)methyl]acetamide (**1**):





(7aS*,10S*,10aS*)-10-(2-hydroxynaphthalen-1-yl)-10,10a-dihydro-7aH-cyclopenta[b]naphtho[1,2-d]furan-9(8H)-one (**2**):



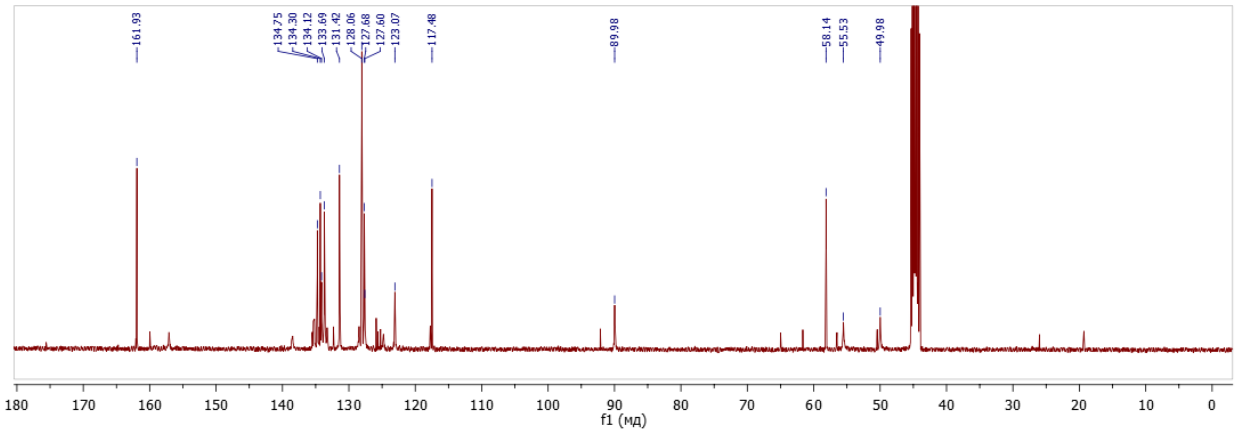
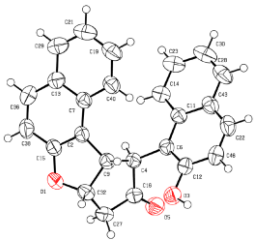


Table 1 Crystal data and structure refinement for (7aS*,10S*,10aS*)-10-(2-hydroxynaphthalen-1-yl)-10,10a-dihydro-7aH-cyclopenta[b]naphtho[1,2-d]furan-9(8H)-one 2.



CCDC	1868665
Empirical formula	$C_{25}H_{18}O_3$
Formula weight	366.39
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	9.66050(10)
b/Å	18.1342(3)
c/Å	20.4799(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3587.78(9)
Z	8
ρ_{calc}g/cm^3	1.357
μ/mm^{-1}	0.707
F(000)	1536.0
Crystal size/mm^3	0.38 × 0.336 × 0.165
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.636 to 152.378
Index ranges	-11 ≤ h ≤ 12, -20 ≤ k ≤ 22, -20 ≤ l ≤ 25
Reflections collected	20305
Independent reflections	3730 [R_{int} = 0.0244, R_{sigma} = 0.0158]
Data/restraints/parameters	3730/0/257
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0388, wR_2 = 0.1007
Final R indexes [all data]	R_1 = 0.0434, wR_2 = 0.1055
Largest diff. peak/hole / e Å^{-3}	0.13/-0.18