Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Three-component synthesis and anticancer evaluation of polycyclic indenopyridines lead to the discovery of a novel indenoheterocycle with potent apoptosis inducing properties

Madhuri Manpadi, Pavel Y. Uglinskii, Shiva K. Rastogi, Karen M. Cotter, Yin-Shan C. Wong, Lisa A. Anderson, Amber J. Ortega, Severine Van slambrouck, Wim F. A. Steelant, Snezna Rogelj, Paul Tongwa, Mikhail Yu. Antipin, Igor V. Magedov,* and Alexander Kornienko*

Departments of Chemistry, New Mexico Institute of Mining and Technology, Socorro, New Mexico 87801, USA, E-mail: akornien@nmt.edu; Fax: +1 505 8355364; Tel: +1 505 8355884
Department of Organic Chemistry, Timiryazev Agriculture Academy, Moscow 127550, Russia, E-mail: ibs@timacad.ru
Departments of Biology, New Mexico Institute of Mining and Technology, Socorro, New Mexico 87801, USA
Department of Natural Sciences, New Mexico Highlands University, Las Vegas, New Mexico 87701, USA
Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russia

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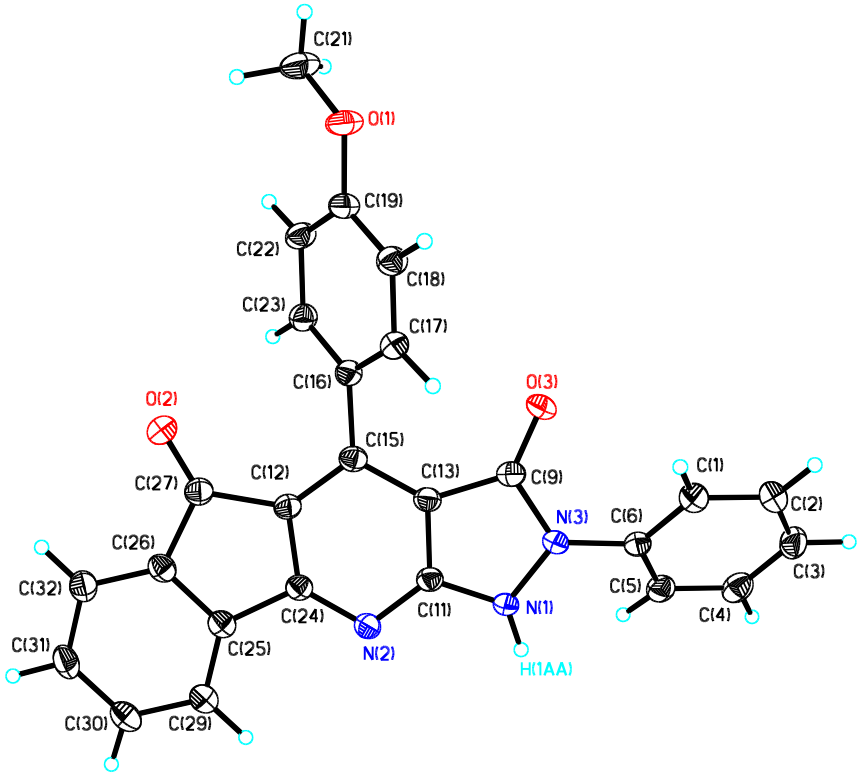
X-ray Crystallographic Data for Compound 27.

X-ray structure determination. Details of the crystal data, data collection and structure refinement parameters for compound **27** presented in **Table 1**. Single crystal X-ray diffraction for **27** experiment was carried out with CCD area detector (graphite monochromated Mo Kα radiation, λ = 0.71073 Å, *ω*-scans with a 0.3° step in *ω* and 10 s per frame exposure) at 250K. Semi-empirical method SADABS[1] was applied for absorption correction. The structure was solved by direct methods and refined by the full-matrix least-squares technique against F^2 with the anisotropic temperature parameters for all non-hydrogen atoms.

All H atoms (except H(1N1), H(1N2), H(2N2), H(1N5), H(2N5), H(1W) and H(2W), were geometrically placed (C—H = 0.95 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The H(1N1), H(1N2), H(2N2), H(1N5), H(2N5), H(1W) and H(2W) atoms were placed in idealized locations, then refined as riding with $U_{iso}(H) = 1.2U_{eq}(N)$ and $U_{iso}(H) = 1.2U_{eq}(O)$ respectively. Data reduction and further calculations were performed using SAINT+[2] and SHELXTL NT[3] program packages.

X-ray structure of 27 (50% probability thermal ellipsoids).



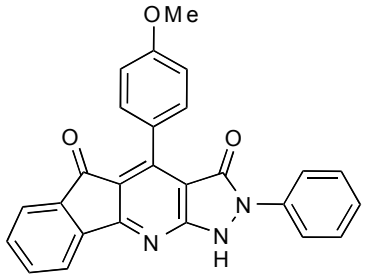


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Table 1. Crystal data and structure refinement for **27**.

Identification code	**27**
Empirical formula	$C_{26}H_{17}N_3O_3$
Formula weight	419.43
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*P bca*
Unit cell dimensions	a = 11.3871(16) Å
	b = 18.131(3) Å
	c = 19.855(3) Å
Volume	4099.2(10) $Å^3$
Z	8
Density (calculated)	1.359 Mg/m^3
Absorption coefficient	0.091 mm^{-1}
F(000)	1744
Crystal size	0.50 x 0.30 x 0.20 mm^3
Theta range for data collection	2.05 to 29.00°.
Index ranges	-15<=h<=15, -24<=k<=24, -27<=l<=27
Reflections collected	69722
Independent reflections	5418 [R(int) = 0.0911]
Completeness to theta = 29.00°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9720 and 0.9459
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5418 / 0 / 353
Goodness-of-fit on F^2	0.998
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.0893
R indices (all data)	R1 = 0.0849, wR2 = 0.1028
Largest diff. peak and hole	0.466 and -0.522 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **27**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)

O(1)	-985(1)	1640(1)	3245(1)	29(1)
O(2)	3188(1)	1752(1)	5109(1)	31(1)
O(3)	2859(1)	-243(1)	2517(1)	32(1)
N(1)	5729(1)	-510(1)	3049(1)	22(1)
N(2)	6052(1)	198(1)	4037(1)	21(1)
N(3)	4815(1)	-570(1)	2577(1)	22(1)
C(1)	4177(2)	-1086(1)	1512(1)	27(1)
C(2)	4159(2)	-1664(1)	1054(1)	32(1)
C(3)	4815(2)	-2296(1)	1174(1)	32(1)
C(4)	5490(2)	-2354(1)	1750(1)	29(1)
C(5)	5503(2)	-1784(1)	2219(1)	25(1)
C(6)	4840(1)	-1154(1)	2099(1)	21(1)
C(9)	3826(1)	-197(1)	2795(1)	23(1)
C(11)	5360(1)	-21(1)	3523(1)	20(1)
C(12)	4292(1)	877(1)	4408(1)	20(1)
C(13)	4194(1)	197(1)	3400(1)	20(1)
C(15)	3604(1)	666(1)	3856(1)	20(1)
C(16)	2385(1)	916(1)	3724(1)	21(1)
C(17)	2083(1)	1158(1)	3077(1)	23(1)
C(18)	952(2)	1394(1)	2936(1)	24(1)
C(19)	95(1)	1379(1)	3437(1)	24(1)
C(21)	-1918(2)	1608(1)	3734(1)	34(1)
C(22)	375(2)	1132(1)	4082(1)	24(1)
C(23)	1521(2)	909(1)	4221(1)	23(1)
C(24)	5481(1)	639(1)	4459(1)	20(1)
C(25)	6026(1)	974(1)	5060(1)	21(1)
C(26)	5194(1)	1423(1)	5376(1)	22(1)
C(27)	4072(2)	1395(1)	4984(1)	23(1)
C(29)	7152(2)	900(1)	5322(1)	25(1)
C(30)	7422(2)	1285(1)	5908(1)	29(1)
C(31)	6595(2)	1734(1)	6223(1)	30(1)
C(32)	5461(2)	1809(1)	5958(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for **27**.

O(1)-C(19)	1.3716(19)		
O(1)-C(21)	1.440(2)	C(18)-H(18A)	1.001(17)
O(2)-C(27)	1.2211(19)	C(19)-C(22)	1.393(2)
O(3)-C(9)	1.2351(19)	C(21)-H(21A)	0.96(2)
N(1)-C(11)	1.3596(19)	C(21)-H(21B)	1.01(2)
N(1)-N(3)	1.4048(18)	C(21)-H(21C)	1.03(2)
N(1)-H(1AA)	0.8800	C(22)-C(23)	1.394(2)
N(2)-C(24)	1.329(2)	C(22)-H(22A)	0.954(18)
N(2)-C(11)	1.3491(19)	C(23)-H(23A)	0.995(16)
N(3)-C(9)	1.383(2)	C(24)-C(25)	1.476(2)
N(3)-C(6)	1.423(2)	C(25)-C(29)	1.389(2)
C(1)-C(2)	1.389(2)	C(25)-C(26)	1.398(2)
C(1)-C(6)	1.393(2)	C(26)-C(32)	1.385(2)
C(1)-H(1A)	0.937(19)	C(26)-C(27)	1.496(2)
C(2)-C(3)	1.388(3)	C(29)-C(30)	1.391(2)
C(2)-H(2A)	0.96(2)	C(29)-H(29A)	0.987(18)
C(3)-C(4)	1.382(3)	C(30)-C(31)	1.394(3)
C(3)-H(3A)	1.003(19)	C(30)-H(30A)	0.935(19)
C(4)-C(5)	1.391(2)	C(31)-C(32)	1.400(3)
C(4)-H(4A)	0.984(19)	C(31)-H(31A)	0.954(19)
C(5)-C(6)	1.390(2)	C(32)-H(32A)	0.966(18)
C(5)-H(5A)	0.936(19)		
C(9)-C(13)	1.459(2)	C(19)-O(1)-C(21)	117.44(14)
C(11)-C(13)	1.407(2)	C(11)-N(1)-N(3)	106.42(12)
C(12)-C(15)	1.400(2)	C(11)-N(1)-H(1AA)	126.8
C(12)-C(24)	1.426(2)	N(3)-N(1)-H(1AA)	126.8
C(12)-C(27)	1.501(2)	C(24)-N(2)-C(11)	111.63(14)
C(13)-C(15)	1.412(2)	C(9)-N(3)-N(1)	110.90(12)
C(15)-C(16)	1.484(2)	C(9)-N(3)-C(6)	126.12(13)
C(16)-C(23)	1.394(2)	N(1)-N(3)-C(6)	119.20(13)
C(16)-C(17)	1.400(2)	C(2)-C(1)-C(6)	119.30(17)
C(17)-C(18)	1.386(2)	C(2)-C(1)-H(1A)	118.6(11)
C(17)-H(17A)	1.015(16)	C(6)-C(1)-H(1A)	122.0(11)
C(18)-C(19)	1.393(2)	C(3)-C(2)-C(1)	120.12(17)

C(3)-C(2)-H(2A)	120.2(12)	C(17)-C(18)-H(18A)	118.3(10)
C(1)-C(2)-H(2A)	119.7(12)	C(19)-C(18)-H(18A)	121.5(10)
C(4)-C(3)-C(2)	120.30(16)	O(1)-C(19)-C(18)	115.08(14)
C(4)-C(3)-H(3A)	121.1(11)	O(1)-C(19)-C(22)	124.78(15)
C(2)-C(3)-H(3A)	118.6(11)	C(18)-C(19)-C(22)	120.12(15)
C(3)-C(4)-C(5)	120.19(17)	O(1)-C(21)-H(21A)	103.0(14)
C(3)-C(4)-H(4A)	120.0(10)	O(1)-C(21)-H(21B)	111.3(11)
C(5)-C(4)-H(4A)	119.8(10)	H(21A)-C(21)-H(21B)	114.0(18)
C(6)-C(5)-C(4)	119.36(16)	O(1)-C(21)-H(21C)	112.4(12)
C(6)-C(5)-H(5A)	118.9(12)	H(21A)-C(21)-H(21C)	104.5(18)
C(4)-C(5)-H(5A)	121.5(12)	H(21B)-C(21)-H(21C)	111.2(16)
C(5)-C(6)-C(1)	120.70(15)	C(19)-C(22)-C(23)	119.31(15)
C(5)-C(6)-N(3)	120.54(14)	C(19)-C(22)-H(22A)	122.0(11)
C(1)-C(6)-N(3)	118.75(15)	C(23)-C(22)-H(22A)	118.6(11)
O(3)-C(9)-N(3)	123.55(15)	C(22)-C(23)-C(16)	121.21(15)
O(3)-C(9)-C(13)	131.12(15)	C(22)-C(23)-H(23A)	119.7(10)
N(3)-C(9)-C(13)	105.28(13)	C(16)-C(23)-H(23A)	119.1(10)
N(2)-C(11)-N(1)	122.31(14)	N(2)-C(24)-C(12)	127.05(14)
N(2)-C(11)-C(13)	126.87(14)	N(2)-C(24)-C(25)	123.56(14)
N(1)-C(11)-C(13)	110.81(13)	C(12)-C(24)-C(25)	109.38(13)
C(15)-C(12)-C(24)	120.24(14)	C(29)-C(25)-C(26)	120.91(15)
C(15)-C(12)-C(27)	132.43(15)	C(29)-C(25)-C(24)	130.56(15)
C(24)-C(12)-C(27)	107.09(13)	C(26)-C(25)-C(24)	108.53(14)
C(11)-C(13)-C(15)	120.47(14)	C(32)-C(26)-C(25)	121.30(16)
C(11)-C(13)-C(9)	106.03(14)	C(32)-C(26)-C(27)	129.69(16)
C(15)-C(13)-C(9)	133.34(14)	C(25)-C(26)-C(27)	109.01(13)
C(12)-C(15)-C(13)	113.65(14)	O(2)-C(27)-C(26)	125.47(15)
C(12)-C(15)-C(16)	125.31(14)	O(2)-C(27)-C(12)	128.51(15)
C(13)-C(15)-C(16)	121.01(14)	C(26)-C(27)-C(12)	105.97(13)
C(23)-C(16)-C(17)	118.60(15)	C(25)-C(29)-C(30)	117.97(16)
C(23)-C(16)-C(15)	122.19(14)	C(25)-C(29)-H(29A)	120.5(10)
C(17)-C(16)-C(15)	119.21(14)	C(30)-C(29)-H(29A)	121.6(10)
C(18)-C(17)-C(16)	120.65(15)	C(29)-C(30)-C(31)	121.21(17)
C(18)-C(17)-H(17A)	118.8(9)	C(29)-C(30)-H(30A)	121.5(11)
C(16)-C(17)-H(17A)	120.5(9)	C(31)-C(30)-H(30A)	117.2(11)
C(17)-C(18)-C(19)	120.10(15)	C(30)-C(31)-C(32)	120.81(16)

C(30)-C(31)-H(31A)	119.8(11)	C(26)-C(32)-H(32A)	120.5(10)
C(32)-C(31)-H(31A)	119.3(11)	C(31)-C(32)-H(32A)	121.7(10)
C(26)-C(32)-C(31)	117.79(16)		

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for paul12. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	17(1)	39(1)	31(1)	3(1)	0(1)	5(1)
O(2)	23(1)	36(1)	34(1)	-10(1)	2(1)	3(1)
O(3)	19(1)	41(1)	36(1)	-13(1)	-10(1)	4(1)
N(1)	14(1)	29(1)	22(1)	-5(1)	-3(1)	3(1)
N(2)	19(1)	25(1)	20(1)	-1(1)	-1(1)	-2(1)
N(3)	16(1)	29(1)	21(1)	-4(1)	-2(1)	0(1)
C(1)	25(1)	31(1)	25(1)	-3(1)	-2(1)	2(1)
C(2)	28(1)	41(1)	28(1)	-9(1)	-4(1)	-1(1)
C(3)	31(1)	31(1)	33(1)	-12(1)	6(1)	-6(1)
C(4)	28(1)	24(1)	33(1)	0(1)	9(1)	-1(1)
C(5)	22(1)	30(1)	22(1)	2(1)	3(1)	-1(1)
C(6)	17(1)	25(1)	21(1)	-1(1)	2(1)	-3(1)
C(9)	18(1)	27(1)	24(1)	-1(1)	0(1)	1(1)
C(11)	17(1)	23(1)	20(1)	1(1)	2(1)	-2(1)
C(12)	18(1)	22(1)	20(1)	1(1)	2(1)	0(1)
C(13)	16(1)	24(1)	21(1)	0(1)	0(1)	-2(1)
C(15)	18(1)	22(1)	21(1)	2(1)	1(1)	-2(1)
C(16)	18(1)	20(1)	24(1)	-2(1)	0(1)	-1(1)
C(17)	20(1)	26(1)	22(1)	-2(1)	2(1)	0(1)
C(18)	23(1)	27(1)	22(1)	1(1)	0(1)	1(1)
C(19)	17(1)	26(1)	28(1)	-1(1)	-2(1)	2(1)
C(21)	18(1)	45(1)	39(1)	3(1)	4(1)	4(1)
C(22)	19(1)	29(1)	24(1)	0(1)	5(1)	1(1)
C(23)	22(1)	26(1)	20(1)	0(1)	1(1)	1(1)

C(24)	19(1)	21(1)	19(1)	2(1)	1(1)	-2(1)
C(25)	22(1)	22(1)	20(1)	2(1)	0(1)	-3(1)
C(26)	23(1)	22(1)	22(1)	2(1)	0(1)	-5(1)
C(27)	21(1)	24(1)	23(1)	0(1)	3(1)	-2(1)
C(29)	24(1)	25(1)	24(1)	0(1)	-2(1)	-3(1)
C(30)	27(1)	32(1)	27(1)	1(1)	-8(1)	-4(1)
C(31)	35(1)	31(1)	24(1)	-7(1)	-4(1)	-7(1)
C(32)	29(1)	25(1)	25(1)	-3(1)	2(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **27**.

Atom	x	y	z	U(eq)
H(1AA)	6407	-743	3040	26
H(1A)	3762(16)	-654(11)	1409(9)	30(5)
H(2A)	3712(18)	-1617(11)	645(11)	44(6)
H(3A)	4797(16)	-2702(10)	831(9)	33(5)
H(4A)	5945(16)	-2806(10)	1836(9)	29(5)
H(5A)	5905(17)	-1828(10)	2628(9)	33(5)
H(17A)	2684(15)	1148(9)	2699(8)	19(4)
H(18A)	783(15)	1595(9)	2477(9)	24(4)
H(21A)	-2560(20)	1844(13)	3507(11)	58(7)
H(21B)	-2086(17)	1083(12)	3875(9)	39(6)
H(21C)	-1755(18)	1940(12)	4148(11)	45(6)
H(22A)	-189(16)	1125(10)	4437(9)	29(5)
H(23A)	1731(14)	747(9)	4684(8)	21(4)
H(29A)	7737(16)	587(9)	5093(8)	24(5)
H(30A)	8158(17)	1242(10)	6114(9)	27(5)
H(31A)	6807(16)	2005(10)	6616(9)	31(5)
H(32A)	4886(16)	2129(10)	6165(9)	25(5)

Table 6. Torsion angles [°] for **27**.

C(11)-N(1)-N(3)-C(9)	-7.58(17)	C(11)-C(13)-C(15)-C(12)	0.4(2)
C(11)-N(1)-N(3)-C(6)	-167.02(13)	C(9)-C(13)-C(15)-C(12)	175.01(17)
C(6)-C(1)-C(2)-C(3)	-1.3(3)	C(11)-C(13)-C(15)-C(16)	178.28(14)
C(1)-C(2)-C(3)-C(4)	-0.1(3)	C(9)-C(13)-C(15)-C(16)	-7.1(3)
C(2)-C(3)-C(4)-C(5)	1.0(3)	C(12)-C(15)-C(16)-C(23)	-47.7(2)
C(3)-C(4)-C(5)-C(6)	-0.6(2)	C(13)-C(15)-C(16)-C(23)	134.64(17)
C(4)-C(5)-C(6)-C(1)	-0.8(2)	C(12)-C(15)-C(16)-C(17)	133.19(17)
C(4)-C(5)-C(6)-N(3)	178.52(15)	C(13)-C(15)-C(16)-C(17)	-44.5(2)
C(2)-C(1)-C(6)-C(5)	1.7(3)	C(23)-C(16)-C(17)-C(18)	0.7(2)
C(2)-C(1)-C(6)-N(3)	-177.56(16)	C(15)-C(16)-C(17)-C(18)	179.88(15)
C(9)-N(3)-C(6)-C(5)	-134.90(17)	C(16)-C(17)-C(18)-C(19)	-1.2(2)
N(1)-N(3)-C(6)-C(5)	21.1(2)	C(21)-O(1)-C(19)-C(18)	177.39(16)
C(9)-N(3)-C(6)-C(1)	44.4(2)	C(21)-O(1)-C(19)-C(22)	-4.5(2)
N(1)-N(3)-C(6)-C(1)	-159.58(15)	C(17)-C(18)-C(19)-O(1)	178.65(15)
N(1)-N(3)-C(9)-O(3)	-170.34(15)	C(17)-C(18)-C(19)-C(22)	0.4(3)
C(6)-N(3)-C(9)-O(3)	-12.6(3)	O(1)-C(19)-C(22)-C(23)	-177.31(15)
N(1)-N(3)-C(9)-C(13)	7.35(18)	C(18)-C(19)-C(22)-C(23)	0.7(3)
C(6)-N(3)-C(9)-C(13)	165.05(14)	C(19)-C(22)-C(23)-C(16)	-1.2(3)
C(24)-N(2)-C(11)-N(1)	-175.86(14)	C(17)-C(16)-C(23)-C(22)	0.4(2)
C(24)-N(2)-C(11)-C(13)	2.8(2)	C(15)-C(16)-C(23)-C(22)	-178.68(15)
N(3)-N(1)-C(11)-N(2)	-176.53(14)	C(11)-N(2)-C(24)-C(12)	-0.2(2)
N(3)-N(1)-C(11)-C(13)	4.59(17)	C(11)-N(2)-C(24)-C(25)	-178.68(14)
N(2)-C(11)-C(13)-C(15)	-3.1(2)	C(15)-C(12)-C(24)-N(2)	-2.2(2)
N(1)-C(11)-C(13)-C(15)	175.76(14)	C(27)-C(12)-C(24)-N(2)	-177.31(15)
N(2)-C(11)-C(13)-C(9)	-179.01(15)	C(15)-C(12)-C(24)-C(25)	176.44(14)
N(1)-C(11)-C(13)-C(9)	-0.19(18)	C(27)-C(12)-C(24)-C(25)	1.35(17)
O(3)-C(9)-C(13)-C(11)	173.12(18)	N(2)-C(24)-C(25)-C(29)	-2.2(3)
N(3)-C(9)-C(13)-C(11)	-4.33(17)	C(12)-C(24)-C(25)-C(29)	179.13(16)
O(3)-C(9)-C(13)-C(15)	-2.1(3)	N(2)-C(24)-C(25)-C(26)	177.97(14)
N(3)-C(9)-C(13)-C(15)	-179.53(17)	C(12)-C(24)-C(25)-C(26)	-0.74(17)
C(24)-C(12)-C(15)-C(13)	1.9(2)	C(29)-C(25)-C(26)-C(32)	0.0(2)
C(27)-C(12)-C(15)-C(13)	175.58(16)	C(24)-C(25)-C(26)-C(32)	179.86(14)
C(24)-C(12)-C(15)-C(16)	-175.88(14)	C(29)-C(25)-C(26)-C(27)	179.92(14)
C(27)-C(12)-C(15)-C(16)	-2.2(3)	C(24)-C(25)-C(26)-C(27)	-0.19(17)

C(32)-C(26)-C(27)-O(2) 3.4(3)	C(26)-C(25)-C(29)-C(30) 0.3(2)
C(25)-C(26)-C(27)-O(2) -176.57(15)	C(24)-C(25)-C(29)-C(30) -179.56(16)
C(32)-C(26)-C(27)-C(12) -179.07(16)	C(25)-C(29)-C(30)-C(31) -0.4(3)
C(25)-C(26)-C(27)-C(12) 0.99(17)	C(29)-C(30)-C(31)-C(32) 0.2(3)
C(15)-C(12)-C(27)-O(2) 1.8(3)	C(25)-C(26)-C(32)-C(31) -0.2(2)
C(24)-C(12)-C(27)-O(2) 176.04(16)	C(27)-C(26)-C(32)-C(31) 179.90(16)
C(15)-C(12)-C(27)-C(26) -175.68(16)	C(30)-C(31)-C(32)-C(26) 0.1(3)
C(24)-C(12)-C(27)-C(26) -1.42(16)	

Symmetry transformations used to generate equivalent atoms.

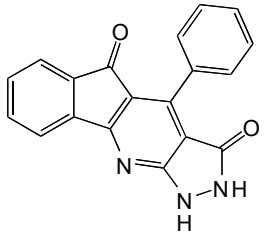
Table 7. Hydrogen bonds in **27**.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1AA	0.880	2.186	118.32	2.716	O3 [x+1/2, y, -z+1/2]

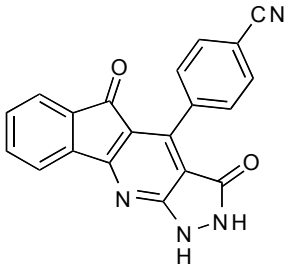
References

1. Sheldrick G.M. SADABS v.2.03, Bruker/Siemens Area Detector Absorption Correction Program, (2003) Bruker AXS, Madison, Wisconsin, USA.
2. SAINTP+ for NT. Data Reduction and Correction Program v. 6.2, (2001) Bruker AXS, Madison, Wisconsin, USA.
3. Sheldrick G.M. SHELXTL NT v. 6.12, Structure Determination Software Suite, (2001) Bruker AXS, Madison, Wisconsin, USA.

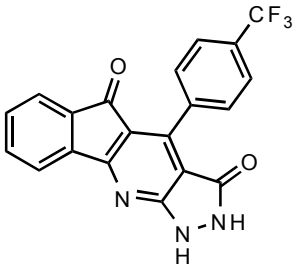
Characterization Data



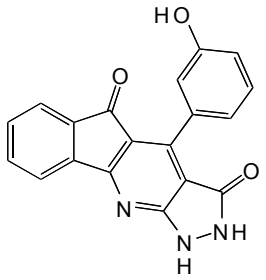
4-phenyl-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (1): 60%; ^{1}H NMR (DMSO-d_6) δ 7.86 (d, 1H, J = 7.4 Hz, Ind-*H*), 7.71 (t, 1H, J = 7.1 Hz, Ind-*H*), 7.58 - 7.44 (m, 7H); ^{13}C NMR δ 189.3, 165.5, 157.1, 154.1, 146.8, 141.9, 137.4, 135.3, 132.0, 131.0, 130.6, 129.5, 127.5, 123.4, 121.2, 117.7, 102.5; HRMS *m/z* (ESI) calcd for $C_{19}H_{11}N_3NaO_2$ $(M + Na)^+$ 336.0749, found 336.0744.



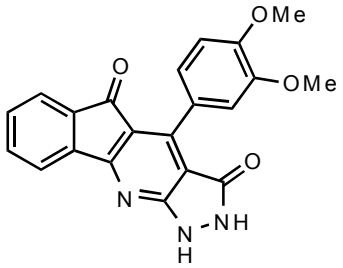
4-(3,5-dioxo-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-4-yl)benzonitrile (2): 55%; ^{1}H NMR (DMSO-d_6) δ 7.94 (d, 2H, J = 8.0 Hz, Ar-*H*), 7.84 (d, 1H, J = 7.1 Hz, Ind-*H*), 7.74 (d, 2H, J = 8.0 Hz, Ar-*H*), 7.69 (t, 1H, J = 7.3 Hz, Ind-*H*), 7.59 - 7.46 (m, 2H, Ind-*H*); ^{13}C NMR δ 189.3, 165.4, 156.9, 154.4, 144.2, 142.1, 137.3, 137.2, 135.6, 132.4, 131.5, 123.7, 121.4, 119.3, 117.9, 112.1, 102.2; HRMS *m/z* (ESI) calcd for $C_{20}H_{10}N_6NaO_2$ $(M + Na)^+$ 361.0701, found 361.0699.



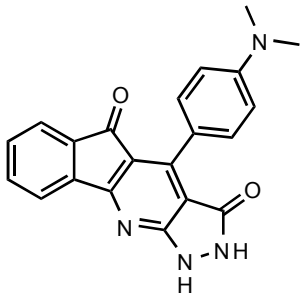
4-(4-(trifluoromethyl)phenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (3): 65%; ^{1}H NMR (DMSO-d_6) δ 7.88 - 7.76 (m, 5H), 7.70 (t, 1H, J = 7.1 Hz, Ind-*H*), 7.58 - 7.51 (m, 2H); ^{13}C NMR δ 189.4, 165.5, 157.0, 154.5, 144.6, 142.1, 137.4, 136.4, 135.6, 132.3, 131.3, 129.9, 124.5, 123.6, 121.4, 117.9, 102.3; HRMS *m/z* (ESI) calcd for $C_{20}H_{10}F_3N_3NaO_2$ $(M + Na)^+$ 404.0623, found 404.0615.



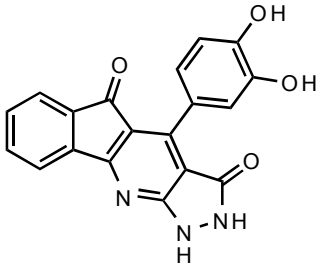
4-(3-hydroxyphenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (4): 64%; ^{1}H NMR (DMSO-d_6) δ 9.44 (s, 1H, O*H*), 7.86 (d, 1H, J = 7.4 Hz, V), 7.68 (t, 1H, J = 6.6 Hz, Ind-*H*), 7.54 (m, 2H), 7.21 (t, 1H, J = 7.7 Hz, Ar-*H*), 6.86 (m, 3H); ^{13}C NMR δ 189.3, 165.5, 157.1, 156.7, 154.9, 157.0, 142.0, 137.4, 135.4, 133.4, 132.2, 128.5, 123.5, 121.3, 121.1, 117.8, 117.3, 116.4, 102.5; HRMS *m/z* (ESI) calcd for $C_{19}H_{11}N_3NaO_3$ $(M + Na)^+$ 352.0698, found 352.0681.



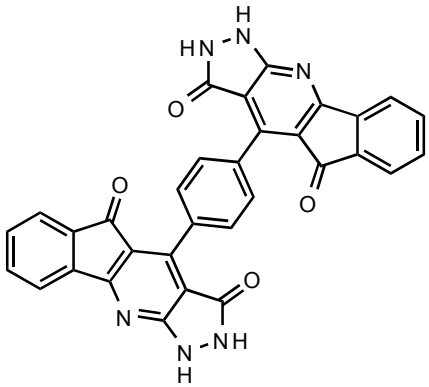
4-(3, 4-dimethoxyphenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (5): 63%; ^{1}H NMR (DMSO-d_6) δ 7.81 (d, 1H, J = 7.2 Hz, Ind-*H*), 7.67 - 7.51 (m, 3H), 7.21(s, 1H, Ar-*H*), 7.14 (d, 1H, J = 8.5 Hz, Ar-*H*), 6.98 (d, 1H, J = 8.5 Hz), 3.81 (s, 3H, OCH_3), 3.73 (s, 3H, OCH_3); ^{13}C NMR δ 189.4, 172.6, 165.7, 157.0, 154.5, 150.3, 147.6, 147.1, 141.9, 137.5, 135.2, 132.0, 124.2, 123.9, 123.9, 123.4, 121.1, 117.6, 115.3, 110.6, 102.3, 56.1; HRMS *m/z* (ESI) calcd for $C_{21}H_{15}N_3O_4$ $(M + H)^+$ 374.1141, found 374.1142.



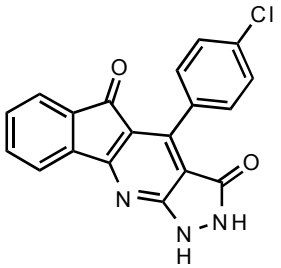
4-(4-(dimethylamino)phenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (6): 67%; ^{1}H NMR (DMSO-d_6) δ 7.83 (d, 1H, J = 7.2 Hz, Ind-*H*), 7.70 - 7.49 (m, 5H), 6.74 (m, 2H, J = 8.2 Hz, Ar-*H*), 3.01 (s, 6H, N(CH_3)$_2$); ^{13}C NMR δ 189.4, 165.8, 157.2, 154.7, 151.7, 148.1, 141.9, 137.6, 135.1, 132.8, 132.0, 123.3, 121.1, 118.7, 117.0, 110.5, 102.1, 40.5; HRMS *m/z* (ESI) calcd for $C_{21}H_{16}N_4O_2$ $(M + H)^+$ 357.1351, found 357.1352.



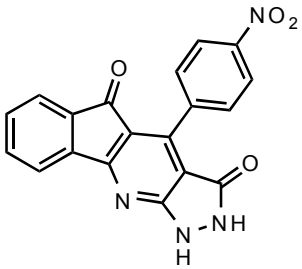
4-(3, 4-dihydroxyphenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (7): 70%; ^{1}H NMR (DMSO-d_6) δ 9.22 (s, 1H, O*H*), 8.94 (s, 1H, O*H*), 7.83 (d, 1H, J = 7.3 Hz, Ind-*H*), 7.69 - 7.51 (m, 3H), 6.99 (s, 1H, Ar-*H*), 6.89 (d, 1H, J = 8.3 Hz, Ar-*H*), 6.75 (d, 1H, J = 8.3 Hz, Ar-*H*); ^{13}C NMR δ 189.4, 166.0, 157.1, 154.6, 148.1, 147.3, 144.3, 142.0, 137.7, 135.3, 132.1, 123.4, 122.9, 121.2, 118.7, 117.5, 114.7, 102.4; HRMS *m/z* (ESI) calcd for $C_{19}H_{11}N_3O_4$ $(M + H)^+$ 346.0828, found 346.0826.



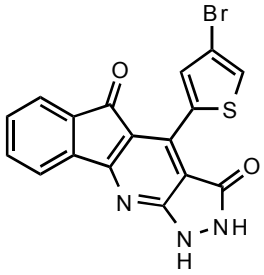
4-[4-(3,5-dioxo-1,2,3,5-tetrahydroindeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-4-yl)phenyl]-1,2-dihydroindeno[1,2-*b*]pyrazolo[4,3-*e*]pyridine-3,5-dione (8): 80%; ^{1}H NMR (DMSO-d_6) δ 7.89 - 7.47 (m, 12H); HRMS *m/z* (ESI) calcd for $C_{32}H_{16}N_6O_4$ $(M + Na)^+$ 571.1131, found 571.1119.



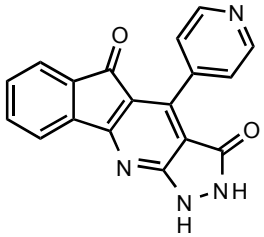
4-(4-chlorophenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (9): 52%; ^{1}H NMR (DMSO-d_6) δ 7.84 (d, 1H, J = 7.2 Hz, Ind-*H*), 7.70 - 7.49 (m, 7H); ^{13}C NMR δ 189.4, 165.5, 157.0, 154.4, 145.2, 142.0, 137.4, 135.5, 134.5, 132.7, 132.3, 130.8, 127.6, 123.6, 121.3, 117.8, 102.3; HRMS *m/z* (ESI) calcd for $C_{19}H_{10}ClN_3O_2$ $(M + H)^+$ 348.0540, found 348.0546.



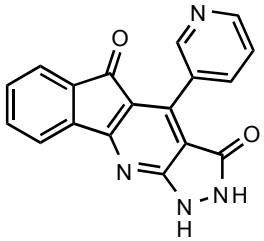
4-(4-nitrophenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (10): 42%; ^{1}H NMR (DMSO-d_6) δ 8.30 (d, 2H, J = 8.5 Hz, Ar-*H*), 7.89 - 7.83 (m, 3H), 7.73 - 7.69 (m, 1H, Ind-*H*), 7.60 - 7.52 (m, 2H); ^{13}C NMR δ 189.4, 172.7, 165.5, 156.9, 154.5, 148.3, 143.7, 142.1, 139.2, 137.3, 135.7, 131.9, 123.7, 122.7, 121.5, 118.0, 102.2; HRMS *m/z* (ESI) calcd for $C_{19}H_{10}N_4O_4$ $(M + H)^+$ 359.0780, found 359.0780.



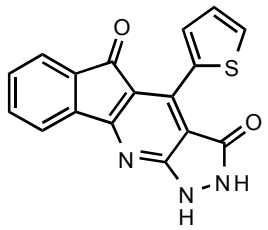
4-(4-bromothiophen-2-yl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (11): 68%; ^{1}H NMR (DMSO-d_6) δ 7.97 (s, 1H, Net-*H*), 7.86 (d, 1H, *J* = 6.9 Hz, Ind-*H*), 7.74 - 7.69 (m, 1H), 7.65 - 7.62 (m, 1H), 7.57 (d, 1H, *J* = 7.2, Ind-*H*), 7.53 - 7.51 (m, 1H); ^{13}C NMR δ 189.0, 167.5, 165.8, 156.8, 154.3, 141.9, 137.3, 135.7, 133.8, 132.4, 127.3, 123.7, 121.4, 118.2, 108.3, 102.1; HRMS *m/z* (ESI) calcd for $C_{17}H_8BrN_3O_2S$ $(M + H)^+$ 397.9599, found 397.9598.



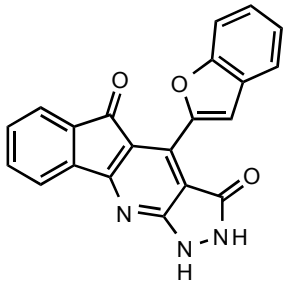
4-(pyridin-4-yl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (12): 61%; ^{1}H NMR (DMSO-d_6) δ 8.68 (d, 2H, *J* = 7.3 Hz, Het-*H*), 7.89 (d, 2H, *J* = 7.4 Hz, Ind-*H*), 7.75 - 7.48 (m, 6H); HRMS m/z (ESI) calcd for $C_{18}H_{10}N_4O_2$ $(M + H)^+$ 315.0882, found 315.0875.



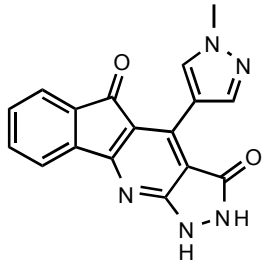
4-(pyridin-3-yl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (13): 55%; ^{1}H NMR (DMSO-d_6) δ 8.80 - 8.76 (m, 1H, Het-*H*), 8.67 (m, 1H, Het-*H*), 8.00 (m, 1H, Het-*H*), 7.89 (d, 1H, *J* = 7.4 Hz, Ind-*H*), 7.75 - 7.48 (m, 6H); ^{13}C NMR δ 189.6, 165.4, 157.0, 154.2, 150.8, 143.2, 141.9, 138.2, 135.6, 132.5, 128.0, 123.9, 121.4, 118.1, 102.6; HRMS *m/z* (ESI) calcd for $C_{18}H_{10}N_4O_2$ $(M + H)^+$ 315.0882, found 315.0883.



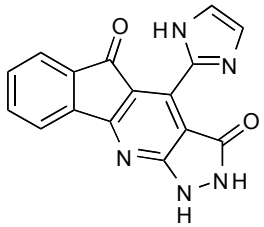
4-(thiophen-2-yl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (14): 53%; ^{1}H NMR (DMSO-d_6) δ 7.85 - 7.83 (m, 7H), 7.20 - 7.17 (m, 1H, Het-*H*); ^{13}C NMR δ 189.1, 165.7, 157.1, 154.6, 141.8, 137.3, 135.5, 132.8, 132.3, 130.1, 126.9, 123.6, 121.3, 117.8, 109.8, 102.3; HRMS *m/z* (ESI) calcd for $C_{17}H_9N_3O_2S$ $(M + H)^+$ 320.0493, found 320.0503.



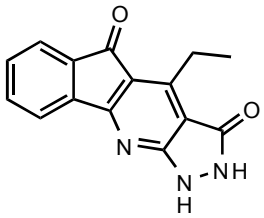
4-(benzofuran-2-yl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (15): 46%; ^{1}H NMR (DMSO-d_6) δ 7.89 (d, 1H, J = 7.2 Hz, Ind-*H*), 7.82 (d, 1H, J = 7.7 Hz, Het-*H*), 7.75 - 7.65 (m, 4H), 7.60 - 7.55 (m, 1H), 7.45 (t, 1H, J = 7.7 Hz, Het-*H*), 7.37 - 7.32 (m, 1H, Het-*H*); ^{13}C NMR δ 188.8, 165.6, 156.9, 155.5, 154.7, 147.6, 141.9, 137.6, 135.9, 132.4, 128.3, 126.5, 123.8, 122.6, 121.5, 119.3, 112.5, 112.0, 104.9, 100.8; HRMS *m/z* (ESI) calcd for $C_{21}H_{11}N_3O_2$ $(M + H)^+$ 354.0878, found 354.0887.



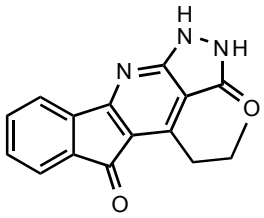
4-(1-methyl-1*H*-pyrazol-4-yl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (16): 55%; ^{1}H NMR (DMSO-d_6) δ 8.42 (s, 1H, Het-*H*), 8.09 (s, 1H, Het-*H*), 7.82 (d, 1H, J = 7.2 Hz, Ind-*H*), 7.71 - 7.52 (m, 3H), 3.95 (s, 3H, N-CH_3); ^{13}C NMR δ 189.5, 165.4, 157.4, 154.9, 152.2, 142.7, 142.0, 137.9, 135.4, 132.5, 123.8, 121.3, 118.9, 116.5, 112.1, 101.4; HRMS *m/z* (ESI) calcd for $C_{17}H_{12}N_5O_2$ $(M + H)^+$ 318.0991, found 318.0987.



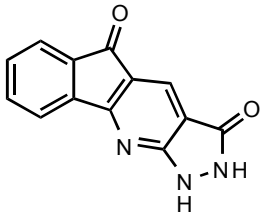
4-(1*H*-imidazol-2-yl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (17): 73%; ^{1}H NMR (DMSO-d_6) δ 9.39 (s, 1H, Het-*H*), 8.38 (s, 1H, Het-*H*), 7.80 - 7.52 (m, 4H, Ind-*H*); ^{13}C NMR δ 186.8, 175.5, 157.2, 154.6, 144.9, 141.7, 136.9, 135.2, 133.7, 132.0, 125.7, 123.4, 121.0, 119.3, 114.6; HRMS *m/z* (ESI) calcd for $C_{16}H_9N_5O_2$ $(M + H)^+$ 304.0834, found 304.0842.



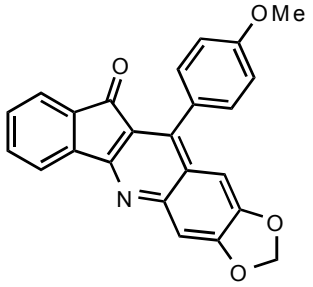
4-ethyl-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (18): 33%; ^{1}H NMR (DMSO-d_6) δ 7.79 (d, 1H, J = 7.2 Hz, Ind-*H*), 7.68 - 7.62 (m, 2H, Ind-*H*), 7.54 - 7.50 (m, 1H, Ind-*H*), 3.34 (q, 2H, J = 7.4 Hz, CH_2CH$_3$), 1.25 (t, 3H, J = 7.4 Hz, CH$_2$CH_3); ^{13}C NMR δ 191.1, 166.3, 158.2, 154.4, 152.2, 142.5, 137.7, 135.4, 132.1, 123.5, 121.3, 118.0, 103.5, 20.8, 15.2; HRMS *m/z* (ESI) calcd for $C_{15}H_{11}N_3O_2$ $(M + H)^+$ 266.0929, found 266.0935.



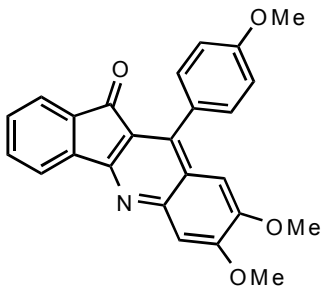
4-propyl-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (19): 43%; ^{1}H NMR (DMSO-d_6) δ 7.81 - 7.53 (m, 4H, Ind-*H*), 3.29 (t, 2H, J = 7.4 Hz, CH_2CH$_2$CH$_3$), 1.70 (m, 2H, CH$_2$CH_2CH$_3$), 0.95 (t, 3H, J = 7.4 Hz, CH$_2$CH$_2$CH_3); ^{13}C NMR δ 191.6, 165.9, 157.8, 155.3, 151.2, 142.3, 137.6, 132.2, 131.0, 121.2, 118.3, 104.2, 29.0, 23.8, 14.2; HRMS *m/z* (ESI) calcd for $C_{16}H_{13}N_3O_2$ $(M + H)^+$ 280.1086, found 280.1088.



1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (20): 34%; ^{1}H NMR (DMSO-d_6) δ 8.24 (s, 1H, C-*H*), 7.84 (d, 1H, *J* = 7.2 Hz, Ind-*H*), 7.73 - 7.68 (m, 2H, Ind-*H*), 7.55 (m, 1H, Ind-*H*); ^{13}C NMR δ 190.8, 190.2, 141.9, 139.7, 138.9, 137.2, 135.8, 128.7, 127.1, 124.2, 122.7, 118.7, 113.7; HRMS *m/z* (ESI)) calcd for $C_{13}H_8N_3O_2$ $(M + H)^+$ 238.0614, found 238.0617.

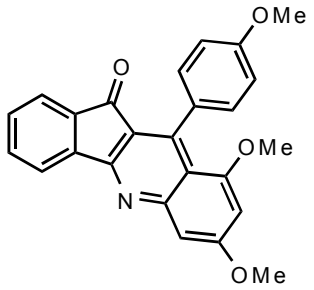


11-(4-methoxyphenyl)-10*H*-[1,3]dioxolo[4,5-*g*]indeno[1,2-*b*]quinolin-10-one (21): 34%; ^{1}H NMR (DMSO-d_6) δ 8.38 (d, 1H, *J* = 7.2 Hz, Ar-*H*), 7.94 (s, 1H, Ar-*H*), 7.75 - 7.49 (m, 3H), 7.36 (s, 1H, Ar-*H*), 7.01 (d, 2H, *J* = 8.5 Hz, Ar-*H*), 6.29 (s, 2H, OCH_2O), 3.84 (s, 3H, OCH_3); ^{13}C NMR δ 192.1, 160.9, 153.3, 151.2, 150.1, 141.5, 135.2, 131.9, 130.9, 128.0, 125.3, 123.7, 118.9, 113.3, 107.0, 103.2, 99.9, 62.2, 57.5, 55.7, 84.5, 49.9; HRMS *m/z* (ESI) calcd for $C_{24}H_{15}NO_4$ $(M + H)^+$ 382.1079, found 382.1075.

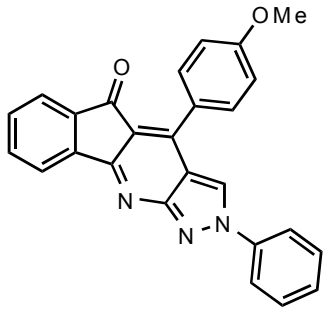


7,8-dimethoxy-10-(4-methoxyphenyl)-11*H*-indeno[1,2-*b*]quinolin-11-one (22): 35%; ^{1}H (DMSO-d_6) δ 7.91 (d, 1H, *J* = 7.7 Hz, Ind-*H*), 7.70 (t, 1H, *J* = 3.4 Hz, Ind-*H*), 7.59 - 7.43 (m, 5H), 7.10 (d, 2H, *J* = 7.7, Ar-*H*), 6.92 (s, 1H, Ar-*H*), 3.97 (s, 3H, OCH_3), 3.89 (s, 3H, OCH_3),

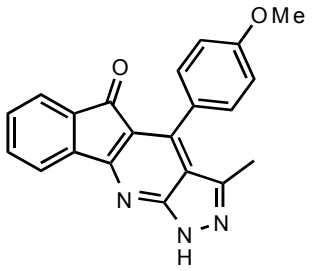
3.66 (s, 3H, OCH_3); ^{13}C NMR δ 190.2, 160.7, 155.7, 154.3, 150.1, 147.8, 146.2, 143.2, 136.9, 135.8, 133.3, 131.7, 128.9, 123.9, 122.5, 121.1, 116.3, 114.0, 109.8, 106.7, 56.3, 56.1, 56.0 ; HRMS *m/z* (ESI) calcd for $C_{25}H_{19}NO_4$ $(M + H)^+$ 398.1393, found 398.1393.



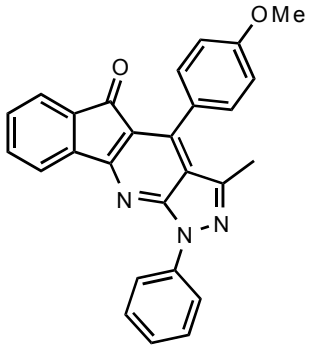
7,9-dimethoxy-10-(4-methoxyphenyl)-11*H*-indeno[1,2-*b*]quinolin-11-one (23): 30%; ^{1}H NMR (DMSO-d6) δ: 7.96 (d, 1H, *J* = 8.0 Hz, Ind-*H*), 7.72 (m, 1H, Ind-*H*), 7.58 (s, 2H), 7.16 (m, 3H), 6.95 (d, 2H, *J* = 8.0, Ar-*H*), 6.55 (s, 1H, Ar-*H*), 3.95 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 3.40 (s, 3H, OCH_3); HRMS m/z (ESI) calcd for $C_{25}H_{19}NO_4$ $(M + H)^+$ 398.1393, found 398.1400.



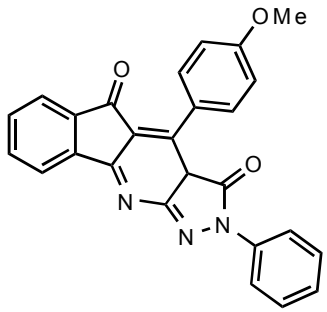
2-phenyl-4-(4-methoxyphenyl)-5H-indeno[1,2-b]pyrazolo[4,3-e]pyridin-5-one (24): 41%; ^{1}H NMR (DMSO-d_6) δ 9.07 (s, 1H, Pyr-*H*), 8.13 (d, 2H, *J* = 8.3 Hz, Ar-*H*), 8.00 (d, 1H, *J* = 7.4 Hz, Ind-*H*), 7.84 - 7.74 (m, 4H), 7.68 - 7.56 (m, 4H), 7.48 (d, 1H, *J* = 7.4 Hz, Ind-*H*), 7.11 (d, 2H, *J* = 8.3 Hz, Ar-*H*), 3.89 (s, 3H, OCH_3); ^{13}C NMR δ 189.7, 165.6, 161.3, 160.4, 146.1, 142.7, 139.8, 138.1, 135.9, 132.6, 132.3, 130.2, 128.9, 127.1, 125.3, 123.8, 121.7, 120.8, 119.3, 116.3, 114.1, 55.8; HRMS *m/z* (ESI) calcd for $C_{26}H_{17}N_3O_2$ $(M + H)^+$ 404.1399, found 404.1398.



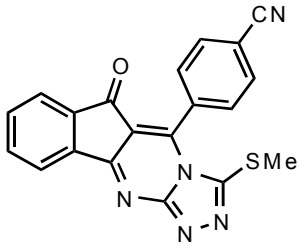
3-methyl-4-(4-methoxyphenyl)-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-5(1*H*)-one (25): 30%; ^{1}H NMR (DMSO-d_6) δ 7.88 (d, 1H, J = 7.2 Hz, Ind-*H*), 7.70 (m, 1H, Ind-*H*), 7.56 - 7.44 (m, 4H), 7.06 (d, 2H, J = 8.3 Hz, Ar-*H*), 3.86 (s, 3H, OCH_3), 1.97 (s, 3H, CH_3); ^{13}C NMR δ 189.7, 164.7, 160.4, 155.2, 146.1, 144.8, 142.3, 137.4, 135.6, 132.2, 131.2, 125.4, 123.6, 121.4, 119.0, 113.6, 55.7, 15.4; HRMS *m/z* (ESI) calcd for $C_{21}H_{15}N_3O_2$ $(M + H)^+$ 342.1242, found 342.1243.



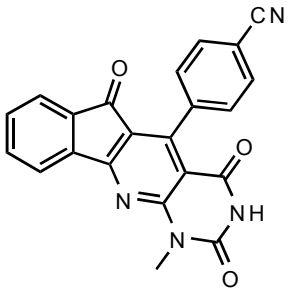
1-phenyl-3-methyl-4-(4-methoxyphenyl)-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-5(1*H*)-one (26): 72%;^{1}H NMR (DMSO-d_6) δ 8.2 (d, 1H, J = 7.6 Hz, Ind-*H*), 7.91 (d, 1H, J = 6.6 Hz, Ind-*H*), 7.71 - 7.37 (m, 10H), 7.06 (d, 1H, J = 7.6 Hz), 3.86 (s, 3H, OCH_3), 2.00 (s, 3H, CH_3); ^{13}C NMR δ 189.5, 165.1, 160.7, 153.0, 146.4, 146.0, 142.1, 139.1, 137.4, 135.7, 133.5, 132.5, 131.2, 129.7, 126.9, 124.7, 123.7, 121.7, 120.2, 115.8, 113.8, 55.8, 15.2; HRMS *m/z* (ESI) calcd for $C_{27}H_{19}N_3O_2$ $(M + H)^+$ 418.1555, found 418.1547.



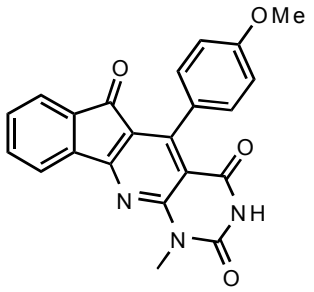
2-phenyl-4-(4-methoxyphenyl)-1,2-dihydro-5H-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-3,5-dione (27): 63%; ^{1}H NMR (DMSO-d_6) δ 7.95 - 7.85 (m, 3H), 7.74 - 7.61(m, 5H), 7.47 (m, 2H), 7.24 (m, 1H, Ind-*H*), 6.99 (d, 2H, J = 8.8 Hz, Ar-*H*), 3.86 (s, 3H, OCH_3); ^{13}C NMR δ 188.5, 180.4, 161.1, 158.5, 151.3, 144.3, 137.9, 136.9, 135.2, 133.2, 133.0, 129.4, 125.7, 123.5, 122.3, 121.9, 120.0, 117.0, 112.7, 106.7, 106.1, 55.7; HRMS *m/z* (ESI) calcd for $C_{26}H_{17}N_3O_3$ $(M + H)^+$ 420.1348, found 420.1357.



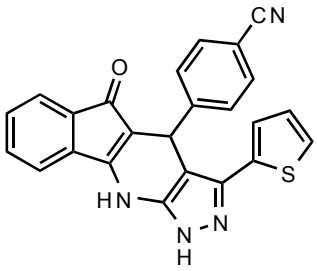
4-[3-(methylsulfanyl)-5-oxo-5*H*-indeno[1,2,4]triazolo[4,3-*a*]pyrimidin-5-yl]benzonitrile (28): 48%; ^{1}H NMR (DMSO-d_6) δ 8.54 (d, 1H, J = 8.5 Hz, Ind-*H*), 8.09 - 7.71 (m, 7H), 2.60 (s, 3H, SCH_3); ^{13}C NMR δ 183.3, 142.9, 140.4, 138.8, 136.8, 136.7, 134.3, 134.0, 132.8, 132.2, 124.5, 123.9, 123.8, 122.9, 118.9, 114.6, 31.2; HRMS m/z (ESI) calcd for $C_{20}H_{12}H_5OS$ $(M + H)^+$ 370.0763, found 370.0779.



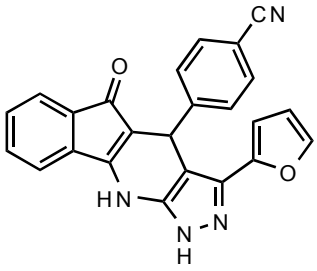
4-(1-methyl-2,4,6-trioxo-2,3,4,6-tetrahydro-1*H*-indeno[2',1':5,6]pyrido[2,3-*d*]pyrimidin-5-yl)benzenecarbonitrile (29): 51%; ^{1}H NMR (DMSO-d_6) δ 11.62 (s, 1H, N*H*), 7.94 (d, 1H, J = 7.4 Hz, Ind-*H*), 7.85 (d, 2H, J = 8.0 Hz, Ar-*H*), 7.77 - 7.28 (m, 5H), 3.65 (s, 3H, NCH_3); ^{13}C NMR δ 188.5, 168.0, 160.5, 150.7, 140.9, 140.7, 136.5, 136.0, 133.6 131.6, 129.2, 124.0, 122.3, 119.4, 111.0, 108.2, 93.9, 70.0, 29.8, 29.4; HRMS *m/z* (ESI) calcd for $C_{22}H_{12}N_4O_3$ $(M+H)^+$ 381.0987, found 381.0984.



5-(4-methoxyphenyl)-1-methyl-1*H*-indeno[2',1':5,6]pyrido[2,3-*d*]pyrimidine-2,4,6(3*H*)-trione (30): 56%; ^{1}H NMR (DMSO-d_6) δ 7.96 (d, 1H, J = 7.4 Hz, Ind-*H*), 7.80 - 7.59 (m, 3H), 7.20 (d, 2H, J = 8.7 Hz, Ar-*H*), 6.93 (d, 2H, J = 8.7 Hz, Ar-*H*), 3.89 (s, 3H, , OCH_3), 3.73 (s, 3H, , NCH_3); HRMS m/z (ESI)) calcd for $C_{22}H_{16}N_3O_4$ $(M + H)^+$ 386.1144, found 386.1141.

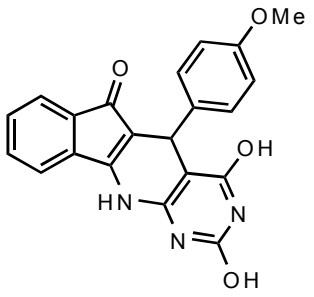


4-(3-(thiophen-2-yl)-5-oxo-1,4,10-trihydro-5*H*-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-4-yl)benzonitrile (31): 65%; ^{1}H NMR (DMSO-d_6) δ 11.4 (s, 1H, N*H*), 7.67 - 7.61 (m, 3H), 7.52 (d, 1H, J = 6.1 Hz, Het-*H*), 7.39 - 7.28 (m, 5H), 7.20 (d, 1H, J = 6.1 Hz, Het-*H*), 7.04 (m, 1H), 5.29 (s, 1H, C-*H*); ^{13}C NMR δ 189.9, 156.9, 151.2, 136.5, 135.2, 132.5, 131.9, 131.2, 129.4, 128.1, 127.8, 127.6, 126.4, 120.6, 119.5, 119.2, 109.29, 105.1, 102.8, 102.0, 69.5, 35.7; HRMS *m/z* (ESI) calcd for $C_{24}H_{14}N_4OS$ $(M + H)^+$ 407.0966, found 407.1005.



4-(3-(furan-2-yl)-5-oxo-1,4,10-trihydro-5*H*-indeno[1,2-*b*]pyrazolo[4,3-*e*]pyridin-4-yl)benzonitrile (32): 61%; ^{1}H NMR (DMSO-d_6) δ 11.49 (s, 1H, N*H*), 7.69 - 7.63 (m, 4H),

7.45 - 7.31 (m, 4H), 7.21 (d, 1H, *J* = 6.9 Hz), 6.54 - 6.49 (m, 2H, Het-*H*), 5.32 (s, 1H, C-*H*); ^{13}C NMR δ 189.9, 157.2, 151.8, 148.9, 144.1, 143.6, 136.8, 135.0, 132.4, 131.7, 130.8, 129.4, 120.3, 119.8, 122.2, 109.3, 108.5, 105.1, 102.4, 82.9, 63.1; HRMS *m/z* (ESI) calcd for $C_{24}H_{14}N_4O_2$ $(M + H)^+$ 391.1195, found 391.1202.



5-(4-methoxyphenyl)-1*H*-indeno[2',1':5,6]pyrido[2,3-*d*]pyrimidine-2,4,6(3*H*)-trione (**33**): 72%; ^{1}H NMR (DMSO-d_6) δ 10.83 (s, 1H, N*H*), 7.46 - 7.14 (m, 8H), 6.77 (d, 2H, *J* = 7.7 Hz, Ar-*H*), 4.62 (s, 1H, C-*H*), 3.67 (s, 3H, , OCH_3); ^{13}C NMR δ 191.4, 163.3, 158.2, 153.7, 150.3, 144.9, 138.0, 136.4, 133.1, 132.6, 130.8, 129.1, 121.3, 119.4, 117.1, 113.9, 110.4, 91.8, 55.5; HRMS *m/z* (ESI) calcd for $C_{21}H_{15}N_3O_4$ $(M + H)^+$ 374.1141, found 374.1151.