Supporting Information

AN EFFICIENT ONE-POT THREE-COMPONENT SYNTHESIS OF HIGHLY FUNCTIONALIZED COUMARIN FUSED INDENODIHYD- ROPYRIDINE AND CHROMENO[4,3-*b*]QUINOLINE DERIVATIVES.

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Bond length (Angstrom)(C25 H19 N O4 S2) (3l)

Selected geometric parameters (Å, °)

S2—O4	1.511(22)	C11—C12	1.400(18)
S2—C25	1.759(29)	C5—C4	1.324(16)
S2—C24	1.765(21)	C15—C14	1.349(16)
S1—C23	1.612(21)	C15—H15	0.930(11)
S1—C20	1.663(16)	C1—C2	1.474(18)
N1—C18	1.376(19)	C1—H1A	0.930(17)
N1—C17	1.384(14)	C10—O2	1.224(17)
N1—H1	0.860(12)	C10—O3	1.343(17)
C21—C22	1.472(13)	C12—C13	1.391(24)
C21—C20	1.572(14)	C12—H12	0.929(15)
C21—H21	0.931(9)	C4—C3	1.376(15)
C18—C7	1.361(19)	C4—H4	0.930(17)
C18—C19	1.481(16)	C3—C2	1.381(26)
C17—C9	1.375(19)	C3—H3	0.929(12)
C17—C16	1.471(18)	C13—C14	1.330(19)
C7—C6	1.459(17)	C13—H13	0.930(13)
C7—C8	1.500(15)	C2—H2	0.93(1)
C9—C10	1.479(16)	C14—H14	0.930(16)
C9—C8	1.503(19)	C22—C23	1.315(15)
C8—C20	1.519(17)	C22—H22	0.931(12)
C8—H8	0.981(15)	C23—H23	0.93(1)
C16—C11	1.394(15)	C24—H24A	0.960(18)
C16—C15	1.397(22)	C24—H24B	0.960(15)
C6—O1	1.199(22)	C24—H24C	0.960(12)
C6—C5	1.588(12)	C25—H25A	0.960(13)
C19—C1	1.373(13)	C25—H25B	0.960(13)
C19—C5	1.430(25)	C25—H25C	0.960(14)
C11—O3	1.340(19)		

Bond Angle

O4—S2—C25	104.27(31)	C14—C15—C16	120.02(72)
O4—S2—C24	107.80(33)	C14—C15—H15	120.00(83)
C25—S2—C24	97.75(40)	C16—C15—H15	119.98(69)
C23—S1—C20	95.67(36)	C19—C1—C2	115.32(63)
C18—N1—C17	117.89(56)	C19—C1—H1A	122.38(63)
C18—N1—H1	121.04(55)	C2—C1—H1A	122.31(83)
C17—N1—H1	121.08(55)	O2—C10—O3	116.91(74)
C22—C21—C20	102.75(45)	O2—C10—C9	124.41(72)
C22—C21—H21	128.63(58)	O3—C10—C9	118.59(76)
C20—C21—H21	128.62(52)	C13—C12—C11	119.18(95)
C7—C18—N1	122.28(52)	C13—C12—H12	120.41(110)
C7—C18—C19	113.22(48)	C11—C12—H12	120.41(104)
N1—C18—C19	124.49(57)	C5—C4—C3	118.11(78)
C9—C17—N1	122.19(56)	C5—C4—H4	120.99(88)

C9—C17—C16	118.13(58)	C3—C4—H4	120.90(82)
N1—C17—C16	119.66(58)	C4—C3—C2	123.44(77)
C18—C7—C6	109.50(52)	C4—C3—H3	118.32(83)
C18—C7—C8	124.34(47)	C2—C3—H3	118.23(90)
C6—C7—C8	126.03(56)	C14—C13—C12	120.27(102)
C17—C9—C10	120.96(60)	C14—C13—H13	119.85(105)
C17—C9—C8	123.60(57)	C12—C13—H13	119.88(108)
C10—C9—C8	115.37(67)	C3—C2—C1	119.11(85)
C7—C8—C9	107.96(54)	C3—C2—H2	120.42(82)
C7—C8—C20	110.00(43)	C1—C2—H2	120.48(84)
C9—C8—C20	110.81(51)	C13—C14—C15	122.34(91)
C7—C8—H8	109.41(47)	C13—C14—H14	118.80(96)
C9—C8—H8	109.32(49)	C15—C14—H14	118.86(89)
C20—C8—H8	109.33(47)	C23—C22—C21	116.23(60)
C11—C16—C15	118.84(60)	C23—C22—H22	121.94(69)
C11—C16—C17	115.67(62)	C21—C22—H22	121.83(59)
C15—C16—C17	125.49(60)	C22—C23—S1	115.05(68)
O1—C6—C7	128.80(64)	C22—C23—H23	122.51(82)
O1—C6—C5	126.88(58)	S1—C23—H23	122.44(59)
C7—C6—C5	104.25(54)	C11—O3—C10	120.08(63)
C8—C20—C21	126.82(46)	S2—C24—H24A	109.48(65)
C8—C20—S1	122.90(46)	S2—C24—H24B	109.49(59)
C21—C20—S1	110.11(38)	H24A—C24—H24B	109.49(72)
C1—C19—C5	121.86(59)	S2—C24—H24C	109.45(67)
C1—C19—C18	132.46(57)	H24A—C24—H24C	109.46(79)
C5—C19—C18	105.63(57)	H24B—C24—H24C	109.46(84)
O3—C11—C16	125.99(64)	S2—C25—H25A	109.48(67)
O3—C11—C12	114.64(74)	S2—C25—H25B	109.51(56)
C16—C11—C12	119.33(77)	H25A—C25—H25B	109.42(85)
C4—C5—C19	122.13(73)	S2—C25—H25C	109.49(68)
C4—C5—C6	130.55(69)	H25A—C25—H25C	109.44(99)
C19—C5—C6	107.31(55)	H25B—C25—H25C	109.48(81)

Bond length (C26 H26 Cl N O4 S) (4b)

Cl1—C20	1.748(12)	C20—C19	1.361(12)
S1—O4	1.554(14)	C19—C18	1.400(14)
S1—C26	1.683(15)	C19—H19	0.93(1)
S1—C25	1.809(13)	C14—C13	1.369(16)
O2—C10	1.207(10)	C14—H14	0.930(9)
C8—C9	1.372(11)	C13—H13	0.929(9)
C8—C10	1.409(12)	C16—H16	0.930(9)
C8—C7	1.528(15)	N1—H1	0.861(6)
C9—N1	1.377(10)	C18—H18	0.930(7)
C9—C12	1.451(15)	O1—C1	1.223(9)
C12—C13	1.389(10)	O3—C10	1.379(15)
C12—C11	1.405(11)	C2—C1	1.488(13)
C7—C6	1.482(13)	C2—C3	1.559(11)
C7—C17	1.516(13)	C2—H2A	0.969(10)
C7—H7	0.980(8)	C2—H2B	0.971(9)
C5—C6	1.352(11)	C3—C23	1.500(12)
C5—N1	1.382(14)	C3—C24	1.520(13)
C5—C4	1.515(13)	C23—H23A	0.961(10)
C6—C1	1.478(15)	C23—H23B	0.959(10)
C17—C22	1.377(11)	C23—H23C	0.960(9)
C17—C18	1.404(11)	C24—H24A	0.960(11)
C4—C3	1.523(14)	C24—H24B	0.961(10)
C4—H4A	0.970(9)	C24—H24C	0.960(9)
C4—H4B	0.970(7)	C25—H25A	0.959(12)
C11—O3	1.370(9)	C25—H25B	0.960(13)
C11—C16	1.381(16)	C25—H25C	0.961(12)
C21—C22	1.358(13)	C26—H26A	0.960(14)
C21—C20	1.362(12)	C26—H26B	0.961(15)

C21—H21	0.930(8)	C26—H26C	0.960(14)
C22—H22	0.930(8)	H1—N1	0.861(6)
C15—C14	1.362(13)	O4—H1	2.050(13)
C15—C16	1.366(13)	O4—N1	2.891(16)
C15—H15	0.930(12)	N1—O4	2.891(16)

Bond Angle

O4—S1—C26	108.53(51)	C14—C13—H13	119.64(82)
O4—S1—C25	100.25(44)	C12—C13—H13	119.66(74)
C26—S1—C25	100.37(61)	C15—C16—C11	119.58(78)
C9—C8—C10	120.32(66)	C15—C16—H16	120.17(85)
C9—C8—C7	121.08(62)	C11—C16—H16	120.25(79)
C10—C8—C7	118.60(62)	C9—N1—C5	121.00(53)
C8—C9—N1	120.51(62)	C9—N1—H1	119.44(59)
C8—C9—C12	120.69(64)	C5—N1—H1	119.56(57)
N1—C9—C12	118.79(57)	C19—C18—C17	119.12(75)
C13—C12—C11	117.38(66)	C19—C18—H18	120.50(74)
C13—C12—C9	125.76(65)	C17—C18—H18	120.38(73)
C11—C12—C9	116.68(59)	C11—O3—C10	122.03(56)
C6—C7—C17	113.60(56)	C1—C2—C3	114.97(57)
C6—C7—C8	110.31(55)	C1—C2—H2A	108.53(58)
C17—C7—C8	110.98(59)	C3—C2—H2A	108.56(61)
C6—C7—H7	107.24(63)	C1—C2—H2B	108.51(68)
C17—C7—H7	107.23(63)	C3—C2—H2B	108.60(67)
C8—C7—H7	107.17(61)	H2A—C2—H2B	107.42(79)
C6—C5—N1	120.78(63)	O1—C1—C6	120.14(63)
C6—C5—C4	123.14(63)	O1—C1—C2	120.70(63)
N1—C5—C4	116.08(55)	C6—C1—C2	119.09(57)
C5—C6—C1	118.47(63)	O2—C10—O3	116.44(64)
C5—C6—C7	123.00(63)	O2—C10—C8	124.89(71)
C1—C6—C7	118.52(56)	O3—C10—C8	118.67(67)
C22—C17—C18	117.46(67)	C23—C3—C24	109.05(69)
C22—C17—C7	123.03(63)	C23—C3—C4	113.71(66)
C18—C17—C7	119.49(65)	C24—C3—C4	109.34(56)
C5—C4—C3	112.64(54)	C23—C3—C2	109.67(65)
C5—C4—H4A	109.15(68)	C24—C3—C2	109.45(59)
C3—C4—H4A	109.02(70)	C4—C3—C2	105.51(55)
C5—C4—H4B	109.07(61)	C3—C23—H23A	109.44(78)
C3—C4—H4B	109.01(61)	C3—C23—H23B	109.49(75)
H4A—C4—H4B	107.82(76)	H23A—C23—H23B	109.46(79)
O3—C11—C16	117.89(65)	C3—C23—H23C	109.46(78)
O3—C11—C12	121.06(63)	H23A—C23—H23C	109.40(85)
C16—C11—C12	121.02(65)	H23B—C23—H23C	109.56(84)
C22—C21—C20	119.17(77)	C3—C24—H24A	109.52(70)
C22—C21—H21	120.45(71)	C3—C24—H24B	109.50(81)
C20—C21—H21	120.38(77)	H24A—C24—H24B	109.47(89)
C21—C22—C17	122.96(67)	C3—C24—H24C	109.49(74)
C21—C22—H22	118.54(79)	H24A—C24—H24C	109.36(85)
C17—C22—H22	118.50(73)	H24B—C24—H24C	109.5(9)
C14—C15—C16	120.26(82)	S1—C25—H25A	109.5(9)
C14—C15—H15	119.85(83)	S1—C25—H25B	109.51(83)
C16—C15—H15	119.89(87)	H25A—C25—H25B	109.42(97)
C19—C20—C21	120.86(74)	S1—C25—H25C	109.42(91)
C19—C20—Cl1	119.72(61)	H25A—C25—H25C	109.50(99)
C21—C20—Cl1	119.41(64)	H25B—C25—H25C	109.48(105)
C20—C19—C18	120.30(77)	S1—C26—H26A	109.49(101)
C20—C19—H19	119.94(89)	S1—C26—H26B	109.45(103)
C18—C19—H19	119.76(91)	H26A—C26—H26B	109.48(126)
C15—C14—C13	121.02(78)	S1—C26—H26C	109.47(107)
C15—C14—H14	119.48(88)	H26A—C26—H26C	109.50(142)
C13—C14—H14	119.50(84)	H26B—C26—H26C	109.44(125)
C14—C13—C12	120.7(7)	N1—H1—O4	165.57(39)

Table 5. The structural comparison between the experimental 3D model and the optimized - B3LYP/6-311++G(d,p) 3D model of *7-(Thiophen-2-yl)-7,13-dihydro-5-oxa-13-aza-indeno[2,1-b] phenanthrene-6,8-dione* (**3l**)

Bond distance R (Å), angle (°)	**Experimental structure**	**DFT structure**
R (C24-C25)	1.596	1.373
R (C25-C26)	1.516	1.426
R (C26-C27)	1.326	1.368
R (C27-S28)	1.561	1.733
R (C24-S28)	1.626	1.743
R (C24-C11)	1.516	1.525
R (C11-C7)	1.510	1.502
R (C11-C12)	1.543	1.532
R (C7-C8)	1.370	1.359
R (C12-C13)	1.380	1.372
R (C8-N22)	1.373	1.374
R (C13-N22)	1.392	1.391
R (C7-C9)	1.449	1.479
R (C9-O10)	1.220	1.219
R (C12-C14)	1.449	1.454
R(C14-O25)	1.220	1.211
angle: C25-C24-C11	126.694	127.894
angle: S28-C24-C11	124.314	121.670
angle: C24-C11-C12	111.942	111.271
angle: C24-C11-C7	109.253	111.383
angle: C11-C12-C14	116.612	116.516
angle: C11-C7-C9	127.616	128.887
dihedral angle: C27-S28-C24-C11	-179.710	-179.759
dihedral angle: C26-C25-C24-C11	179.863	179.919
dihedral angle: C25-C24-C11-C12	-88.788	90.021
dihedral angle: C25-C24-C11-C7	152.164	-30.066
dihedral angle: S28-C24-C11-C7	-27.639	150.171
dihedral angle: S28-C24-C11-C12	91.408	-89.742
dihedral angle: C24-C11-C12-	80.107	78.944

C14 dihedral angle: C24-C11-C7-C9	-77.511	-75.689

Table 6. The structural comparison between the experimental 3D model and the optimized DFT -B3LYP/6-311++G(d,p) 3D model of *10,10-Dimethyl-7-(4-chlorophenyl)-7,10,11,12-tetrahydro-9H -chromeno[4,3-b]quinoline-6,8-dione* **(4b)**

Bond distance R (Å), angle (°)	**Experimental structure**	**DFT structure**
R (C19-C6)	1.536	1.534
R (C6-C2)	1.511	1.521
R (C6-C7)	1.500	1.518
R (C2-C3)	1.338	1.357
R (C7-C8)	1.370	1.370
R (C3-N17)	1.373	1.388
R (C8-N17)	1.341	1.387
R (C2-C4)	1.467	1.469
R (C4-O5)	1.216	1.227
R (C4-C1)	1.495	1.527
R (C3-C37)	1.488	1.508
R (C1-C36)	1.527	1.543
R (C37-C36)	1.533	1.547
R (C36-C38)	1.513	1.542
R (C36-C42)	1.566	1.538
angle: C19-C6-C7	110.955	112.002
angle: C19-C6-C2	113.263	111.426
angle: C38-C36-C37	111.237	110.501
angle: C38-C36-C1	110.173	110.460
angle: C38-C36-C42	108.518	109.049
angle: C42-C36-C37	108.551	109.205
angle: C42-C36-C1	111.110	109.884
dihedral angle: C32-C19-C6-C7	-118.329	-127.844
dihedral angle: C20-C19-C6-C2	-60.778	-70.142
dihedral angle: C19-C6-C7-C8	-107.593	-104.467
dihedral angle: C19-C6-C2-C3	108.440	104.370
dihedral angle: C19-C6-C2-C4	-71.362	-75.683
dihedral angle: C38-C36-C37-C3	-68.224	72.512
dihedral angle: C38-C36-C1-C4	70.417	-68.202
dihedral angle: C42-C36-C37-	172.446	-167.540

C3 dihedral angle: C42-C36-C1-C4	-169.282	171.442