Supporting Information

Prioritization before dereplication, an effective strategy to target new metabolites in whole extract: Ghosalin from *Murraya paniculata* root

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S.1. Flow chart of isolation scheme



S.2. TIC of LC-HRMS of crude



S.3. HPLCs of crude on cartridge column for fractionation.



S.4. HPLCs of Ghosalin (1).

<Chromatogram>



S.5. Chemical structures of compounds isolated from *M. paniculata*



S.6. Data NMR

Ghosalin (1): Rectangular crystals, SC-XRD analysis HRESIMS m/z 321.1331 [M+H]⁺ calcd for $C_{17}H_{20}O_6+H^+$ ¹H NMR (500 MHz, CDCl₃) δ 7.53(d, 1H, J=10), 7.33(d, 1H, J=10), 6.80(d, 1H, J=5), 6.17(d, 1H, J=10)

1H, J=10), 5.49(d, 1H, J=5), 4.94(d, 1H, J=10), 4.89(s, 1H), 4.78(s, 1H), 3.86(s, 3H), 1.63(d, 6H, J=20), 1.47(s, 3H). 13 C NMR (126 MHz, CDCl₃) δ 161.4, 160.4, 154.1, 143.6, 141.5, 129.3, 113.4, 113.2, 111.9, 109.6, 108.1, 81.6, 72.7, 56.3, 27.4, 27.1, 17.6.

Osthenone (2). Transparent needles. HRESIMS m/z 245.0793 [M+H]⁺ (calcd for C₁₄H₁₂O₄+H⁺, 245.0803)

Murranlongin (3): 20 mg, White powder, HRMESIMS m/z 259.0948 [M+H]⁺ (calcd for C₁₅H₁₄O₄+H⁺, 259.0965). ¹H NMR (500 MHz, MeOD) δ 10.13 (s, 1H), 7.81 (d, 1H, J=10), 7.53 (d, 1H, J=10), 6.99 (d, 1H, J=10), 6.12 (d, 1H, J=10), 3.76 (s, 3H), 2.36 (s, 3H), 1.70 (s, 3H). ¹³C NMR (126 MHz, MeOD) δ 189.9, 161.9, 161.3, 160.4, 152.5, 144.8, 129.4, 129.1, 113.1, 112.8, 112, 108, 55.5, 23.7, 18.4. Minumicrolin (4) 35 mg, White particles, HRMESIMS m/z 299.0891 [M+Na]⁺ (calcd for C₁₅H₁₆O₅ +Na⁺, 299.0890). ¹H NMR (600 MHz, CDCl₃) δ 7.77(d, 1H, J=10), 7.54(d, 1H, J=10), 7.03(d, 1H, J=5), 6.39(d, 1H, J=10), 5.56(t, 1H, J=5), 5.11(d, 2H, J=10), 4.66(d, 1H, J=10), 4.11(s, 3H), 2.03(s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 161, 160.8, 153.8, 145.6, 144.3, 129, 117, 114.3, 113.9, 113.7, 108.5, 78.9, 69, 56.9, 18.5.

S.7. DNP search for compounds in *M. paniculata*

S.8. DNP search for aromatic compounds in *M. paniculata*

S.9. DNP search for coumarin compounds in *M. paniculata*

Spectral information of compound 1



S.10. UV Spectra of compound 1



S.11. X-ray data of compound 1

Table 2 Fractional Atomic Coordinates (×10 ⁴) and Equivalent Isotropic Displacement Parameters (Å ² ×10 ³) for							
ov_SK-IIA_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.							
Atom	x	у	Z	U(eq)			
0001	7709(3)	5231(3)	4139(2)	62.8(6)			
0002	6225(3)	6132(3)	1716(2)	65.3(7)			
0003	8365(3)	6785(3)	888(2)	76.1(8)			
0004	3711(3)	9865(3)	2777(3)	83.5(9)			
0005	9715(4)	3131(4)	4682(3)	98.0(10)			
C006	6391(4)	6375(4)	4394(3)	57.4(8)			
C007	6244(4)	7521(4)	2135(3)	56.6(8)			
C008	7969(4)	7554(4)	1943(3)	58.4(8)			
C009	5695(4)	7538(4)	3440(3)	56.8(8)			
C00A	4366(4)	8727(5)	3723(4)	66.8(9)			
СООВ	8114(4)	9136(4)	1684(4)	66.9(9)			
C00C	8538(5)	4010(5)	5003(4)	73.0(10)			
C00D	5798(4)	6311(5)	5591(3)	65.8(9)			
COOE	6580(5)	5019(6)	6477(3)	78.4(12)			
COOF	7495(5)	5728(5)	875(3)	70.0(10)			
C00G	3783(5)	8705(6)	4914(4)	81.5(12)			
СООН	7869(5)	3939(6)	6220(4)	79.6(12)			
C00I	4484(5)	7504(6)	5811(4)	83.0(13)			
0001	8678(6)	9682(6)	2608(5)	143.5(17)			
СООК	2310(5)	11057(6)	2986(6)	100.8(16)			
COOL	8509(7)	4124(6)	1317(6)	110.1(18)			
С00М	6798(7)	5922(8)	-409(4)	120(2)			
COON	7609(9)	10036(7)	440(5)	127(2)			

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for ov_SK-IIA_auto. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+]$.						
Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
0001	55.6(13)	75.8(16)	54.3(13)	-6.7(11)	10.1(10)	-17.3(11)
0002	66.7(15)	82.5(16)	60.2(13)	-23.7(12)	21.3(11)	-36.9(12)
O003	81.8(17)	88.4(18)	75.3(17)	-31.4(14)	36.2(13)	-43.3(14)
0004	61.5(16)	76.8(18)	103(2)	-19.3(16)	13.2(14)	-4.7(13)
O005	71.7(19)	104(2)	94(2)	6.4(18)	13.7(16)	0.5(17)
C006	48.2(17)	76(2)	56.4(18)	-22.5(16)	13.4(14)	-25.8(16)
C007	50.8(18)	65(2)	56.4(18)	-12.5(15)	7.7(13)	-19.9(15)
C008	52.7(18)	69(2)	56.3(18)	-10.9(15)	10.4(14)	-22.2(15)
C009	47.7(17)	70(2)	58.3(18)	-18.4(16)	11.4(14)	-22.1(15)
C00A	56(2)	72(2)	80(2)	-29(2)	14.2(17)	-22.9(17)
COOB	60(2)	69(2)	76(2)	-9.6(18)	5.8(16)	-24.5(17)
C00C	64(2)	90(3)	66(2)	-3(2)	-0.6(17)	-28(2)
C00D	62(2)	95(3)	53.1(19)	-23.6(18)	13.6(15)	-37.2(19)
COOE	82(3)	125(4)	47.5(19)	-16(2)	9.9(17)	-58(3)
C00F	83(3)	79(2)	62(2)	-26.1(18)	30.1(18)	-38(2)
C00G	68(2)	93(3)	91(3)	-43(3)	29(2)	-23(2)
С00Н	72(3)	110(3)	61(2)	2(2)	0.5(18)	-40(2)
C00I	78(3)	123(4)	67(2)	-44(3)	28(2)	-46(3)
000J	141(4)	138(4)	175(4)	-61(3)	20(3)	-60(3)
СООК	56(2)	82(3)	160(5)	-29(3)	18(3)	-10(2)
COOL	129(4)	76(3)	126(4)	-24(3)	62(3)	-27(3)
C00M	140(5)	193(6)	65(3)	-40(3)	31(3)	-97(5)
C00N	187(6)	108(4)	96(4)	25(3)	-27(4)	-78(4)

Table 4 Bond Lengths for ov_SK-IIA_auto.					
Atom Atom		Length/Å			
0001	C006	1.369(4)			
0001	C00C	1.382(5)			
0002	C007	1.426(4)			
0002	C00F	1.435(4)			
O003	C008	1.427(4)			
O003	C00F	1.408(4)			
O004	C00A	1.358(5)			
0004	С00К	1.423(5)			
O005	C00C	1.191(5)			
C006	C009	1.383(5)			
C006	C00D	1.408(5)			
C007	C008	1.530(4)			
C007	C009	1.506(4)			
C008	С00В	1.493(5)			
C009	C00A	1.408(5)			
C00A	C00G	1.397(6)			
COOB	000J	1.347(6)			
C00B	C00N	1.485(6)			

Table 4 Bond Lengths for ov_SK-IIA_auto.					
Atom	Atom	Length/Å			
C00C	С00Н	1.454(6)			
C00D	C00E	1.423(6)			
C00D	C00I	1.380(6)			
COOE	С00Н	1.322(6)			
C00F	COOL	1.493(7)			
C00F	C00M	1.499(6)			
C00G	C00I	1.365(7)			

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Table 5 Bond Angles for ov_SK-IIA_auto.						
Atom	Atom	Atom	Angle/°			
C006	0001	C00C	123.8(3)			
C007	0002	C00F	108.4(2)			
COOF	O003	C008	109.5(2)			
C00A	0004	СООК	118.6(4)			
0001	C006	C009	117.4(3)			
0001	C006	C00D	119.3(3)			
C009	C006	C00D	123.3(3)			
0002	C007	C008	103.6(3)			
0002	C007	C009	110.1(3)			
C009	C007	C008	115.9(3)			
O003	C008	C007	101.5(3)			
O003	C008	COOB	110.7(3)			
С00В	C008	C007	113.5(3)			
C006	C009	C007	122.8(3)			
C006	C009	C00A	116.8(3)			
C00A	C009	C007	120.3(3)			
0004	C00A	C009	115.9(3)			
0004	C00A	C00G	123.3(4)			
C00G	C00A	C009	120.8(4)			
0001	COOB	C008	117.7(4)			
0001	COOB	C00N	123.4(4)			
COON	COOB	C008	118.9(4)			
0001	C00C	С00Н	115.8(4)			
O005	C00C	0001	117.3(4)			
O005	C00C	С00Н	126.9(4)			
C006	C00D	COOE	117.8(4)			
C00I	C00D	C006	117.3(4)			
C00I	C00D	COOE	124.9(4)			
соон	COOE	C00D	121.9(4)			
0002	C00F	COOL	108.1(3)			
0002	C00F	C00M	109.7(4)			
0003	COOF	0002	106.5(3)			
O003	C00F	COOL	111.8(4)			
0003	COOF	C00M	107.7(3)			

Table 5 Bond Angles for ov_SK-IIA_auto.					
Atom Atom Atom Angle/°					
COOL	C00F	С00М	112.8(4)		
C00I	C00G	C00A	119.9(4)		
C00E	СООН	C00C	121.2(4)		
C00G	C00I	C00D	121.9(4)		

A B C D Angle/° 0001 C006 C009 C007 5.0(5) 0001 C006 C009 C00A -178.4(3) 0001 C006 C00D C00E -1.8(5) 0001 C006 C00D C00E -2.4(6) 0002 C007 C008 C003 31.5(3) 0002 C007 C008 C008 150.3(3) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B C001 178.6(4) 0003 C008 C00B C001 178.6(4) 0003 C008 C00B C001 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 O011 C00C C00H 3.8(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C007 O022 C00F<	Table 6 Torsion Angles for ov_SK-IIA_auto.					
0001 C006 C009 C007 5.0(5) 0001 C006 C009 C00A -178.4(3) 0001 C006 C00D C00E -1.8(5) 0001 C006 C00D C00E -2.4(6) 0002 C007 C008 C003 31.5(3) 0002 C007 C008 C008 54.2(4) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B C001 178.6(4) 0003 C008 C00B C001 178.6(4) 0003 C008 C00B C001 178.6(4) 0004 C00A C00C C00H 177.6(4) C006 C001 C00C C00H 3.8(5) C006 C001 C00C C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C006 C00D C00F C00L 126.0(4) C007 C002	Α	B	C	D	Angle/°	
0001 C006 C009 C00A -178.4(3) 0001 C006 C00D C00E -1.8(5) 0001 C006 C00D C00I 178.9(3) 0001 C00C C00H C00E -2.4(6) 0002 C007 C008 C00B 150.3(3) 0002 C007 C009 C006 54.2(4) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B C001 -143.2(4) 0003 C008 C00B C001 178.6(4) 0004 C00A C00E 177.6(4) 0005 C00C C00H C00E 177.6(4) 0006 O001 C00C C00H 3.8(5) 0006 C009 C00A C00G -0.7(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00F C00H 3.1(6) C007 O002 C00F	0001	C006	C009	C007	5.0(5)	
O001 C006 C00D C00E -1.8(5) O001 C006 C00D C00I 178.9(3) O001 C00C C00H C00E -2.4(6) O002 C007 C008 O003 31.5(3) O002 C007 C008 C00B 150.3(3) O002 C007 C009 C00A -122.2(3) O003 C008 C00B O0J -143.2(4) O003 C008 C00B C00N 37.8(5) O004 C00A C00G C0II 178.6(4) O005 C00C C00H C00E 177.6(4) C006 O001 C00C C00H 3.8(5) C006 C00D C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C007 O002 C00F C00L 126.0(4) C007 C002 C00F C00L 126.0(4) C007 C002	0001	C006	C009	C00A	-178.4(3)	
0001 C006 C00D C001 178.9(3) 0001 C00C C00H C00E -2.4(6) 0002 C007 C008 0003 31.5(3) 0002 C007 C008 C00B 150.3(3) 0002 C007 C009 C006 54.2(4) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B O00J -143.2(4) 0003 C008 C00B C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) 0006 O001 C00C C00H 3.8(5) C006 C001 C00C C00H 3.8(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C007 O002 C00F C00L 126.0(4) C007 C002 C00F C00L 126.0(4) C007 C008	0001	C006	COOD	COOE	-1.8(5)	
0001 C00C C00H C00E -2.4(6) 0002 C007 C008 C00B 150.3(3) 0002 C007 C009 C006 54.2(4) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B 000J -143.2(4) 0003 C008 C00B C00N 37.8(5) 0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 O001 C00C C00H 3.8(5) C006 C001 C00C C00H 3.8(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00L 126.0(4) C007 C008	0001	C006	C00D	C00I	178.9(3)	
0002 C007 C008 O003 31.5(3) 0002 C007 C008 C00B 150.3(3) 0002 C007 C009 C006 54.2(4) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B O00J -143.2(4) 0003 C008 C00B C00N 37.8(5) 0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 O001 C00C C00H 3.8(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C007 O002 C00F C00A -0.3(6) C007 O002 C00F C00H -110.6(4) C007 C008	0001	C00C	C00H	C00E	-2.4(6)	
0002 C007 C008 C008 150.3(3) 0002 C007 C009 C006 54.2(4) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B O00J -143.2(4) 0003 C008 C00B C00N 37.8(5) 0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 O001 C00C C00H 3.8(5) C006 O001 C00C C00H 3.8(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C007 O002 C00F C00G -0.3(6) C007 O002 C00F C00H 3.1(6) C007 C002 C00F C00H 110.6(4) C007 C008	0002	C007	C008	0003	31.5(3)	
0002 C007 C009 C006 54.2(4) 0002 C007 C009 C00A -122.2(3) 0003 C008 C00B O00J -143.2(4) 0003 C008 C00B C00N 37.8(5) 0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 O001 C00C C00H 3.8(5) C006 C001 C00C C00H 3.8(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00L 126.0(4) C007 C008 C00B O0J 103.4(4) C007 C008 C00A C00G 175.9(3) C007 C009	0002	C007	C008	C00B	150.3(3)	
0002 C007 C009 C00A -122.2(3) 0003 C008 C00B O00J -143.2(4) 0003 C008 C00B C00N 37.8(5) 0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 O001 C00C C00H 3.8(5) C006 C009 C00A O004 179.3(3) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C007 O002 C00F O003 5.7(4) C007 O002 C00F C00H -110.6(4) C007 C008 C00B O0J 103.4(4) C007 C009 C00A C00G 175.9(3) C007 C009	0002	C007	C009	C006	54.2(4)	
0003 C008 C00B O00J -143.2(4) 0003 C008 C00B C00N 37.8(5) 0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 O001 C00C C00B -176.2(3) C006 O001 C00C C00H 3.8(5) C006 C009 C00A C00G -176.2(3) C006 C009 C00A C00H 3.8(5) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C006 C00D C00F C00G -0.3(6) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00M -110.6(4) C007 C008 C00B C00J 103.4(4) C007 C009	0002	C007	C009	C00A	-122.2(3)	
0003 C008 C00B C00N 37.8(5) 0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 0001 C00C C00H 3.8(5) C006 C001 C00C C00H 3.8(5) C006 C009 C00A O004 179.3(3) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C007 O002 C00F C00G -0.3(6) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00L 126.0(4) C007 C008 C00B O0J 103.4(4) C007 C008 C00A C00G 175.9(3) C007 C009 C00A C00G 175.9(3) C008 O003	0003	C008	C00B	000J	-143.2(4)	
0004 C00A C00G C00I 178.6(4) 0005 C00C C00H C00E 177.6(4) C006 0001 C00C 0005 -176.2(3) C006 0001 C00C C00H 3.8(5) C006 C009 C00A 0004 179.3(3) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00I C00G -0.3(6) C007 O002 C00F O003 5.7(4) C007 O002 C00F C00H -110.6(4) C007 O002 C00F C00M -110.6(4) C007 C008 C00B C00N -75.6(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003	0003	C008	C00B	C00N	37.8(5)	
O005 COOC COOH COOE 177.6(4) CO06 OO11 COOC OO05 -176.2(3) CO06 OO01 COOC COOH 3.8(5) CO06 CO09 COOA OO04 179.3(3) CO06 CO09 COOA COOG -0.7(5) CO06 COOD COOE COOH 3.1(6) CO06 COOD COOE COOH 3.1(6) CO06 COOD COOE COOH 3.1(6) CO07 OO22 COOF OO03 5.7(4) CO07 OO22 COOF COOL 126.0(4) CO07 OO22 COOF COOM -110.6(4) CO07 CO08 COOB OOJ 103.4(4) CO07 CO09 COOA OOQ4 -4.0(5) CO07 CO09 COOA COOG 175.9(3) CO08 OO03 COOF COOL -101.8(4) CO08 CO07	0004	C00A	C00G	C00I	178.6(4)	
C006 O001 C00C O005 -176.2(3) C006 O001 C00C C00H 3.8(5) C006 C009 C00A O004 179.3(3) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C007 O002 C00F O003 5.7(4) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00L 126.0(4) C007 C008 C00B O00J 103.4(4) C007 C009 C00A C00G 175.9(3) C007 C009 C00A C00G 175.9(3) C008 O003 C00F C00L -101.8(4) C008 C007	0005	C00C	C00H	COOE	177.6(4)	
C006 O001 CO0C C00H 3.8(5) C006 C009 C00A O004 179.3(3) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00G -0.3(6) C007 O002 C00F O003 5.7(4) C007 O002 C00F C00M -110.6(4) C007 O002 C00F C00M -110.6(4) C007 C008 C00B O00J 103.4(4) C007 C008 C00B C00N -75.6(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00L -101.8(4) C008 C007	C006	0001	C00C	0005	-176.2(3)	
C006 C009 C00A O004 179.3(3) C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C006 C00D C00F C00G -0.3(6) C007 O002 C00F O003 5.7(4) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00M -110.6(4) C007 C008 C00B O00J 103.4(4) C007 C008 C00B C00N -75.6(5) C007 C009 C00A C00G 175.9(3) C007 C009 C00A C00G 175.9(3) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00L -101.8(4) C008 C007 C009 C00A 120.6(4) C008 C007	C006	0001	C00C	С00Н	3.8(5)	
C006 C009 C00A C00G -0.7(5) C006 C00D C00E C00H 3.1(6) C006 C00D C00E C00H 3.1(6) C006 C00D C00I C00G -0.3(6) C007 O002 C00F O003 5.7(4) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00M -110.6(4) C007 C008 C00B O0J 103.4(4) C007 C008 C00B C00N -75.6(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00L -101.8(4) C008 C007 C009 C00A 120.6(4) C008 C007 C009 C00A 120.6(4) C009 C006	C006	C009	C00A	0004	179.3(3)	
CO06 CO0D CO0E CO0H 3.1(6) CO06 CO0D CO0I CO0G -0.3(6) CO07 OO02 CO0F OO03 5.7(4) CO07 OO02 CO0F CO0L 126.0(4) CO07 OO02 CO0F CO0M -110.6(4) CO07 CO08 CO0B OO0J 103.4(4) CO07 CO08 CO0B CO0N -75.6(5) CO07 CO09 CO0A OO04 -4.0(5) CO07 CO09 CO0A CO0G 175.9(3) CO08 OO03 CO0F CO0L -101.8(4) CO08 OO03 CO0F CO0L -101.8(4) CO08 OO03 CO0F CO0L -101.8(4) CO08 CO07 CO09 CO0A 120.6(4) CO08 CO07 CO09 CO0A 120.6(4) CO09 CO06 CO0D CO06 -63.0(4) CO09 CO06 <td>C006</td> <td>C009</td> <td>C00A</td> <td>C00G</td> <td>-0.7(5)</td>	C006	C009	C00A	C00G	-0.7(5)	
C006 C00D C00I C00G -0.3(6) C007 O002 C00F O003 5.7(4) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00L 126.0(4) C007 O002 C00F C00M -110.6(4) C007 C008 C00B O00J 103.4(4) C007 C008 C00B C00N -75.6(5) C007 C009 C00A O004 -4.0(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00M 133.7(4) C008 C007 C009 C00A 120.6(4) C008 C007 C009 C00A 120.6(4) C009 C006	C006	C00D	C00E	С00Н	3.1(6)	
C007 O002 CO0F O003 5.7(4) C007 O002 CO0F CO0L 126.0(4) C007 O002 CO0F CO0M -110.6(4) C007 C008 CO0B O00J 103.4(4) C007 C008 CO0B CO0N -75.6(5) C007 C009 C00A C00G 175.9(3) C008 O003 CO0F C00L -101.8(4) C008 C007 C009 C00A -63.0(4) C008 C007 C009 C00A 120.6(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00I -2.0(5) C009 C006 C00D C00I -2.0(5) C009 C007<	C006	C00D	C00I	C00G	-0.3(6)	
CO07 OO02 CO0F COOL 126.0(4) CO07 OO02 CO0F CO0M -110.6(4) CO07 CO08 CO0B OO0J 103.4(4) CO07 CO08 CO0B OO0J 103.4(4) CO07 CO08 CO0B CO0N -75.6(5) CO07 CO09 CO0A OO04 -4.0(5) CO07 CO09 CO0A CO0G 175.9(3) CO08 OO03 CO0F OO02 16.0(4) CO08 OO03 CO0F CO0L -101.8(4) CO08 OO03 CO0F CO0M 133.7(4) CO08 CO07 CO09 CO0A 120.6(4) CO08 CO07 CO09 CO0A 120.6(4) CO09 CO06 CO0D CO0E 177.3(3) CO09 CO06 CO0D CO0I -2.0(5) CO09 CO07 CO08 OO03 152.3(3)	C007	0002	C00F	0003	5.7(4)	
C007 O002 CO0F C00M -110.6(4) C007 C008 C00B OOJ 103.4(4) C007 C008 C00B C00N -75.6(5) C007 C009 C00A O004 -4.0(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00L -101.8(4) C008 C007 C009 C00A 133.7(4) C008 C007 C009 C00A 120.6(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C007	0002	C00F	COOL	126.0(4)	
C007 C008 C00B O00J 103.4(4) C007 C008 C00B C00N -75.6(5) C007 C009 C00A O004 -4.0(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00M 133.7(4) C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C007	0002	C00F	C00M	-110.6(4)	
C007 C008 C00B C00N -75.6(5) C007 C009 C00A O004 -4.0(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00M 133.7(4) C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C007	C008	C00B	000J	103.4(4)	
C007 C009 C00A O004 -4.0(5) C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00M 133.7(4) C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C007	C008	C00B	COON	-75.6(5)	
C007 C009 C00A C00G 175.9(3) C008 O003 C00F O002 16.0(4) C008 O003 C00F C00L -101.8(4) C008 O003 C00F C00M 133.7(4) C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C007	C009	C00A	0004	-4.0(5)	
C008 O003 CO0F O002 16.0(4) C008 O003 CO0F CO0L -101.8(4) C008 O003 CO0F CO0L -101.8(4) C008 O003 CO0F CO0M 133.7(4) C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C007	C009	C00A	C00G	175.9(3)	
C008 O003 CO0F C00L -101.8(4) C008 O003 CO0F C00M 133.7(4) C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C008	0003	C00F	0002	16.0(4)	
C008 O003 COOF COOM 133.7(4) C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C008	0003	C00F	COOL	-101.8(4)	
C008 C007 C009 C006 -63.0(4) C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C008	0003	C00F	C00M	133.7(4)	
C008 C007 C009 C00A 120.6(4) C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C008	C007	C009	C006	-63.0(4)	
C009 C006 C00D C00E 177.3(3) C009 C006 C00D C00I -2.0(5) C009 C007 C008 O003 152.3(3)	C008	C007	C009	C00A	120.6(4)	
C009 C006 C00D C001 -2.0(5) C009 C007 C008 O003 152.3(3)	C009	C006	C00D	COOE	177.3(3)	
C009 C007 C008 O003 152.3(3)	C009	C006	C00D	C00I	-2.0(5)	
	C009	C007	C008	0003	152.3(3)	
C009 C007 C008 C00B -89.0(4)	C009	C007	C008	C00B	-89.0(4)	
C009 C00A C00G C00I -1.4(6)	C009	C00A	C00G	C00I	-1.4(6)	
COOA COOG COOI COOD 1.9(6)	C00A	C00G	C00I	C00D	1.9(6)	

Table 6 Torsion Angles for ov_SK-IIA_auto.					
Α	В	С	D	Angle/°	
C00C	0001	C006	C009	179.1(3)	
C00C	0001	C006	C00D	-1.7(5)	
C00D	C006	C009	C007	-174.2(3)	
C00D	C006	C009	C00A	2.4(5)	
C00D	COOE	С00Н	C00C	-0.9(6)	
COOE	C00D	C00I	C00G	-179.5(4)	
C00F	0002	C007	C008	-23.2(4)	
C00F	0002	C007	C009	-147.8(3)	
C00F	O003	C008	C007	-29.3(4)	
C00F	O003	C008	C00B	-150.1(3)	
C00I	C00D	COOE	СООН	-177.6(4)	
СООК	0004	C00A	C009	176.5(3)	
С00К	0004	C00A	C00G	-3.4(6)	

Table 7 Hydrogen Atom Coordinates (Å×10 ⁴) and Isotropic Displacement Parameters (Å ² ×10 ³) for ov_SK- IIA auto.						
Atom	x	у	Z	U(eq)		
H007	5512.29	8389.57	1599.04	68		
H008	8665.1	6969.03	2656.48	70		
НООВ	9207.92	8725.6	1410.64	80		
HOOE	6172.58	4932.38	7261.01	94		
H00G	2918.51	9508.39	5094.55	98		
ноон	8356.19	3119.6	6827.69	96		
H00I	4064.34	7489.26	6593.06	100		
H00A	1929.06	11725.77	2224.83	151		
Н00С	2564.05	11630.32	3580.83	151		
H00D	1492.73	10618.21	3293.96	151		
HOOF	8989.17	4079.33	2114.91	165		
НООК	9336.79	3811.69	745.09	165		
HOOL	7852.6	3451.62	1376.13	165		
Н00М	6175.85	5228.87	-440.1	180		
HOON	7650.05	5705.03	-974.9	180		
Н00О	6120.25	6957.55	-632.86	180		
НООР	8267.87	9522.69	-167.81	190		
H00Q	7726.52	11038.71	422.08	190		
HOOR	6505.61	10127.61	261.87	190		
НООЈ	8840(70)	10680(40)	2610(50)	121(19)		





S.12. ¹H NMR spectrum of compound 1 in $CDCl_3$

S.13. ¹³C NMR spectrum of compound 1 in $CDCI_3$



S.14. DEPT-135 NMR spectrum of compound 1 in $CDCI_3$



S.15. HSQC spectrum of compound 1 in $CDCI_3$



S.16. HMBC spectrum of compound 1 in $CDCI_3$



S.17: $^{1}H^{-1}H$ COSY NMR spectrum of compound 1 in CDCl₃



S.18. NOESY spectrum of compound 1 in CDCl₃









Spectral information of compound 3

S.20. UV Spectra of compound 3









S.22. ¹³C NMR spectrum of compound 3 in CD_3OD



S.23. DEPT-135 NMR spectrum of compound 3 in CD₃OD



S.24. HSQC spectrum of compound 3 in CD₃OD



S.25. HMBC spectrum of compound 3 in CD₃OD



S.26. 1 H- 1 H COSY NMR spectrum of compound 3 in CD₃OD



S.27. NOESY spectrum of compound 3 in CD₃OD



Spectral information of compound 4





S.29. ¹H NMR spectrum of compound 4 in CDCl₃



S.31. DEPT-135 NMR spectrum of compound 4 in $CDCI_3$



S.32. HSQC spectrum of compound 4 in CDCl₃



S.33. HMBC spectrum of compound 4 in CDCl₃



S.34. 1 H- 1 H COSY NMR spectrum of compound 4 in CDCl₃



S 35. Calculation for DoU

[•] a compound which contains elements other than carbon and hydrogen:

$$DoU=\frac{2C+2+N-X-H}{2}$$

C is the number of carbons

N is the number of nitrogens

 \boldsymbol{X} is the number of halogens (F, Cl, Br, I)

 \boldsymbol{H} is the number of hydrogens