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Reactions of functionally substituted bicyclo[4.2.2]deca-2,4,7,9-tetraenes with *m*-chloroperbenzoic acid and *in vitro* evaluation of product cytotoxicity against tumor cells

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Contents

Experimental Section

The ^{1}H, ^{13}C spectra were measured in $CDCl_3$ on a Bruker Avance-500 spectrometer (500 MHz for ^{1}H, 125 MHz for ^{13}C). X-Ray diffraction analysis was performed on an XCaliburEos four-circle automated diffractometer (graphite monochromator, MoKα radiation, λ = 0.71073 Å, w-scan mode, $2\theta_{max}$ = 62°). The data were collected and treated using the CrysAlis^{Pro}OxfordDiffractionLtd. program package, version 1.171.36.20. The structures were solved by the direct method and refined by the full-matrix least-squares method in the anisotropic approximation for non-hydrogen atoms. The hydrogen atoms were located on electron density maps and refined in the isotropic approximation. The refinement was done using SHELX97 program package. Mass spectra were recorded on a MALDI TOF/TOF Autoflex-III Bruker mass spectrometer using 2,5-dihydroxybenzoic acid (2,5-DHB) and α-cyano-4-hydroxycinnamic acid (HCCA) as a matrix in positive ion mode. Elemental analyses were measured on a 1106 Carlo Erba apparatus. IR spectra were recorded on spectrometer as liquid films and are reported in wavenumbers (cm^{-1}). All solvents were dried and freshly distilled before use. *m*-Chloroperbenzoic acid (70-75%, balance 3-Chlorobenzoic acid and water) were purchased from commercial sources and used without further purification.

*Synthesis of oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trienes **2a-f** and dihydroxybicyclo[4.3.1]deca-2,4,7(8)-trienes **3a,b**, **4a,b** (general procedure).* At 0 °C, mCPBA (2.8 mmol) was added to a mixture of cycloadduct **1a-f** (2 mmol) in $CHCl_3$ (46 ml). The mixture was stirred for 3 hours at 0 °C, 3 hours at 40 °C and for 12 hours at room temperature. Then $NaHCO_3$ (4 mmol) was added, and after being stirred for 1 hour at 0 °C, the mixture was washed with 1 *M* NaOH (23 ml) and brine (2×10 ml). The aqueous layer was extracted with CH_2Cl_2 (3×15 ml) and the combined extracts were dried over $MgSO_4$, filtered, and concentrated. Column chromatography on silica gel (petroleum ether → petroleum ether / EtOAc 10:1 for **2a-f**, petroleum ether → petroleum ether / EtOAc 5:1 for **3a,b, 4a,b**) afforded the target products.

*2-[4-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)butyl]-1H-isoindole-1,3(2H)-dione **2a**:* Yield 0.160 g (23%), colorless oil. R_f 0.48 (petroleum ether → petroleum ether / ethyl acetate 10:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.85 (dd, *J* = 5.4 Hz, *J* = 3.0 Hz, 2H), 7.72 (dd, *J* = 5.4 Hz, *J* = 3.1 Hz, 2H), 5.83-6.12 (m, 4H), 5.45 (dd, *J* = 9.4 Hz, *J* = 6.7 Hz, 1H), 5.23-5.29 (m, 1H), 3.68 (t, *J* = 7.1 Hz, 2H), 3.18-3.27 (m, 1H), 3.03-3.12 (m, 2H), 1.94-2.02 (m, 1H), 1.63-1.74 (m, 2H), 1.37-1.48 (m, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.4 (2C), 135.6, 133.9 (2C), 133.7, 132.1 (2C), 127.3, 125.7, 123.2 (2C), 120.8, 117.4, 61.1, 59.0, 37.9, 37.8, 35.7, 32.3, 28.6, 21.2 ppm. IR (liquid film): 3465, 3020, 2928, 2865, 1714, 1396, 1038 cm^{-1}. MALDI-TOF: 347 $[M]^+$. Anal. Calcd for $C_{22}H_{21}NO_3$: C, 76.06; H, 6.09; N, 4.03. Found: C, 75.95; H, 6.04; N, 3.95.

*2-[4-(7,10-Dihydroxybicyclo[4.3.1]deca-2,4,8-trien-1-yl)butyl]-1H-isoindole-1,3(2H)-dione **3a**:* Yield 0.168 g (23%), colorless oil. R_f 0.52 (petroleum ether → petroleum ether / ethyl acetate 5:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (dd, *J* = 5.1 Hz, *J* = 3.1 Hz, 2H), 7.73 (dd, *J* = 5.2 Hz, *J* = 3.0 Hz, 2H), 6.15 (dd, *J* = 9.9 Hz, *J* = 5.2 Hz, 1H), 5.71-5.81 (m, 2H), 5.64 (dd, *J* = 11.4 Hz, *J* = 7.1 Hz, 1H), 5.53 (d, *J* = 11.4 Hz, 1H), 5.36 (d, *J* = 9.9 Hz, 1H), 4.06-4.15 (m, 2H), 3.74 (td, *J* = 6.8 Hz, *J* = 2.6 Hz, 2H), 3.31 (d, *J* = 4.0 Hz, 1H), 1.98-2.08 (m, 1H), 1.63-1.85 (m, 2H), 1.40-1.59 (m, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.8 (2C), 134.7, 134.0 (2C), 132.0 (2C), 130.5, 130.2, 126.6, 124.9, 123.7, 123.3 (2C), 69.9, 66.6, 48.0, 45.3, 38.5, 37.4, 29.4, 20.3 ppm. IR (liquid film): 3460, 3026, 2935, 2865, 1770, 1712, 1398, 1072 cm^{-1}. MALDI-TOF: 365 $[M]^+$. Anal. Calcd for $C_{22}H_{23}NO_4$: C, 72.31; H, 6.34; N, 3.83. Found: C, 72.21; H, 6.25; N, 3.76.

*2-[4-(9,10-Dihydroxybicyclo[4.3.1]deca-2,4,7-trien-1-yl)butyl]-1H-isoindole-1,3(2H)-dione **4a**:* Yield 0.168 g (23%), colorless oil. R_f 0.56 (petroleum ether → petroleum ether / ethyl acetate 5:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (dd, *J* = 5.4 Hz, *J* = 3.0 Hz, 2H), 7.73 (dd, *J* = 5.4 Hz, *J* = 3.0 Hz, 2H), 6.19 (ddd, *J* = 10.0 Hz, *J* = 5.6 Hz, *J* = 1.8 Hz, 1H), 5.95 (t, *J* = 10.0 Hz, 1H), 5.84 (dd, *J* = 10.6 Hz, *J* = 7.0 Hz, 1H), 5.77 (dd, *J* = 12.2 Hz, *J* = 6.8 Hz, 1H), 5.51 (dd, *J* = 9.9 Hz, *J* = 4.5 Hz, 1H), 5.24 (d, *J* = 12.2 Hz, 1H), 3.97 (d, *J* = 3.3 Hz, 1H), 3.65-3.84 (m, 2H), 3.54 (d, *J* = 5.3 Hz, 1H), 3.29-3.36 (m, 1H), 2.40 (td, *J* = 13.2 Hz, *J* = 4.5 Hz, 1H), 1.66-1.89 (m, 2H), 1.23-1.61 (m, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.9 (2C), 136.2, 134.0 (2C), 132.0

(2C), 130.0, 128.3, 126.1, 123.9, 123.3 (2C), 121.2, 70.3 (2C), 47.9, 44.4, 37.2, 33.8, 29.1, 19.9 ppm. IR (liquid film): 3459, 3020, 2938, 2865, 1770, 1712, 1398, 1072 cm^{-1}. MALDI-TOF: 365 $[M]^+$. Anal. Calcd for $C_{22}H_{23}NO_4$: C, 72.31; H, 6.34; N, 3.83. Found: C, 72.20; H, 6.26; N, 3.76.

Methyl 4-(8-oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)butanoate ***2b****:* Yield 0.103 g (21%), colorless oil. R_f 0.50 (petroleum ether → petroleum ether / ethyl acetate 10:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.85-6.11 (m, 4H), 5.46 (dd, *J* = 9.4 Hz, *J* = 6.7 Hz, 1H), 5.25-5.30 (m, 1H), 3.67 (s, 3H), 3.22-3.27 (m, 1H), 3.06-3.12 (m, 2H), 2.26-2.40 (m, 2H), 1.94-2.01 (m, 1H), 1.64-1.79 (m, 2H), 1.37-1.46 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 173.8, 135.5, 133.7, 127.3, 125.7, 120.7, 117.4, 61.0, 58.7, 51.5, 38.0, 35.7, 33.8, 32.1, 19.4 ppm. IR (liquid film): 3460, 3020, 2914, 1732, 1435, 1173, 1035 cm^{-1}. MALDI-TOF: 246 $[M]^+$. Anal. Calcd for $C_{15}H_{18}O_3$: C, 73.15; H, 7.37. Found: C, 73.00; H, 7.31.

Methyl 4-(7,10-dihydroxybicyclo[4.3.1]deca-2,4,8-trien-1-yl)butanoate ***3b*** *and methyl 4-(9,10-dihydroxybicyclo[4.3.1]deca-2,4,7-trien-1-yl)butanoate* ***4b*** (1:1 mixture): Yield 0.232 g (44%), colorless oil. R_f 0.58 (petroleum ether → petroleum ether / ethyl acetate 5:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.12-6.20 (m, 2H), 5.97 (t, *J* = 10.0 Hz, 1H), 5.75-5.89 (m, 4H), 5.64-5.70 (m, 1H), 5.49-5.57 (m, 2H), 5.24-5.30 (m, 2H), 4.25 (s, 1H), 4.00-4.06 (m, 2H), 3.68-3.74 (m, 7H), 3.29-3.39 (m, 2H), 2.31-2.55 (m, 3H), 2.09-2.17 (m, 1H), 1.54-1.81 (m, 8H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.3, 174.9, 135.5, 133.9, 130.9, 130.1, 129.3, 127.9, 127.1, 126.1, 125.3, 124.1, 123.5, 121.5, 70.6, 69.9, 69.8, 66.6, 52.0, 51.7, 47.8, 47.5, 45.2, 44.5, 38.1, 34.1, 33.9, 33.1, 18.2, 17.7 ppm. IR (liquid film): 3468, 3021, 2910, 1736, 1435, 1178, 1034 cm^{-1}. MALDI-TOF: 264 $[M]^+$. Anal. Calcd for $C_{15}H_{20}O_4$: C, 68.16; H, 7.63. Found: C, 68.01; H, 7.58.

3-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)propanenitrile ***2c****:* Yield 0.287 g (72%), white needles, m.p. = 96-97 °C. R_f 0.39 (petroleum ether → petroleum ether / ethyl acetate 10:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.87-6.16 (m, 4H), 5.45 (dd, *J* = 9.5 Hz, *J* = 6.7 Hz, 1H), 5.25-5.32 (m, 1H), 3.25-3.29 (m, 1H), 3.15-3.20 (m, 1H), 3.09 (t, *J* = 7.7 Hz, 1H), 2.32-2.45 (m, 2H), 2.21-2.30 (m, 1H), 1.86-1.92 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 134.5, 133.5, 127.5, 126.4, 120.2, 119.5, 117.4, 59.8, 58.8, 37.9, 35.4, 28.7, 12.0 ppm. IR (liquid film): 3021, 2924, 2855, 1650, 1400, 1315, 1015 cm^{-1}. MALDI-TOF: 199 $[M]^+$. Anal. Calcd for $C_{13}H_{13}NO$: C, 78.36; H, 6.58; N, 7.03. Found: C, 78.27; H, 6.53; N, 6.98.

4-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)butanenitrile ***2d*****:** Yield 0.290 g (68%), white needles, m.p. = 100-101 °C. R_f 0.40 (petroleum ether → petroleum ether / ethyl acetate 10:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.87-6.10 (m, 4H), 5.46 (dd, *J* = 9.4 Hz, *J* = 6.7 Hz, 1H), 5.25-5.32 (m, 1H), 3.22-3.29 (m, 1H), 3.09-3.12 (m, 1H), 3.04 (t, *J* = 7.7 Hz, 1H), 2.31-2.46 (m, 2H), 2.03-2.09 (m, 1H), 1.67-1.80 (m, 2H), 1.55-1.61 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.0, 133.7, 127.4, 126.0, 120.5, 119.4, 117.4, 60.5, 58.5, 38.1, 35.6, 31.5, 20.2, 17.2

ppm. IR (liquid film): 3021, 2920, 2856, 1655, 1400, 1311, 1014 cm^{-1}. MALDI-TOF: 213 $[M]^+$. Anal. Calcd for $C_{14}H_{15}NO$: C, 78.84; H, 7.09; N, 6.57. Found: C, 78.73; H, 7.06; N, 6.53.

2-[2-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)ethyl]-1H-isoindole-1,3(2H)-dione ***2e****:* Yield 0.453 g (71%), colorless oil. R_f 0.42 (petroleum ether → petroleum ether / ethyl acetate 10:1). ^1H NMR (500 MHz, $CDCl_3$): δ 7.83 (dd, *J* = 5.4 Hz, *J* = 3.1 Hz, 2H), 7.70 (dd, *J* = 5.4 Hz, *J* = 3.0 Hz, 2H), 6.06-6.14 (m, 1H), 5.95-6.02 (m, 1H), 5.84-5.91 (m, 2H), 5.46 (dd, *J* = 9.4 Hz, *J* = 6.8 Hz, 1H), 5.23-5.26 (m, 1H), 3.82-3.90 (m, 1H), 3.68-3.78 (m, 1H), 3.27 (t, *J* = 7.6 Hz, 1H), 3.19-3.24 (m, 1H), 3.15-3.18 (m, 1H), 2.26-2.31 (m, 1H), 1.92 (dt, *J* = 14.8 Hz, *J* = 8.1 Hz, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.2 (2C), 135.3, 133.9 (2C), 133.8, 132.2 (2C), 127.2, 126.0, 123.2 (2C), 120.6, 117.3, 59.7, 58.0, 37.7, 35.5, 33.5, 31.1 ppm. IR (liquid film): 3463, 3020, 2925, 2863, 1710, 1396, 1034 cm^{-1}. MALDI-TOF: 319 $[M]^+$. Anal. Calcd for $C_{20}H_{17}NO_3$: C, 75.22; H, 5.37; N, 4.39. Found: C, 75.10; H, 5.31; N, 4.35.

Methyl 3-(8-oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)propanoate ***2f****:* Yield 0.311 g (67%), colorless oil. R_f 0.45 (petroleum ether → petroleum ether / ethyl acetate 10:1). ^1H NMR (500 MHz, $CDCl_3$): δ 5.87-6.11 (m, 4H), 5.46 (dd, *J* = 9.4 Hz, *J* = 6.7 Hz, 1H), 5.25-5.31 (m, 1H), 3.68 (s, 3H), 3.22-3.28 (m, 1H), 3.12 (dt, *J* = 3.1 Hz, *J* = 1.4 Hz, 1H), 3.01-3.06 (m, 1H), 2.33-2.39 (m, 2H), 2.19-2.28 (m, 1H), 1.83-1.92 (m, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 173.6, 135.3, 133.6, 127.3, 125.9, 120.6, 117.4, 60.5, 58.6, 51.7, 38.5, 35.6, 28.5, 27.7 ppm. IR (liquid film): 3460, 3021, 2919, 1731, 1437, 1173, 1036 cm^{-1}. MALDI-TOF: 232 $[M]^+$. Anal. Calcd for $C_{14}H_{16}O_3$: C, 72.39; H, 6.94. Found: C, 72.29; H, 6.89.

Crystal data for 2c

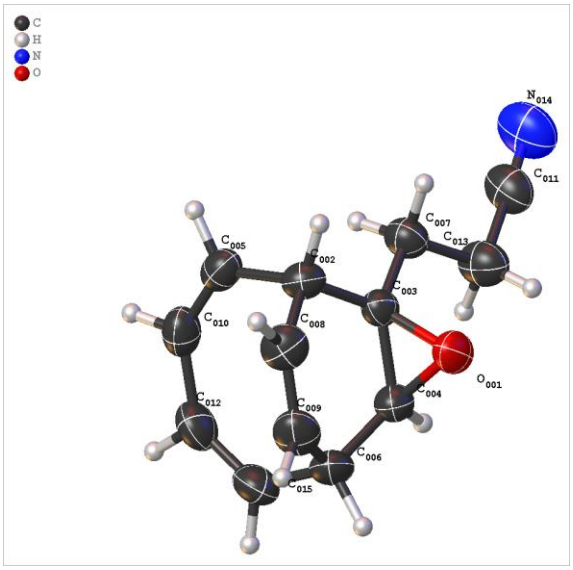


Figure S1. Geometry of molecule 2c

Table S1. Crystal data and structure refinement for **2c**.	
Identification code	**GGF-748-26 (2c)**
Empirical formula	$C_{13}H_{13}NO$
Formula weight	199.24
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	7.8596(11)
b/Å	14.0911(14)
c/Å	19.2901(19)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2136.4(4)
Z	8
ρ_{calc}g cm^{-3}	1.239
μ/mm^{-1}	0.079
F(000)	848.0
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.222 to 58.274
Index ranges	$-9 \leq h \leq 5$, $-17 \leq k \leq 19$, $-26 \leq l \leq 24$
Reflections collected	6175
Independent reflections	2523 [R_{int} = 0.0240, R_{sigma} = 0.0350]
Data/restraints/parameters	2523/0/188
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0554, wR_2 = 0.1436
Final R indexes [all data]	R_1 = 0.0831, wR_2 = 0.1709
Largest diff. peak/hole / e Å^{-3}	0.21/-0.27

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for GGF-748-26. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.				
Atom	***x***	***y***	***z***	**U(eq)**
$O_{(001)}$	2925.0(16)	5299.3(9)	405.5(6)	50.0(4)
$C_{(002)}$	3659(2)	3578.6(12)	560.3(9)	40.4(4)
$C_{(003)}$	3676(2)	4580.6(11)	847.8(8)	36.7(4)
$C_{(004)}$	2039(2)	4994.1(13)	1023.8(9)	42.0(4)
$C_{(005)}$	3809(2)	2882.7(12)	1153.0(9)	45.1(4)
$C_{(006)}$	452(2)	4405.7(14)	929.7(10)	49.0(5)
$C_{(007)}$	5329(2)	4856.4(13)	1181.9(10)	45.0(4)
$C_{(008)}$	2068(2)	3354.9(14)	165.1(9)	49.6(5)
$C_{(009)}$	600(3)	3726.3(14)	339.0(10)	52.3(5)
$C_{(010)}$	2757(3)	2772.7(14)	1682.2(10)	50.4(5)
$C_{(011)}$	7075(3)	6086.0(15)	1724.5(10)	54.8(5)
$C_{(012)}$	1155(3)	3207.2(14)	1887.0(11)	55.1(5)
$C_{(013)}$	5380(3)	5857.9(15)	1460.7(13)	57.7(5)
$N_{(014)}$	8399(3)	6244.6(15)	1925.7(10)	74.7(6)
$C_{(015)}$	152(3)	3863.8(14)	1595.0(11)	56.1(5)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for GGF-748-26. 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}**
$O_{(001)}$	44.4(8)	51.1(7)	54.4(7)	17.6(6)	0.3(6)	2.3(6)
$C_{(002)}$	35.9(9)	45.8(9)	39.6(9)	-5.3(7)	-1.5(7)	4.1(7)
$C_{(003)}$	34.1(9)	39.2(8)	36.8(8)	4.6(7)	0.9(6)	0.5(7)
$C_{(004)}$	38.6(10)	39.7(9)	47.8(9)	1.9(8)	5.9(7)	3.6(7)
$C_{(005)}$	42.9(10)	37.9(9)	54.5(10)	-2.1(8)	-9.1(8)	2.9(8)
$C_{(006)}$	30.6(9)	51.4(10)	64.9(11)	7.0(9)	1.6(8)	6.2(8)
$C_{(007)}$	38.4(10)	47.7(10)	48.8(9)	-5.2(8)	0.0(8)	-3.7(8)
$C_{(008)}$	49.6(12)	54.4(10)	44.7(9)	-6.1(9)	-10.3(8)	-0.8(9)
$C_{(009)}$	42.3(11)	59.2(11)	55.4(11)	3.7(9)	-15.0(9)	-4.7(9)
$C_{(010)}$	55.8(12)	42.7(10)	52.6(10)	10.5(8)	-9.9(9)	-5.5(9)
$C_{(011)}$	57.2(13)	53.7(11)	53.4(11)	-16.8(9)	5.0(9)	-12.6(9)
$C_{(012)}$	58.0(13)	54.8(11)	52.5(11)	9.6(9)	11.5(9)	-10.8(10)
$C_{(013)}$	48.8(12)	56.5(12)	67.8(13)	-16.5(11)	-1.0(11)	-5.4(9)
$N_{(014)}$	67.4(13)	81.9(13)	74.8(12)	-24.4(11)	-3.7(10)	-21.1(11)
$C_{(015)}$	42.1(11)	58.1(11)	68.0(12)	1.5(10)	16.8(10)	-4.7(9)

Table S4. Bond Lengths for GGF-748-26.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
$O_{(001)}$	$C_{(003)}$	1.450(2)		$C_{(006)}$	$C_{(009)}$	1.493(3)
$O_{(001)}$	$C_{(004)}$	1.447(2)		$C_{(006)}$	$C_{(015)}$	1.512(3)
$C_{(002)}$	$C_{(003)}$	1.517(2)		$C_{(007)}$	$C_{(013)}$	1.511(3)
$C_{(002)}$	$C_{(005)}$	1.511(3)		$C_{(008)}$	$C_{(009)}$	1.310(3)
$C_{(002)}$	$C_{(008)}$	1.498(2)		$C_{(010)}$	$C_{(012)}$	1.455(3)
$C_{(003)}$	$C_{(004)}$	1.453(2)		$C_{(011)}$	$C_{(013)}$	1.462(3)
$C_{(003)}$	$C_{(007)}$	1.501(2)		$C_{(011)}$	$N_{(014)}$	1.133(3)
$C_{(004)}$	$C_{(006)}$	1.508(3)		$C_{(012)}$	$C_{(015)}$	1.339(3)
$C_{(005)}$	$C_{(010)}$	1.322(3)				

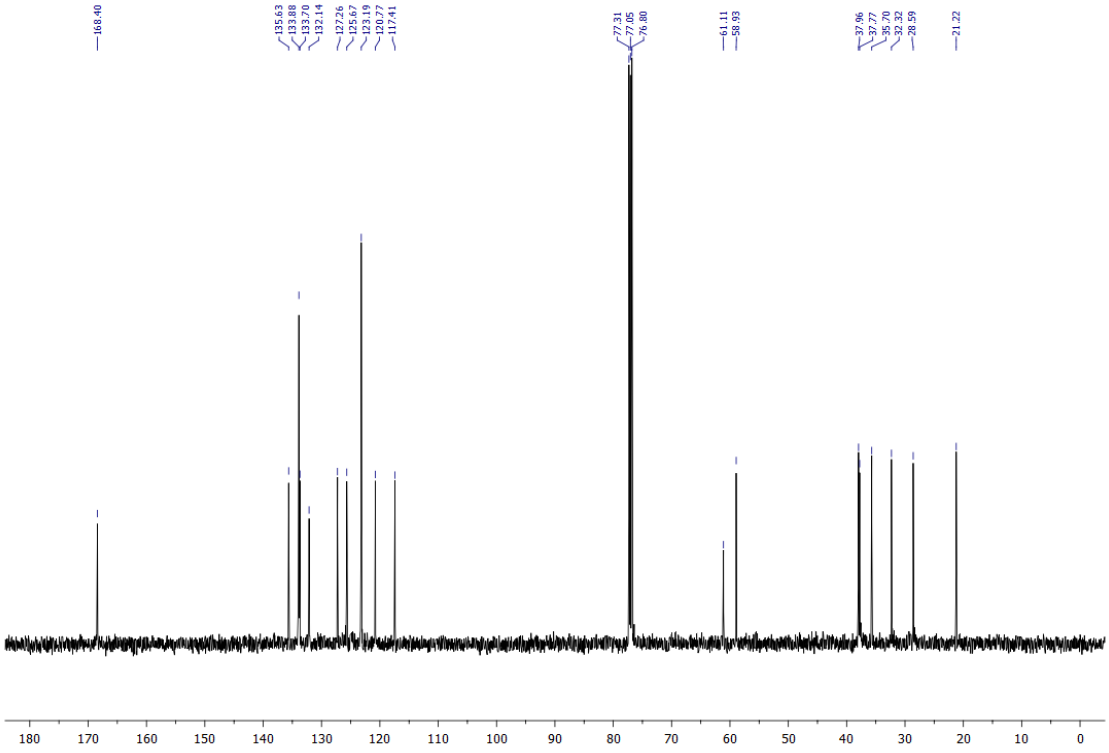
Table S5. Bond Angles for GGF-748-26.								
Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
$C_{(004)}$	$O_{(001)}$	$C_{(003)}$	60.21(10)		$C_{(010)}$	$C_{(005)}$	$C_{(002)}$	127.69(18)
$C_{(005)}$	$C_{(002)}$	$C_{(003)}$	109.08(13)		$C_{(004)}$	$C_{(006)}$	$C_{(015)}$	107.72(16)
$C_{(008)}$	$C_{(002)}$	$C_{(003)}$	112.89(14)		$C_{(009)}$	$C_{(006)}$	$C_{(004)}$	112.32(16)
$C_{(008)}$	$C_{(002)}$	$C_{(005)}$	108.27(15)		$C_{(009)}$	$C_{(006)}$	$C_{(015)}$	109.64(16)
$O_{(001)}$	$C_{(003)}$	$C_{(002)}$	115.57(13)		$C_{(003)}$	$C_{(007)}$	$C_{(013)}$	114.70(16)
$O_{(001)}$	$C_{(003)}$	$C_{(004)}$	59.79(11)		$C_{(009)}$	$C_{(008)}$	$C_{(002)}$	121.36(18)
$O_{(001)}$	$C_{(003)}$	$C_{(007)}$	115.09(14)		$C_{(008)}$	$C_{(009)}$	$C_{(006)}$	121.36(18)
$C_{(004)}$	$C_{(003)}$	$C_{(002)}$	116.81(15)		$C_{(005)}$	$C_{(010)}$	$C_{(012)}$	134.52(19)
$C_{(004)}$	$C_{(003)}$	$C_{(007)}$	124.21(15)		$N_{(014)}$	$C_{(011)}$	$C_{(013)}$	178.6(2)
$C_{(007)}$	$C_{(003)}$	$C_{(002)}$	113.91(14)		$C_{(015)}$	$C_{(012)}$	$C_{(010)}$	133.29(18)
$O_{(001)}$	$C_{(004)}$	$C_{(003)}$	60.00(10)		$C_{(011)}$	$C_{(013)}$	$C_{(007)}$	110.72(18)
$O_{(001)}$	$C_{(004)}$	$C_{(006)}$	117.54(16)		$C_{(012)}$	$C_{(015)}$	$C_{(006)}$	127.88(18)
$C_{(003)}$	$C_{(004)}$	$C_{(006)}$	118.92(16)					

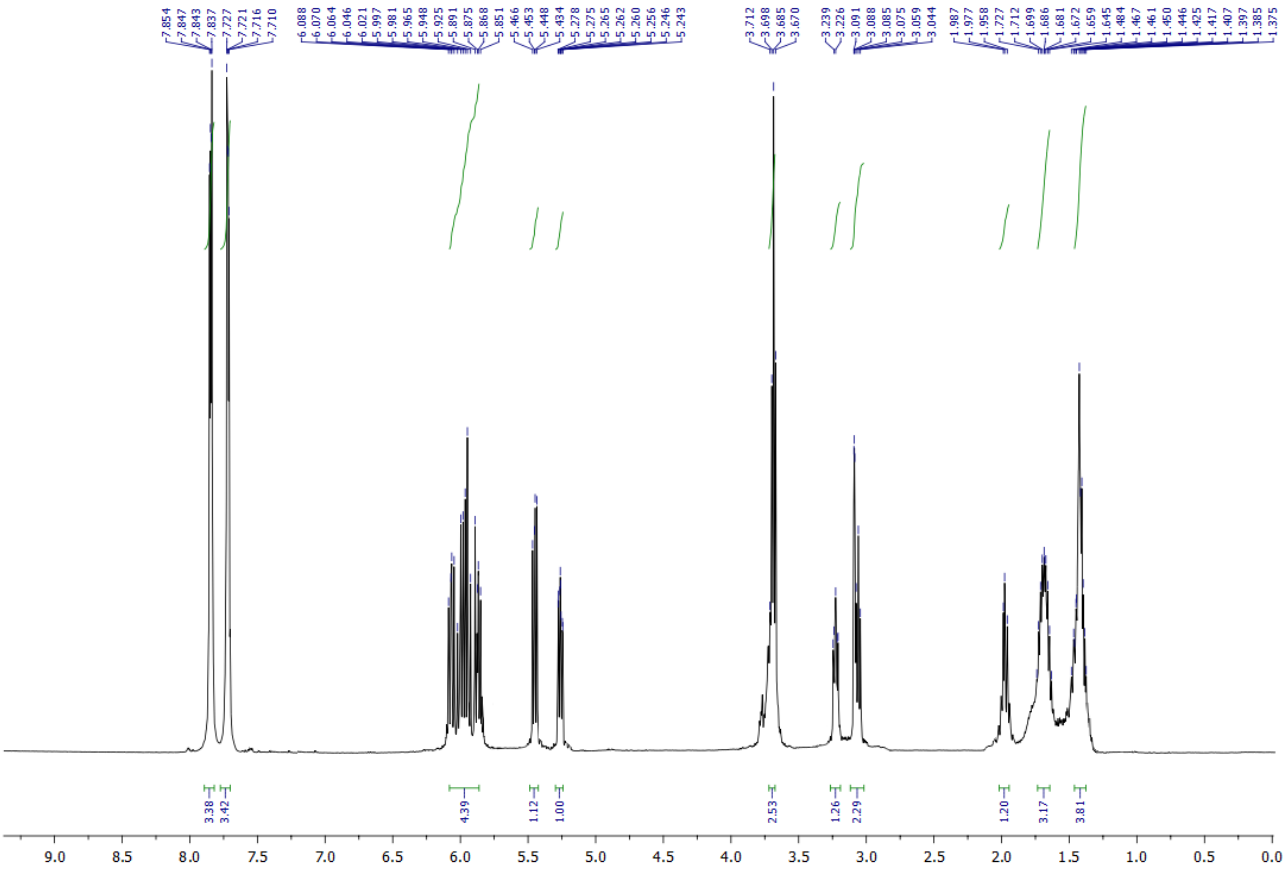
Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for GGF-748-26.				
Atom	***x***	***y***	***z***	**U(eq)**
$H_{(004)}$	2000(20)	5481(14)	1372(10)	47(5)
$H_{(008)}$	2180(30)	2846(16)	-239(11)	71(6)
$H_{(010)}$	3050(30)	2304(17)	1992(12)	66(6)
$H_{(002)}$	4630(20)	3521(12)	255(9)	47(5)
$H_{(006)}$	-570(30)	4830(14)	841(9)	54(5)
$H_{(012)}$	730(30)	2958(14)	2326(11)	64(6)
$H_{(00A)}$	6240(30)	4800(16)	820(12)	76(7)
$H_{(005)}$	4810(30)	2464(15)	1149(10)	63(6)
$H_{(00B)}$	5620(30)	4415(14)	1536(11)	63(6)
$H_{(015)}$	-890(30)	3999(18)	1812(12)	76(7)
$H_{(009)}$	-470(30)	3566(15)	96(11)	74(6)
$H_{(01A)}$	4630(30)	5900(20)	1884(15)	102(9)
$H_{(01B)}$	4940(40)	6310(20)	1114(15)	112(10)

Crystal Data for $C_{13}H_{13}NO$ (*M* =199.24 g mol^{-1}): orthorhombic, space group Pbca (no. 61), *a* = 7.8596(11) Å, *b* = 14.0911(14) Å, *c* = 19.2901(19) Å, *V* = 2136.4(4) Å^3, *Z* = 8, *T* = 293(2) K, μ(MoKα) = 0.079 mm^{-1}, *Dcalc* = 1.239 g cm^{-3}, 6175 reflections measured (4.222° ≤ 2Θ ≤ 58.274°), 2523 unique (R_{int} = 0.0240, R_{sigma} = 0.0350) which were used in all calculations. The final R_1 was 0.0554 (I > 2σ(I)) and wR_2 was 0.1709 (all data).
Refinement model description
Number of restraints - 0, number of constraints - unknown.
Details:
This report has been created with Olex2, compiled on 2018.05.29 svn.r3508 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

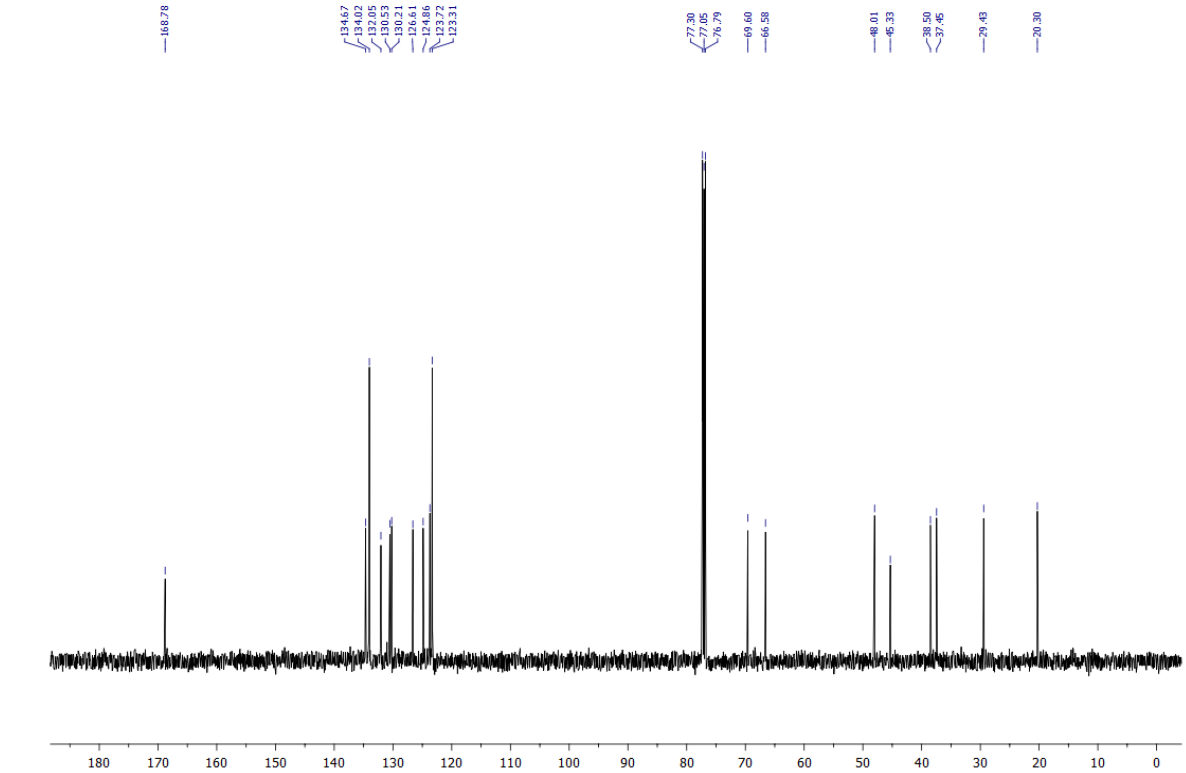
Copies of NMR spectra

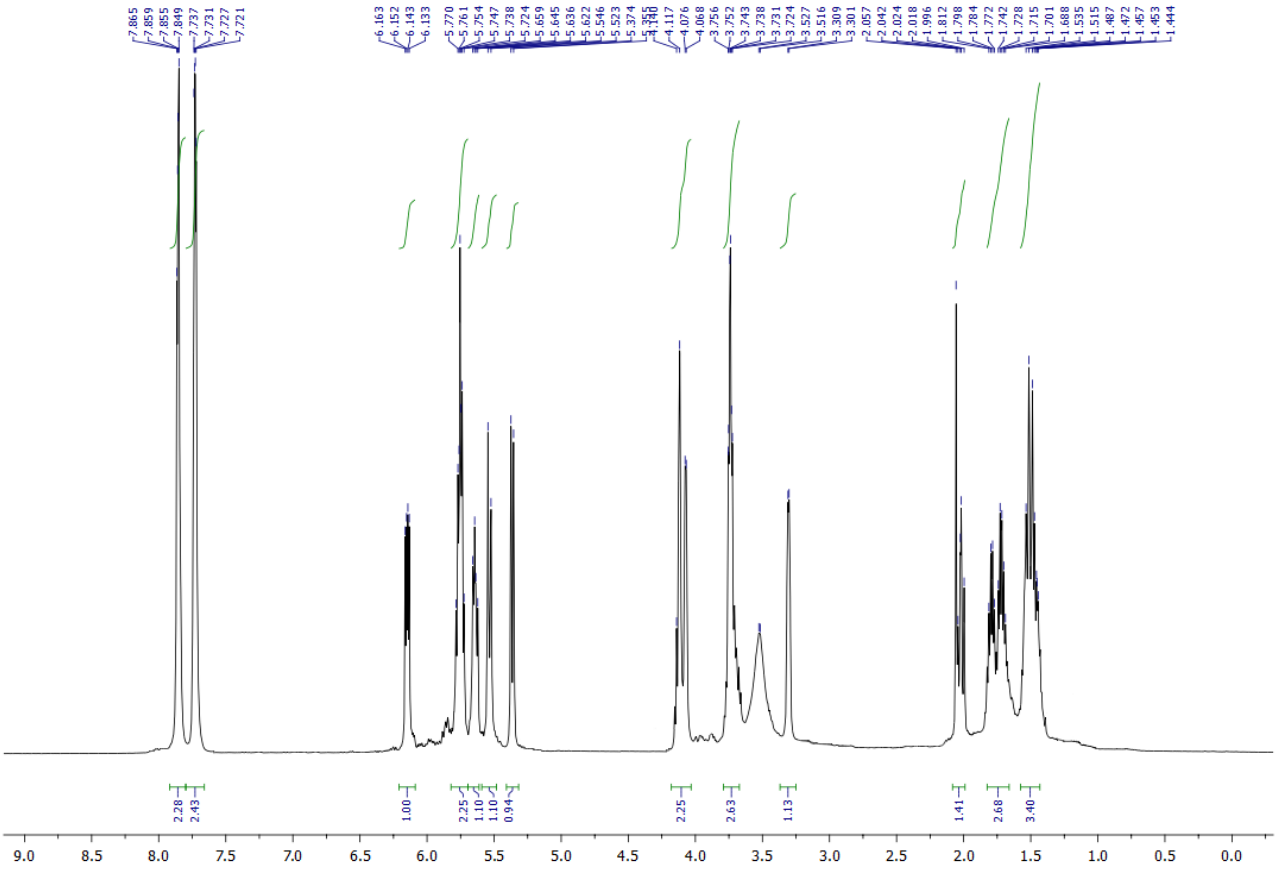
2-[4-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)butyl]-1*H*-isoindole-1,3(2*H*)-dione (2a):



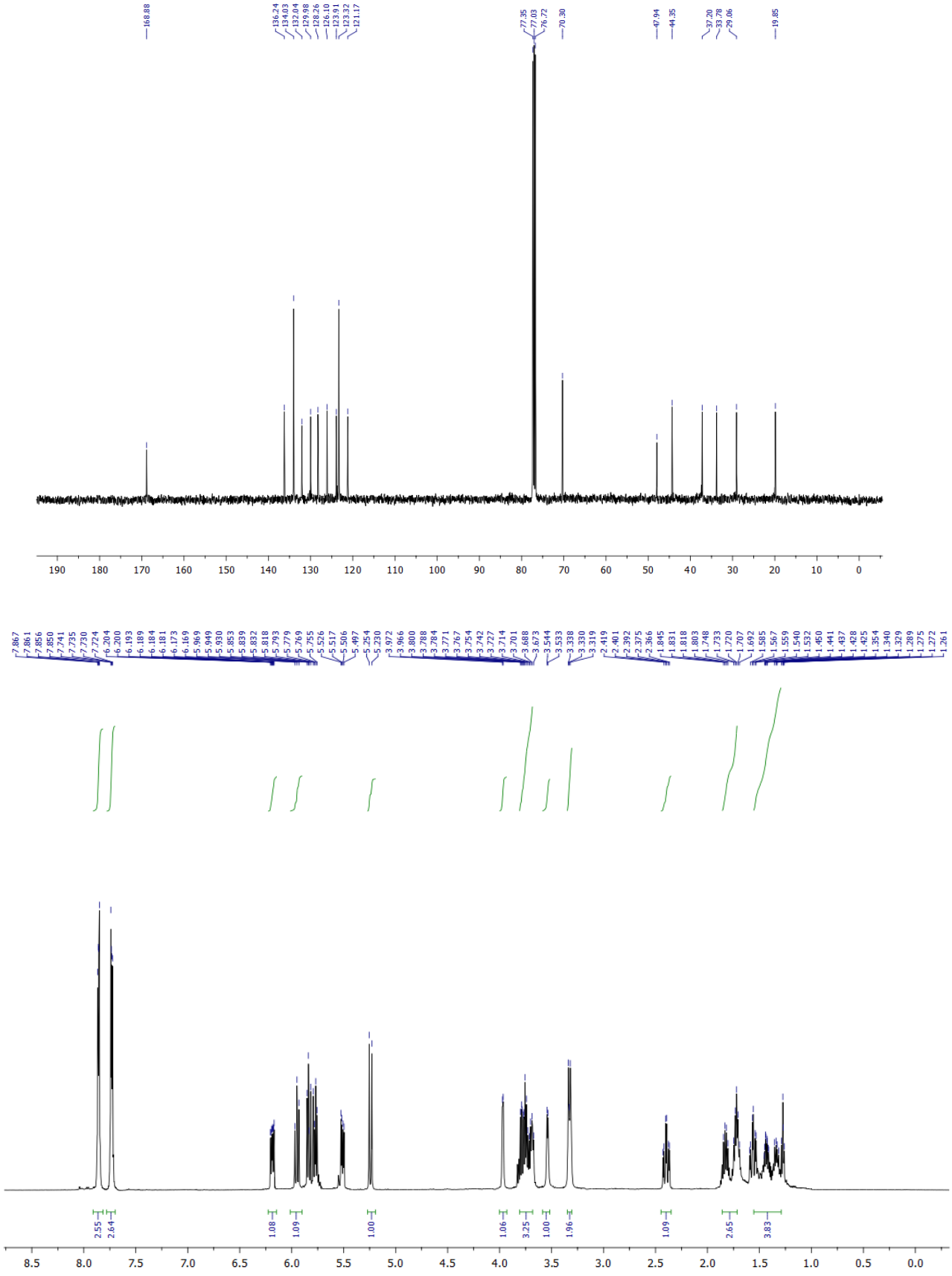


2-[4-(7,10-Dihydroxybicyclo[4.3.1]deca-2,4,8-trien-1-yl)butyl]-1*H*-isoindole-1,3(2*H*)-dione (3a):

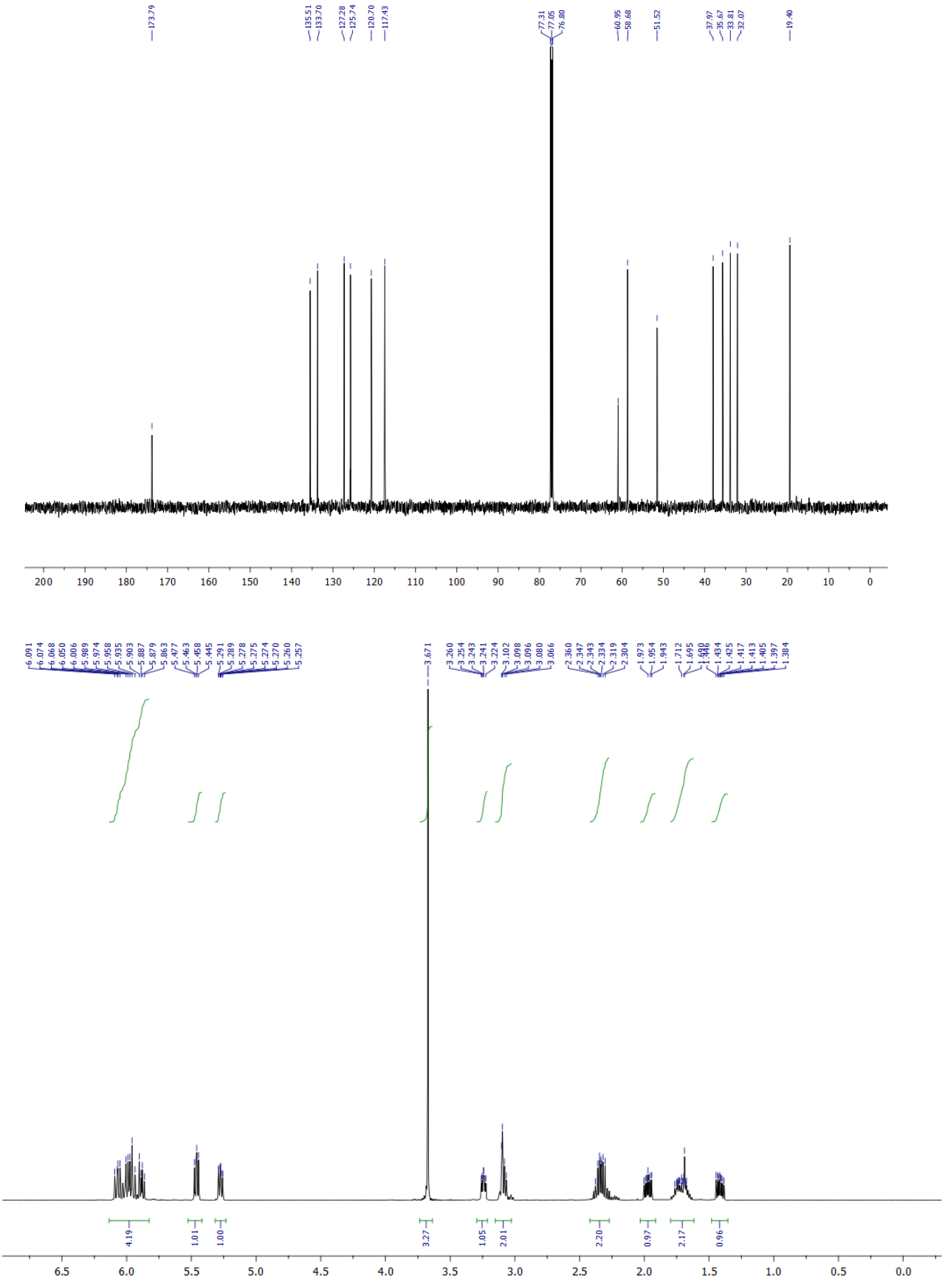




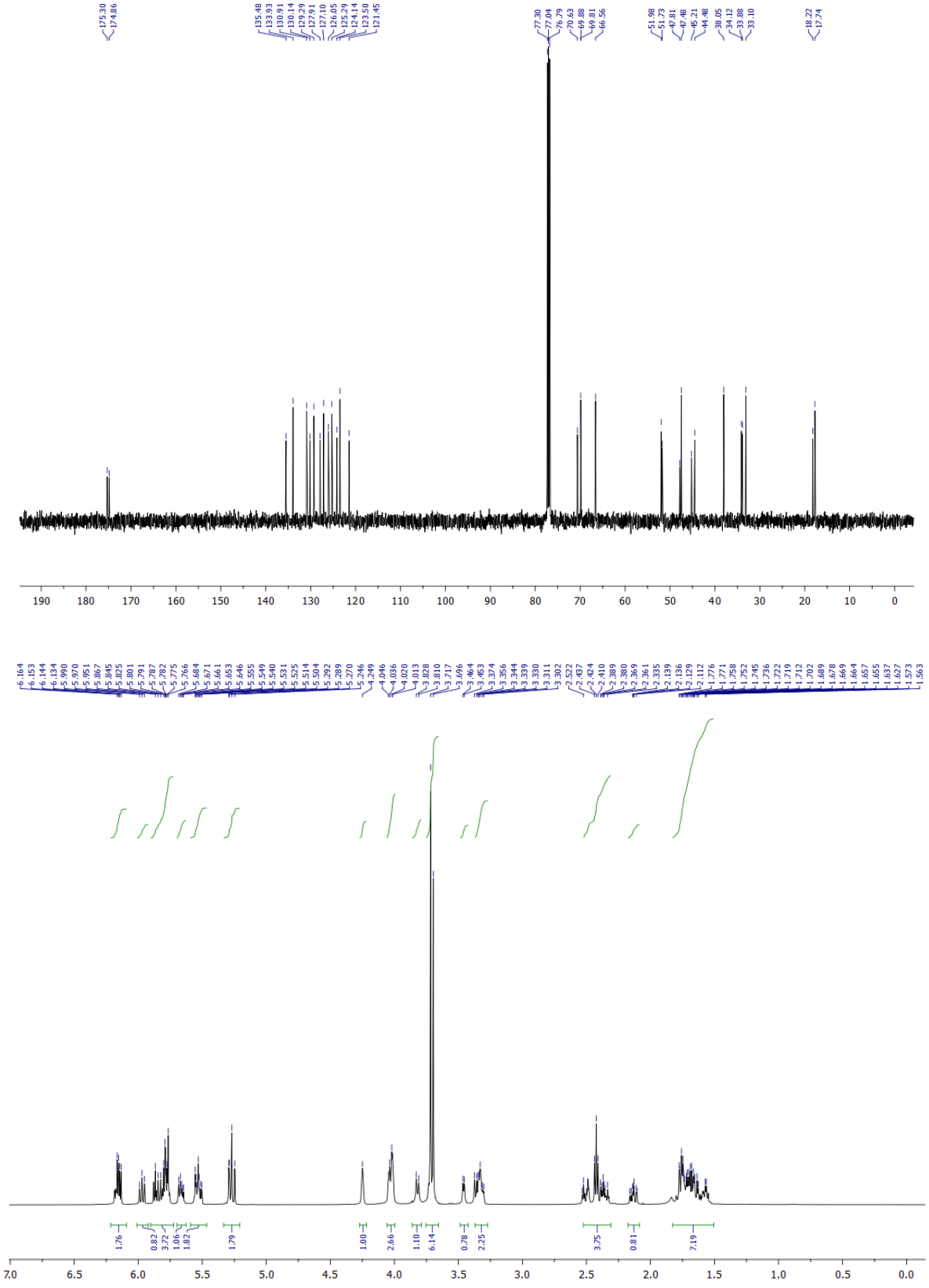
2-[4-(9,10-Dihydroxybicyclo[4.3.1]deca-2,4,7-trien-1-yl)butyl]-1*H*-isoindole-1,3(2*H*)-dione (4a):



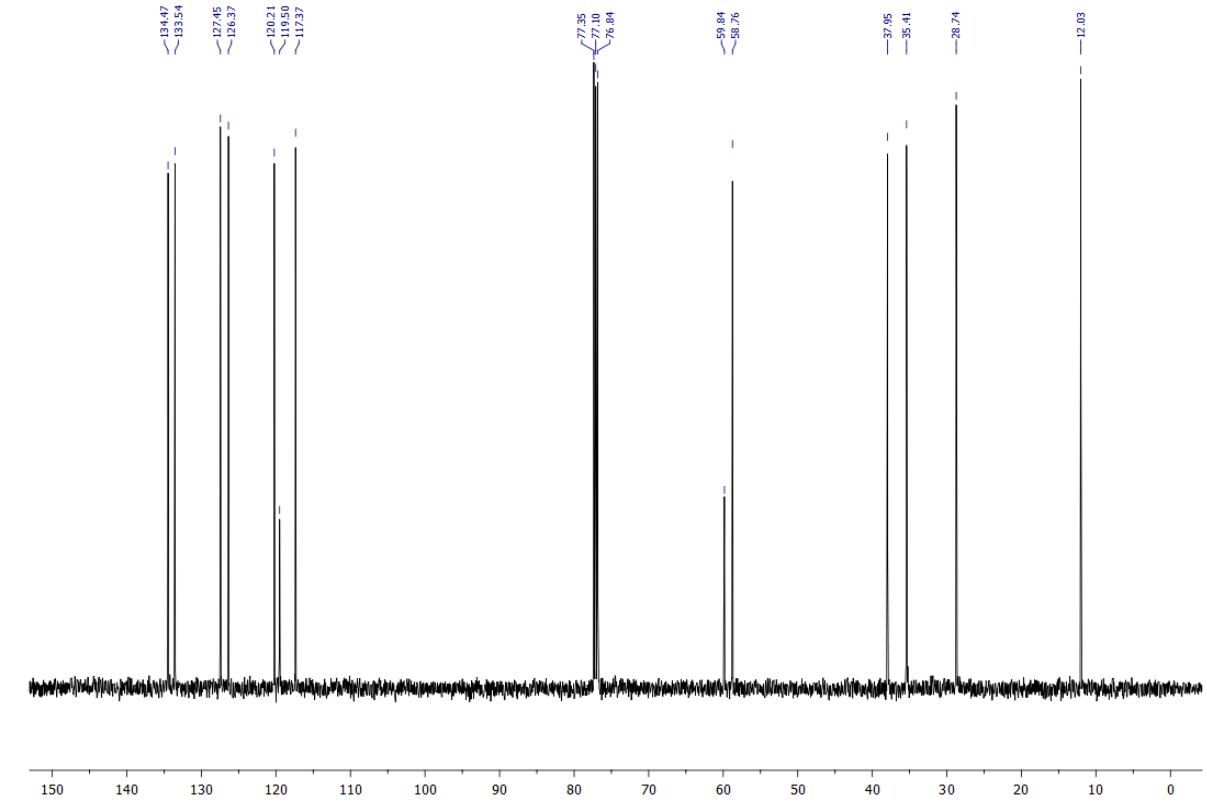
Methyl 4-(8-oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)butanoate (2b):

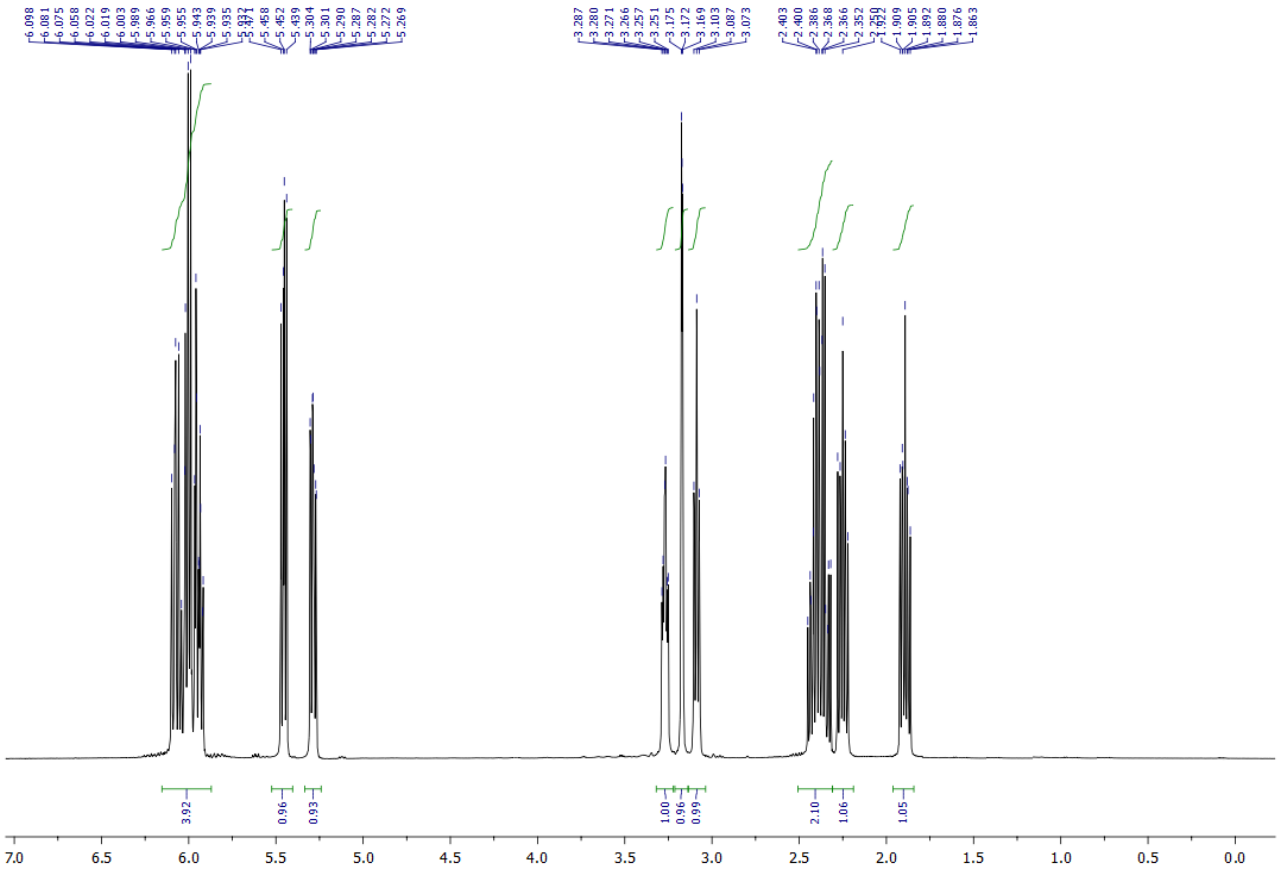


Methyl 4-(7,10-dihydroxybicyclo[4.3.1]deca-2,4,8-trien-1-yl)butanoate (3b) and methyl 4-(9,10-dihydroxybicyclo[4.3.1]deca-2,4,7-trien-1-yl)butanoate (4b), ratio 1:1:

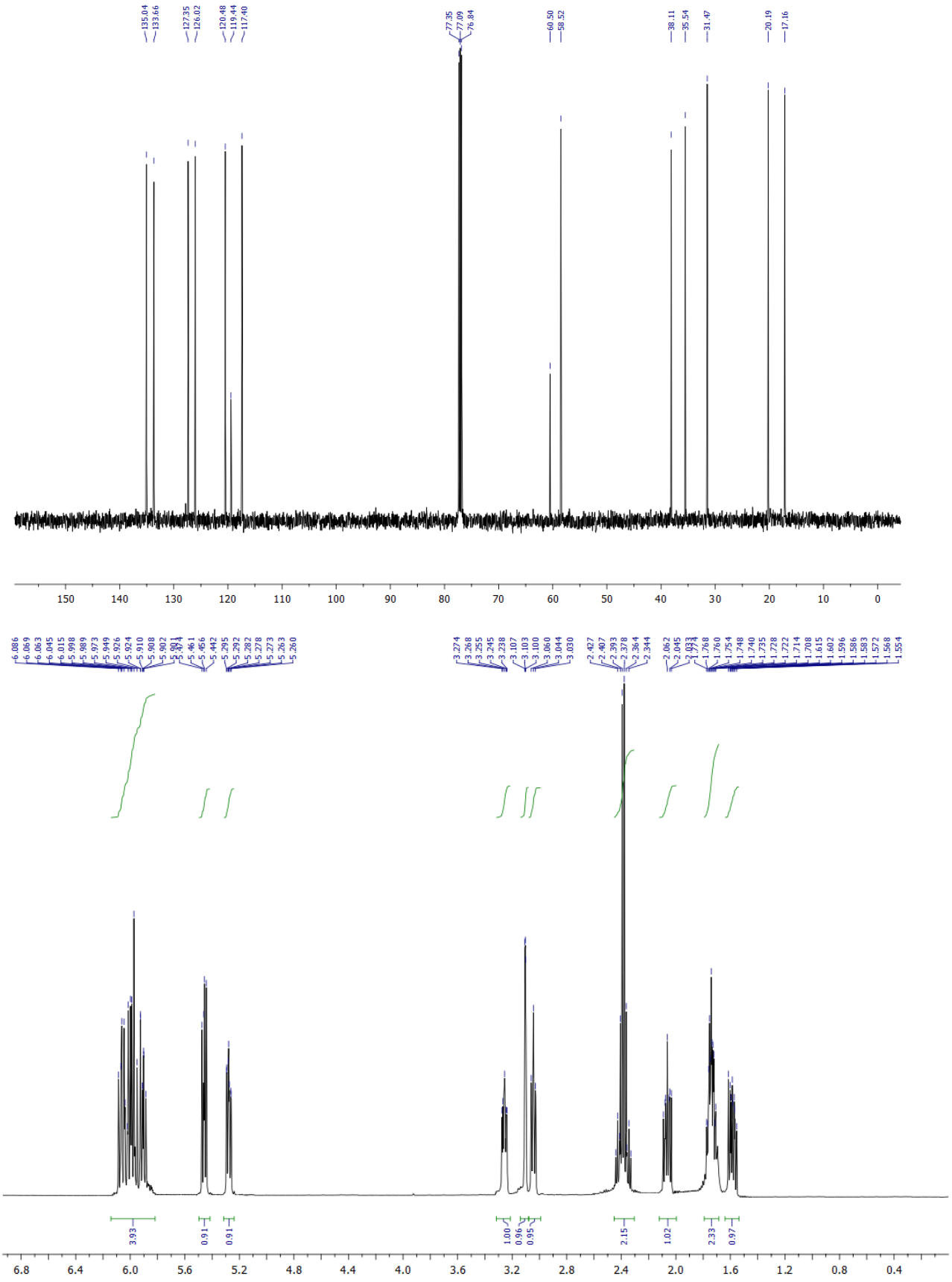


3-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)propanenitrile (2c):

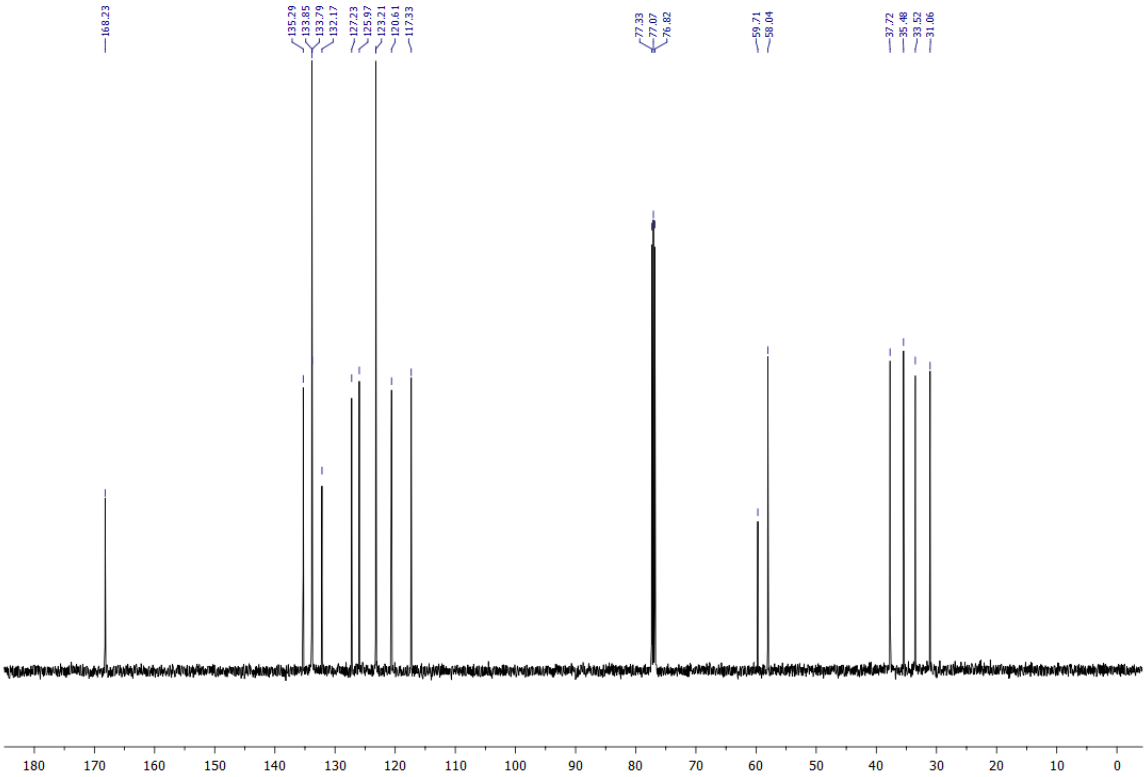


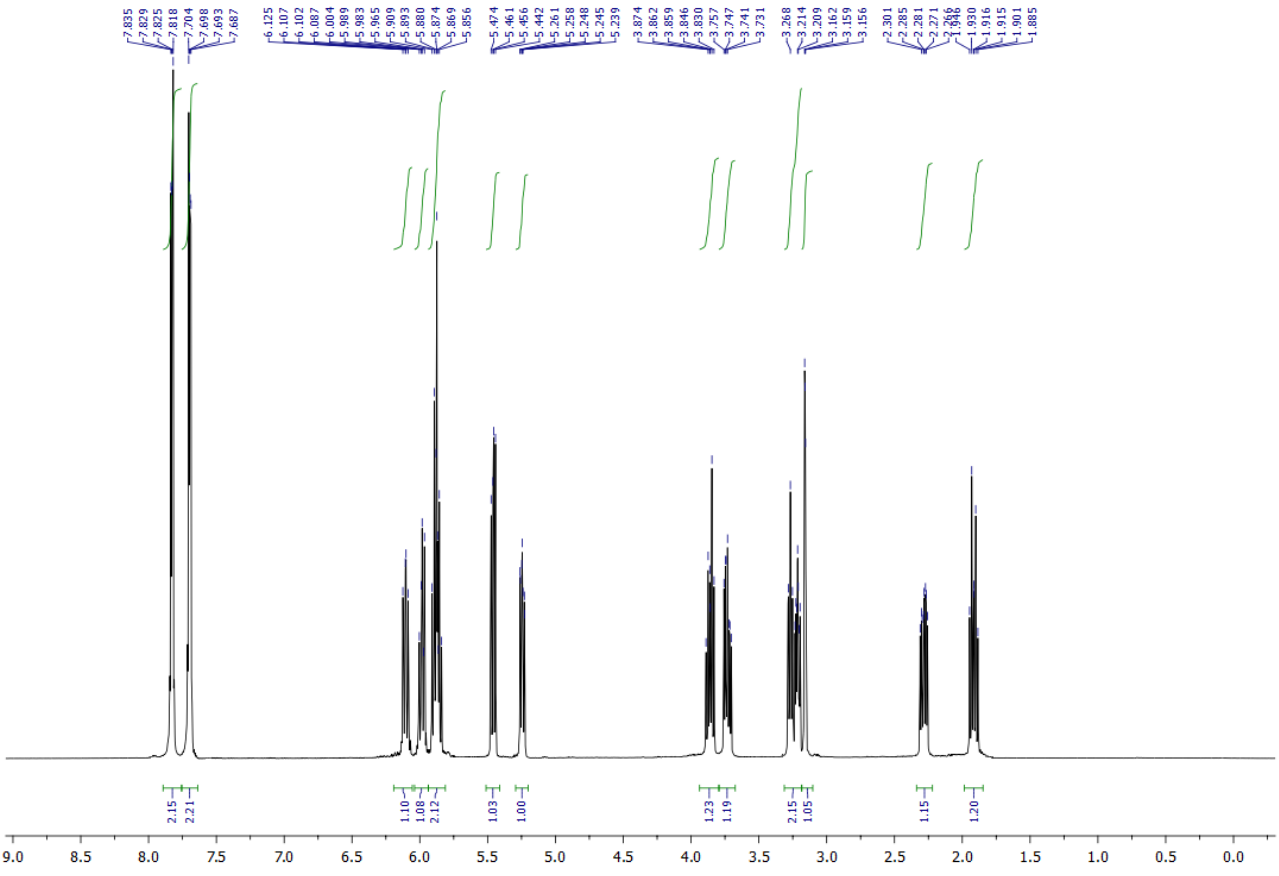


4-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)butanenitrile (2d):

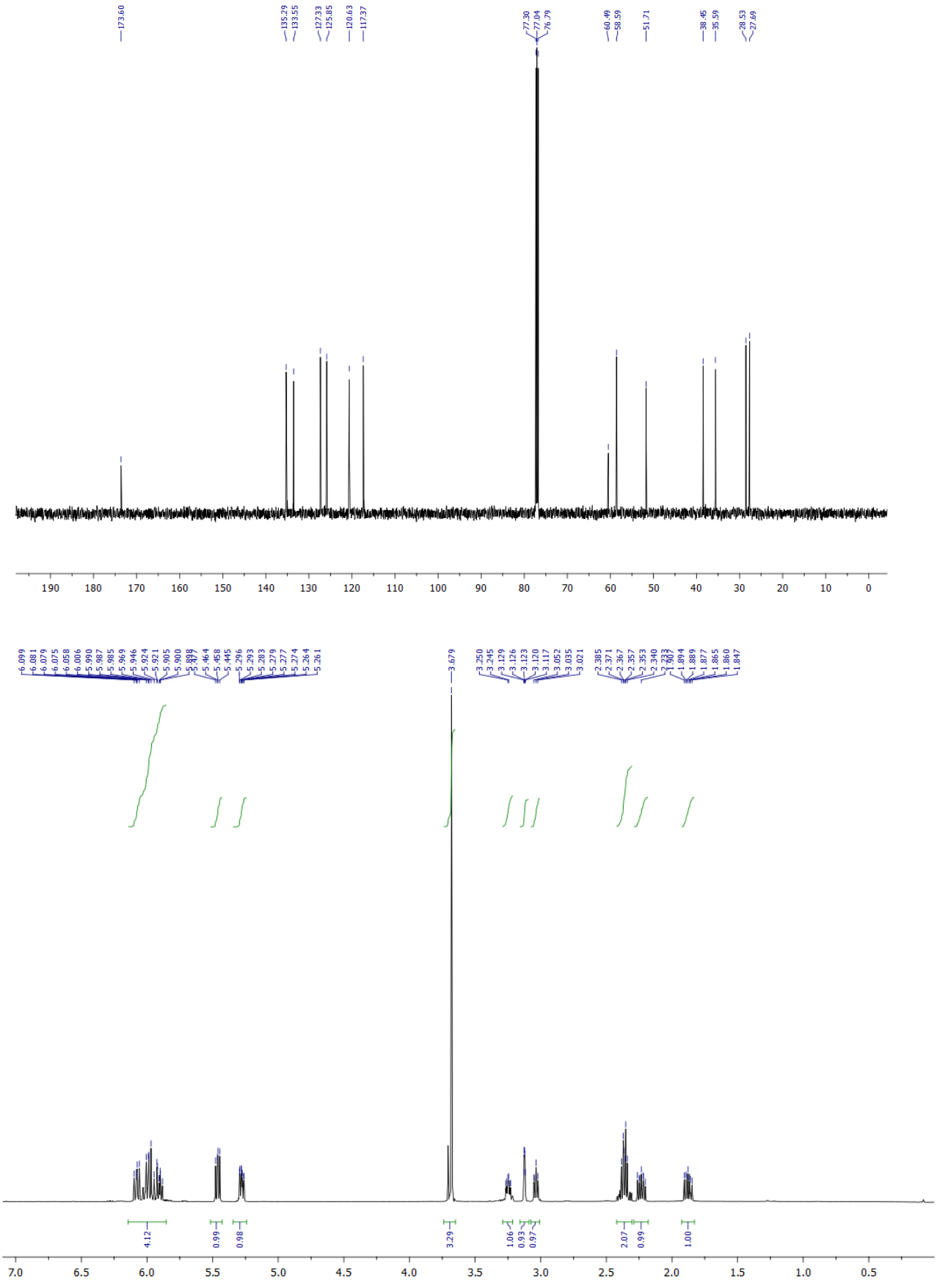


2-[2-(8-Oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)ethyl]-1*H*-isoindole-1,3(2*H*)-dione (2e):





Methyl 3-(8-oxatricyclo[4.3.2.0^{7,9}]undeca-2,4,10-trien-7-yl)propanoate (2f):



Biology Studies

Cell Culturing Cells (Jurkat, K562, HL60, U937) were purchased from Russian Cell Culture Collection (Institute of Cytology of the Russian Academy of Sciences) and cultured according to standard mammalian tissue culture protocols and sterile technique. All cell lines used in the study were tested and shown to be free of mycoplasma and viral contamination. The cells were maintained in RPMI 1640 (Jurkat, K562, HL60, U937) (Gibco) supplemented with 4 mM glutamine, 10% FBS (Sigma) and 100 units per ml penicillin-streptomycin (Sigma). All types of cells were grown in an atmosphere of 5 % CO_2 at 37 °C. The cells were subcultured at 2-3 days intervals. The cells were then seeded in 24 well plates at 5×104 cells per well and incubated overnight. Jurkat, K562, HL60, U937 cells were subcultured at 2 day intervals with a seeding density of 1×105 cells per 24 well plates in RPMI with 10% FBS.

Cytotoxicity Assay

Viability (live/dead) assessment was performed by staining cells with 7-AAD (7-Aminoactinomycin D, Biolegend). After treatment, the cells were harvested, washed 1-2 times with phosphate-buffered saline (PBS) and centrifuged at 400 *g* for 5 minutes. The cell pellets were re-suspended in 200 uL of flow cytometry staining buffer (PBS without Ca^{2+} and Mg^{2+}, 2.5% FBS) and stained with 5 uL of 7-AAD staining solution for 15 minutes at room temperature in the dark. Samples were acquired on NovoCyteTM 2000 FlowCytometry System (ACEA) equipped with 488 nm argon laser. Detection of 7-AAD emission was collected through a 675/30 nm filter in FL4 channel.