Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Divergent Synthesis of prenylated carbazole alkaloids (+)-S-Mahanimbine led to the discovery of Notch activator

Yedukondalu Nalli,[a,b] Gaurav Gupta,[a,c] Janhavi Nadkarni,[c] Vivek Kumar Gupta,[d] Sajad Hussain Syed,*[,a,c] and Asif Ali*[,a,b]

[a]Academy of Scientific and Innovative Research

[b]Natural Product Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India.

[c]Pharmacology division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India.

[d]Post Graduate Department of Physics and Electronics, University of Jammu, Jammu Tawi 2006, India.

Corresponding Author

**E-mail:* asifali@iiim.ac.in; asifchem73@gmail.com

Tel.: +91-191-2569222. Fax: +91-191-25693331.

Table of Contents

Divergent Synthesis of (+)-(*S*)-Mahanimbine (1).....SI-03

X-ray diffraction analysis of compound **2** SI-04-10

X-ray diffraction analysis of compound **5** SI-10-16

^{1}H NMR Spectra of **1** and **2**.....SI-17

^{13}C NMR Spectra of **2** &^{1}H NMR Spectra of **3**.....SI-18

^{13}C NMR Spectra of **3** & ^{1}H NMR Spectra of **4** SI-19

^{13}C NMR Spectra of **4** & HREIMS of **5** SI-20

^{1}H & ^{13}C NMR Spectra of **5** SI-21

DEPT 135 NMR of **5** & HREIMS of **6** SI-22

^{1}H &^{13}C NMR Spectra of **6** SI-23

DEPT & HSQC NMR Spectra of **6** SI-24

COSY & HMBC of **6** SI-25

^{1}H & ^{13}C NMR Spectra of **7**.....SI-26

HREIMS & ^{1}H NMR of **8**.....SI-27

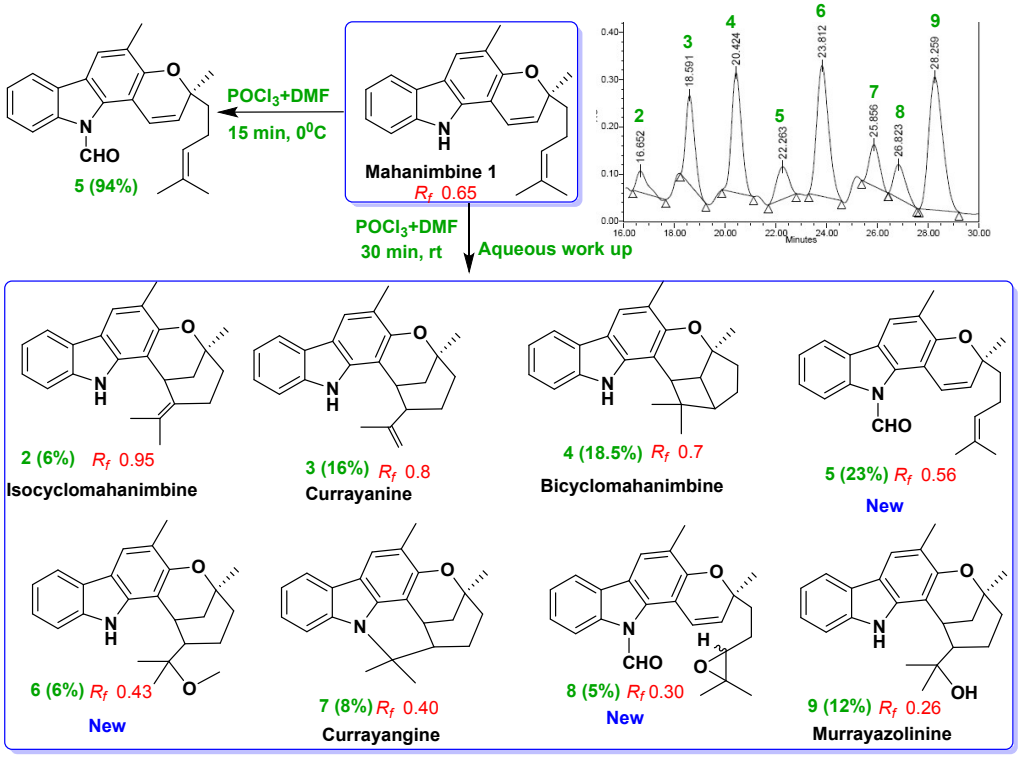
^{13}C & DEPT NMR Spectra of **8**.....SI-28

HSQC & COSY NMR Spectra of **8**.....SI-29

HMBC of **8** & ^{1}H NMR of **9** SI-30

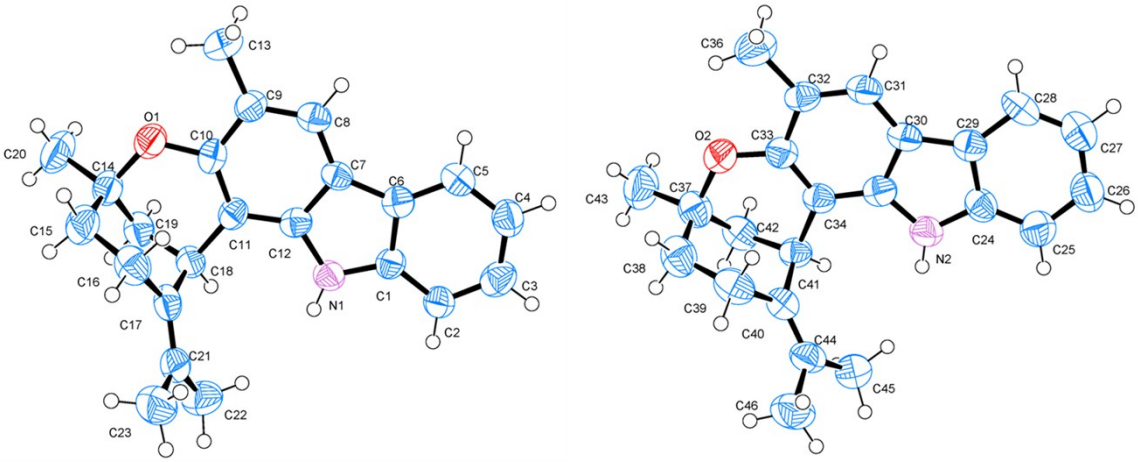
^{13}C NMR Spectra of **9**.....SI-31

Supporting Fig. (SF) 1: Divergent Synthesis of (+)-(*S*)-Mahanimbine (1) by Vilsmeier-Haack reaction and Characterization Data for Compounds (2-9).



$POCl_3$ (0.5 mL, 5 mmol) was added drop wise to ice-cold dry DMF (20 mL) in a 150ml round bottle flask and stirred for 10–15 min at 0°C. The mixture was degassed by vacuum under a nitrogen atmosphere and brought to the room temperature before adding (drop by drop over a period of 5 minutes) 1ml DMF solution of compound **1** (0.5 g, 1.51 mmmol) and stirred for 30 min. The reaction mixture was cooled; distilled water (50 ml) was added and further stirred for 5 min. The aqueous layer was extracted with ethyl acetate (60 mL x 3) and the combined organic extracts were dried over Na_2SO_4, filtered, and concentrated in *vacuo* to give 510 mg of dry residue. TLC [(Hex: EtOAc 9:1)] of the reaction mixture exhibited very close R_f difference in which the compounds **2** (30 mg, 6%) isolated from fraction 3 (R_f = 0.95), **3** (79 mg, 16%, Fr. 4, R_f = 0.8), **4** (92.5 mg, 18.5%, Fr. 5, R_f = 0.7) and **5** (118 mg, 23% Fr. 6, R_f = 0.56) were purified by silica gel chromatography (230-400 mesh) eluting with a gradient of hexane/EtOAc (94:6, v/v). Remaining fraction 7, was the mixture of compound **6** and **7** (74 mg), which was purified by semi-preparative HPLC using waters spherisorb reversed-phase (C_{18}, 250 X 10 mm, 5µm) column eluting with acetonitrile at a flow rate of 2.5 mL min^{-1} to give **6** (29 mg, 6%) with a t_R of 14.60 min., **7** (38 mg, 8%) with a t_R of 19.26 min. The fraction 9 (90 mg) mixture of compound **8** & **9** which were purified by semi-preparative HPLC eluting with a mixture of acetonitrile and H_2O 9:1 (v/v) at a flow rate of 3.0 mL min^{-1} to yield **8** (26 mg, 5%) with a t_R of 13.8 min., **9** (57 mg, 12%) with a t_R of 17.2 min.

Compound 2: X-ray crystallographic Data of 5,7-Dimethyl-2-(propan-2-yl-idene)-1,2,3,4,5,13-hexahydro-1,5-methano-oxocino[3,2-a]carbazole (2): X-ray intensity data of 2884 and 7064 reflections were collected on *X'calibur* CD area-detector diffractometer equipped with graphite monochromated MoKα radiation (λ = 0.71073 Å). The crystal used for data collection was of dimensions 0.30 x 0.20 x 0.20 mm. The cell dimensions were determined by least-squares fit of angular settings of 966 reflections in the θ range 3.8–28.6°**.** Data were corrected for Lorentz, polarisation and absorption factors. The crystallographic data are summarized in Table 1.



2a **2b**

Fig. S1: CCDC No. 1058032 of compound **2** which crystallized in monoclinic space group $P2_1/c$ with two molecules a = 8.4284 (6) Å, b=18.5039 (14) Å, c = 23.3119 (16) Å; α = 90^0, β = 93.85^0 , γ = 90^0. These two molecules are present in unit cell.

Table 1. Crystal and diffraction parameter

Empirical formula	$C_{46}H_{50}N_2O_2$
Crystal habit	Rod, Colourless
CCDC no:	1058032
Crystal size [mm]	0.36 × 0.21 × 0.18
Crystallizing solvent	Hexane: EtOAc (1:1)
Space group	Monoclinic, $P2_{1/c}$
a [Å]	8.4284 (6)
b [Å]	18.5039 (14)
c [Å]	23.3119 (16)
α,β,γ [°]	90.0, 93.85, 90.0
Volume [$Å^3$]	3627.5 (5)
Z / *Z'*	Z: 4 Z': 0
Molecular weight	662.88
Density [calc.]	1.214 Mg m^{-3}
F (000)	1424
Radiation	Mo *K*α radiation, λ = 0.71073 Å

Temperature	293K
θ Range [°]	3.8–28.6°
Scan type	ω scans
Measured reflections	14007
R_{int}	0.070
Independent reflections	7064
Observed reflections [$\|F\| > 4\sigma(F)$]	2884
Final *R* / *wR2* [%]	0.079
Final *wR2* [%]	0.227
Goodness - of - fit (S)	0.99
Restraints / Parameters	0/452

Table 2. Atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.3032 (3)	0.38494 (15)	0.52985 (12)	0.0500 (8)
H1	0.2273	0.4137	0.5184	0.060*
C1	0.4503 (4)	0.40571 (19)	0.55442 (15)	0.0469 (9)
C2	0.5080 (4)	0.4742 (2)	0.56501 (15)	0.0545 (10)
H2	0.4464	0.5147	0.5556	0.065*
C3	0.6617 (5)	0.4809 (2)	0.59035 (17)	0.0647 (11)
H3	0.7029	0.5266	0.5987	0.078*
C4	0.7542 (4)	0.4202 (2)	0.60329 (16)	0.0610 (11)
H4	0.8570	0.4258	0.6198	0.073*
C5	0.6953 (4)	0.3519 (2)	0.59188 (15)	0.0545 (10)
H5	0.7578	0.3116	0.6010	0.065*
C6	0.5428 (4)	0.3434 (2)	0.56679 (14)	0.0471 (9)
C7	0.4447 (4)	0.28217 (19)	0.54958 (14)	0.0437 (9)
C8	0.4700 (4)	0.20798 (19)	0.54916 (15)	0.0497 (9)
H8	0.5669	0.1894	0.5638	0.060*
C9	0.3531 (4)	0.1614 (2)	0.52726 (16)	0.0511 (9)
C10	0.2067 (4)	0.1922 (2)	0.50599 (15)	0.0498 (9)
C11	0.1741 (4)	0.2653 (2)	0.50584 (15)	0.0469 (9)
C12	0.2986 (4)	0.30936 (19)	0.52676 (14)	0.0460 (9)
C13	0.3800 (5)	0.0820 (2)	0.5230 (2)	0.0765 (13)
H13A	0.2853	0.0593	0.5063	0.115*
H13B	0.4054	0.0626	0.5606	0.115*
H13C	0.4664	0.0731	0.4991	0.115*
O1	0.0964 (3)	0.14175 (13)	0.48452 (11)	0.0609 (7)
C14	-0.0597 (4)	0.1670 (2)	0.46159 (17)	0.0569 (10)
C15	-0.0510 (5)	0.1828 (2)	0.39755 (17)	0.0683 (12)
H15A	-0.1575	0.1926	0.3810	0.082*
H15B	-0.0124	0.1400	0.3789	0.082*
C16	0.0563 (4)	0.2465 (2)	0.38472 (16)	0.0633 (11)
H16A	0.1665	0.2332	0.3935	0.076*
H16B	0.0430	0.2583	0.3441	0.076*
C17	0.0165 (4)	0.3118 (2)	0.41982 (16)	0.0516 (10)
C18	0.0149 (4)	0.2937 (2)	0.48334 (15)	0.0504 (9)

H18	-0.0117	0.3370	0.5049	0.060*
C19	-0.1059 (4)	0.2344 (2)	0.49272 (16)	0.0560 (10)
H19A	-0.1089	0.2245	0.5335	0.067*
H19B	-0.2110	0.2501	0.4783	0.067*
C20	-0.1701 (5)	0.1037 (2)	0.4711 (2)	0.0842 (14)
H20A	-0.1367	0.0625	0.4500	0.126*
H20B	-0.2769	0.1164	0.4581	0.126*
H20C	-0.1663	0.0921	0.5114	0.126*
C21	-0.0134 (4)	0.3776 (2)	0.39641 (18)	0.0584 (10)
C22	-0.0703 (5)	0.4393 (2)	0.4310 (2)	0.0804 (13)
H22A	-0.0847	0.4812	0.4069	0.121*
H22B	0.0069	0.4496	0.4621	0.121*
H22C	-0.1697	0.4267	0.4462	0.121*
C23	0.0090 (5)	0.3928 (2)	0.33417 (18)	0.0855 (14)
H23A	-0.0186	0.4422	0.3256	0.128*
H23B	-0.0582	0.3613	0.3105	0.128*
H23C	0.1181	0.3846	0.3265	0.128*
N2	0.2039 (3)	0.71475 (16)	0.26890 (13)	0.0589 (9)
H2A	0.2743	0.6958	0.2485	0.071*
C24	0.0611 (4)	0.6826 (2)	0.28099 (17)	0.0558 (10)
C25	-0.0004 (5)	0.6172 (2)	0.26339 (17)	0.0686 (12)
H25	0.0533	0.5876	0.2390	0.082*
C26	-0.1452 (5)	0.5966 (2)	0.28302 (19)	0.0741 (13)
H26	-0.1890	0.5522	0.2719	0.089*
C27	-0.2256 (5)	0.6412 (3)	0.31901 (19)	0.0724 (12)
H27	-0.3221	0.6261	0.3321	0.087*
C28	-0.1653 (4)	0.7069 (2)	0.33551 (17)	0.0629 (12)
H28	-0.2201	0.7362	0.3599	0.075*
C29	-0.0209 (4)	0.7301 (2)	0.31570 (15)	0.0523 (10)
C30	0.0760 (4)	0.7939 (2)	0.32405 (15)	0.0495 (9)
C31	0.0607 (4)	0.8602 (2)	0.35122 (15)	0.0558 (10)
H31	-0.0293	0.8691	0.3711	0.067*
C32	0.1748 (4)	0.9128 (2)	0.34940 (15)	0.0535 (10)
C33	0.3142 (4)	0.8976 (2)	0.32030 (15)	0.0541 (10)
C34	0.3389 (4)	0.8324 (2)	0.29499 (15)	0.0500 (9)
C35	0.2153 (4)	0.7825 (2)	0.29499 (15)	0.0519 (10)
C36	0.1599 (5)	0.9867 (2)	0.37530 (19)	0.0816 (14)
H36A	0.2530	1.0146	0.3688	0.122*
H36B	0.1493	0.9823	0.4159	0.122*
H36C	0.0677	1.0105	0.3578	0.122*
O2	0.4205 (3)	0.95376 (14)	0.31953 (11)	0.0664 (8)
C37	0.5706 (4)	0.9437 (2)	0.29202 (18)	0.0643 (11)
C38	0.5487 (5)	0.9632 (2)	0.22933 (19)	0.0736 (12)
H38A	0.6522	0.9648	0.2135	0.088*
H38B	0.5031	1.0113	0.2259	0.088*
C39	0.4421 (5)	0.9108 (2)	0.19340 (16)	0.0675 (12)
H39A	0.3323	0.9191	0.2017	0.081*

H39B	0.4514	0.9211	0.1530	0.081*
C40	0.4819 (4)	0.8320 (2)	0.20433 (16)	0.0547 (10)
C41	0.4942 (4)	0.8166 (2)	0.26788 (14)	0.0515 (10)
H41	0.5224	0.7657	0.2742	0.062*
C42	0.6219 (4)	0.8648 (2)	0.29922 (17)	0.0628 (11)
H42A	0.6330	0.8523	0.3397	0.075*
H42B	0.7237	0.8574	0.2830	0.075*
C43	0.6867 (5)	0.9946 (2)	0.3234 (2)	0.0911 (15)
H43A	0.6994	0.9811	0.3633	0.137*
H43B	0.6469	1.0431	0.3203	0.137*
H43C	0.7877	0.9918	0.3068	0.137*
C44	0.5061 (4)	0.7835 (2)	0.16427 (17)	0.0622 (11)
C45	0.5445 (5)	0.7049 (2)	0.1761 (2)	0.0826 (14)
H45A	0.5577	0.6803	0.1405	0.124*
H45B	0.4593	0.6829	0.1952	0.124*
H45C	0.6412	0.7015	0.2002	0.124*
C46	0.4935 (5)	0.8021 (3)	0.10045 (17)	0.0890 (15)
H46A	0.5152	0.7598	0.0785	0.134*
H46B	0.5693	0.8391	0.0931	0.134*
H46C	0.3882	0.8192	0.0896	0.134*

Table 3. Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0528 (18)	0.0455 (18)	0.0508 (18)	0.0081 (15)	-0.0022 (14)	-0.0060 (16)
C1	0.055 (2)	0.041 (2)	0.044 (2)	0.0005 (18)	0.0001 (17)	-0.0081 (18)
C2	0.060 (2)	0.048 (2)	0.055 (2)	0.001 (2)	-0.0086 (19)	-0.005 (2)
C3	0.083 (3)	0.051 (3)	0.060 (3)	-0.006 (2)	0.004 (2)	-0.008 (2)
C4	0.057 (2)	0.070 (3)	0.055 (2)	-0.009 (2)	-0.0049 (18)	0.000 (2)
C5	0.052 (2)	0.060 (3)	0.051 (2)	0.006 (2)	-0.0008 (18)	0.002 (2)
C6	0.056 (2)	0.051 (2)	0.0341 (18)	0.0013 (19)	0.0045 (16)	-0.0022 (18)
C7	0.047 (2)	0.047 (2)	0.0364 (18)	0.0054 (18)	0.0014 (16)	0.0029 (18)
C8	0.052 (2)	0.050 (2)	0.048 (2)	0.0091 (19)	0.0039 (17)	0.0014 (19)
C9	0.053 (2)	0.043 (2)	0.057 (2)	-0.0016 (19)	0.0052 (18)	0.000 (2)
C10	0.052 (2)	0.050 (2)	0.048 (2)	-0.0092 (19)	0.0041 (17)	-0.008 (2)
C11	0.054 (2)	0.043 (2)	0.044 (2)	-0.0016 (18)	0.0043 (17)	-0.0090 (18)
C12	0.056 (2)	0.042 (2)	0.0402 (19)	0.0047 (19)	0.0062 (17)	-0.0041 (18)
C13	0.086 (3)	0.041 (2)	0.102 (3)	0.004 (2)	-0.005 (3)	-0.001 (2)
O1	0.0587 (16)	0.0490 (16)	0.0744 (18)	-0.0034 (13)	0.0013 (13)	-0.0082 (14)
C14	0.052 (2)	0.052 (2)	0.066 (3)	-0.003 (2)	0.001 (2)	-0.012 (2)
C15	0.075 (3)	0.059 (3)	0.070 (3)	-0.001 (2)	-0.002 (2)	-0.021 (2)
C16	0.067 (2)	0.074 (3)	0.049 (2)	0.007 (2)	0.0014 (19)	-0.011 (2)
C17	0.0374 (19)	0.060 (3)	0.057 (2)	0.0003 (19)	-0.0031 (17)	-0.014 (2)
C18	0.047 (2)	0.049 (2)	0.055 (2)	0.0071 (18)	-0.0041 (17)	-0.0110 (19)
C19	0.049 (2)	0.062 (3)	0.057 (2)	-0.001 (2)	0.0022 (18)	-0.007 (2)
C20	0.074 (3)	0.061 (3)	0.118 (4)	-0.023 (2)	0.009 (3)	-0.014 (3)
C21	0.042 (2)	0.058 (3)	0.074 (3)	-0.002 (2)	-0.0069 (19)	-0.001 (2)
C22	0.082 (3)	0.054 (3)	0.104 (4)	0.013 (2)	0.002 (3)	0.001 (3)

C23	0.086 (3)	0.090 (4)	0.078 (3)	-0.009 (3)	-0.011 (2)	0.023 (3)
N2	0.064 (2)	0.052 (2)	0.062 (2)	0.0031 (17)	0.0190 (17)	-0.0011 (17)
C24	0.058 (2)	0.053 (2)	0.057 (2)	0.000 (2)	0.0085 (19)	0.010 (2)
C25	0.078 (3)	0.063 (3)	0.065 (3)	-0.003 (2)	0.008 (2)	0.000 (2)
C26	0.073 (3)	0.075 (3)	0.075 (3)	-0.018 (3)	0.008 (2)	0.007 (3)
C27	0.065 (3)	0.074 (3)	0.080 (3)	-0.007 (2)	0.014 (2)	0.012 (3)
C28	0.049 (2)	0.084 (3)	0.058 (2)	0.002 (2)	0.0156 (19)	0.016 (2)
C29	0.057 (2)	0.054 (2)	0.045 (2)	0.004 (2)	0.0033 (18)	0.008 (2)
C30	0.049 (2)	0.056 (2)	0.045 (2)	0.0112 (19)	0.0103 (17)	0.005 (2)
C31	0.057 (2)	0.059 (3)	0.053 (2)	0.010 (2)	0.0163 (19)	0.001 (2)
C32	0.062 (2)	0.051 (2)	0.049 (2)	0.013 (2)	0.0064 (19)	0.000 (2)
C33	0.059 (2)	0.054 (2)	0.051 (2)	0.000 (2)	0.0077 (19)	0.000 (2)
C34	0.055 (2)	0.051 (2)	0.044 (2)	0.006 (2)	0.0064 (17)	0.0057 (19)
C35	0.066 (2)	0.047 (2)	0.043 (2)	0.009 (2)	0.0036 (18)	0.0072 (19)
C36	0.091 (3)	0.068 (3)	0.087 (3)	0.014 (3)	0.018 (3)	-0.011 (3)
O2	0.0673 (17)	0.0563 (17)	0.0769 (19)	-0.0029 (15)	0.0144 (15)	-0.0102 (16)
C37	0.054 (2)	0.067 (3)	0.072 (3)	0.001 (2)	0.005 (2)	0.008 (3)
C38	0.075 (3)	0.062 (3)	0.084 (3)	0.005 (2)	0.007 (2)	0.018 (3)
C39	0.069 (3)	0.082 (3)	0.050 (2)	0.010 (2)	0.002 (2)	0.018 (2)
C40	0.052 (2)	0.060 (3)	0.053 (2)	-0.001 (2)	0.0080 (18)	0.004 (2)
C41	0.056 (2)	0.054 (2)	0.046 (2)	0.0056 (19)	0.0043 (18)	0.0023 (19)
C42	0.058 (2)	0.071 (3)	0.058 (2)	0.006 (2)	0.0025 (19)	0.013 (2)
C43	0.089 (3)	0.082 (4)	0.101 (4)	-0.024 (3)	-0.003 (3)	-0.009 (3)
C44	0.050 (2)	0.084 (3)	0.054 (2)	-0.003 (2)	0.0110 (19)	-0.004 (2)
C45	0.090 (3)	0.074 (3)	0.086 (3)	-0.006 (3)	0.027 (3)	-0.015 (3)
C46	0.094 (3)	0.120 (4)	0.055 (3)	-0.013 (3)	0.011 (2)	-0.004 (3)

Table 4. Geometric parameters

Bond Length (Å)

N1—C1	1.385 (4)	N2—C24	1.388 (4)
N1—C12	1.401 (4)	N2—C35	1.394 (4)
C1—C2	1.373 (5)	C24—C25	1.369 (5)
C1—C6	1.411 (5)	C24—C29	1.407 (5)
C2—C3	1.393 (5)	C25—C26	1.385 (5)
C3—C4	1.389 (5)	C26—C27	1.386 (5)
C4—C5	1.377 (5)	C27—C28	1.363 (5)
C5—C6	1.385 (4)	C28—C29	1.398 (5)
C6—C7	1.443 (5)	C29—C30	1.442 (5)
C7—C8	1.389 (4)	C30—C31	1.390 (5)
C7—C12	1.401 (4)	C30—C35	1.411 (4)
C8—C9	1.380 (5)	C31—C32	1.371 (5)
C9—C10	1.418 (5)	C32—C33	1.424 (4)
C9—C13	1.492 (5)	C32—C36	1.504 (5)
C10—C11	1.380 (5)	C33—C34	1.366 (5)
C10—O1	1.388 (4)	C33—O2	1.372 (4)
C11—C12	1.391 (4)	C34—C35	1.391 (5)
C11—C18	1.503 (4)	C34—C41	1.520 (4)
O1—C14	1.463 (4)	O2—C37	1.468 (4)

C14—C19	1.508 (5)	C37—C38	1.504 (5)
C14—C15	1.528 (5)	C37—C43	1.512 (5)
C14—C20	1.522 (5)	C37—C42	1.530 (5)
C15—C16	1.528 (5)	C38—C39	1.533 (5)
C16—C17	1.509 (5)	C39—C40	1.512 (5)
C17—C21	1.352 (5)	C40—C44	1.322 (5)
C17—C18	1.519 (5)	C40—C41	1.506 (5)
C18—C19	1.523 (4)	C41—C42	1.544 (5)
C21—C22	1.495 (5)	C44—C45	1.511 (5)
C21—C23	1.502 (5)	C44—C46	1.524 (5)
Bond Angles (°)			
C1—N1—C12	108.6 (3)	C24—N2—C35	109.4 (3)
C2—C1—N1	128.8 (3)	C25—C24—N2	129.4 (4)
C2—C1—C6	122.2 (3)	C25—C24—C29	122.2 (4)
N1—C1—C6	109.0 (3)	N2—C24—C29	108.4 (3)
C1—C2—C3	117.8 (4)	C24—C25—C26	118.0 (4)
C4—C3—C2	120.8 (4)	C27—C26—C25	120.9 (4)
C5—C4—C3	120.7 (3)	C28—C27—C26	120.9 (4)
C4—C5—C6	119.9 (4)	C27—C28—C29	119.8 (4)
C5—C6—C1	118.5 (3)	C28—C29—C24	118.1 (4)
C5—C6—C7	134.8 (3)	C28—C29—C30	134.8 (4)
C1—C6—C7	106.6 (3)	C24—C29—C30	107.0 (3)
C8—C7—C12	118.9 (3)	C31—C30—C35	117.2 (3)
C8—C7—C6	133.8 (3)	C31—C30—C29	135.7 (3)
C12—C7—C6	107.2 (3)	C35—C30—C29	107.2 (3)
C9—C8—C7	120.9 (3)	C32—C31—C30	121.7 (3)
C8—C9—C10	117.5 (3)	C31—C32—C33	118.5 (3)
C8—C9—C13	122.1 (3)	C31—C32—C36	123.8 (3)
C10—C9—C13	120.3 (3)	C33—C32—C36	117.7 (3)
C11—C10—O1	122.0 (3)	C34—C33—O2	123.0 (3)
C11—C10—C9	124.3 (3)	C34—C33—C32	122.3 (4)
O1—C10—C9	113.7 (3)	O2—C33—C32	114.7 (3)
C10—C11—C12	115.3 (3)	C33—C34—C35	116.8 (3)
C10—C11—C18	121.1 (3)	C33—C34—C41	120.7 (3)
C12—C11—C18	123.5 (3)	C35—C34—C41	122.6 (3)
C11—C12—N1	128.4 (3)	C34—C35—N2	128.8 (3)
C11—C12—C7	123.1 (3)	C34—C35—C30	123.3 (3)
N1—C12—C7	108.6 (3)	N2—C35—C30	108.0 (3)
C10—O1—C14	118.8 (3)	C33—O2—C37	119.5 (3)
O1—C14—C19	110.1 (3)	O2—C37—C38	109.9 (3)
O1—C14—C15	108.5 (3)	O2—C37—C43	105.0 (3)
C19—C14—C15	110.1 (3)	C38—C37—C43	110.8 (4)
O1—C14—C20	104.1 (3)	O2—C37—C42	108.6 (3)
C19—C14—C20	112.7 (3)	C38—C37—C42	110.5 (4)
C15—C14—C20	111.1 (3)	C43—C37—C42	111.9 (3)
C14—C15—C16	114.0 (3)	C37—C38—C39	114.1 (3)
C17—C16—C15	110.8 (3)	C40—C39—C38	113.7 (3)

C21—C17—C16	123.0 (4)	C44—C40—C41	124.2 (4)
C21—C17—C18	125.3 (3)	C44—C40—C39	125.4 (4)
C16—C17—C18	111.7 (3)	C41—C40—C39	110.4 (3)
C11—C18—C17	110.6 (3)	C40—C41—C34	111.6 (3)
C11—C18—C19	106.7 (3)	C40—C41—C42	110.8 (3)
C17—C18—C19	110.4 (3)	C34—C41—C42	106.5 (3)
C14—C19—C18	109.3 (3)	C37—C42—C41	108.5 (3)
C17—C21—C22	121.9 (4)	C40—C44—C45	124.5 (4)
C17—C21—C23	121.8 (4)	C40—C44—C46	122.1 (4)
C22—C21—C23	116.4 (4)	C45—C44—C46	113.3 (4)

Compound 5: X-ray crystallographic Data of 3,5-Dimethyl-3-(4-methylpent-3-en-1-yl)pyrano[3,2-a]-carbazole-11(3H)-carbaldehyde.

X-ray intensity data of 3858 reflections (of which 1967 unique) were collected on *X'calibur* CD area-detector diffractometer equipped with graphite monochromated MoKα radiation (λ = 0.71073 Å). The crystal used for data collection was of dimensions 0.30 x 0.20 x 0.20 mm. The cell dimensions were determined by least-squares fit of angular settings of 966 reflections in the θ range 3.97 to 23.11°**.** The intensities were measured by ω scan mode for θ ranges 3.63 to 26.00 °. 1130 reflections were treated as observed (I > 2σ(I)). Data were corrected for Lorentz, polarisation and absorption factors. The structure was solved by direct methods using SHELXS97 [1]. All non-hydrogen atoms of the molecule were located in the best E-map. All the hydrogen atoms were geometrically fixed and allowed to ride on the corresponding non-hydrogen atoms with C-H= 0.93-0.98 Å, and $U_{iso} = 1.5U_{eq}$ of the attached C atom for methyl H atoms and 1.2 U_{eq} for other H atoms. Full-matrix least-squares refinement was carried out using SHELXL97 [1]. The final refinement cycles converged to an R = 0.0531 and wR (F^2) = 0.1069 for 1130 observed data. Residual electron densities ranged from -0.152 to 0.121 eÅ^{-3}. Atomic scattering factors were taken from International Tables for X-ray Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4).

The geometry of the molecule was calculated using the PLATON [2] and PARST [3] software's. The crystallographic data are summarized in Table 1.

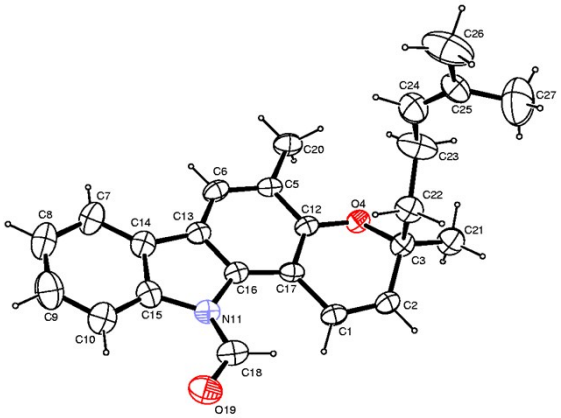


Fig. S2: CCDC No. 975379 of compound **5** and *ORTEP* view of the molecule with displacement ellipsoids drawn at 50% probability level H atoms are shown as small spheres of arbitrary radii.

1. Hubschle, C. B.; Sheldrick, G. M.; Dittrich, B. *J. Appl. Crystallogr.* **2011,** 44, 1281-1284.
2. Spek, A. L. *Acta Crystallogr. D Biol. Crystallogr.* **2009**, 65, 148-155.
3. Nardelli, M. *J. of App. Crystallogr.***1995***,* 28, 659.

Table 1. Crystal and diffraction parameter

Empirical formula	C_{24} H_{25} NO_2
Crystal habit	White
Crystal size [mm]	0.3 x 0.2 x 0.2
Crystallizing solvent	Ethyl acetate
CCDC No.	975379
Space group	Monoclinic, P 2_1
a [Å]	5.6204(5)
b [Å]	25.209(3)
c [Å]	6.9669(6)
α,β,γ [°]	90.0^0 , 93.88^0, 90.0^0
Volume [$Å^3$]	984.835
Z / *Z*′	Z: 2 Z': 0
Molecular weight	359.45
Density [calc.]	1.212 Mg m^{-3}
F (000)	384
Radiation	Mo *K*α radiation, λ = 0.71073 Å
Temperature [ºC]	25
θ Range [º]	4.0-23.1
Scan type	ω scans
Measured reflections	3858
R_{int}	0.036
Independent reflections	1967
Observed reflections [| F | >4σ(F)]	1130

Final *R* / *wR2* [%]	0.053
Final *wR2* [%]	0.107
Goodness - of - fit (S)	0.93
$\Delta\rho_{max}$ / $\Delta\rho_{min}$ [e Å^{-3}]	0.12 e Å^{-3}/ -0.15 e Å^{-3}
Restraints / Parameters	1/248

Table 2. Atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0671 (7)	0.2946 (2)	0.7095 (6)	0.0540 (12)
H1	-0.0161	0.3172	0.6237	0.065*
C2	0.1400 (7)	0.2471 (2)	0.6492 (6)	0.0559 (12)
H2	0.1158	0.2374	0.5206	0.067*
C3	0.2606 (7)	0.21015 (19)	0.7921 (6)	0.0547 (12)
O4	0.4138 (4)	0.24196 (13)	0.9270 (4)	0.0513 (8)
C5	0.4081 (7)	0.30001 (19)	1.1895 (6)	0.0492 (12)
C6	0.3082 (7)	0.34310 (19)	1.2757 (7)	0.0559 (13)
H6	0.3732	0.3552	1.3940	0.067*
C7	-0.0268 (9)	0.4423 (2)	1.4166 (9)	0.0792 (17)
H7	0.0920	0.4370	1.5142	0.095*
C8	-0.2008 (11)	0.4810 (3)	1.4341 (10)	0.096 (2)
H8	-0.1977	0.5021	1.5437	0.115*
C9	-0.3797 (11)	0.4881 (3)	1.2876 (11)	0.098 (2)
H9	-0.4955	0.5139	1.3029	0.117*
C10	-0.3911 (9)	0.4586 (2)	1.1215 (9)	0.0766 (16)
H10	-0.5120	0.4635	1.0254	0.092*
N11	-0.1889 (6)	0.38368 (15)	0.9547 (5)	0.0517 (10)
C12	0.3082 (7)	0.28389 (19)	1.0087 (6)	0.0451 (11)
C13	0.1092 (7)	0.36890 (18)	1.1863 (6)	0.0504 (12)
C14	-0.0342 (8)	0.41214 (19)	1.2529 (7)	0.0588 (13)
C15	-0.2131 (8)	0.4209 (2)	1.1041 (8)	0.0591 (13)
C16	0.0139 (7)	0.35179 (18)	1.0075 (6)	0.0472 (11)
C17	0.1171 (7)	0.31069 (17)	0.9075 (6)	0.0461 (12)
C18	-0.3574 (8)	0.3731 (2)	0.8077 (7)	0.0651 (14)
H18	-0.3430	0.3418	0.7391	0.078*
O19	-0.5247 (6)	0.40230 (15)	0.7615 (5)	0.0781 (11)
C20	0.6215 (7)	0.2715 (2)	1.2820 (7)	0.0674 (16)
H201	0.7603	0.2804	1.2157	0.101*
H202	0.5951	0.2339	1.2749	0.101*
H203	0.6451	0.2821	1.4143	0.101*
C21	0.4295 (8)	0.1735 (2)	0.7013 (8)	0.0741 (16)
H211	0.5450	0.1938	0.6376	0.111*
H212	0.3424	0.1512	0.6094	0.111*
H213	0.5095	0.1518	0.7989	0.111*
C22	0.0757 (7)	0.1814 (2)	0.9056 (7)	0.0624 (14)
H221	-0.0190	0.1587	0.8179	0.075*
H222	-0.0308	0.2077	0.9548	0.075*
C23	0.1785 (8)	0.1477 (3)	1.0743 (9)	0.095 (2)

H231	0.2603	0.1173	1.0241	0.114*
H232	0.2953	0.1685	1.1505	0.114*
C24	-0.0095 (10)	0.1281 (3)	1.2033 (9)	0.0864 (17)
H24	-0.0512	0.1516	1.2986	0.104*
C25	-0.1180 (8)	0.0835 (2)	1.1977 (8)	0.0684 (15)
C26	-0.3046 (10)	0.0685 (3)	1.3288 (11)	0.136 (3)
H262	-0.2436	0.0416	1.4161	0.203*
H263	-0.4419	0.0552	1.2545	0.203*
H261	-0.3489	0.0991	1.4003	0.203*
C27	-0.0764 (14)	0.0422 (3)	1.0568 (12)	0.156 (4)
H271	-0.0050	0.0575	0.9485	0.233*
H272	-0.2255	0.0260	1.0145	0.233*
H273	0.0285	0.0158	1.1148	0.233*

Table 3. Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.047 (2)	0.069 (4)	0.045 (3)	-0.003 (2)	-0.006 (2)	0.005 (3)
C2	0.055 (3)	0.066 (3)	0.045 (3)	-0.004 (3)	-0.005 (2)	-0.002 (3)
C3	0.042 (2)	0.067 (3)	0.054 (3)	-0.002 (2)	0.000 (2)	-0.005 (3)
O4	0.0389 (14)	0.064 (2)	0.0504 (18)	-0.0014 (15)	-0.0021 (14)	-0.0026 (18)
C5	0.045 (2)	0.060 (3)	0.042 (3)	-0.007 (2)	-0.001 (2)	0.012 (3)
C6	0.055 (2)	0.070 (4)	0.042 (3)	-0.019 (3)	-0.003 (2)	0.001 (3)
C7	0.072 (3)	0.089 (4)	0.077 (4)	-0.010 (3)	0.008 (3)	-0.027 (4)
C8	0.103 (4)	0.091 (5)	0.094 (5)	-0.004 (4)	0.025 (4)	-0.034 (4)
C9	0.079 (4)	0.087 (5)	0.129 (6)	0.010 (4)	0.019 (4)	-0.019 (5)
C10	0.068 (3)	0.080 (4)	0.082 (4)	-0.009 (3)	0.008 (3)	-0.010 (4)
N11	0.0457 (18)	0.056 (3)	0.053 (2)	-0.0063 (18)	0.0019 (19)	0.005 (2)
C12	0.039 (2)	0.057 (3)	0.040 (3)	-0.010 (2)	0.005 (2)	0.005 (3)
C13	0.047 (2)	0.056 (3)	0.048 (3)	-0.011 (2)	0.006 (2)	0.006 (3)
C14	0.053 (3)	0.061 (3)	0.064 (3)	-0.012 (3)	0.012 (3)	-0.003 (3)
C15	0.053 (3)	0.055 (3)	0.071 (3)	-0.006 (3)	0.015 (3)	0.002 (3)
C16	0.043 (2)	0.054 (3)	0.044 (3)	-0.008 (2)	0.002 (2)	0.004 (3)
C17	0.038 (2)	0.054 (3)	0.045 (3)	-0.008 (2)	-0.004 (2)	0.011 (3)
C18	0.053 (3)	0.081 (4)	0.061 (3)	-0.012 (3)	-0.001 (3)	0.012 (3)
O19	0.0559 (18)	0.089 (3)	0.088 (3)	0.0084 (19)	-0.0048 (19)	0.013 (2)
C20	0.052 (2)	0.085 (4)	0.063 (3)	-0.004 (3)	-0.015 (2)	0.011 (3)
C21	0.059 (3)	0.087 (4)	0.076 (4)	0.009 (3)	-0.001 (3)	-0.005 (3)
C22	0.039 (2)	0.072 (4)	0.075 (4)	-0.003 (2)	-0.005 (2)	0.005 (3)
C23	0.059 (3)	0.109 (5)	0.115 (5)	-0.016 (3)	-0.009 (3)	0.052 (4)
C24	0.091 (4)	0.076 (4)	0.091 (5)	0.012 (4)	0.002 (4)	0.000 (4)
C25	0.056 (3)	0.056 (3)	0.094 (4)	0.006 (3)	0.008 (3)	0.012 (4)
C26	0.096 (4)	0.145 (7)	0.173 (7)	0.029 (4)	0.059 (5)	0.085 (6)
C27	0.175 (8)	0.116 (7)	0.177 (9)	-0.036 (6)	0.026 (7)	-0.046 (7)

Table 4. Geometric parameters

Bond Length (Å)

C1—C2	1.342 (6)	C13—C14	1.451 (6)
C1—C17	1.447 (6)	C14—C15	1.412 (6)
C1—H1	0.9300	C16—C17	1.396 (6)

C2—C3	1.492 (6)	C18—O19	1.220 (5)
C2—H2	0.9300	C18—H18	0.9300
C3—O4	1.469 (5)	C20—H201	0.9600
C3—C21	1.496 (6)	C20—H202	0.9600
C3—C22	1.530 (6)	C20—H203	0.9600
O4—C12	1.356 (5)	C21—H211	0.9600
C5—C6	1.379 (6)	C21—H212	0.9600
C5—C12	1.404 (5)	C21—H213	0.9600
C5—C20	1.505 (6)	C22—C23	1.533 (6)
C6—C13	1.402 (6)	C22—H221	0.9700
C6—H6	0.9300	C22—H222	0.9700
C7—C14	1.368 (6)	C23—C24	1.515 (7)
C7—C8	1.393 (7)	C23—H231	0.9700
C7—H7	0.9300	C23—H232	0.9700
C8—C9	1.395 (9)	C24—C25	1.278 (7)
C8—H8	0.9300	C24—H24	0.9300
C9—C10	1.374 (8)	C25—C27	1.462 (8)
C9—H9	0.9300	C25—C26	1.486 (7)
C10—C15	1.390 (6)	C26—H262	0.9600
C10—H10	0.9300	C26—H263	0.9600
N11—C18	1.373 (5)	C26—H261	0.9600
N11—C15	1.416 (6)	C27—H271	0.9600
N11—C16	1.423 (5)	C27—H272	0.9600
C12—C17	1.416 (5)	C27—H273	0.9600
C13—C16	1.391 (6)		
Bond Angles ((^{o})			
C2—C1—C17	120.4 (4)	C16—C17—C12	115.6 (4)
C2—C1—H1	119.8	C16—C17—C1	128.6 (4)
C17—C1—H1	119.8	C12—C17—C1	115.6 (4)
C1—C2—C3	118.8 (4)	O19—C18—N11	124.1 (5)
C1—C2—H2	120.6	O19—C18—H18	118.0
C3—C2—H2	120.6	N11—C18—H18	118.0
O4—C3—C2	107.8 (4)	C5—C20—H201	109.5
O4—C3—C21	104.3 (3)	C5—C20—H202	109.5
C2—C3—C21	112.1 (4)	H201—C20—H202	109.5
O4—C3—C22	108.5 (3)	C5—C20—H203	109.5
C2—C3—C22	110.3 (3)	H201—C20—H203	109.5
C21—C3—C22	113.5 (4)	H202—C20—H203	109.5
C12—O4—C3	116.1 (3)	C3—C21—H211	109.5
C6—C5—C12	118.0 (4)	C3—C21—H212	109.5
C6—C5—C20	121.7 (4)	H211—C21—H212	109.5
C12—C5—C20	120.3 (4)	C3—C21—H213	109.5
C5—C6—C13	120.5 (4)	H211—C21—H213	109.5
C5—C6—H6	119.7	H212—C21—H213	109.5
C13—C6—H6	119.7	C3—C22—C23	115.2 (4)
C14—C7—C8	118.7 (6)	C3—C22—H221	108.5
C14—C7—H7	120.7	C23—C22—H221	108.5

C8—C7—H7	120.7	C3—C22—H222	108.5
C7—C8—C9	120.1 (6)	C23—C22—H222	108.5
C7—C8—H8	119.9	H221—C22—H222	107.5
C9—C8—H8	119.9	C24—C23—C22	113.2 (4)
C10—C9—C8	122.4 (6)	C24—C23—H231	108.9
C10—C9—H9	118.8	C22—C23—H231	108.9
C8—C9—H9	118.8	C24—C23—H232	108.9
C9—C10—C15	116.8 (5)	C22—C23—H232	108.9
C9—C10—H10	121.6	H231—C23—H232	107.8
C15—C10—H10	121.6	C25—C24—C23	128.2 (6)
C18—N11—C15	125.5 (4)	C25—C24—H24	115.9
C18—N11—C16	125.7 (4)	C23—C24—H24	115.9
C15—N11—C16	107.5 (4)	C24—C25—C27	123.4 (6)
O4—C12—C5	116.3 (4)	C24—C25—C26	124.1 (6)
O4—C12—C17	120.1 (4)	C27—C25—C26	112.5 (6)
C5—C12—C17	123.5 (4)	C25—C26—H262	109.5
C16—C13—C6	120.1 (4)	C25—C26—H263	109.5
C16—C13—C14	109.3 (4)	H262—C26—H263	109.5
C6—C13—C14	130.6 (5)	C25—C26—H261	109.5
C7—C14—C15	120.3 (5)	H262—C26—H261	109.5
C7—C14—C13	134.2 (5)	H263—C26—H261	109.5
C15—C14—C13	105.5 (4)	C25—C27—H271	109.5
C10—C15—C14	121.6 (5)	C25—C27—H272	109.5
C10—C15—N11	128.5 (5)	H271—C27—H272	109.5
C14—C15—N11	109.6 (4)	C25—C27—H273	109.5
C13—C16—C17	121.9 (4)	H271—C27—H273	109.5
C13—C16—N11	108.0 (4)	H272—C27—H273	109.5
C17—C16—N11	130.0 (4)		

Torsional Angles (º)			
C17—C1—C2—C3	3.5 (6)	C18—N11—C15—C10	-9.0 (7)
C1—C2—C3—O4	-38.0 (5)	C16—N11—C15—C10	-176.6 (4)
C1—C2—C3—C21	-152.3 (4)	C18—N11—C15—C14	165.7 (4)
C1—C2—C3—C22	80.2 (5)	C16—N11—C15—C14	-1.8 (5)
C2—C3—O4—C12	51.4 (5)	C6—C13—C16—C17	-3.0 (6)
C21—C3—O4—C12	170.8 (4)	C14—C13—C16—C17	179.4 (4)
C22—C3—O4—C12	-68.0 (4)	C6—C13—C16—N11	178.2 (4)
C12—C5—C6—C13	1.6 (6)	C14—C13—C16—N11	0.7 (5)
C20—C5—C6—C13	180.0 (4)	C18—N11—C16—C13	-166.8 (4)
C14—C7—C8—C9	0.7 (9)	C15—N11—C16—C13	0.7 (4)
C7—C8—C9—C10	-0.9 (10)	C18—N11—C16—C17	14.5 (6)
C8—C9—C10—C15	-0.6 (9)	C15—N11—C16—C17	-177.9 (4)
C3—O4—C12—C5	153.2 (3)	C13—C16—C17—C12	6.6 (6)
C3—O4—C12—C17	-30.3 (5)	N11—C16—C17—C12	-174.9 (4)
C6—C5—C12—O4	178.9 (4)	C13—C16—C17—C1	-168.1 (4)
C20—C5—C12—O4	0.4 (5)	N11—C16—C17—C1	10.4 (7)
C6—C5—C12—C17	2.5 (5)	O4—C12—C17—C16	177.3 (3)
C20—C5—C12—C17	-175.9 (4)	C5—C12—C17—C16	-6.5 (5)

C5—C6—C13—C16	-1.3 (6)	O4—C12—C17—C1	-7.3 (5)
C5—C6—C13—C14	175.6 (4)	C5—C12—C17—C1	168.9 (4)
C8—C7—C14—C15	1.0 (7)	C2—C1—C17—C16	-164.2 (4)
C8—C7—C14—C13	-178.8 (5)	C2—C1—C17—C12	21.1 (6)
C16—C13—C14—C7	178.1 (5)	C15—N11—C18—O19	17.5 (7)
C6—C13—C14—C7	0.9 (8)	C16—N11—C18—O19	-177.2 (4)
C16—C13—C14—C15	-1.7 (5)	O4—C3—C22—C23	-54.7 (6)
C6—C13—C14—C15	-178.9 (4)	C2—C3—C22—C23	-172.6 (5)
C9—C10—C15—C14	2.3 (7)	C21—C3—C22—C23	60.7 (6)
C9—C10—C15—N11	176.4 (5)	C3—C22—C23—C24	169.6 (5)
C7—C14—C15—C10	-2.5 (7)	C22—C23—C24—C25	95.4 (8)
C13—C14—C15—C10	177.3 (4)	C23—C24—C25—C27	-0.5 (10)
C7—C14—C15—N11	-177.7 (4)	C23—C24—C25—C26	-178.6 (5)
C13—C14—C15—N11	2.2 (5)		

Figure S1: ^{1}H NMR spectrum of compound Mahanimbine (**1**) ($CDCl_3$, 400 MHz)

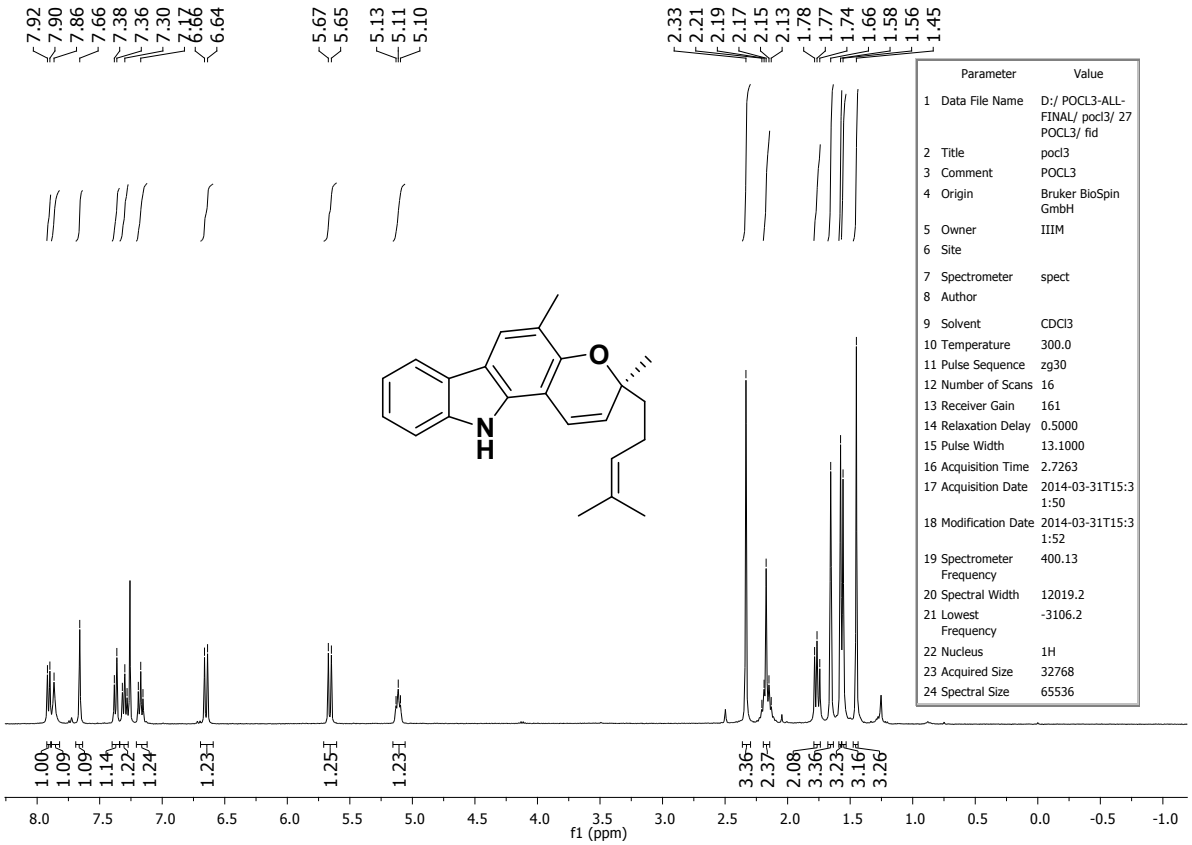


Figure S2: ^{1}H NMR spectrum of Isocyclomahanimbine (**2**) ($CDCl_3$, 400 MHz)

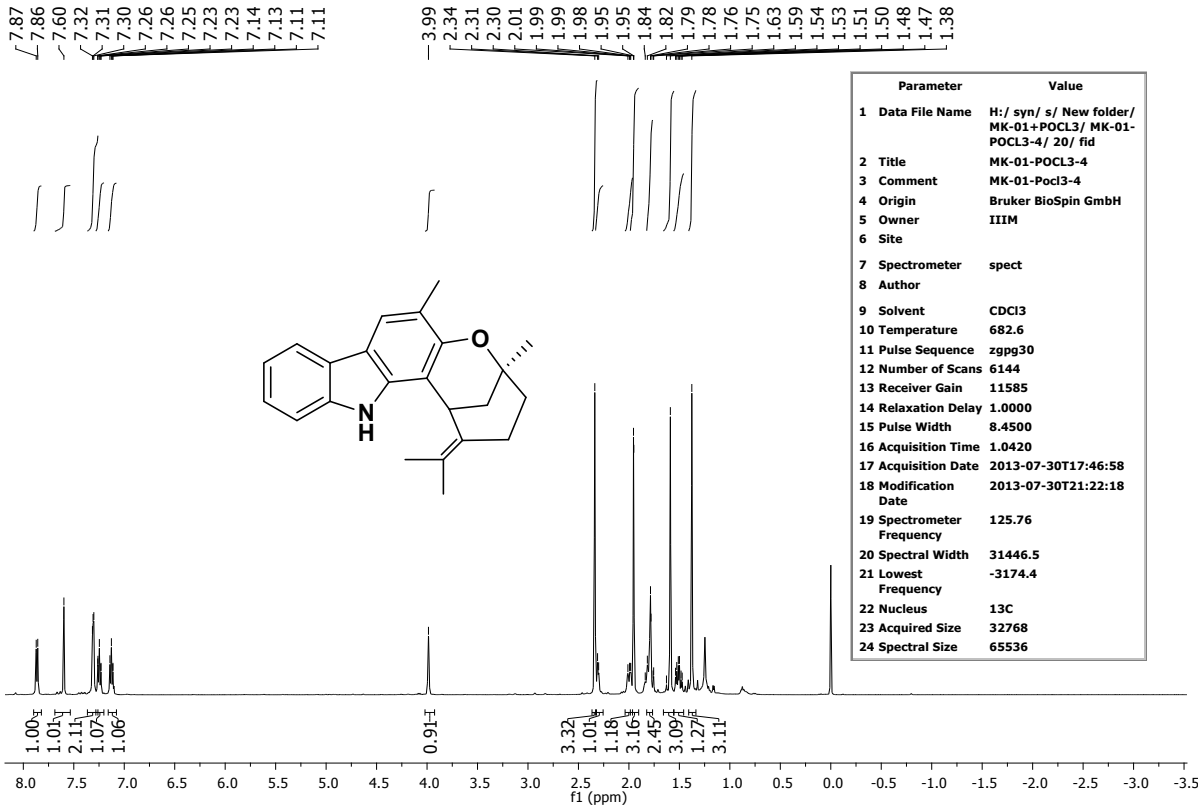


Figure S3: ^{13}C NMR spectrum of Isocyclomahanimbine (**2**) ($CDCl_3$, 125 MHz)

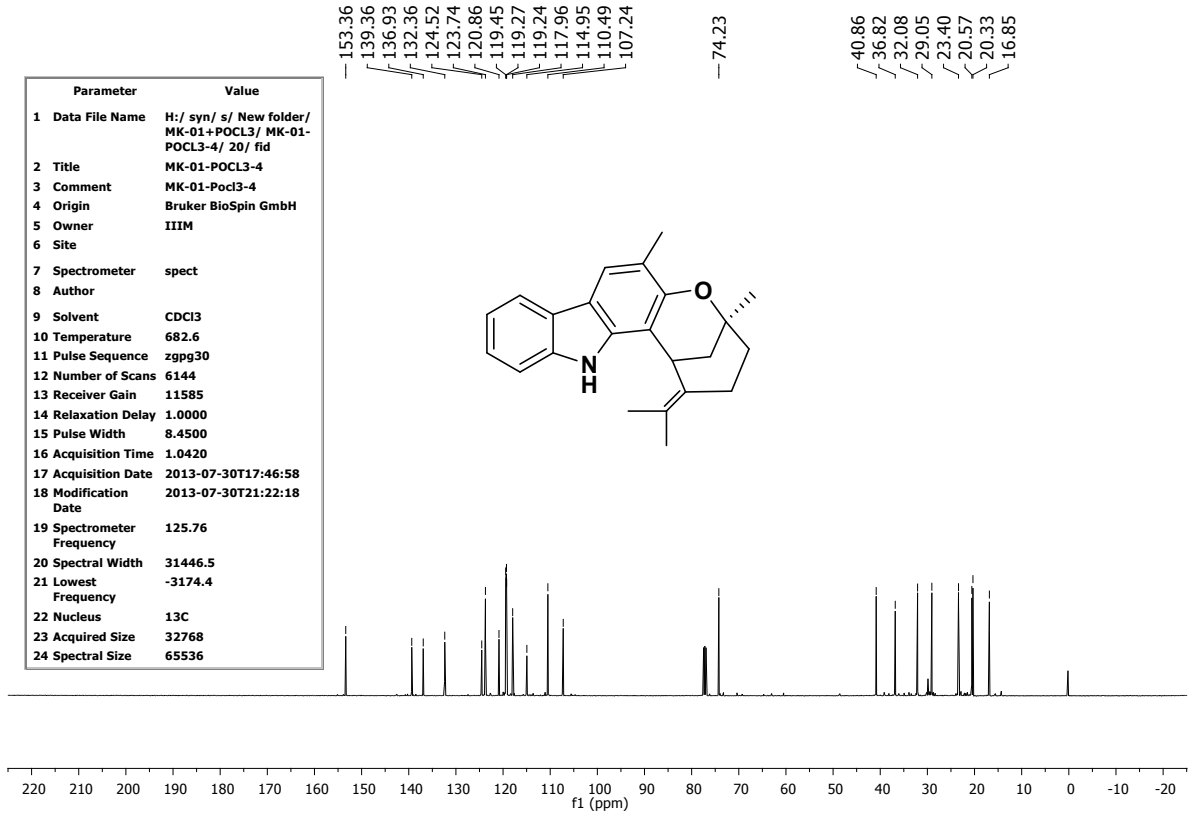


Figure S4: ^{1}H NMR spectrum of Curryanin (**3**) ($CDCl_3$, 500 MHz)

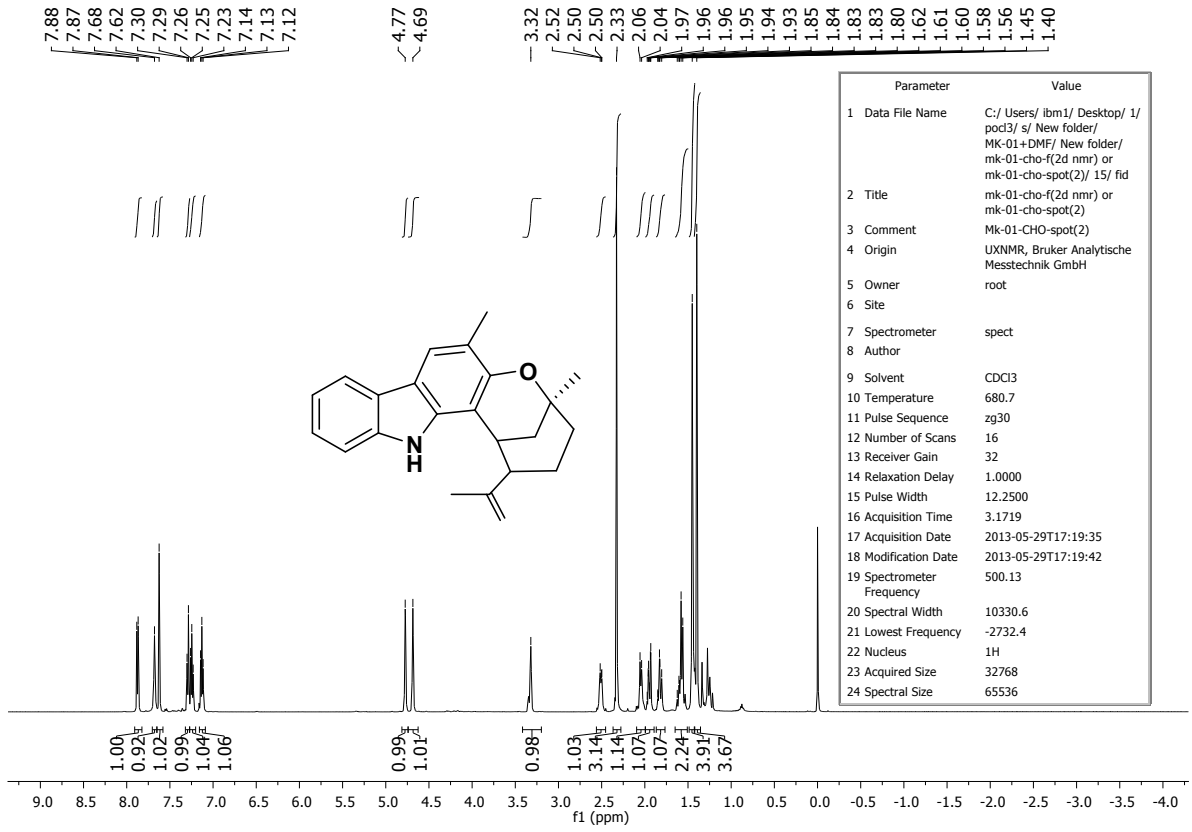
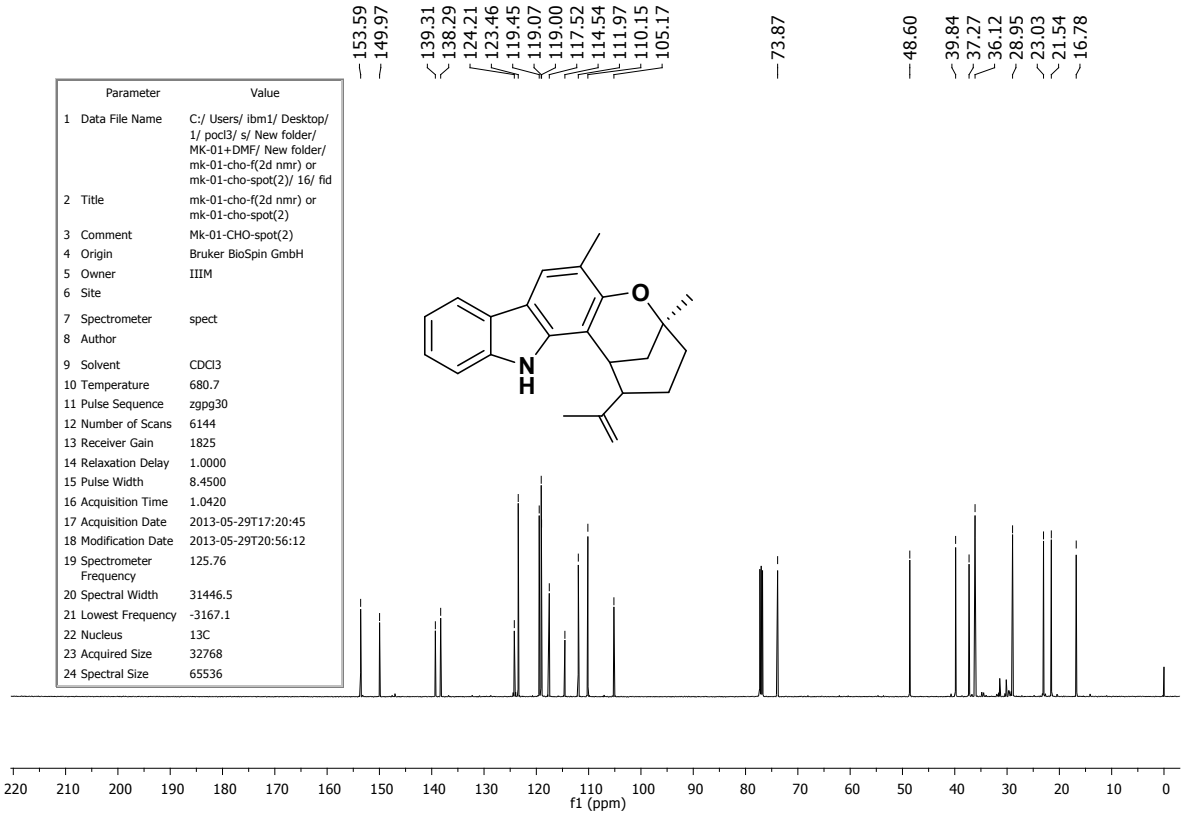
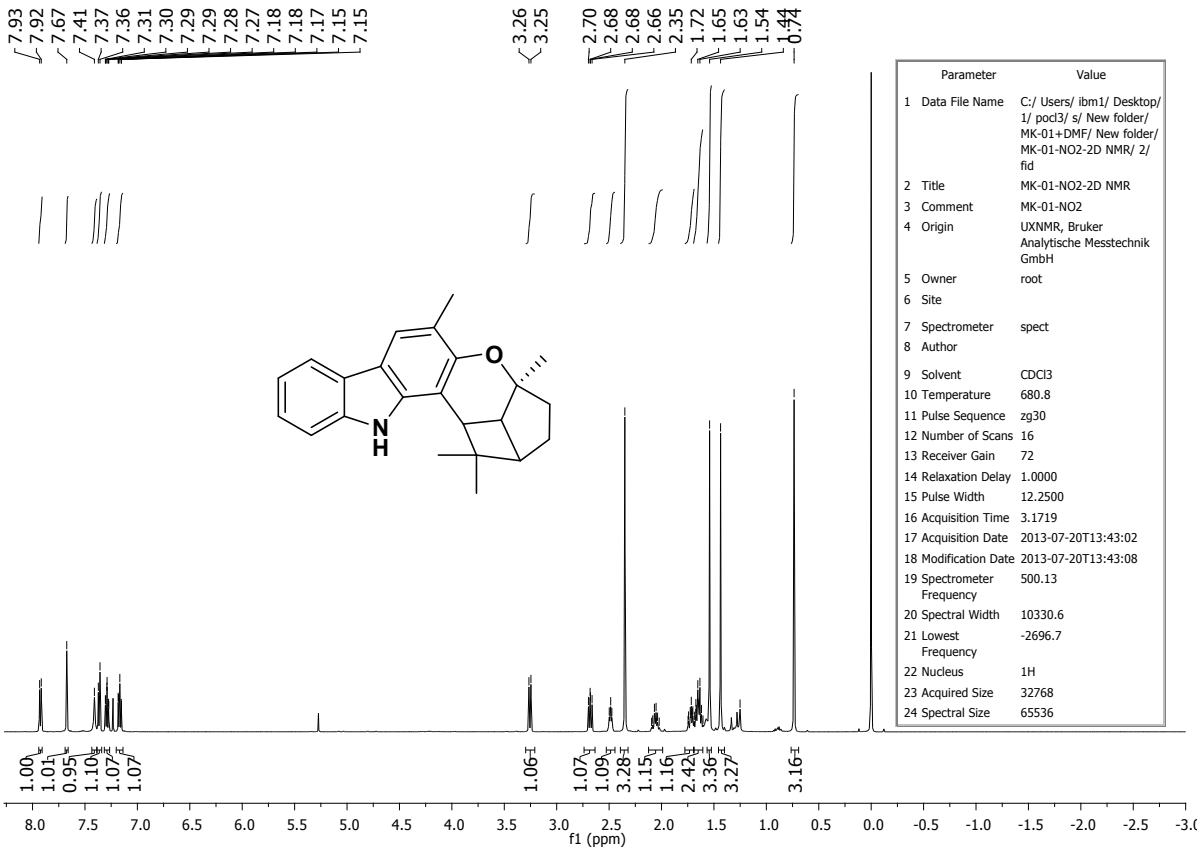


Figure S5: ^{13}C NMR spectrum of Curryanin (**3**) ($CDCl_3$, 125 MHz)



	Parameter	Value
1	Data File Name	C:/ Users/ ibm1/ Desktop/ 1/ pocl3/ s/ New folder/ MK-01+DMF/ New folder/ mk-01-cho-f(2d nmr) or mk-01-cho-spot(2)/ 16/ fid
2	Title	mk-01-cho-f(2d nmr) or mk-01-cho-spot(2)
3	Comment	Mk-01-CHO-spot(2)
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.7
11	Pulse Sequence	zgpg30
12	Number of Scans	6144
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-05-29T17:20:45
18	Modification Date	2013-05-29T20:56:12
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3167.1
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure S6: ^{1}H NMR spectrum of Bicyclomahanimbine (**4**), ($CDCl_3$, 500 MHz)



	Parameter	Value
1	Data File Name	C:/ Users/ ibm1/ Desktop/ 1/ pocl3/ s/ New folder/ MK-01+DMF/ New folder/ MK-01-NO2-2D NMR/ 2/ fid
2	Title	MK-01-NO2-2D NMR
3	Comment	MK-01-NO2
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.8
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	72
14	Relaxation Delay	1.0000
15	Pulse Width	12.2500
16	Acquisition Time	3.1719
17	Acquisition Date	2013-07-20T13:43:02
18	Modification Date	2013-07-20T13:43:08
19	Spectrometer Frequency	500.13
20	Spectral Width	10330.6
21	Lowest Frequency	-2696.7
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure S7: ^{13}C NMR spectrum of Bicyclomahanimbine (**4**), ($CDCl_3$, 125 MHz)

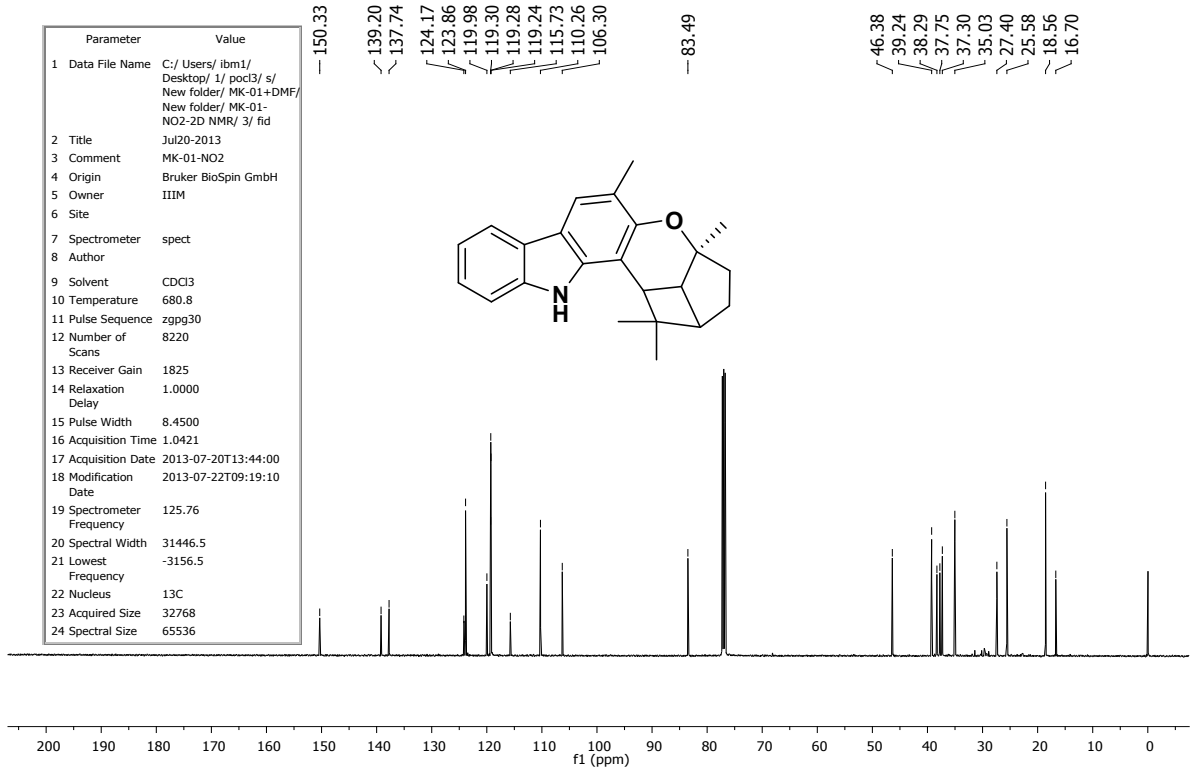


Figure S7: HRESIMS spectroscopic data of compound **5**

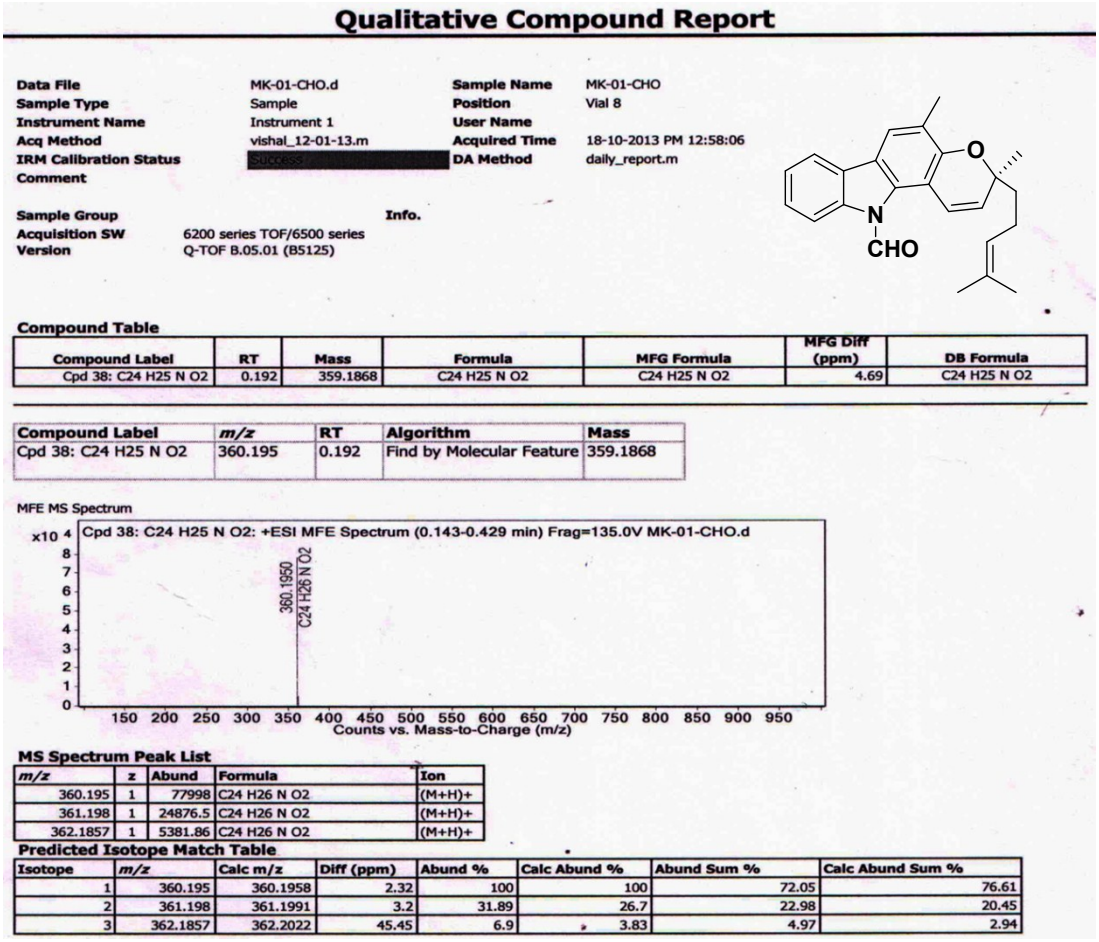


Figure S8: ^{1}H NMR spectrum of compound **5** ($CDCl_3$, 400 MHz)

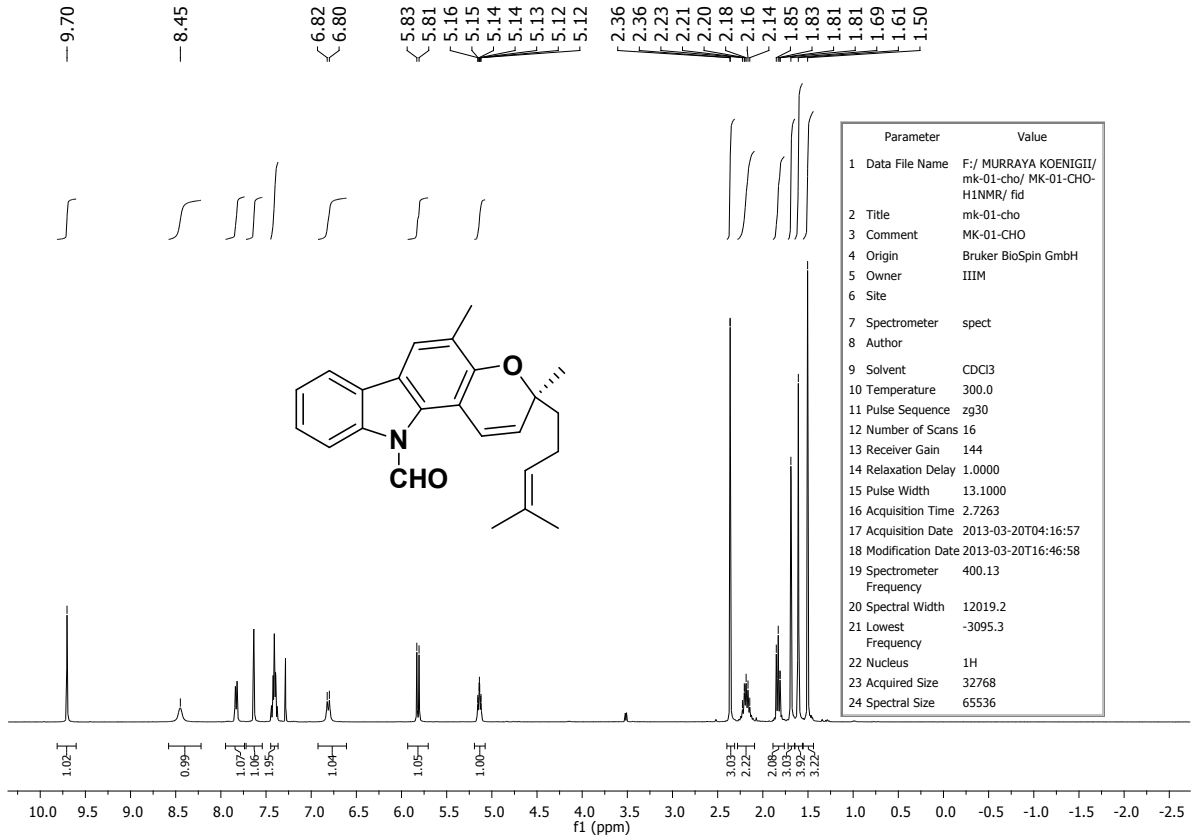


Figure S9: ^{13}C NMR spectrum of compound **5** ($CDCl_3$, 100 MHz)

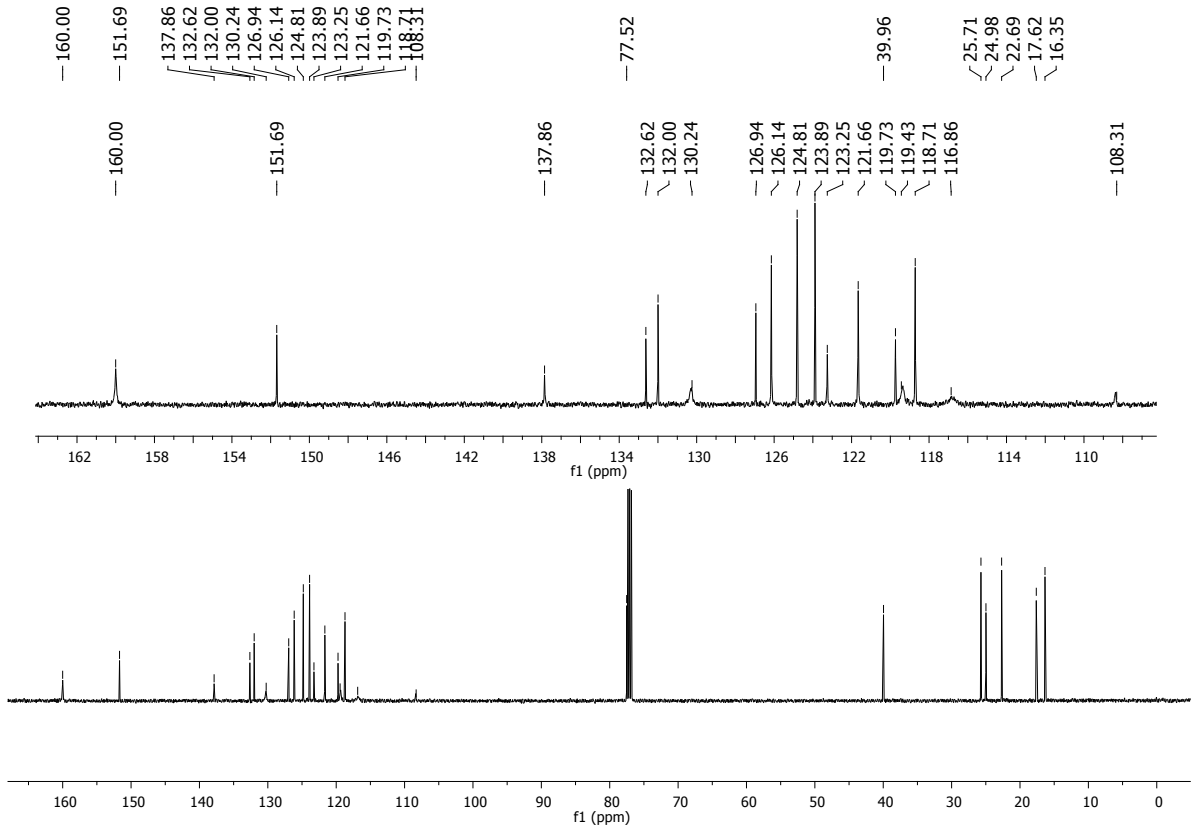


Figure S10: DEPT-135 spectrum of compound **5**

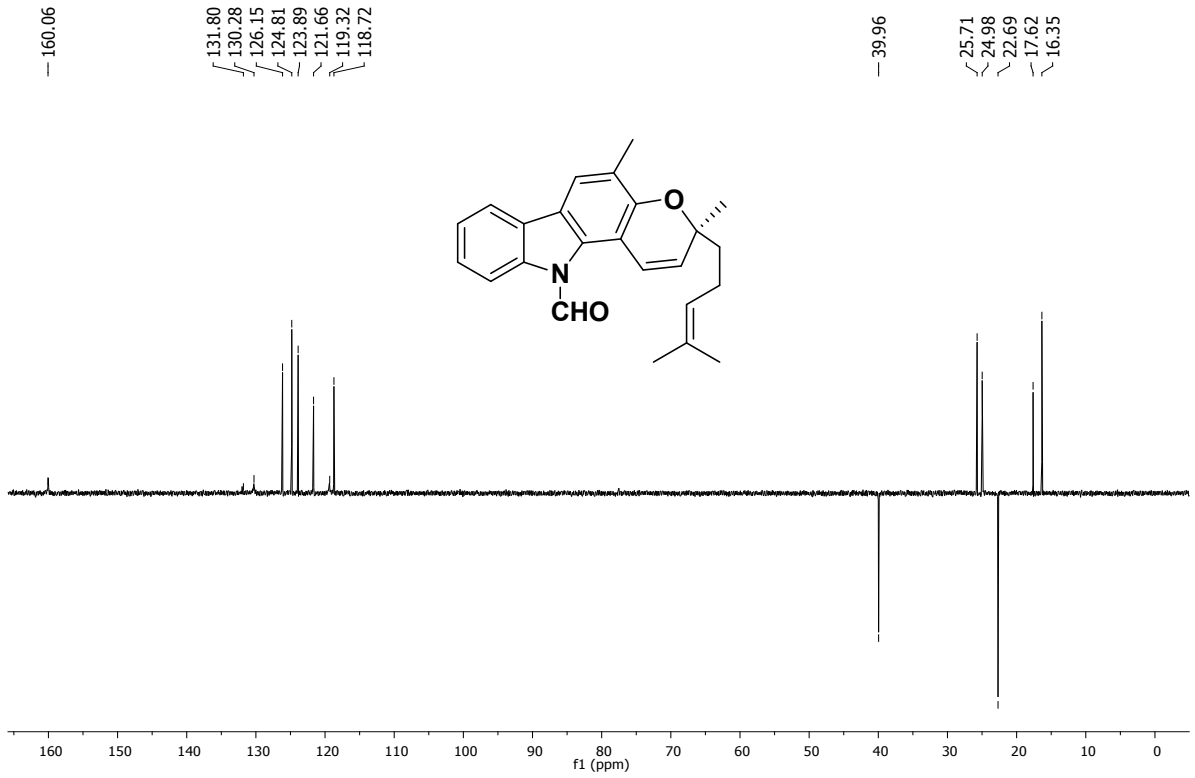
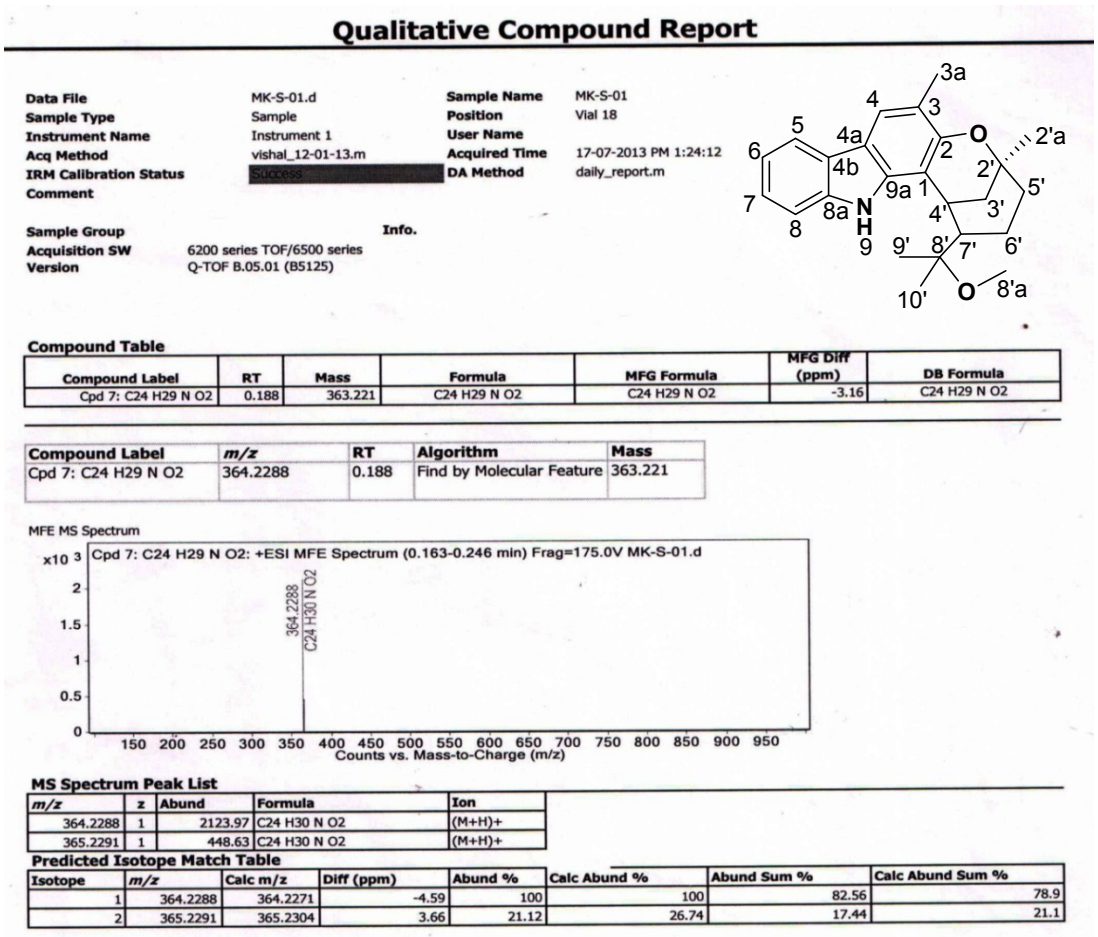


Figure S11: HRESIMS spectroscopic data of compound **6**



Qualitative Compound Report

Data File	MK-S-01.d	**Sample Name**	MK-S-01
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	17-07-2013 PM 1:24:12
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C24 H29 N O2	0.188	363.221	C24 H29 N O2	C24 H29 N O2	-3.16	C24 H29 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C24 H29 N O2	364.2288	0.188	Find by Molecular Feature	363.221

MFE MS Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
364.2288	1	2123.97	C24 H30 N O2	(M+H)+
365.2291	1	448.63	C24 H30 N O2	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	364.2288	364.2271	-4.59	100	100	82.56	78.9
2	365.2291	365.2304	3.66	21.12	26.74	17.44	21.1

Figure S13: ^{1}H NMR spectrum of compound **6** ($CDCl_3$, 500 MHz)

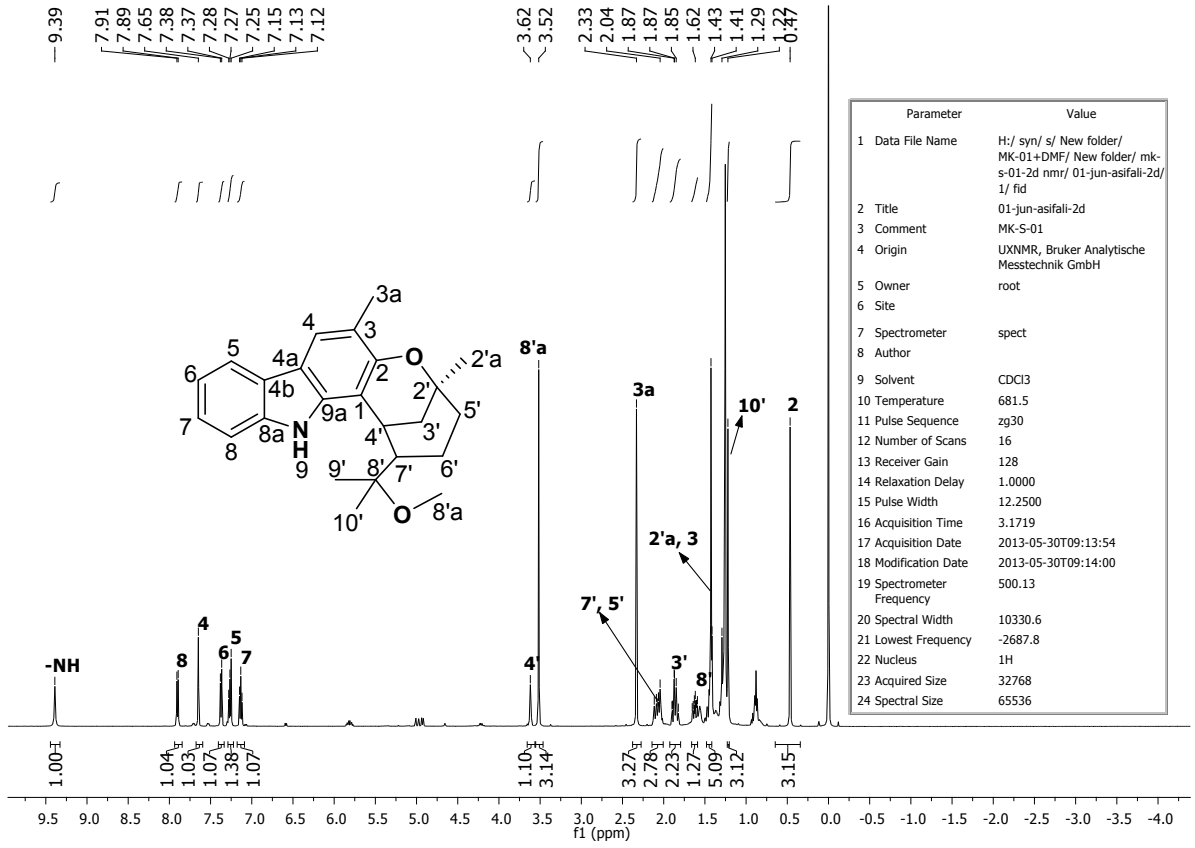


Figure S14: S19. ^{13}C NMR spectrum of compound **6** ($CDCl_3$, 125 MHz)

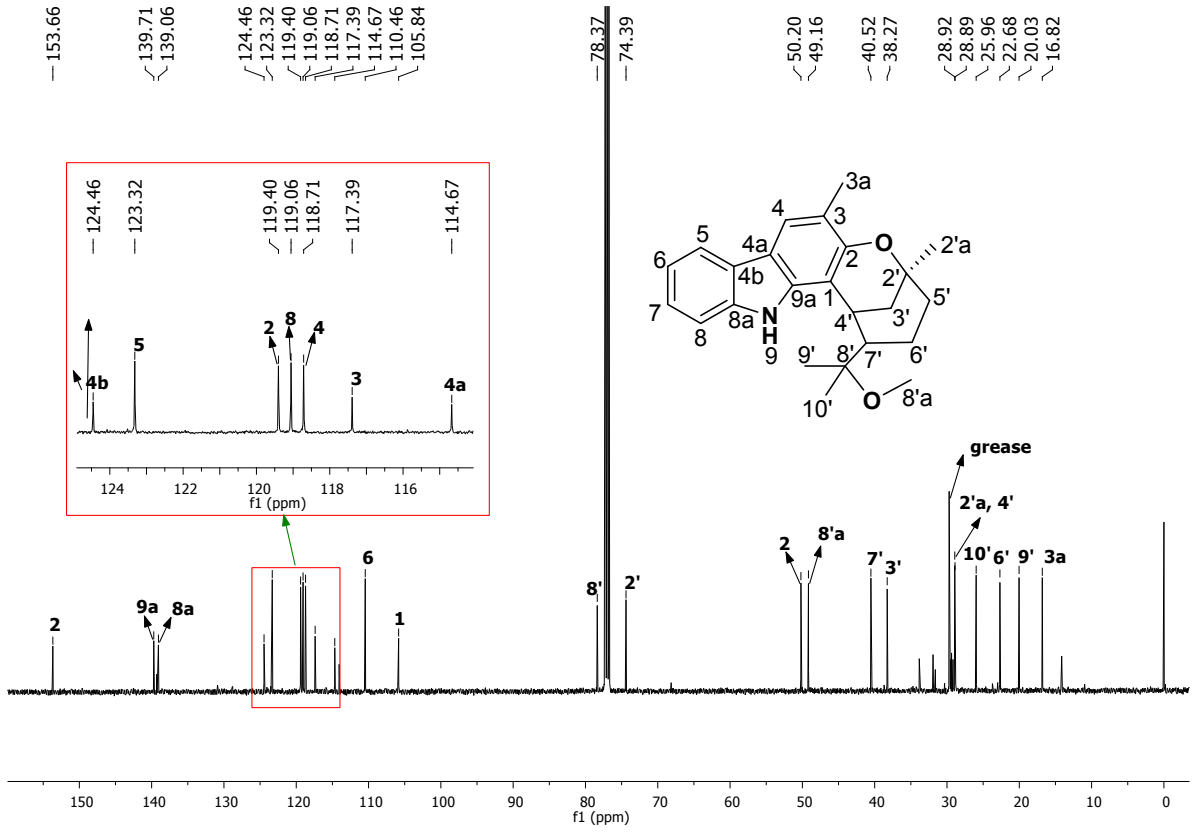


Figure S15: DEPT-135 spectrum of compound **6** ($CDCl_3$, 125 MHz)

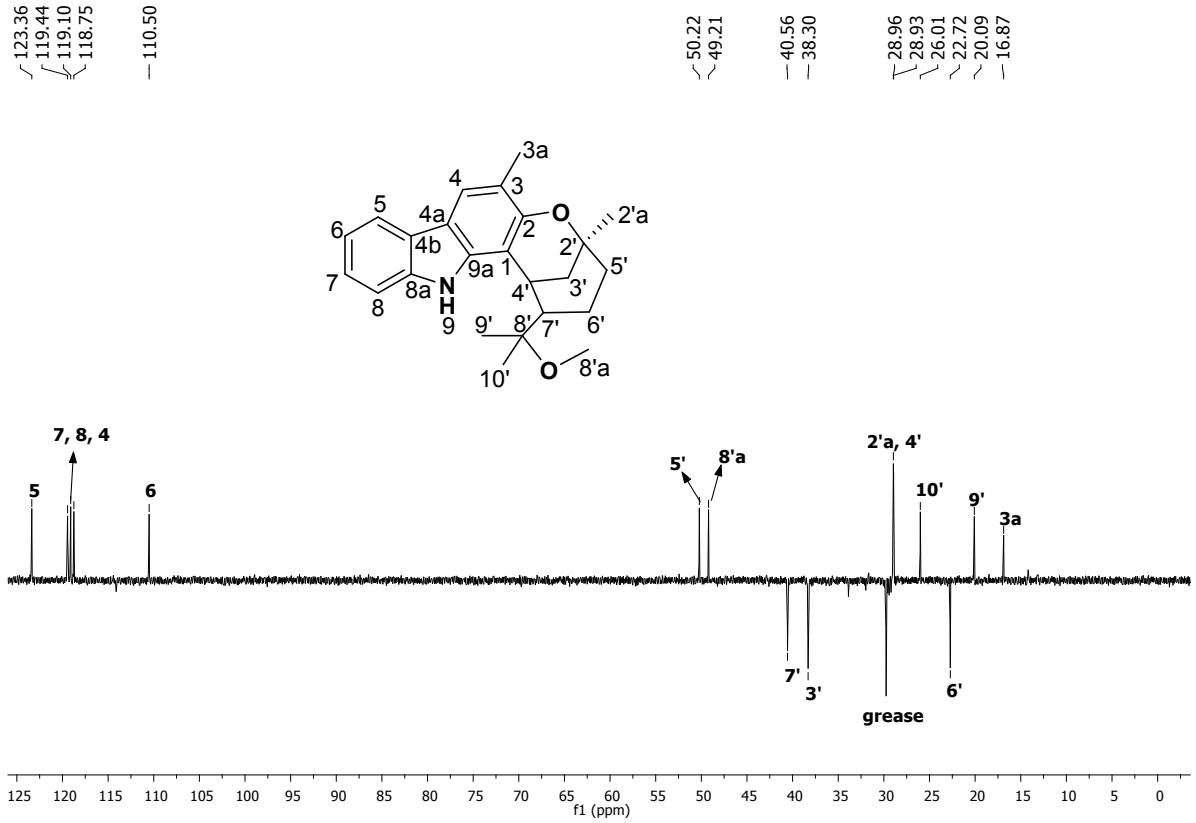


Figure S16: HSQC spectrum of compound **6** ($CDCl_3$, 125 MHz)

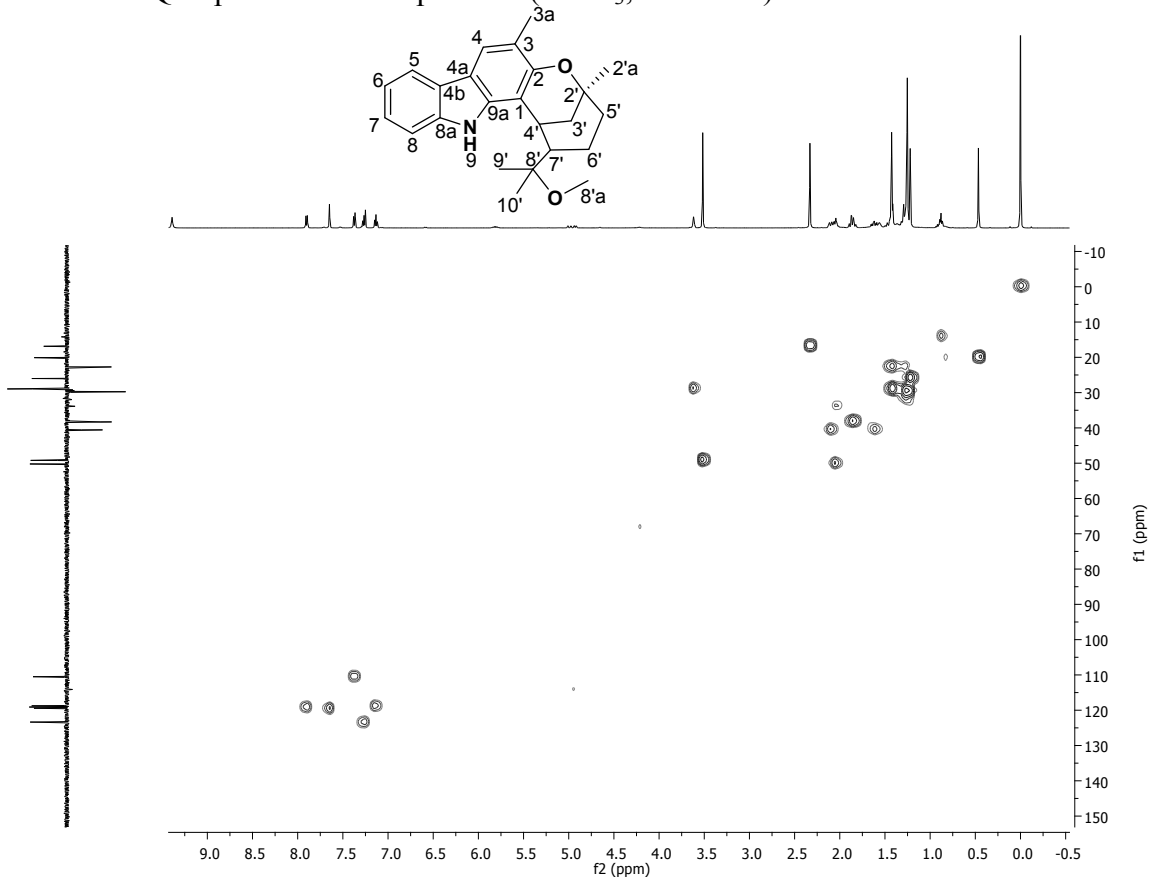


Figure S17: S22. COSY spectrum of compound **6**

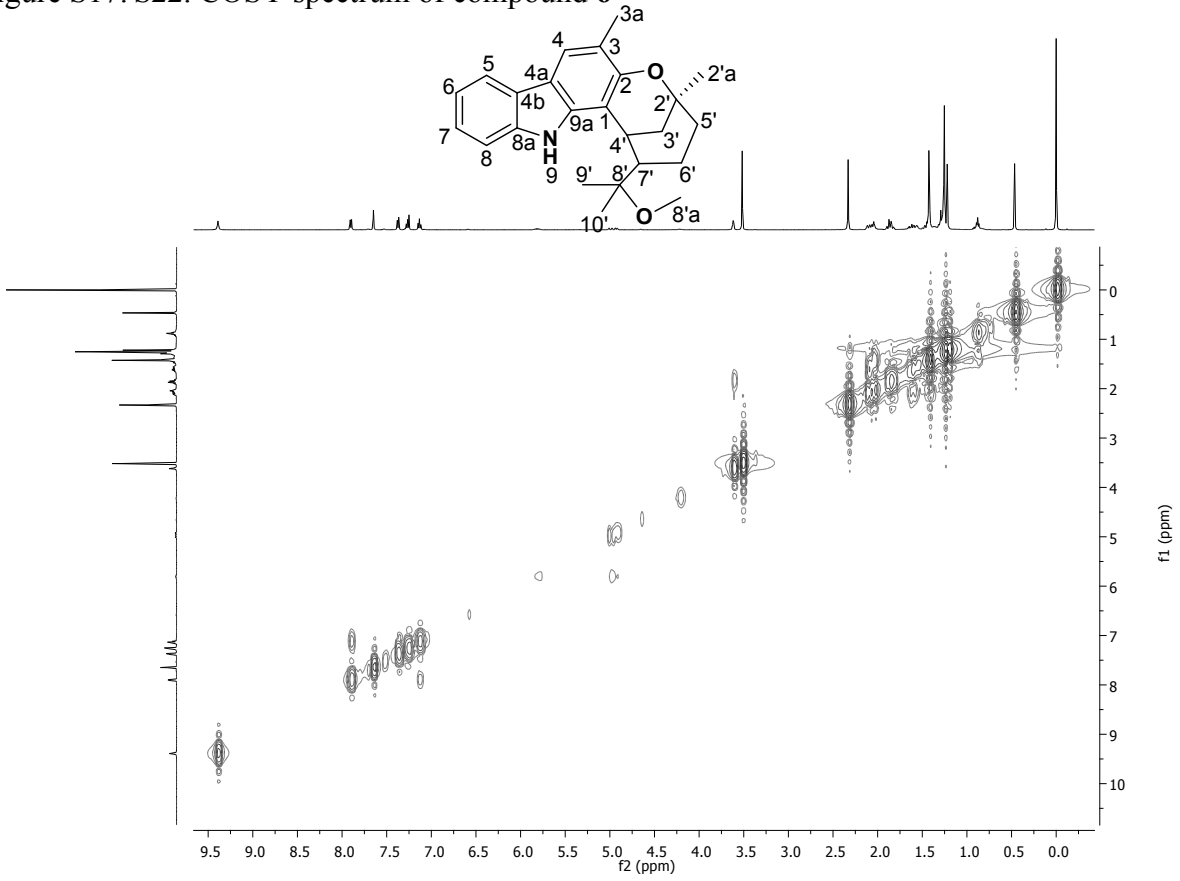


Figure S18: HMBC spectrum of compound **6**

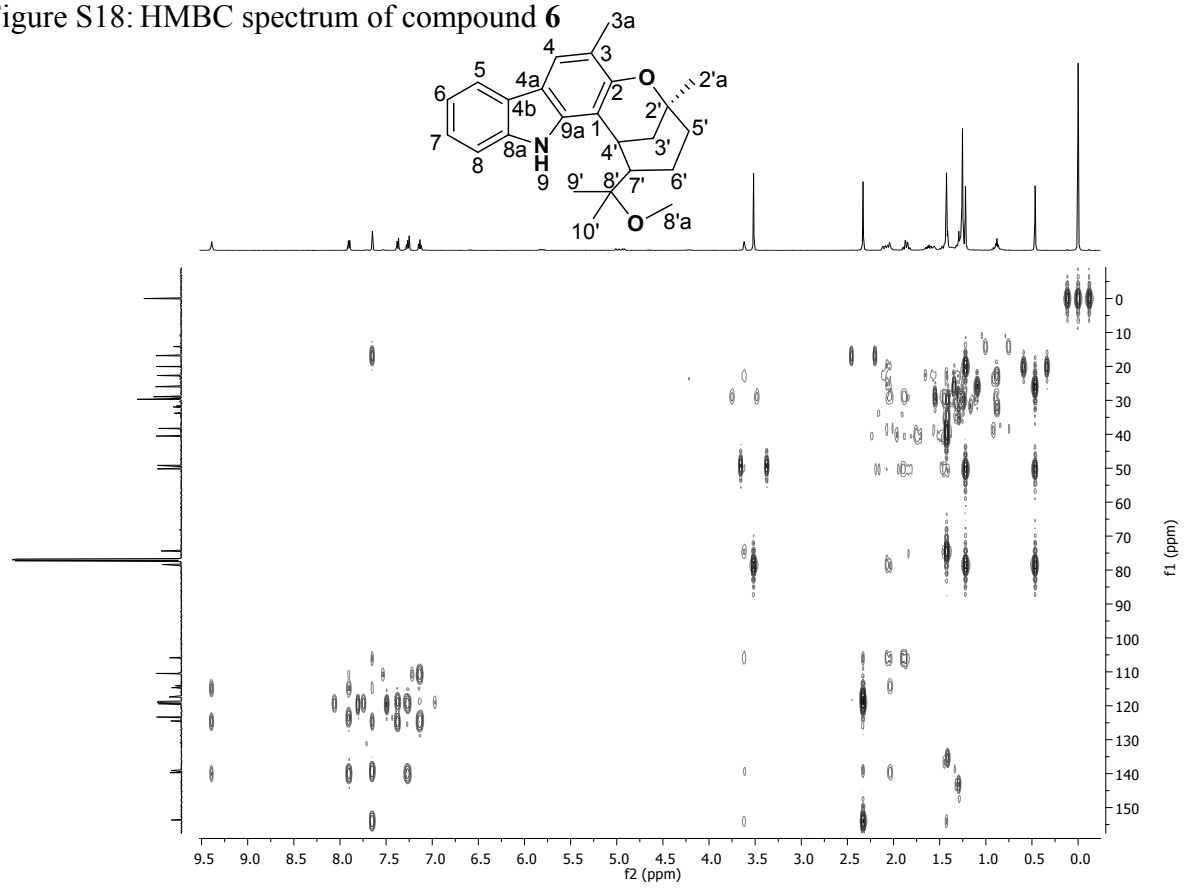
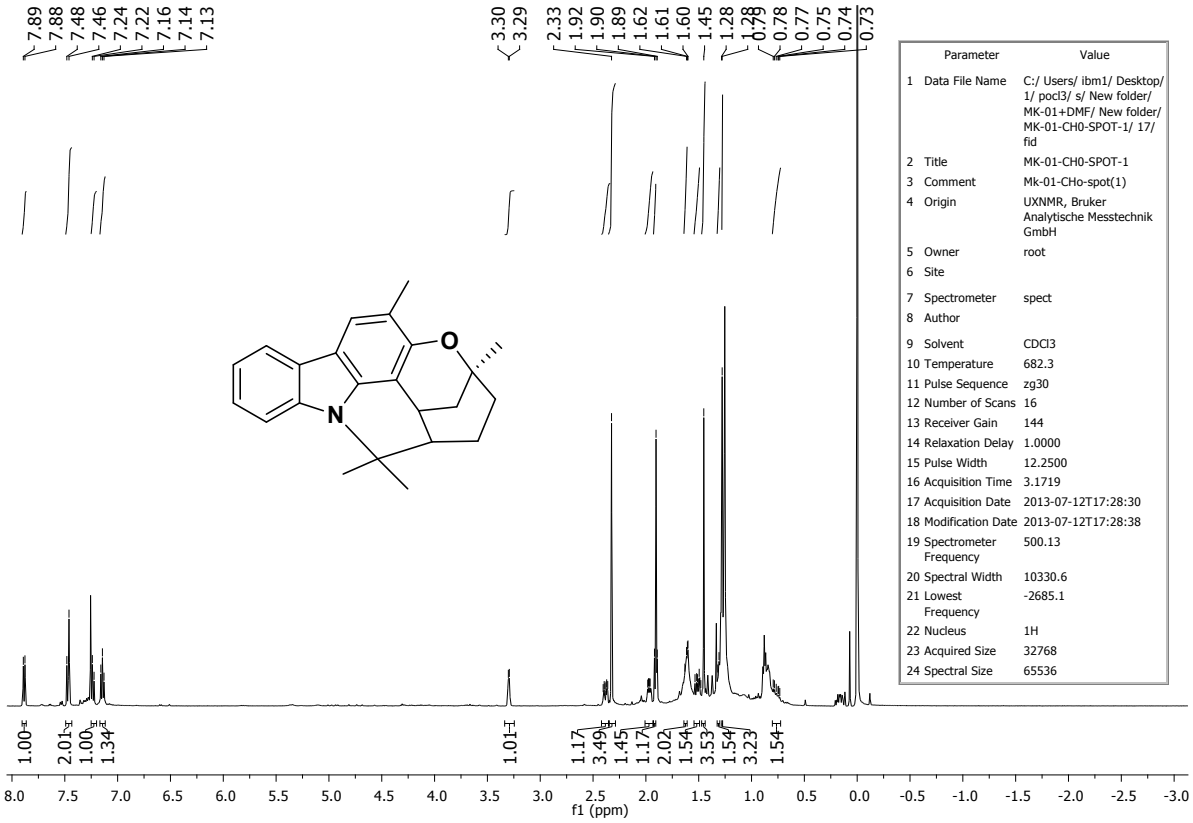
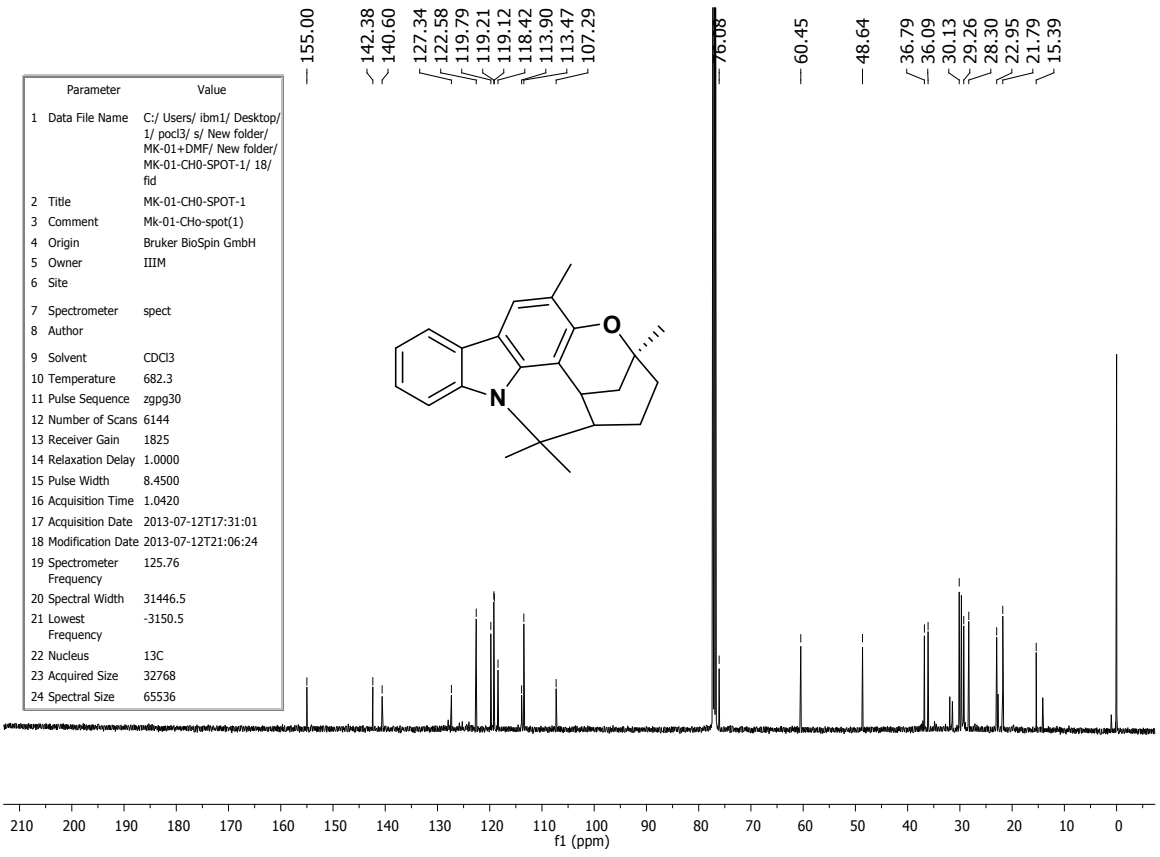


Figure S19: ^{1}H NMR spectrum of Curryangin (**7**) ($CDCl_3$, 500 MHz)



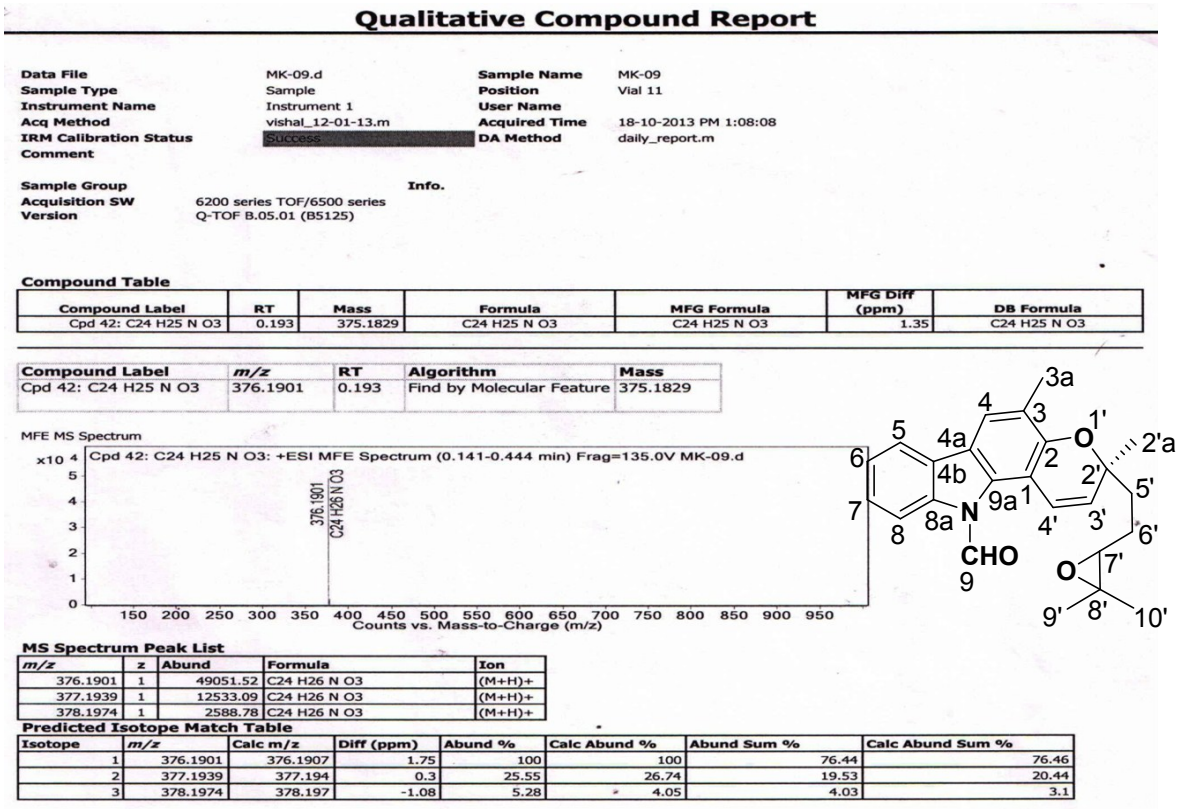
	Parameter	Value
1	Data File Name	C:/ Users/ ibm1/ Desktop/ 1/ pocl3/ s/ New folder/ MK-01+DMF/ New folder/ MK-01-CH0-SPOT-1/ 17/ fid
2	Title	MK-01-CH0-SPOT-1
3	Comment	Mk-01-CHo-spot(1)
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	682.3
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	144
14	Relaxation Delay	1.0000
15	Pulse Width	12.2500
16	Acquisition Time	3.1719
17	Acquisition Date	2013-07-12T17:28:30
18	Modification Date	2013-07-12T17:28:38
19	Spectrometer Frequency	500.13
20	Spectral Width	10330.6
21	Lowest Frequency	-2685.1
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure S20: ^{13}C NMR spectrum of Curryangin (7) ($CDCl_3$, 125 MHz)



	Parameter	Value
1	Data File Name	C:/ Users/ ibm1/ Desktop/ 1/ pocl3/ s/ New folder/ MK-01+DMF/ New folder/ MK-01-CH0-SPOT-1/ 18/ fid
2	Title	MK-01-CH0-SPOT-1
3	Comment	Mk-01-CHo-spot(1)
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	682.3
11	Pulse Sequence	zgpg30
12	Number of Scans	6144
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-07-12T17:31:01
18	Modification Date	2013-07-12T21:06:24
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3150.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure S21: HRESIMS spectroscopic data of compound **8**



Qualitative Compound Report

Data File	MK-09.d	**Sample Name**	MK-09
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	18-10-2013 PM 1:08:08
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

Sample Group	**Info.**
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 42: C24 H25 N O3	0.193	375.1829	C24 H25 N O3	C24 H25 N O3	1.35	C24 H25 N O3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 42: C24 H25 N O3	376.1901	0.193	Find by Molecular Feature	375.1829

MFE MS Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
376.1901	1	49051.52	C24 H26 N O3	(M+H)+
377.1939	1	12533.09	C24 H26 N O3	(M+H)+
378.1974	1	2588.78	C24 H26 N O3	(M+H)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	376.1901	376.1907	1.75	100	100	76.44	76.46
2	377.1939	377.194	0.3	25.55	26.74	19.53	20.44
3	378.1974	378.197	-1.08	5.28	4.05	4.03	3.1

Figure S22: ^{1}H NMR spectrum of compound **8** ($CDCl_3$, 400 MHz)

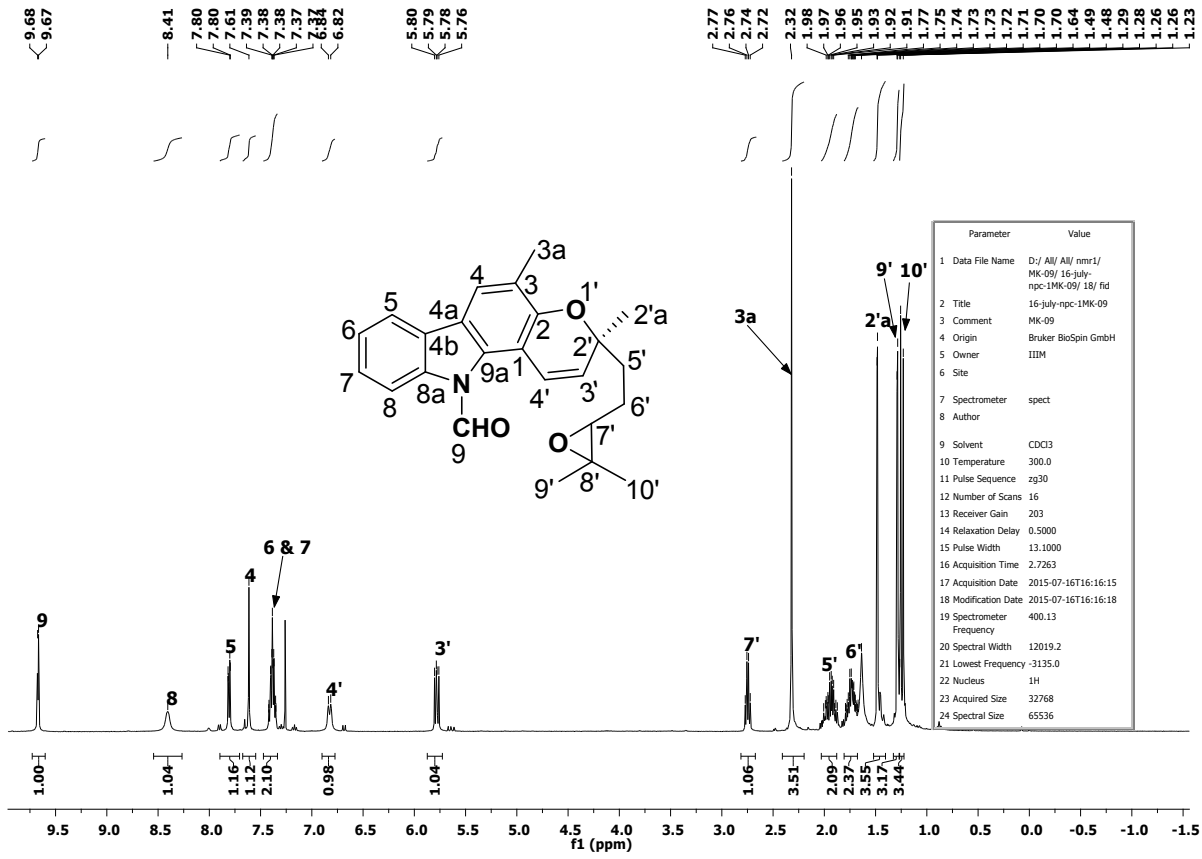


Figure S23: ^{13}C NMR spectrum of compound **8** ($CDCl_3$, 125 MHz)

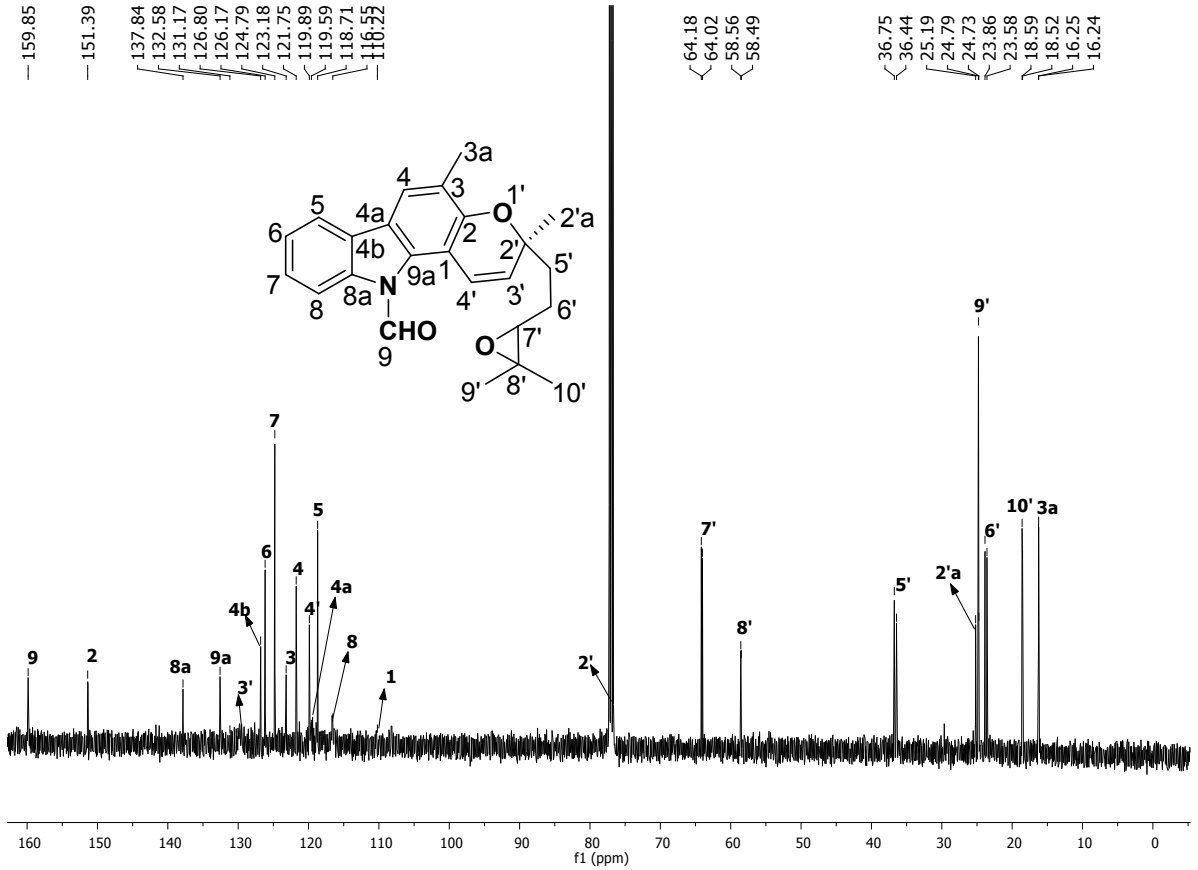


Figure S24: DEPT-135 spectrum of compound **8**

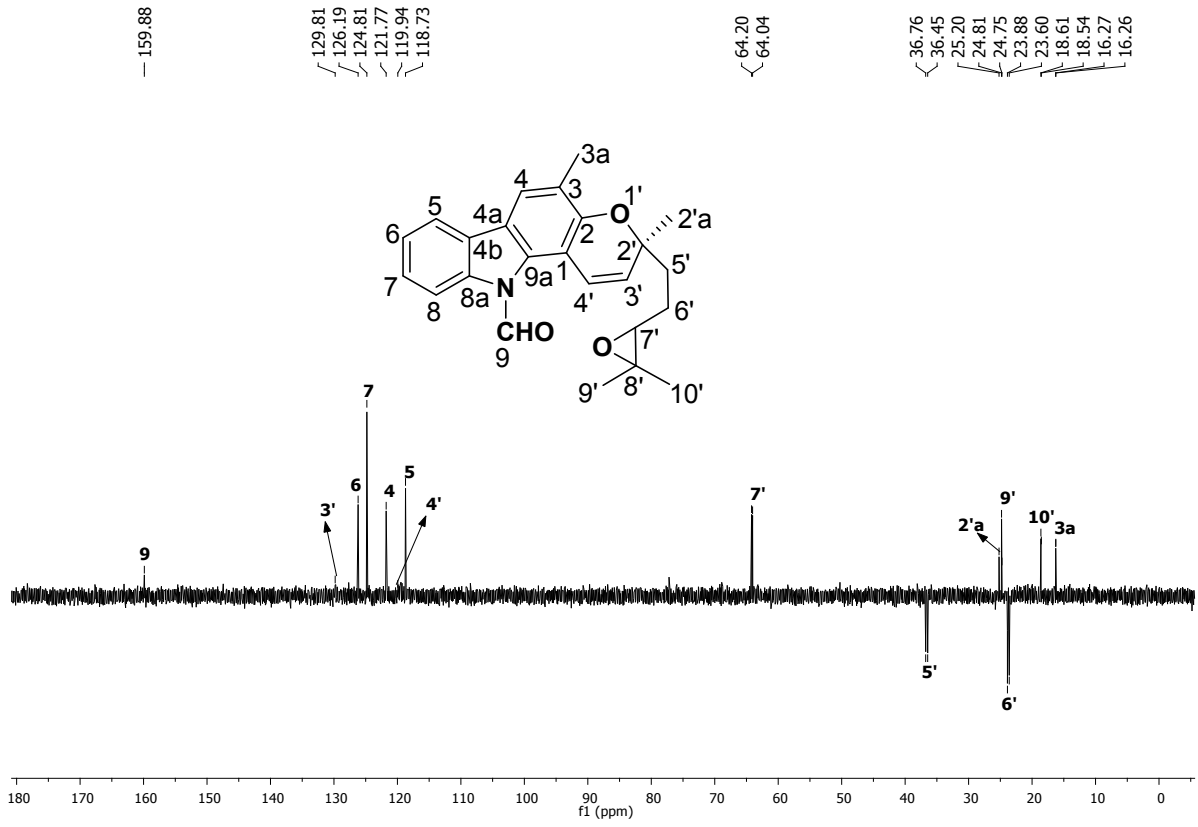


Figure S25: HSQC spectrum of compound **8**

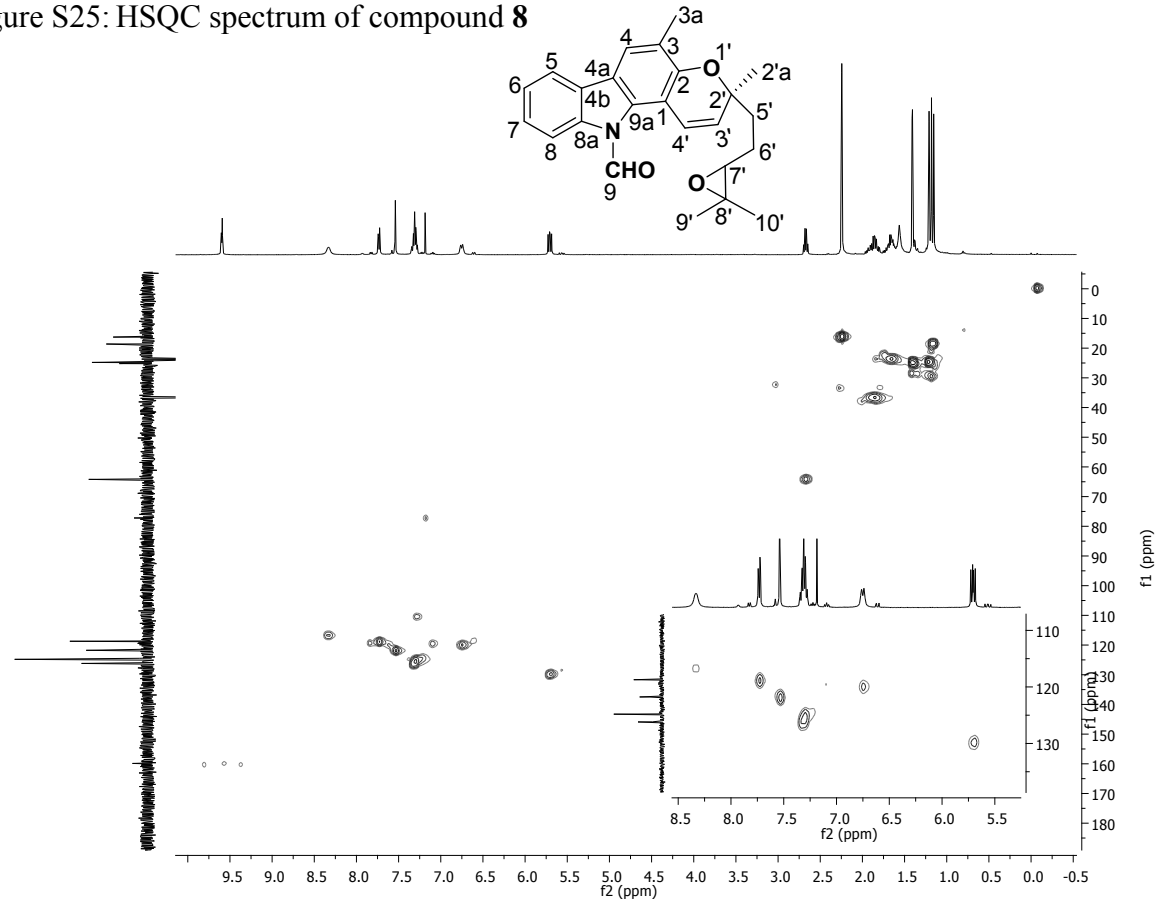


Figure S26: COSY spectrum of compound **8**

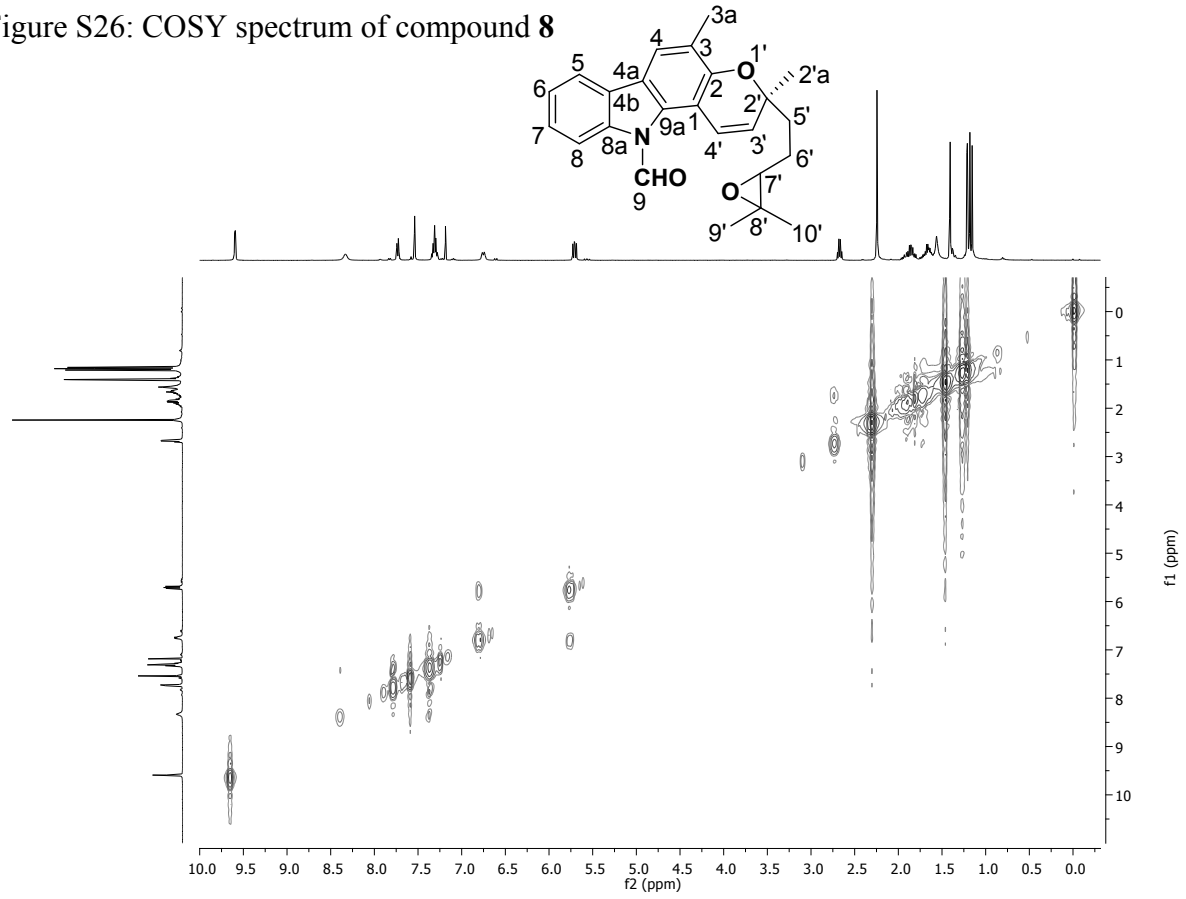


Figure S27: HMBC spectrum of compound **8**

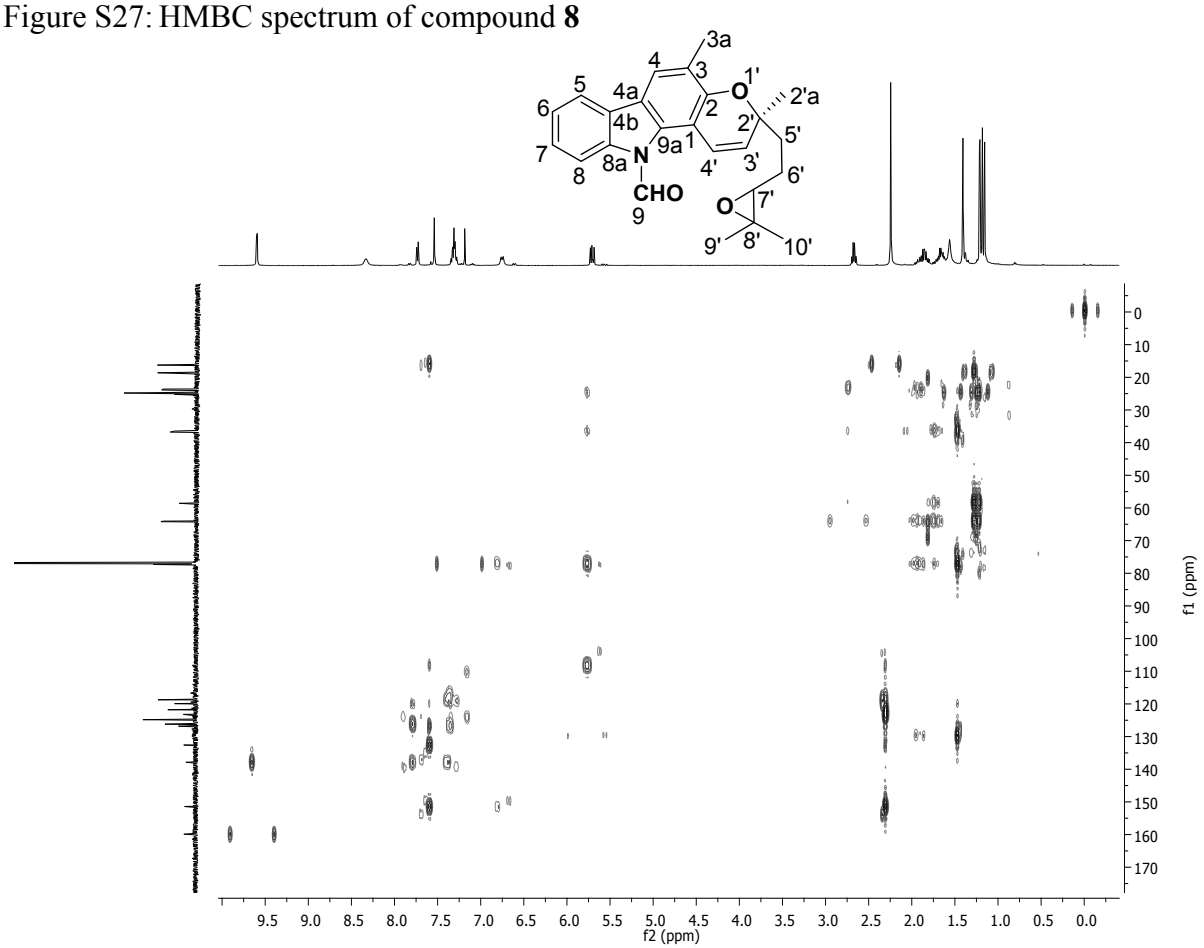


Figure S28: ^{1}H NMR spectrum of Murrayazolinine (**9**) ($CDCl_3$, 400 MHz)

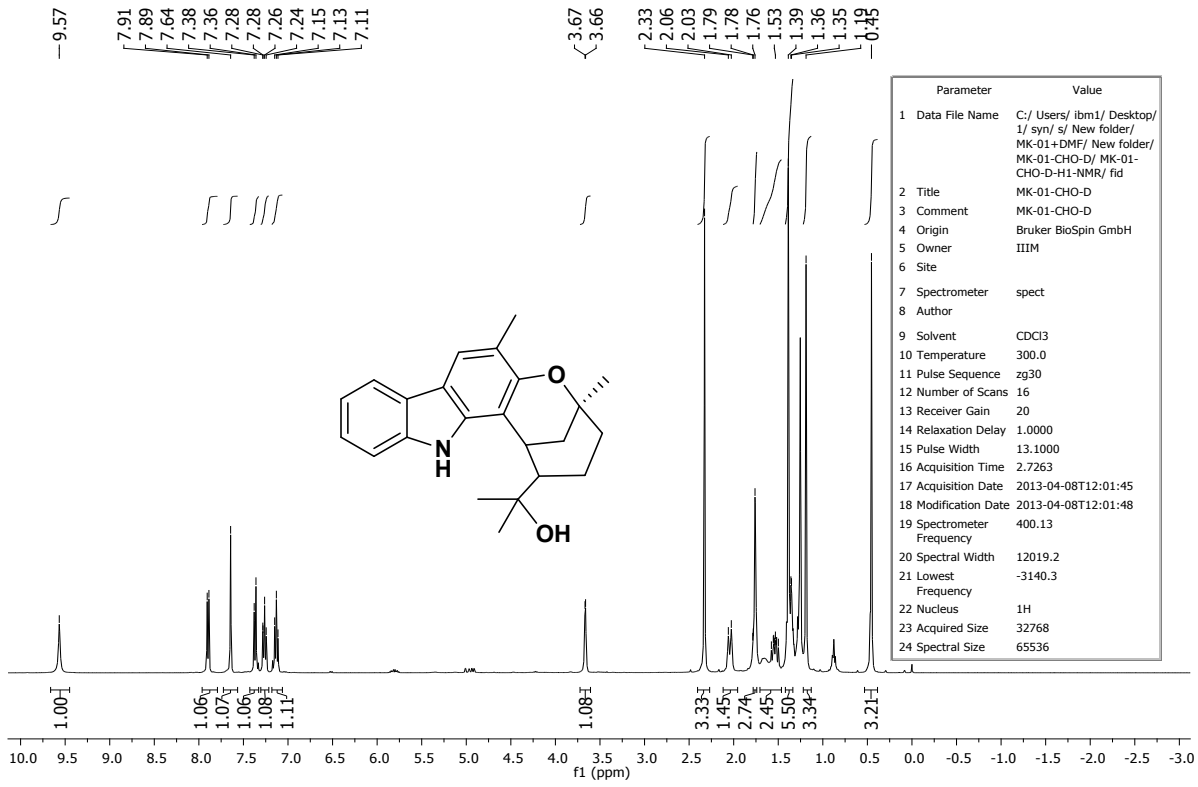
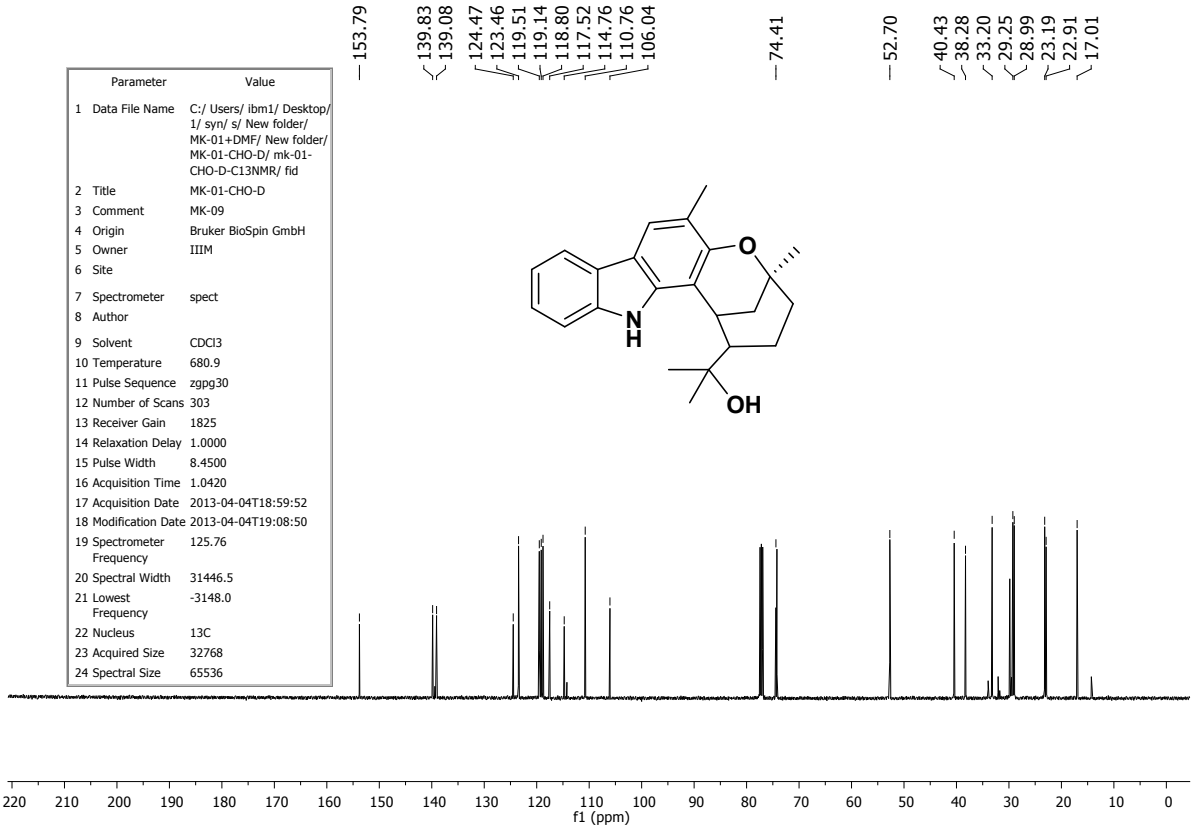


Figure S29: ^{13}C NMR spectrum of Murrayazolinine (**9**) ($CDCl_3$, 125 MHz)



	Parameter	Value
1	Data File Name	C:/ Users/ ibm1/ Desktop/ 1/ syn/ s/ New folder/ MK-01+DMF/ New folder/ MK-01-CHO-D/ mk-01-CHO-D-C13NMR/ fid
2	Title	MK-01-CHO-D
3	Comment	MK-09
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.9
11	Pulse Sequence	zgpg30
12	Number of Scans	303
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-04-04T18:59:52
18	Modification Date	2013-04-04T19:08:50
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536