Supporting Information

$POCl_3$-mediated Cyclization of (+)-*S*-Mahanimbine Led to the Divergent Synthesis of Natural Product Derivatives with Antiplasmodial Activity.

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Figure S1: HRESIMS of compound **2**

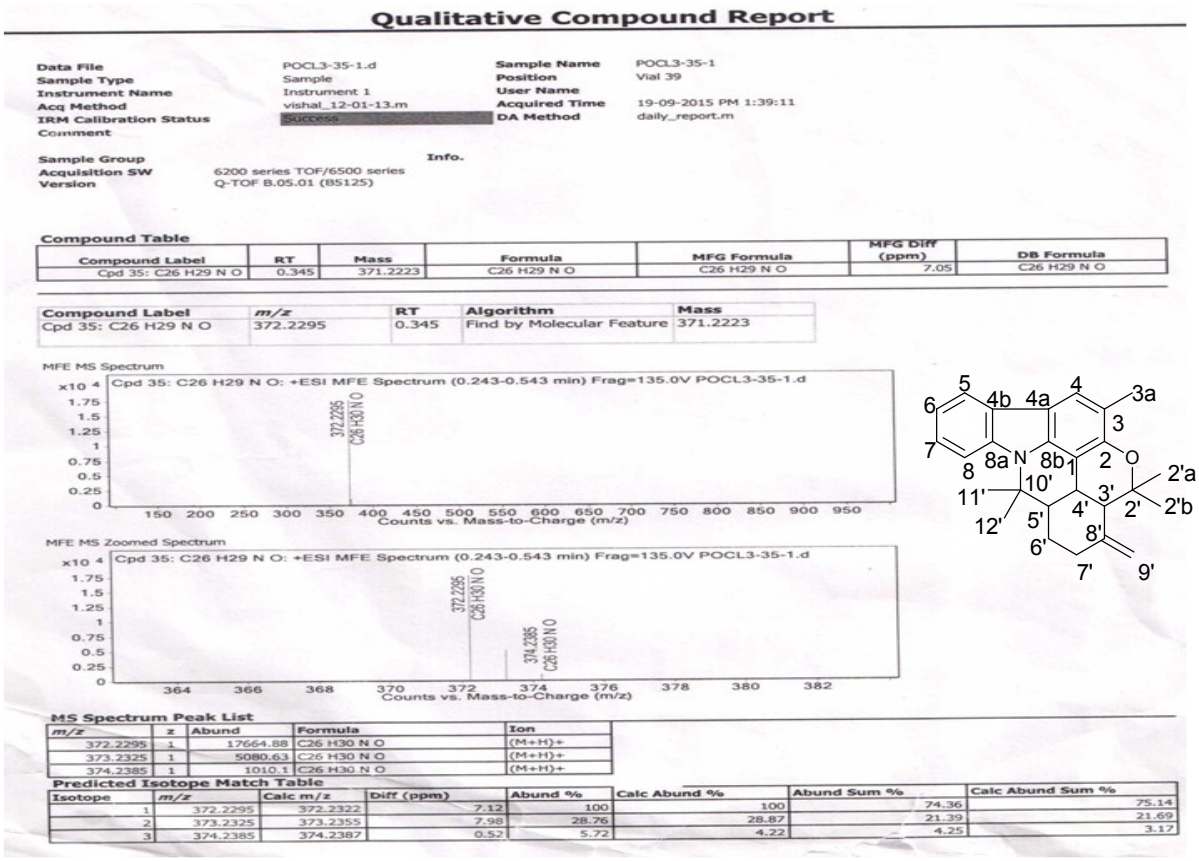


Figure S2: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **2**

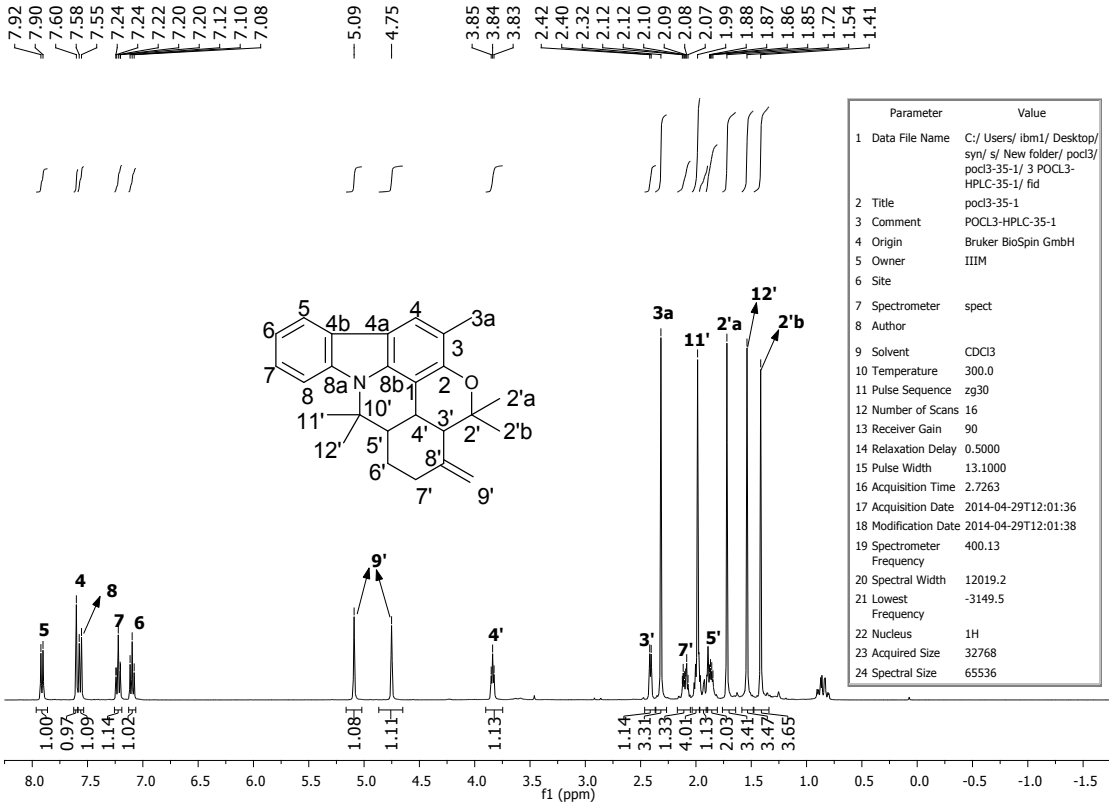


Figure S3: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **2**

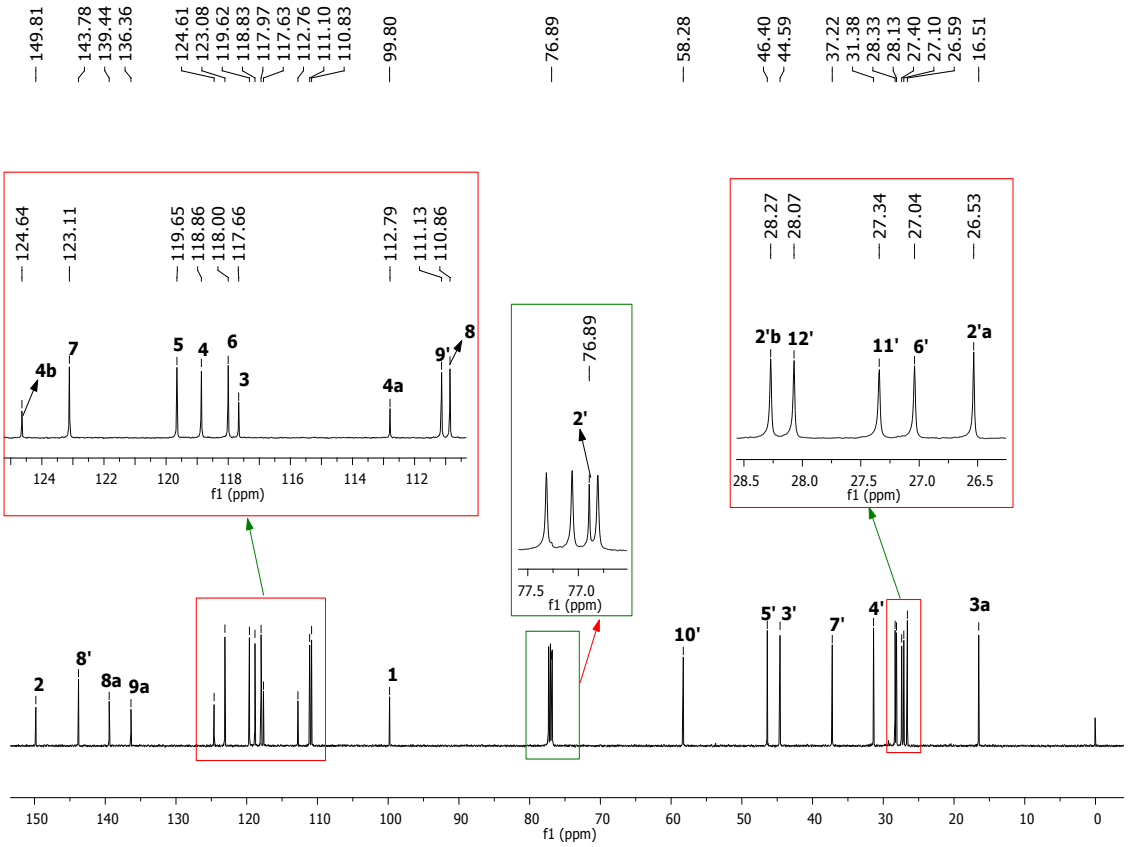


Figure S4: DEPT-135 (100 MHz, $CDCl_3$) spectrum of compound **2**

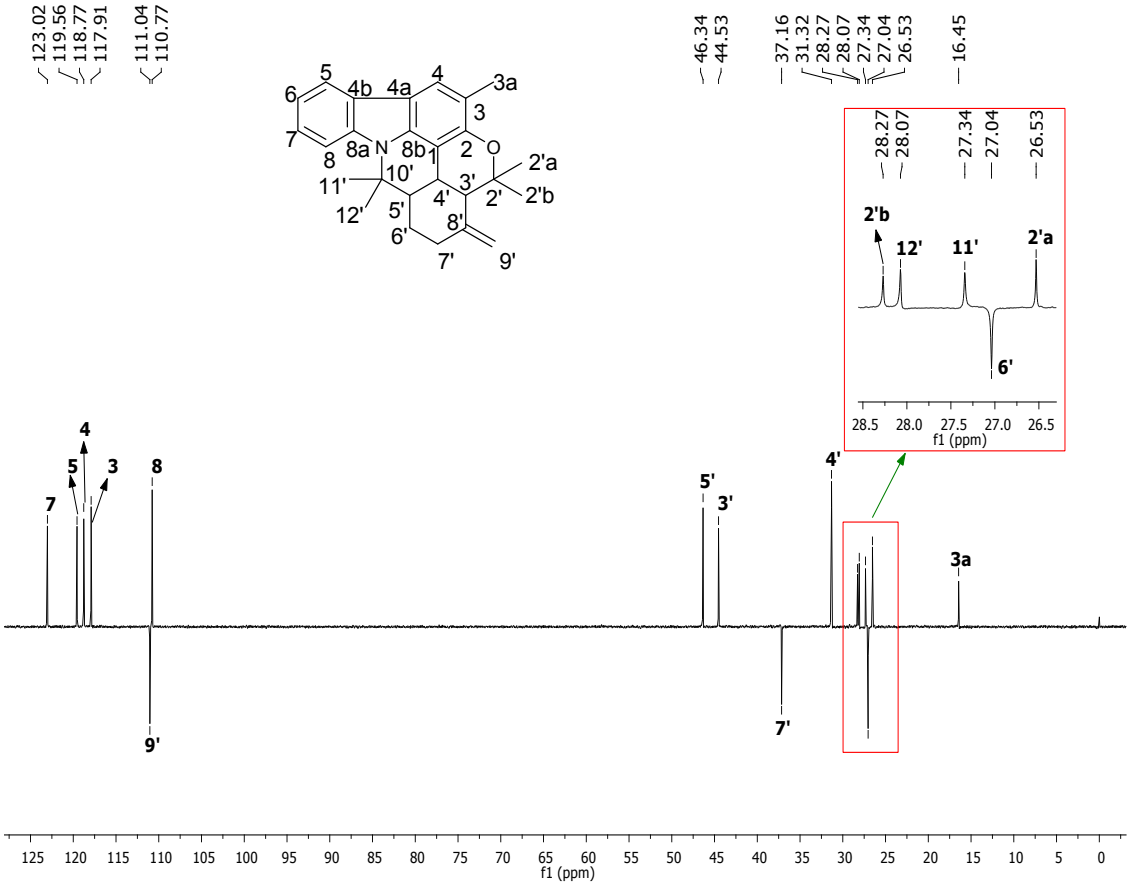


Figure S5: COSY spectrum of compound **2**

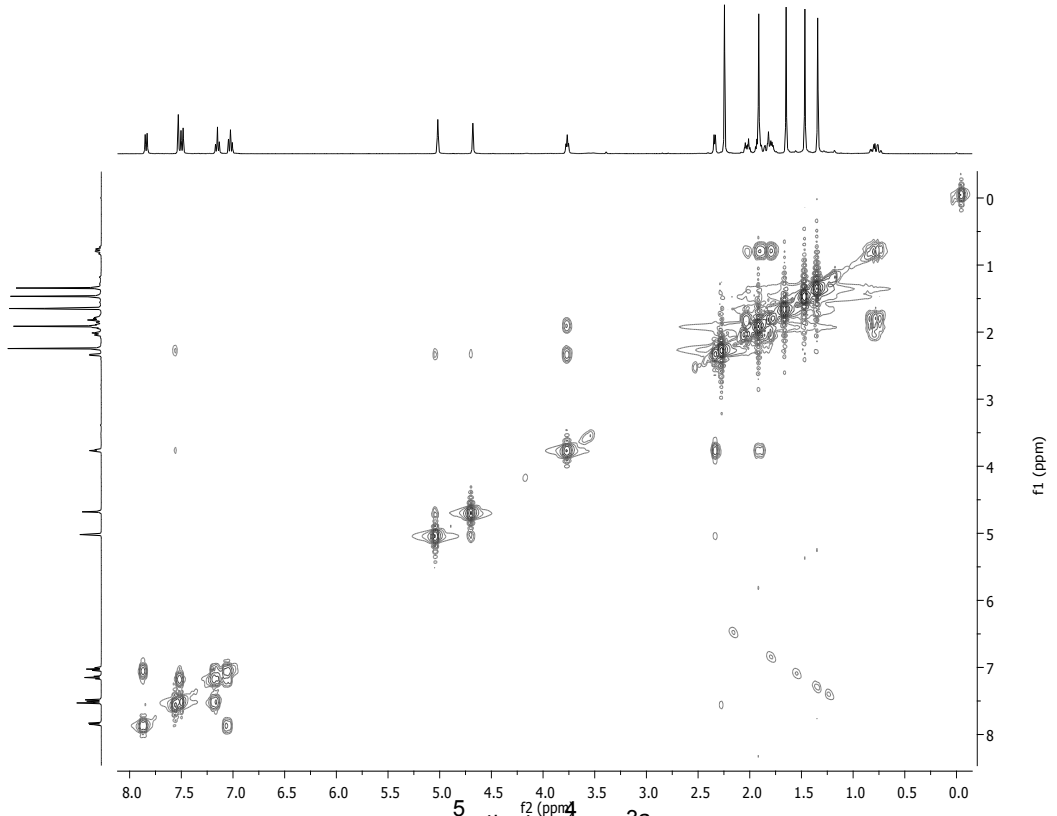
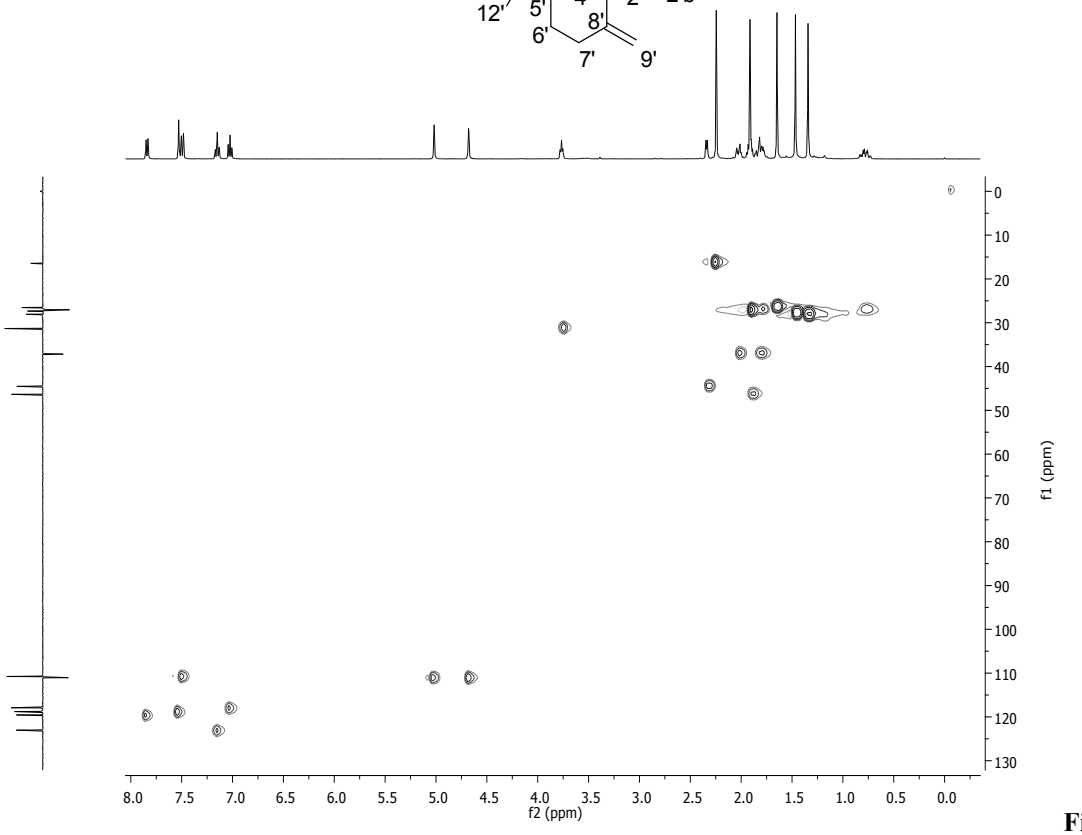


Figure S6: HSQC spectrum of compound **2**



Figu

re S7: HMBC spectrum of compound **2**

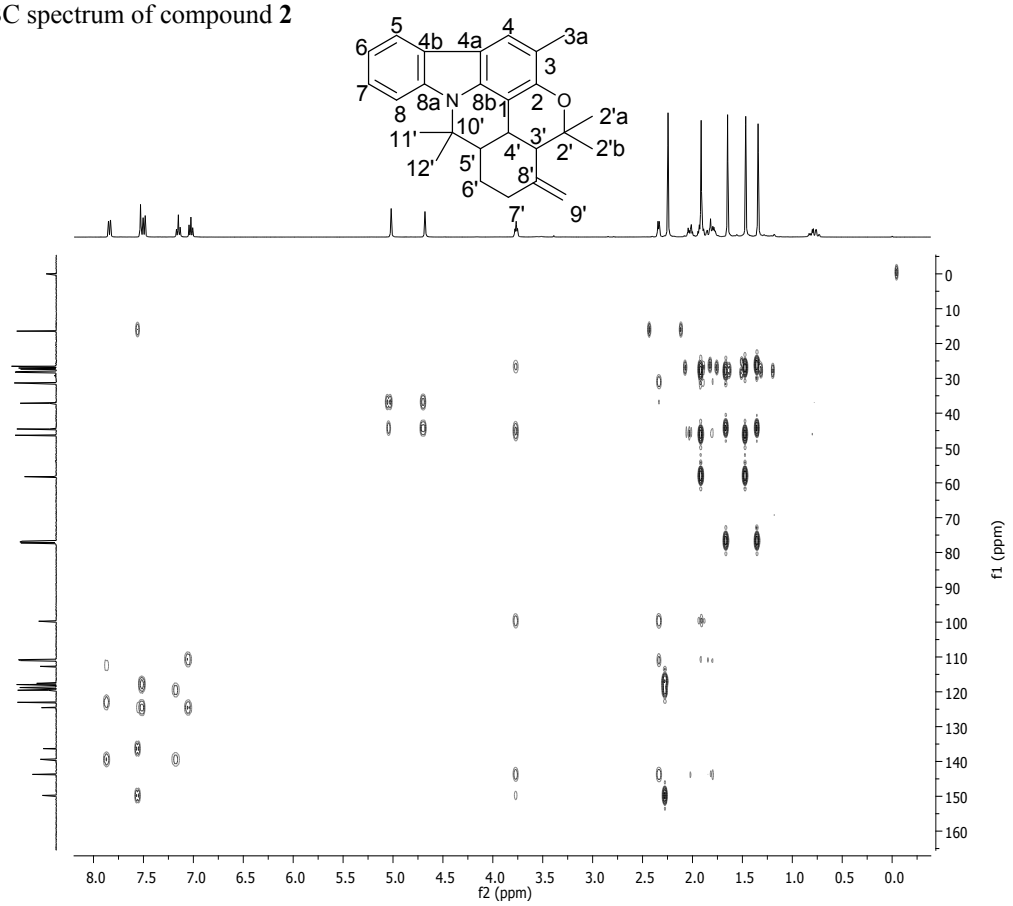


Figure S8: NOESY spectrum of compound **2**

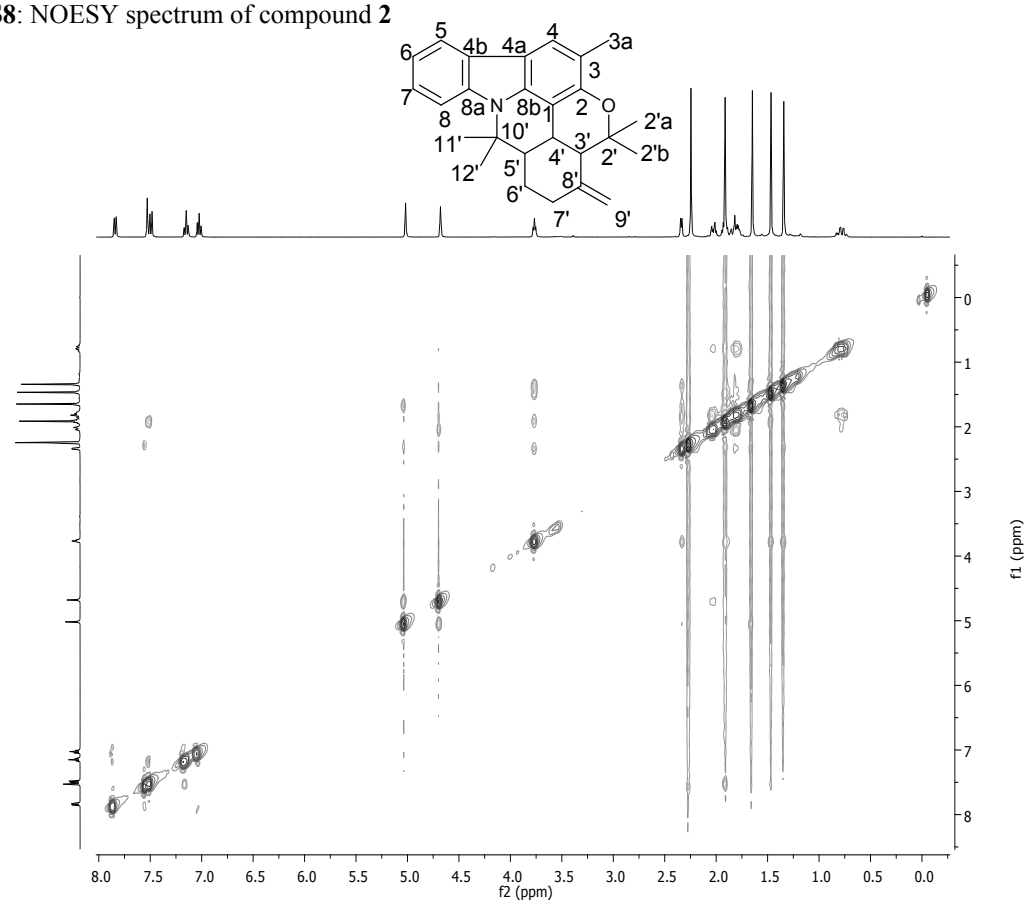
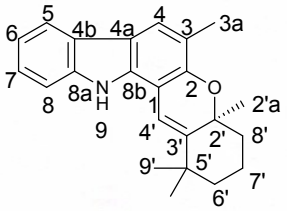


Figure S9: HRESIMS spectroscopic data of compound **4**

Qualitative Compound Report

Data File	MK-POCl3-3.d	**Sample Name**	MK-POCl3-3
Sample Type	Sample	**Position**	Vial 70
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	17-10-2013 PM 12:14:56
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)

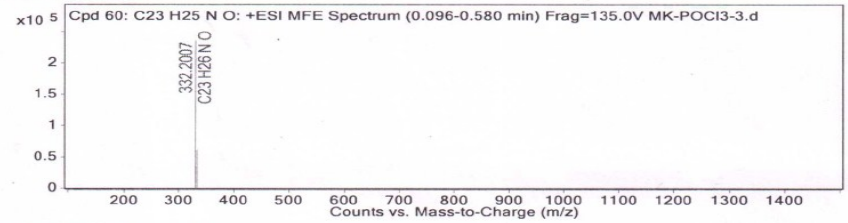


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 60: C23 H25 N O	0.195	331.1933	C23 H25 N O	C23 H25 N O	0.88	C23 H25 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 60: C23 H25 N O	332.2007	0.195	Find by Molecular Feature	331.1933

MFE MS Spectrum



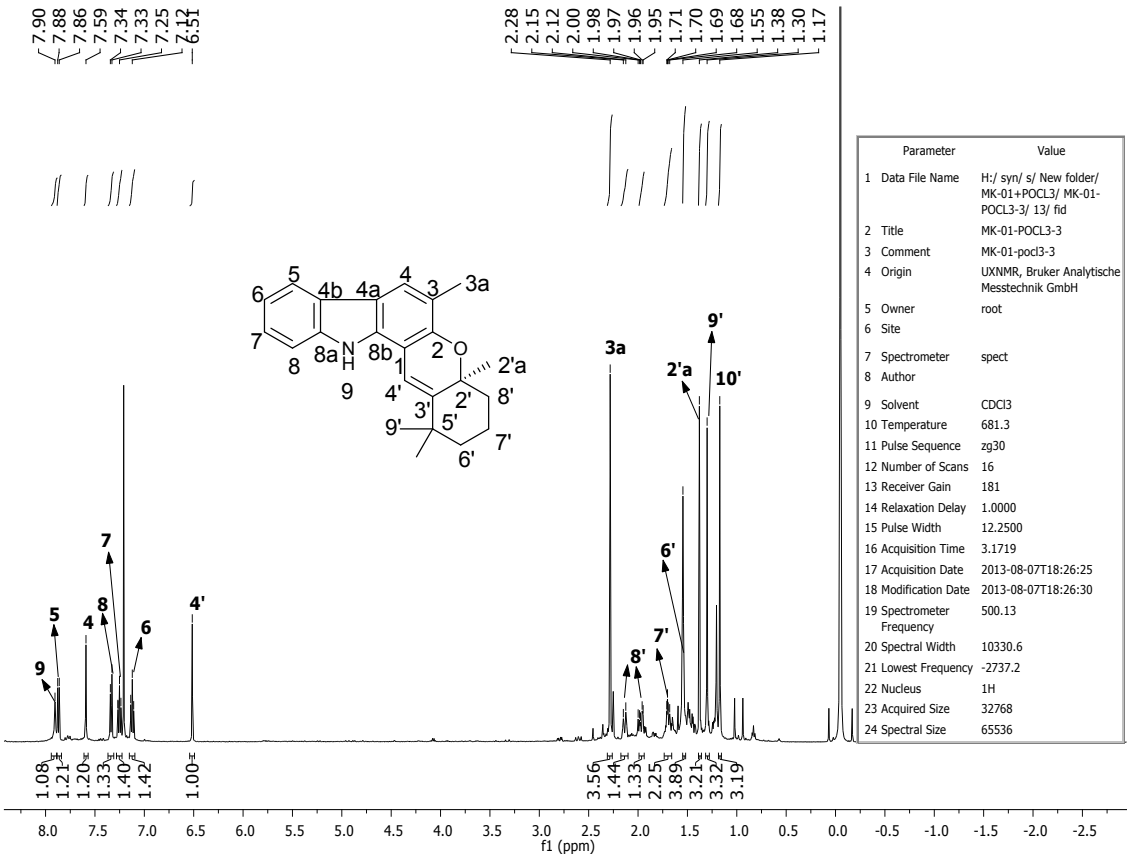
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
332.2007	1	236465.36	C23 H26 N O	(M+H)+
333.2037	1	62547.96	C23 H26 N O	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	332.2007	332.2009	0.69	100	100	79.08	79.63
2	333.2037	333.2042	1.6	26.45	25.58	20.92	20.37

Figure S10: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4**



Figu

re S11: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4**

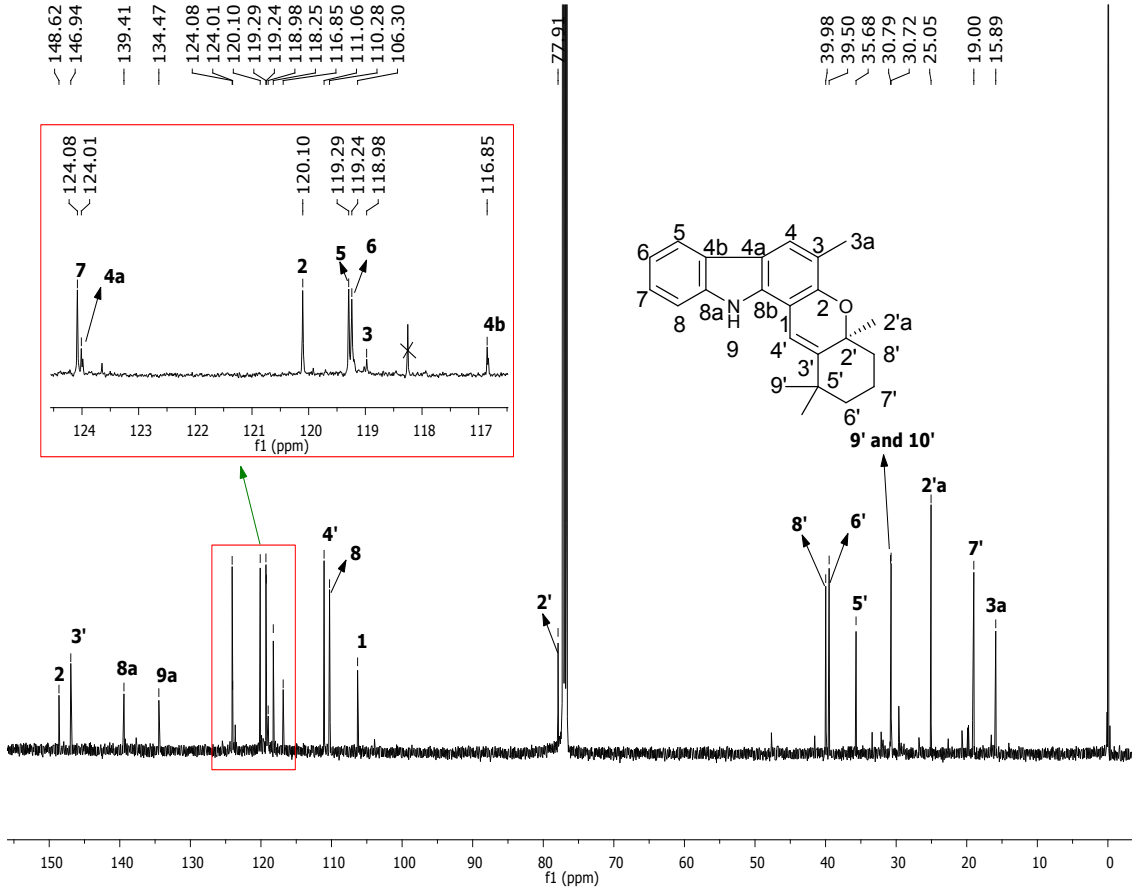
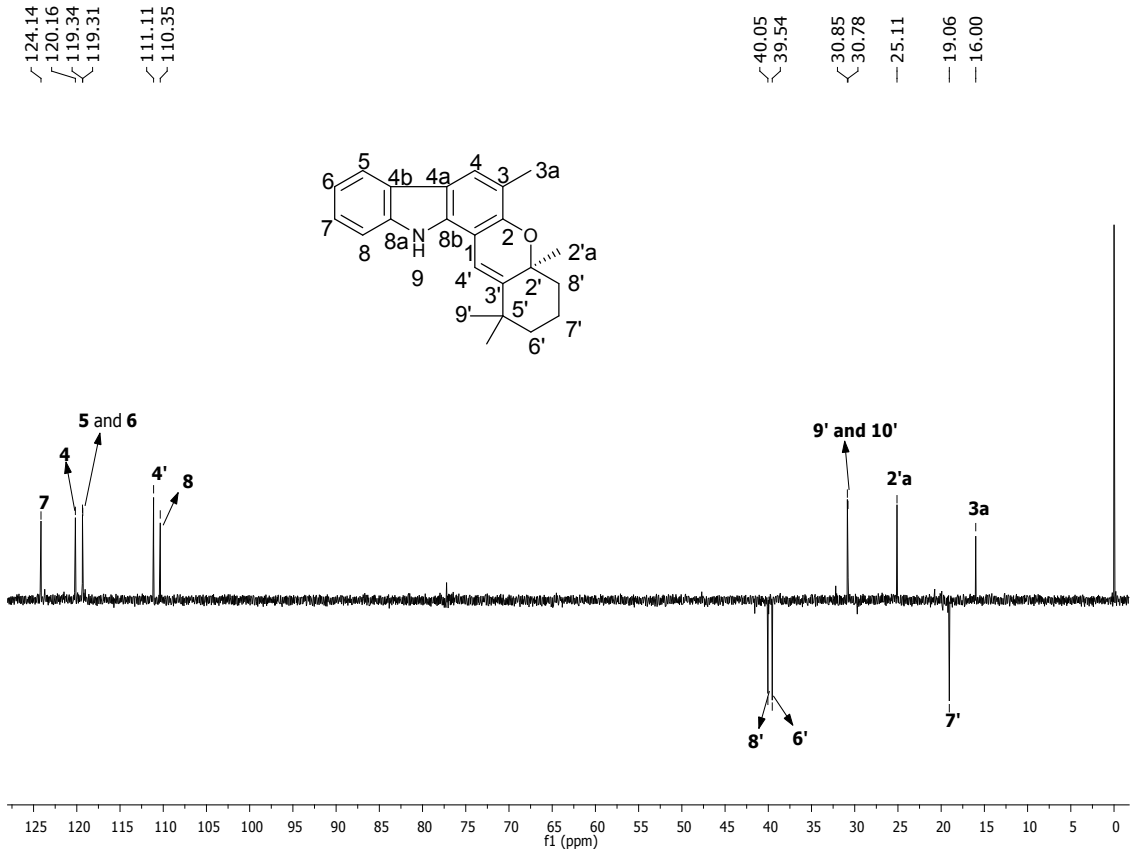


Figure S12: DEPT-135 (100 MHz, $CDCl_3$) spectrum of compound **4**



Figu

re S13: COSY spectrum of compound **4**

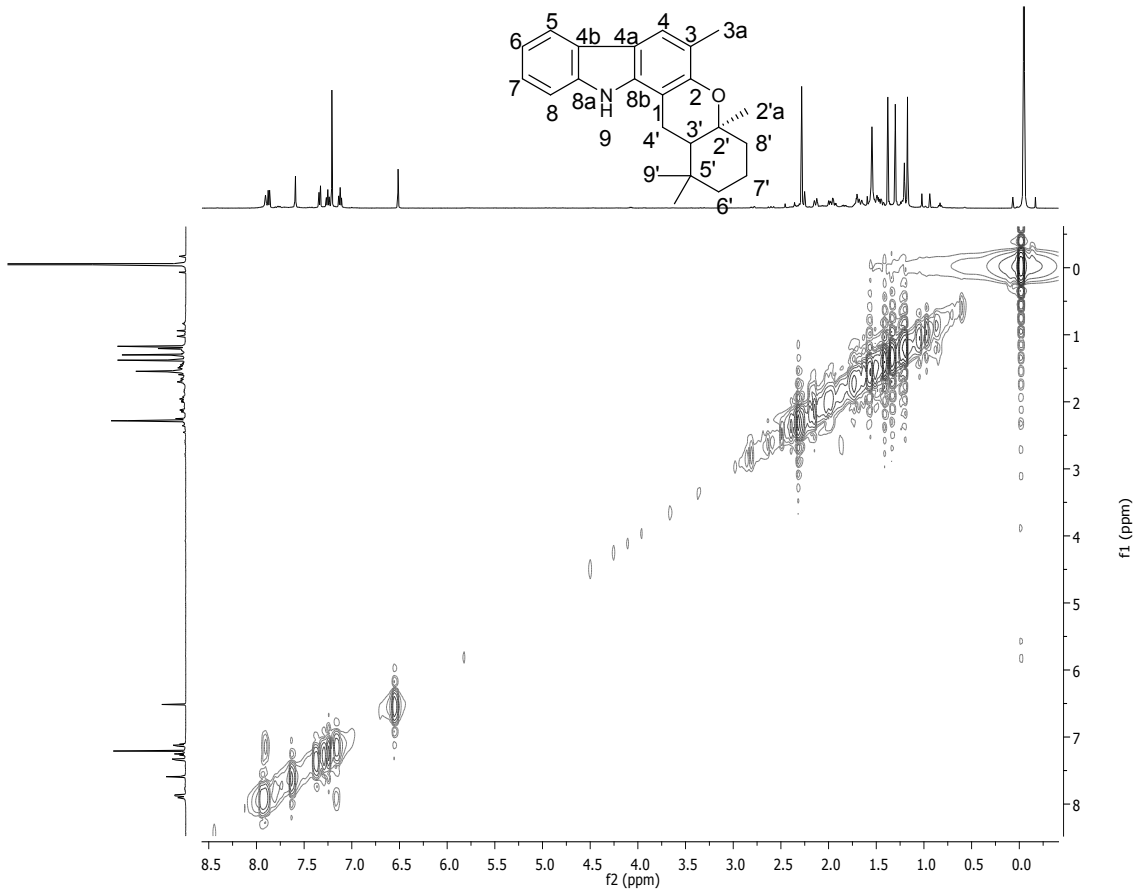
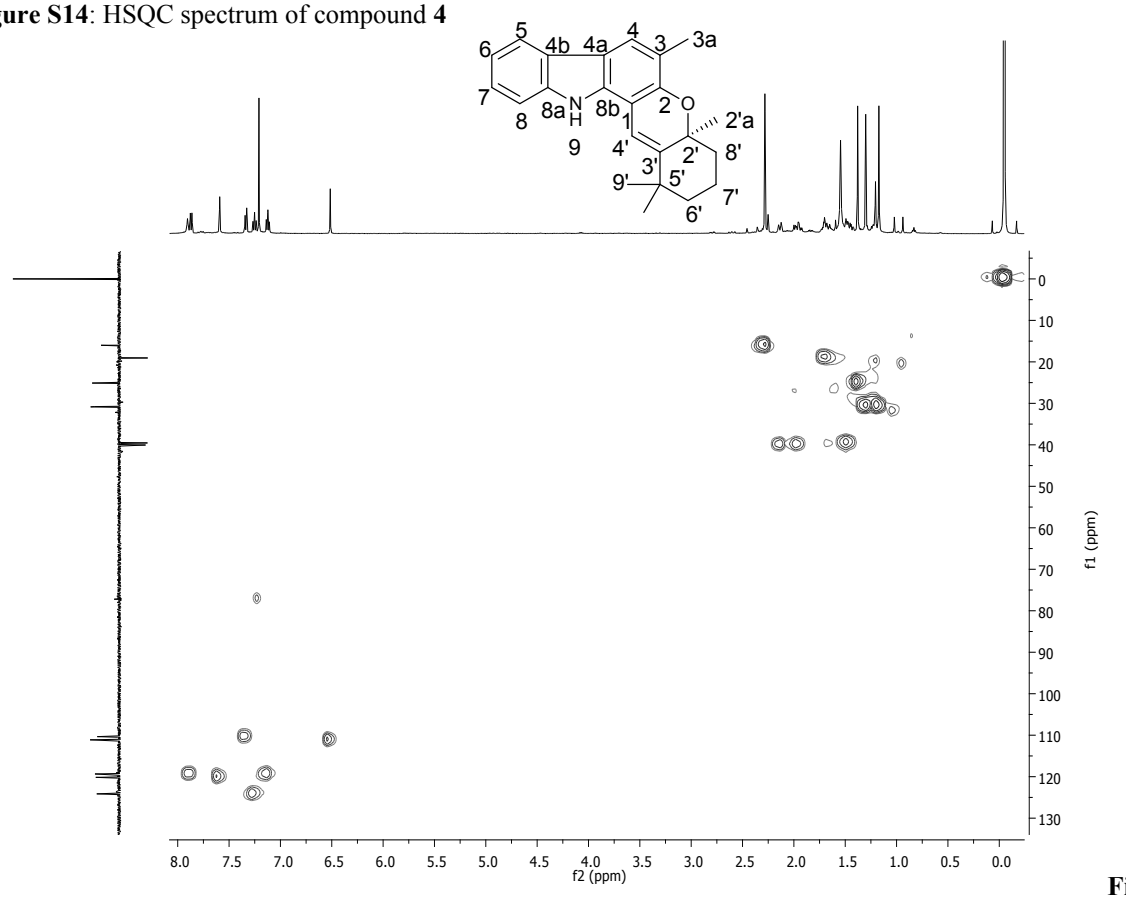


Figure S14: HSQC spectrum of compound **4**



Figu

re S15: HMBC spectrum of compound **4**

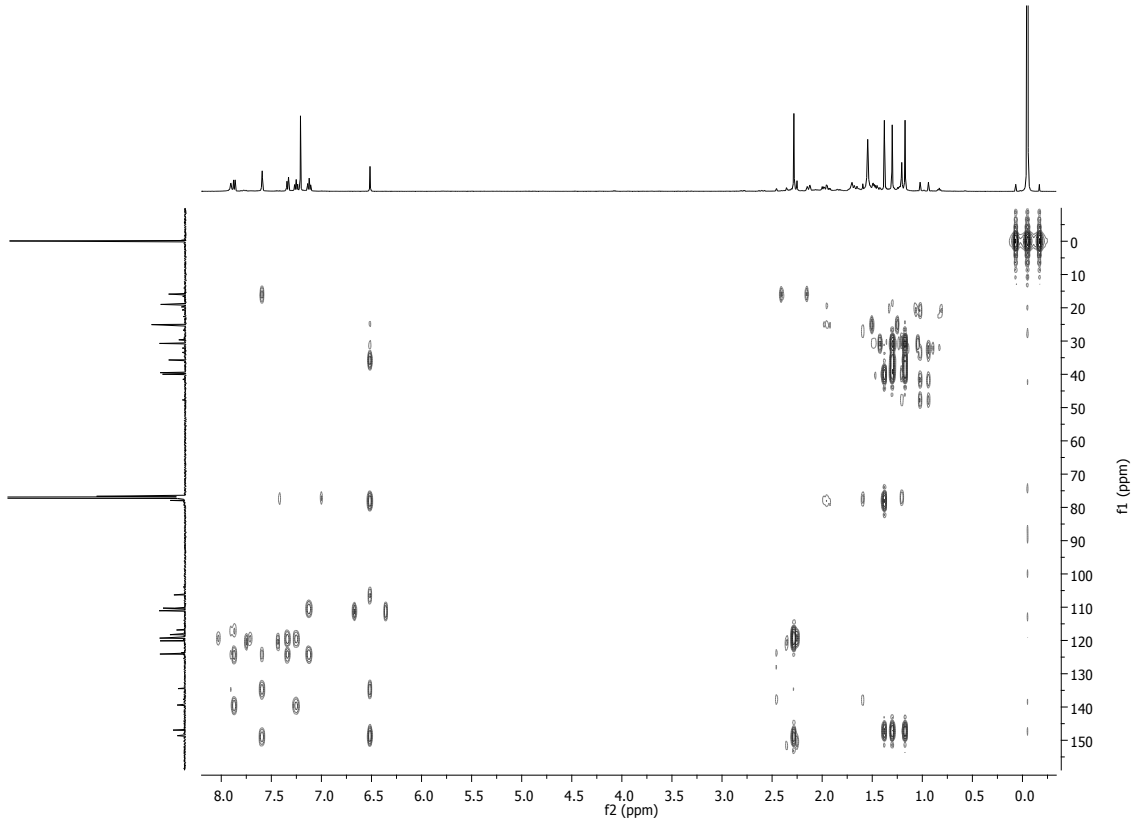
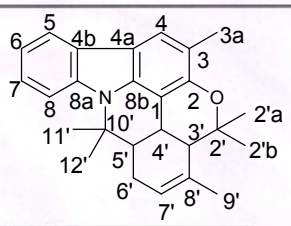


Figure S16: HRESIMS of compound **6**

Qualitative Compound Report

Data File	POCL3-35-2.d	Sample Name	POCL3-35-2
Sample Type	Sample	Position	Vial 38
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_12-01-13.m	Acquired Time	19-09-2015 PM 1:36:53
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)		

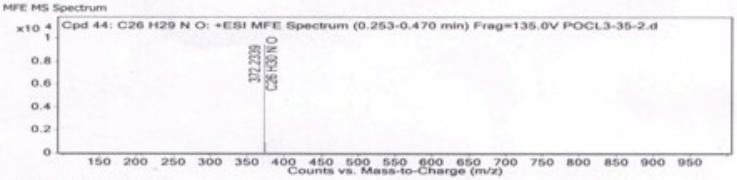


Compound Table

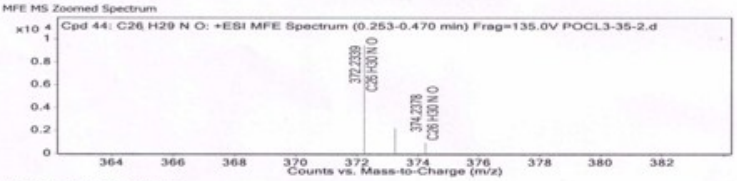
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 44: C26 H29 N O	0.343	371.2263	C26 H29 N O	C26 H29 N O	-3.72	C26 H29 N O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 44: C26 H29 N O	372.2339	0.343	Find by Molecular Feature	371.2263

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
372.2339	1	9482.85	C26 H30 N O	(M+H)+
373.2366	1	2242.05	C26 H30 N O	(M+H)+
374.2378	1	972.83	C26 H30 N O	(M+H)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	372.2339	372.2322	-4.56	100	100	74.68	75.14
2	373.2366	373.2355	-2.82	23.64	28.87	17.66	21.69
3	374.2378	374.2387	2.46	10.26	4.22	7.66	3.17

Figure S17: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6**

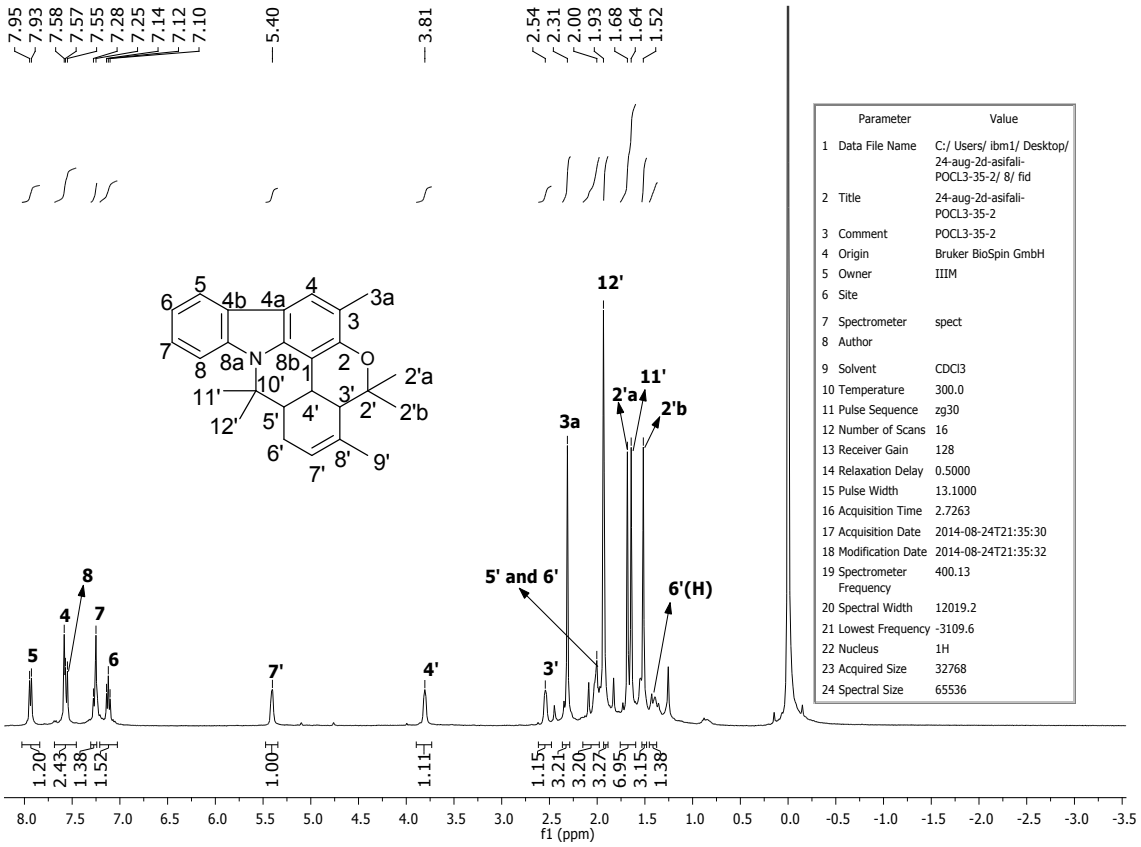
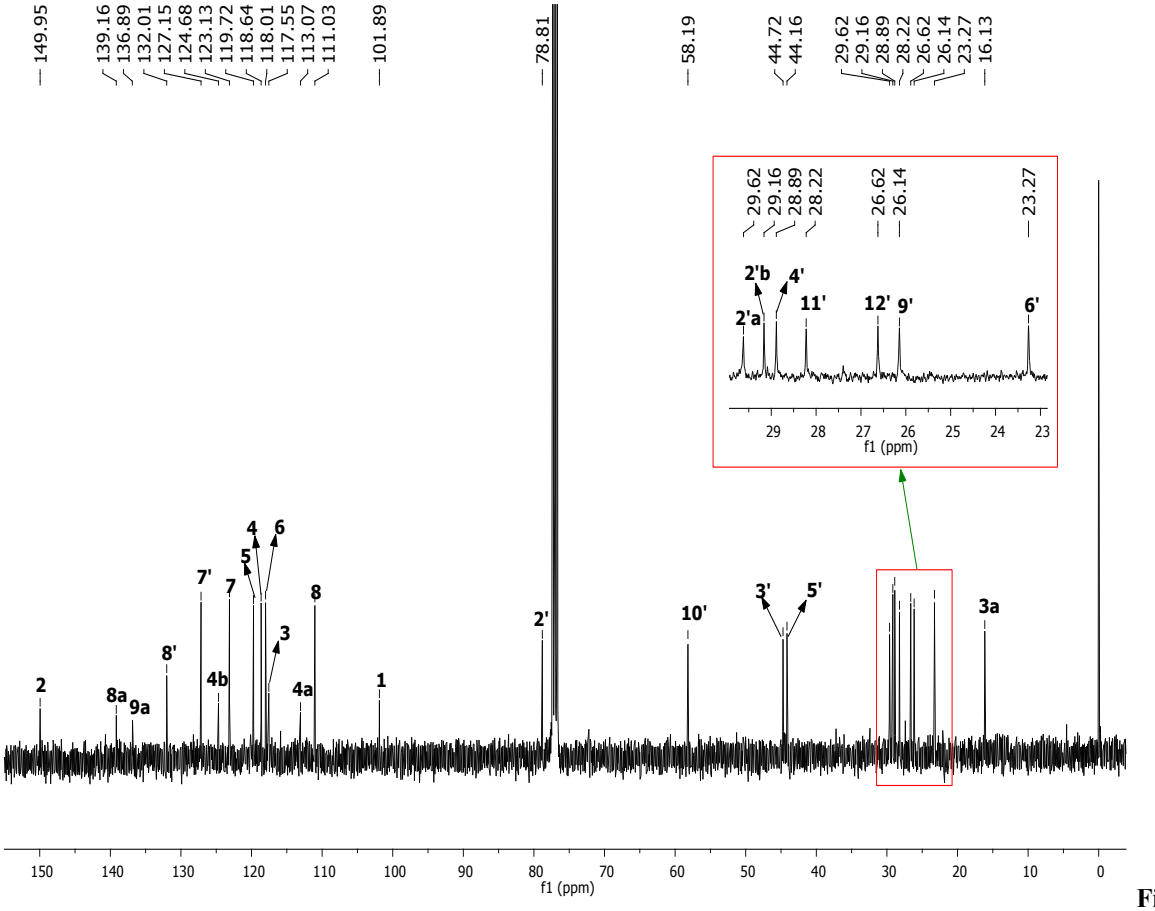


Figure S18: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6**



Figu

re S19: DEPT-135 (100 MHz, $CDCl_3$) spectrum of compound **6**

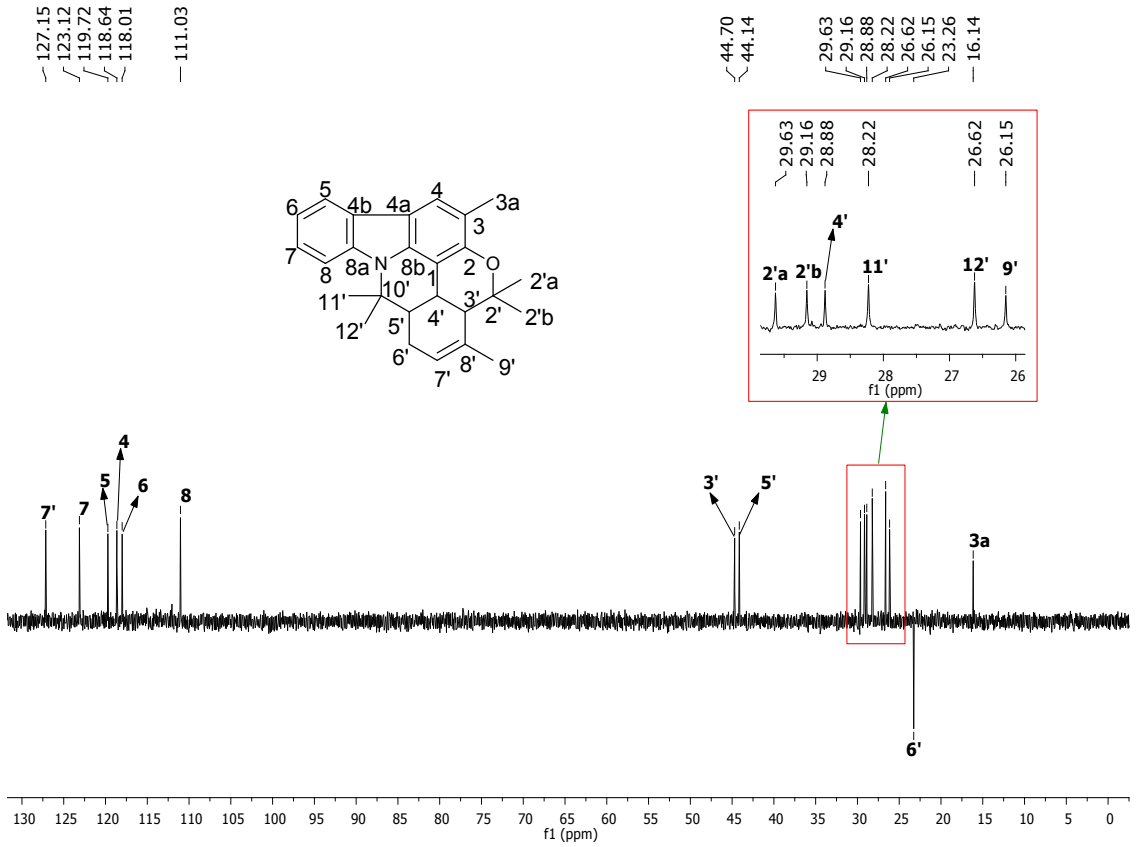
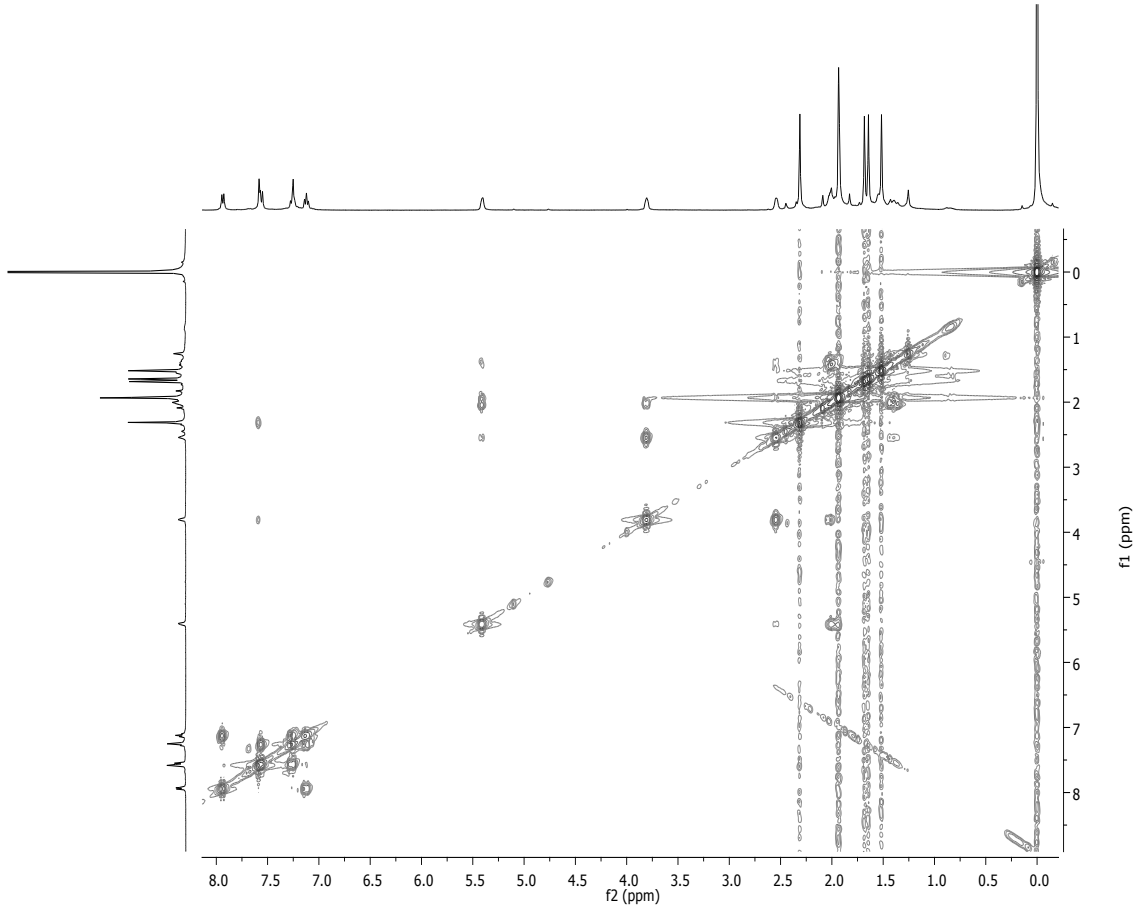


Figure S20: COSY spectrum of compound **6**



Figu

re S21: HSQC spectrum of compound **6**

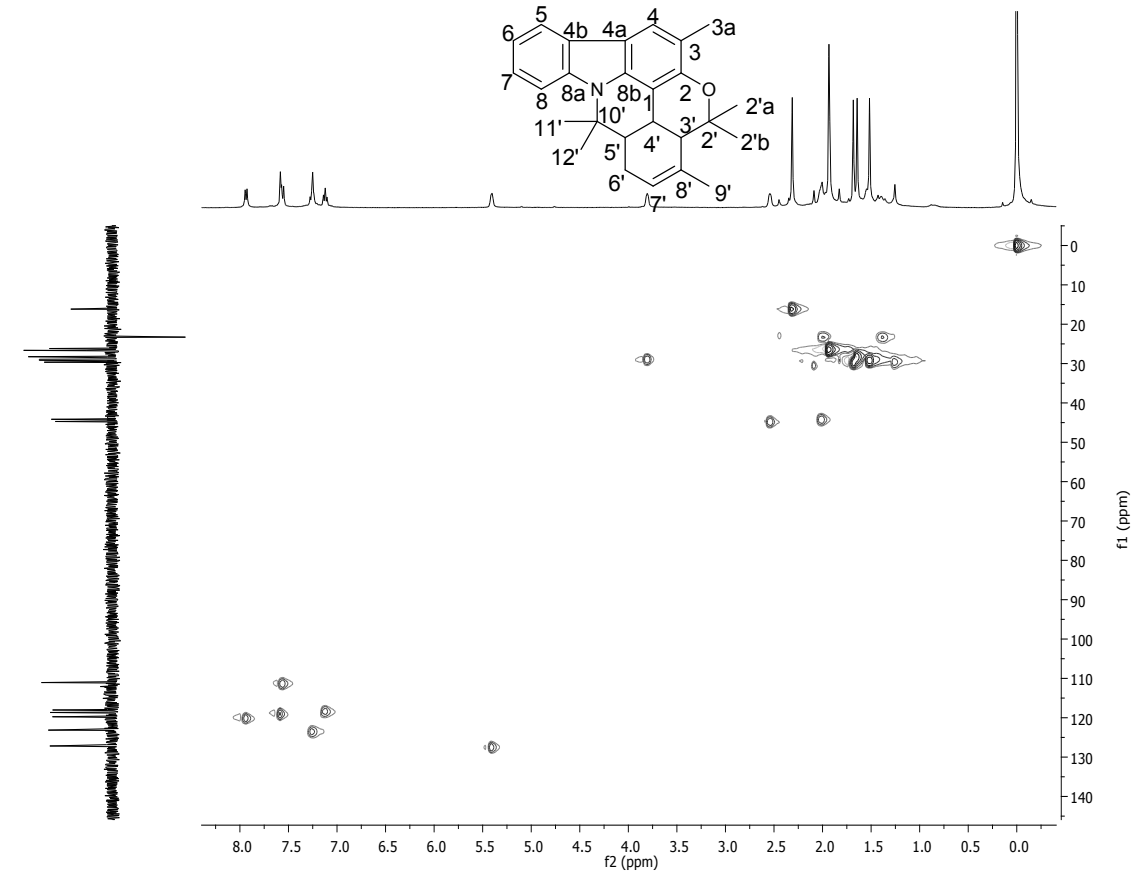


Figure S22: HMBC spectrum of compound **6**

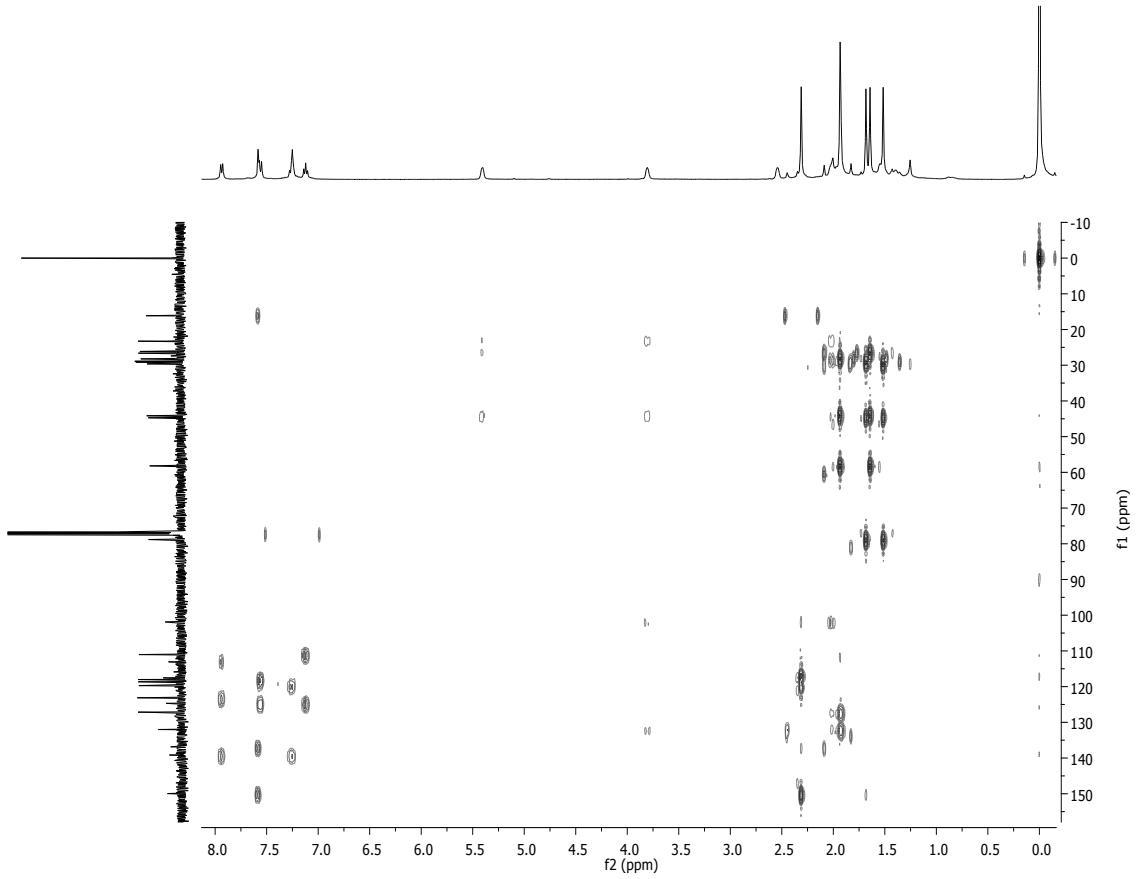


Figure S23: NOESY spectrum of compound **6**

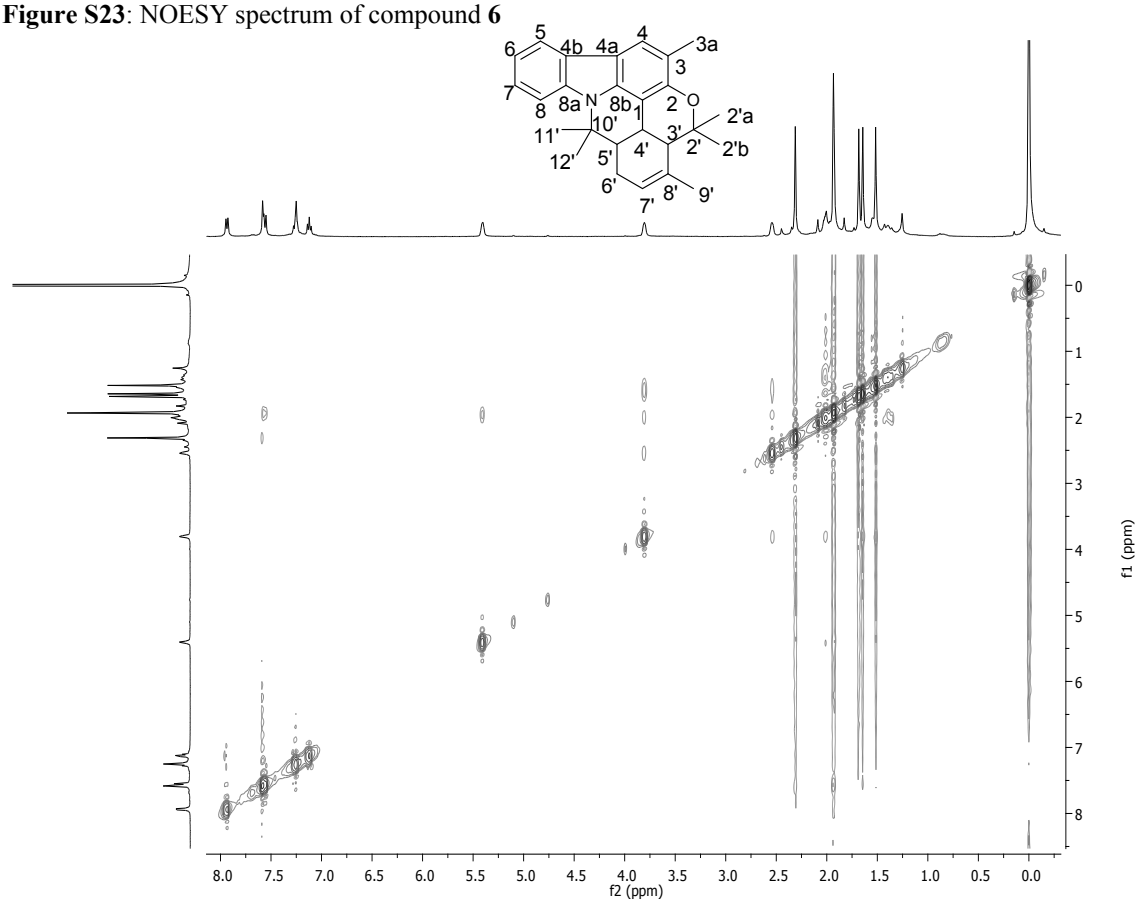


Figure S24: HRESIMS of compound **7**

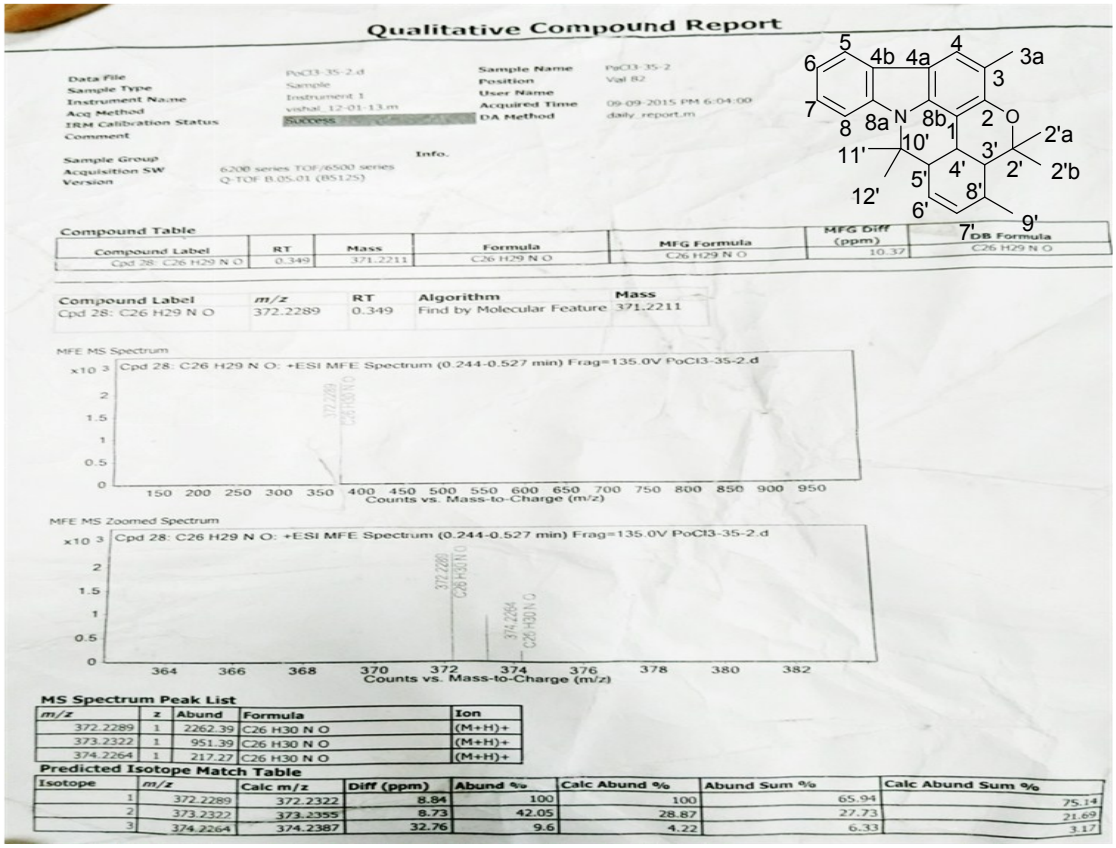


Figure S25: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7**

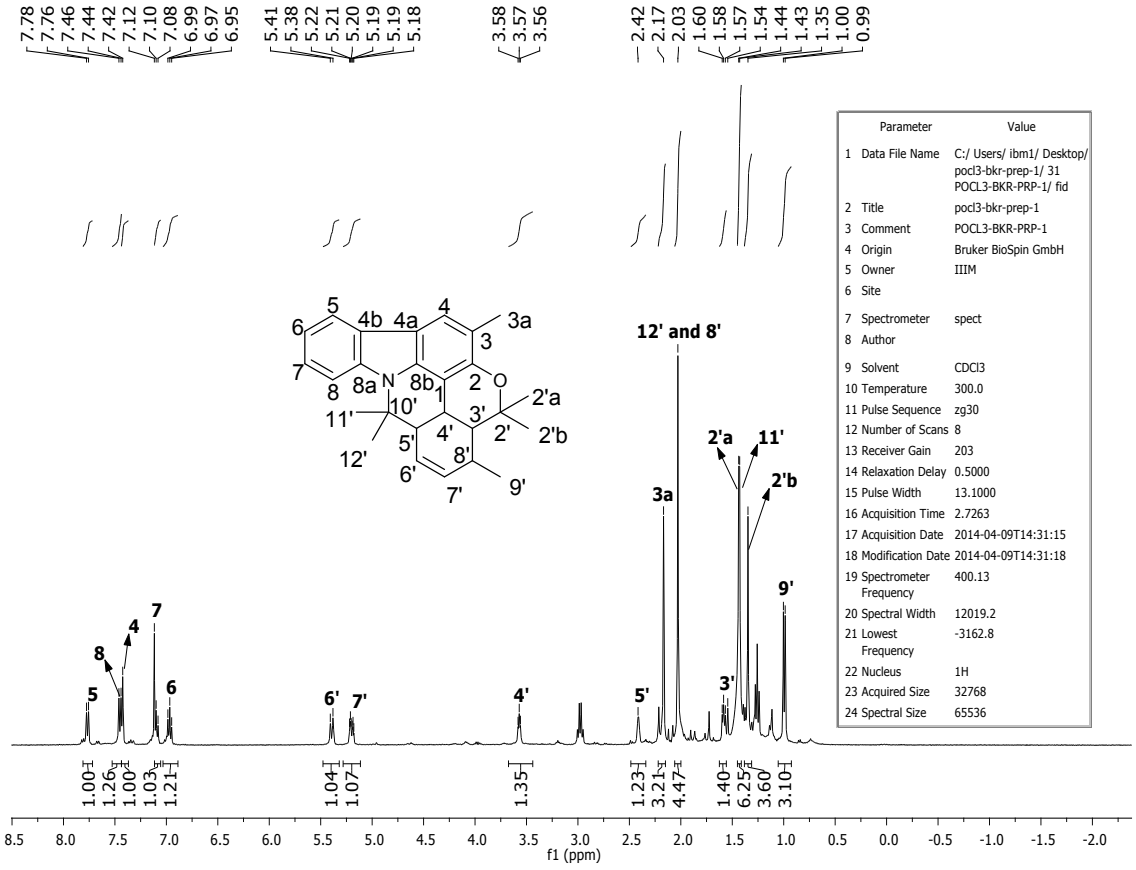


Figure S26: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7**

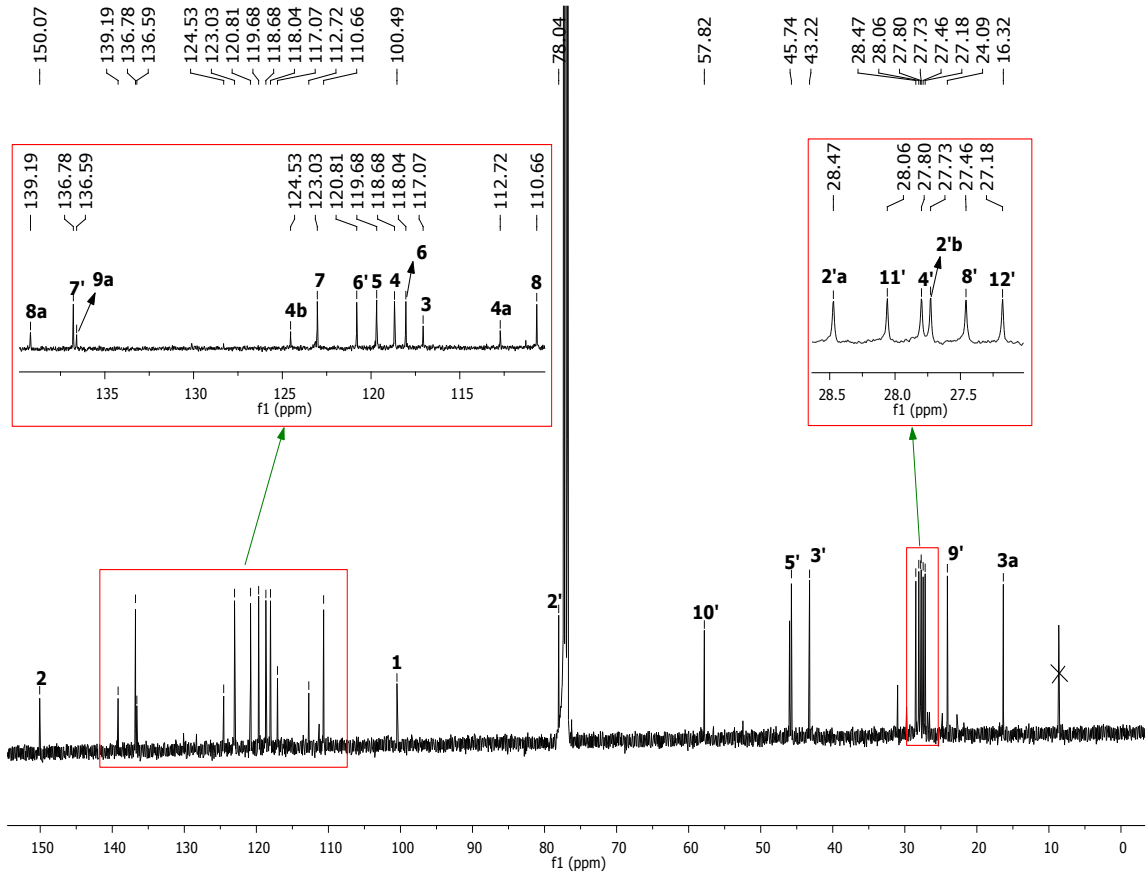


Figure S27: DEPT-135 (100 MHz, $CDCl_3$) spectrum of compound **7**

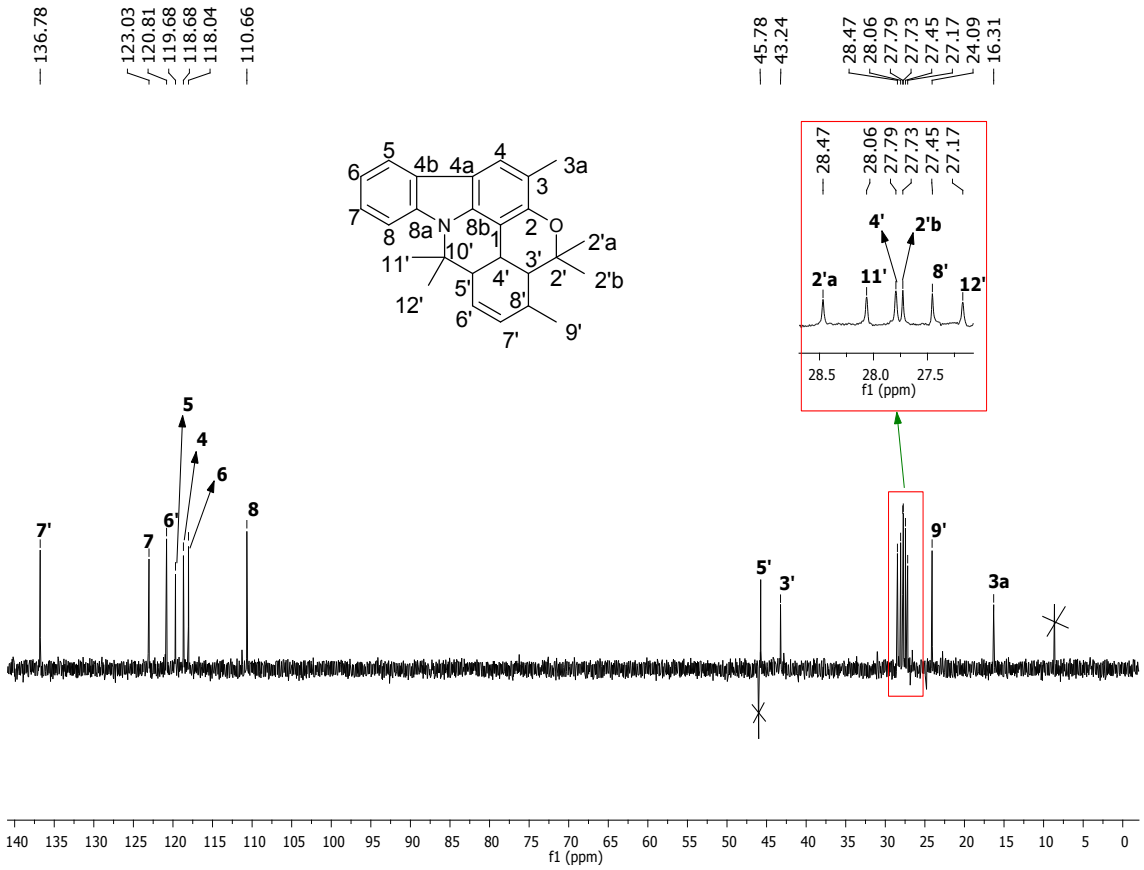


Figure S28: COSY spectrum of compound **7**

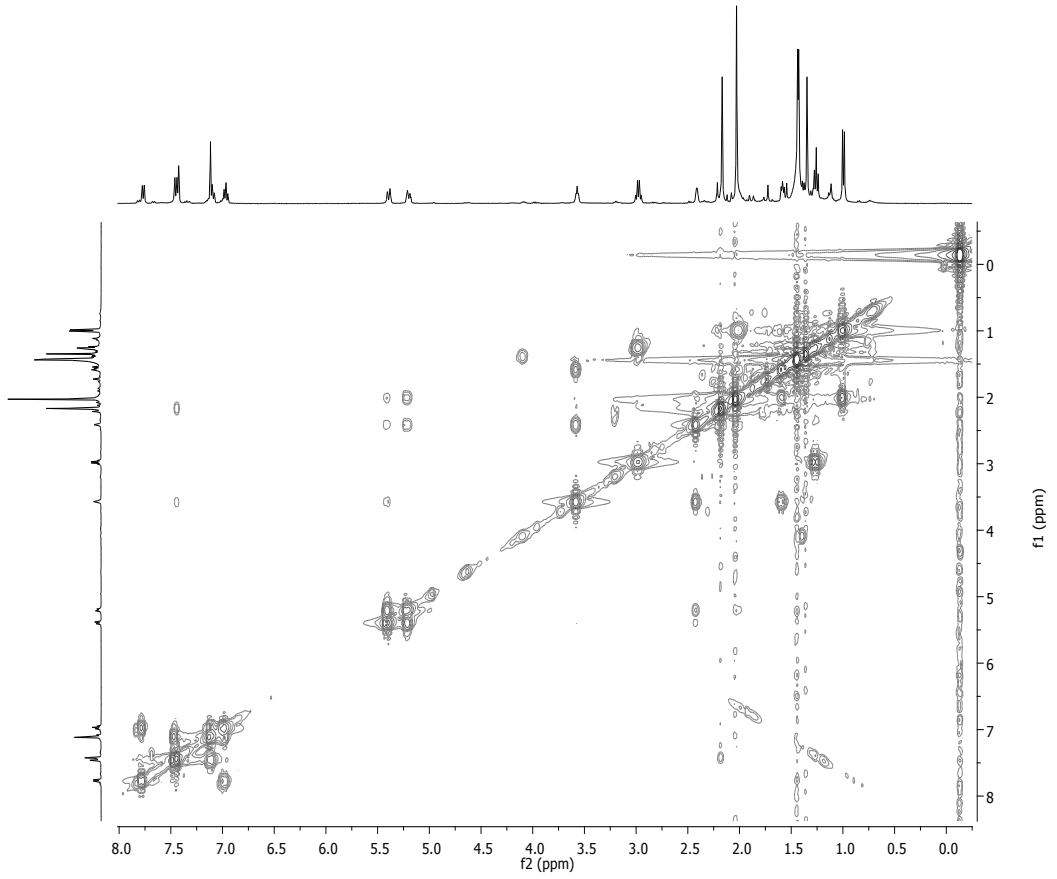


Figure S29: HSQC spectrum of compound **7**

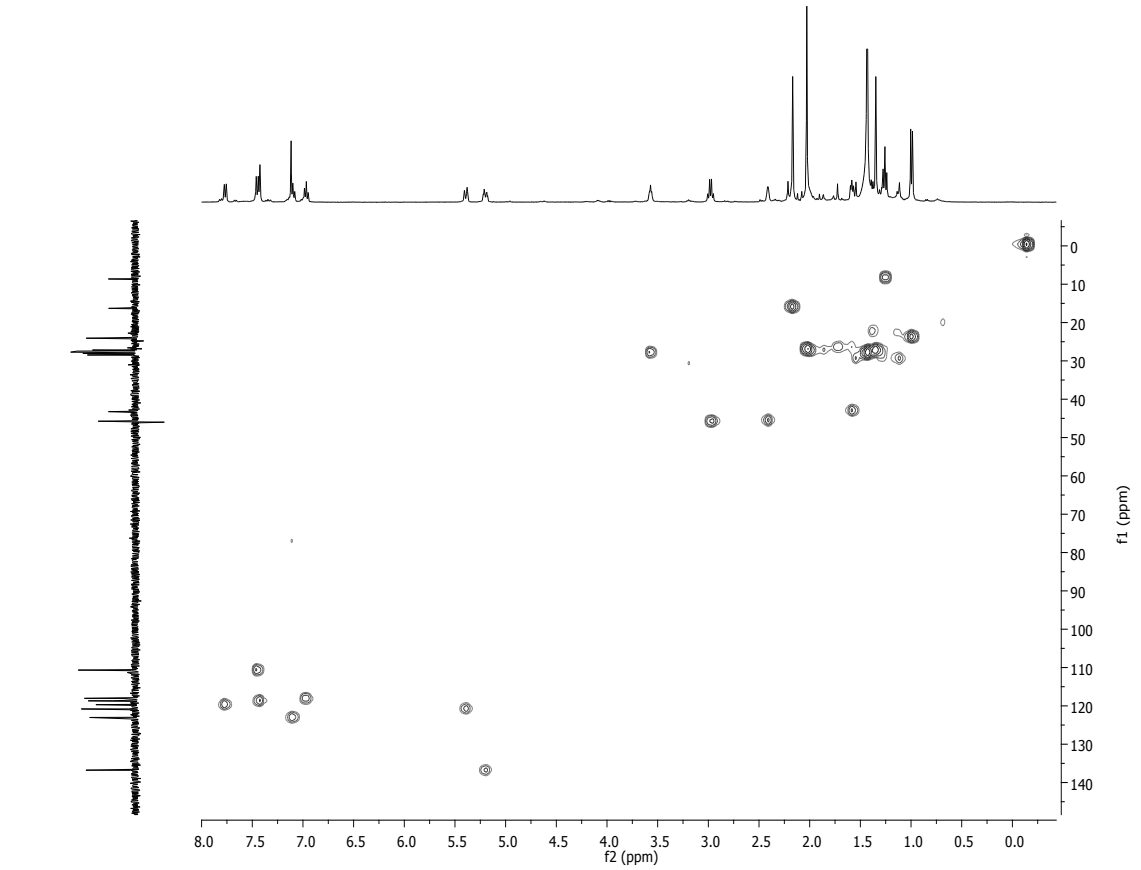


Figure S30: HMBC spectrum of compound **7**

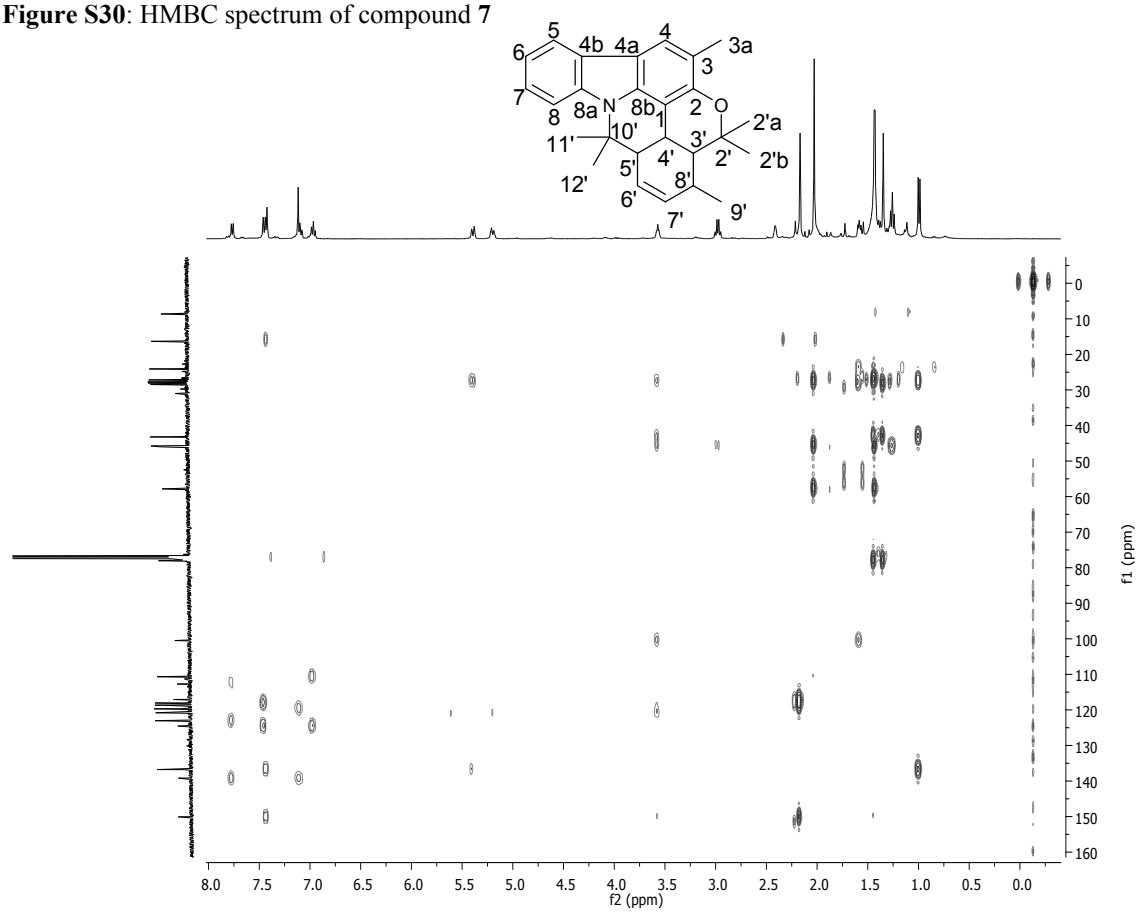


Figure S31: NOESY spectrum of compound **7**

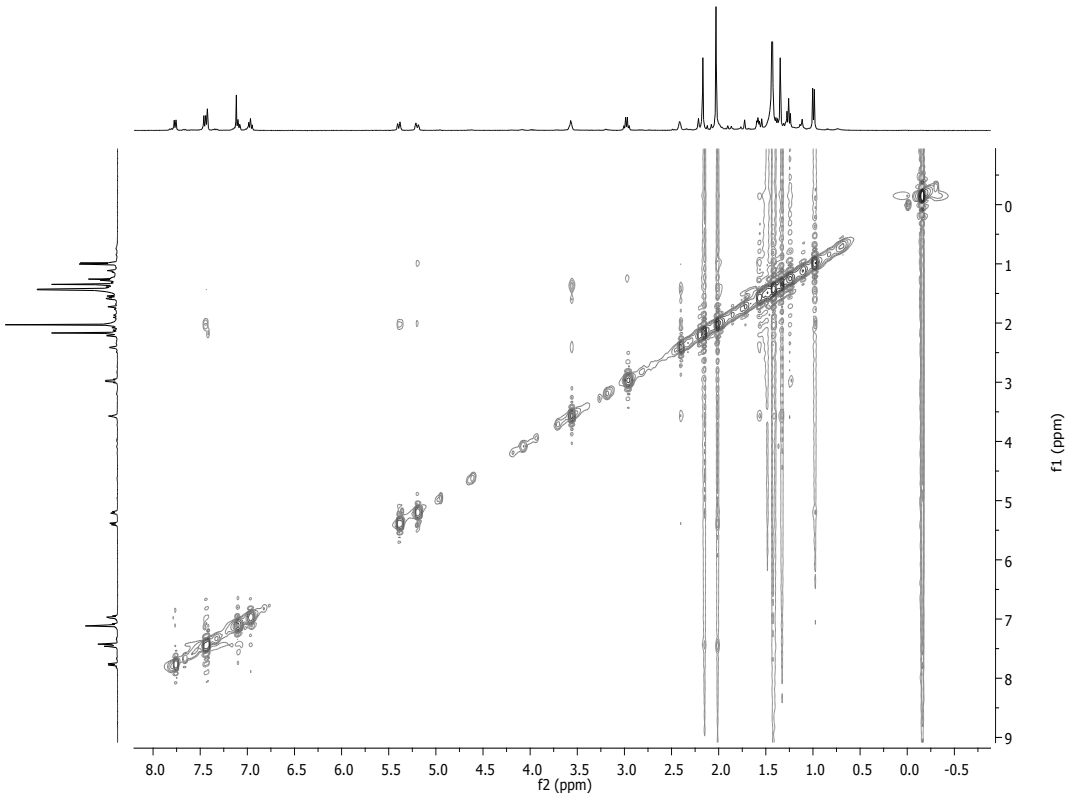
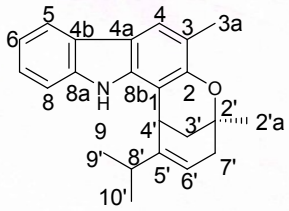


Figure S32: HRESIMS spectroscopic data of compound **8**

Qualitative Compound Report

Data File	MK-01-POCI3-1.d	**Sample Name**	MK-01-POCI3-1
Sample Type	Sample	**Position**	Vial 67
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	17-10-2013 PM 12:02:00
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)		

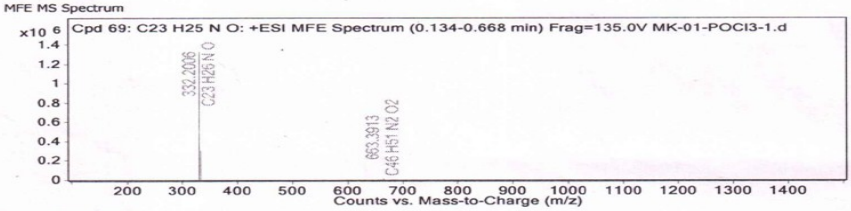


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 69: C23 H25 N O	0.196	331.1934	C23 H25 N O	C23 H25 N O	0.52	C23 H25 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 69: C23 H25 N O	332.2006	0.196	Find by Molecular Feature	331.1934

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
332.2006	1	1333111.5	C23 H26 N O	(M+H)+
333.2041	1	309328.63	C23 H26 N O	(M+H)+
334.2087	1	43345.84	C23 H26 N O	(M+H)+
663.3913	1	13639.02	C46 H51 N2 O2	(2M+H)+
664.3956	1	6630.53	C46 H51 N2 O2	(2M+H)+
665.4012	1	1893.93	C46 H51 N2 O2	(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	332.2006	332.2009	0.74	100	100	79.08	77.57
2	333.2041	333.2042	0.18	23.2	25.58	18.35	19.84
3	334.2087	334.2073	-3.99	3.25	3.34	2.57	2.59

Figure S33: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **8**

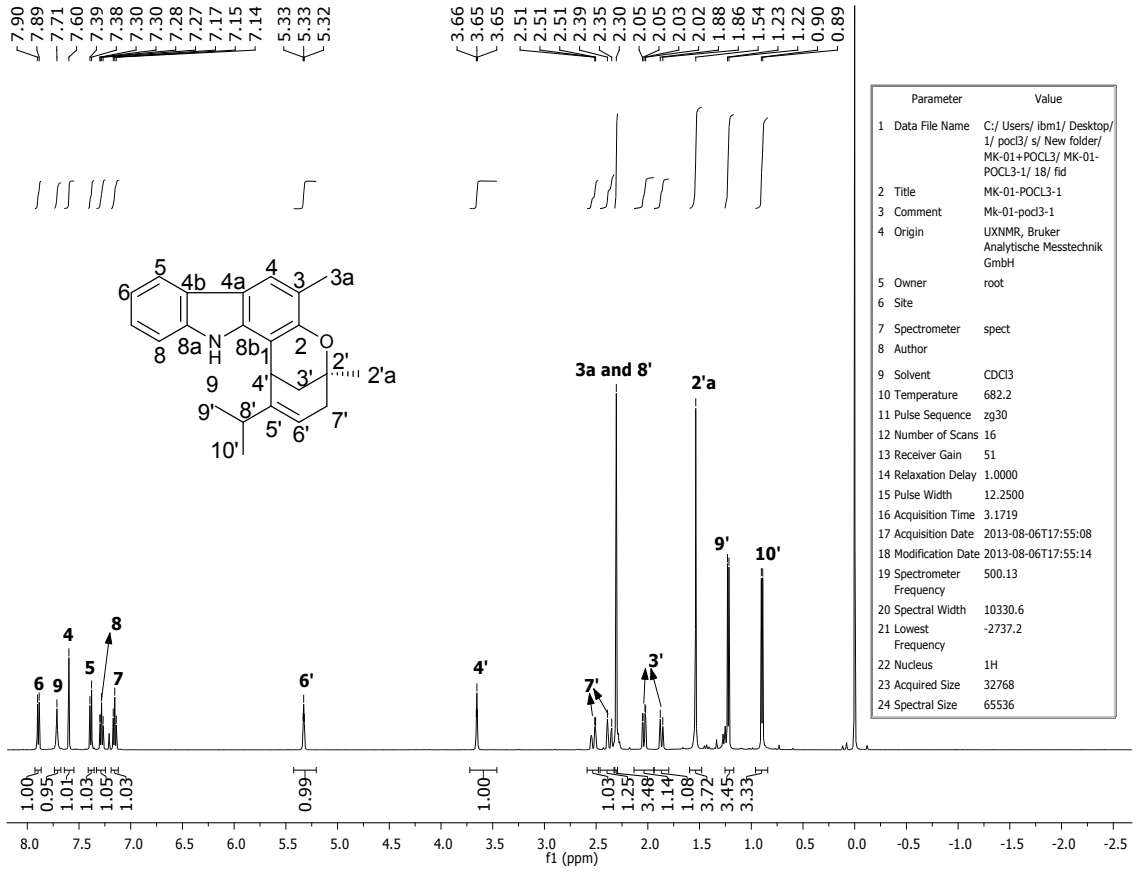


Figure S34: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **8**

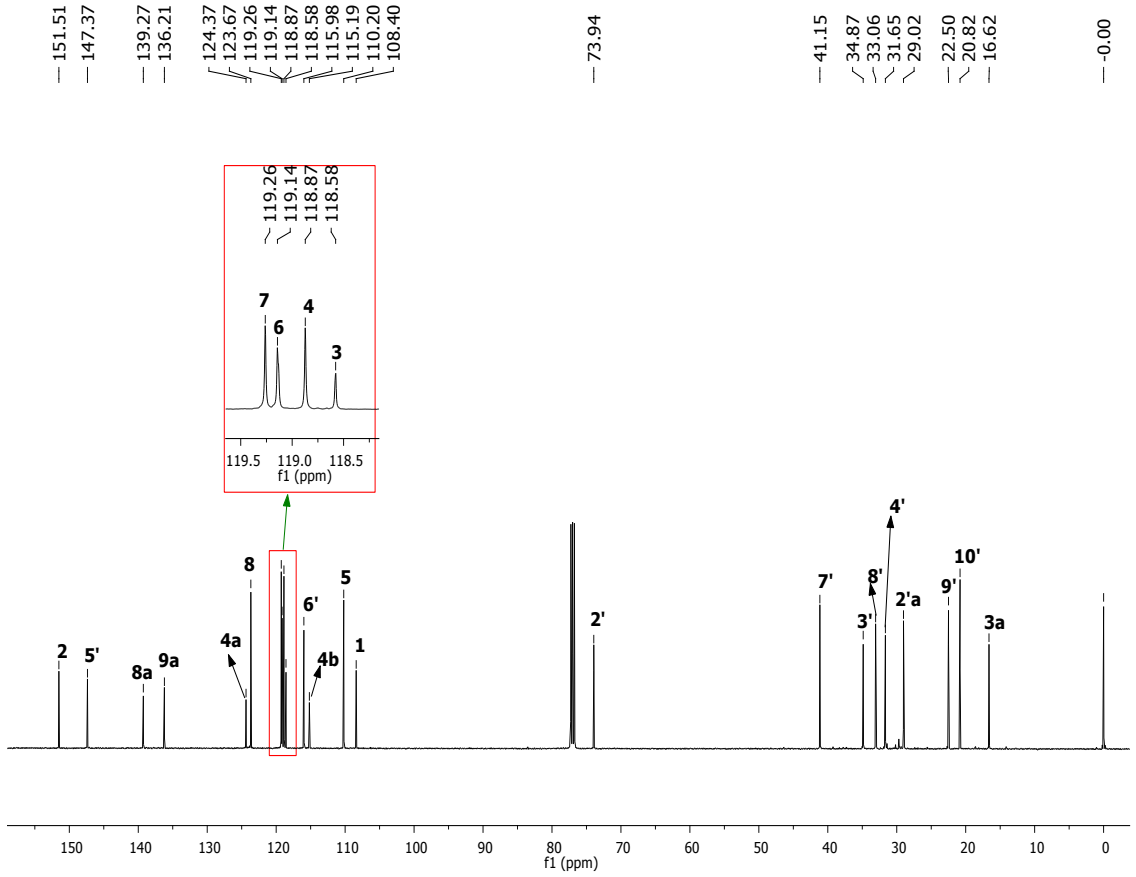


Figure S35: DEPT-135 (100 MHz, $CDCl_3$) spectrum of compound **8**

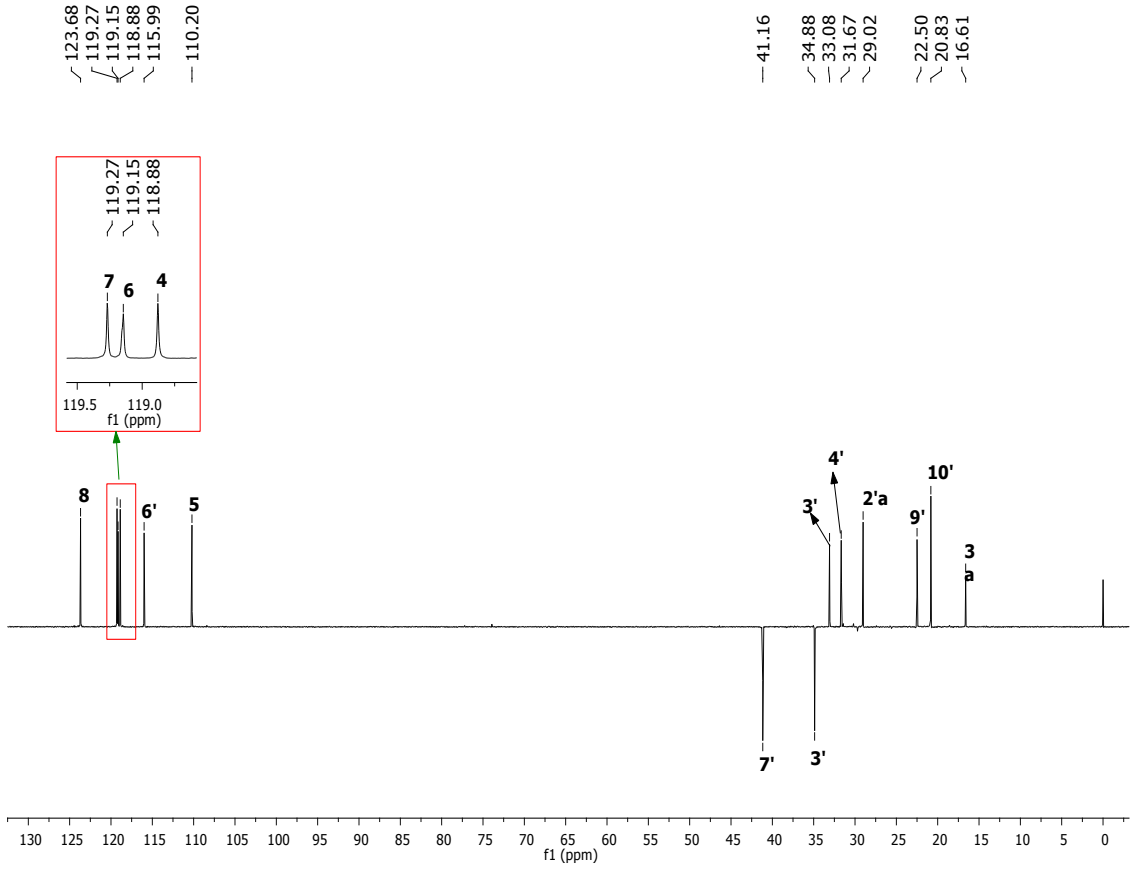


Figure S36: COSY spectrum of compound **8**

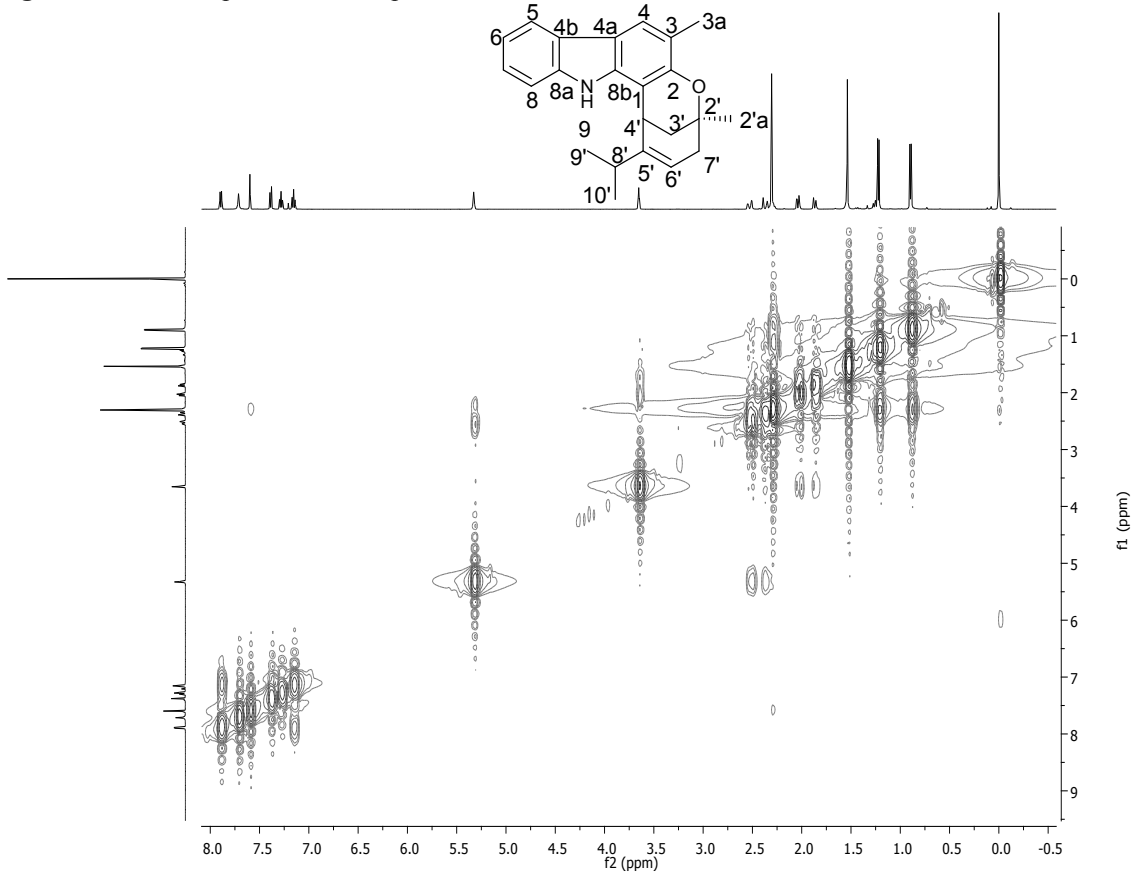


Figure S37: HSQC spectrum of compound **8**

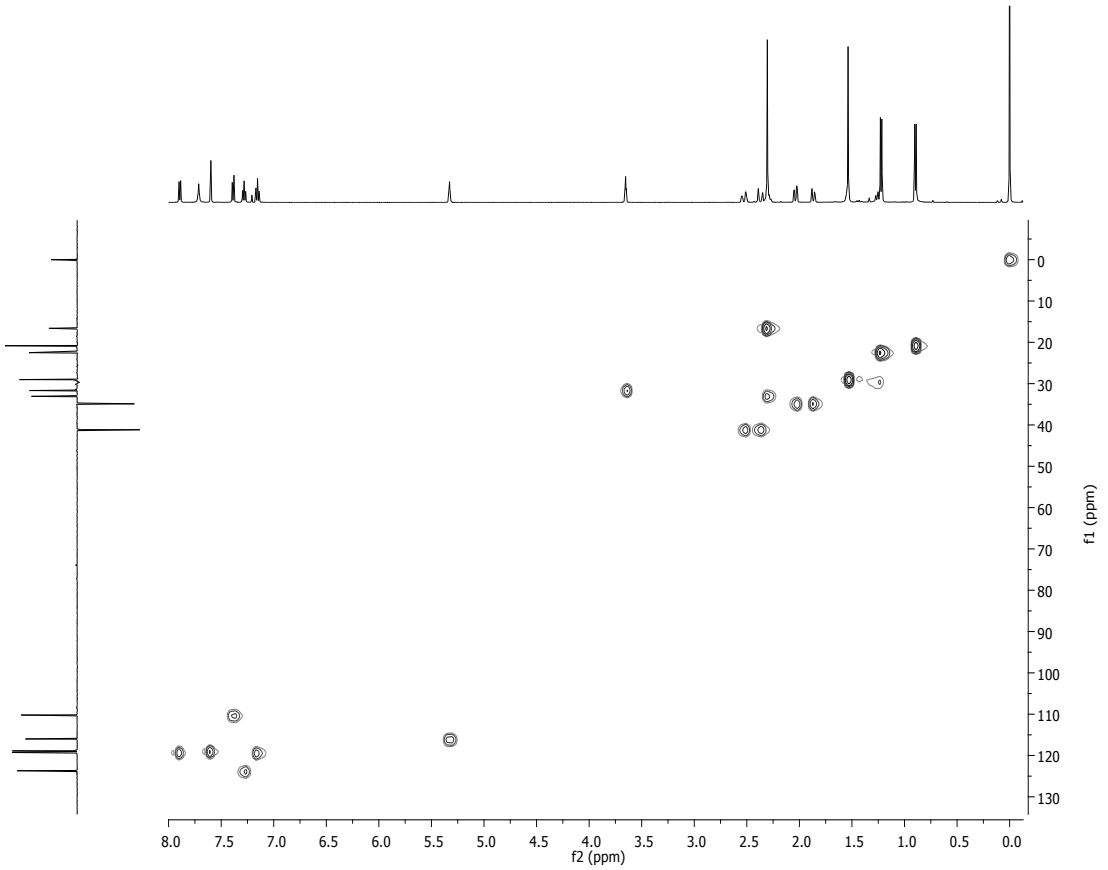


Figure S38: HMBC spectrum of compound **8**

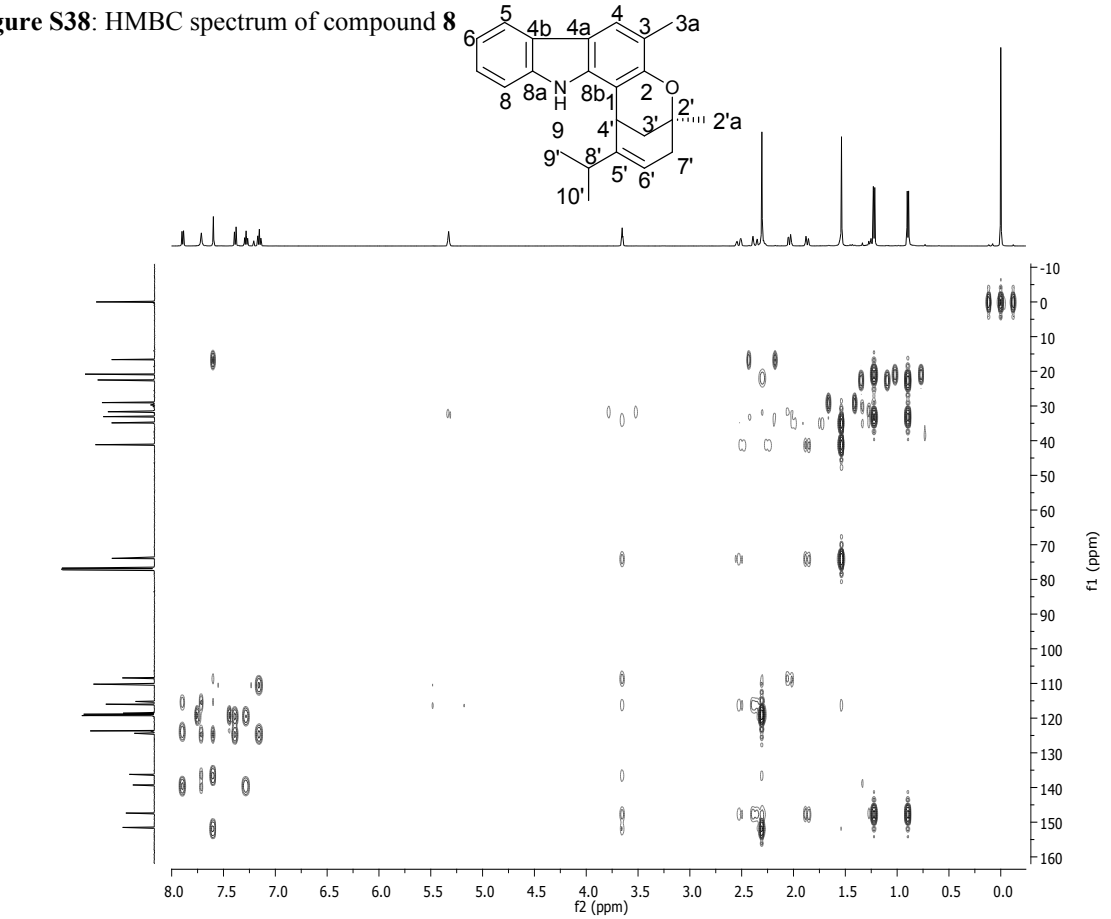
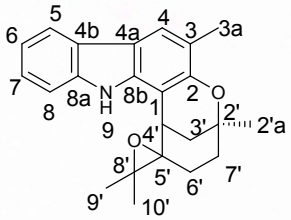


Figure S39: HRESIMS spectroscopic data of compound **11**

Qualitative Compound Report

Data File	MK-01-POCl3-9.d	**Sample Name**	MK-01-POCl3-9
Sample Type	Sample	**Position**	Vial 69
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	17-10-2013 PM 12:10:35
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)

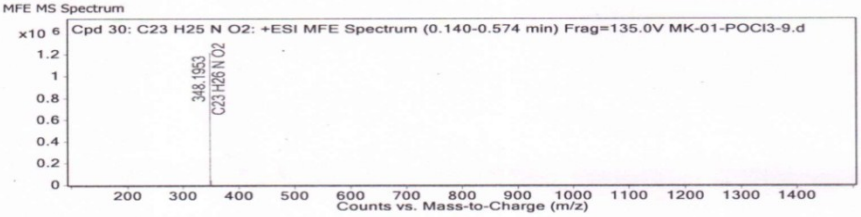


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C23 H25 N O2	0.192	347.1881	C23 H25 N O2	C23 H25 N O2	1.25	C23 H25 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C23 H25 N O2	348.1953	0.192	Find by Molecular Feature	347.1881

MFE MS Spectrum



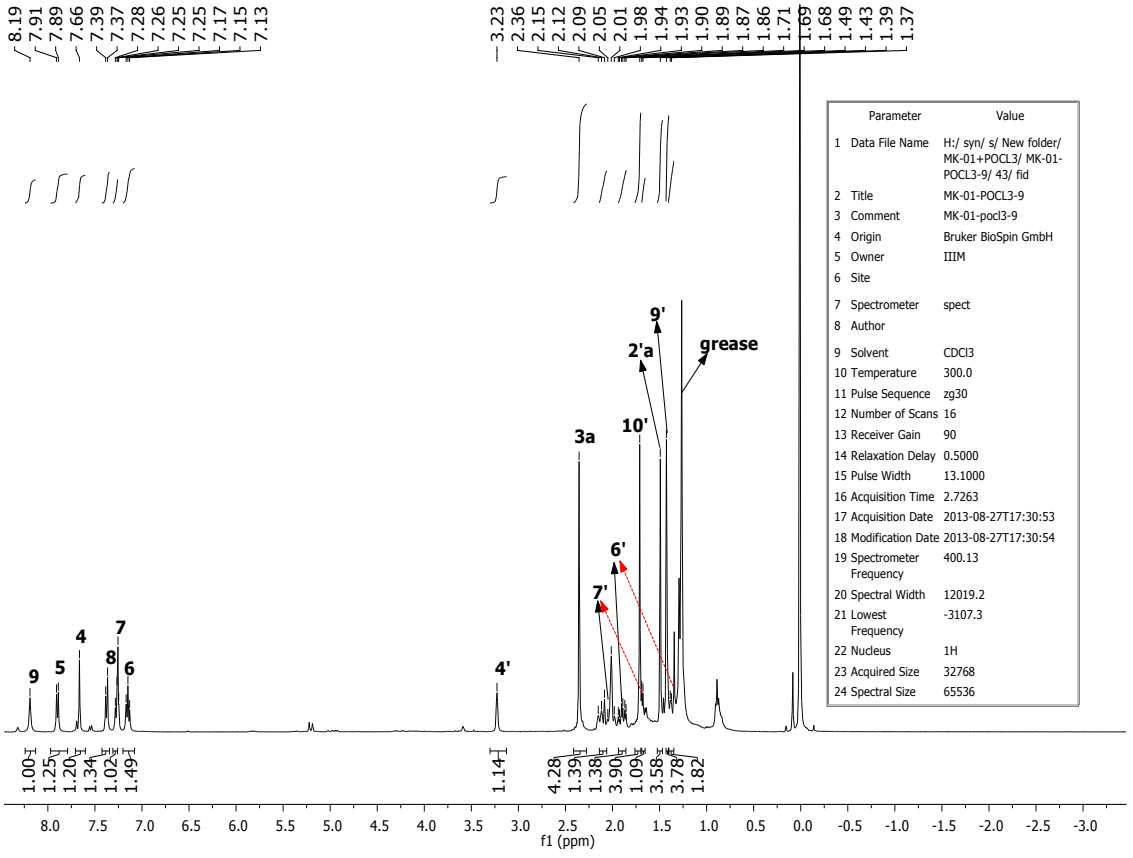
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
348.1953	1	1215104.13	C23 H26 N O2	(M+H)+
349.1989	1	287613.75	C23 H26 N O2	(M+H)+
350.2019	1	38484.71	C23 H26 N O2	(M+H)+
351.2046	1	4371.57	C23 H26 N O2	(M+H)+
352.2038	1	979.02	C23 H26 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	348.1953	348.1958	1.4	100	100	78.57	77.19
2	349.1989	349.1991	0.62	23.67	25.62	18.6	19.77
3	350.2019	350.2021	0.67	3.17	3.56	2.49	2.75
4	351.2046	351.205	1.13	0.36	0.35	0.28	0.27
5	352.2038	352.2078	11.37	0.08	0.03	0.06	0.02

Figure S40: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11**



Parameter	Value
1 Data File Name	H:/ syn/ s/ New folder/ MK-01+POCL3/ MK-01-POCL3-9/ 43/ fid
2 Title	MK-01-POCL3-9
3 Comment	MK-01-pocl3-9
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	90
14 Relaxation Delay	0.5000
15 Pulse Width	13.1000
16 Acquisition Time	2.7263
17 Acquisition Date	2013-08-27T17:30:53
18 Modification Date	2013-08-27T17:30:54
19 Spectrometer Frequency	400.13
20 Spectral Width	12019.2
21 Lowest Frequency	-3107.3
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

Figure S41: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **11**

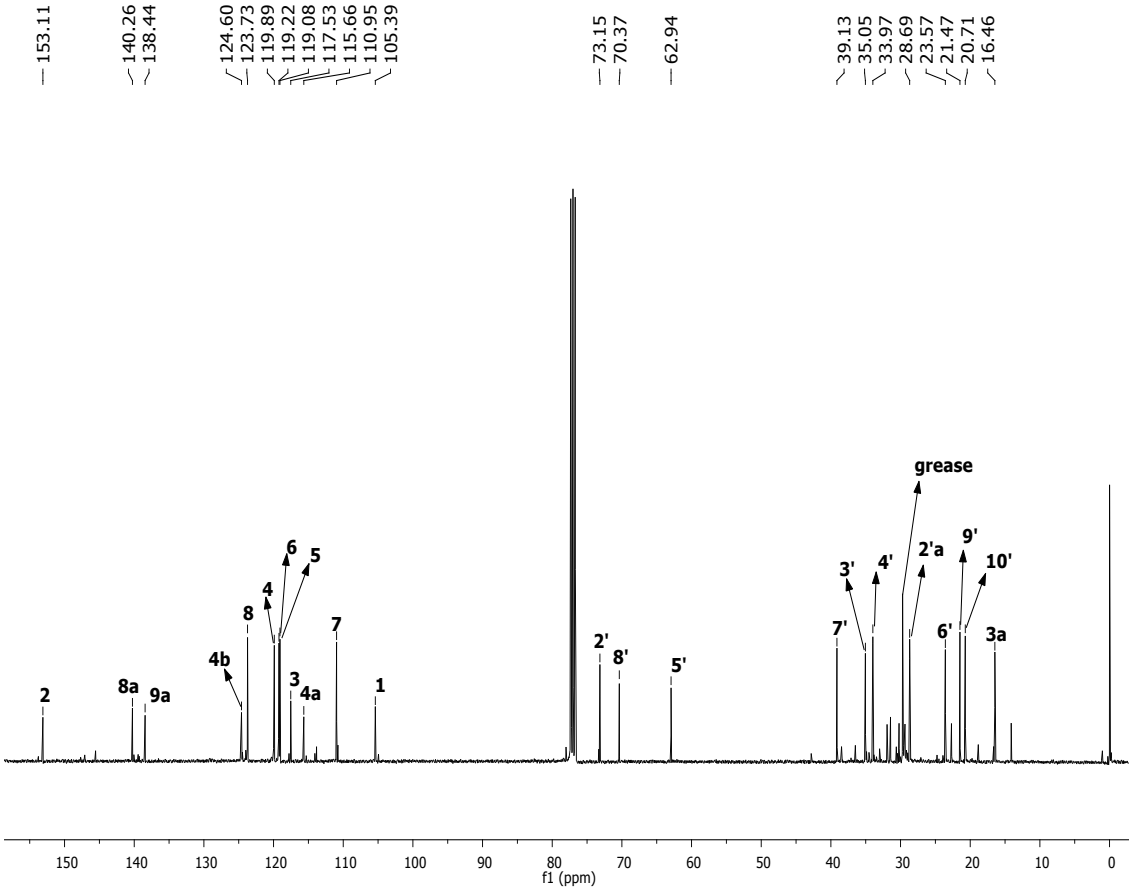


Figure S42: DEPT-135 (100 MHz, $CDCl_3$) spectrum of compound **11**

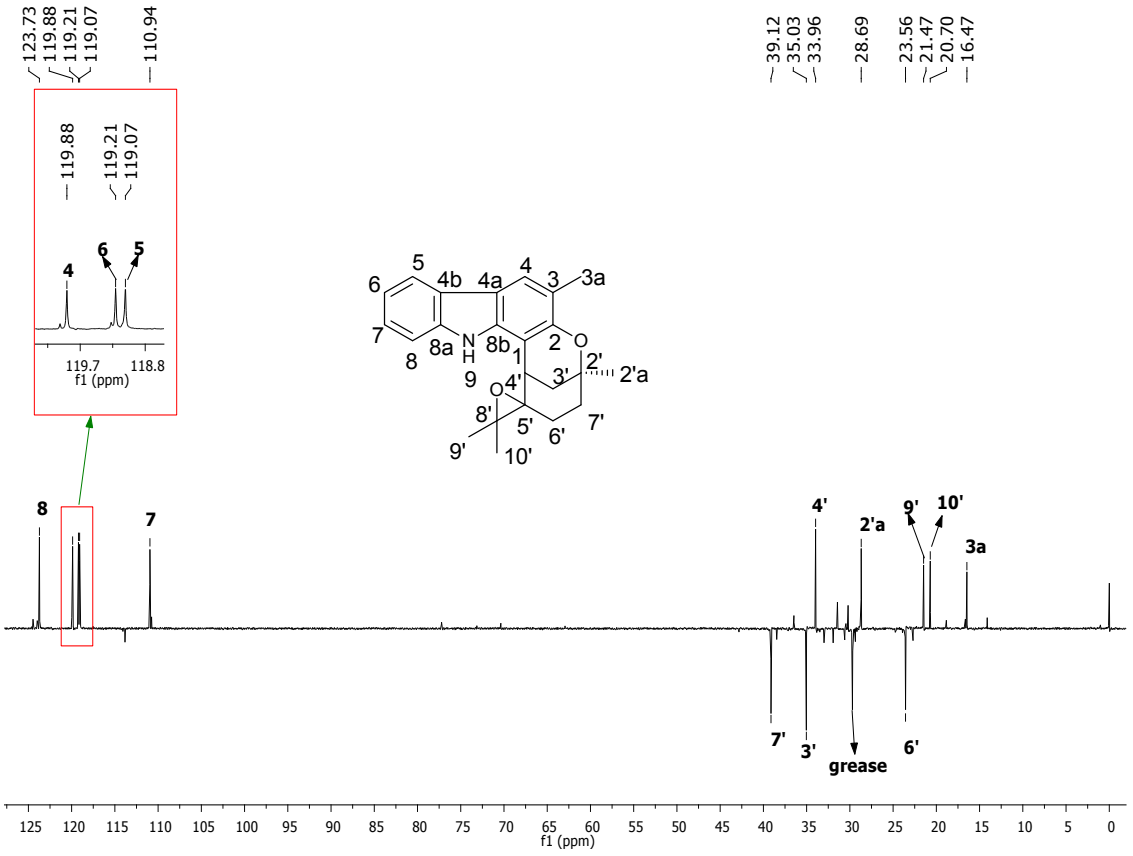


Figure S43: COSY spectrum of compound **11**

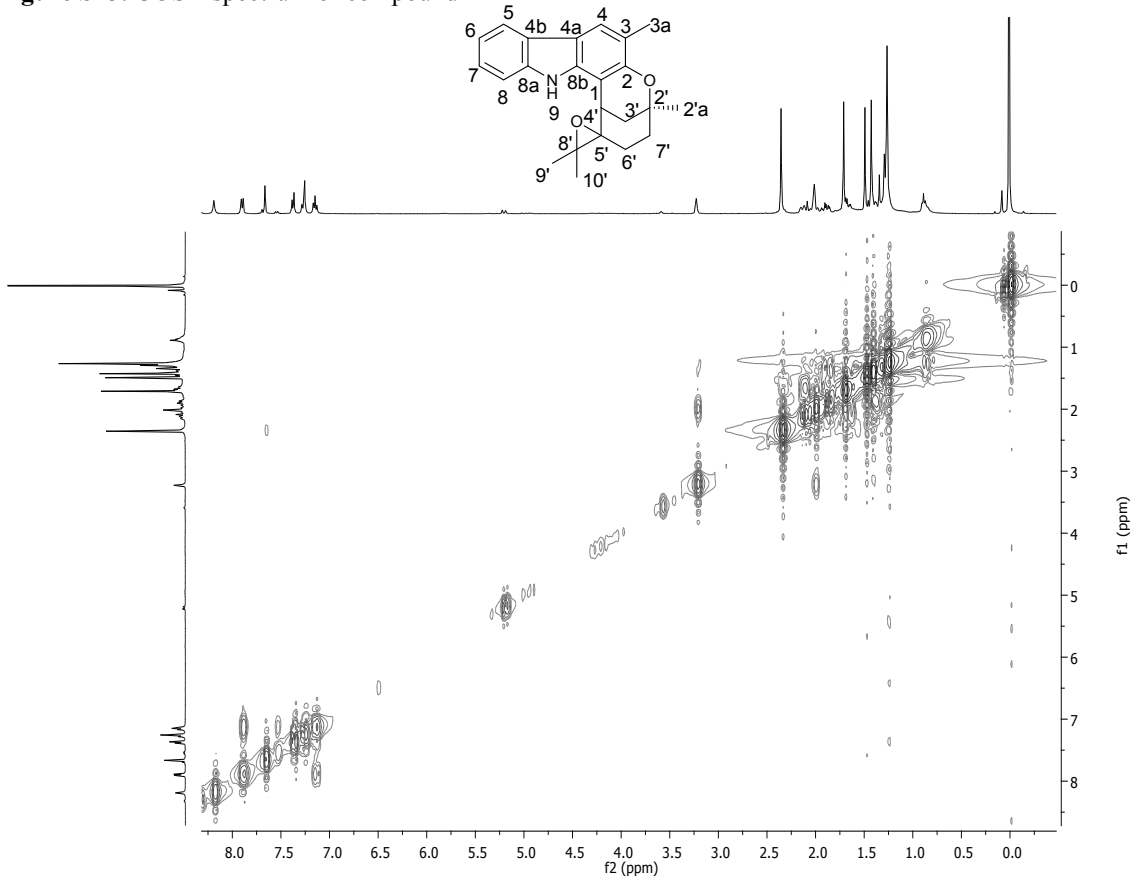


Figure S44: HSQC spectrum of compound **11**

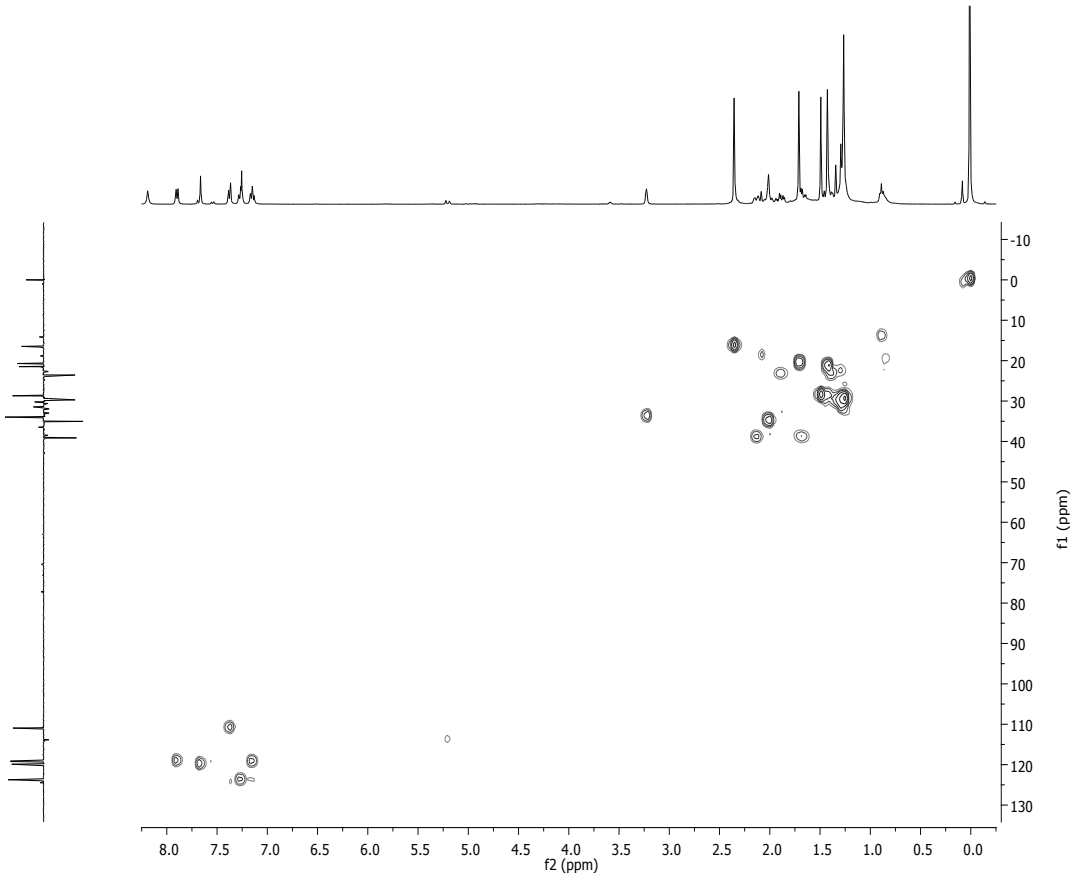


Figure S45: HMBC spectrum of compound **11**

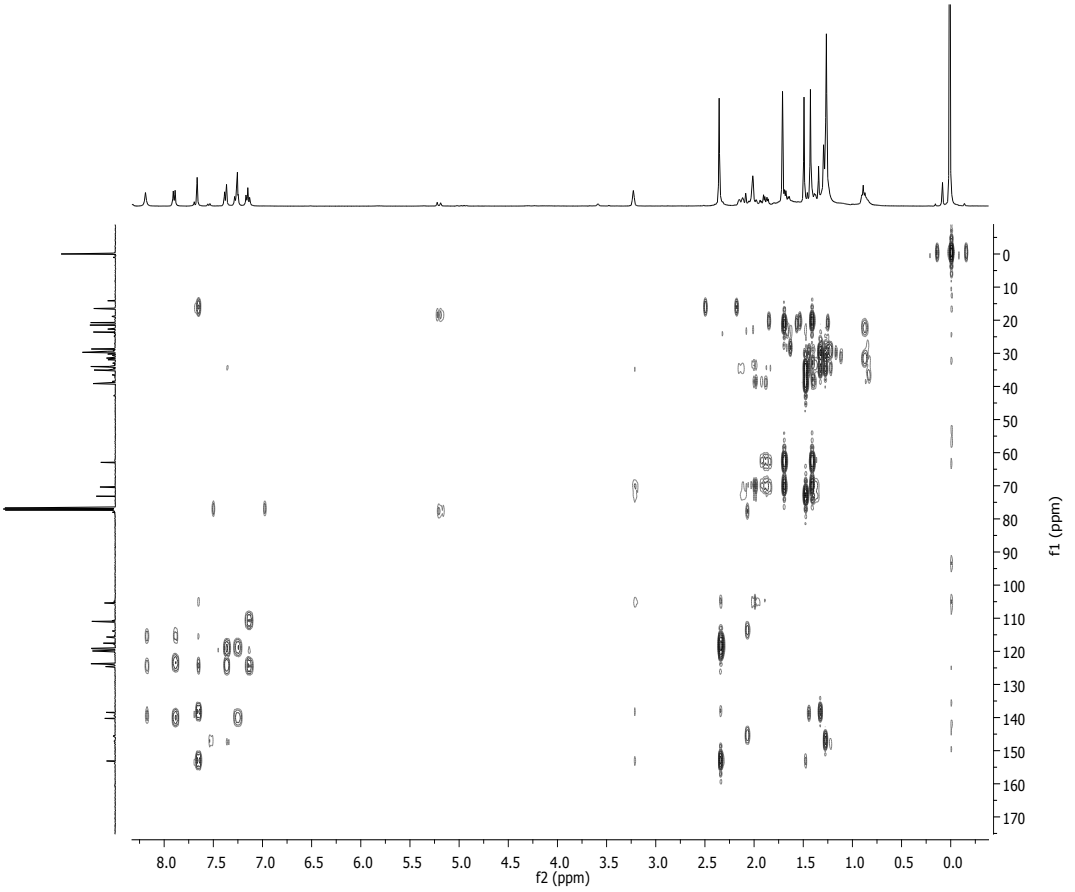


Figure S46: NOESY spectrum of compound **11**

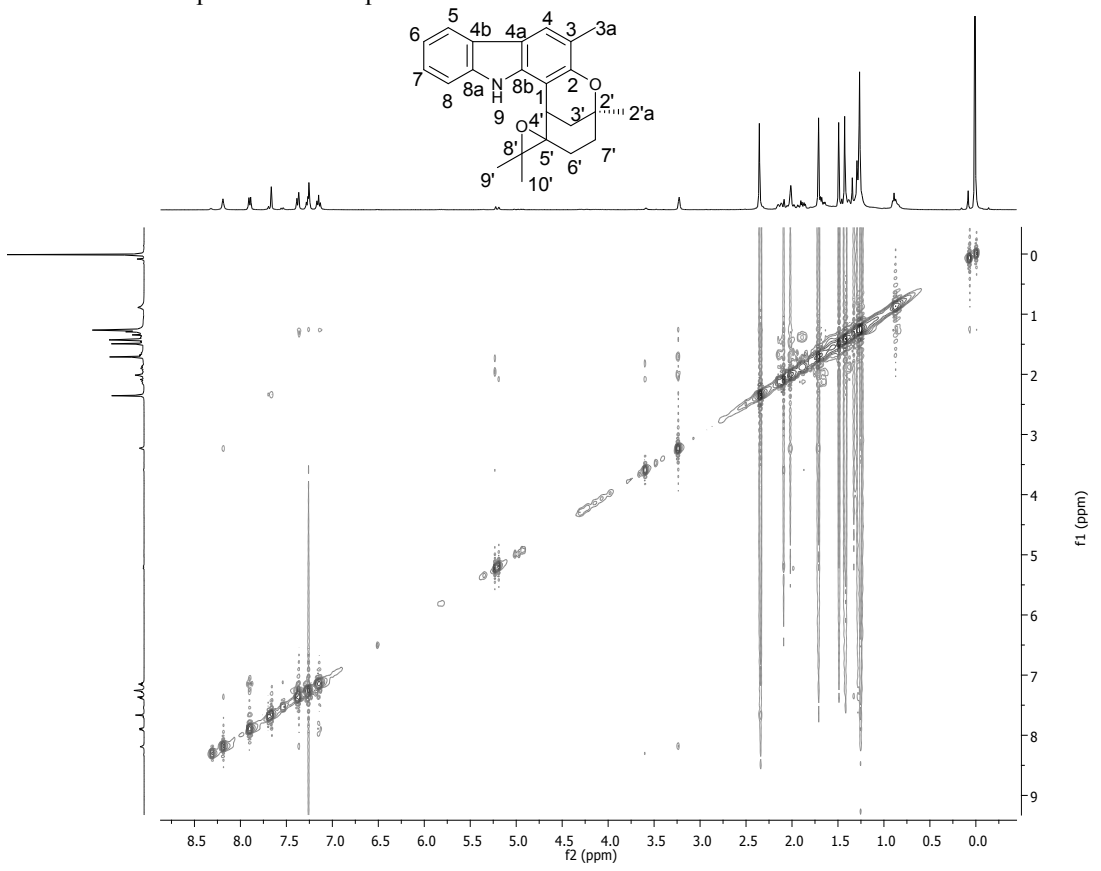
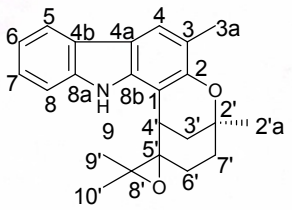


Figure S47: HRESIMS spectroscopic data of compound **12**

Qualitative Compound Report

Data File	MK-01-POCL3-12.d	**Sample Name**	MK-01-POCL3-12
Sample Type	Sample	**Position**	Vial 56
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	15-10-2013 PM 1:56:45
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)

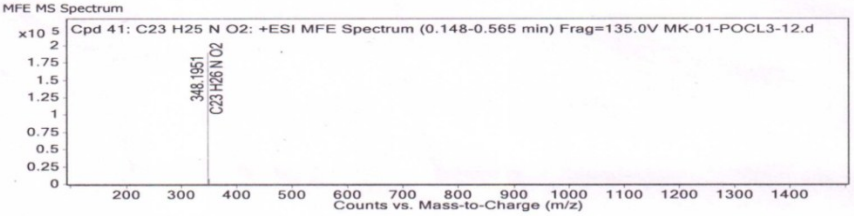


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 41: C23 H25 N O2	0.194	347.1877	C23 H25 N O2	C23 H25 N O2	2.5	C23 H25 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 41: C23 H25 N O2	348.1951	0.194	Find by Molecular Feature	347.1877

MFE MS Spectrum



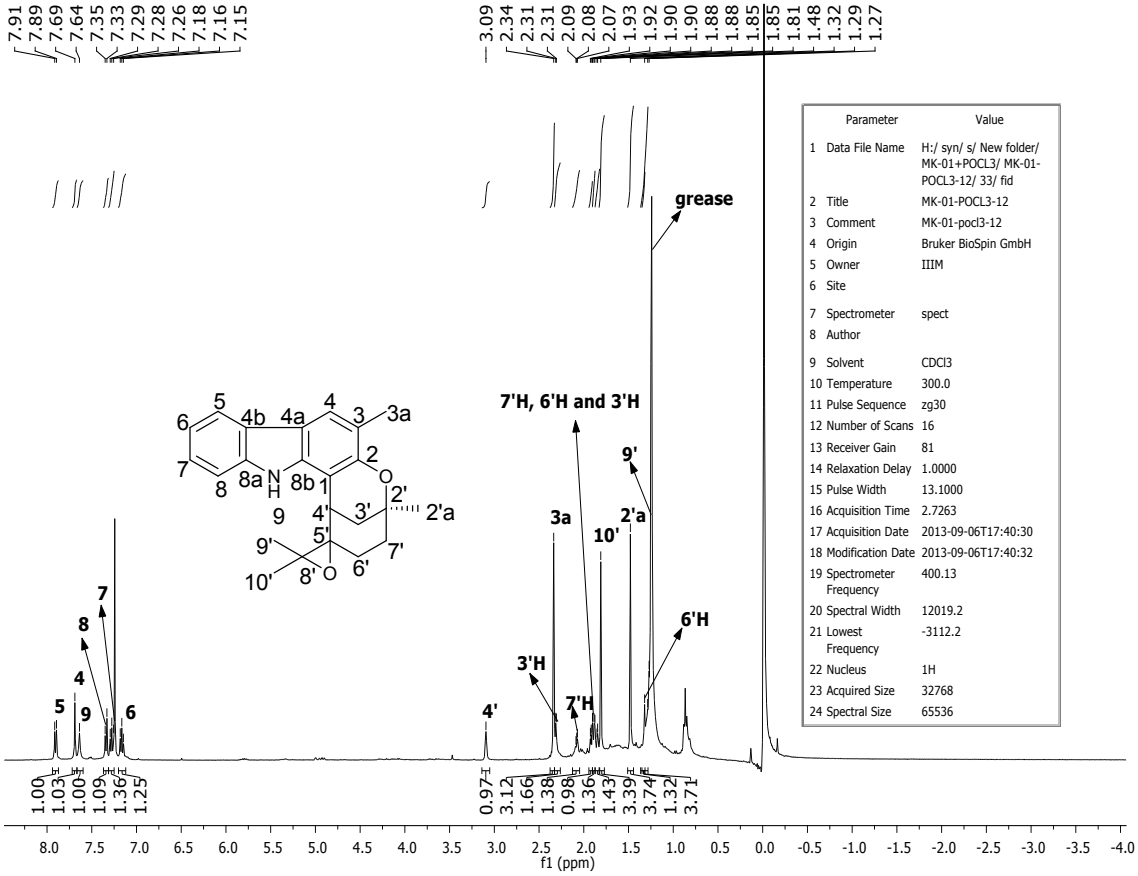
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
348.1951	1	189020.31	C23 H26 N O2	(M+H)+
349.1985	1	51534.26	C23 H26 N O2	(M+H)+
350.1983	1	7894.74	C23 H26 N O2	(M+H)+
351.1892	1	1868.1	C23 H26 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	348.1951	348.1958	1.93	100	100	75.51	77.21
2	349.1985	349.1991	1.7	27.26	25.62	20.59	19.78
3	350.1983	350.2021	10.82	4.18	3.56	3.15	2.75
4	351.1892	351.205	45.11	0.99	0.35	0.75	0.27

Figure S48: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **12**



	Parameter	Value
1	Data File Name	H:/ syn/ s/ New folder/ MK-01+POCL3/ MK-01-POCL3-12/ 33/ fid
2	Title	MK-01-POCL3-12
3	Comment	MK-01-pocl3-12
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	81
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2013-09-06T17:40:30
18	Modification Date	2013-09-06T17:40:32
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3112.2
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure S49: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **12**

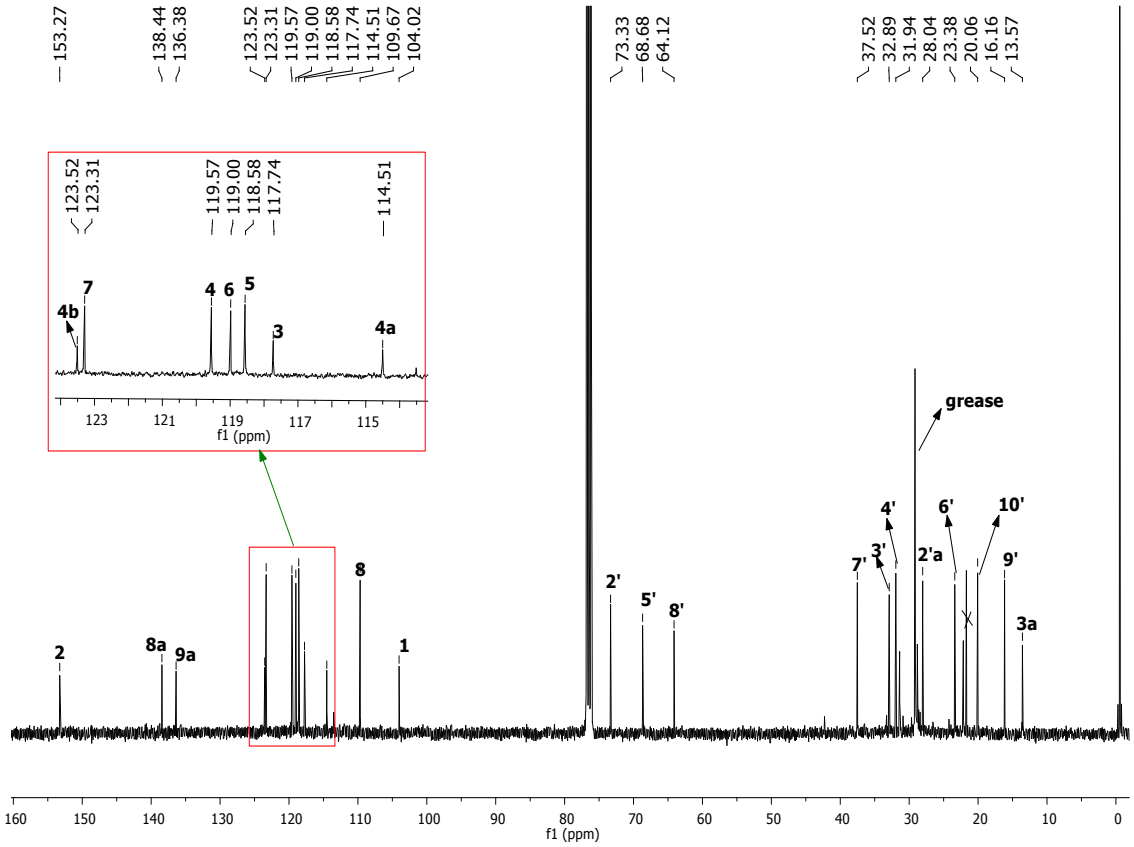


Figure S50: DEPT-135 (100 MHz, $CDCl_3$) spectrum of compound **12**

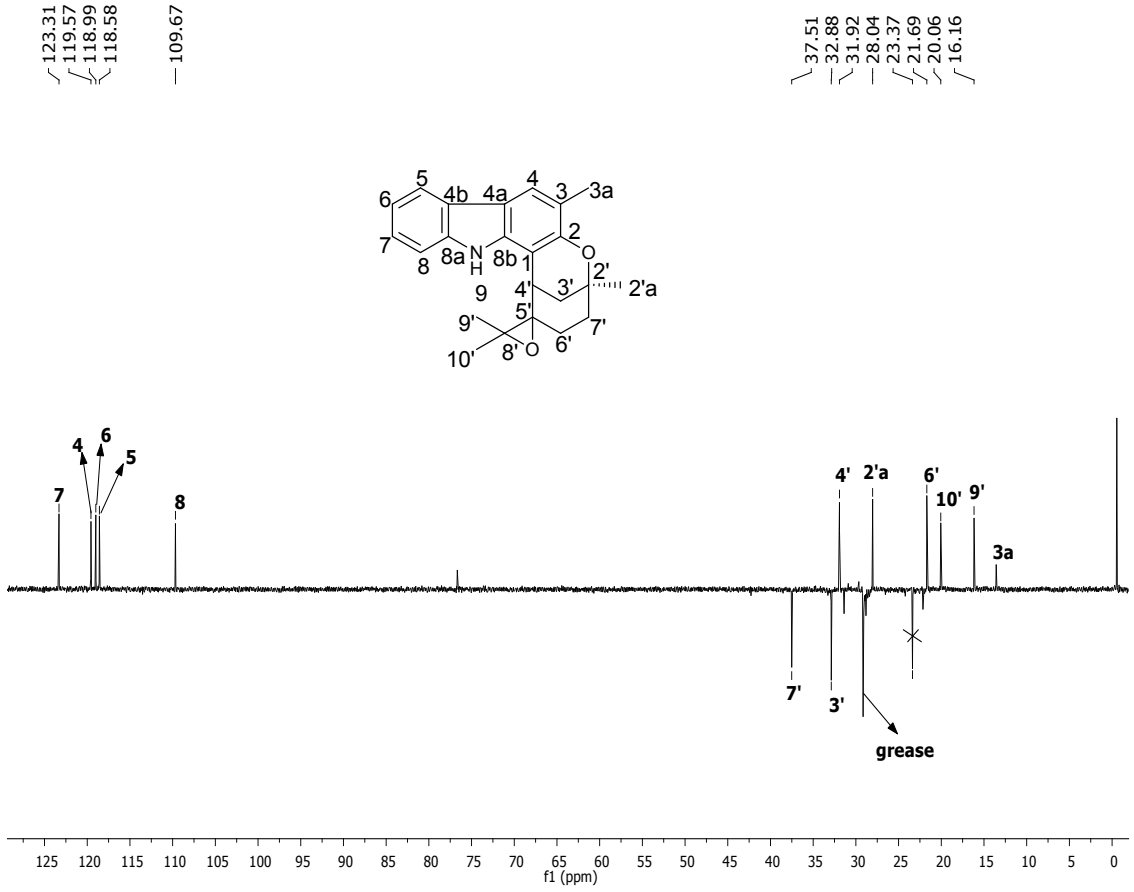


Figure S51: COSY spectrum of compound **12**

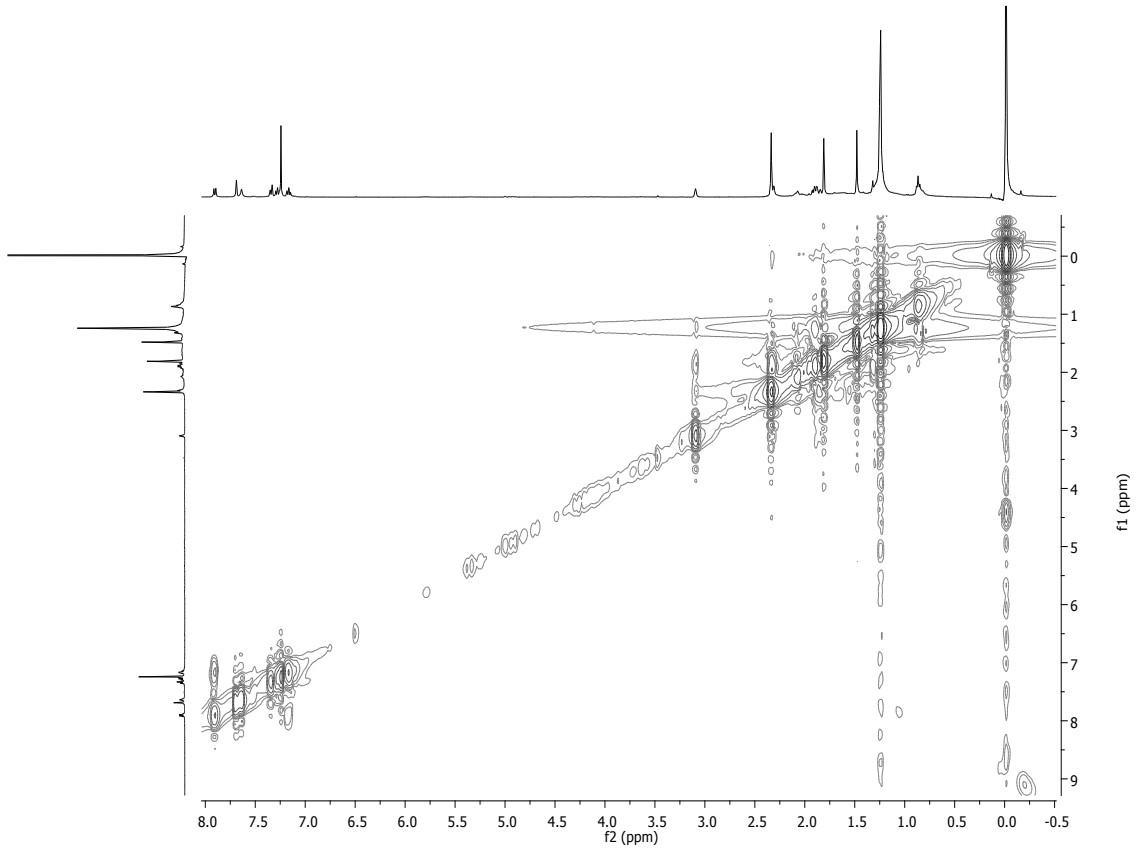


Figure S52: HSQC spectrum of compound **12**

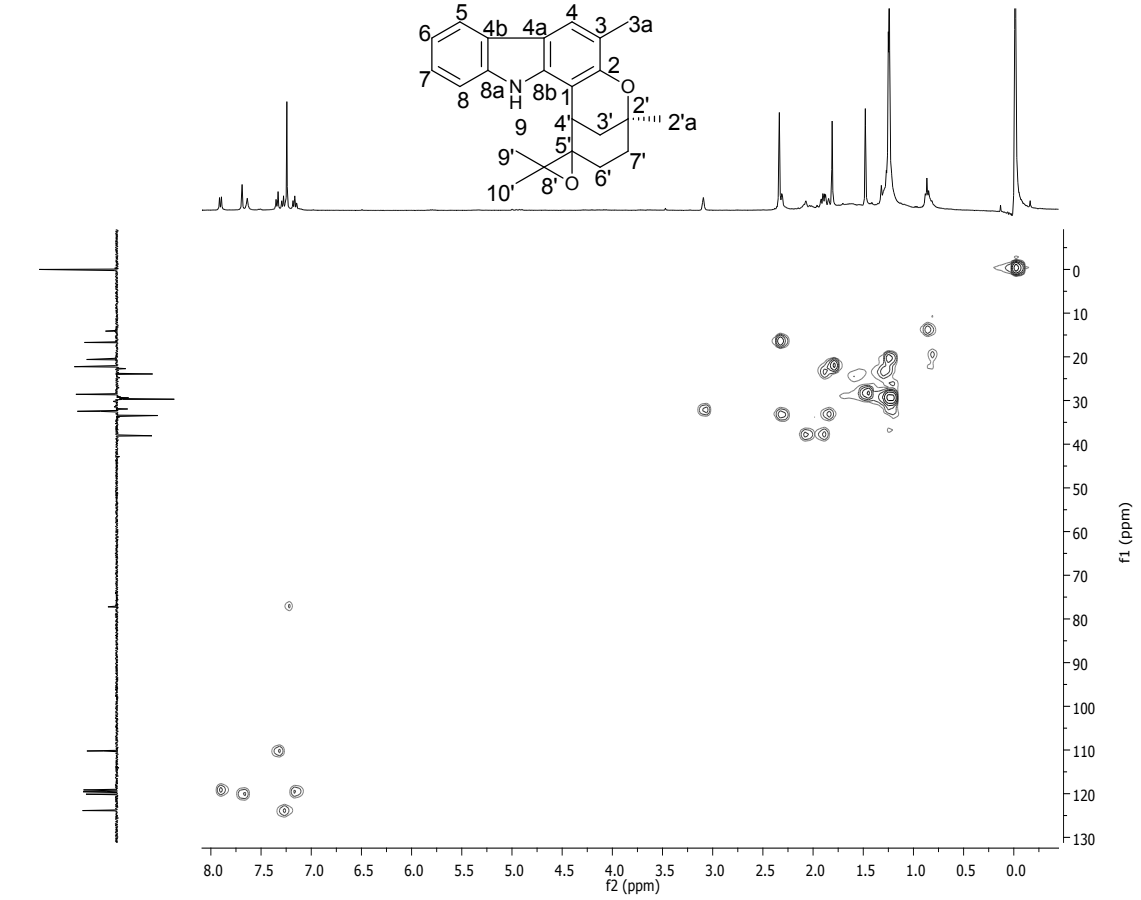


Figure S53: HMBC spectrum of compound **12**

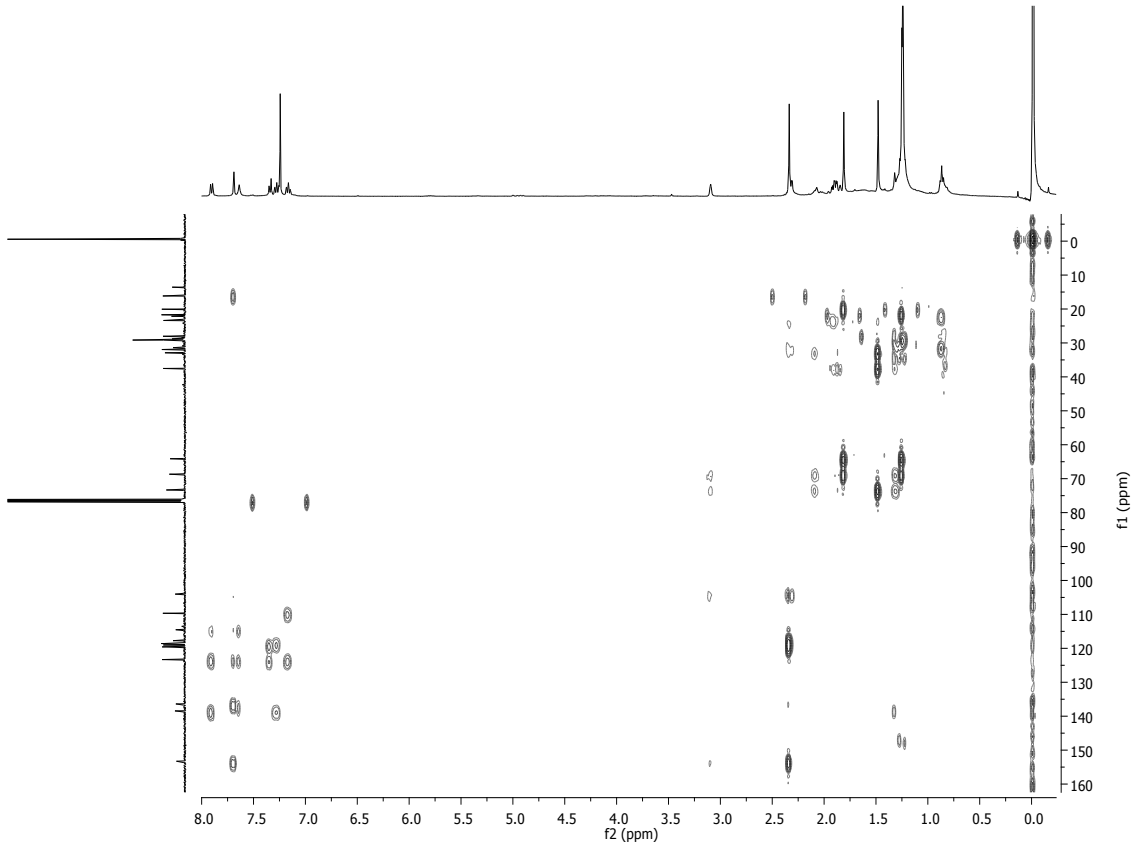
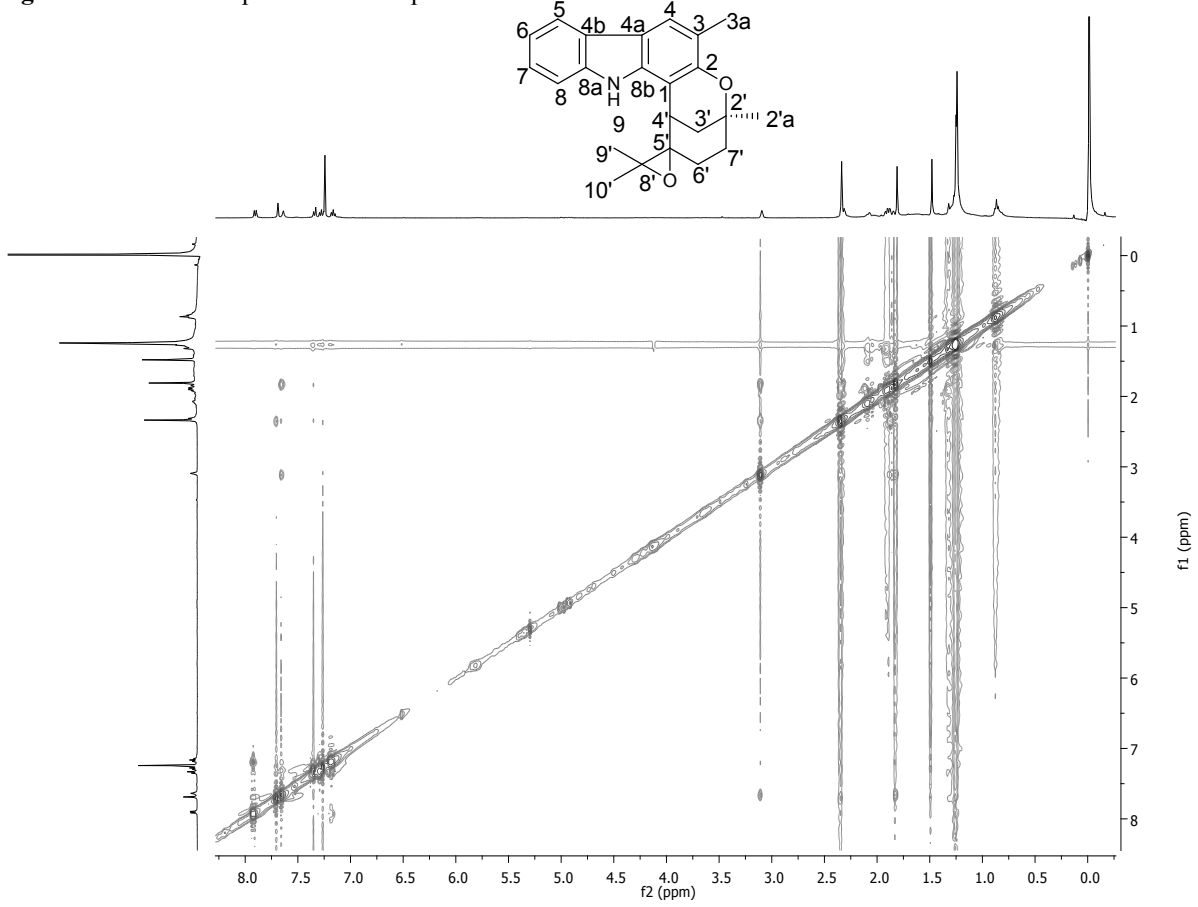


Figure S54: NOESY spectrum of compound **12**



X-ray crystallographic Data of 2:

The compound crystallizes in the monoclinic space group P 21 with the following unit-cell parameters: a=11.5077(10), b=12.2620(7), c= 15.7286(11) Å, β= 109.805(9) and Z = 4. The crystal structure was solved by direct methods using single-crystal X-ray diffraction data collected at room temperature and refined by full-matrix least-squares procedures to a final R-value of 0.0463 for 2582 observed reflections.

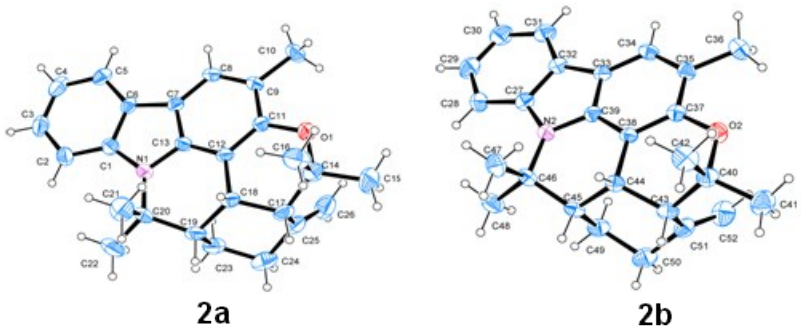


Fig. S55: CCDC No. 1435339 of compound **2** which crystallized in monoclinic space group $P2_1/c$ with two molecules a = 11.5077(10) Å, b = 12.2620(7) Å, c = 15.7286(11) Å; $\alpha = 90^0$, $\beta = 109.805^0$, $\gamma = 90^0$. These two molecules are present in unit cell.

Crystal structure determination and refinement

X-ray intensity data of 7542 reflections (of which 3844 unique) were collected on *X'calibur* CCD 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 intensities were measured by ω scan mode for θ ranges 3.60 to 25.00°. 2582 reflections were treated as observed ($I > 2\sigma(I)$). Data were corrected for Lorentz, polarisation and absorption factors. The structure was solved by direct methods using SHELXS97. All non-hydrogen atoms of the molecule were located in the best E-map. Full-matrix least-squares refinement was carried out using SHELXL97. The final refinement cycles converged to an R = 0.0463 and $wR(F^2) = 0.0787$ for the observed data. Residual electron densities ranged from $-0.142 < \Delta\rho < 0.136$ eÅ^{-3}. Atomic scattering factors were taken from International Tables for X-ray Crystallography. An ORTEP view of the compound with atomic labelling is shown in Figure S84. The geometry of the molecule was calculated using the WinGX, PARST and PLATON software.

Table S1: Crystal and experimental data of compound **2**.

Crystal description	white block
Crystal size	0.3 X 0.2 X 0.2 mm
CCDC No:	1435339
Empirical formula	$C_{26}H_{29}NO$
Formula weight	371.50
Radiation, Wavelength	Mo *K*α, 0.71073 Å
Unit cell dimensions	a = 11.5077(10), b = 12.2620(7), c = 15.7286(11) Å, α = 90.00°, β = 109.805(9)°, γ = 90.00°
Crystal system	monoclinic
Space group	P 21
Unit cell volume	2088.1(3)
No. of molecules per unit cell, Z	4
Temperature	293(2) K
Absorption coefficient	0.071 mm^{-1}
F(000)	800
Scan mode	ω scan
θ range for entire data collection	3.60 <θ< 25.00
Range of indices	h= -12 to 13, k=-13 to 14, l= -17 to 18
Reflections collected / unique	7542/ 3844
Reflections observed (I > 2σ (I))	2582
R_{int}	0.0347
R_{sigma}	0.0591
Structure determination	Direct methods
Refinement	Full-matrix least-squares on F^2
No. of parameters refined	515
Final R	0.0463
wR(F^2)	0.0787
Weight	$1/1/[\sigma^2(F_o^2)+(0.0312P)^2+0.0000P]$ Where $P=[F_o^2+2F_c^2]/3$
Goodness-of-fit	1.031
Final residual electron density	$-0.142 < \Delta\rho < 0.136$ eÅ^{-3}
Measurement	*X'calibur system-Oxford diffraction make, U.K*
Software for structure solution:	SHELXS97
Software for refinement:	SHELXL97
Software for molecular plotting:	ORTEP-3, PLATON
Software for geometrical calculation	PLATON

Table S2. Atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.3398(2)	0.39568(18)	0.12303(14)	0.0551(6)
N2	0.7225(3)	0.3886(2)	0.05854(17)	0.0484(7)
C21	0.5220(3)	0.3964(2)	0.08089(19)	0.0397(8)
C22	0.4523(3)	0.3525(3)	0.1287(2)	0.0455(9)
C23	0.4958(4)	0.2659(3)	0.1896(2)	0.0466(9)
C23A	0.4160(4)	0.2248(3)	0.2419(2)	0.0707(12)
H23A	0.4584	0.1674	0.2818	0.106
H23B	0.3396	0.1975	0.2004	0.106
H23C	0.3994	0.2835	0.2765	0.106
C24	0.6102(4)	0.2224(3)	0.2010(2)	0.0513(10)
H24	0.6385	0.1639	0.2402	0.062
C24A	0.6846(3)	0.2643(2)	0.1551(2)	0.0417(9)
C24B	0.8060(3)	0.2440(3)	0.1511(2)	0.0480(9)
C25	0.8978(4)	0.1692(3)	0.1927(2)	0.0639(11)
H25	0.8861	0.1191	0.2334	0.077
C26	1.0059(4)	0.1689(4)	0.1739(3)	0.0795(13)
H26	1.0680	0.1193	0.2026	0.095
C27	1.0221(4)	0.2417(3)	0.1128(3)	0.0753(12)
H27	1.0949	0.2392	0.0997	0.090
C28	0.9339(4)	0.3188(3)	0.0700(3	0.0623(11)
H28	0.9469	0.3677	0.0289	0.075
C28A	0.8255(4)	0.3209(3)	0.0901(2)	0.0492(9)
C28B	0.6381(3)	0.3509(2)	0.0961(2)	0.0417(8)
C22'	0.2891(3)	0.4807(3)	0.0553(2)	0.0537(10)
C22A	0.2276(3)	0.4220(3)	-0.0337(2)	0.0709(12)
H22A	0.2861	0.3741	-0.0458	0.106
H22B	0.1990	0.4746	-0.0816	0.106
H22C	0.1589	0.3803	-0.0301	0.106
C22B	0.1907(4)	0.5382(3)	0.0836(3)	0.0795(13)
H22D	0.1426	0.4850	0.1017	0.119
H22E	0.1379	0.5796	0.0336	0.119
H22F	0.2297	0.5863	0.1332	0.119
C23'	0.3924(3)	0.5582(3)	0.0517(2)	0.0483(9)
H23'	0.3549	0.6140	0.0061	0.058
C24'	0.4848(3)	0.4929(2)	0.01974(19)	0.0412(8)
H24'	0.4409	0.4663	-0.0415	0.049
C25'	0.5994(3)	0.5556(3)	0.04(2)	0.0491(9)
H25'	0.5709	0.6099	-0.0302	0.059
C26'	0.6600(3)	0.6179(3)	0.1056(2)	0.0582(10)
H26A	0.7254	0.6640	0.0997	0.070
H26B	0.6962	0.5671	0.1547	0.070
C27'	0.5632(4)	0.6877(3)	0.1261(3)	0.0730(13)
H27A	0.6017	0.7297	0.27	0.088
H27B	0.5268	0.7383	0.0768	0.088
C28'	0.4646(4)	0.6158(3)	0.1382(3)	0.0570(10)
C29'	0.4592(4)	0.5992(3	0.2190(3)	0.0837(14)
H29A	0.5166	0.6321	0.2690	0.100
H29B	0.3980	0.5546	0.2264	0.100
C30'	0.6918(3)	0.4803(3)	-0.0062(2)	0.0530(10)
C30A	0.6338(4)	0.4344(3)	-0.1016(2)	0.0719(12)
H30A	0.6898	0.3838	-0.1137	0.108
H30B	0.6169	0.4930	-0.1446	0.108
H30C	0.5581	0.3978	-0.1064	0.108
C30B	0.8073(4)	0.5454(3)	-0.0020(3)	0.0757(13)
H30D	0.8610	0.5513	0.0596	0.114*
H30E	0.7835	0.6170	-0.0264	0.114*

H30F	0.8499	0.5087	-0.0368	0.114*
O1	0.6688(2)	0.05355(19)	0.47431(16)	0.0651(7)
N1	1.0643(3)	0.0260(2)	0.43051(18)	0.0538(8)
C1	0.8680(3)	0.0524(3)	0.45647(19)	0.0439(9)
C2	0.7470(3)	0.0168(3)	0.4321(2)	0.0471(9)
C3	0.6991(3)	-0.0619(3)	0.3643(2)	0.0462(9)
C3A	0.5677(3)	-0.0993(3)	0.3438(3)	0.0708(12)
H3A1	0.5453	-0.1478	0.2929	0.106*
H3A2	0.5136	-0.0373	0.3300	0.106*
H3A3	0.5604	-0.1368	0.3953	0.106*
C4	0.7726(3)	-0.1030(3)	0.3190(2)	0.0489(9)
H4	0.7404	-0.1533	0.2727	0.059*
C4A	0.8960(3)	-0.0696(2)	0.3424(2)	0.0429(9)
C4B	0.9966(3)	-0.0918(3)	0.3099(2)	0.0474(9)
C5	1.0080(4)	-0.1527(3)	0.2400(2)	0.0608(11)
H5	0.9412	-0.1932	0.2036	0.073*
C6	1.1178(5)	-0.1541(4)	0.2235(3)	0.0785(14)
H6	1.1261	-0.1959	0.1766	0.094
C7	1.2163(4)	-0.0924(4)	0.2777(3)	0.0791(13)
H7	1.2897	-0.0932	0.2653	0.095
C8	1.2104(4)	-0.0303(3)	0.3487(3)	0.0698(12)
H8	1.2782	0.0095	0.3843	0.084*
C8A	1.0992(4)	-0.0292(3)	0.3656(2)	0.0525(10)
C8B	0.9399(3)	0.0047(3)	0.4121(2)	0.0449(9)
C2'	0.7115(4)	0.1459(3)	0.5348(3)	0.0698(12)
C20A	0.6915(4)	0.2485(3)	0.4757(3)	0.0869(14)
H20A	0.7290	0.2385	0.4303	0.130*
H20B	0.7284	0.3101	0.5127	0.130*
H20C	0.6046	0.2612	0.4472	0.130*
C20B	0.6254(4)	0.1534(4)	0.5897(3)	0.1062(17)
H20D	0.5413	0.1484	0.5500	0.159*
H20E	0.6379	0.2218	0.6213	0.159*
H20F	0.6427	0.0947	0.6326	0.159*
C3'	0.8489(4)	0.1314(3)	0.5928(2)	0.0618(11)
H3'	0.8733	0.1949	0.6328	0.074*
C4'	0.9231(3)	0.1348(3)	0.5282(2)	0.0529(10)
H4'	0.9107	0.2068	0.4995	0.063*
C5'	C 1.0633(4)	0.1157(3)	0.5705(2)	0.0602(11)
H5'	H 1.0974	0.1793	0.6085	0.072*
C6'	C 1.0896(4)	0.0168(3)	0.6334(2)	0.0760(13)
H6'1	H 1.0647	-0.0491	0.5977	0.091*
H6'2	H 1.1777	0.0122	0.6661	0.091*
C7'	C 1.0208(5)	0.0249(4)	.7002(3)	0.0910(15)
H7'1	H 1.0394	-0.0384	0.7395	0.109*
H7'2	H 1.0478	0.0893	0.7375	0.109*
C8'	C 0.8831(5)	0.0312(4)	0.6509(3)	0.0708(12)
C9'	C 0.8119(5)	-0.0489(4)	0.6580(3)	0.0962(16)
H9'1	H 0.7281	-0.0480	0.6242	0.115*
H9'2	H 0.8450	-0.1067	0.6970	0.115*
C10'	C 1.1260(4)	0.1118(3)	0.4969(2)	0.0639(11)
C11'	C 1.1107(4)	0.2215(3)	0.4472(3)	0.0926(16)
H11A	H 1.1561	0.2201	0.4060	0.139*
H11B	H 1.1415	0.2791	0.4903	0.139*
H11C	H 1.0248	0.2338	0.4141	0.139*
C12'	C 1.2638(4)	0.0874(4)	0.5414(3)	0.1028(17)
H12A	H 1.2744	0.0133	0.5623	0.154*
H12B	H 1.2985	0.1358	0.5917	0.154*
H12C	H 1.3050	0.0979	0.4982	0.154*

Table S3. Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O2	0.0456(17)	0.0620(15)	0.0587(15)	0.0027(13)	0.0191(12)	0.0004(14)
N2	0.052(2)	0.0475(16)	0.0488(17)	0.0082(15)	0.0218(15)	0.0036(17)
C21	0.052(2)	0.0330(17)	0.0316(17)	-0.0007(15)	0.0115(16)	-0.0020(18)
C22	0.049(3)	0.045(2)	0.0394(19)	-0.0012(17)	0.0098(17)	-0.0018(19)
C23	0.054(3)	0.047(2)	0.0404(19)	0.0009(18)	0.07(18)	-0.0067(19)
C23A	0.078(3)	0.074(3)	0.065(2)	0.012(2)	0.031(2)	-0.008(3)
C24	0.065(3)	0.042(2)	0.044(2)	0.0091(17)	0.0146(19)	-0.002(2)
C24A	0.048(2)	0.0343(17)	0.0398(18)	0.0020(16)	0.0106(17)	-0.0008(17)
C24B	0.050 (3)	0.044 (2)	0.047(2)	-0.0019(17)	0.0122(17)	0.0057(19)
C25	0.067(3)	0.056(2)	0.063(2)	0.007(2)	0.015(2)	0.012(2)
C26	0.073(4)	0.071(3)	0.089(3)	0.007(3)	0.021(3)	0.023(3)
C27	0.056(3)	0.080(3)	0.094(3)	-0.004(3)	0.030(2)	0.014(3)
C28	0.056(3)	0.064(2)	0.074(3)	0.001(2)	0.030(2)	0.001(2)
C28A	0.048(3)	0.049(2)	0.050(2)	-0.0033(18)	0.0159(18)	0.002(2)
C28B	0.045(2)	0.040(2)	0.0381(18)	-0.0020(16)	0.0122(16)	0.0014(17)
C22'	0.045(2)	0.054(2)	0.054(2)	0.0042(19)	0.0069(18)	0.007(2)
C22A	0.050(3)	0.082(3)	0.067(3)	-0.006(2)	0.003(2)	-0.009(2)
C22B	0.058(3)	0.080(3)	0.098(3)	0.000(3)	0.022(2)	0.013(3)
C23'	0.050(2)	0.0413(19)	0.045(2)	0.0047(17)	0.0054(17)	0.0021(18)
C24'	0.043(2)	0.0400(18)	0.0349(17)	0.0010(16)	0.0064(15)	-0.0012(17)
C25'	0.056(3)	0.0399(18)	0.047(2)	0.0103(17)	0.0125(17)	0.0007(19)
C26'	0.052(3)	0.047(2)	0.069(2)	-0.0045(19)	0.011(2)	-0.009(2)
C27'	0.075(3)	0.056(3)	0.081(3)	-0.020(2)	0.016(2)	-0.006(2)
C28'	0.057(3)	0.051(2)	0.060(2)	-0.013(2)	0.016(2)	0.002(2)
C29'	0.085(4)	0.096(3)	0.066(3)	-0.029(3)	0.021(3)	-0.014(3)
C30'	0.062(3)	0.049(2)	0.049(2)	0.0131(18)	0.0205(18)	-0.003(2)
C30A	0.093(3)	0.080(3)	0.049(2)	0.008(2)	0.033(2)	-0.001(2)
C30B	0.069(3)	0.063(3)	0.105(3)	0.018(2)	0.043(3)	-0.007(2)
O1	0.0555(18)	0.0756(17)	0.0694(16)	-0.0263(14)	0.0278(14)	-0.0113(15)
N1	0.045(2)	0.0621(19)	0.0518(17)	-0.0033(16)	0.0134(15)	-0.0110(17)
C1	0.048(2)	0.047(2)	0.0335(18)	-0.0064(16)	0.0095(16)	-0.0077(19)
C2	0.049(2)	0.050(2)	0.0422(19)	-0.0064(18)	0.0146(17)	-0.0012(19)
C3	0.038(2)	0.0478(19)	0.048(2)	-0.0054(18)	0.0085(17)	-0.0085(18)
C3A	0.049(3)	0.078(3)	0.083(3)	-0.018(2)	0.019(2)	-0.017(2)
C4	0.053(3)	0.0455(19)	0.0406(19)	-0.0038(17)	0.0054(17)	-0.007(2)
C4A	0.051(2)	0.0397(19)	0.0341(18)	0.0005(16)	0.0101(17)	-0.0050(18)
C4B	0.053(3)	0.052(2)	0.0392(19)	0.0117(18)	0.011(18)	0.007(2)
C5	0.074(3)	0.067(2)	0.040(2)	0.0099(19)	0.017(2)	0.014(2)
C6	0.088(4)	0.103(4)	0.054(3)	0.018(2)	0.037(3)	0.034(3)
C7	0.060(3)	0.118(4)	0.069(3)	0.026(3)	0.034(2)	0.017(3)
C8	0.054(3)	0.094(3)	0.063(3)	0.011(2)	0.021(2)	-0.007(3)
C8A	0.051(3)	0.058(2)	0.048(2)	0.0112(19)	0.0158(19)	-0.001(2)
C8B	0.043(2)	0.046(2)	0.042(2)	0.0026(17)	0.0093(17)	-0.0074(18)
C2'	0.073(3)	0.068(3)	0.073(3)	-0.031(2)	0.031(2)	-0.007(2)
C20A	0.072(3)	0.081(3)	0.096(3)	-0.022(3)	0.013(2)	0.012(3)
C20B	0.092(4)	0.127(4)	0.118(4)	-0.049(3)	0.060(3)	-0.005(3)
C3'	0.073(3)	0.065(3)	0.047(2)	-0.021(2)	0.020(2)	-0.012(2)
C4'	0.059(3)	0.050(2)	0.043(2)	-0.0052(17)	0.0092(18)	-0.007(2)
C5'	0.062(3)	0.061(2)	0.047(2)	-0.011(2)	0.004(2)	-0.017(2)
C6'	0.071(3)	0.086(3)	0.057(2)	-0.008(2)	0.004(2)	-0.001(2)
C7'	0.118(5)	0.092(3)	0.051(3)	0.001(2)	0.014(3)	0.001(3)
C8'	0.094(4)	0.077(3)	0.047(2)	-0.009(2)	0.031(2)	-0.011(3)
C9'	0.129(5)	0.094(3)	0.085(3)	-0.001(3)	0.061(3)	-0.012(3)
C10'	0.047(3)	0.074(3)	0.064(2)	-0.014(2)	0.009(2)	-0.024(2)
C11'	0.116(5)	0.066(3)	0.105(3)	-0.011(3)	0.048(3)	-0.034(3)
C12'	0.047(3)	0.145(4)	0.102(3)	-0.033(3)	0.007(2)	-0.026(3)

O2—C22	1.373(4)	O1—C2	1.363(4)
O2—C22'	1.463(4)	O1—C2'	1.454(4)
N2—C28B	1.376(4)	N1—C8B	1.386(4)
N2—C28A	1.394(4)	N1—C8A	1.392(4)
N2—C30'	1.476(4)	N1—C10'	1.483(4)
C21—C22	1.381(4)	C1—C8B	1.380(4)
C21—C28B	1.391(4)	C1—C2	1.384(4)
C21—C24'	1.492(4)	C1—C4'	1.488(4)
C22—C23	1.405(4)	C2—C3	1.405(4)
C23—C24	1.374(5)	C3—C4	1.373(4)
C23—C23A	1.511(4)	C3—C3A	1.507(4)
C23A—H23A	0.96	C3A—H3A1	0.96
C23A—H23B	0.96	C3A—H3A2	0.96
C23A—H23C	0.96	C3A—H3A3	0.96
C24—C24A	1.392(4)	C4—C4A	1.402(5)
C24—H24	0.93	C4—H4	0.93
C24A—C28B	1.392(4)	C4A—C8B	1.383(4)
C24A—C24B	1.441(5)	C4A—C4B	1.441(5)
C24B—C25	1.384(5)	C4B—C5	1.372(5)
C24B—C28A	1.417(4)	C4B—C8A	1.432(5)
C25—C26	1.373(5)	C5—C6	1.373(5)
C25—H25	0.93	C5—H5	0.93
C26—C27	1.369(5)	C6—C7	1.388(6)
C26—H26	0.93	C6—H6	0.93
C27—C28	1.384(5)	C7—C8	1.373(5)
C27—H27	0.93	C7—H7	0.93
C28—C28A	1.388(5)	C8—C8A	1.392(5)
C28—H28	0.93	C8—H8	0.93
C22'—C22A	1.519(4)	C2'—C20B	1.522(5)
C22'—C22B	1.523(5)	C2'—C20A	1.535(5)
C22'—C23'	1.537(5)	C2'—C3'	1.545(5)
C22A—H22A	0.96	C20A—H20A	0.96
C22A—H22B	0.96	C20A—H20B	0.96
C22A—H22C	0.96	C20A—H20C	0.96
C22B—H22D	0.96	C20B—H20D	0.96
C22B—H22E	0.96	C20B—H20E	0.96
C22B—H22F	0.96	C20B—H20F	0.96
C23'—C28'	1.508(4)	C3'—C8'	1.502(6)
C23'—C24'	1.545(4)	C3'—C4'	1.532(5)
C23'—H23'	0.98	C3'—H3'	0.98
C24'—C25'	1.534(4)	C4'—C5'	1.540(5)
C24'—H24'	0.98	C4'—H4'	0.98
C25'—C26'	1.521(4)	C5'—C6'	1.529(5)
C25'—C30'	1.551(5)	C5'—C10'	1.559(5)
C25'—H25'	0.98	C5'—H5'	0.98
C26'—C27'	1.524(5)	C6'—C7'	1.520(5)
C26'—H26A	0.97	C6'—H6'1	0.97
C26'—H26B	0.97	C6'—H6'2	0.97
C27'—C28'	1.499(5)	C7'—C8'	1.512(6)
C27'—H27A	0.97	C7'—H7'1	0.97
C27'—H27B	0.97	C7'—H7'2	0.97
C28'—C29'	1.308(5)	C8'—C9'	1.308(5)
C29'—H29A	0.93	C9'—H9'1	0.93
C29'—H29B	0.93	C9'—H9'2	0.93
C30'—C30A	1.528(4)	C10'—C12'	1.530(5)
C30'—C30B	1.533(5)	C10'—C11'	1.535(5)
C30A—H30A	0.96	C11'—H11A	0.96
C30A—H30B	0.96	C11'—H11B	0.96
C30A—H30C	0.96	C11'—H11C	0.96

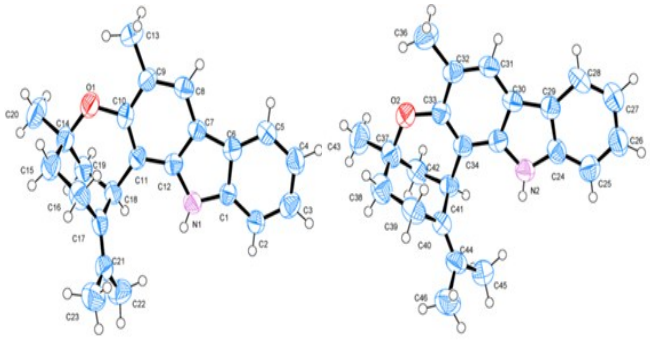
C30B—H30D	0.96	C12'—H12A	0.96
C30B—H30E	0.96	C12'—H12B	0.96
C30B—H30F	0.96	C12'—H12C	0.96
Bond Angles (º)			
C22— O2— C22'	117.1(3)	C2— O1— C2'	116.3(3)
C28B— N2— C28A	106.6(3)	C8B— N1— C8A	106.9(3)
C28B— N2— C30'	120.9(3)	C8B— N1— C10'	119.7(3)
C28A— N2— C30'	132.4(3)	C8A— N1— C10'	132.2(3)
C22— C21— C28B	116.8(3)	C8B— C1— C2	116.4(3)
C22— C21— C24'	124.5(3)	C8B— C1— C4'	119.8(3)
C28B— C21— C24'	118.5(3)	C2— C1— C4'	123.7(3)
O2— C22— C21	121.6(3)	O1— C2— C1	122.0(3)
O2— C22— C23	116.5(3)	O1— C2— C3	116.2(3)
C21— C22— C23	121.8(3)	C1— C2— C3	121.8(3)
C24— C23— C22	119.1(3)	C4— C3— C2	119.6(3)
C24— C23— C23A	122.1(3)	C4— C3— C3A	121.8(3)
C22— C23— C23A	118.8(4)	C2— C3— C3A	118.6(3)
C23— C23A— H23A	109.5	C3— C3A— H3A1	109.5
C23— C23A— H23B	109.5	C3— C3A— H3A2	109.5
H23A— C23A— H23B	109.5	H3A1— C3A— H3A2	109.5
C23— C23A— H23C	109.5	C3— C3A— H3A3	109.5
H23A— C23A— H23C	109.5	H3A1— C3A H3A3	109.5
H23B— C23A— H23C	109.5	H3A2— C3A— H3A3	109.5
C23— C24— C24A	121.3(3)	C3— C4— C4A	120.3(3)
C23— C24— H24	119.4	C3— C4— H4	119.9
C24A— C24— H24	119.4	C4A— C4— H4	119.9
C28B— C24A— C24	117.5(3)	C8B— C4A— C4	117.7(3)
C28B— C24A— C24B	105.2(3)	C8B— C4A— C4B	106.5(3)
C24— C24A— C24B	137.2(3)	C4— C4A— C4B	135.7(3)
C25— C24B— C28A	119.4(4)	C5— C4B— C8A	120.0(4)
C25— C24B— C24A	133.6(3)	C5— C4B— C4A	133.9(4)
C28A— C24B— C24A	107.0(3)	C8A— C4B— C4A	106.1(3)
C26— C25— C24B	120.2(4)	C4B— C5— C6	120.1(4)
C26— C25— H25	119.9	C4B— C5— H5	120
C24B— C25— H25	119.9	C6— C5— H5	120
C27— C26— C25	119.8(4)	C5— C6— C7	119.3(4)
C27— C26— H26	120.1	C5— C6— H6	120.3
C25— C26— H26	120.1	C7— C6 H6	120.3
C26— C27— C28	122.4(4)	C8— C7 C6	123.1(4)
C26— C27— H27	118.8	C8— C7 H7	118.4
C28— C27— H27	118.8	C6— C7— H7	118.5
C27— C28— C28A	118.0(4)	C7— C8— C8A	117.6(4)
C27— C28— H28	121	C7— C8— H8	121.2
C28A— C28— H28	121	C8A— C8— H8	121.2
C28— C28A— N2	130.7(3)	C8— C8A— N1	131.1(4)
C28— C28A— C24B	120.2(3)	C8— C8A— C4B	119.9(3)
N2— C28A— C24B	109.1(3)	N1— C8A— C4B	109.0(3)
N2— C28B— C21	124.6(3)	C1— C8B— C4A	124.1(3)
N2— C28B— C24A	112.0(3)	C1— C8B— N1	124.6(3)
C21— C28B— C24A	123.4(3)	C4A— C8B— N1	111.3(3)
O2—C22'— C22A	106.2(3)	O1— C2'— C20B	106.1(3)
O2— C22'— C22B	105.6(3)	O1— C2'— C20A	107.1(3)
C22A— C22'— C22B	109.2(3)	C20B— C2'— C20A	107.6(4)
O2— C22'— C23'	110.2(3)	O1— C2'— C3'	110.3(3)
C22A— C22'— C23'	112.6(3)	C20B— C2'— C3'	113.9(3)
C22B— C22'— C23'	112.7(3)	C20A— C2'— C3'	111.4(4)
C22'— C22A— H22A	109.5	C2'— C20A— H20A	109.5
C22'— C22A— H22B	109.5	C2'— C20A— H20B	109.5
H22A— C22A— H22B	109.5	H20A— C20A— H20B	109.5

C22'— C22A— H22C	109.5	C2'— C20A— H20C	109.5
H22A— C22A— H22C	109.5	H20A— C20A— H20C	109.5
H22B— C22A— H22C	109.5	H20B— C20A— H20C	109.5
C22'— C22B— H22D	109.5	C2'— C20B— H20D	109.5
C22'— C22B— H22E	109.5	C2'— C20B— H20E	109.5
H22D— C22B— H22E	109.5	H20D— C20B— H20E	109.5
C22'— C22B— H22F	109.5	C2'— C20B— H20F	109.5
H22D— C22B— H22F	109.5	H20D— C20B— H20F	109.5
H22E— C22B— H22F	109.5	H20E— C20B— H20F	109.5
C28'— C23'— C22'	117.0(3)	C8'— C3'— C4'	109.7(3)
C28'— C23'— C24'	107.9(3)	C8'— C3'— C2'	117.2(4)
C22'— C23'— C24'	108.5(3)	C4'— C3'— C2'	107.1(3)
C28'— C23'— H23'	107.7	C8'— C3'— H3'	107.5
C22'— C23' H23'	107.7	C4'— C3'— H3'	107.5
C24'— C23'— H23'	107.7	C2'— C3'— H3'	107.5
C21— C24'— C25'	110.3(3)	C1— C4'— C3'	107.1(3)
C21— C24'— C23'	106.2(3)	C1— C4'— C5'	109.8(3)
C25'— C24'— C23'	115.8(3)	C3'— C4'— C5'	116.5(3)
C21— C24'— H24'	108.1	C1— C4'— H4'	107.7
C25'— C24'— H24'	108.1	C3'— C4'— H4'	107.7
C23'— C24'— H24'	108.1	C5'— C4'— H4'	107.7
C26'— C25'— C24'	111.7(3)	C6'— C5'— C4'	110.5(3)
C26'— C25'— C30'	112.3(3)	C6'— C5'— C10'	114.6(3)
C24'— C25'— C30'	111.7(3)	C4'— C5'— C10'	111.4(3)
C26'— C25'— H25'	106.9	C6'— C5'— H5'	106.6
C24'— C25'— H25'	106.9	C4'— C5'— H5'	106.6
C30'— C25'— H25'	106.9	C10'— C5'— H5'	106.6
C25'— C26'— C27'	109.2(3)	C7'— C6'— C5'	111.1(4)
C25'— C26'— H26A	109.8	C7'— C6'— H6'1	109.4
C27'— C26'— H26A	109.8	C5'— C6'— H6'1	109.4
C25'— C26'— H26B	109.8	C7'— C6'— H6'2	109.4
C27'— C26'— H26B	109.8	C5'— C6'— H6'2	109.4
H26A— C26'— H26B	108.3	H6'1— C6'— H6'2	108
C28'— C27'— C26'	109.6(3)	C8'— C7'— C6'	110.5(3)
C28'— C27'— H27A	109.7	C8'— C7'— H7'1	109.6
C26'— C27'— H27A	109.7	C6'— C7'— H7'1	109.6
C28'— C27'— H27B	109.7	C8'— C7'— H7'2	109.6
C26'— C27'— H27B	109.7	C6'— C7'— H7'2	109.6
H27A— C27'— H27B	108.2	H7'—1 C7'— H7'2	108.1
C29'— C28'— C27'	120.1(4)	C9'— C8'— C3'	128.6(5)
C29'— C28'— C23'	127.6(4)	C9'— C8'— C7'	119.7(5)
C27'— C28'— C23'	111.7(3)	C3'— C8'— C7'	111.5(4)
C28'— C29'— H29A	120	C8'— C9'— H9'1	120
C28'— C29'— H29B	120	C8'— C9'— H9'2	120
H29A— C29'— H29B	120	H9'1— C9'— H9'2	120
N2— C30'— C30A	108.7(3)	N1— C10'— C12'	111.0(3)
N2— C30'— C30B	111.5(3)	N1— C10'— C11'	108.5(3)
C30A— C30'— C30B	108.5(3)	C12'— C10'— C11'	109.1(4)
N2— C30'— C25'	107.9(3)	N1— C10'— C5'	108.2(3)
C30A— C30'— C25'	110.7(3)	C12'— C10'— C5'	109.6(3)
C30B— C30'— C25'	109.7(3)	C11'— C10'— C5'	110.5(3)
C30'— C30A— H30A	109.5	C10'— C11'— H11A	109.5
C30'— C30A— H30B	109.5	C10'— C11'— H11B	109.5
H30A— C30A— H30B	109.5	H11A— C11'— H11B	109.5
C30'— C30A— H30C	109.5	C10'— C11'— H11C	109.5
H30A— C30A— H30C	109.5	H11A— C11'— H11C	109.5
H30B— C30A— H30C	109.5	H11B— C11'— H11C	109.5
C30'— C30B— H30D	109.5	C10'— C12'— H12A	109.5
C30'— C30B— H30E	109.5	C10'— C12'— H12B	109.5

H30D— C30B— H30E	109.5	H12A— C12'— H12B	109.5
C30'— C30B— H30F	109.5	C10'— C12'— H12C	109.5
H30D— C30B— H30F	109.5	H12A— C12'— H12C	109.5
H30E— C30B— H30F	109.5	H12B— C12'— H12C	109.5

X-ray crystallographic data of compound 3:

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 4.



3a **3b**

Fig. S56: ORTEP of (CCDC No. 1058032) compound **3** which crystallized in monoclinic space group $P2_1/c$ with two molecules a = 8.4284 (6) Å, b=18.5039 (14) Å = 23.3119 (16) Å; $\alpha = 90^0$, $\beta = 93.85^0$, $\gamma = 90^0$. These two molecules are present in unit cell.

Table S4: Crystal and diffraction parameters of **3.**

Empirical formula	$C_{46}H_{50}N_2O_2$
Crystal habit	Rodolourless
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 S5. 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	0.58	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)	0.68 (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	-0.012	0.4422	0.3256	0.128*
H23B	-0.0582	0.3613	0.3105	0.128*
H23C	0.14	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 S6. Atomic displacement parameters (Å²)

	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 S7. 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 (º)			
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)

Figure S57: ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound mahanimbine (**1**)

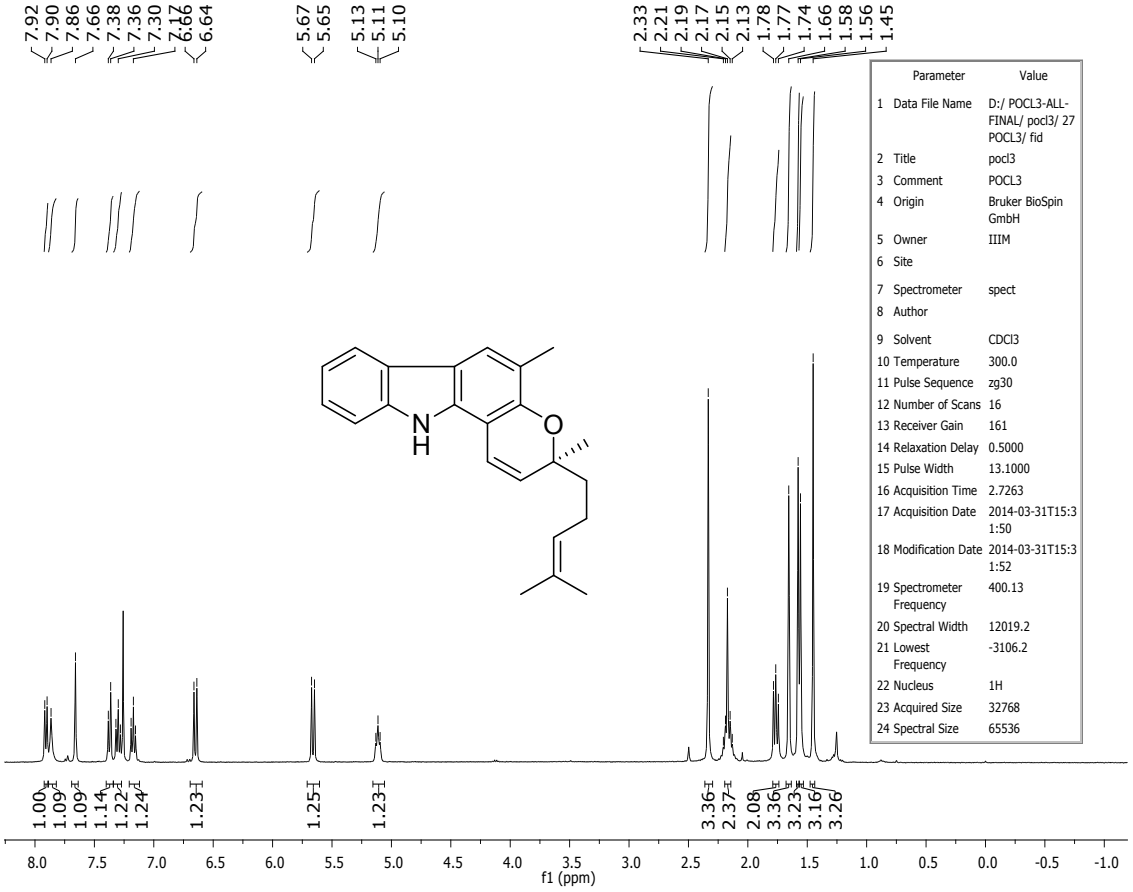


Figure S58: ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of isocyclomahanimbine (**3**)

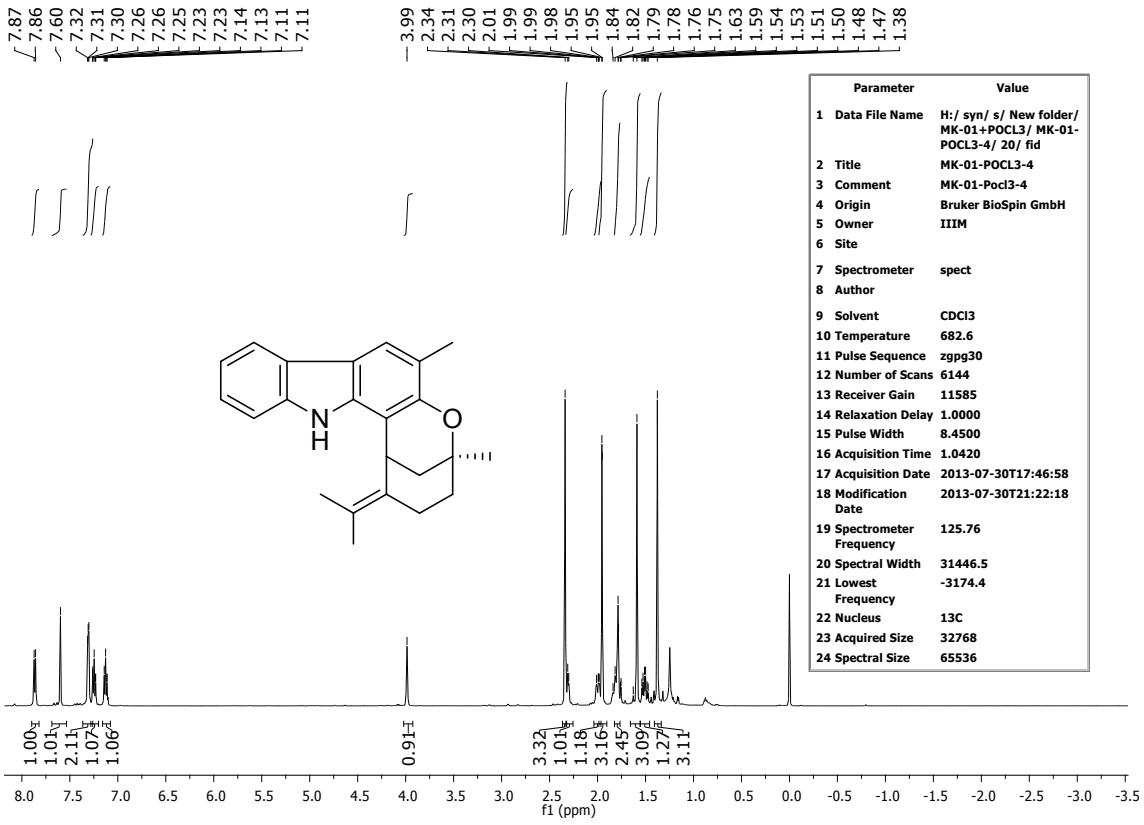
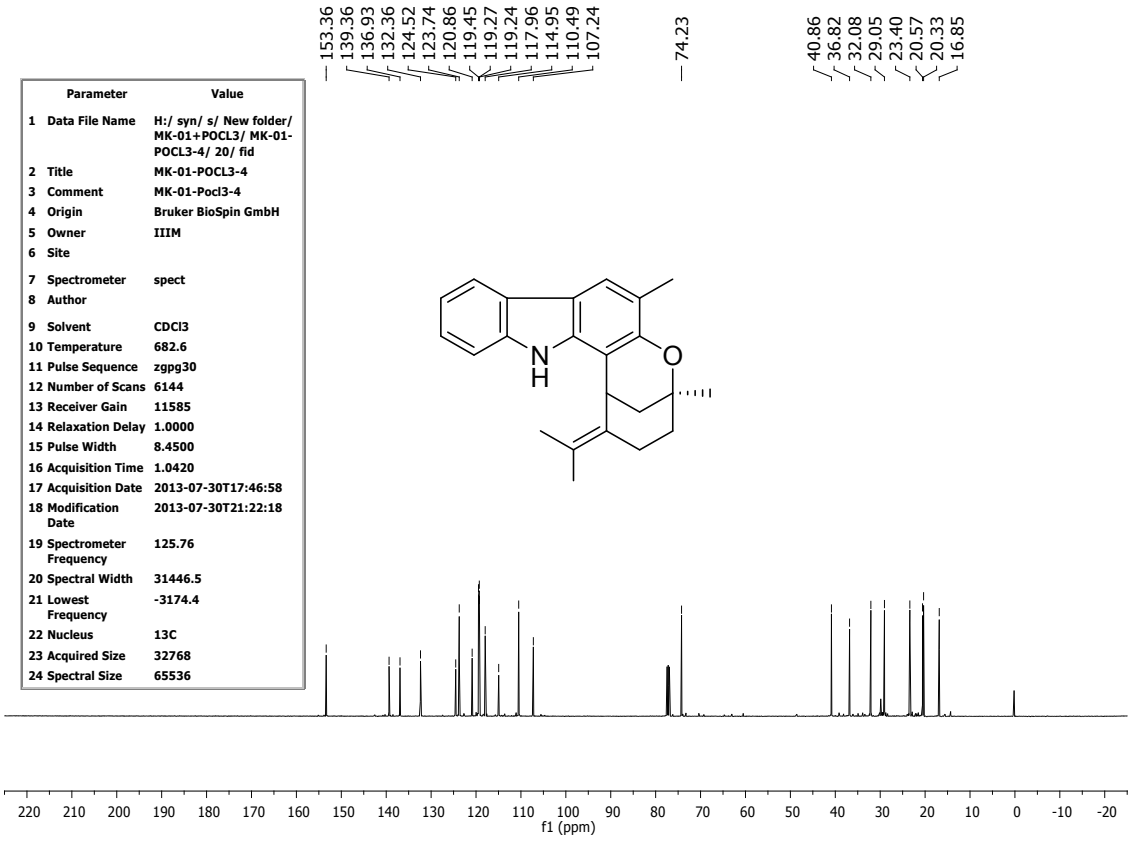


Figure S59: ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of Isocyclomahanimbine (**3**)



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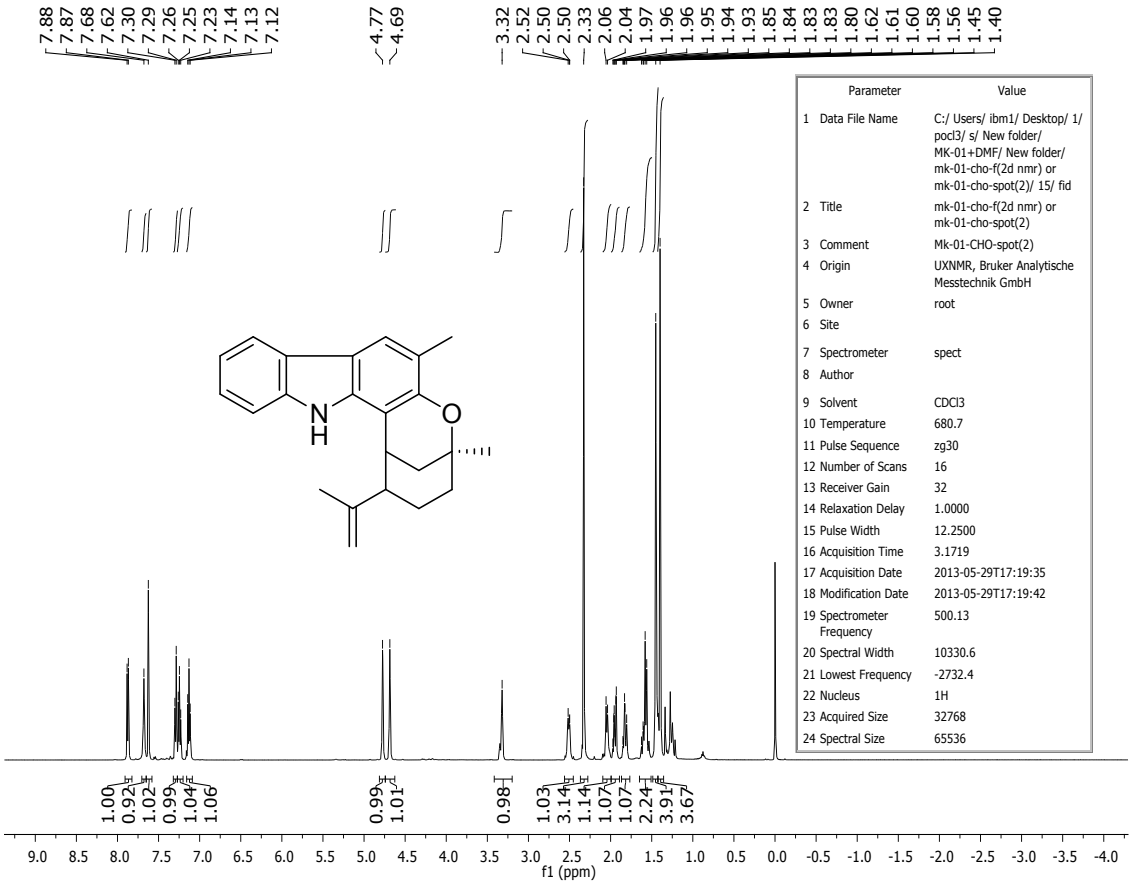
3	Comment	MK-01-Pocl3-4
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	682.6
11	Pulse Sequence	zgpg30
12	Number of Scans	6144
13	Receiver Gain	11585
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-07-30T17:46:58
18	Modification Date	2013-07-30T21:22:18
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3174.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure S60: ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of curryanin (**5**)



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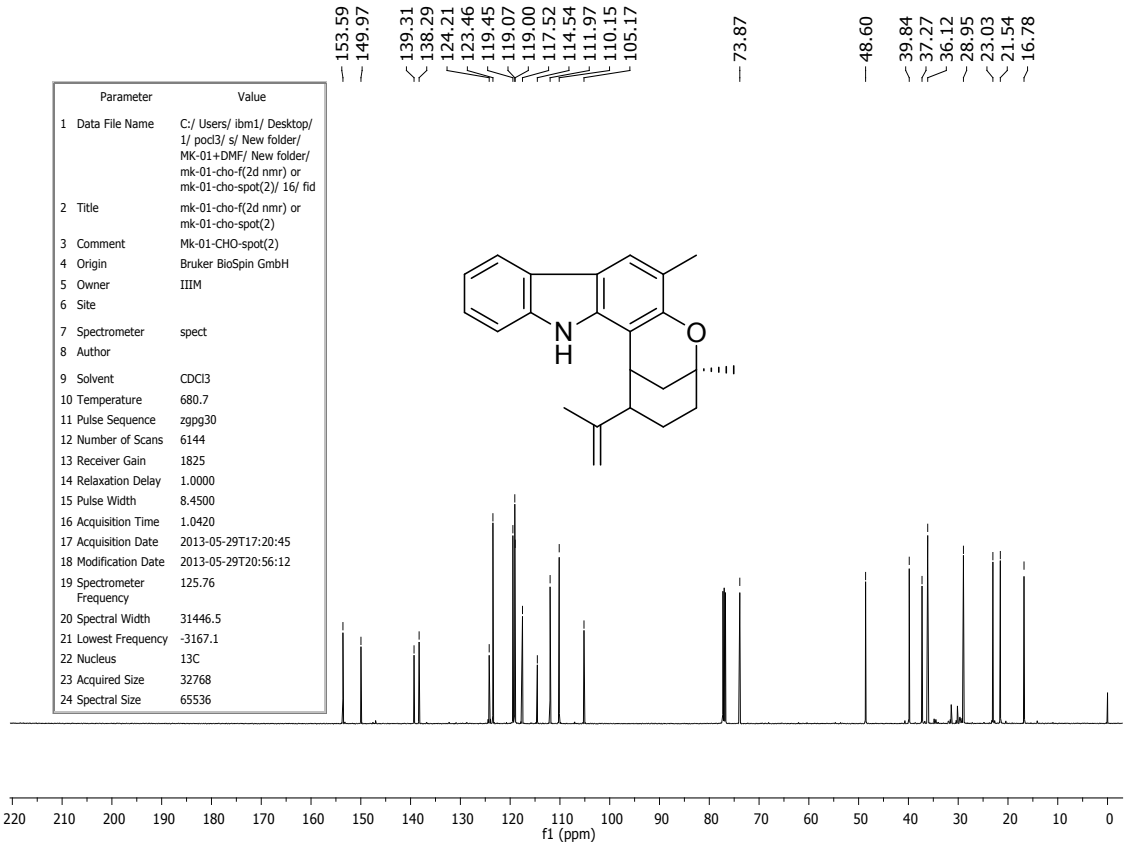
2	Title	mk-01-cho-f(2d nmr) or mk-01-cho-spot(2)
3	Comment	Mk-01-CHO-spot(2)
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.7
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	32
14	Relaxation Delay	1.0000
15	Pulse Width	12.2500
16	Acquisition Time	3.1719
17	Acquisition Date	2013-05-29T17:19:35
18	Modification Date	2013-05-29T17:19:42
19	Spectrometer Frequency	500.13
20	Spectral Width	10330.6
21	Lowest Frequency	-2732.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure S61: ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of Curryanin (**5**)



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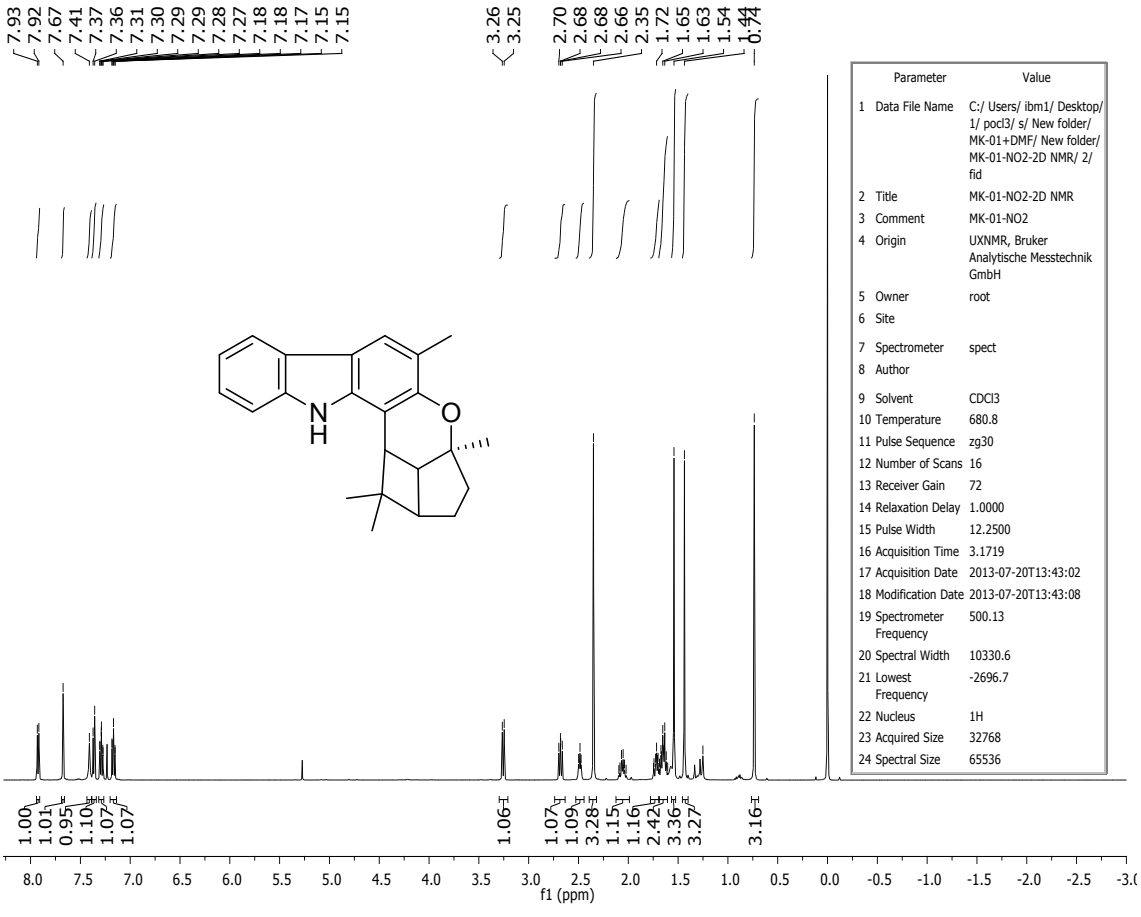
3	Comment	Mk-01-CHO-spot(2)
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.7
11	Pulse Sequence	zgpg30
12	Number of Scans	6144
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition 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 S62: ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of bicyclomahanimbine (**9**)



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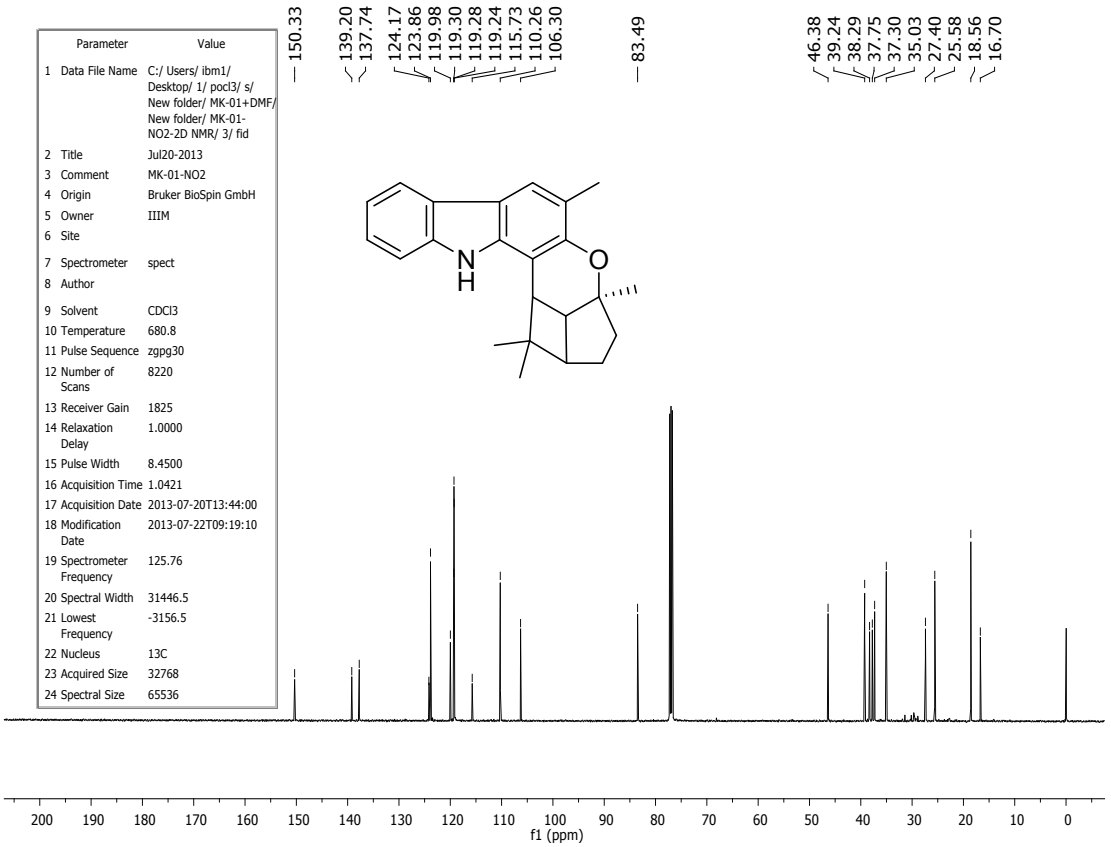
3	Comment	MK-01-NO2
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.8
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	72
14	Relaxation Delay	1.0000
15	Pulse Width	12.2500
16	Acquisition Time	3.1719
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 S63: ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of bycyclomahanimbine (**9**)



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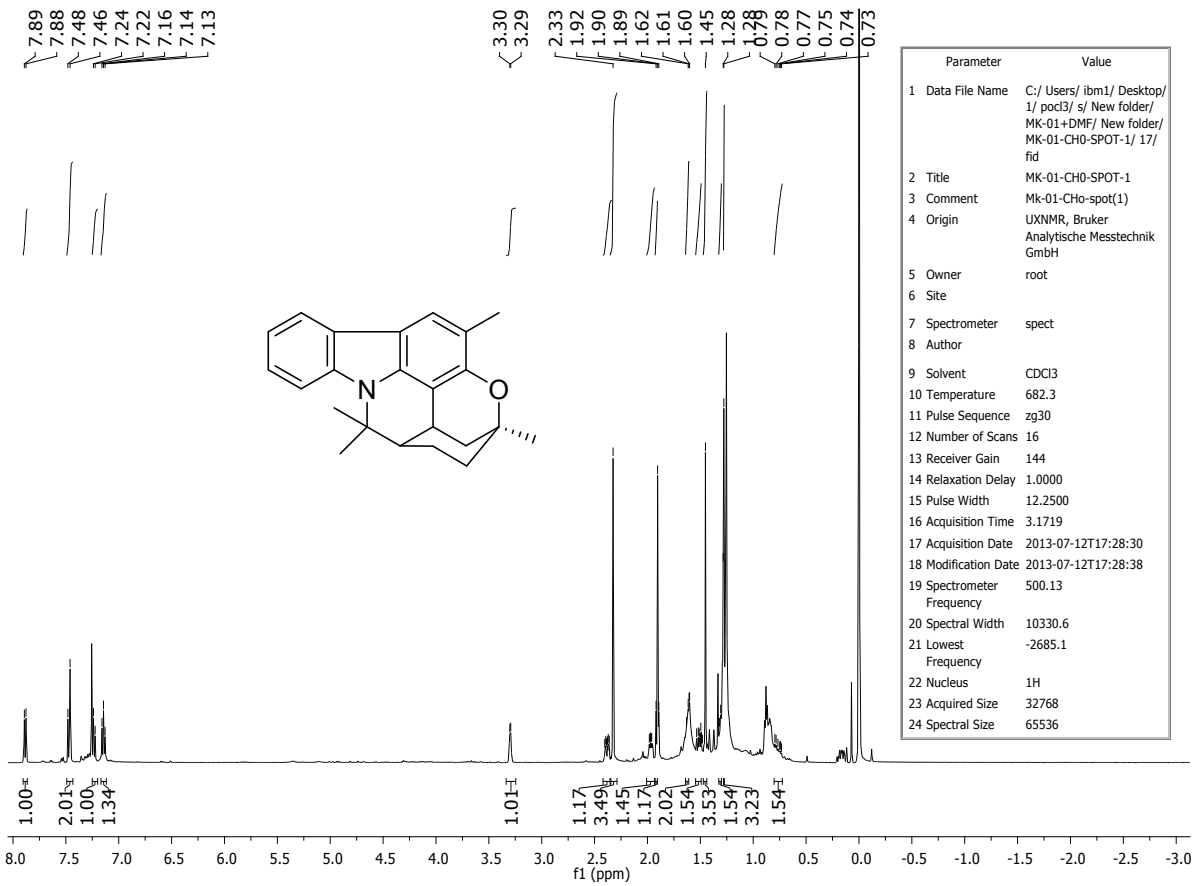
2 Title	Jul20-2013
3 Comment	MK-01-NO2
4 Origin	Bruker BioSpin GmbH
5 Owner	IIIM
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	680.8
11 Pulse Sequence	zgpg30
12 Number of Scans	8220
13 Receiver Gain	1825
14 Relaxation Delay	1.0000
15 Pulse Width	8.4500
16 Acquisition Time	1.0421
17 Acquisition Date	2013-07-20T13:44:00
18 Modification Date	2013-07-22T09:19:10
19 Spectrometer Frequency	125.76
20 Spectral Width	31446.5
21 Lowest Frequency	-3156.5
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Figure S64: ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of curryangin (**10**)



Parameter	Value
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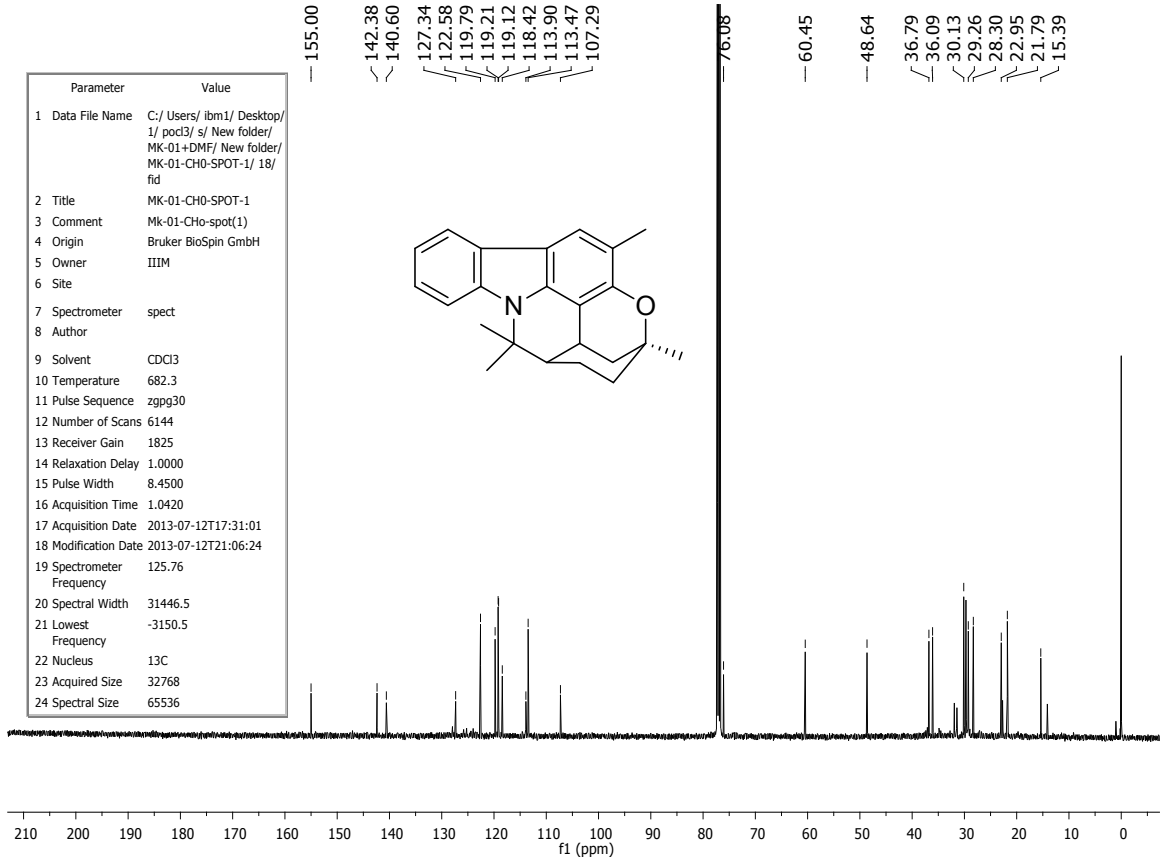
3 Comment	Mk-01-CHo-spot(1)
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	682.3
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	144
14 Relaxation Delay	1.0000
15 Pulse Width	12.2500
16 Acquisition Time	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 S65: ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of curryangin (**10**)



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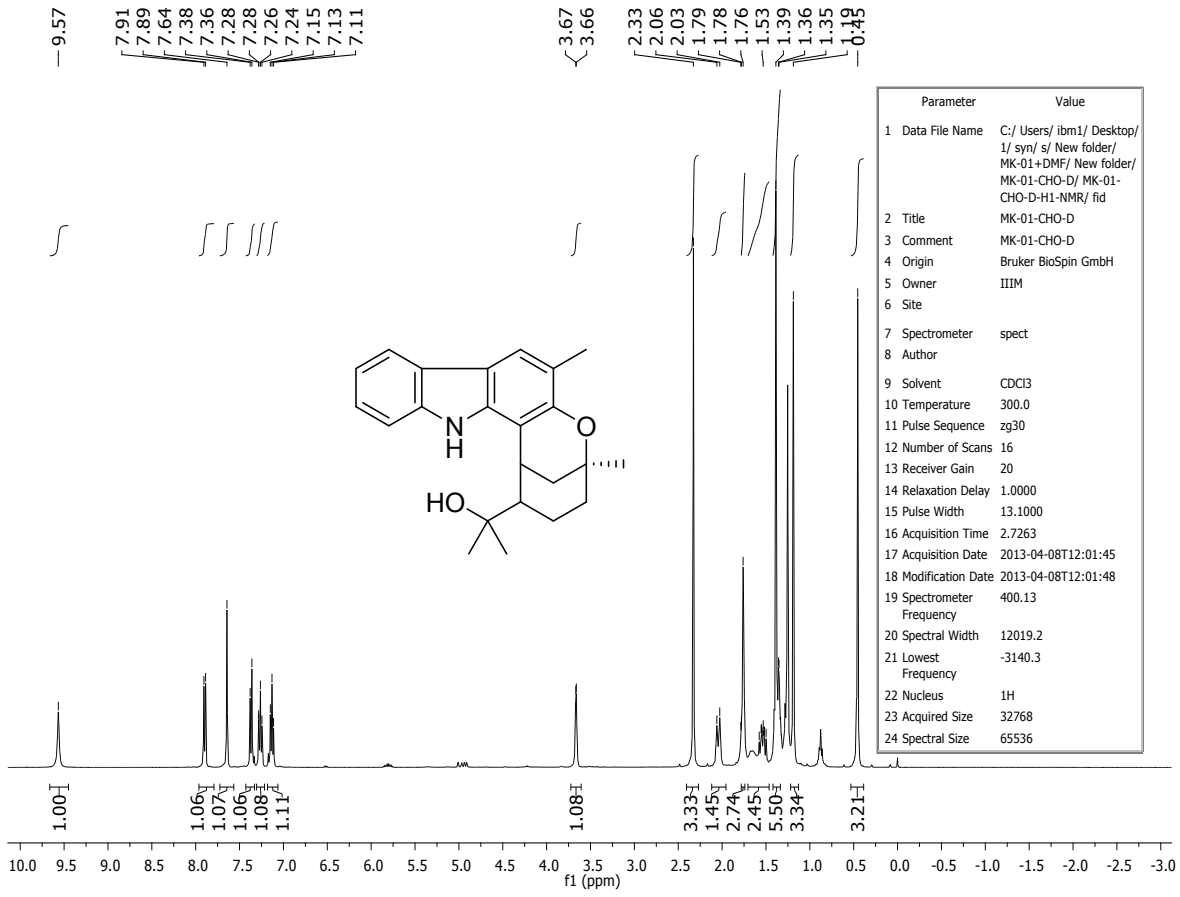
3	Comment	Mk-01-CHo-spot(1)
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	682.3
11	Pulse Sequence	zgpg30
12	Number of Scans	6144
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition 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 S66: ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of murrayazolinine (**13**)



	Parameter	Value
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2	Title	MK-01-CHO-D
3	Comment	MK-01-CHO-D
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	20
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2013-04-08T12:01:45
18	Modification Date	2013-04-08T12:01:48
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3140.3
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure S67: ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of murrayazolinine (**13**)