Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information

Four new carbazole alkaloids from *Murraya koenigii* depicting anti-inflammatory and anti-microbial activity

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[e]Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu-Tawi, J&K 180001, India.

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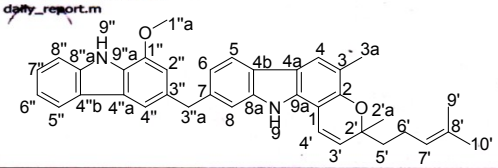
Contents

Figure S1: HRESIMS spectrum of murrayakonine A (**1**)

Qualitative Compound Report

Data File	MK-345-2.d	**Sample Name**	MK-345-2
Sample Type	Sample	**Position**	Vial 16
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-04-2015 PM 4:58:06
IRM Calibration Status		**DA Method**	daily_report.m
Comment			
Sample Group	**Info.**		
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

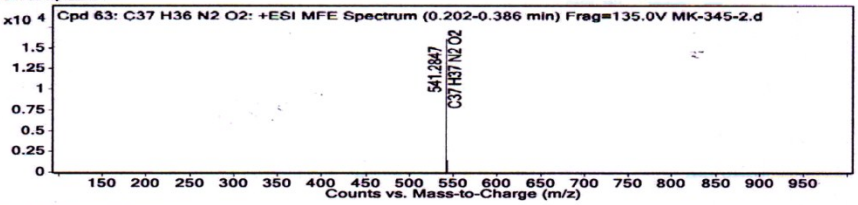


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 63: C37 H36 N2 O2	0.272	540.2774	C37 H36 N2 O2	C37 H36 N2 O2	0.55	C37 H36 N2 O2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 63: C37 H36 N2 O2	541.2847	0.272	Find by Molecular Feature	540.2774

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
541.2847	1	16082.85	C37 H37 N2 O2	(M+H)+
542.2877	1	5978.06	C37 H37 N2 O2	(M+H)+
543.2916	1	1451.46	C37 H37 N2 O2	(M+H)+

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	541.2847	541.285	0.45	100	100	68.4	66.69
2	542.2877	542.2882	1.05	37.17	41.25	25.43	27.51
3	543.2916	543.2914	-0.43	9.02	8.7	6.17	5.8

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

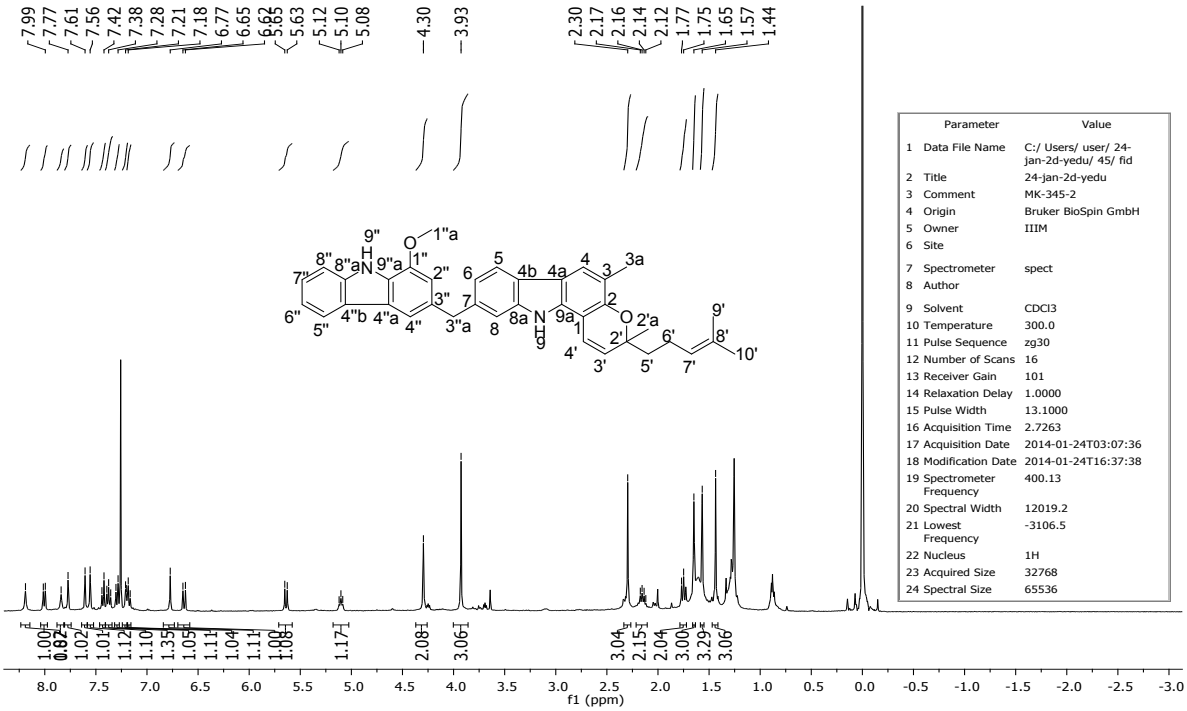


Figure S3: Expansion (0-6.4 ppm) of ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of murrayakonine A (**1**)

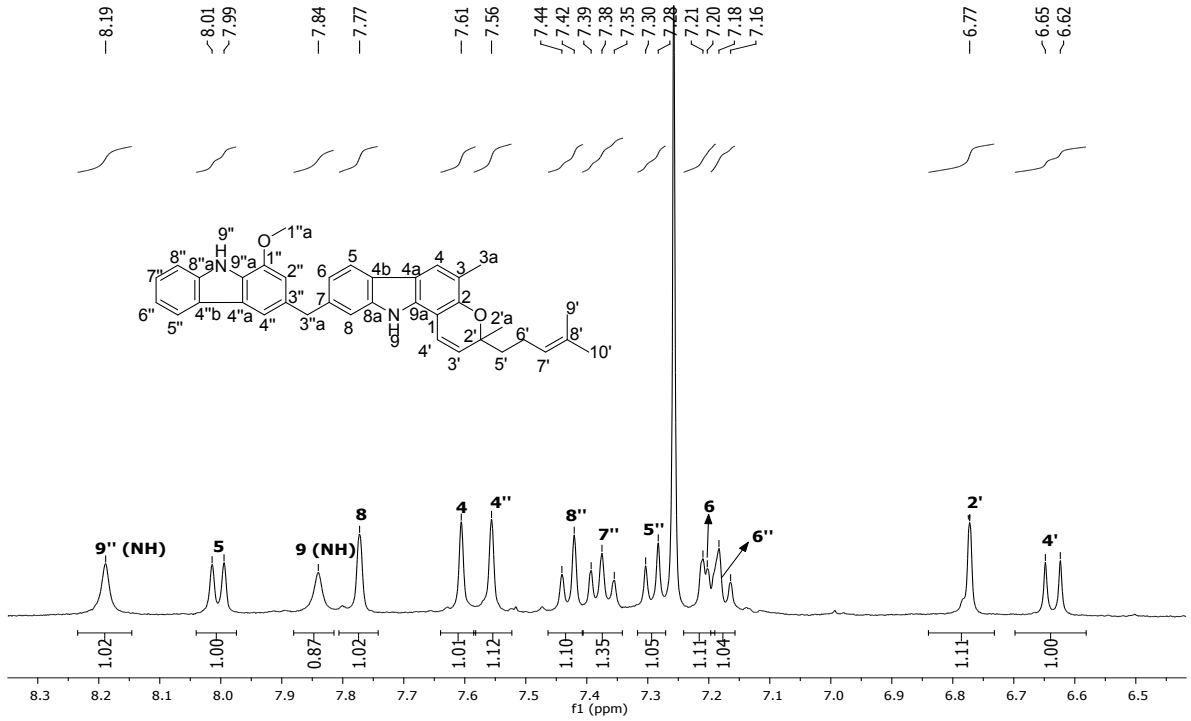


Figure S4: Expansion (6.5-8.3 ppm) of ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of murrayakonine A (**1**)

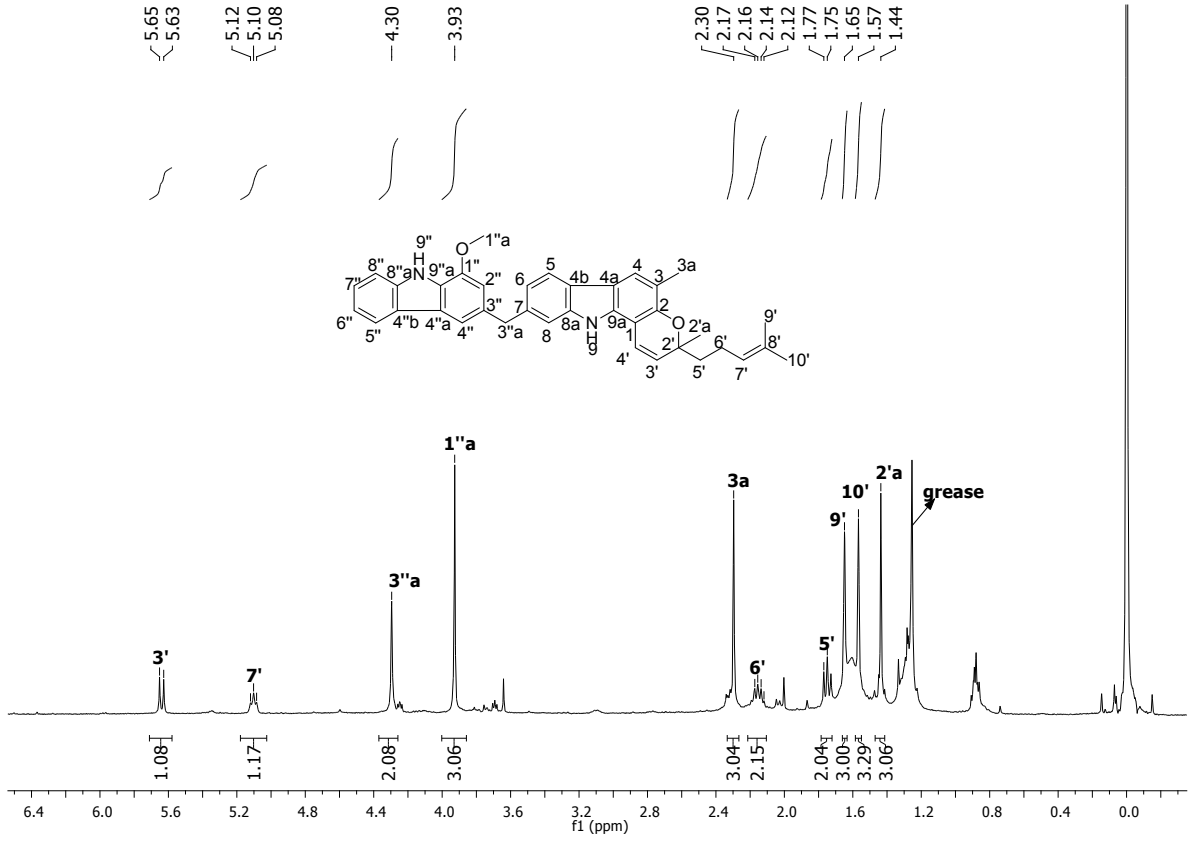


Figure S5: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of murrayakonine A (**1**)

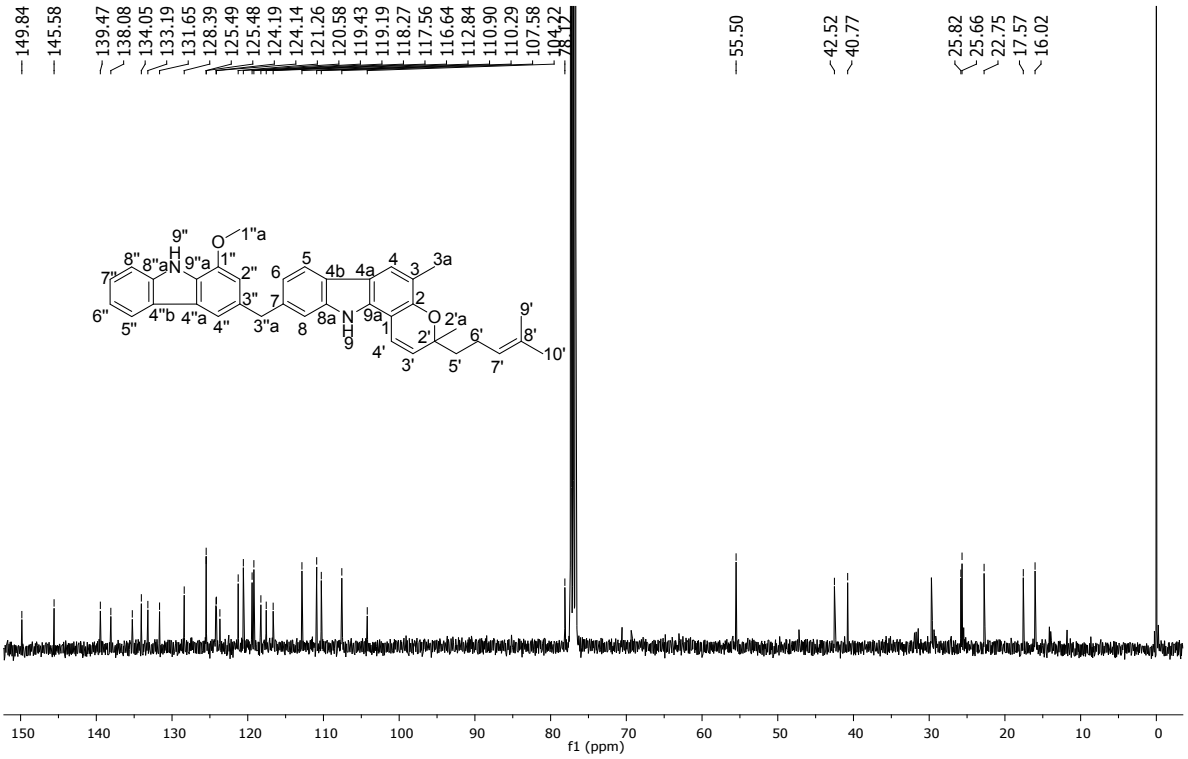


Figure S6: Expansion (0-80 ppm) of ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of murrayakonine A (**1**)

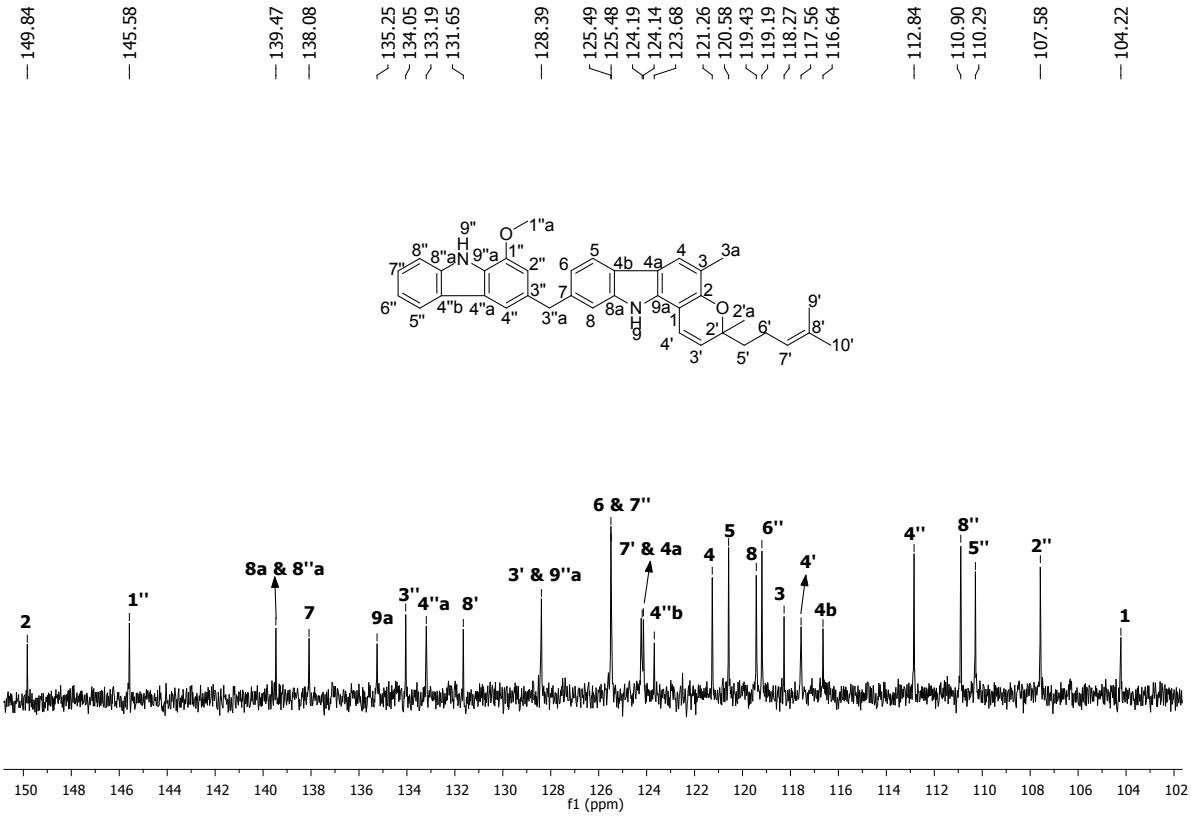


Figure S7: Expansion (102-150 ppm) of ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of murrayakonine A (**1**)

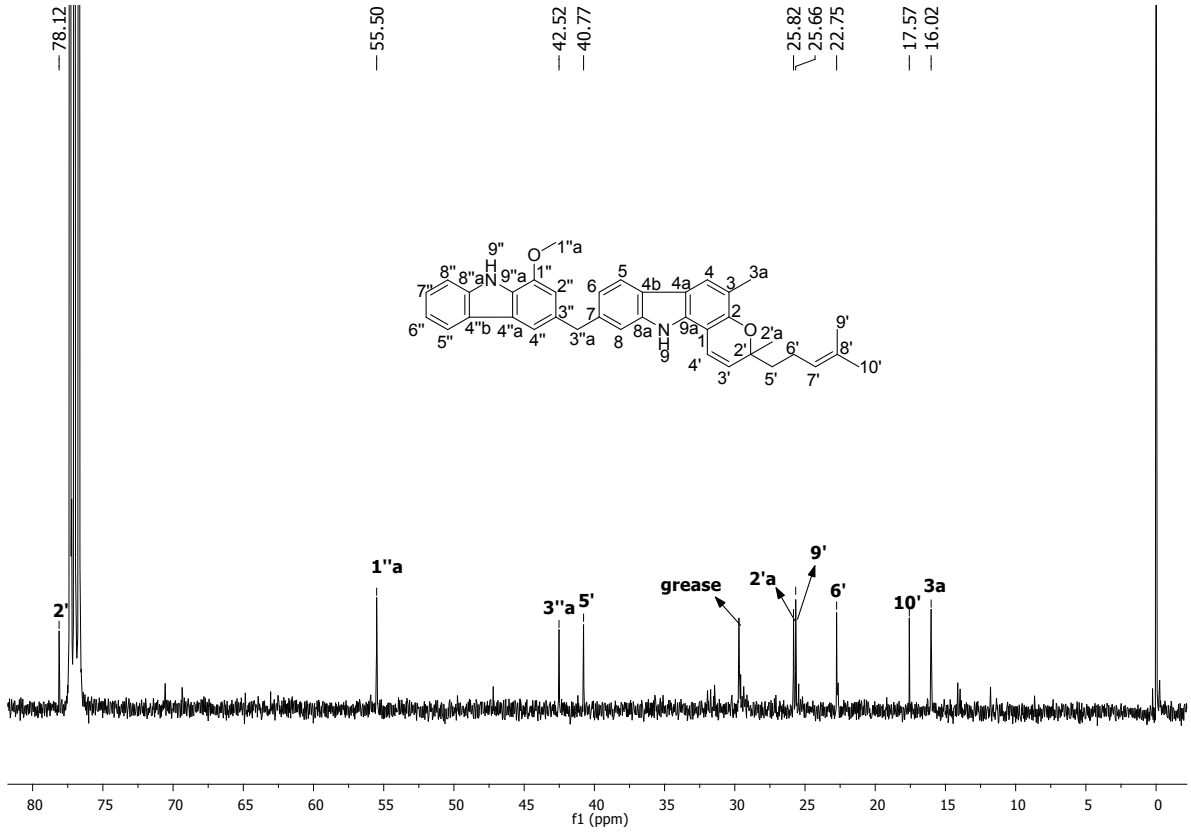


Figure S8: Expansion (102-150 ppm) of ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of murrayakonine A (**1**)

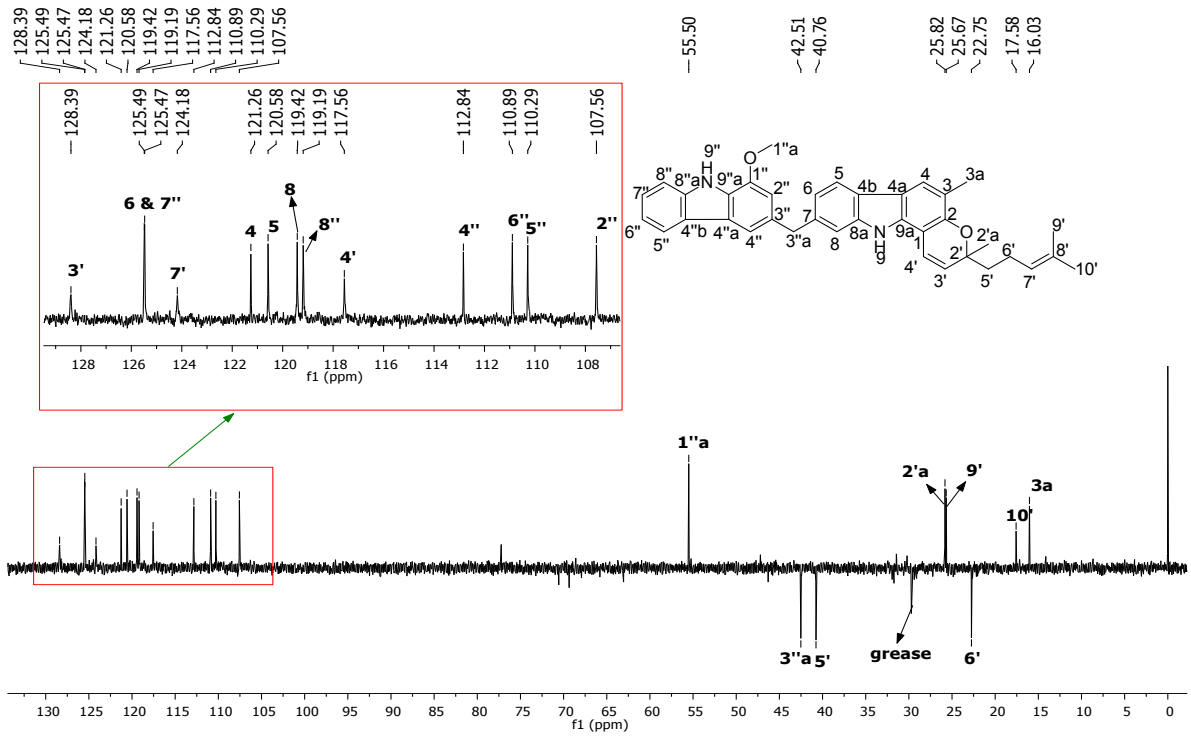


Figure S9: COSY spectrum of murrayakonine A (**1**)

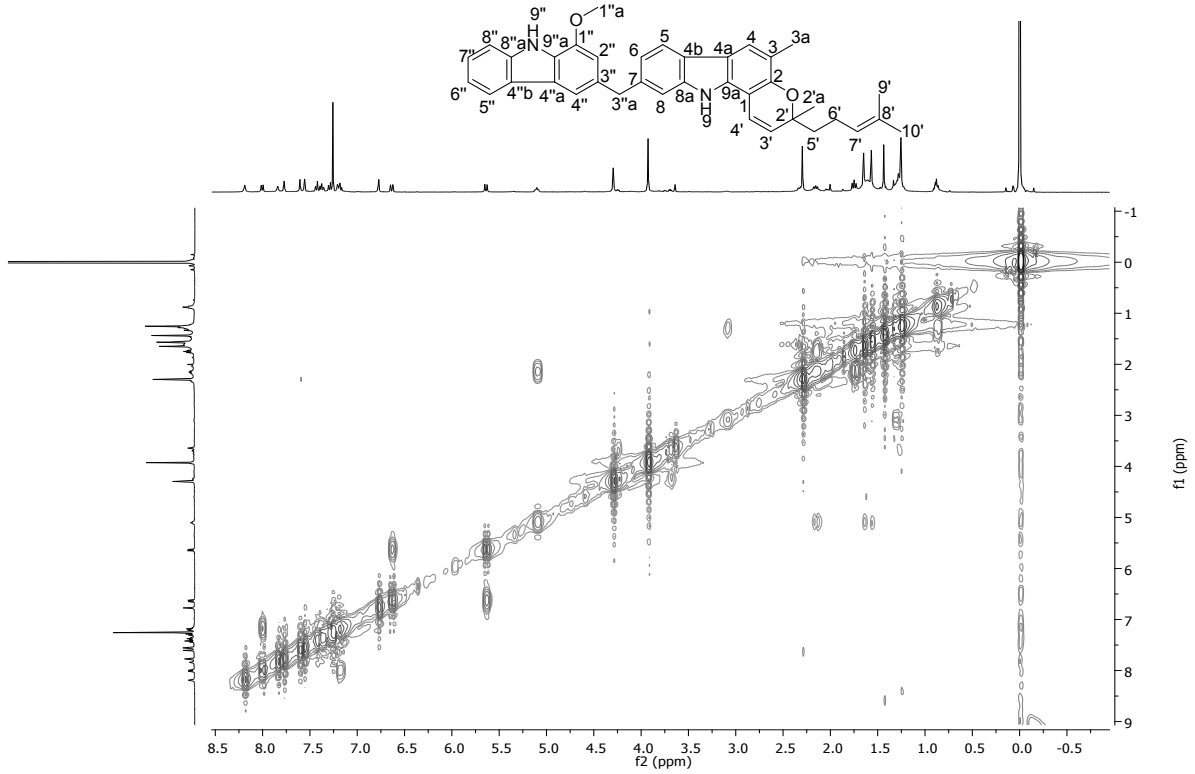


Figure S10: HSQC spectrum of murrayakonine A (**1**)

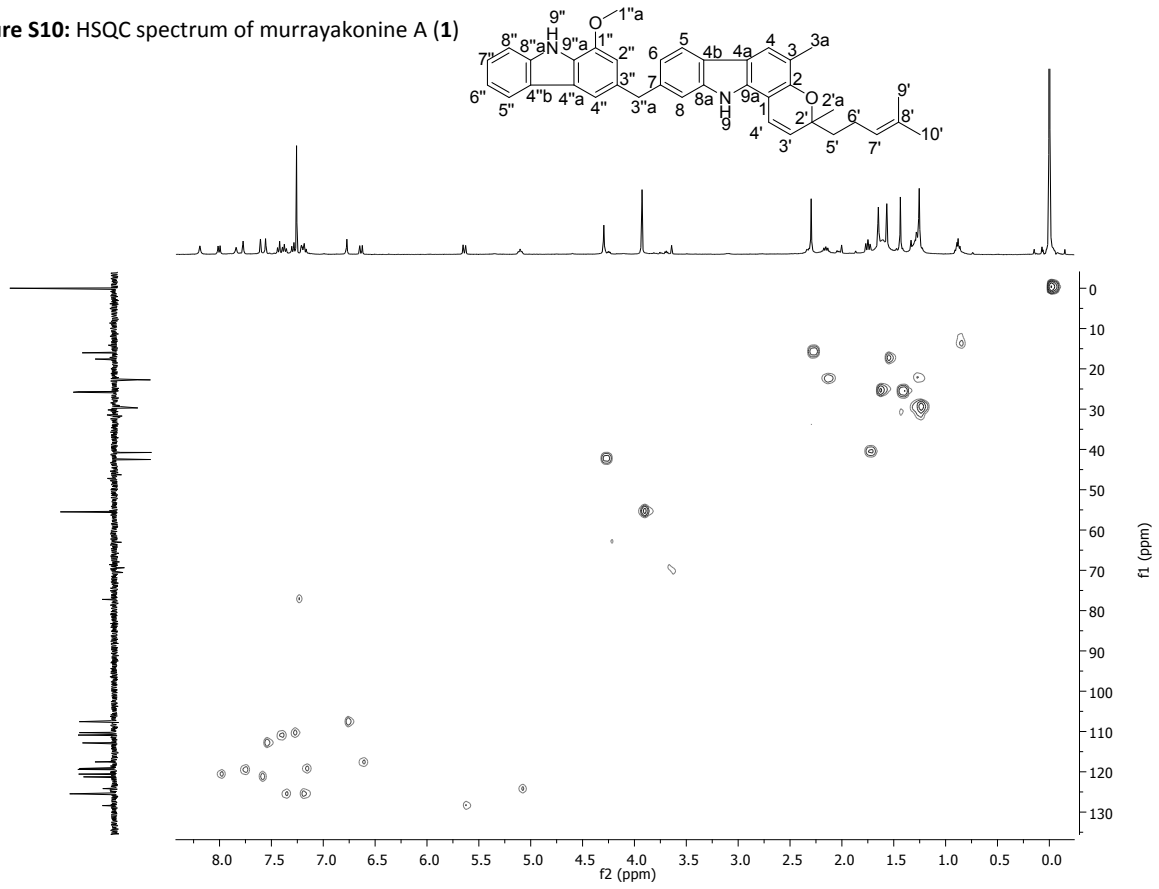


Figure S11: HMBC spectrum of murrayakonine A (**1**)

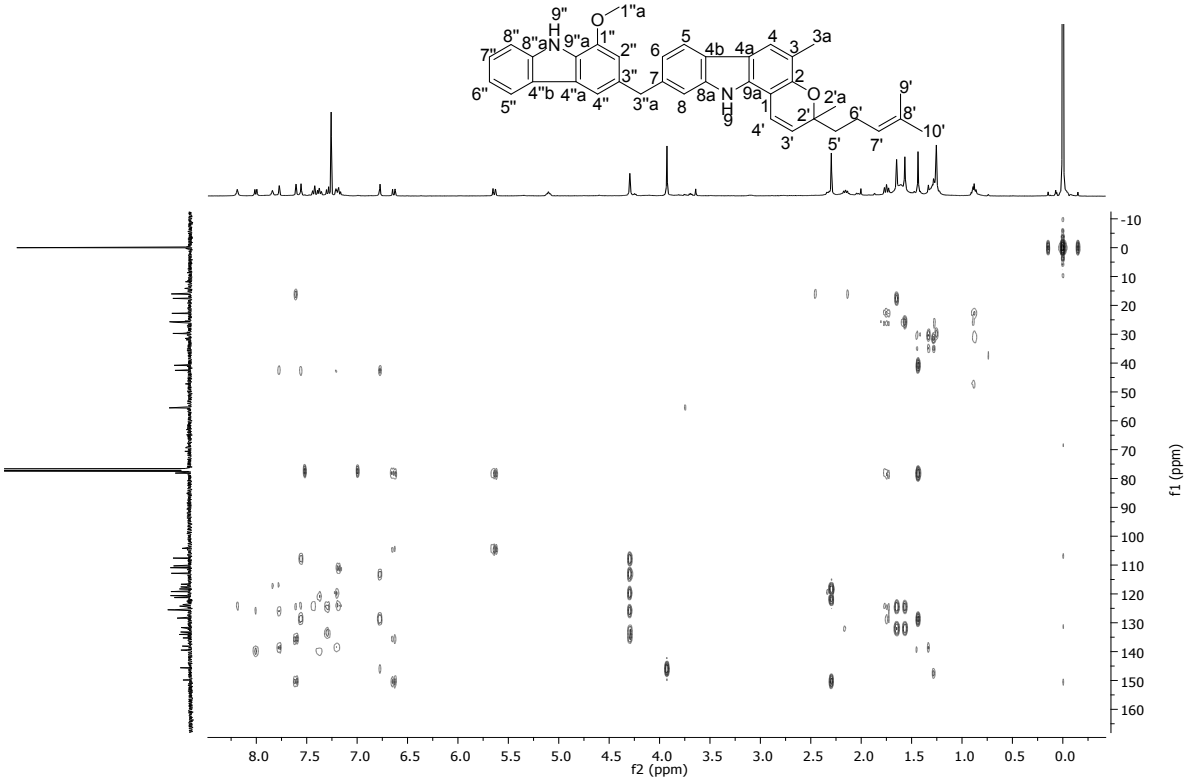


Figure S12: NOESY spectrum of murrayakonine A (**1**)

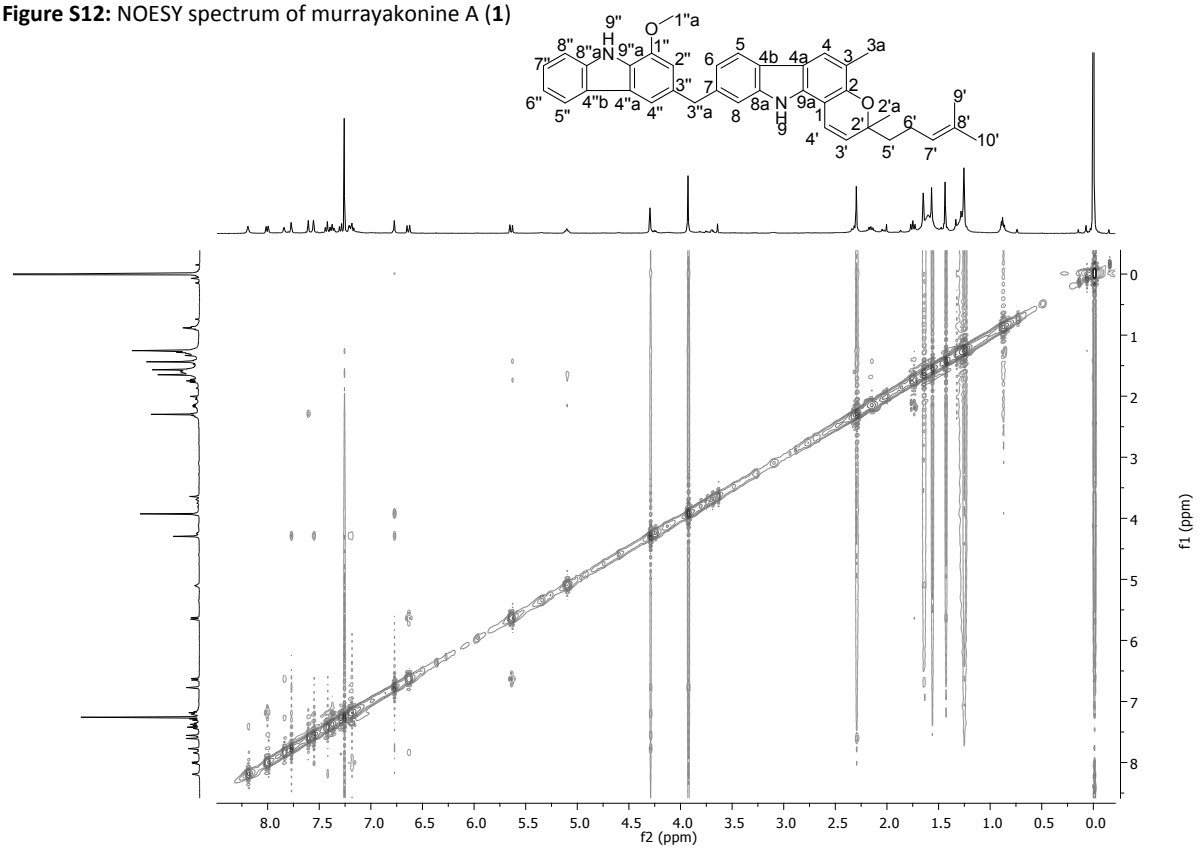


Figure S13: UV spectrum of murrayakonine A (**1**)

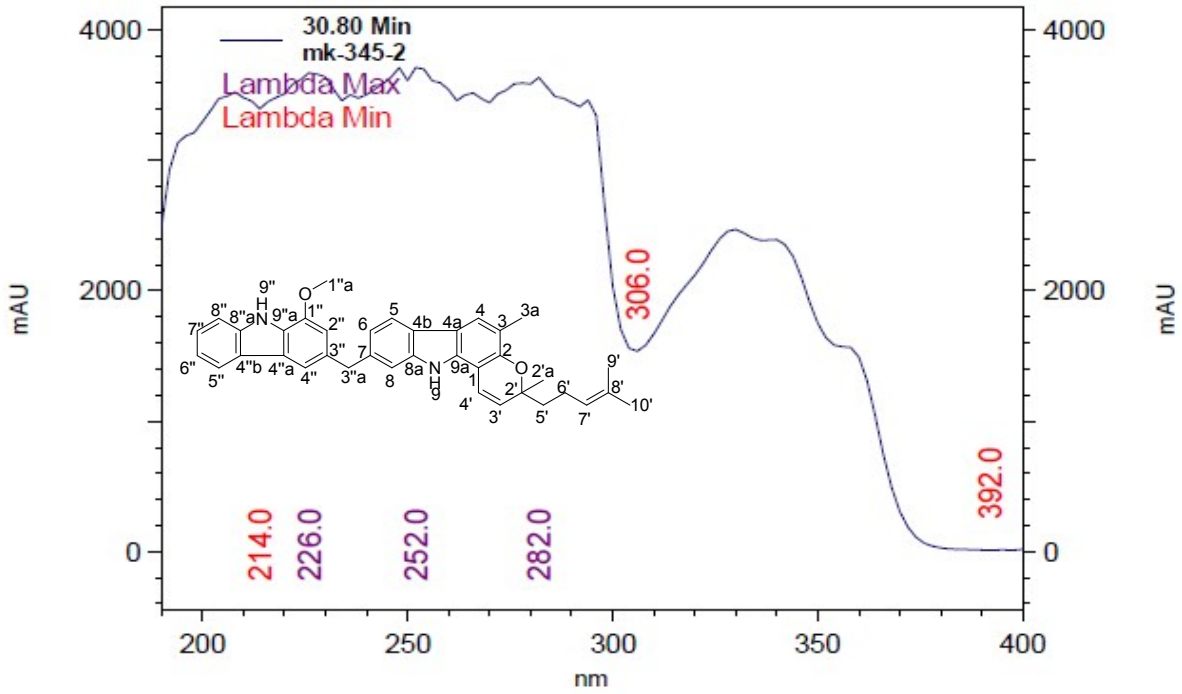


Figure S14: HRESIMS spectroscopic data of murrayakonine B (**2**)

Qualitative Compound Report

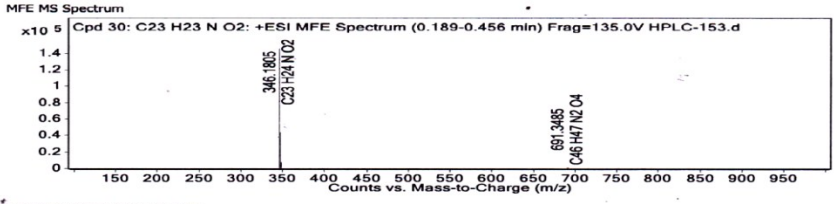
Data File	HPLC-153.d	**Sample Name**	HPLC-153
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-04-2015 PM 4:52:51
IRM Calibration Status	[redacted]	**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition 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 H23 N O2	0.271	345.1731	C23 H23 N O2	C23 H23 N O2	-0.76	C23 H23 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C23 H23 N O2	346.1805	0.271	Find by Molecular Feature	345.1731

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
346.1805	1	145236.5	C23 H24 N O2	(M+H)+
347.1836	1	43624.99	C23 H24 N O2	(M+H)+
348.1863	1	7077.46	C23 H24 N O2	(M+H)+
691.3485	1	749.4	C46 H47 N2 O4	(2M+H)+
692.3578	1	432.72	C46 H47 N2 O4	(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	346.1805	346.1802	-0.95	100	100	74.12	77.43
2	347.1836	347.1835	-0.32	30.04	25.59	22.26	19.82
3	348.1863	348.1865	0.49	4.87	3.55	3.61	2.75

Figure S15: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of murrayakonine B (**2**)

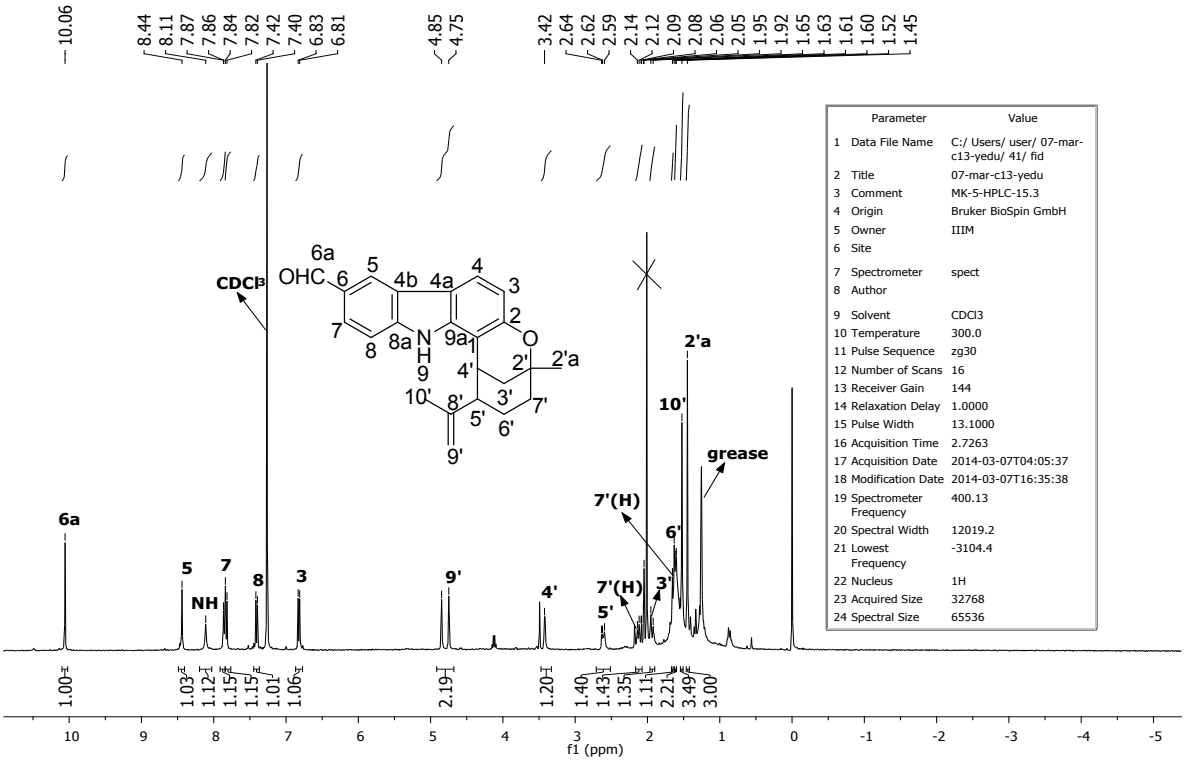


Figure S16: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of murrayakonine B (**2**)

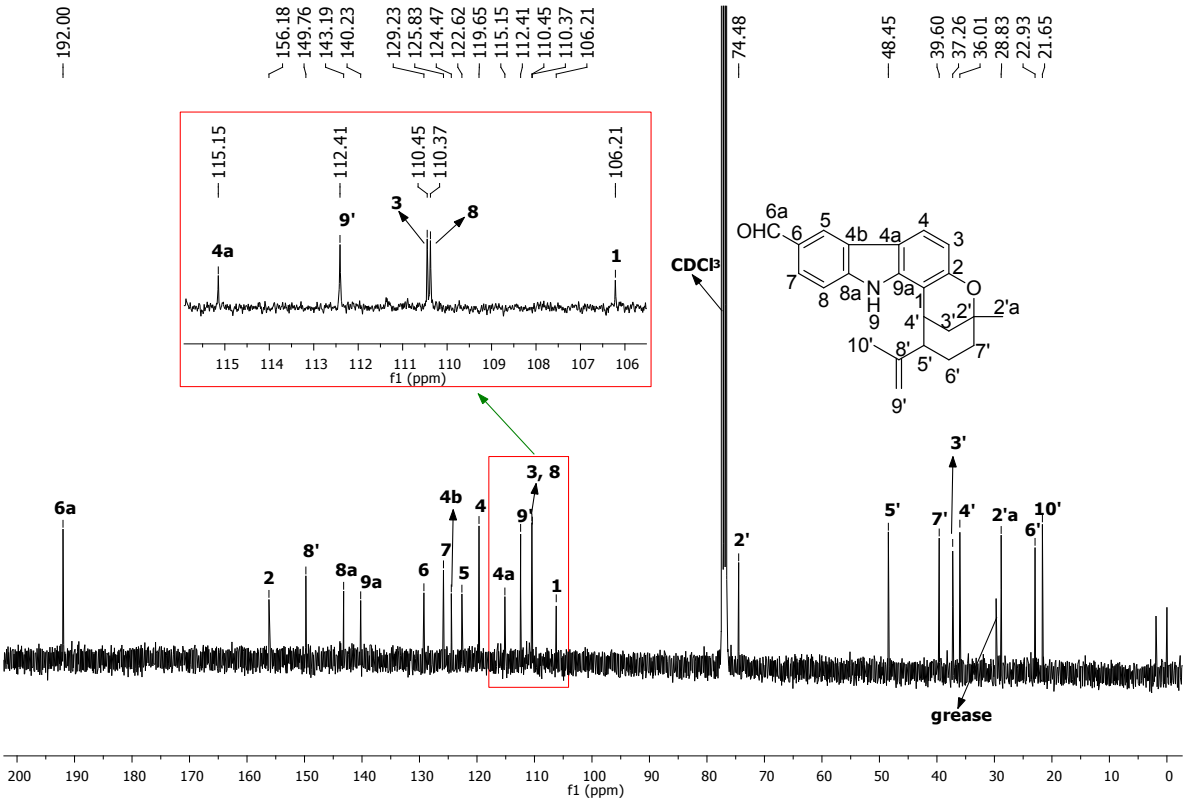


Figure S17: DEPT-135 (100 MHz, $CDCl_3$) spectrum of of murrayakonine B (**2**)

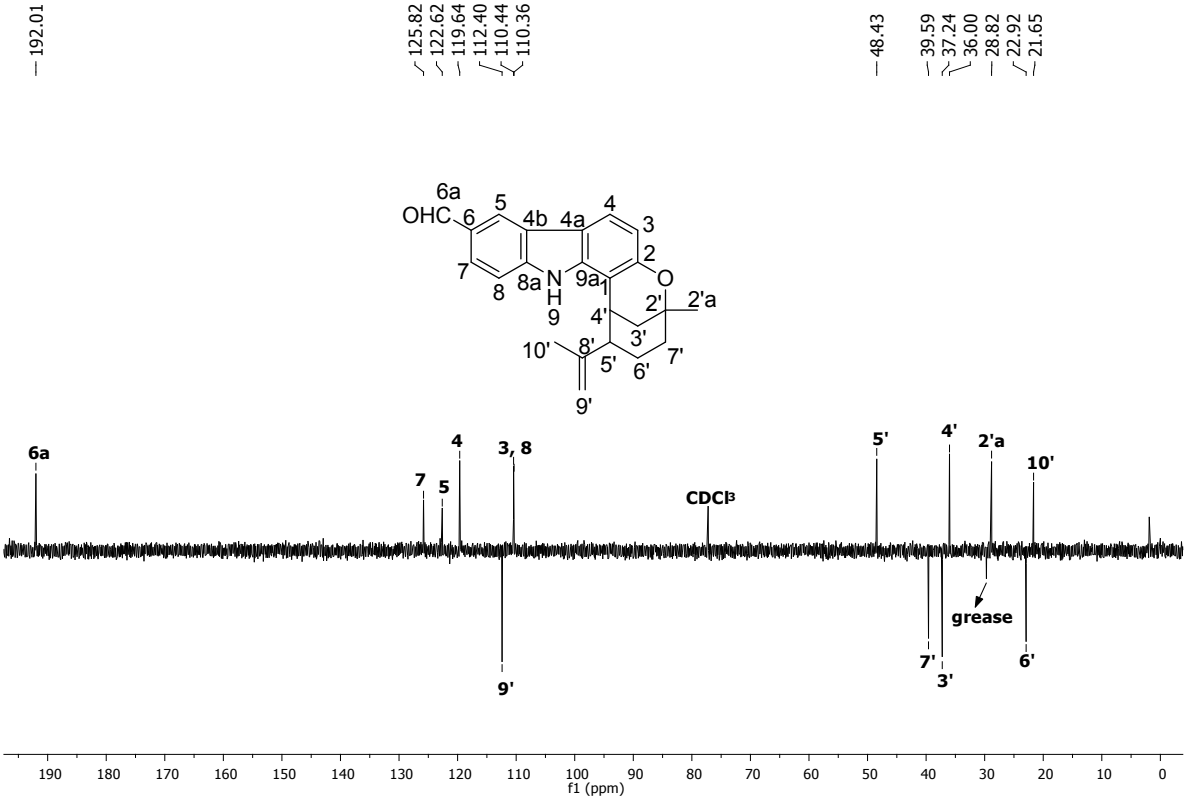


Figure S18: COSY spectrum of murrayakonine B (**2**)

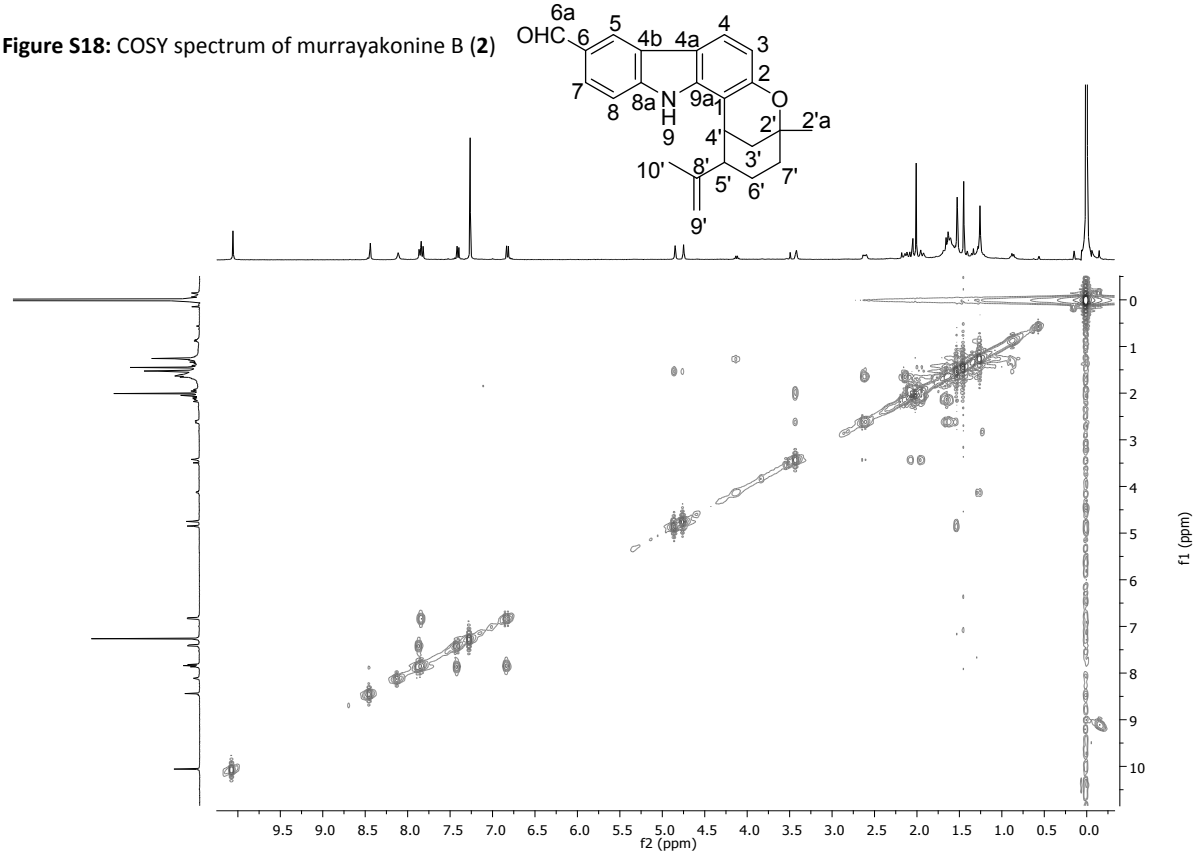


Figure S19: HSQC spectrum of murrayakonine B (**2**)

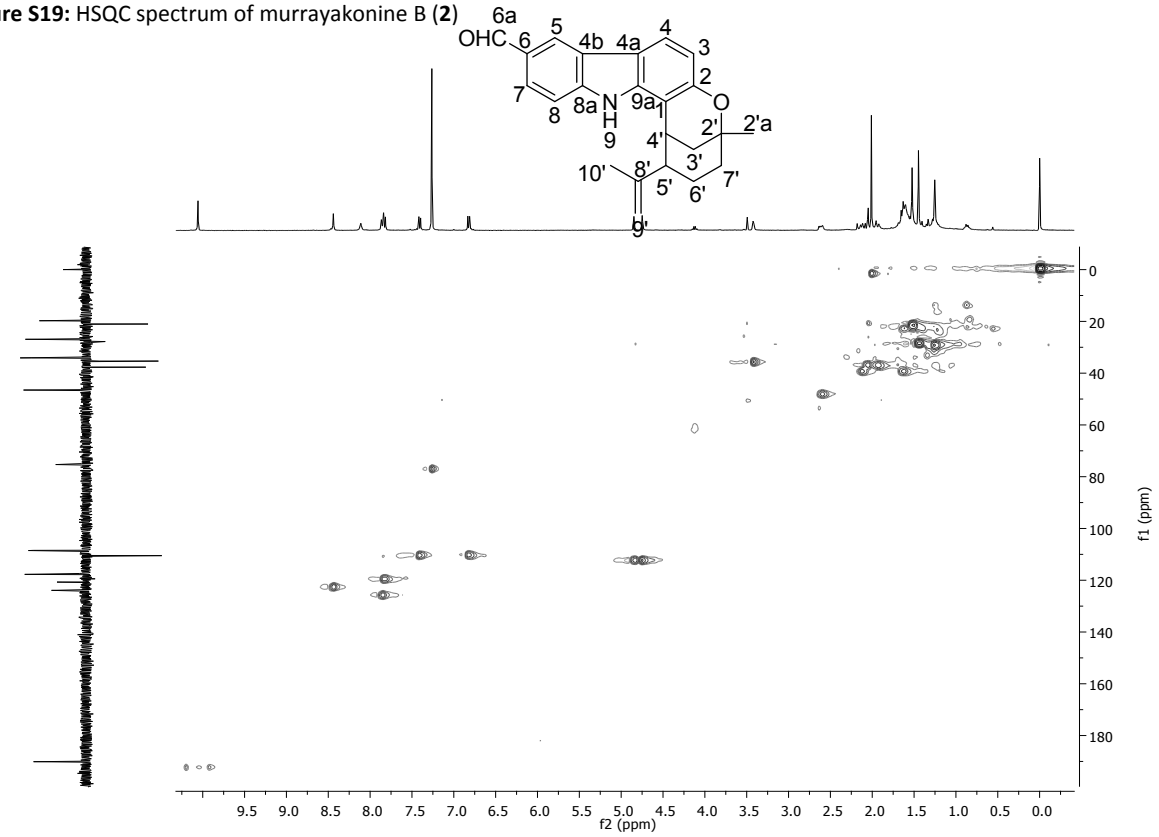


Figure S20: HMBC spectrum of murrayakonine B (**2**)

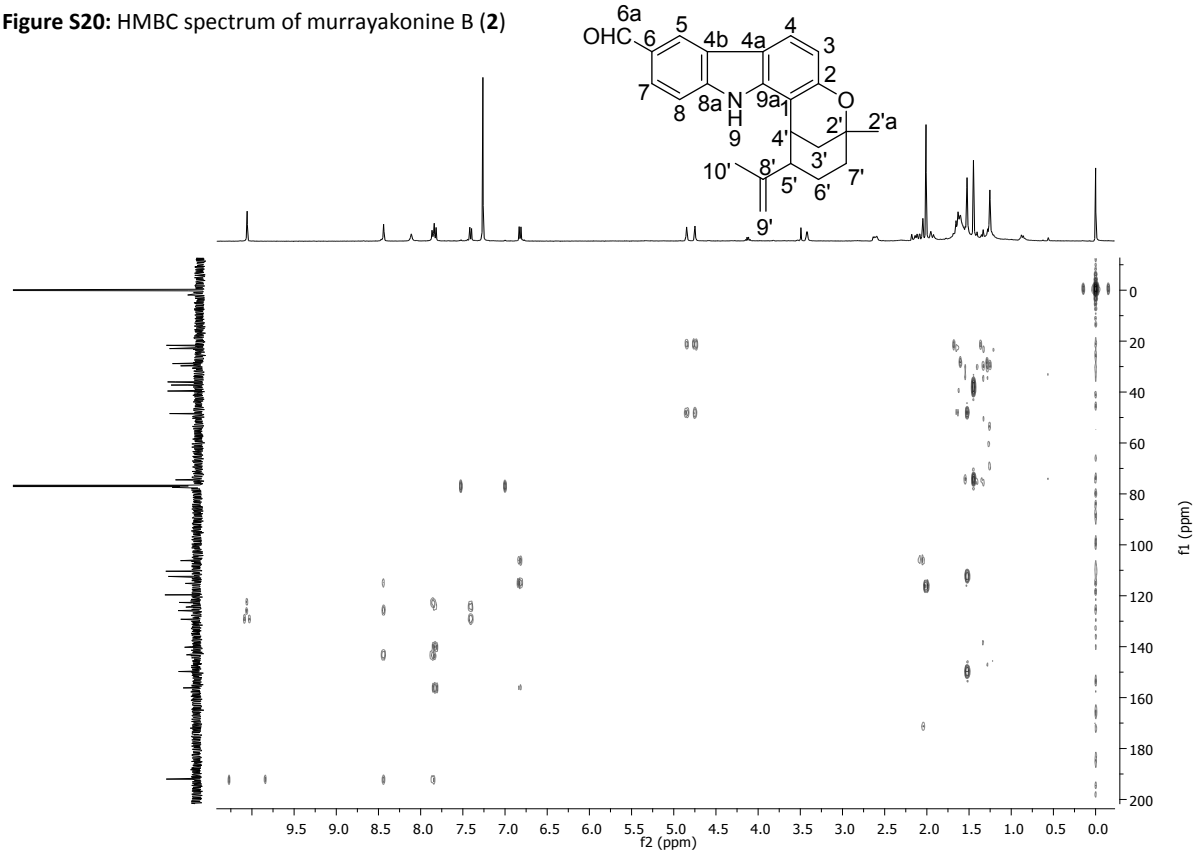


Figure S21: UV spectrum of murrayakonine B (**2**)

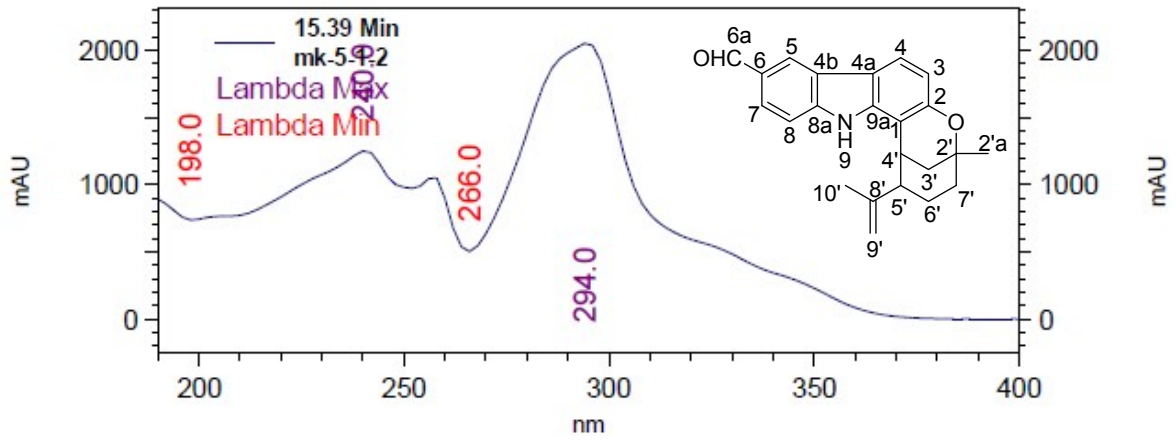


Figure S22: HPLC chromatogram of Sub fraction Fr.2.5 (Semi preparative HPLC Eclipse XDB-C-18; 5µm, 250x9.4 mm; 100%ACN, 30 min; 1 mL/min)

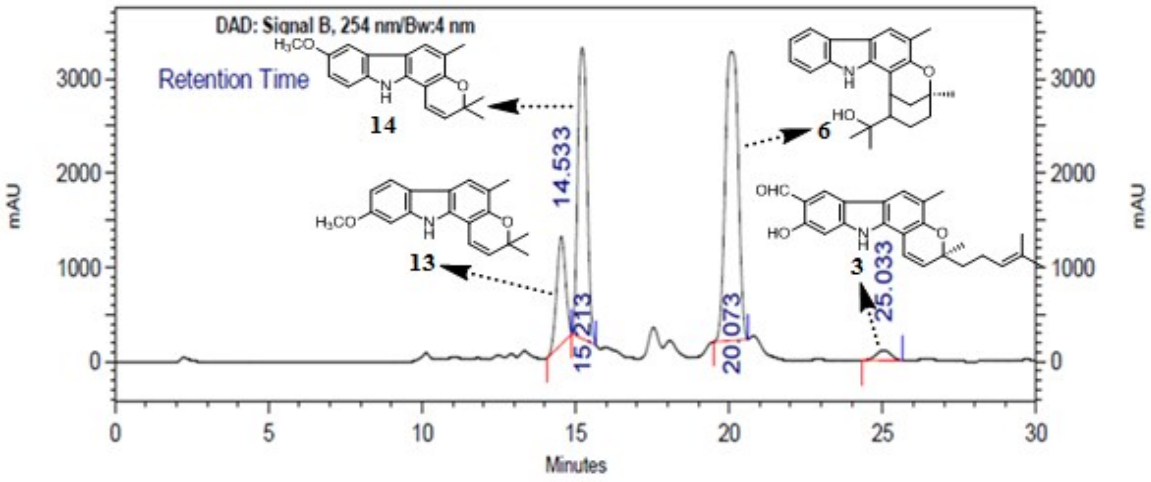


Figure S23: HPLC chromatogram of sub fraction Fr.4.3 (Semi preparative HPLC Eclipse XDB-C-18; 5µm, 250x9.4 mm; 100%ACN, 15 min; 1 mL/min)

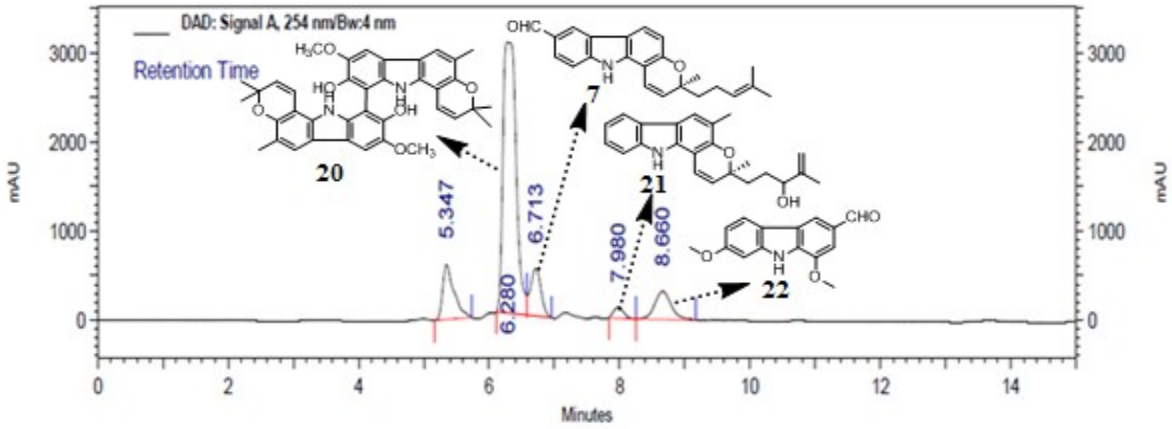
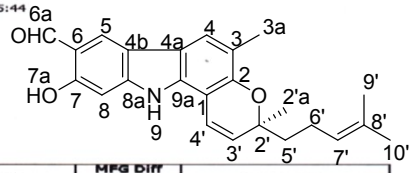


Figure S24: HRESIMS spectroscopic data of murrayakonine C (**3**)

Qualitative Compound Report

Data File	LH20-4.d	**Sample Name**	LH20-4
Sample Type	Sample	**Position**	Vial 19
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-04-2015 PM 5:05:44
IRM Calibration Status		**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

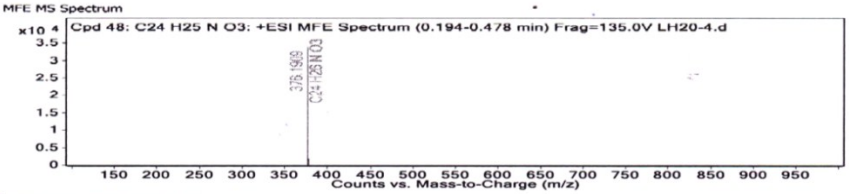


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 48: C24 H25 N O3	0.274	375.1838	C24 H25 N O3	C24 H25 N O3	-0.83	C24 H25 N O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 48: C24 H25 N O3	376.1909	0.274	Find by Molecular Feature	375.1838

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
376.1909	1	33656.43	C24 H26 N O3	(M+H)+
377.1945	1	10939.08	C24 H26 N O3	(M+H)+
378.1988	1	1817.45	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	376.1909	376.1907	-0.47	100	100	72.52	76.46
2	377.1945	377.194	-1.24	32.5	26.74	23.57	20.44
3	378.1988	378.197	-4.89	5.4	4.05	3.92	3.1

--- End Of Report ---

Figure S25: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of murrayakonine C (**3**)

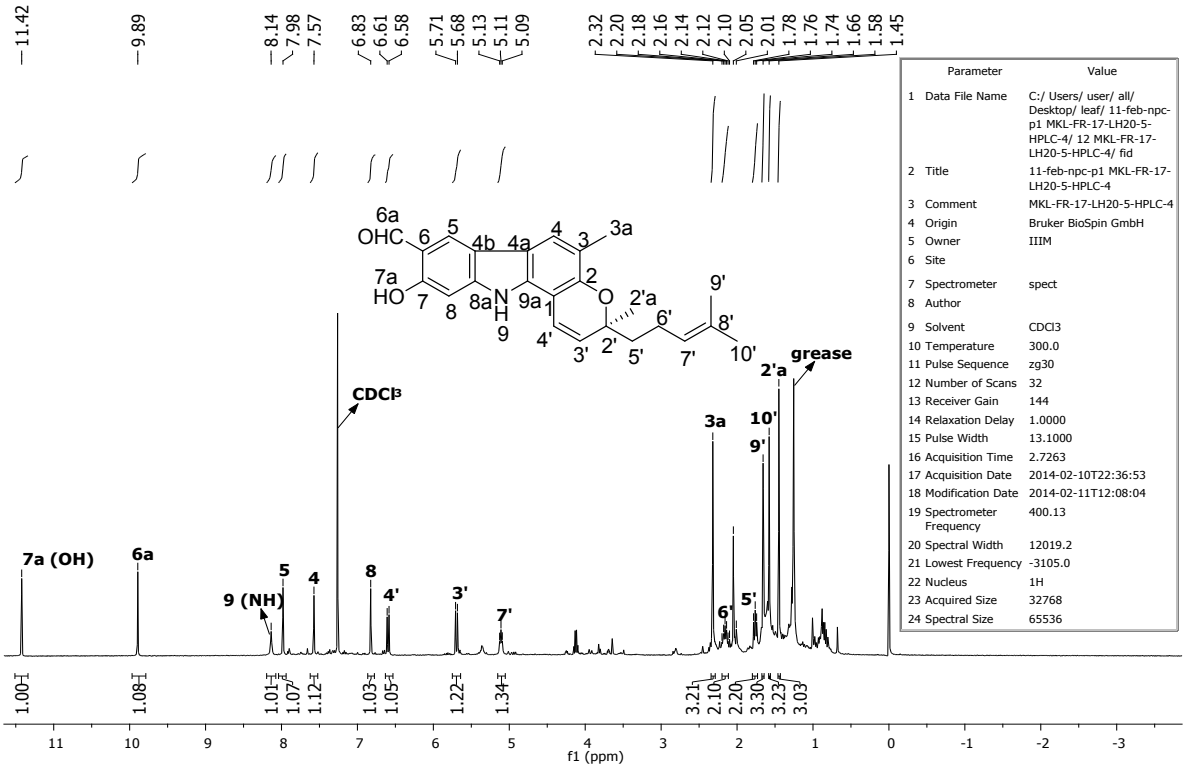


Figure S26: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of murrayakonine C (**3**)

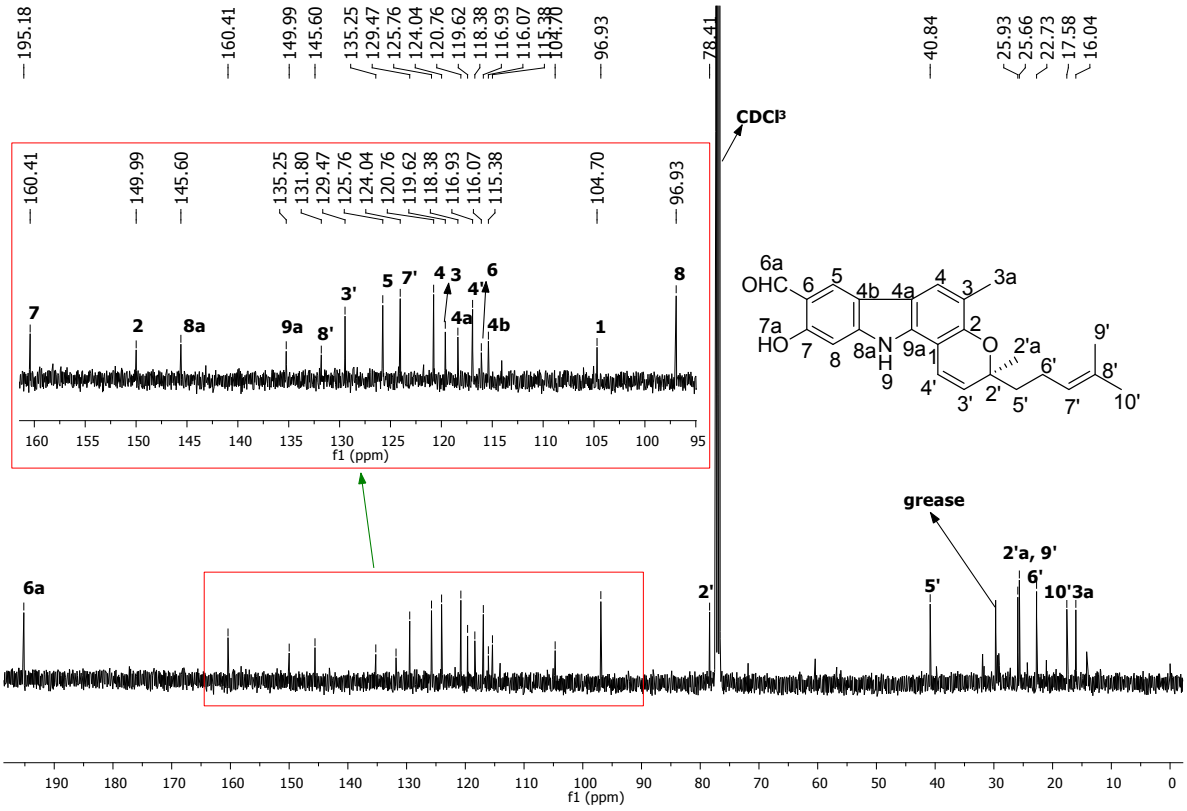


Figure S27: DEPT-135 (100 MHz, $CDCl_3$) spectrum of murrayakonine C (**3**)

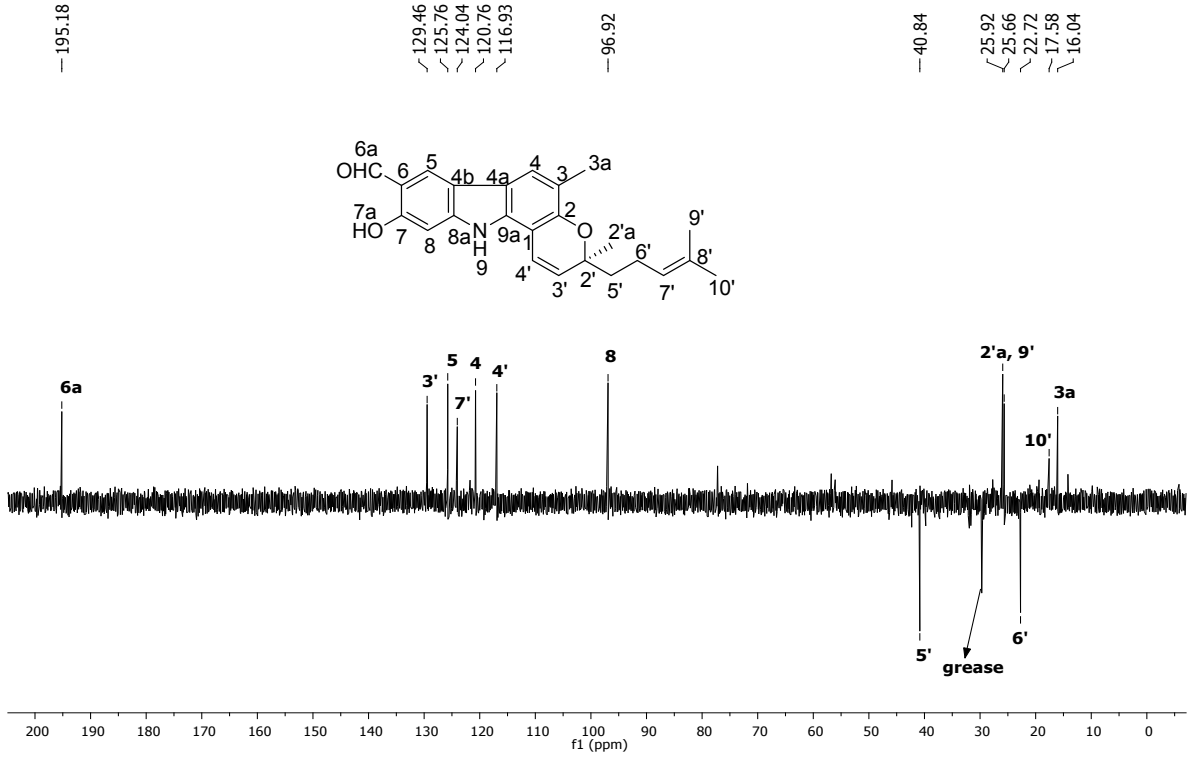
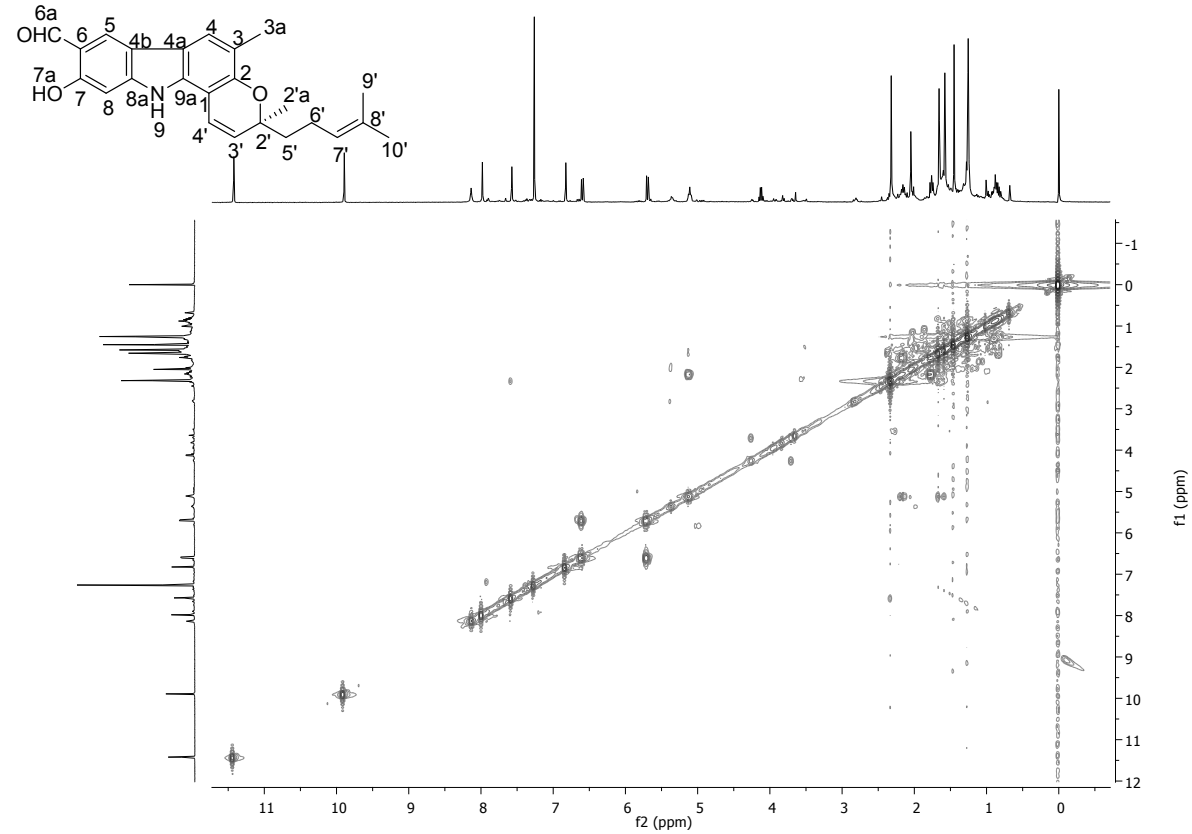


Figure S28: COSY spectrum of murrayakonine C (**3**)



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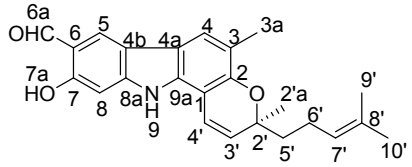


re S29: HSQC spectrum of murrayakonine C (**3**)

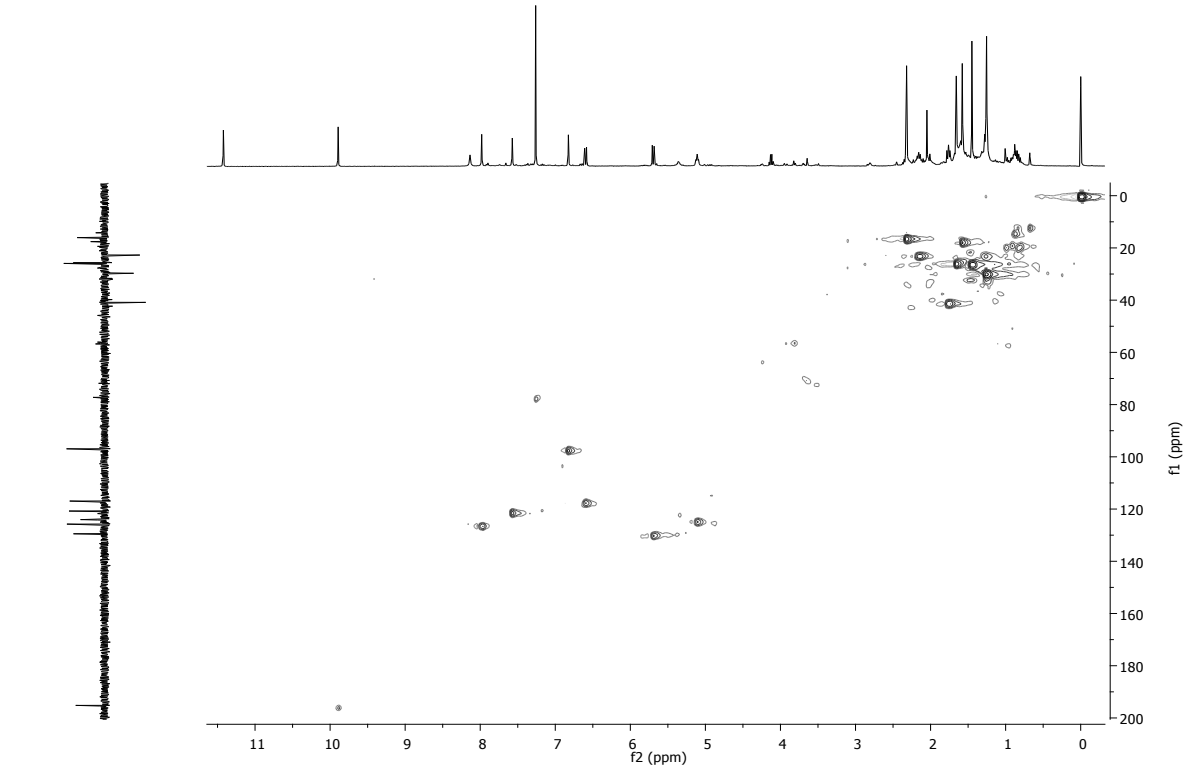


Figure S30: HMBC spectrum of murrayakonine C (**3**)

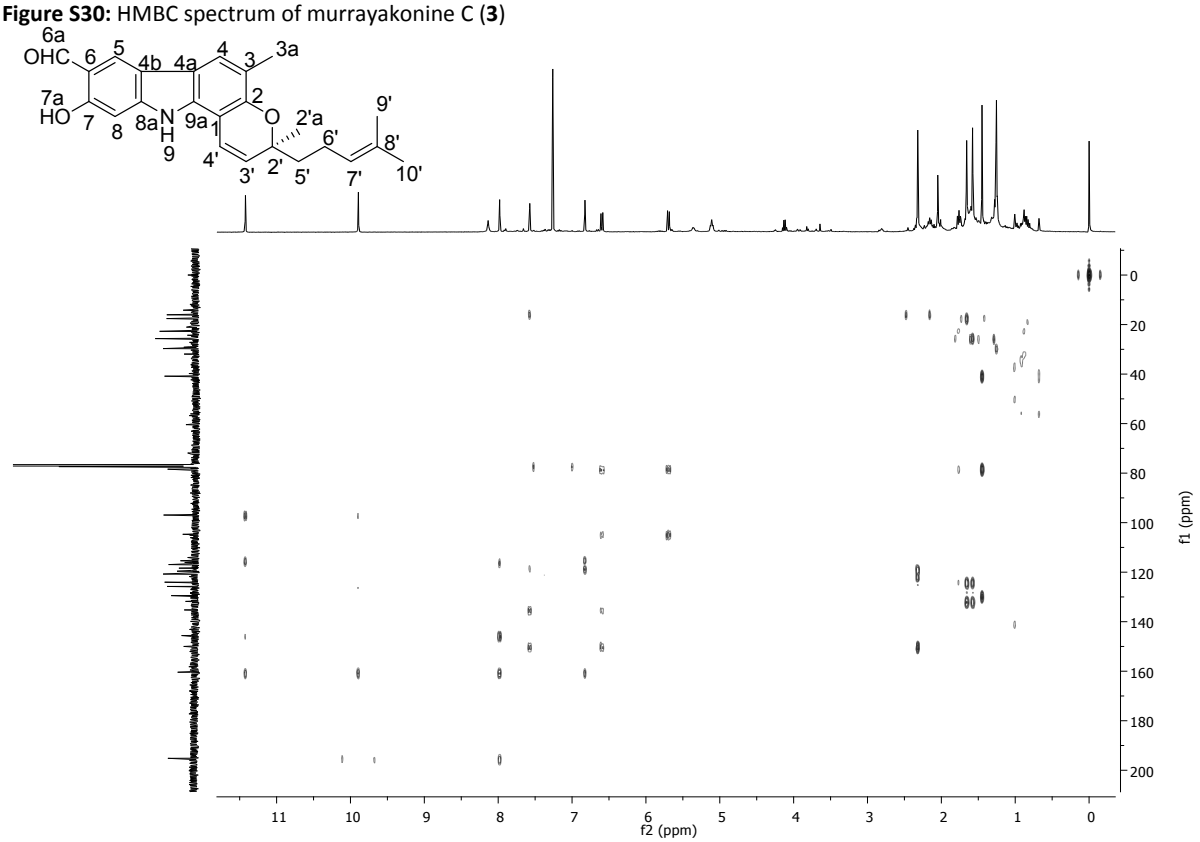


Figure S31: NOESY spectrum of murrayakonine C (**3**)

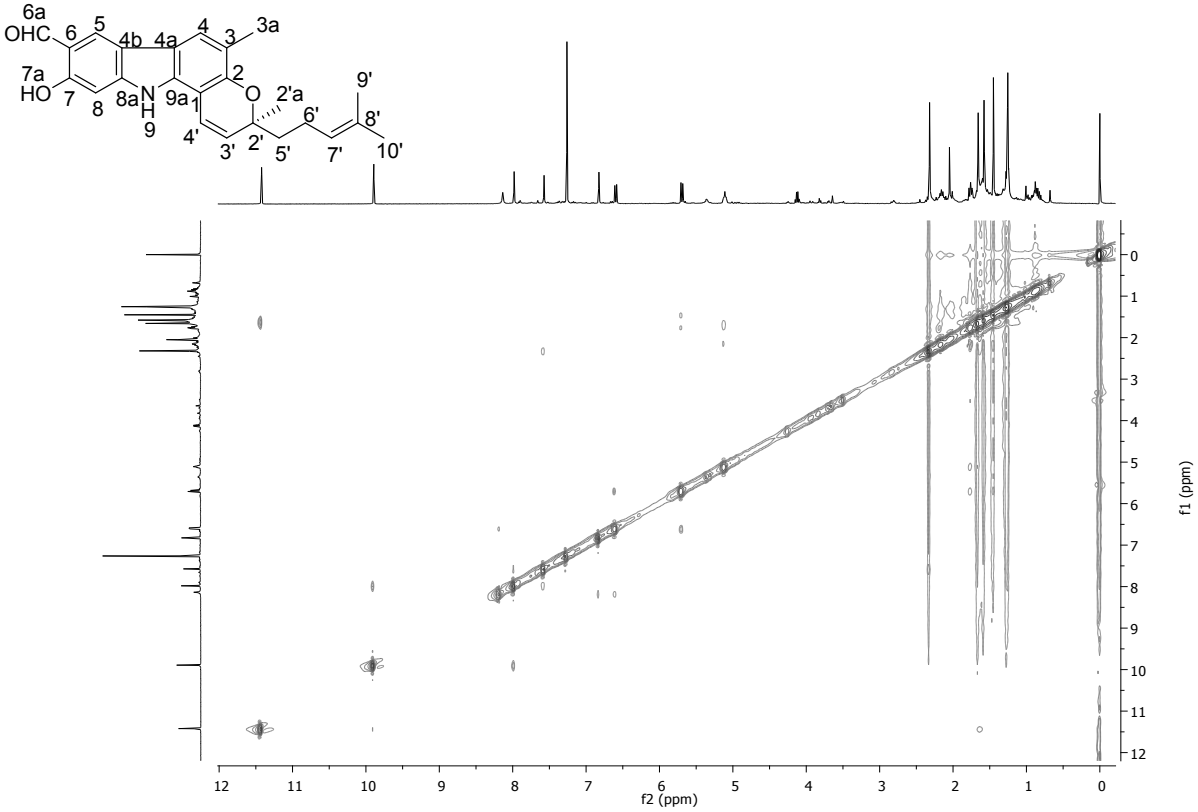


Figure S32: UV spectrum of murrayakonine C (**3**)

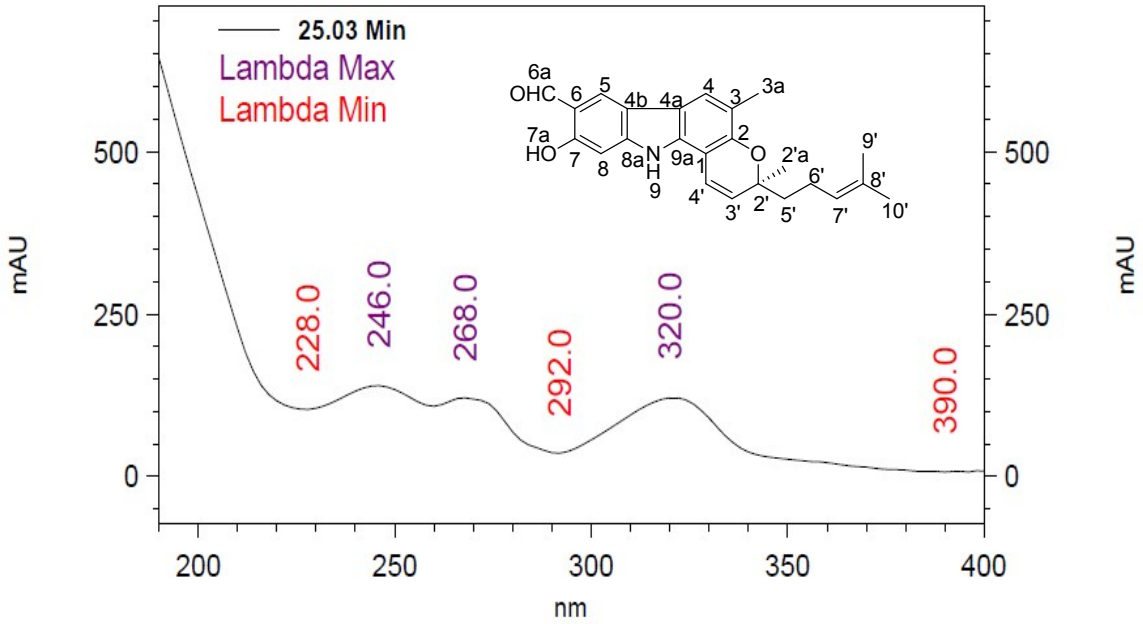


Figure S33: CD spectrum (in MeOH) of murrayakonine C (**3**)

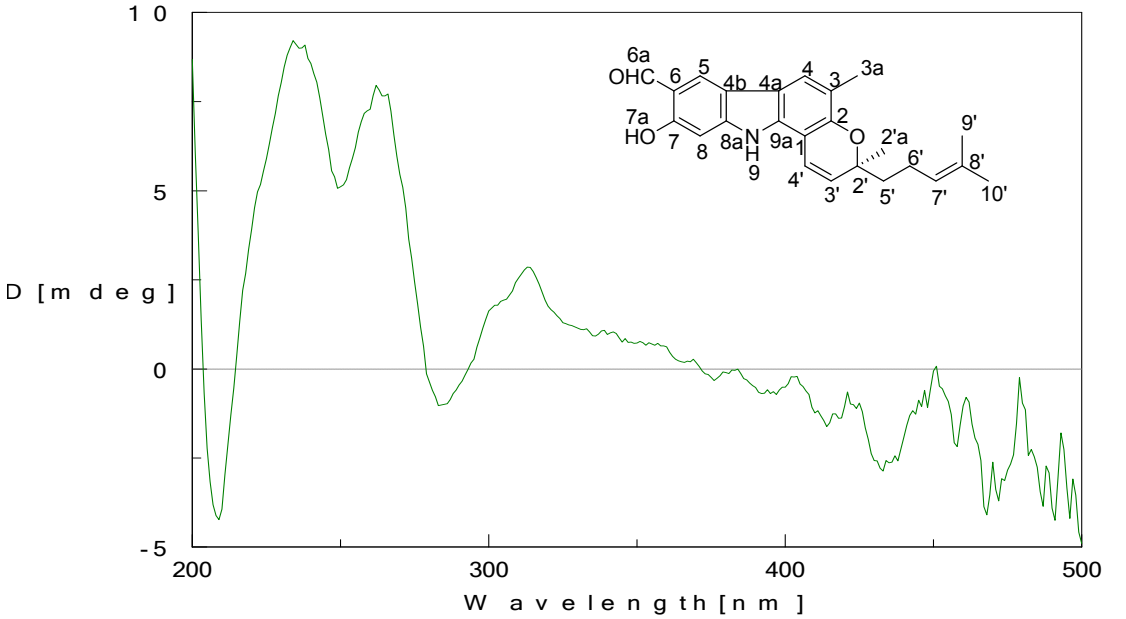
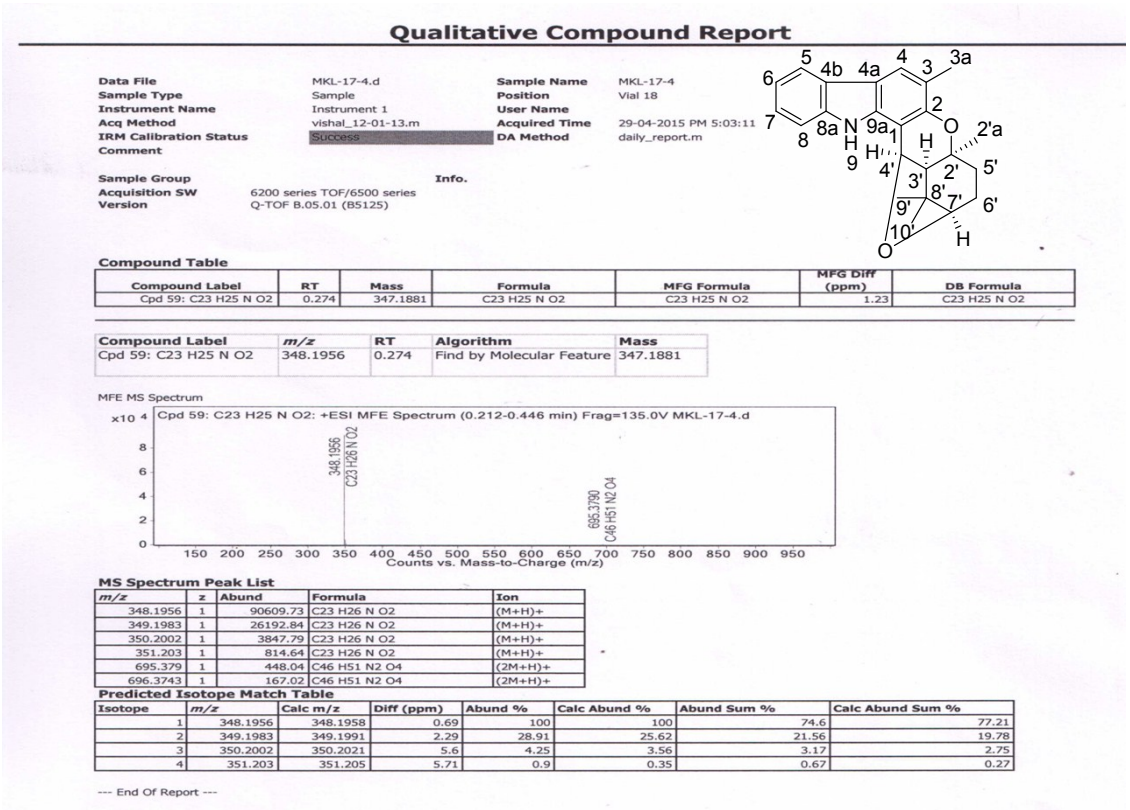


Figure S34: HRESIMS spectroscopic data of murrayakonine D (**4**)



Qualitative Compound Report

Data File	MKL-17-4.d	**Sample Name**	MKL-17-4
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-04-2015 PM 5:03:11
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 59: C23 H25 N O2	0.274	347.1881	C23 H25 N O2	C23 H25 N O2	1.23	C23 H25 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 59: C23 H25 N O2	348.1956	0.274	Find by Molecular Feature	347.1881

MFE MS Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
348.1956	1	90609.73	C23 H26 N O2	(M+H)+
349.1983	1	26192.84	C23 H26 N O2	(M+H)+
350.2002	1	3847.79	C23 H26 N O2	(M+H)+
351.203	1	814.64	C23 H26 N O2	(M+H)+
695.379	1	448.04	C46 H51 N2 O4	(2M+H)+
696.3743	1	167.02	C46 H51 N2 O4	(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	348.1956	348.1958	0.69	100	100	74.6	77.21
2	349.1983	349.1991	2.29	28.91	25.62	21.56	19.78
3	350.2002	350.2021	5.6	4.25	3.56	3.17	2.75
4	351.203	351.205	5.71	0.9	0.35	0.67	0.27

--- End Of Report ---

Figure S35: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of murrayakonine D (**4**)

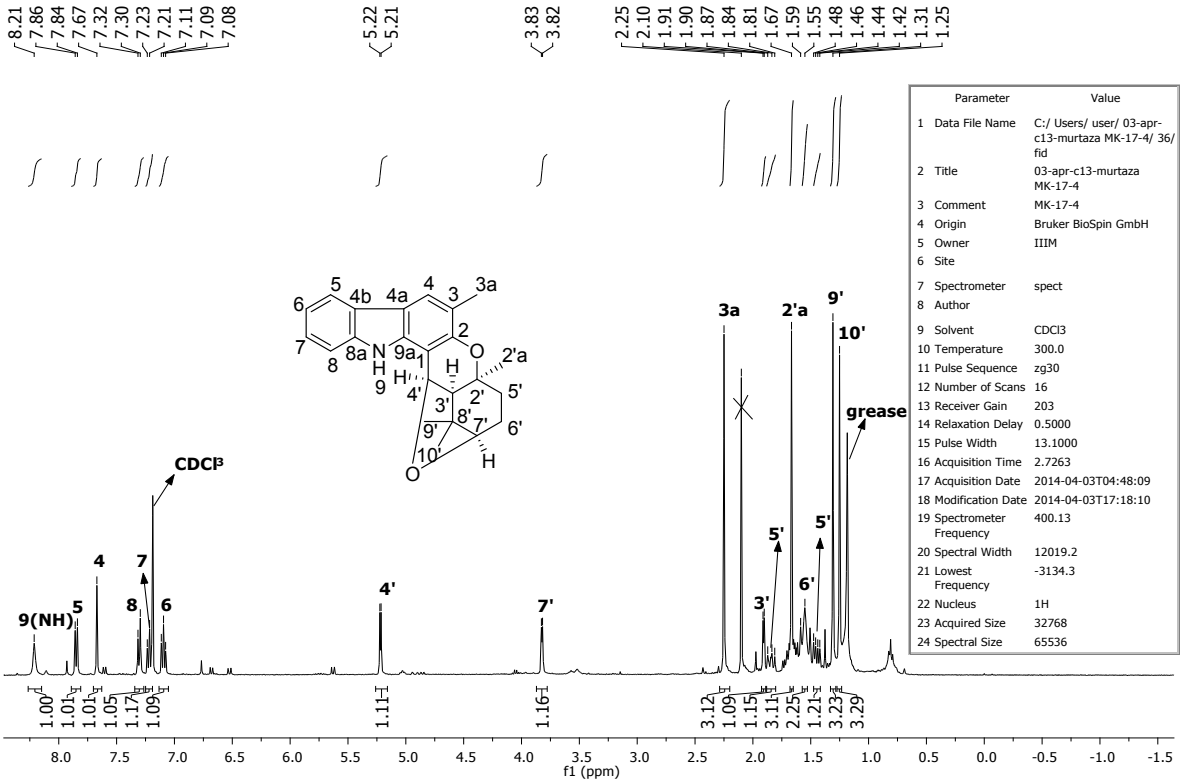


Figure S36: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of murrayakonine D (**4**)

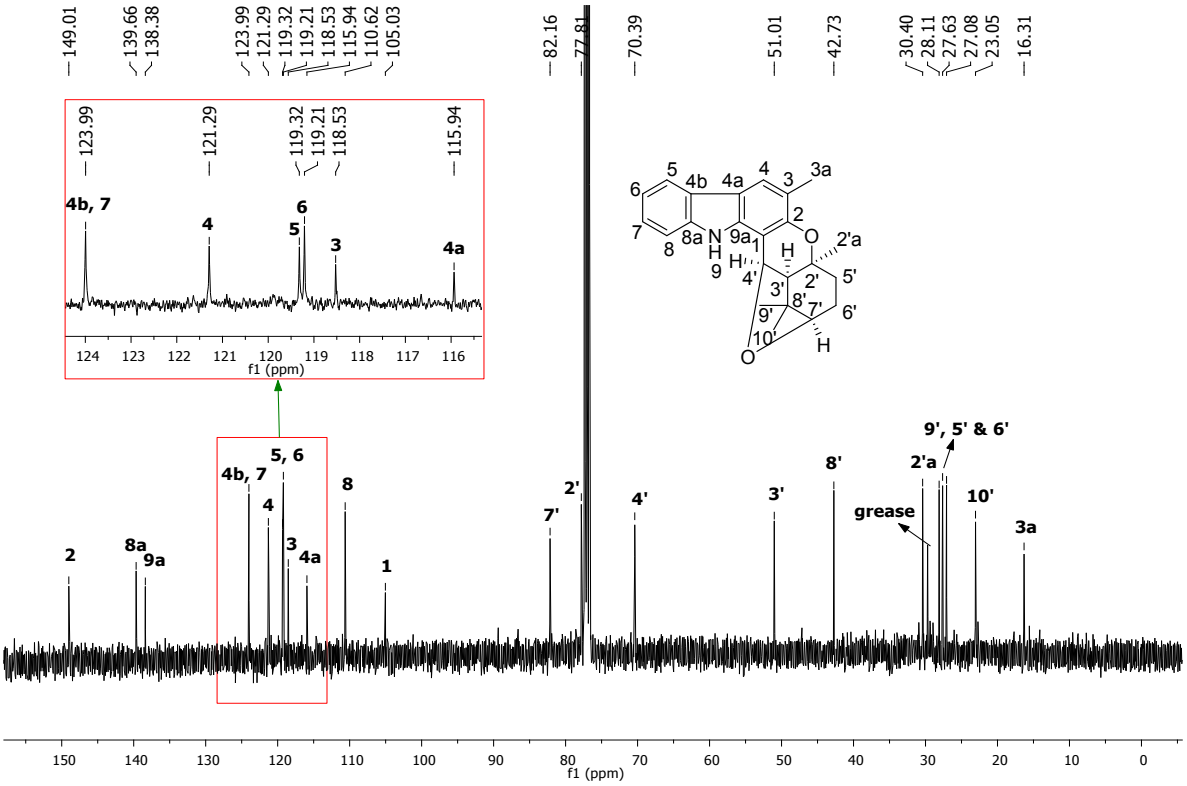


Figure S37: DEPT-135 (100 MHz, $CDCl_3$) spectrum of murrayakonine D (**4**)

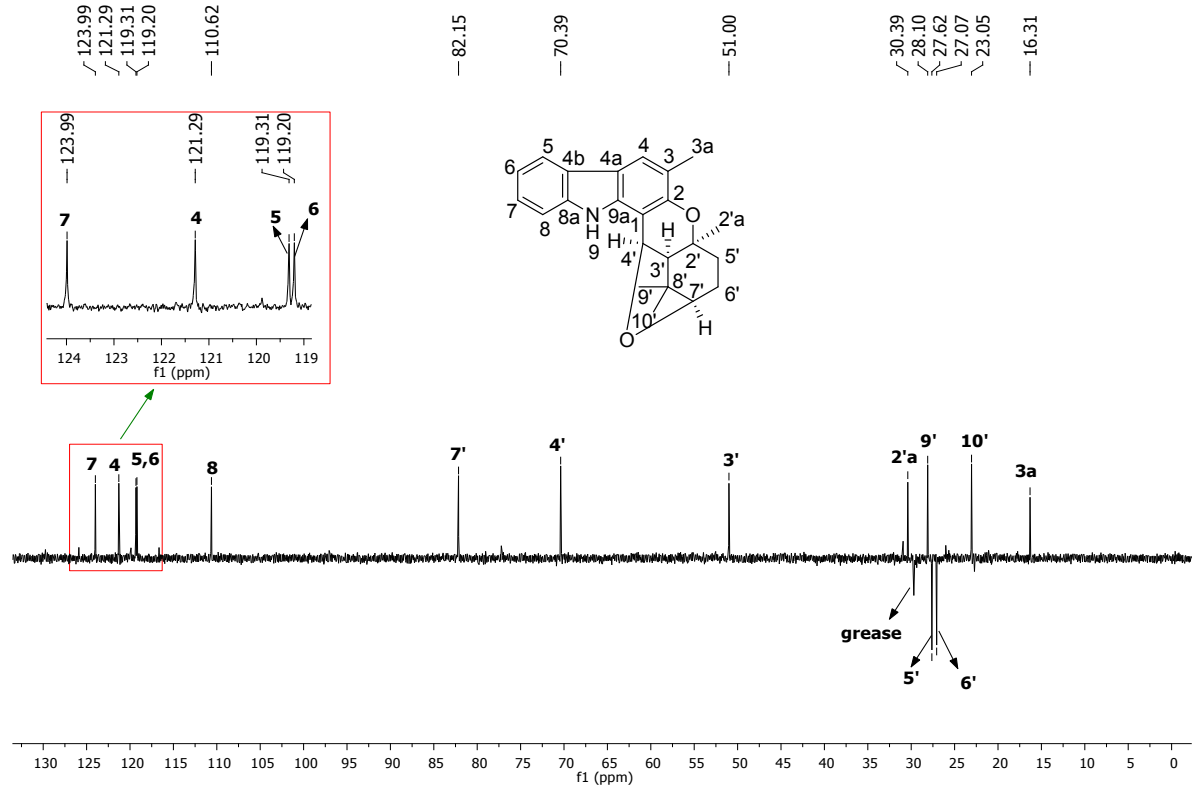


Figure S38: COSY spectrum of murrayakonine D (**4**)

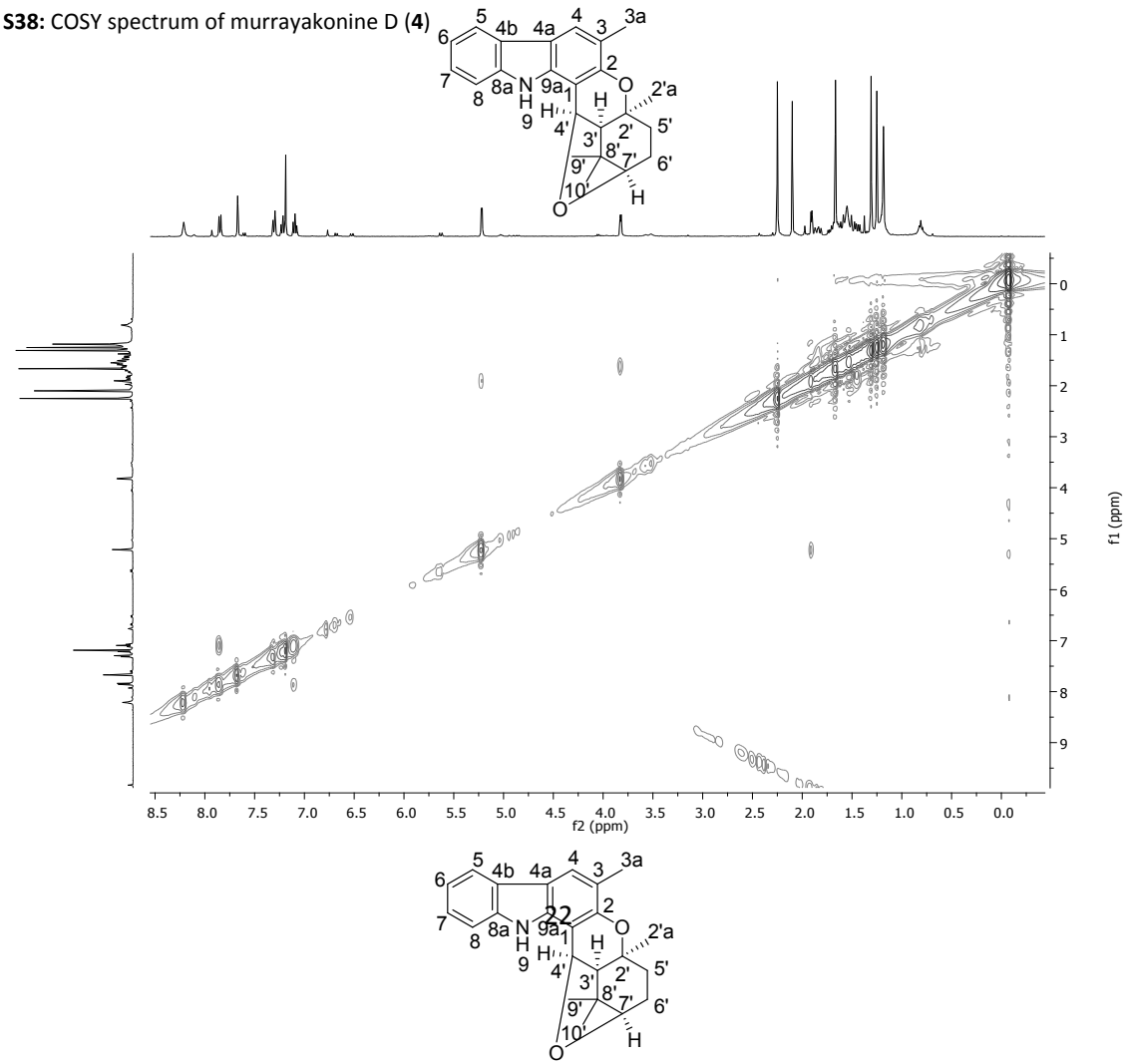


Figure S39: HSQC spectrum of murrayakonine D (**4**)

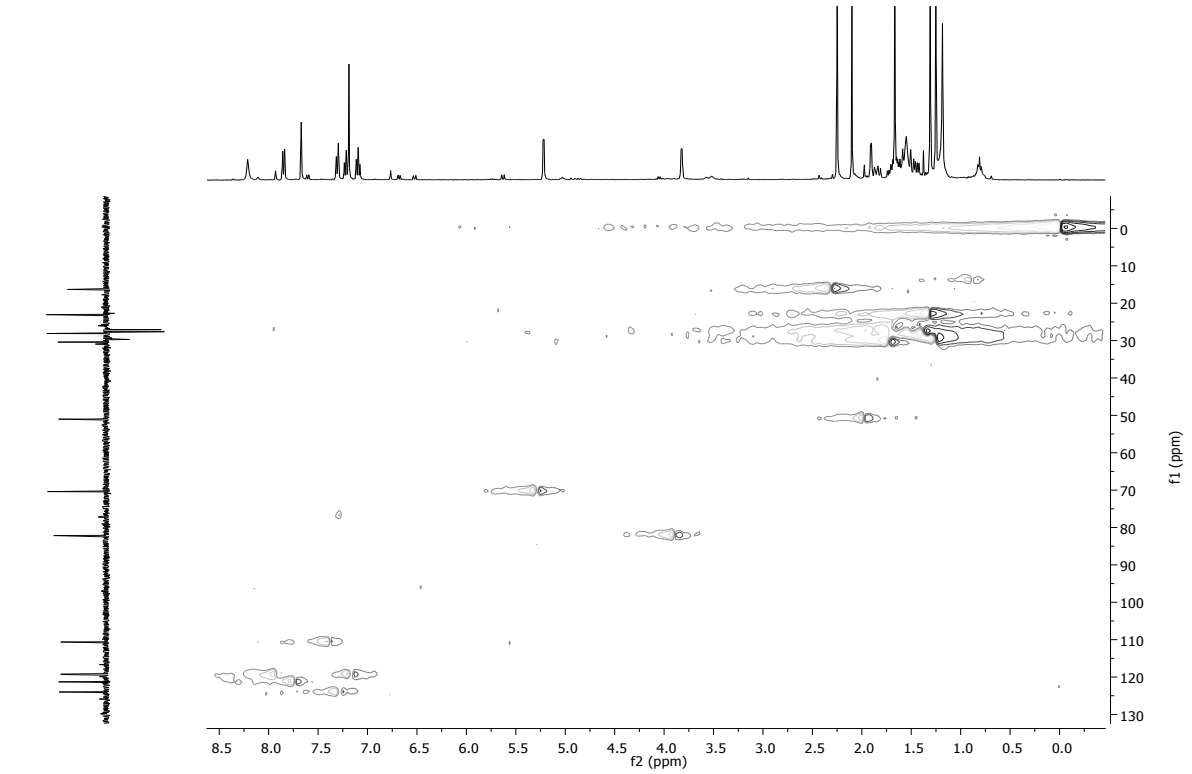


Figure S40: HMBC spectrum of murrayakonine D (**4**)

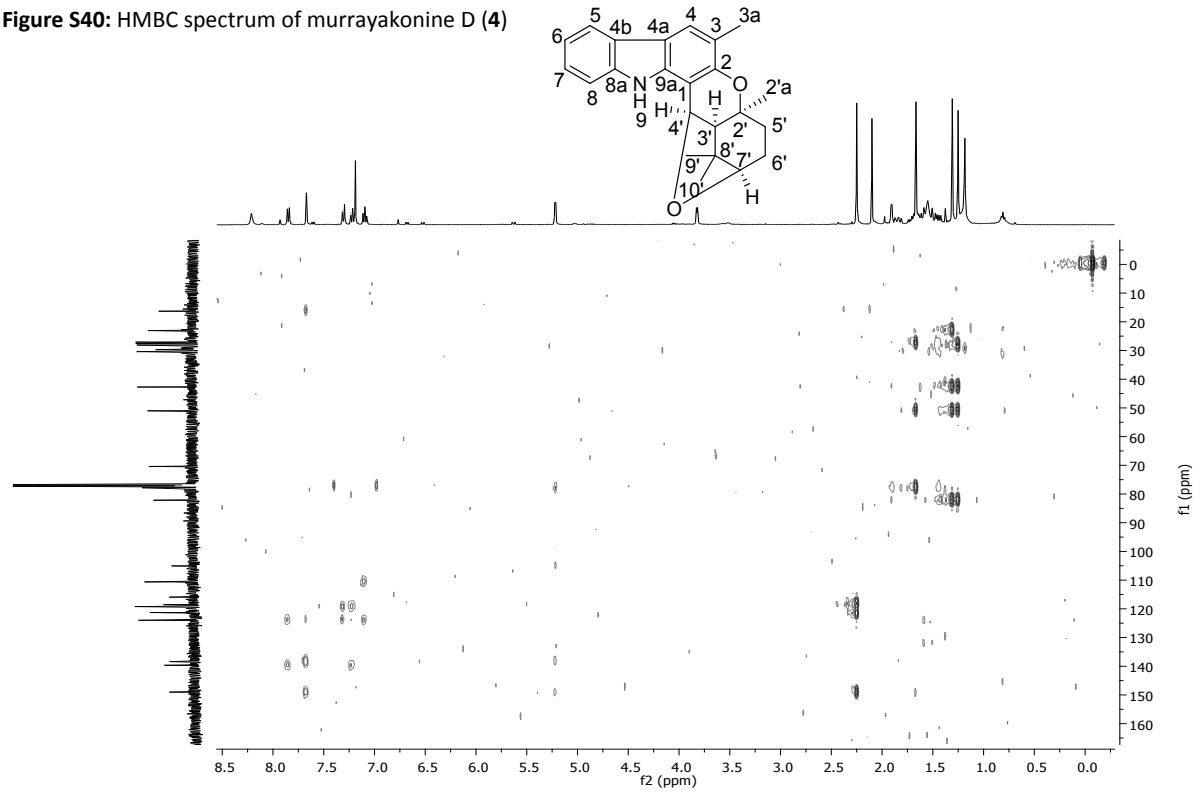


Figure S41: NOESY spectrum of murrayakonine D (**4**)

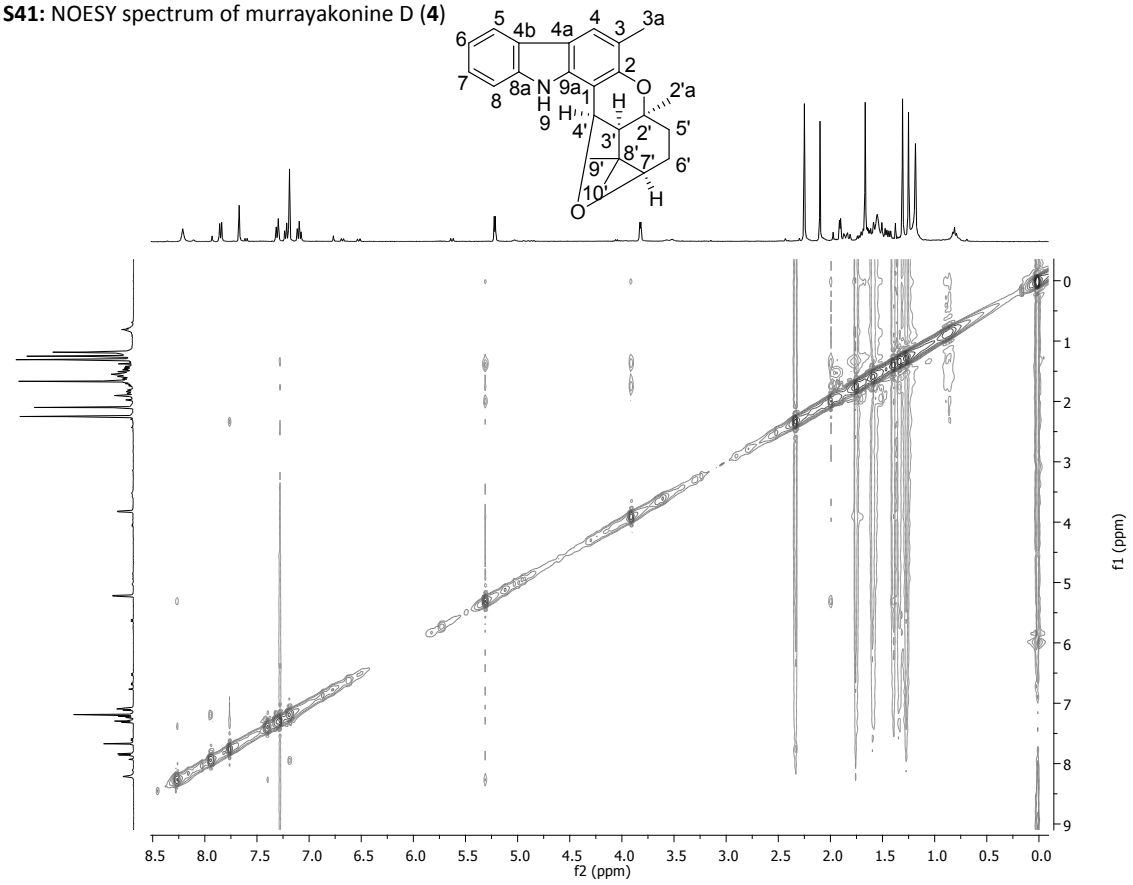


Figure S42: UV spectrum of murrayakonine D (**4**)