Supporting Information for

Melokhanines A–J, Bioactive Monoterpenoid Indole Alkaloids with Diverse Skeletons from *Melodinus khasianus*

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Table S1. Key MOs transitions, percentage of transitions, excitation energies, oscillator strengths, and rotatory strengths in the ECD spectra of most stable conformer at TDDFT/B3LYP/6-311++G(2d,2p) level in PCM model in MeOH.

MOs	%	λ/nm	*ΔE*/ev	*f*	R^a
89(HOMO)→90(LUMO)	92.18	272.7(266)[b]	4.55	0.0346	6.36
89(HOMO)→91(LUMO+1)	2.01				
85→90	26.50	245.9(241)[b]	5.04	0.1234	-51.62
85→91	2.34				
87→90	2.81				
89→90	3.98				
89(HOMO)→91(LUMO+1)	59.37				
85→91	12.28	219.7(210)[b]	5.65	0.0262	13.74
86→90	14.19				
86→91	13.32				
87(HOMO-2)→91(LUMO+1)	53.23				

[a]Rotatory strength in length form (10^{-40} cgs). [b]Experimental values in parentheses.

Table S2. Calculation of $[\alpha]_D$ for (7*R*,20*R*,21*S*)-**1** of Conformers **a1**-**a4**

conformer	P(%)[a]	Calcd.[b]	$[\alpha]_D$
a1	0.486	102.59	49.86
a2	0.425	53.81	22.88
a3	0.068	58.27	3.967
a4	0.018	77.94	1.444
Conformational average		78.12	

[a]From *ΔG* values at 298 K. [b]Calculated values of specific rotations in degrees·[dm·g/cm^3]$^{-1}$ at B3LYP/6-311++G(2d,2p) level in PCM model.

Table S3. The experimental ECD data of Melokhanine A (**1**)

Wave-length	CD data	Wave-length	CD data	Wave-length	CD data	Wave-length	CD data	Wave-length	CD data
400	-0.02454	358	-0.05949	316	-0.44458	274	0.35894	232	-11.7899
399	-0.10658	357	-0.04681	315	-0.48777	273	0.62314	231	-10.8497
398	-0.08107	356	-0.04172	314	-0.52004	272	1.04721	230	-9.98711
397	-0.08222	355	-0.10841	313	-0.54266	271	1.54964	229	-9.10985
396	0.01232	354	-0.11213	312	-0.51557	270	2.03991	228	-8.16928
395	0.04066	353	-0.10587	311	-0.5934	269	2.46922	227	-7.07126
394	0.06009	352	-0.0084	310	-0.66284	268	2.84798	226	-5.96185
393	0.0383	351	0.04119	309	-0.74582	267	2.96315	225	-4.73081
392	0.0247	350	0.08345	308	-0.82857	266	3.04473	224	-3.22019
391	-0.03551	349	0.12765	307	-0.90575	265	2.98743	223	-1.317
390	-0.08894	348	0.13657	306	-0.96303	264	2.9281	222	1.11926
389	-0.12107	347	0.05831	305	-1.04453	263	2.68242	221	4.02792
388	-0.1165	346	-0.01378	304	-1.0791	262	2.26377	220	7.42881
387	-0.13	345	-0.05939	303	-1.09274	261	1.73251	219	10.7964
386	-0.08945	344	-0.05804	302	-1.06489	260	1.04049	218	14.1117
385	-0.06692	343	-0.00858	301	-1.05199	259	0.22471	217	17.3205
384	-0.02377	342	0.03319	300	-0.99227	258	-0.61823	216	20.0945
383	-0.02396	341	0.02521	299	-0.92973	257	-1.4802	215	22.6644
382	-0.03626	340	0.097	298	-0.83628	256	-2.39997	214	24.9859
381	-0.07901	339	0.05434	297	-0.86965	255	-3.59643	213	26.9247
380	-0.12485	338	-0.0022	296	-0.84492	254	-4.86258	212	28.5001
379	-0.13745	337	-0.01675	295	-0.85621	253	-6.16195	211	29.3741
378	-0.09792	336	-0.03823	294	-0.83924	252	-7.69765	210	29.9798
377	-0.0831	335	0.04407	293	-0.80547	251	-9.07797	209	29.6678
376	-0.04865	334	0.05661	292	-0.7436	250	-10.439	208	28.8777
375	-0.05827	333	0.0117	291	-0.65346	249	-11.7692	207	27.2705
374	-0.0806	332	0.03837	290	-0.51067	248	-12.9956	206	25.3727
373	-0.04487	331	0.00791	289	-0.47887	247	-14.0452	205	23.2045
372	-0.06042	330	0.01619	288	-0.46622	246	-14.8556	204	20.9693
371	-0.01615	329	0.00139	287	-0.46832	245	-15.5975	203	18.6477
370	0.00698	328	-0.03716	286	-0.50188	244	-16.19	202	16.662
369	0.01728	327	-0.0285	285	-0.44465	243	-16.5015	201	14.3531
368	-0.01851	326	-0.06878	284	-0.44729	242	-16.6912	200	12.1114
367	-0.07332	325	-0.15871	283	-0.3939	241	-16.8263	199	9.7303
366	-0.10066	324	-0.1476	282	-0.39176	240	-16.7908	198	7.72122
365	-0.09099	323	-0.1237	281	-0.39234	239	-16.4302	197	5.70776
364	-0.09319	322	-0.08376	280	-0.2806	238	-15.9561	196	5.28094
363	-0.07107	321	-0.11191	279	-0.14393	237	-15.4341	195	4.80055
362	-0.05116	320	-0.12732	278	-0.05388	236	-14.799		
361	-0.03866	319	-0.22974	277	0.04346	235	-14.1291		
360	-0.01951	318	-0.31565	276	0.17407	234	-13.3289		
359	-0.03112	317	-0.421	275	0.22605	233	-12.6409		

Table S4. The experimental and calculated VCD data of Melokhanine A (**1**)

Wave-number	Experimental Data for **1**	Wave-number	Calcd. Data for (7*R*,20*R*,21*S*)-**1**	Wave-number	Calcd. Data for (7*R*,20*S*,21*R*)-**1**
1000	-9.36E-07	999	-1.13E-06	1000	1.96E-06
1002	-7.27E-07	1003	-1.30E-06	1002	2.28E-06
1004	-5.95E-07	1007	-1.34E-06	1004	2.72E-06
1006	-5.06E-07	1011	-1.20E-06	1006	3.33E-06
1008	-4.61E-07	1015	-1.42E-06	1008	4.13E-06
1010	-4.47E-07	1019	-1.99E-06	1010	5.13E-06
1012	-4.66E-07	1023	-1.88E-06	1012	6.21E-06
1014	-5.24E-07	1027	-8.79E-07	1014	7.17E-06
1016	-6.29E-07	1031	3.29E-07	1016	7.88E-06
1018	-8.43E-07	1035	1.86E-06	1018	8.36E-06
1020	-1.24E-06	1039	3.46E-06	1020	8.60E-06
1022	-1.97E-06	1043	3.46E-06	1022	8.37E-06
1024	-3.20E-06	1047	3.46E-06	1024	7.48E-06
1026	-4.29E-06	1051	3.46E-06	1026	6.13E-06
1028	-3.65E-06	1055	3.46E-06	1028	4.62E-06
1030	-2.18E-06	1059	3.46E-06	1030	3.06E-06
1032	-1.12E-06	1063	-1.08E-06	1032	1.42E-06
1034	-4.21E-07	1067	-2.24E-06	1034	-3.51E-07
1036	1.13E-07	1071	-1.01E-06	1036	-2.19E-06
1038	7.02E-07	1075	-9.11E-07	1038	-3.86E-06
1040	1.77E-06	1079	-3.00E-05	1040	-4.81E-06
1042	4.25E-06	1083	-9.88E-06	1042	-4.34E-06
1044	7.55E-06	1087	-5.47E-06	1044	-2.33E-06
1046	7.95E-06	1091	-3.64E-06	1046	5.33E-07
1048	5.41E-06	1095	-6.15E-07	1048	3.19E-06
1050	3.26E-06	1099	-8.67E-06	1050	4.85E-06
1052	2.08E-06	1103	-9.84E-06	1052	5.40E-06
1054	1.54E-06	1107	-9.72E-06	1054	5.39E-06
1056	1.60E-06	1111	-8.06E-06	1056	5.48E-06
1058	2.09E-06	1115	-2.70E-06	1058	5.92E-06
1060	1.69E-06	1119	9.15E-06	1060	6.84E-06
1062	8.82E-07	1123	1.17E-05	1062	8.26E-06
1064	2.74E-07	1127	1.65E-05	1064	1.01E-05
1066	-1.56E-07	1131	1.36E-05	1066	1.18E-05
1068	-5.16E-07	1135	8.85E-06	1068	1.26E-05
1070	-8.80E-07	1139	6.10E-06	1070	1.18E-05
1072	-1.31E-06	1143	5.00E-06	1072	9.34E-06
1074	-1.89E-06	1147	5.07E-06	1074	9.34E-06
1076	-2.75E-06	1151	6.27E-06	1076	2.91E-06
1078	-4.11E-06	1155	8.73E-06	1078	-1.01E-07
1080	-6.45E-06	1159	1.13E-05	1080	-2.60E-06
1082	-1.06E-05	1163	1.22E-05	1082	-4.18E-06
1084	-1.73E-05	1167	1.34E-05	1084	-4.63E-06

1086	-2.25E-05	1171	1.44E-05	1086	-4.24E-06
1088	-1.77E-05	1175	1.62E-05	1088	-3.56E-06
1090	-8.74E-06	1179	8.23E-06	1090	-2.97E-06
1092	-1.28E-06	1183	9.42E-06	1092	-2.59E-06
1094	2.88E-06	1187	2.83E-06	1094	-2.41E-06
1096	1.84E-06	1191	1.34E-05	1096	-2.37E-06
1098	-1.15E-06	1195	9.40E-06	1098	-2.35E-06
1100	-4.26E-06	1199	5.78E-06	1100	-2.28E-06
1102	-8.23E-06	1203	1.66E-07	1102	-2.13E-06
1104	-1.33E-05	1207	-7.29E-06	1104	-1.98E-06
1106	-1.56E-05	1211	-1.55E-05	1106	-1.91E-06
1108	-1.31E-05	1215	-1.84E-05	1108	-2.00E-06
1110	-1.14E-05	1219	-1.33E-05	1110	-2.30E-06
1112	-1.30E-05	1223	-8.04E-06	1112	-2.87E-06
1114	-1.69E-05	1227	-4.98E-06	1114	-3.74E-06
1116	-1.68E-05	1231	-3.28E-06	1116	-4.90E-06
1118	-1.07E-05	1235	-2.30E-06	1118	-6.25E-06
1120	-4.75E-06	1239	-1.94E-06	1120	-7.46E-06
1122	-3.76E-07	1243	-3.19E-06	1122	-8.01E-06
1124	3.59E-06	1247	-6.96E-06	1124	-7.54E-06
1126	8.52E-06	1251	-1.08E-05	1126	-6.30E-06
1128	1.61E-05	1255	-1.30E-05	1128	-4.90E-06
1130	2.72E-05	1259	-1.11E-05	1130	-3.73E-06
1132	3.39E-05	1263	-7.75E-06	1132	-2.89E-06
1134	2.67E-05	1267	-5.87E-06	1134	-2.32E-06
1136	1.65E-05	1271	-5.48E-06	1136	-1.97E-06
1138	1.02E-05	1275	-3.78E-06	1138	-1.79E-06
1140	6.77E-06	1279	-1.13E-06	1140	-1.77E-06
1142	4.85E-06	1283	-7.21E-07	1142	-1.87E-06
1144	3.75E-06	1287	-2.48E-06	1144	-1.99E-06
1146	3.13E-06	1291	-1.89E-07	1146	-1.95E-06
1148	2.83E-06	1295	-3.80E-07	1148	-1.53E-06
1150	2.75E-06	1299	-3.44E-06	1150	-6.87E-07
1152	2.90E-06	1303	-6.48E-06	1152	4.30E-07
1154	3.30E-06	1307	-6.48E-06	1154	1.69E-06
1156	4.10E-06	1311	-2.65E-07	1156	3.07E-06
1158	5.54E-06	1315	1.22E-06	1158	4.63E-06
1160	8.14E-06	1319	1.88E-06	1160	6.39E-06
1162	1.23E-05	1323	2.62E-06	1162	8.23E-06
1164	1.58E-05	1327	3.96E-06	1164	9.87E-06
1166	1.45E-05	1331	5.31E-06	1166	1.10E-05
1168	1.19E-05	1335	6.64E-06	1168	1.19E-05
1170	1.19E-05	1339	7.72E-06	1170	1.26E-05
1172	1.50E-05	1343	1.21E-05	1172	1.33E-05
1174	2.01E-05	1347	6.91E-06	1174	1.36E-05
1176	2.05E-05	1351	4.24E-06	1176	1.38E-05

1178	1.44E-05	1355	9.54E-07	1178	1.42E-05
1180	8.76E-06	1359	9.52E-07	1180	1.50E-05
1182	5.75E-06	1363	1.18E-06	1182	1.56E-05
1184	5.81E-06	1367	1.51E-06	1184	1.55E-05
1186	8.13E-06	1371	1.57E-06	1186	1.43E-05
1188	1.28E-05	1375	7.64E-07	1188	1.24E-05
1190	2.07E-05	1379	3.82E-07	1190	1.02E-05
1192	2.79E-05	1383	-2.05E-06	1192	7.93E-06
1194	2.47E-05	1387	-2.29E-06	1194	6.01E-06
1196	1.66E-05	1391	-1.46E-06	1196	4.44E-06
1198	1.15E-05	1395	-1.44E-05	1198	3.16E-06
1200	9.81E-06	1399	-3.43E-06	1200	2.07E-06
1202	1.05E-05	1403	-7.03E-06	1202	1.09E-06
1204	1.07E-05	1407	-1.15E-05	1204	1.60E-07
1206	6.98E-06	1411	-1.50E-05	1206	-7.12E-07
1208	2.10E-06	1415	-3.30E-05	1208	-1.44E-06
1210	-2.29E-06	1419	-1.64E-05	1210	-1.88E-06
1212	-7.14E-06	1423	-1.28E-05	1212	-1.98E-06
1214	-1.42E-05	1427	-7.96E-06	1214	-1.87E-06
1216	-2.53E-05	1431	-2.99E-06	1216	-1.71E-06
1218	-3.73E-05	1435	-3.44E-06	1218	-1.59E-06
1220	-3.57E-05	1439	-2.74E-06	1220	-1.56E-06
1222	-2.35E-05	1443	-2.53E-06	1222	-1.63E-06
1224	-1.41E-05	1447	-2.17E-06	1224	-1.84E-06
1226	-8.82E-06	1451	-1.29E-06	1226	-2.29E-06
1228	-5.85E-06	1455	-4.44E-07	1228	-3.10E-06
1230	-4.10E-06	1459	2.39E-07	1230	-4.34E-06
1232	-2.99E-06	1463	8.77E-07	1232	-5.98E-06
1234	-2.22E-06	1467	1.60E-06	1234	-7.83E-06
1236	-1.62E-06	1471	2.58E-06	1236	-9.48E-06
1238	-1.05E-06	1475	4.12E-06	1238	-1.04E-05
1240	-4.33E-07	1479	7.01E-06	1240	-1.06E-05
1242	1.65E-07	1483	1.23E-05	1242	-1.05E-05
1244	9.38E-07	1487	5.08E-05	1244	-1.04E-05
1246	2.19E-06	1491	1.91E-05	1246	-1.06E-05
1248	2.19E-06	1495	1.08E-05	1248	-1.04E-05
1250	-2.00E-06	1499	5.65E-06	1250	-9.59E-06
1252	-7.98E-06	1503	5.03E-06	1252	-8.13E-06
1254	-1.14E-05	1507	6.30E-06	1254	-6.47E-06
1256	-1.31E-05	1511	8.14E-06	1256	-4.96E-06
1258	-1.72E-05	1515	9.26E-06	1258	-3.69E-06
1260	-2.21E-05	1519	9.15E-06	1260	-2.63E-06
1262	-2.00E-05	1523	9.22E-06	1262	-1.73E-06
1264	-1.33E-05	1527	7.40E-06	1264	-9.15E-07
1266	-8.47E-06	1531	4.98E-06	1266	-2.16E-07
1268	-5.78E-06	1535	3.47E-06	1268	2.57E-07

1270	-4.33E-06	1539	2.63E-06	1270	3.41E-07
1272	-3.59E-06	1543	1.99E-06	1272	-1.70E-09
1274	-3.29E-06	1547	1.47E-06	1274	-6.32E-07
1276	-3.35E-06	1551	1.12E-06	1276	-1.37E-06
1278	-3.85E-06	1555	8.91E-07	1278	-2.06E-06
1280	-4.99E-06	1559	7.32E-07	1280	-2.49E-06
1282	-7.07E-06	1563	6.18E-07	1282	-2.41E-06
1284	-9.65E-06	1567	5.30E-07	1284	-1.74E-06
1286	-1.12E-05	1571	4.68E-07	1286	-6.80E-07
1288	-1.22E-05	1575	4.17E-07	1288	4.89E-07
1290	-1.13E-05	1579	3.83E-07	1290	1.43E-06
1292	-8.41E-06	1583	3.50E-07	1292	1.73E-06
1294	-6.33E-06	1587	3.22E-07	1294	1.11E-06
1296	-5.71E-06	1591	2.98E-07	1296	-2.21E-07
1298	-6.43E-06	1595	2.76E-07	1298	-1.78E-06
1300	-8.74E-06	1599	2.53E-07	1300	-3.18E-06
1302	-1.21E-05	1603	2.27E-07	1302	-4.37E-06
1304	-1.25E-05			1304	-5.52E-06
1306	-8.70E-06			1306	-6.71E-06
1308	-5.21E-06			1308	-7.87E-06
1310	-3.03E-06			1310	-8.79E-06
1312	-1.61E-06			1312	-9.37E-06
1314	-4.67E-07			1314	-9.55E-06
1316	7.64E-07			1316	-9.33E-06
1318	2.27E-06			1318	-8.91E-06
1320	3.30E-06			1320	-8.53E-06
1322	2.84E-06			1322	-8.21E-06
1324	2.13E-06			1324	-7.70E-06
1326	1.93E-06			1326	-6.85E-06
1328	2.27E-06			1328	-5.81E-06
1330	3.21E-06			1330	-4.83E-06
1332	4.71E-06			1332	-4.04E-06
1334	6.23E-06			1334	-3.48E-06
1336	7.85E-06			1336	-3.11E-06
1338	8.82E-06			1338	-2.90E-06
1340	8.20E-06			1340	-2.76E-06
1342	7.83E-06			1342	-2.61E-06
1344	6.75E-06			1344	-2.37E-06
1346	4.55E-06			1346	-2.05E-06
1348	2.85E-06			1348	-1.75E-06
1350	1.85E-06			1350	-1.57E-06
1352	1.28E-06			1352	-1.50E-06
1354	9.18E-07			1354	-1.51E-06
1356	7.07E-07			1356	-1.59E-06
1358	5.88E-07			1358	-1.75E-06
1360	5.48E-07			1360	-1.99E-06

1362	5.65E-07	1362	-2.24E-06
1364	6.71E-07	1364	-2.38E-06
1366	9.21E-07	1366	-2.33E-06
1368	1.30E-06	1368	-2.26E-06
1370	1.64E-06	1370	-2.43E-06
1372	2.07E-06	1372	-2.96E-06
1374	2.96E-06	1374	-3.86E-06
1376	3.69E-06	1376	-4.98E-06
1378	2.93E-06	1378	-6.08E-06
1380	1.68E-06	1380	-6.72E-06
1382	8.33E-07	1382	-6.54E-06
1384	1.32E-07	1384	-5.69E-06
1386	-1.43E-06	1386	-4.67E-06
1388	-4.05E-06	1388	-3.88E-06
1390	-5.18E-06	1390	-3.41E-06
1392	-3.60E-06	1392	-3.19E-06
1394	-1.60E-06	1394	-3.16E-06
1396	1.52E-07	1396	-3.31E-06
1398	1.80E-06	1398	-3.63E-06
1400	2.50E-06	1400	-4.16E-06
1402	1.28E-06	1402	-4.96E-06
1404	-9.21E-07	1404	-6.08E-06
1406	-3.18E-06	1406	-7.58E-06
1408	-5.88E-06	1408	-9.39E-06
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1414	-1.80E-05	1414	-1.22E-05
1416	-2.13E-05	1416	-1.11E-05
1418	-2.00E-05	1418	-9.62E-06
1420	-1.85E-05	1420	-8.19E-06
1422	-2.13E-05	1422	-6.96E-06
1424	-2.63E-05	1424	-5.83E-06
1426	-2.37E-05	1426	-4.66E-06
1428	-1.48E-05	1428	-3.48E-06
1430	-8.69E-06	1430	-2.41E-06
1432	-5.70E-06	1432	-1.48E-06
1434	-4.05E-06	1434	-7.30E-07
1436	-3.04E-06	1436	-2.06E-07
1438	-2.40E-06	1438	9.73E-08
1440	-2.00E-06	1440	2.54E-07
1442	-1.79E-06	1442	3.58E-07
1444	-1.78E-06	1444	4.70E-07
1446	-2.03E-06	1446	5.99E-07
1448	-2.66E-06	1448	7.57E-07
1450	-3.42E-06	1450	9.46E-07
1452	-3.18E-06	1452	1.17E-06

1454	-2.11E-06	1454	1.44E-06
1456	-1.25E-06	1456	1.76E-06
1458	-7.16E-07	1458	2.15E-06
1460	-3.72E-07	1460	2.62E-06
1462	-1.23E-07	1462	3.22E-06
1464	8.52E-08	1464	3.97E-06
1466	2.65E-07	1466	4.90E-06
1468	4.41E-07	1468	6.07E-06
1470	6.26E-07	1470	7.43E-06
1472	8.29E-07	1472	9.10E-06
1474	1.06E-06	1474	1.12E-05
1476	1.33E-06	1476	1.38E-05
1478	1.65E-06	1478	1.66E-05
1480	2.03E-06	1480	1.92E-05
1482	2.63E-06	1482	2.12E-05
1484	4.02E-06	1484	2.30E-05
1486	6.65E-06	1486	2.45E-05
1488	1.09E-05	1488	2.46E-05
1490	1.81E-05	1490	2.21E-05
1492	3.03E-05	1492	1.68E-05
1494	4.33E-05	1494	1.04E-05
1496	3.68E-05	1496	4.68E-06
1498	1.69E-05	1498	8.61E-07
1500	4.97E-06	1500	-1.10E-06
1502	7.05E-07	1502	-1.95E-06
1504	-1.19E-06	1504	-2.32E-06
1506	-7.13E-07	1506	-2.35E-06
1508	1.86E-06	1508	-1.72E-06
1510	4.47E-06	1510	-1.95E-08
1512	5.21E-06	1512	2.48E-06
1514	5.45E-06	1514	4.81E-06
1516	8.77E-06	1516	6.16E-06
1518	1.34E-05	1518	6.34E-06
1520	1.25E-05	1520	5.67E-06
1522	8.67E-06	1522	4.66E-06
1524	8.47E-06	1524	3.69E-06
1526	1.11E-05	1526	2.90E-06
1528	1.40E-05	1528	2.28E-06
1530	1.23E-05	1530	1.82E-06
1532	8.14E-06	1532	1.47E-06
1534	5.23E-06	1534	1.22E-06
1536	3.59E-06	1536	1.04E-06
1538	2.68E-06	1538	9.08E-07
1540	2.22E-06	1540	8.05E-07
1542	2.06E-06	1542	7.23E-07
1544	2.04E-06	1544	6.54E-07

1546	1.78E-06	1546	5.96E-07
1548	1.34E-06	1548	5.45E-07
1550	1.01E-06	1550	5.02E-07
1552	8.00E-07	1552	4.65E-07
1554	6.57E-07	1554	4.33E-07
1556	5.55E-07	1556	4.04E-07
1558	4.79E-07	1558	3.84E-07
1560	4.18E-07	1560	3.62E-07
1562	3.68E-07	1562	3.43E-07
1564	3.29E-07	1564	3.25E-07
1566	2.96E-07	1566	3.10E-07
1568	2.68E-07	1568	2.96E-07
1570	2.44E-07	1570	2.88E-07
1572	2.26E-07	1572	2.77E-07
1574	2.07E-07	1574	2.67E-07
1576	1.91E-07	1576	2.59E-07
1578	1.86E-07	1578	2.51E-07
1580	1.73E-07	1580	2.44E-07
1582	1.61E-07	1582	2.38E-07
1584	1.95E-07	1584	2.32E-07
1586	2.02E-07	1586	2.28E-07
1588	1.93E-07	1588	2.24E-07
1590	1.84E-07	1590	2.19E-07
1592	1.77E-07	1592	2.16E-07
1594	1.70E-07	1594	2.14E-07
1596	1.64E-07	1596	2.13E-07
1598	1.58E-07	1598	2.12E-07
1600	1.52E-07	1600	2.12E-07

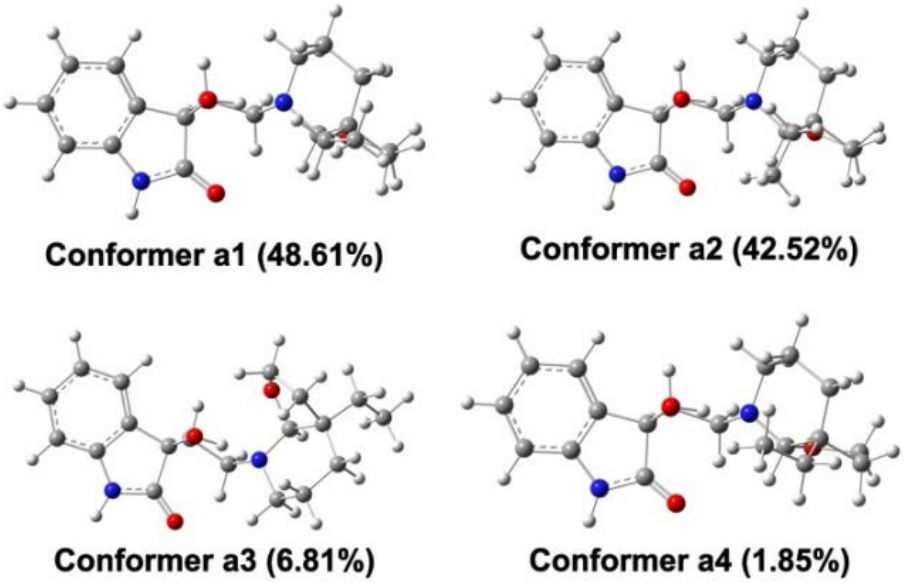


Figure S1. Most stable conformers of (7*R*,20*R*,21*S*)-**1** optimized at the DFT/B3LYP/6-311++G(2d,2p) level of theory. Relative populations are in parentheses.

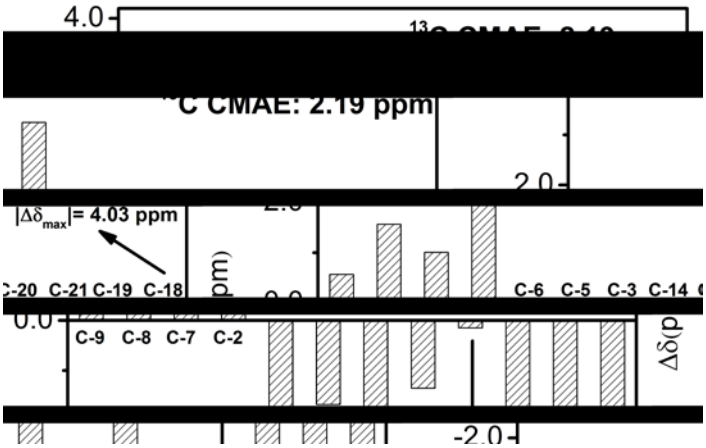


Figure S2. The relative errors between the recorded and Boltzmann-averaged ^{13}C NMR data at the SCRF-mPW1PW91/6-311++(2d,2p)//B3LYP/6-311++(2d,2p) level.

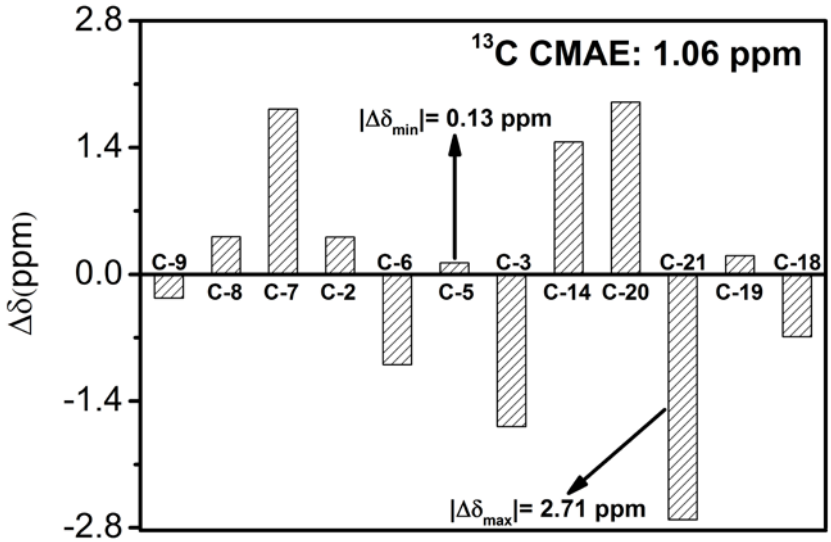
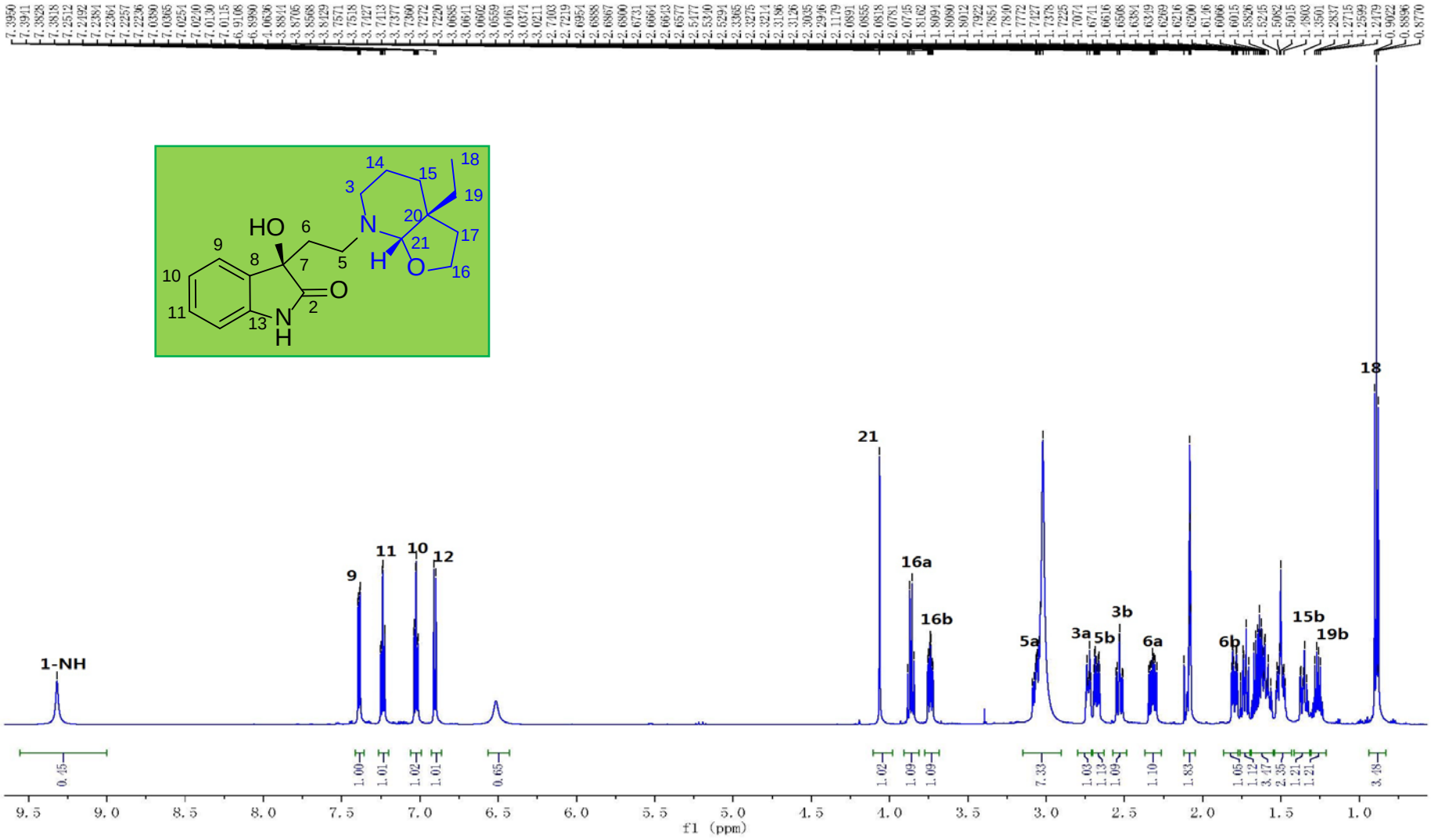


Figure S3. The Boltzmann averaged ^{13}C NMR chemical shifts (ppm, relative to TMS), and its relative errors between the recorded and computed ^{13}C NMR data at the SCRF-mPW1PW91/6-311++(2d,2p)//B3LYP/6-311++(2d,2p) level. The obtained equation was $\delta_{corr} = 0.96527 \times \delta_{calc} - 2.1228$. An intercept of – 2.1228 and a Slope of 0.96527 were the corresponding least-squares parameters obtained by the linear correlation plots between experimental and calculated data. The δ_{calc} represents values of chemical shifts for ^{13}C for each carbon atom.

Note: The relative errors and corrected mean absolute error (CMAE) were calculated from the theoretical data compared to experiment data. The calculated ^{13}C NMR value of C-20 was 44.4 ppm, which was very close to the experimental value of 42.5 ppm (the absolute $\Delta\delta_{min}$ was 0.15 ppm). The largest deviation for C-21 might have been caused by sensitivity of chemical shifts to nitrogen and oxygen atoms of strongly electron withdrawing groups. A clear correlation ($|\Delta\delta_{max}|$ = 2.71 ppm is less than 5.0 ppm) between theoretical and experimental data revealed that the gauge including atomic orbital (GIAO) method can be utilized for the determination of the C-20 and C-21 configurations of compound **1**.

Figure S4. ^{1}H NMR spectrum of Melokhanine A (**1**) (Acetone-d_6)



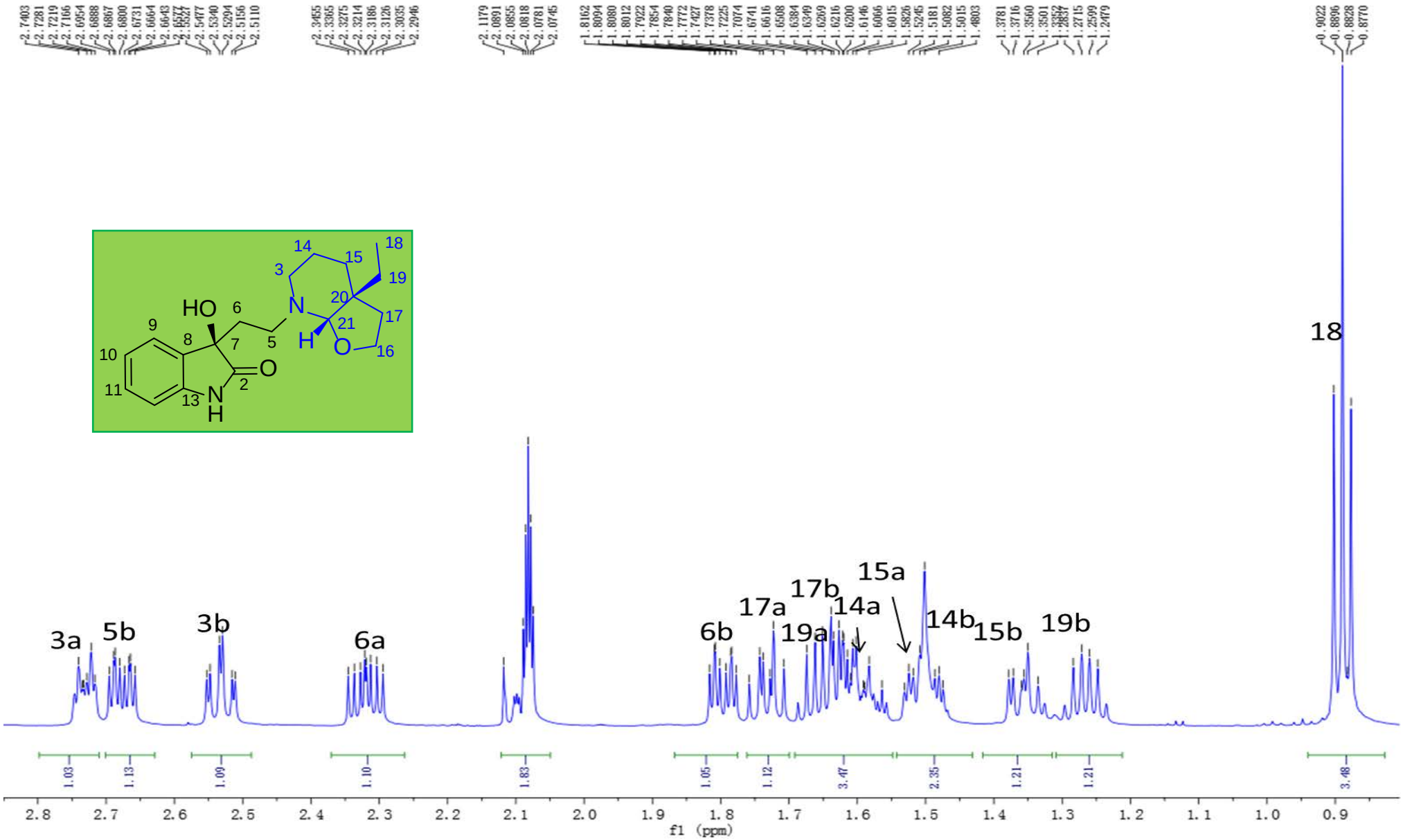

3a
5b
3b
6a
6b
17a
19a
17b
14a
15a
14b
15b
19b
18
1.03
1.13
1.09
1.10
1.83
1.05
1.12
3.47
2.35
1.21
1.21
3.48
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
f1 (ppm)

Figure S5. ^{13}C NMR spectrum of Melokhanine A (**1**) (Acetone-d_6)

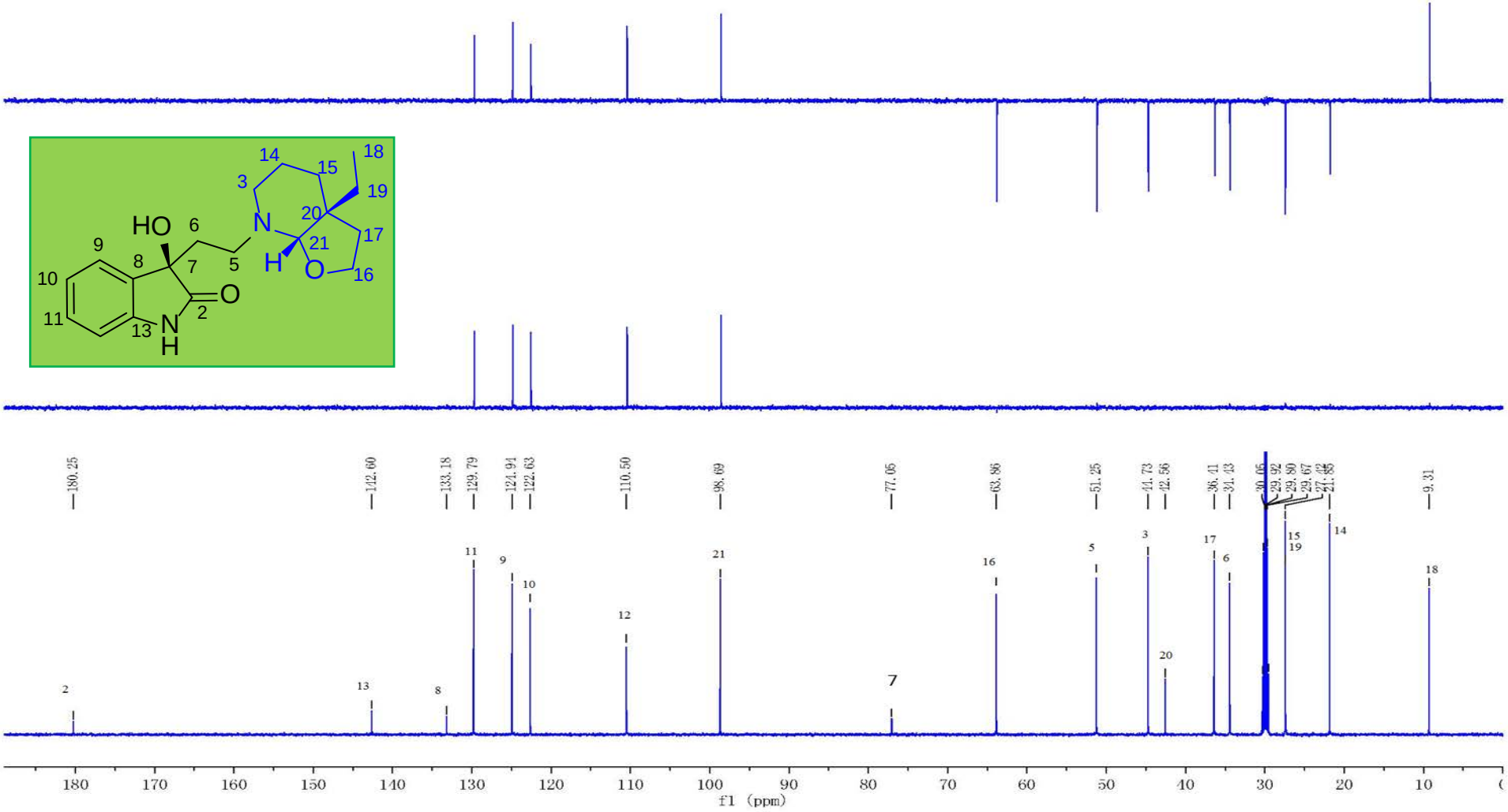
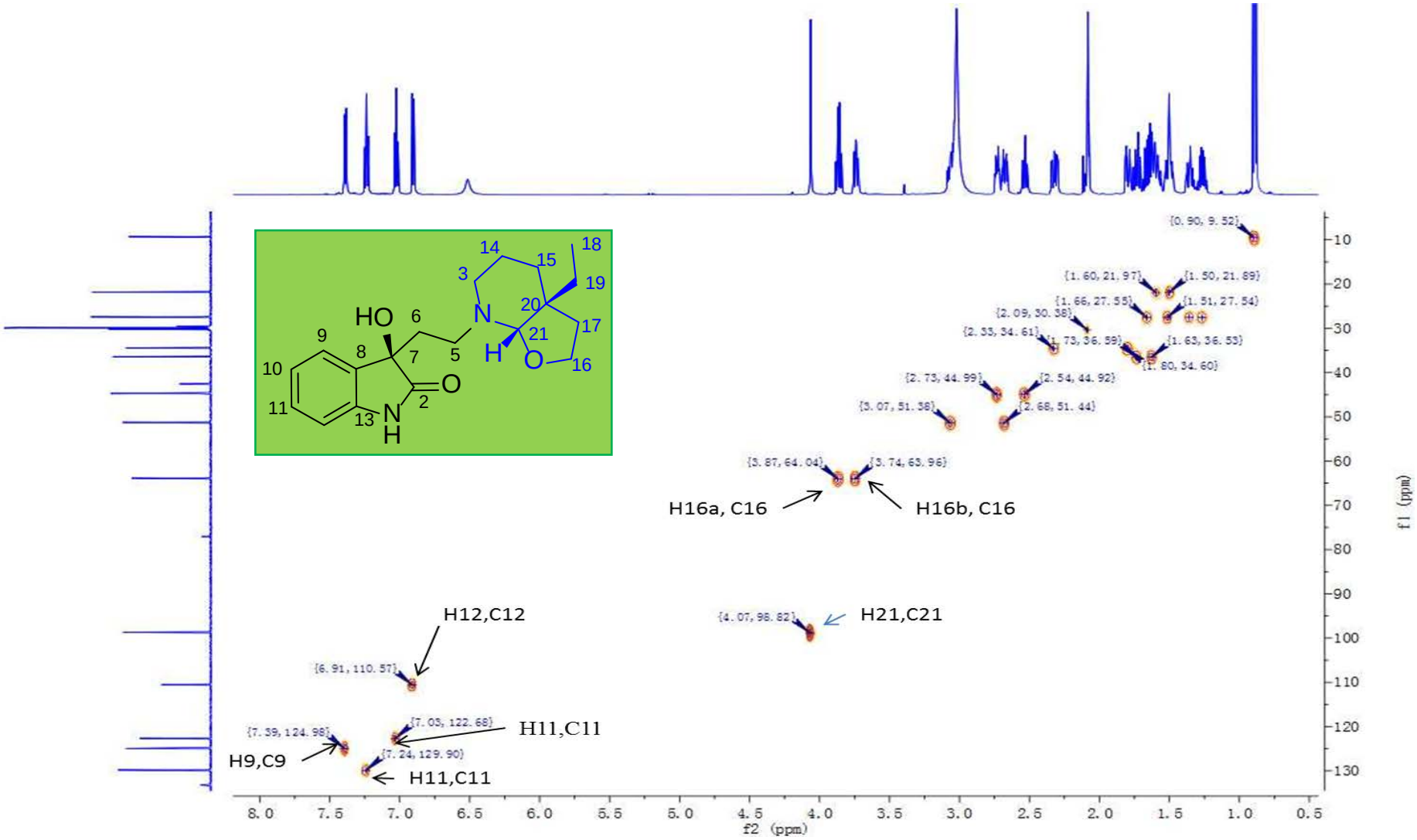


Figure S6. HSQC spectrum of Melokhanine A (**1**) (Acetone-d_6)



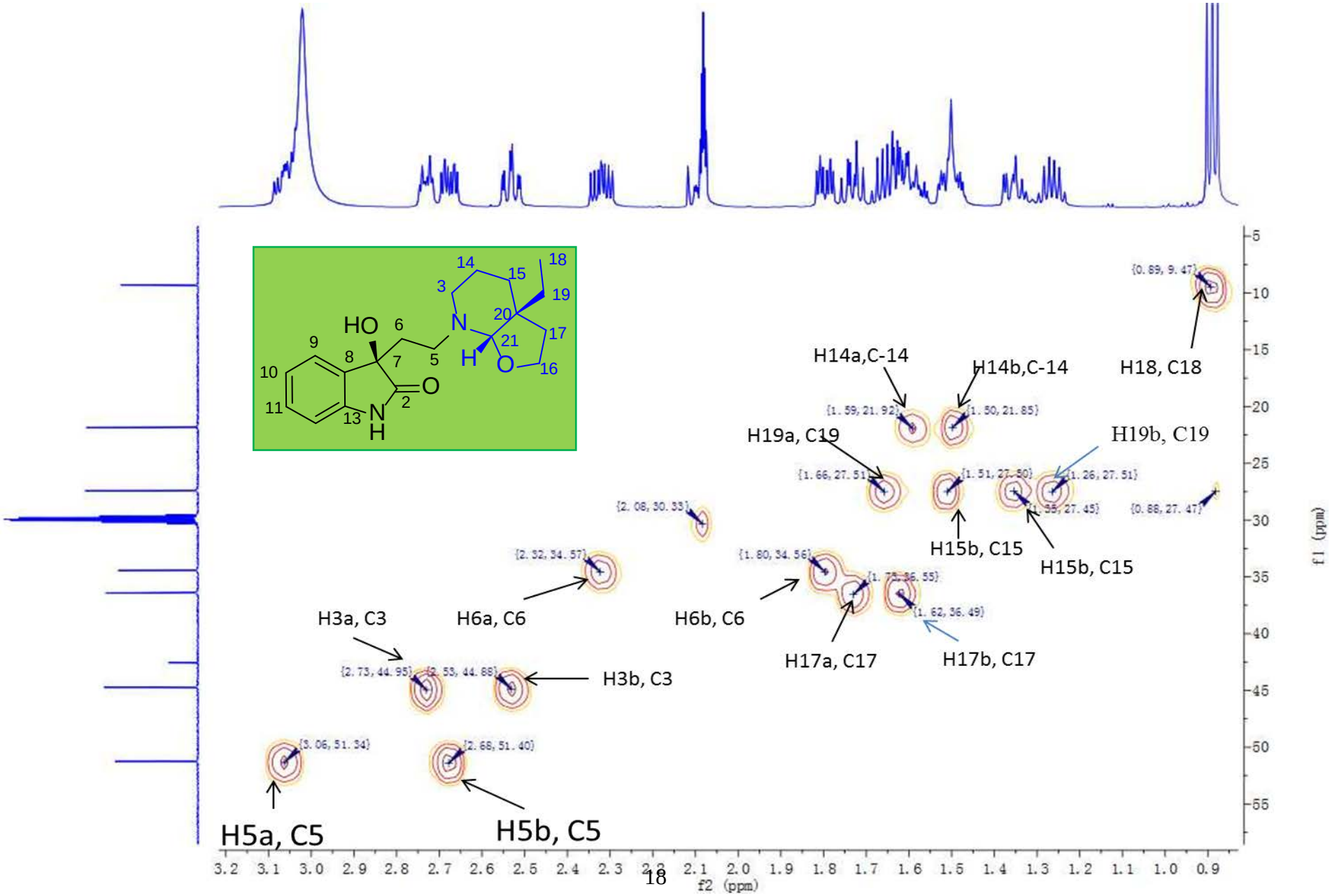
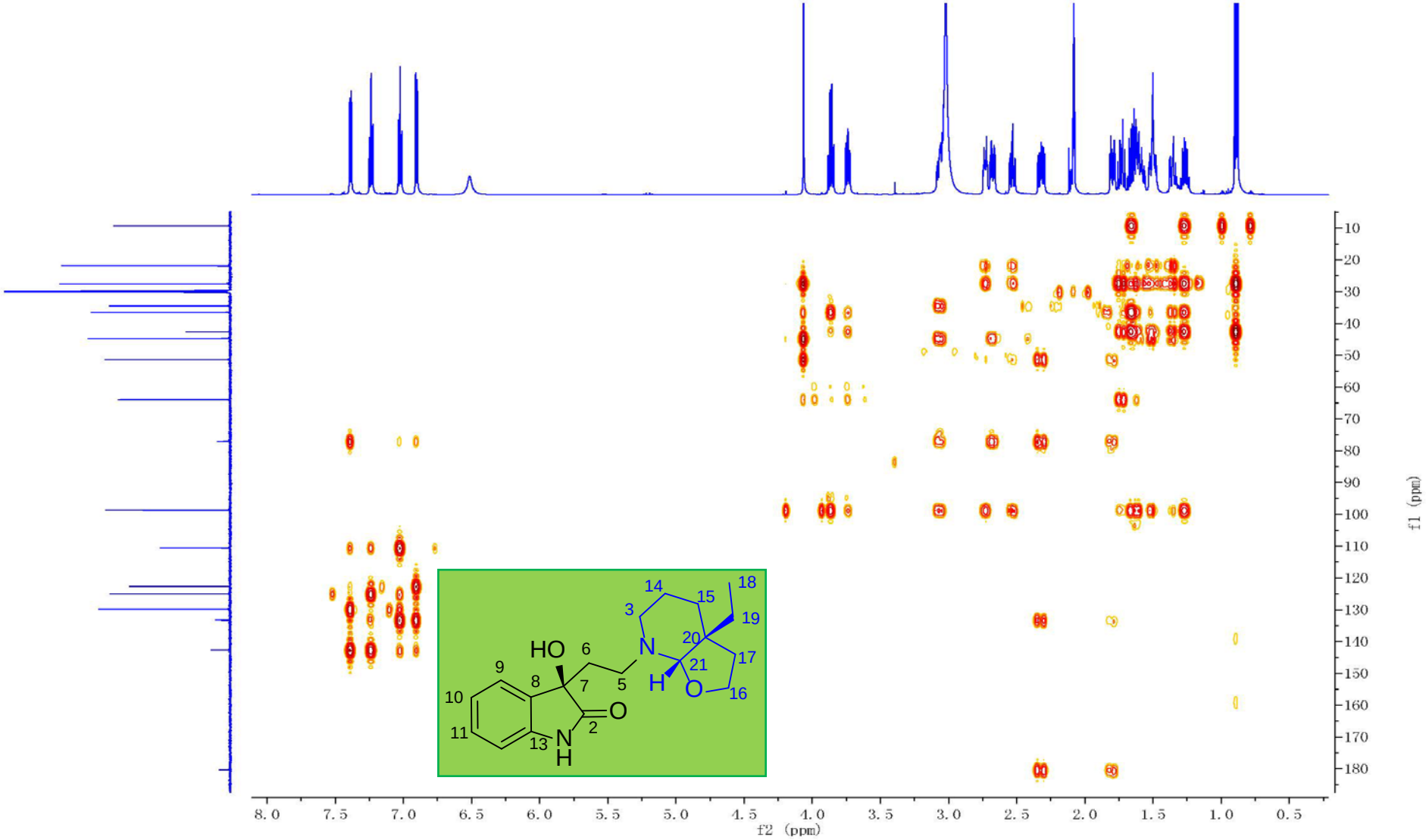

H14a,C-14
H14b,C-14
H18, C18
H19a, C19
H19b, C19
H15b, C15
H15b, C15
H3a, C3
H6a, C6
H6b, C6
H17a, C17
H17b, C17
H3b, C3
H5a, C5
H5b, C5
f2 (ppm)
f1 (ppm)

Figure S7. HMBC spectrum of Melokhanine A (**1**) (Acetone-d_6)



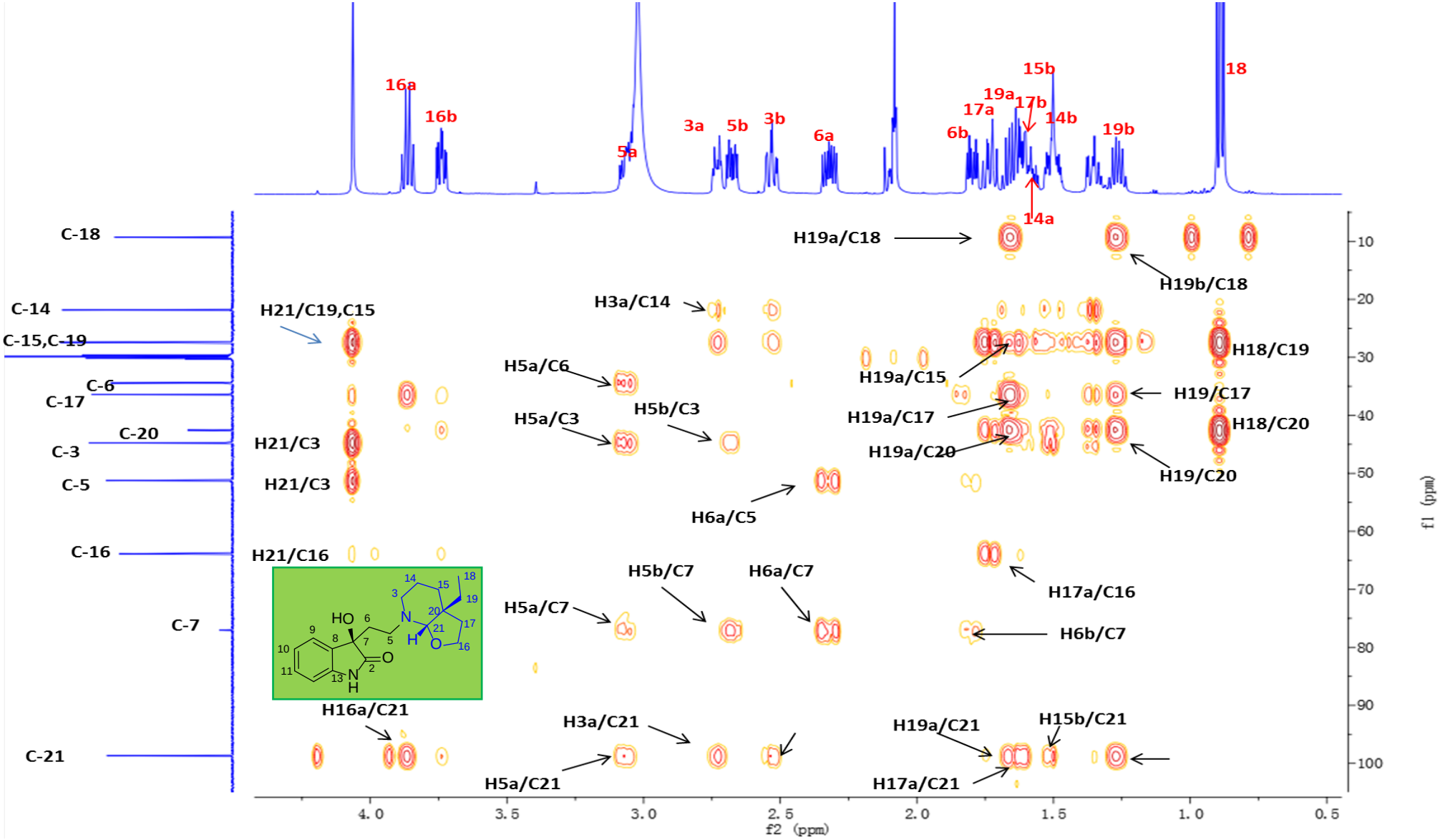
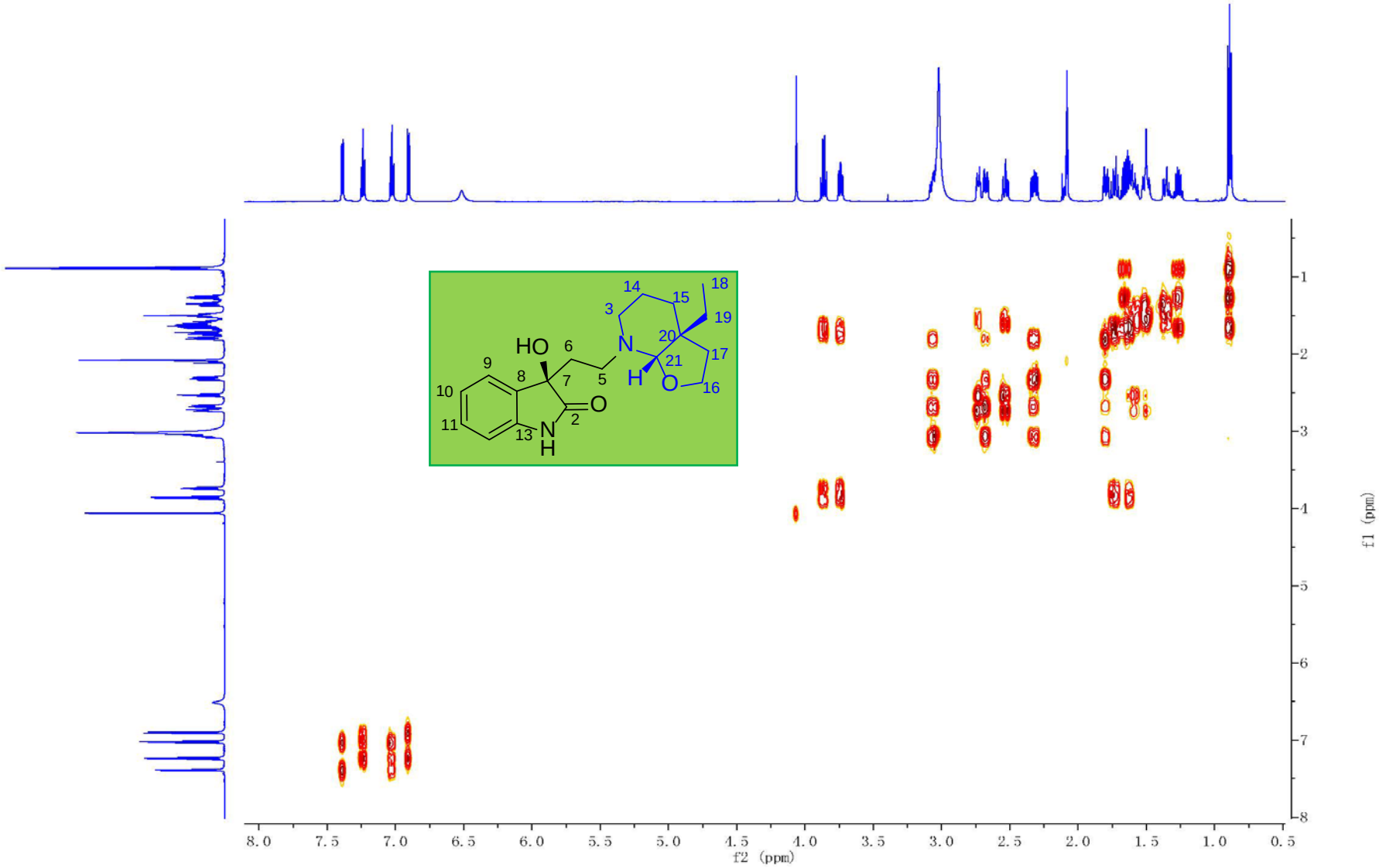

16a
16b
5a
3a
5b
3b
6a
6b
17a
19a
17b
15b
14b
14a
19b
18
C-18
C-14
C-15,C-19
C-6
C-17
C-20
C-3
C-5
C-16
C-7
C-21
H19a/C18
H19b/C18
H21/C19,C15
H3a/C14
H18/C19
H5a/C6
H19a/C15
H19/C17
H5b/C3
H5a/C3
H19a/C17
H18/C20
H21/C3
H19a/C20
H19/C20
H21/C3
H6a/C5
H21/C16
H5b/C7
H6a/C7
H17a/C16
H5a/C7
H6b/C7
H16a/C21
H3a/C21
H19a/C21
H15b/C21
H5a/C21
H17a/C21
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
f1 (ppm)

Figure S8. ^{1}H-^{1}H COSY spectrum of Melokhanine A (**1**) (Acetone-d_6)



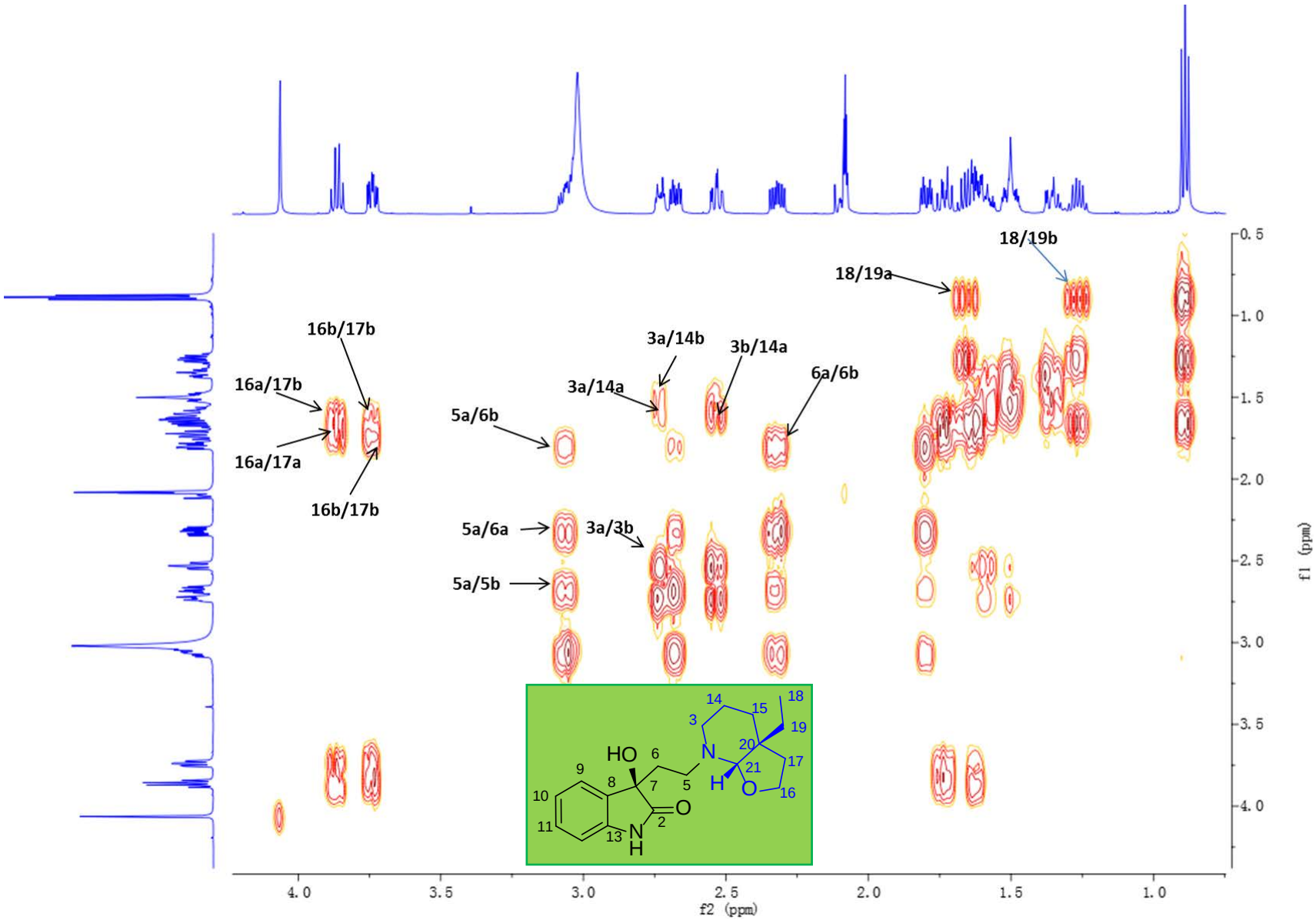
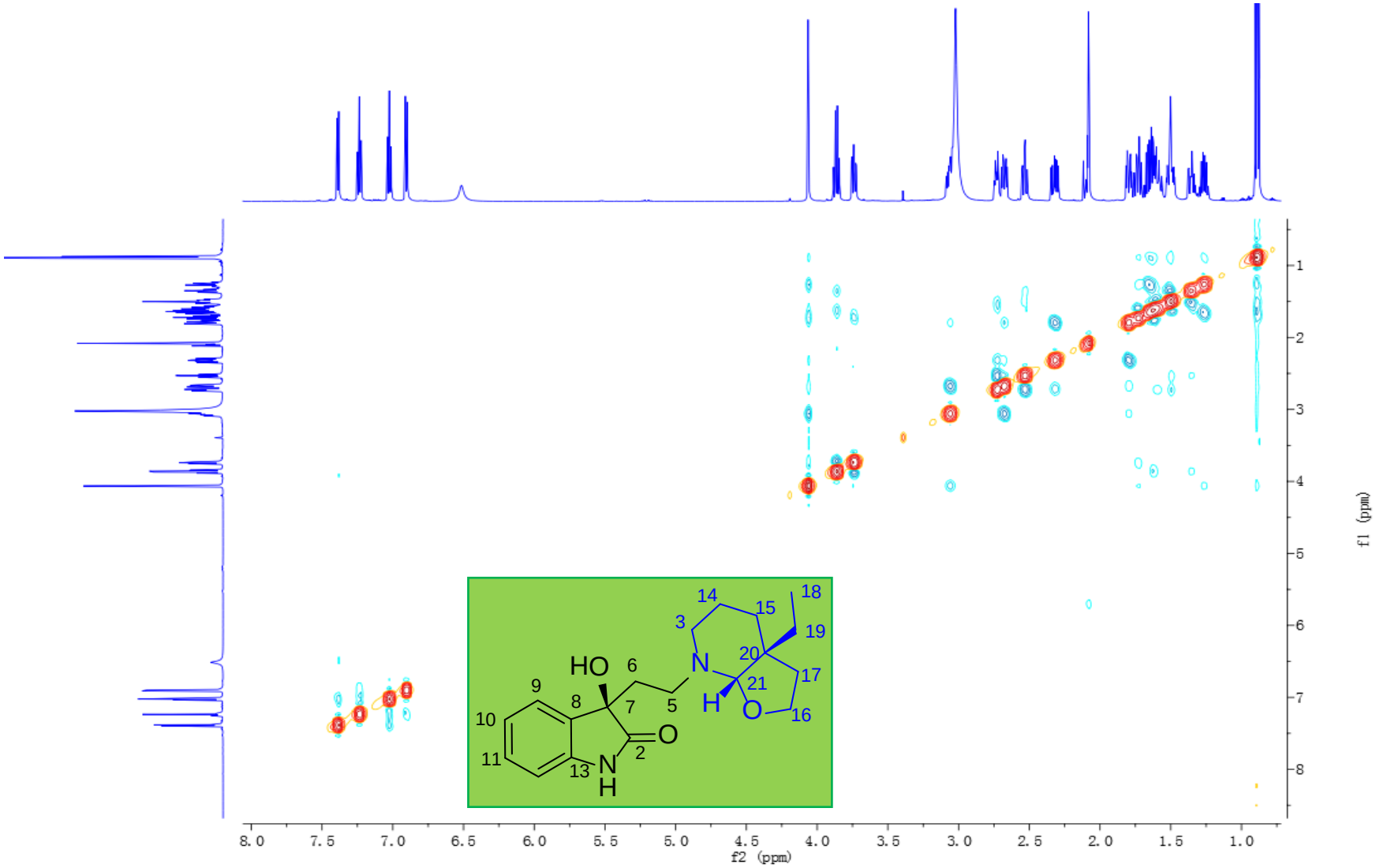

18/19b
18/19a
16b/17b
3a/14b
3b/14a
6a/6b
16a/17b
3a/14a
5a/6b
16a/17a
16b/17b
5a/6a
3a/3b
5a/5b
HO
N
H
O
N
H
O
f2 (ppm)
f1 (ppm)

Figure S9. ROESY spectrum of Melokhanine A (**1**) (Acetone-d_6)



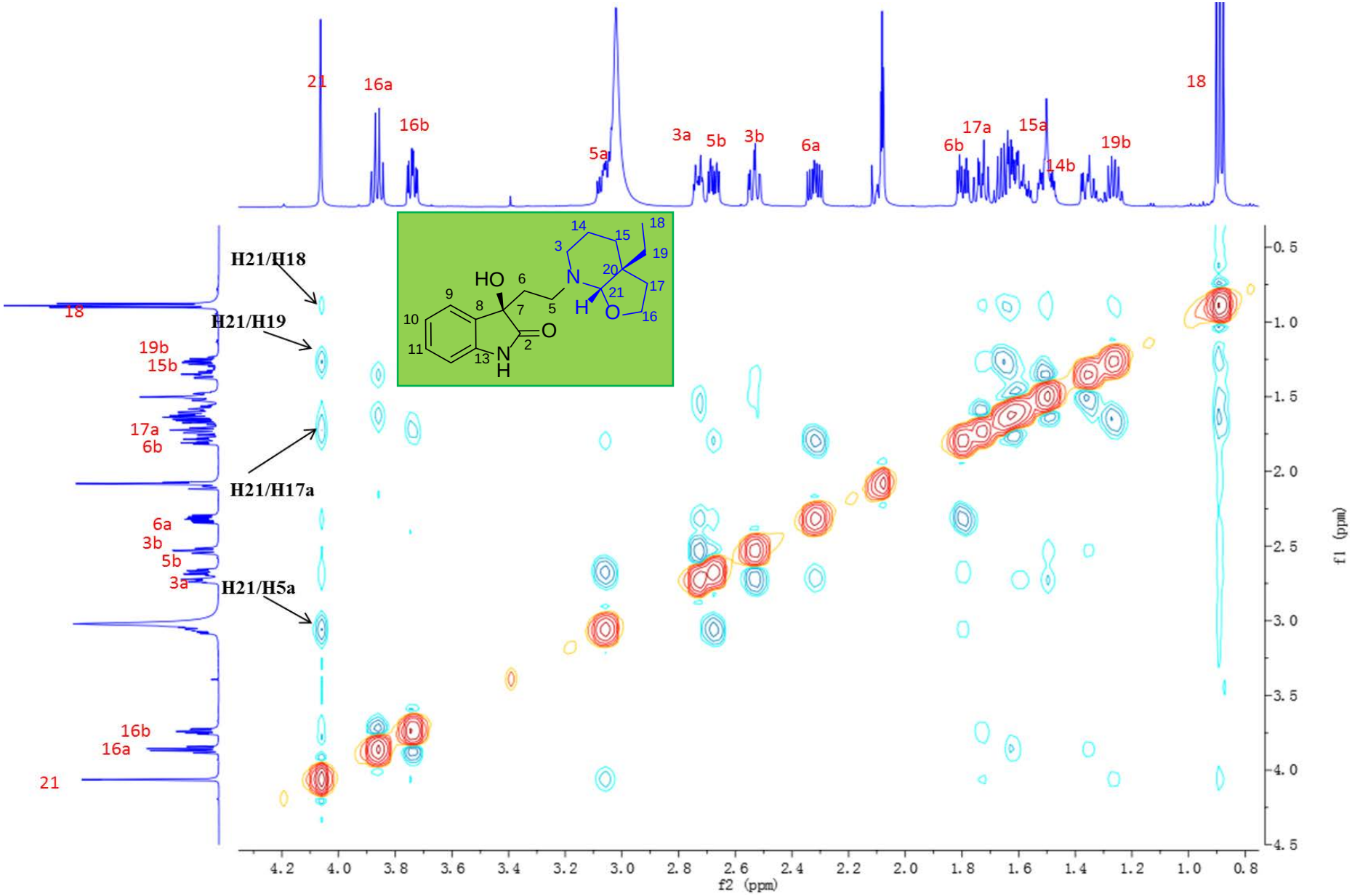
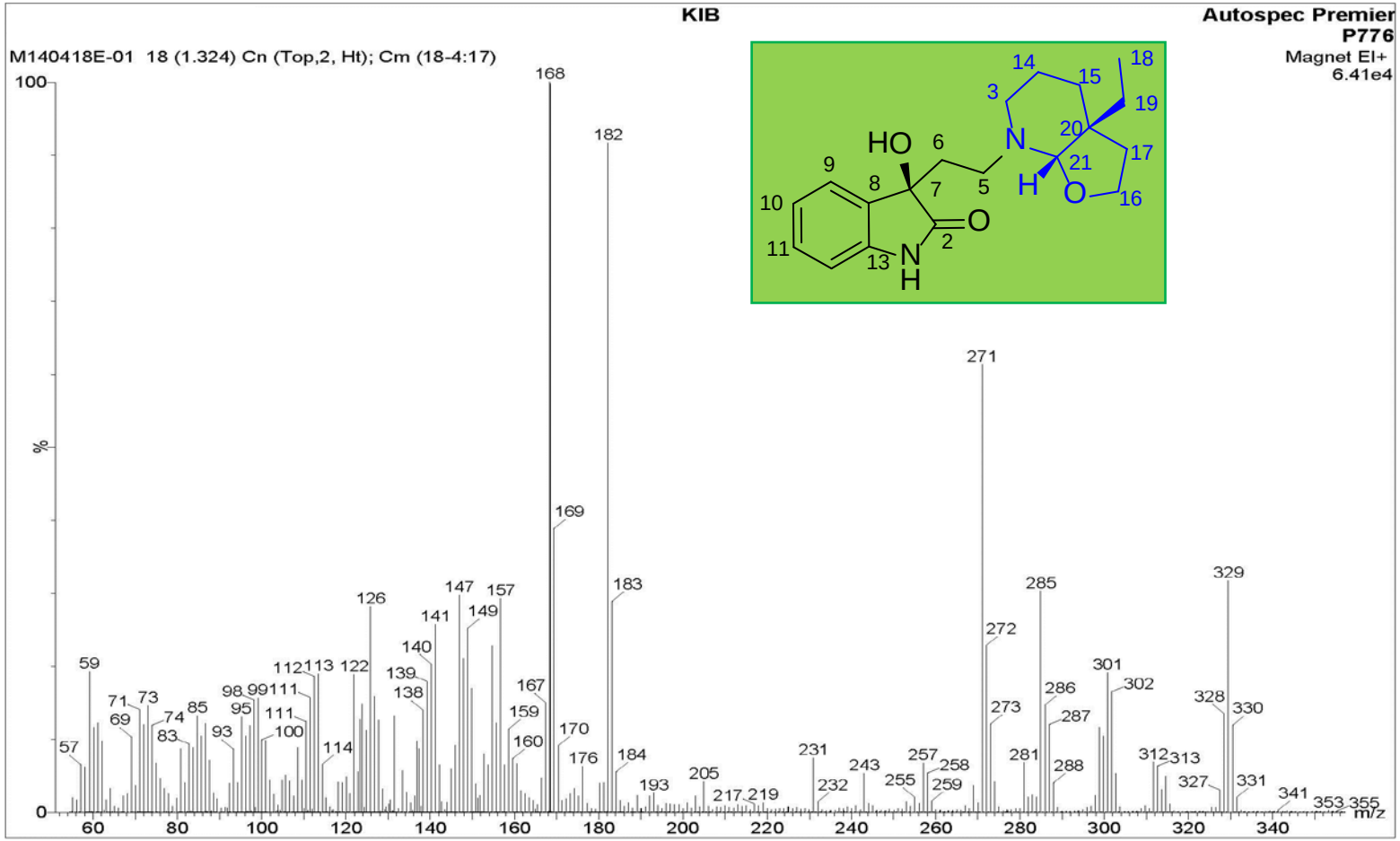

21
16a
16b
5a
3a
5b
3b
6a
6b
17a
15a
14b
19b
18
H21/H18
H21/H19
H21/H17a
H21/H5a
19b
15b
17a
6b
6a
3b
5b
3a
16b
16a
21
18
HO
N
H
O
O
N
H
f2 (ppm)
f1 (ppm)

Figure S10. MS and HREIMS data of Melokhanine A (**1**)



Elemental Composition Report **Page 1**

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Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
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Elements Used:
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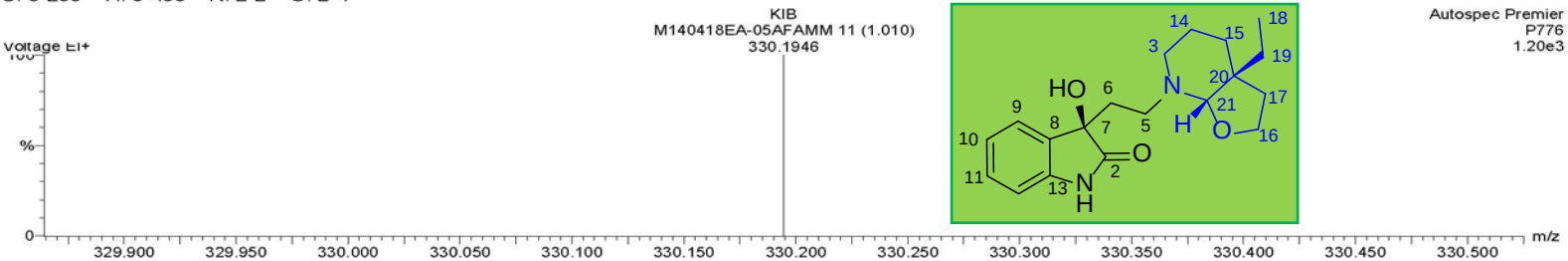

Autospec Premier
P776
1.20e3

Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Figure S11. IR spectrum of Melokhanine A (**1**)

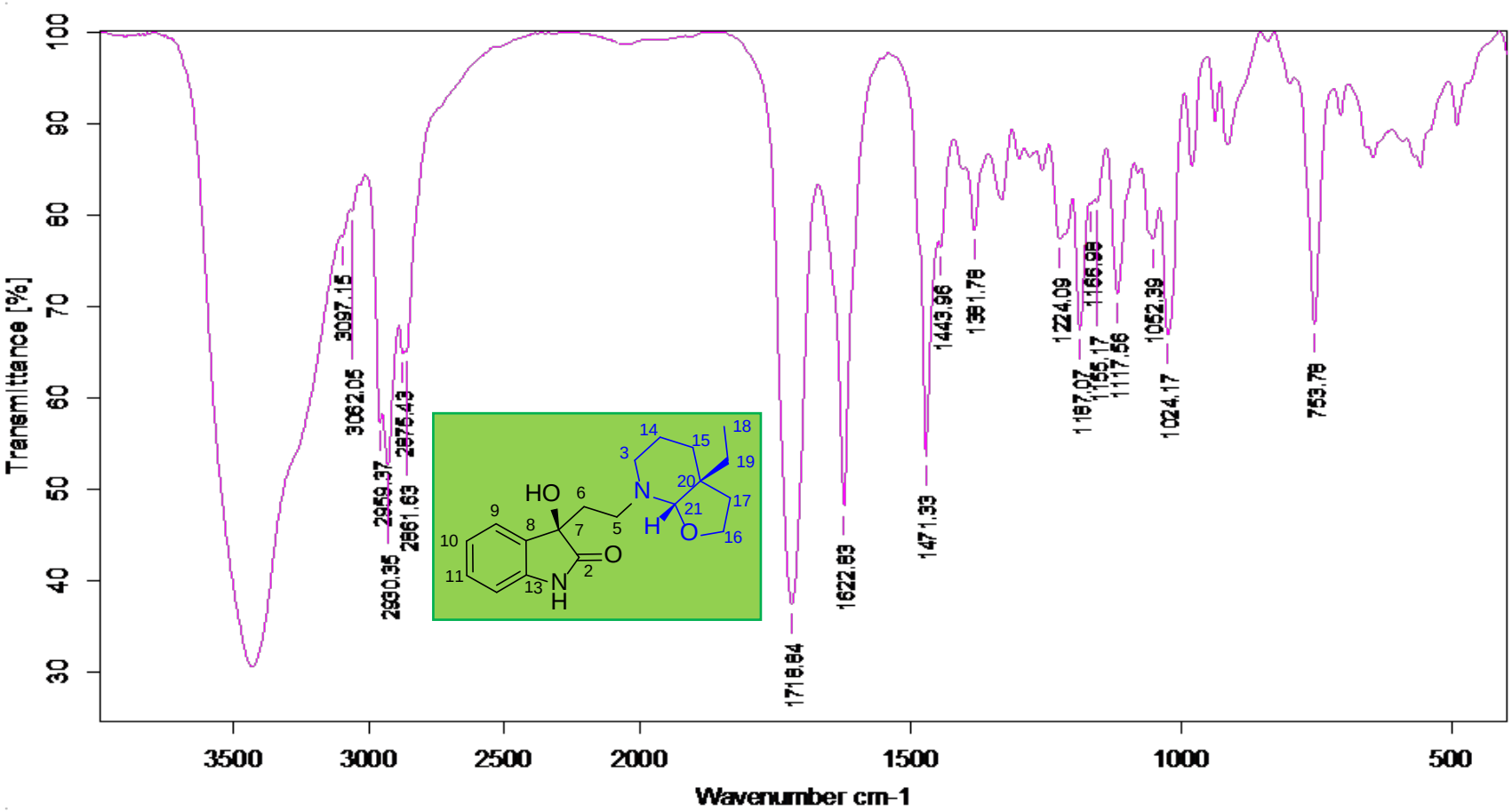


Figure S12. UV spectrum of Melokhanine A (**1**)

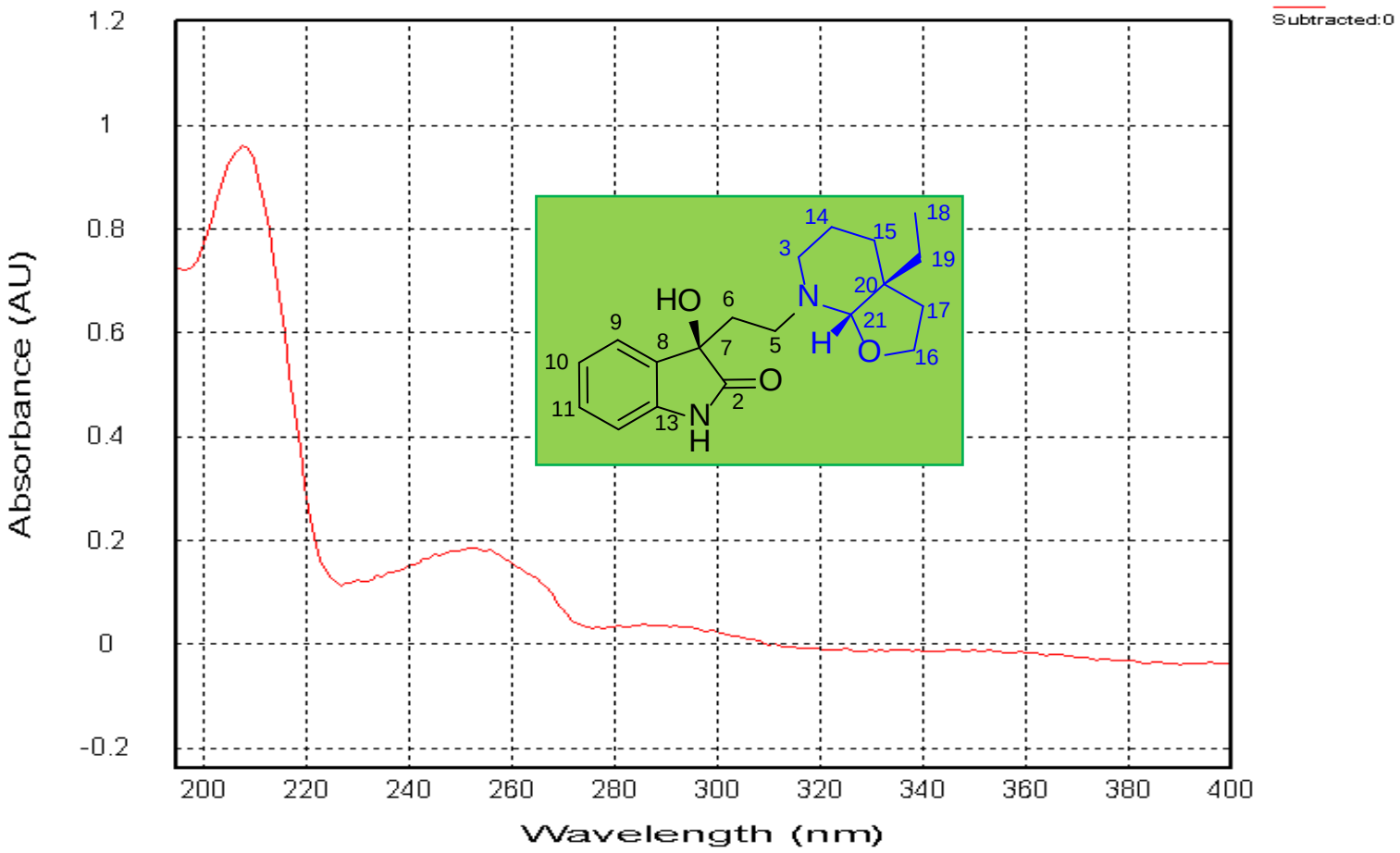


Figure S13. CD spectrum of Melokhanine A (**1**)

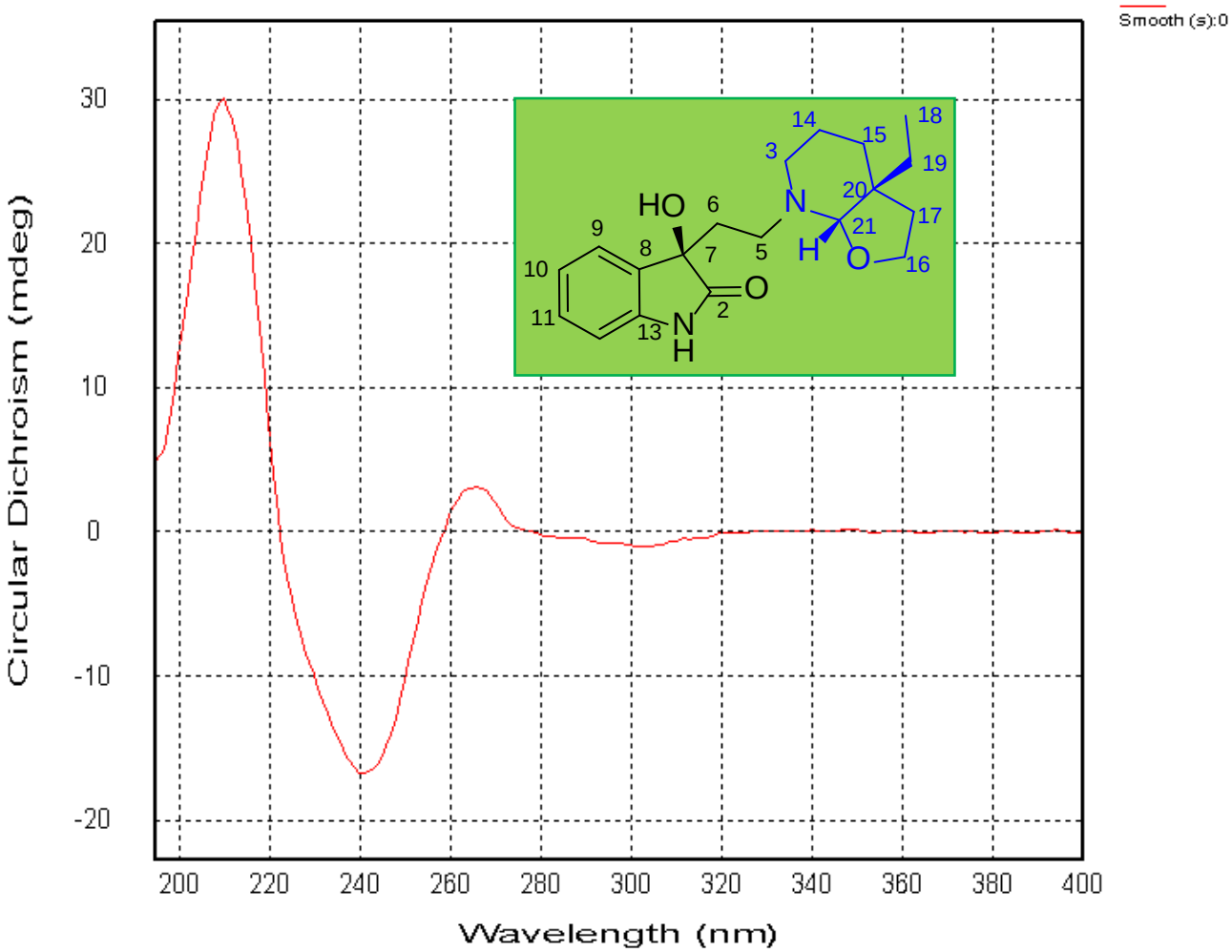


Figure S14. ^{1}H NMR spectrum of Melokhanine B (**2**) (Acetone-d_6)

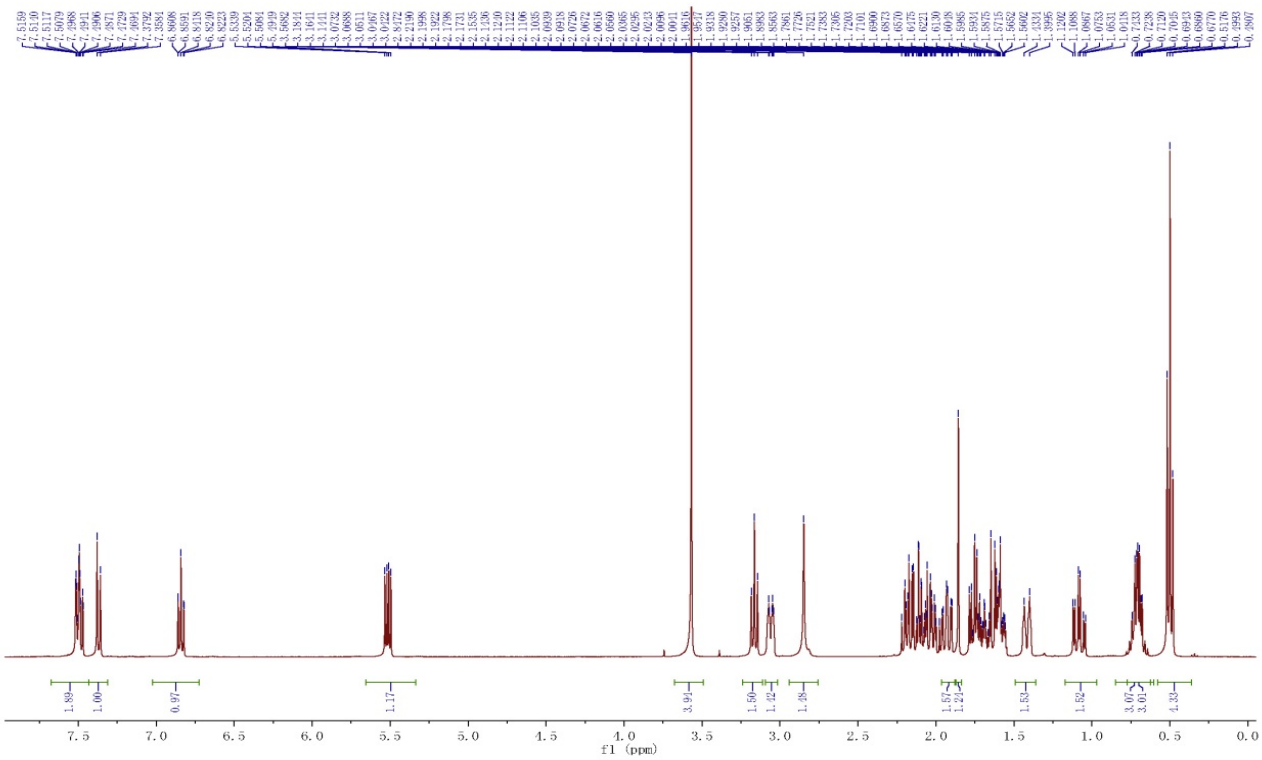


Figure S15. ^{13}C NMR spectrum of Melokhanine B (**2**) (Acetone-d_6)

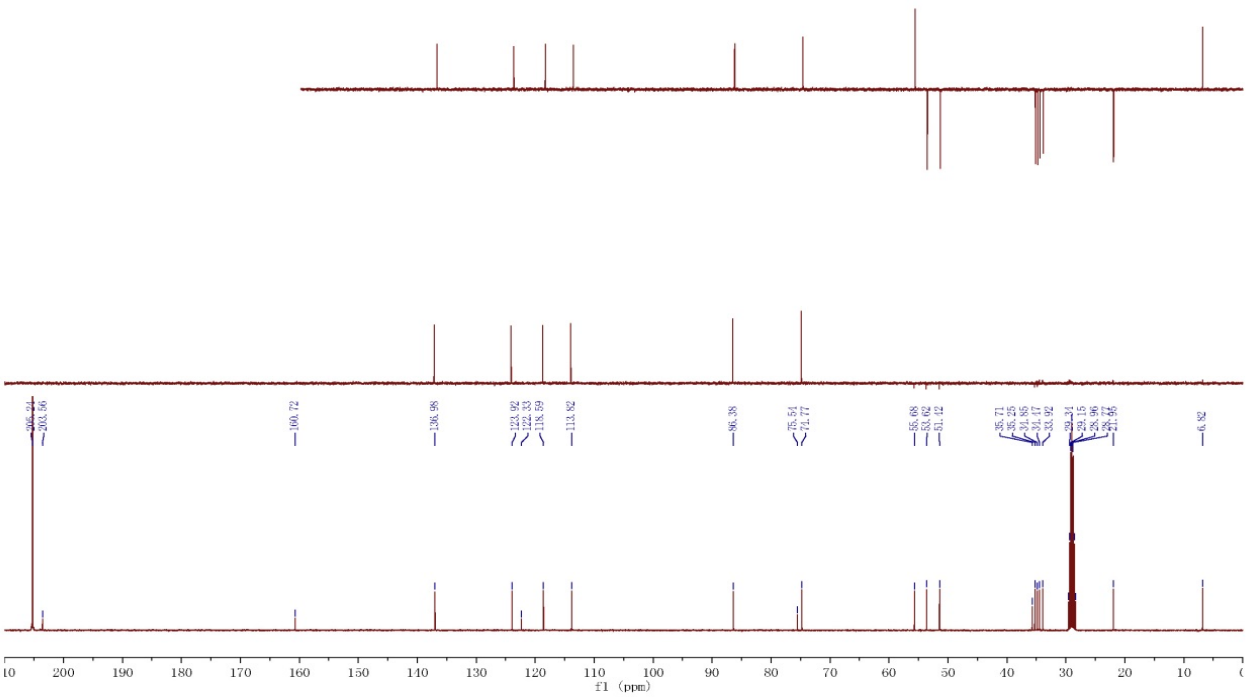


Figure S16. HSQC spectrum of Melokhanine B (**2**) (Acetone-d_6)

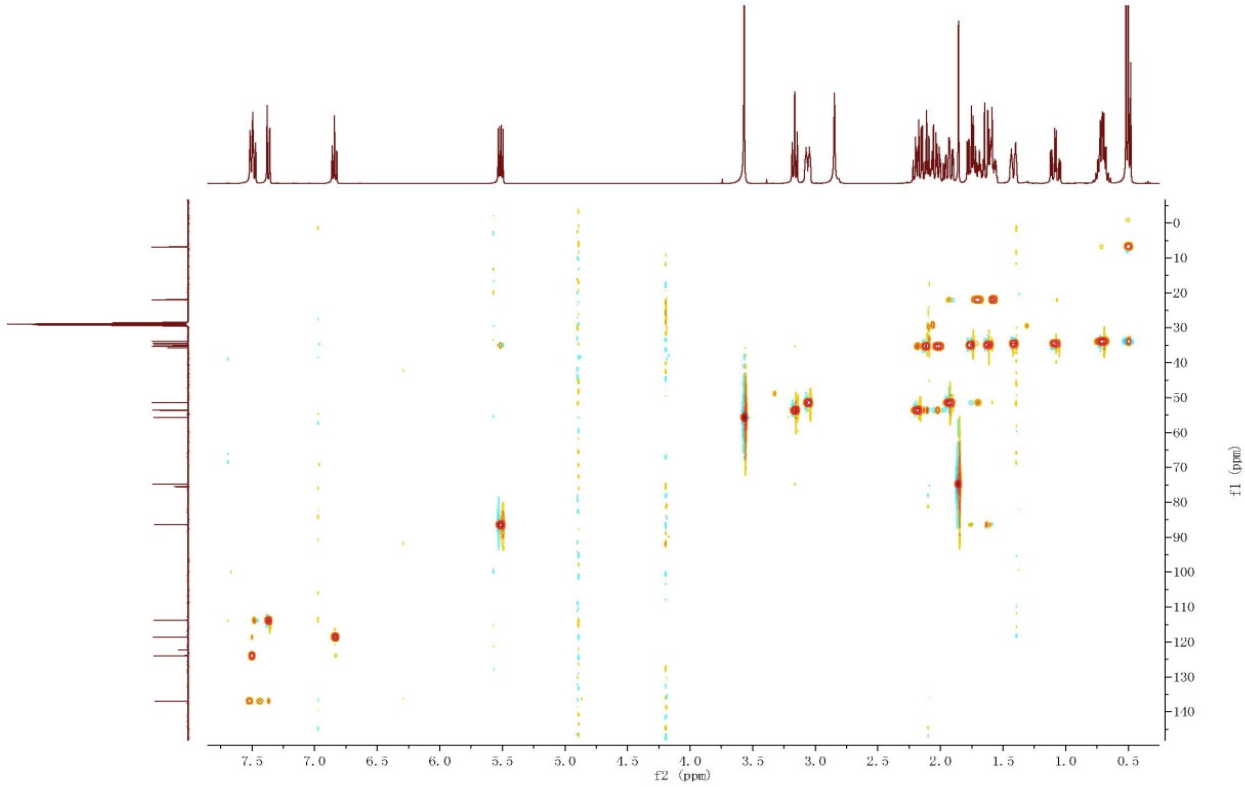


Figure S17. HMBC spectrum of Melokhanine B (**2**) (Acetone-d_6)

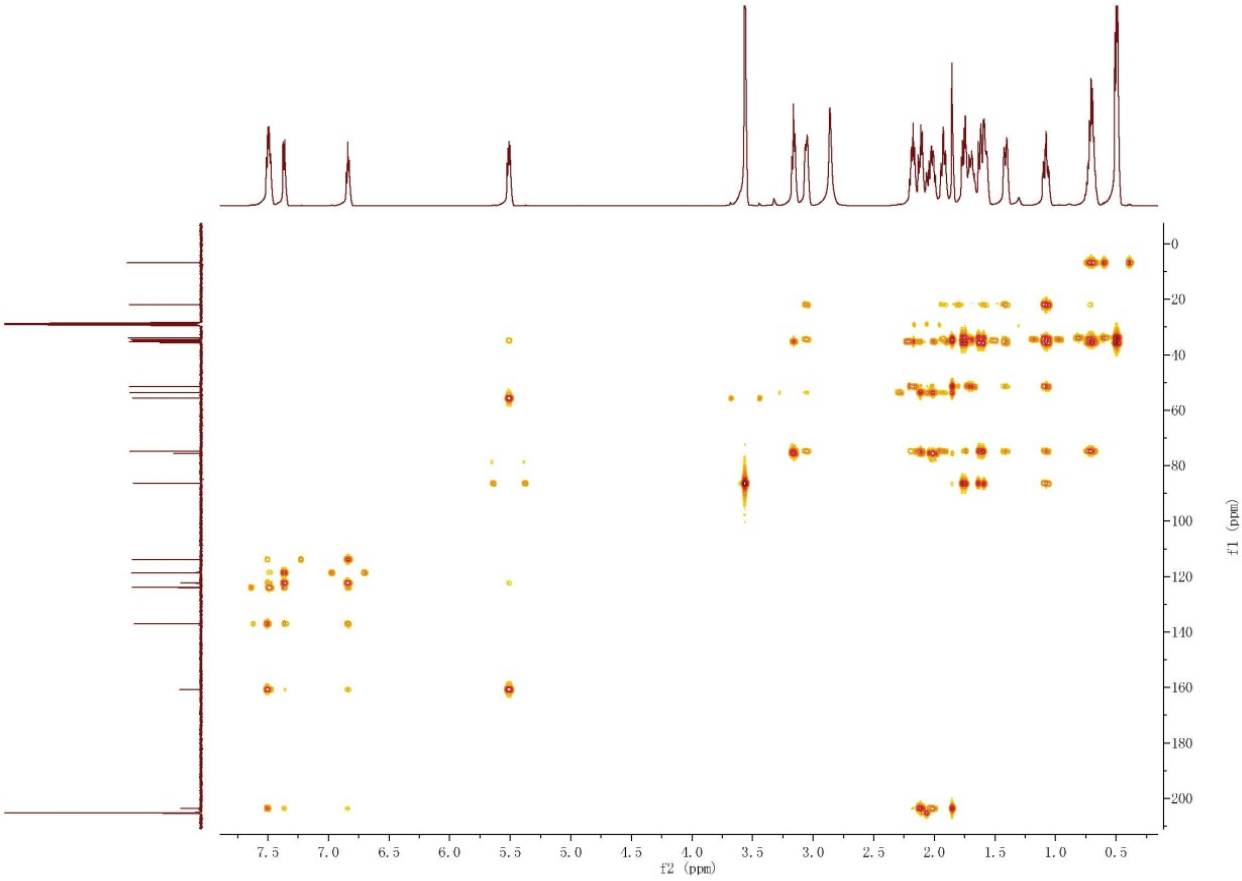


Figure S18. ^{1}H-^{1}H COSY spectrum of Melokhanine B (**2**) (Acetone-d_6)

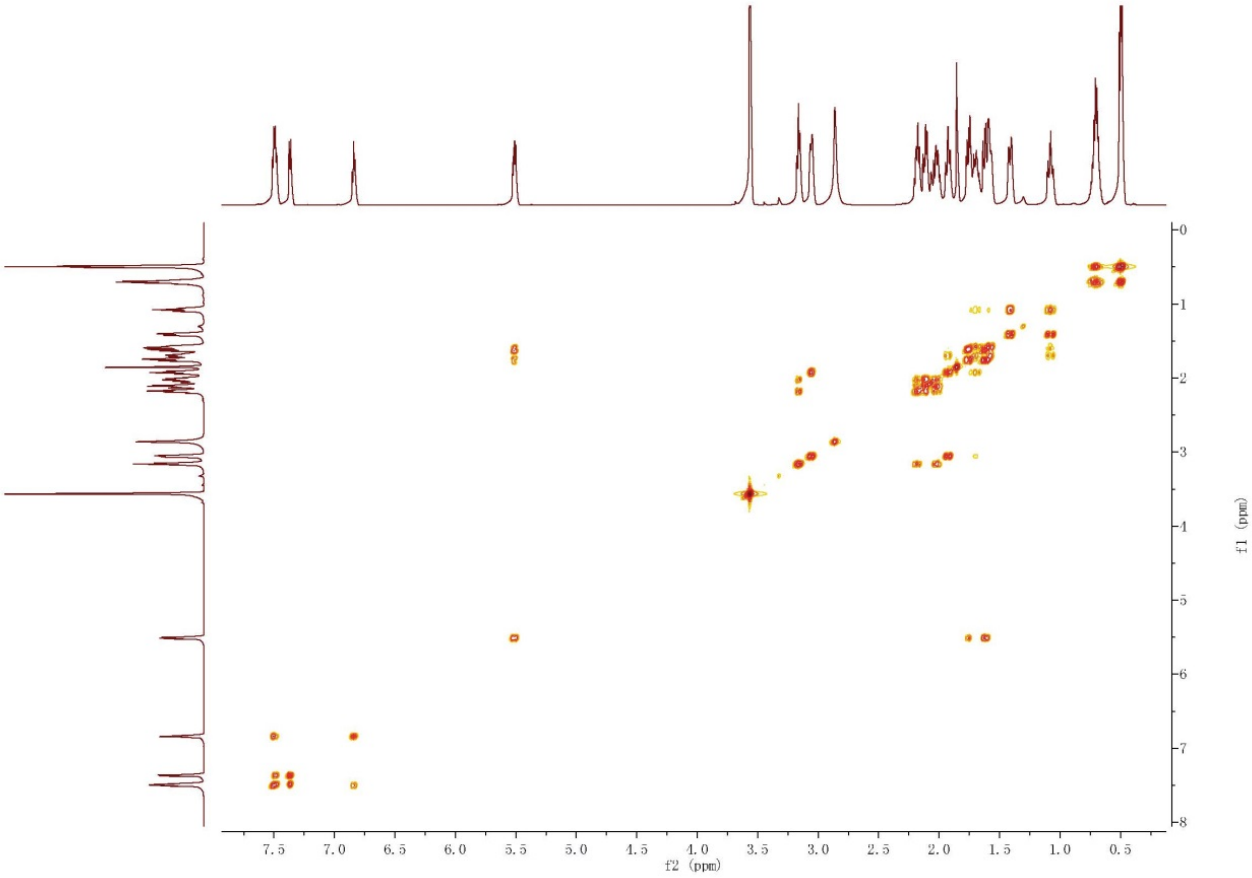


Figure S19. ROESY spectrum of Melokhanine B (**2**) (Acetone-d_6)

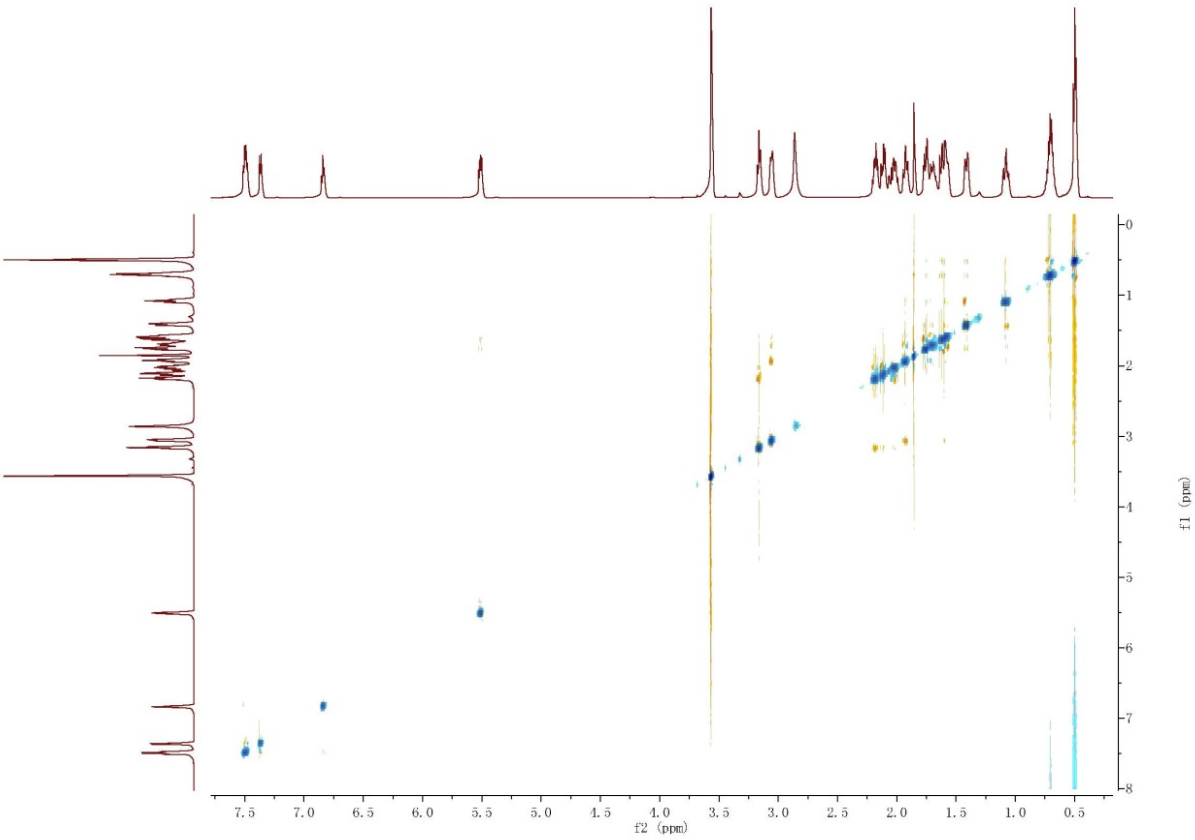


Figure S20. HREIMS spectrum of Melokhanine B (**2**)

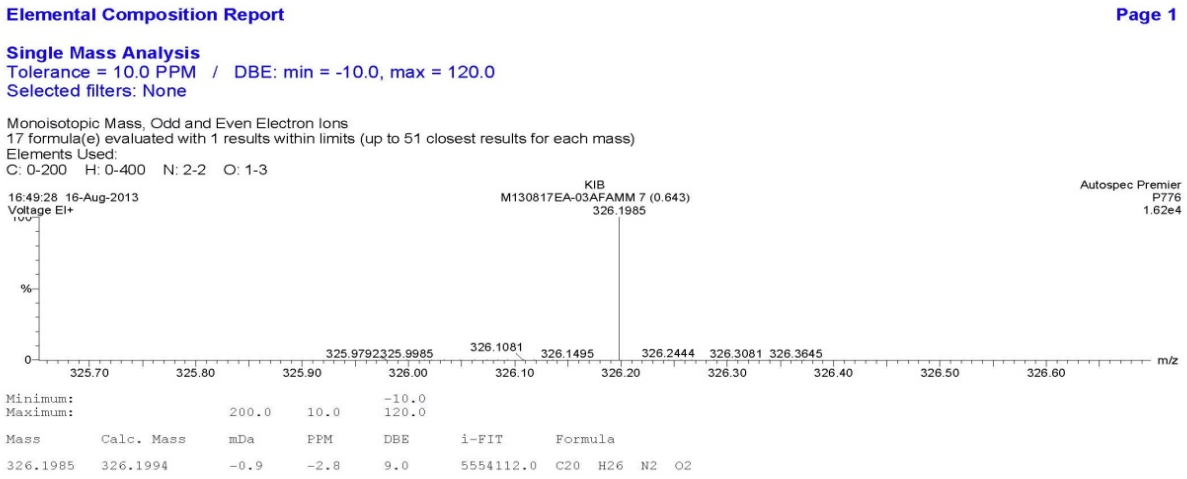
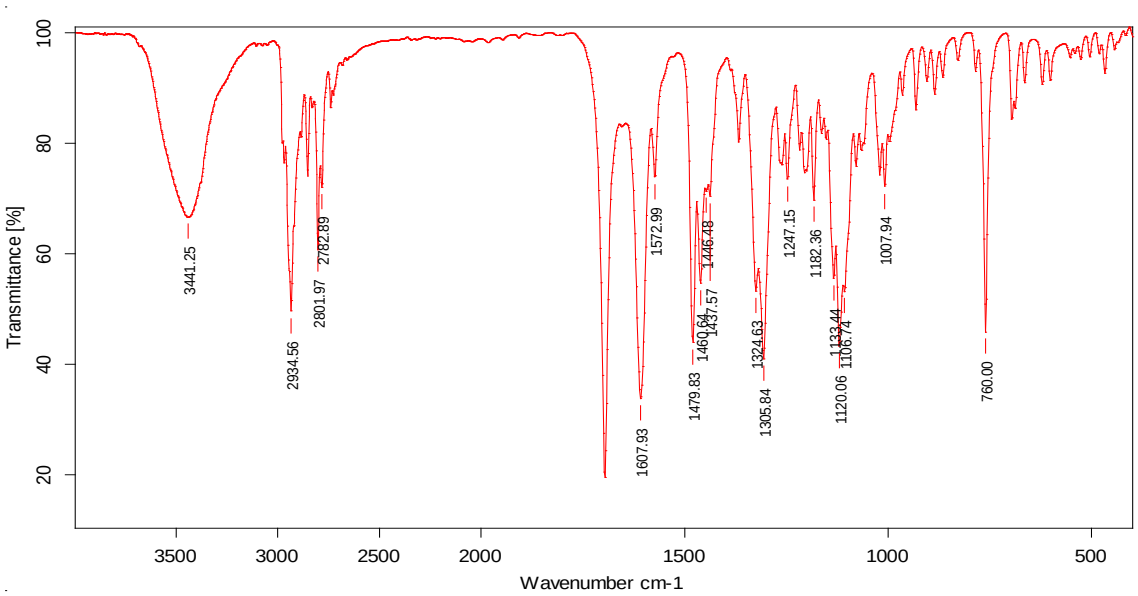


Figure S21. IR spectrum spectrum of Melokhanine B (**2**)



Sample : MHA-3	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2013	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 130925IR12	Zerofilling : 2	Acquisition : Double Sided,Forv	

Figure S22 ^{1}H NMR spectrum of Melokhanine C (**3**) (DMSO-d_6)

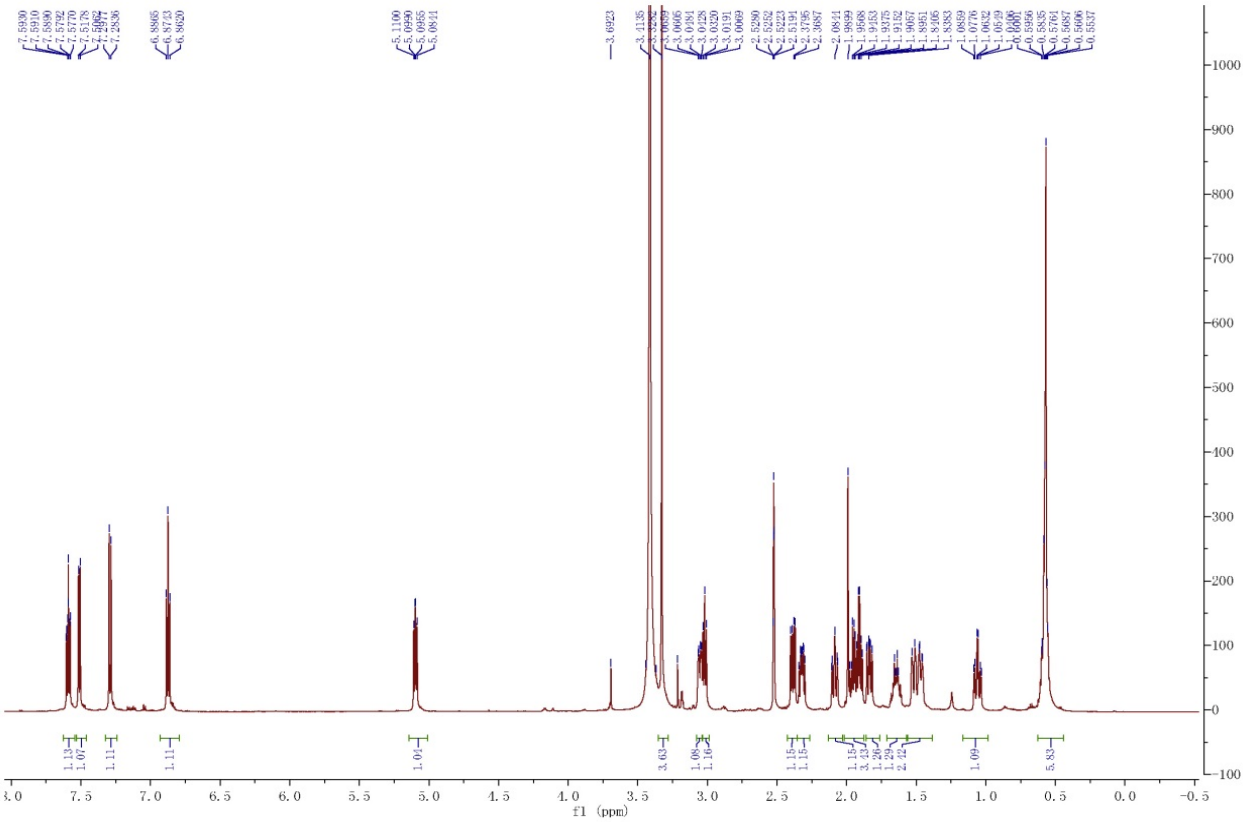


Figure S23. ^{13}C NMR spectrum of Melokhanine B (**2**) (Acetone-d_6)

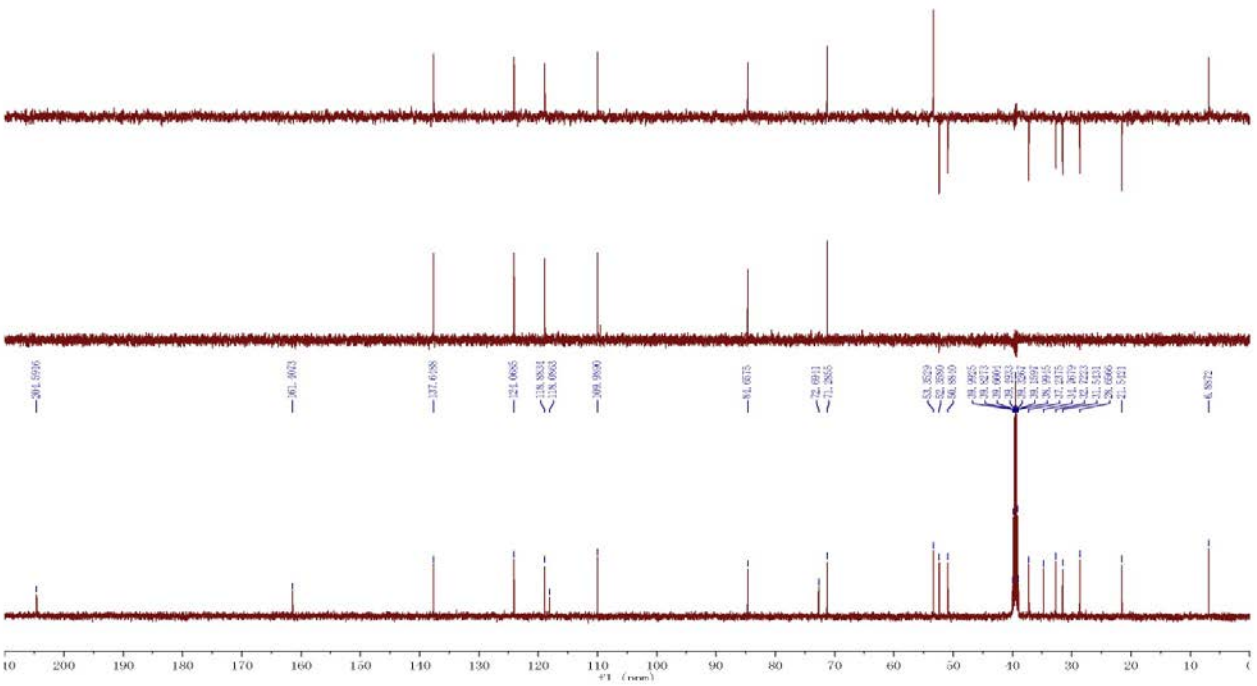


Figure S24. HSQC spectrum of Melokhanine C (**3**) (DMSO-d_6)

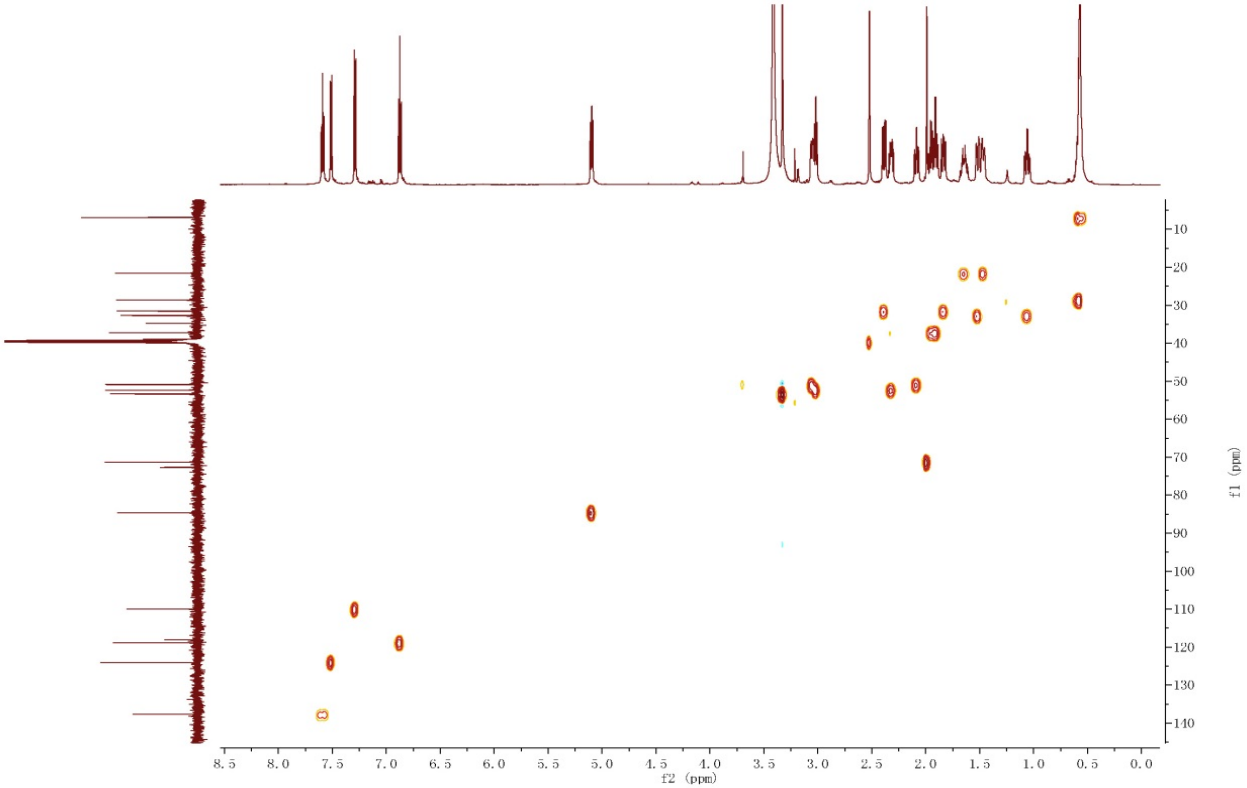


Figure S25. HMBC spectrum of Melokhanine C (**3**) (DMSO-d_6)

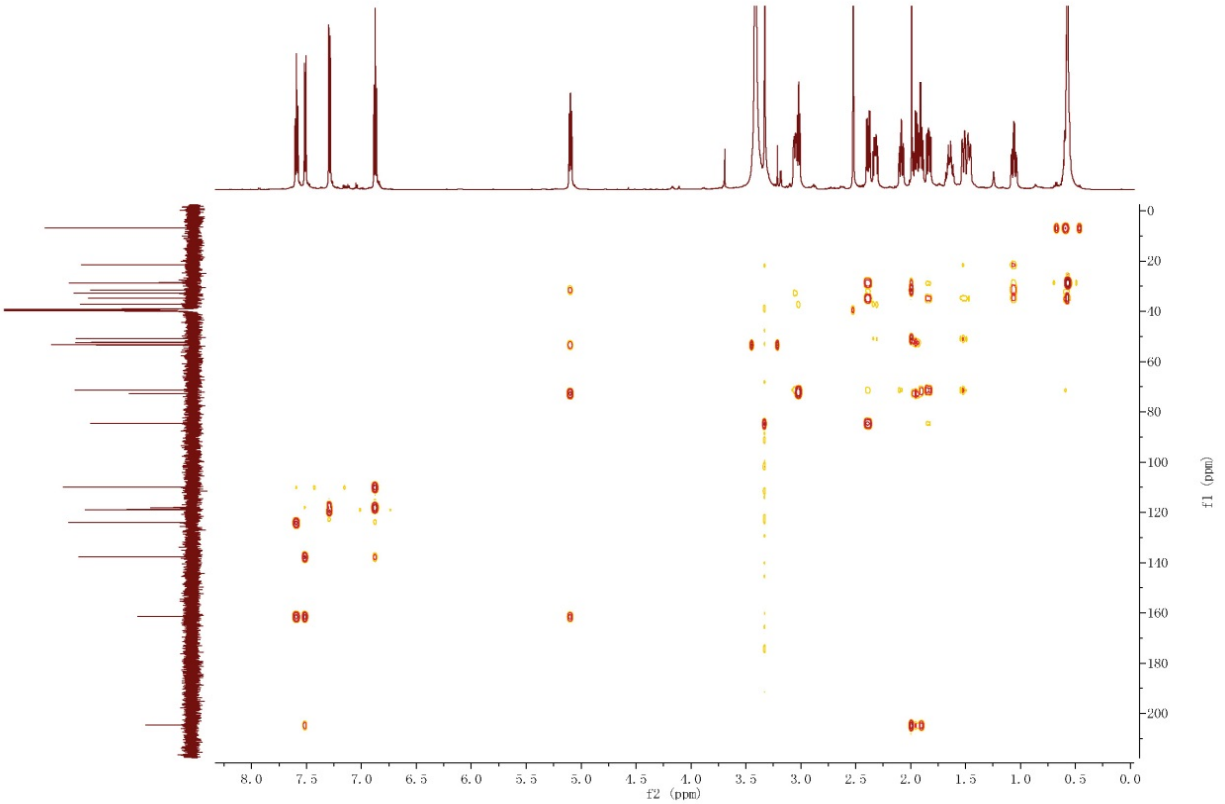


Figure S26. ^{1}H-^{1}H COSY spectrum of Melokhanine C (**3**) (DMSO-d_6)

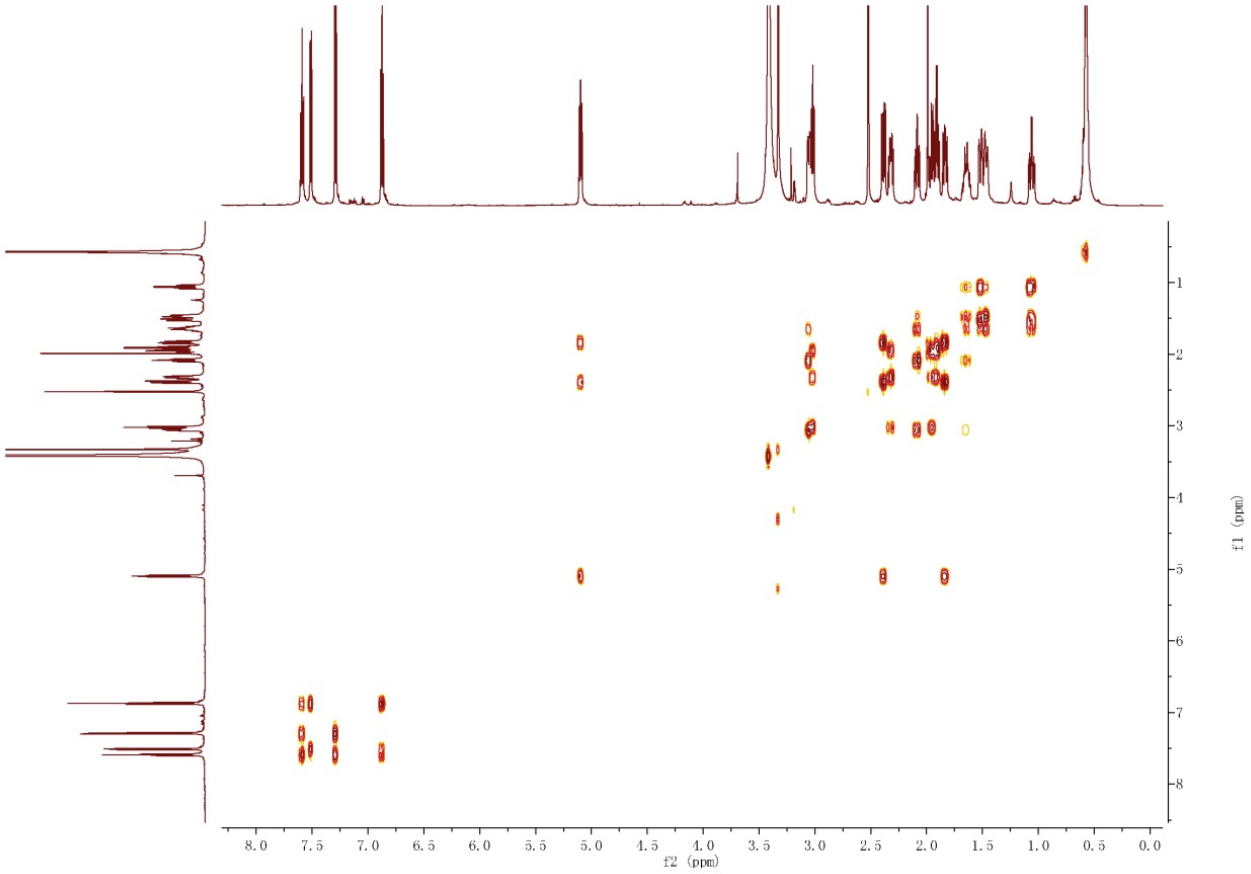


Figure S27. ROESY spectrum of Melokhanine C (**3**) (DMSO-d_6)

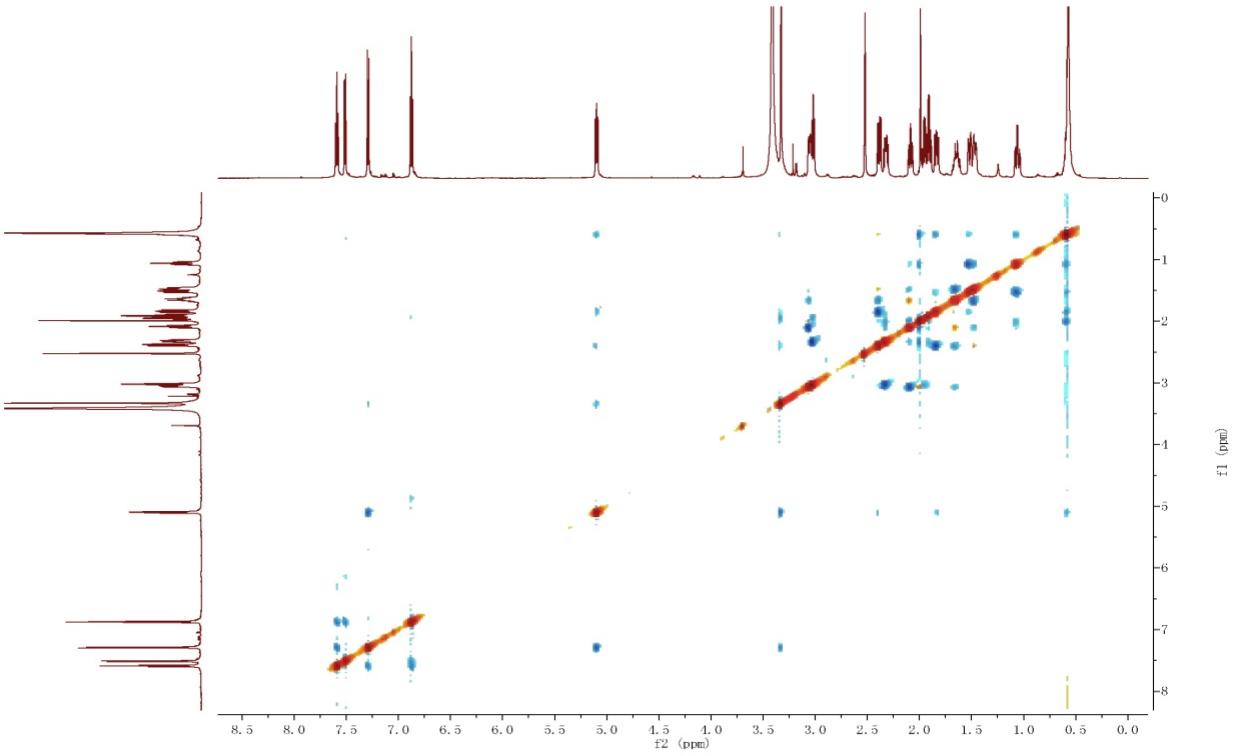
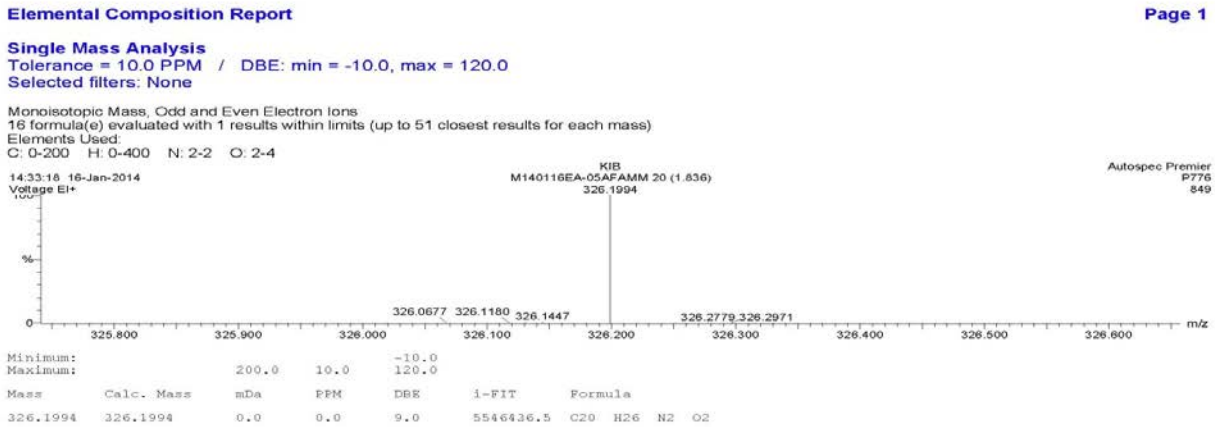


Figure S28. HREIMS spectrum of Melokhanine C (**3**)



Elemental Composition Report Page 1

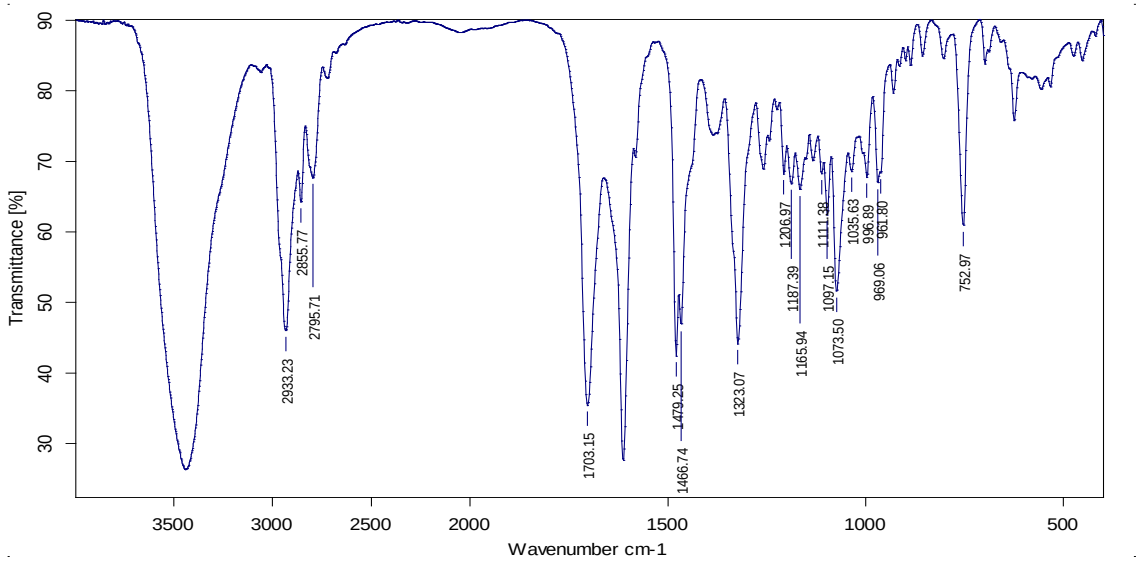
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 N: 2-2 O: 2-4

14:33:18 16-Jan-2014 Voltage EI+
KIB M140116EA-05AFAMM 20 (1.836)
Autospec Premier P776 849

Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.1994	326.1994	0.0	0.0	9.0	5546436.5	C20 H26 N2 O2

Figure S29. IR spectrum spectrum of Melokhanine C (**3**)



Sample : wmha-23a	Frequency Range : 399.246 - 3996.32	Measured on : 20/01/2014	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 140120IR3	Zerofilling : 2	Acquisition : Double Sided,Forv	

Figure S30. ^{1}H NMR spectrum of Melokhanine D (**4**) (Acetone-d_6)

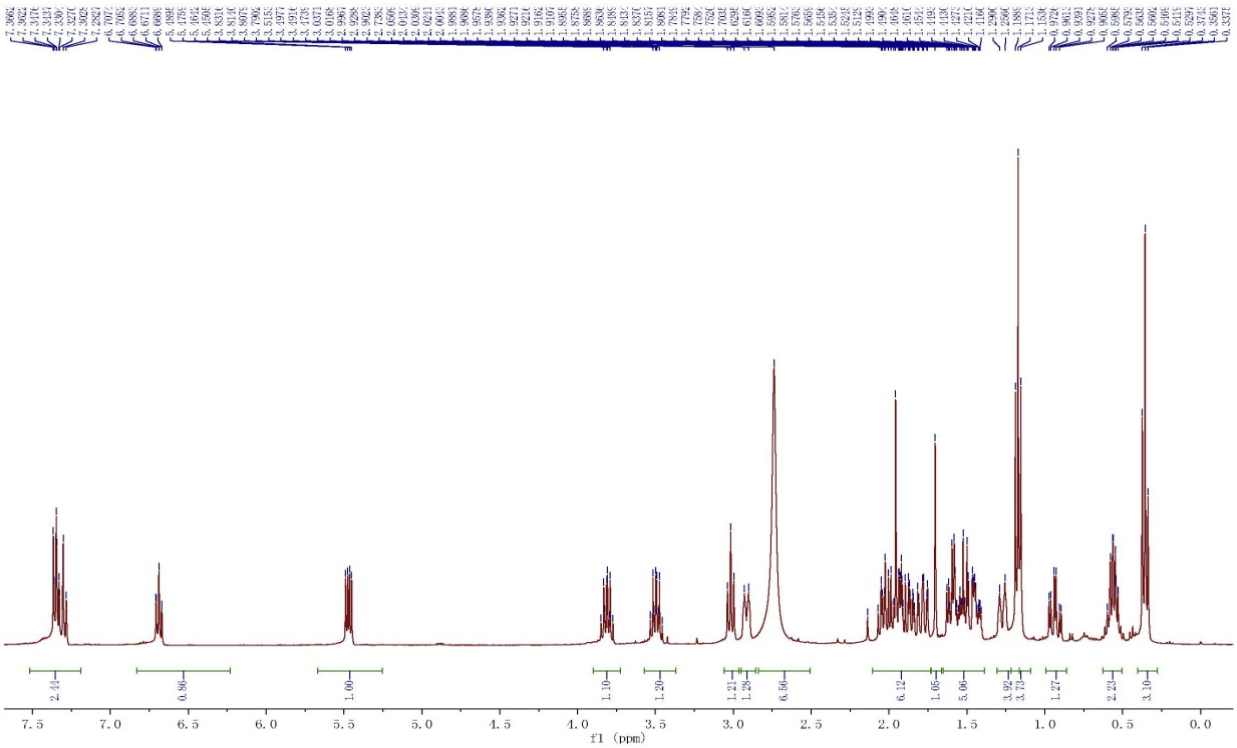


Figure S31. ^{13}C NMR spectrum of Melokhanine D (**4**) (Acetone-d_6)

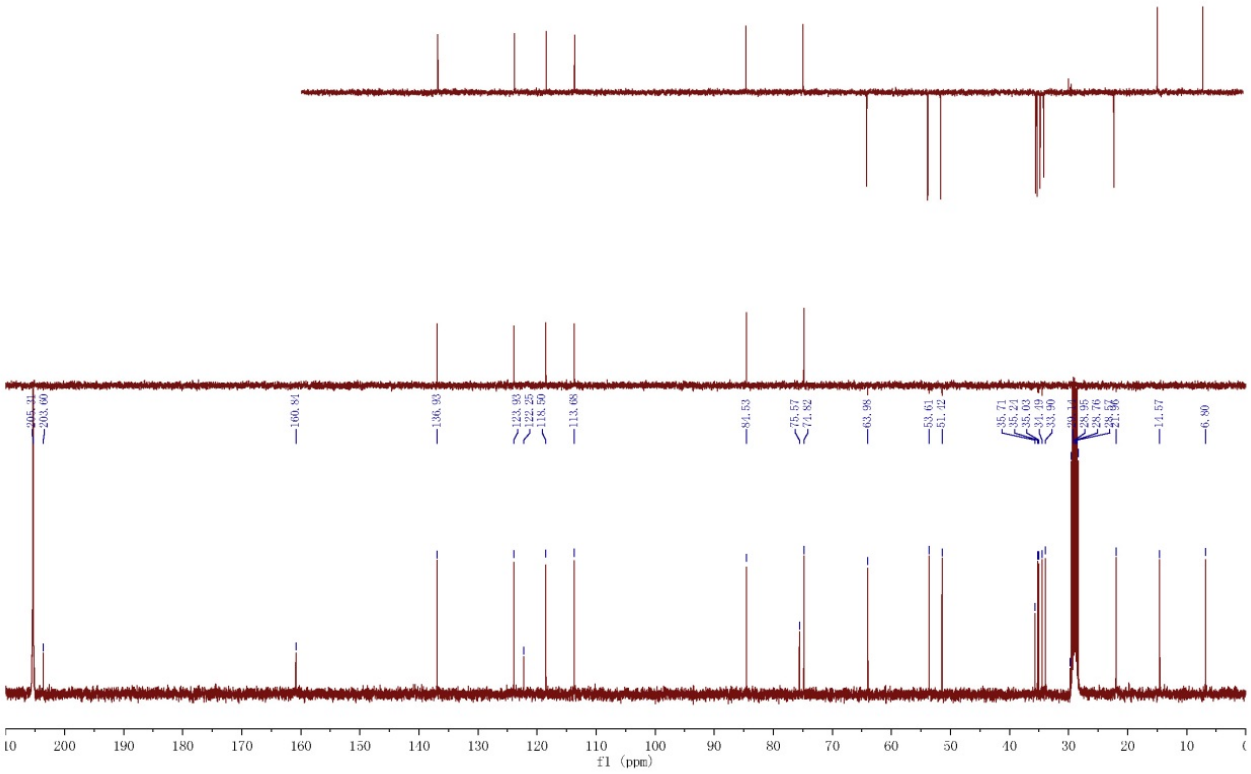


Figure S32. HSQC spectrum of Melokhanine D (**4**) (Acetone-d_6)

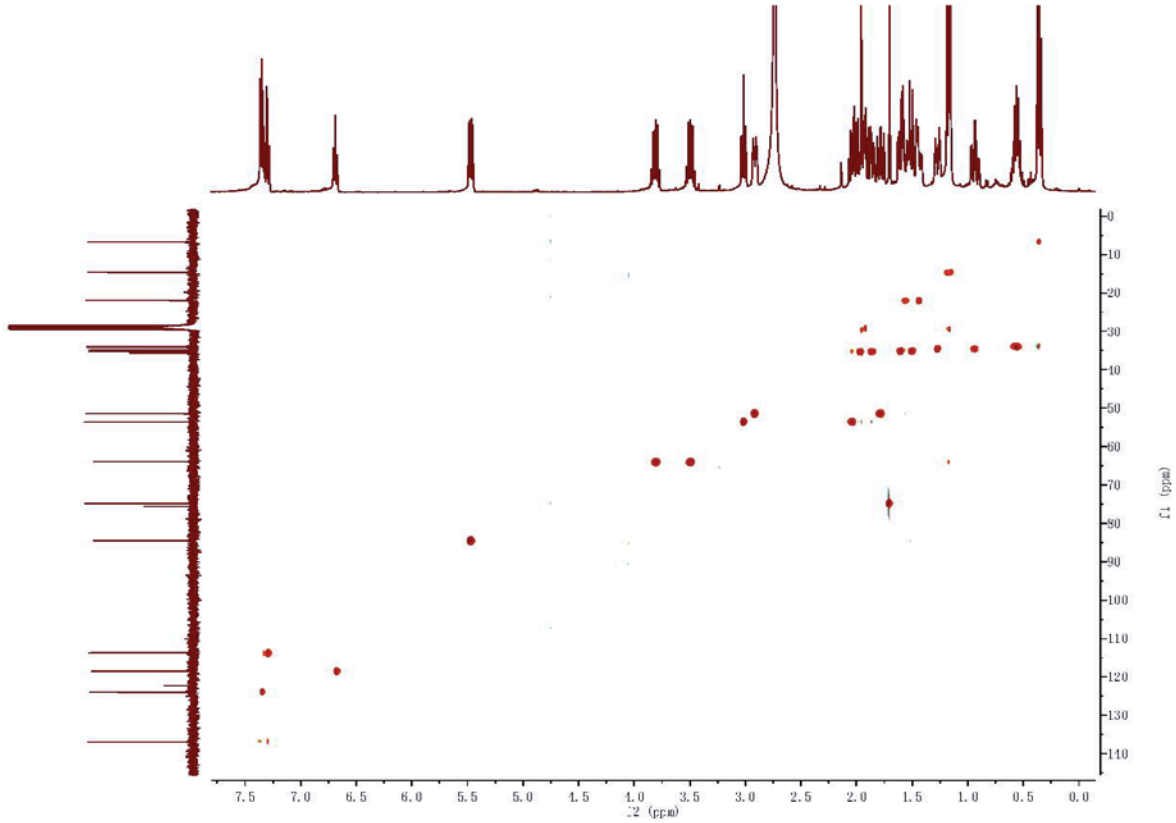


Figure S33. HMBC spectrum of Melokhanine D (**4**) (Acetone-d_6)

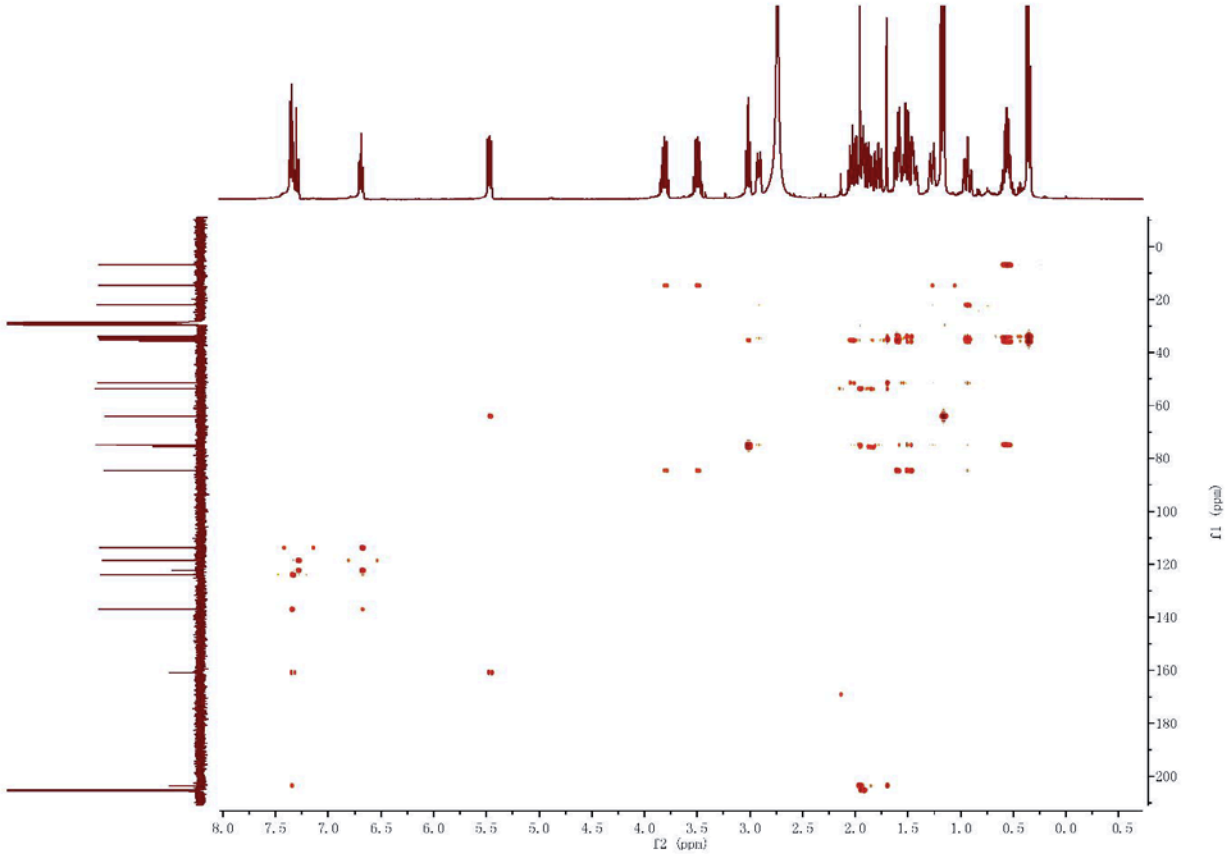


Figure S34. ROESY spectrum of Melokhanine D (**4**) (Acetone-d_6)

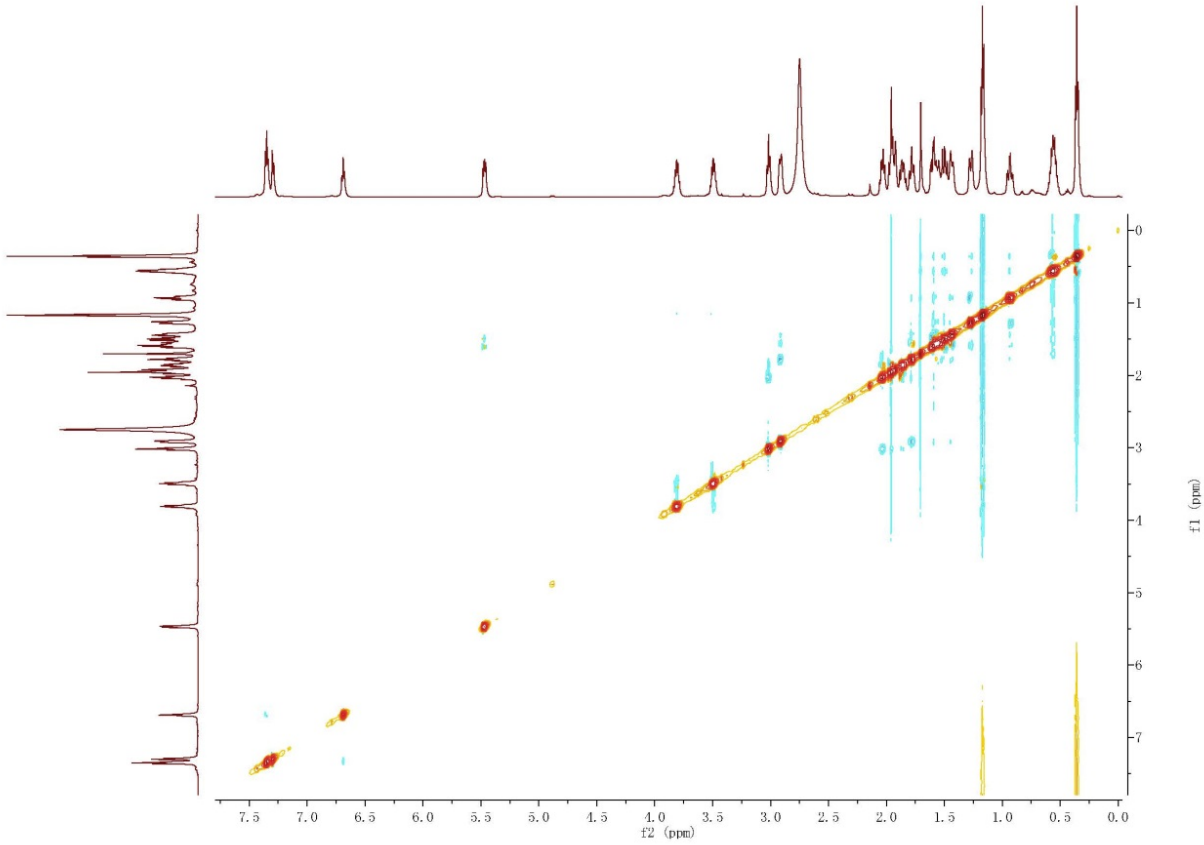
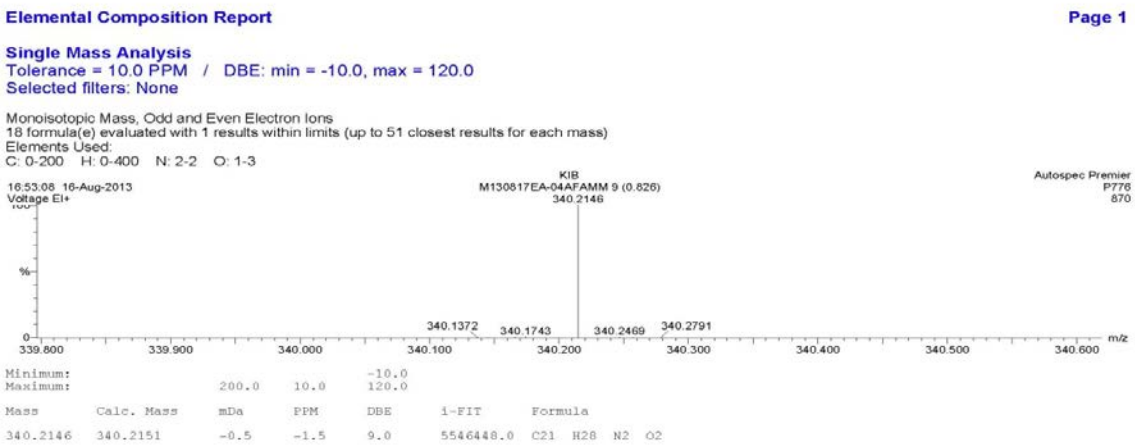


Figure S35. HREIMS spectrum of D (**4**)



Elemental Composition Report Page 1

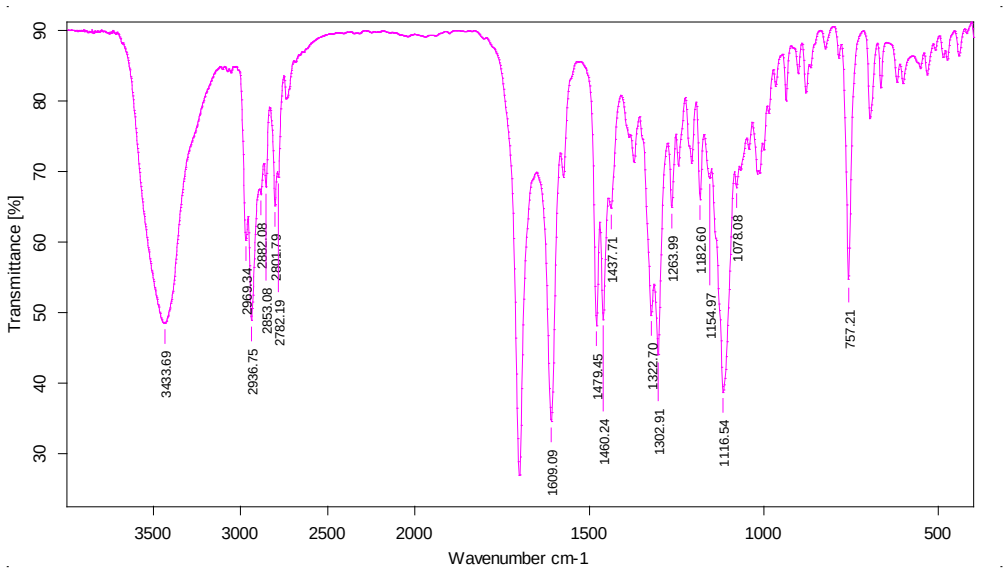
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 N: 2-2 O: 1-3

16:53:08 16-Aug-2013
Voltage EI+
KIB
M130817EA-04AFAMM 9 (0.826)
340.2146
Autospec Premier
P776
870

Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
340.2146	340.2151	-0.5	-1.5	9.0	5546448.0	C21 H28 N2 O2

Figure S36. IR spectrum spectrum of Melokhanine D (**4**)



Sample : MHA-4	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2013	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 130925IR13	Zerofilling : 2	Acquisition : Double Sided,Forw	

Figure S37. ^{1}H NMR spectrum of Melokhanine E (**5**) (Acetone-d_6)

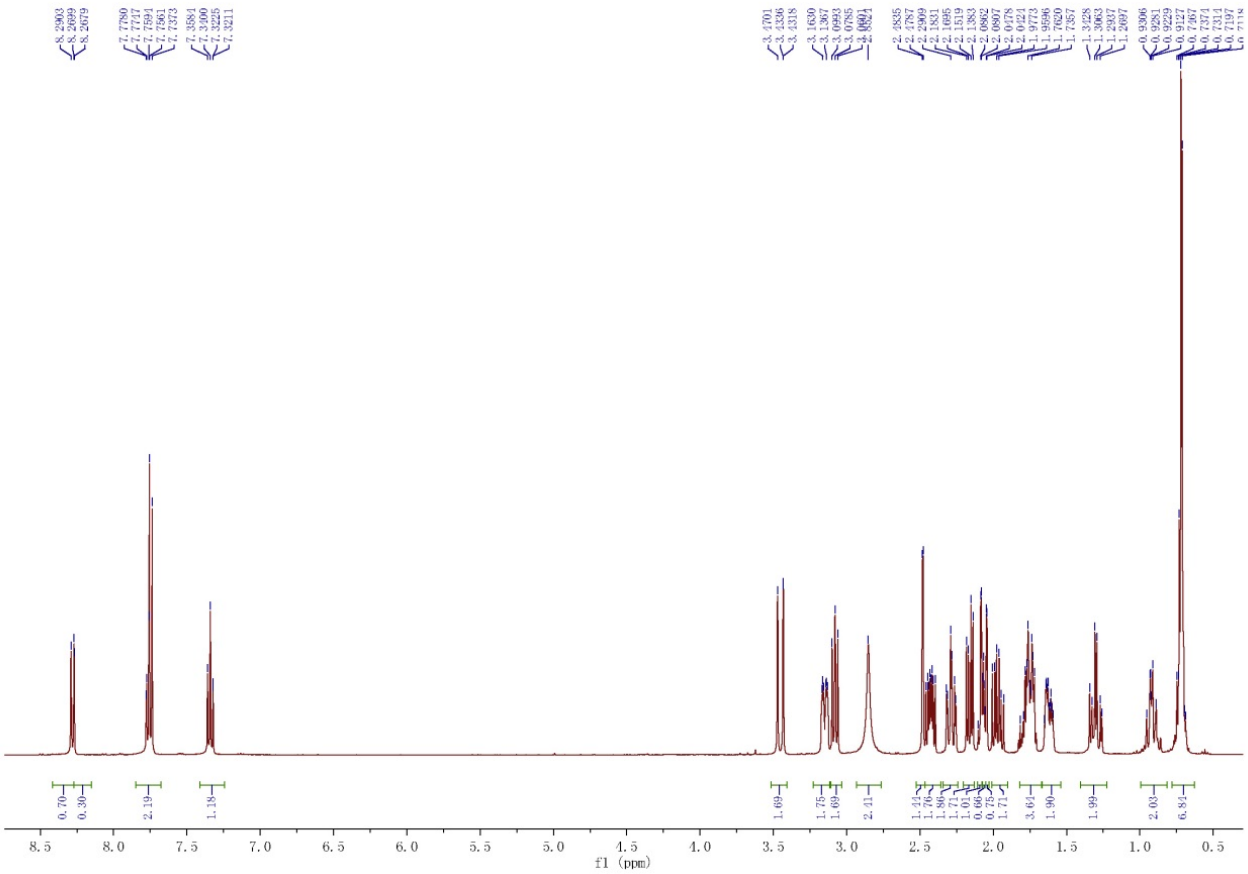


Figure S38. ^{13}C NMR spectrum of Melokhanine E (**5**) (Acetone-d_6)

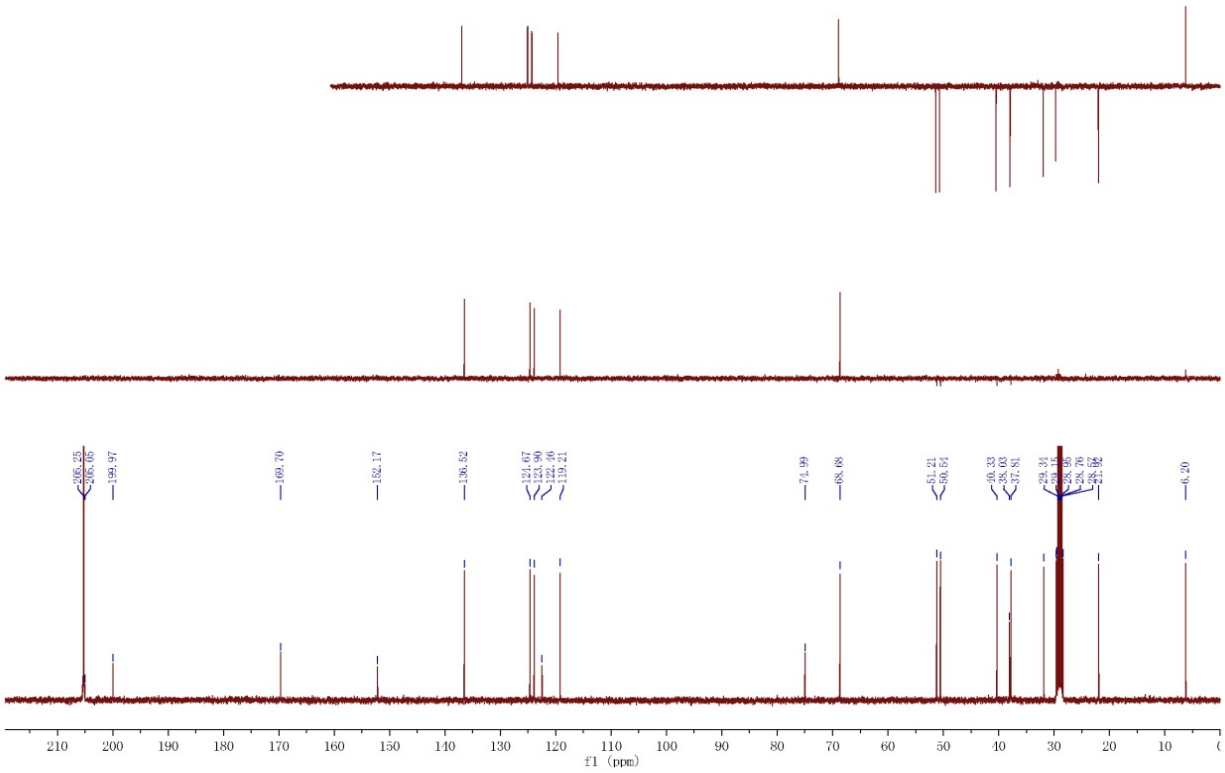


Figure S39. HSQC spectrum of Melokhanine E (**5**) (Acetone-d_6)

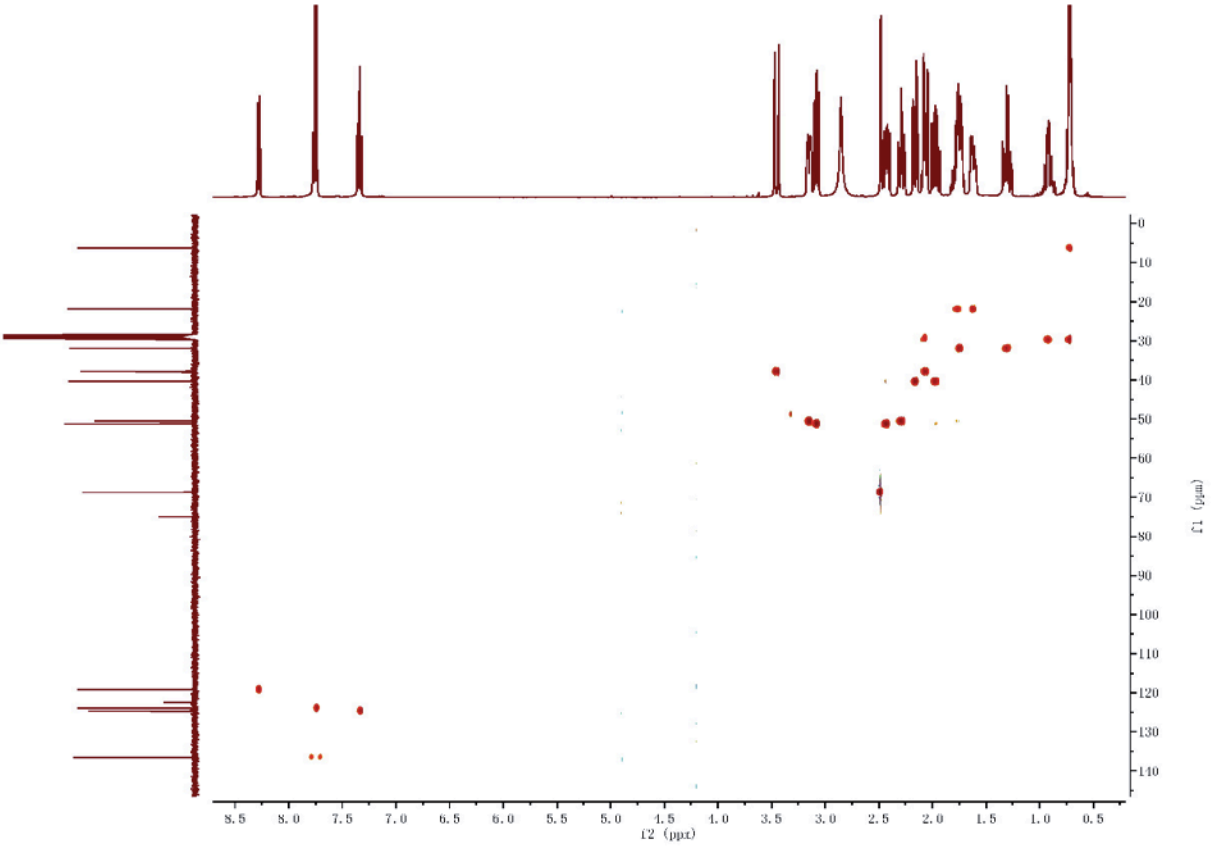


Figure S40. HMBC spectrum of Melokhanine E (**5**) (Acetone-d_6)

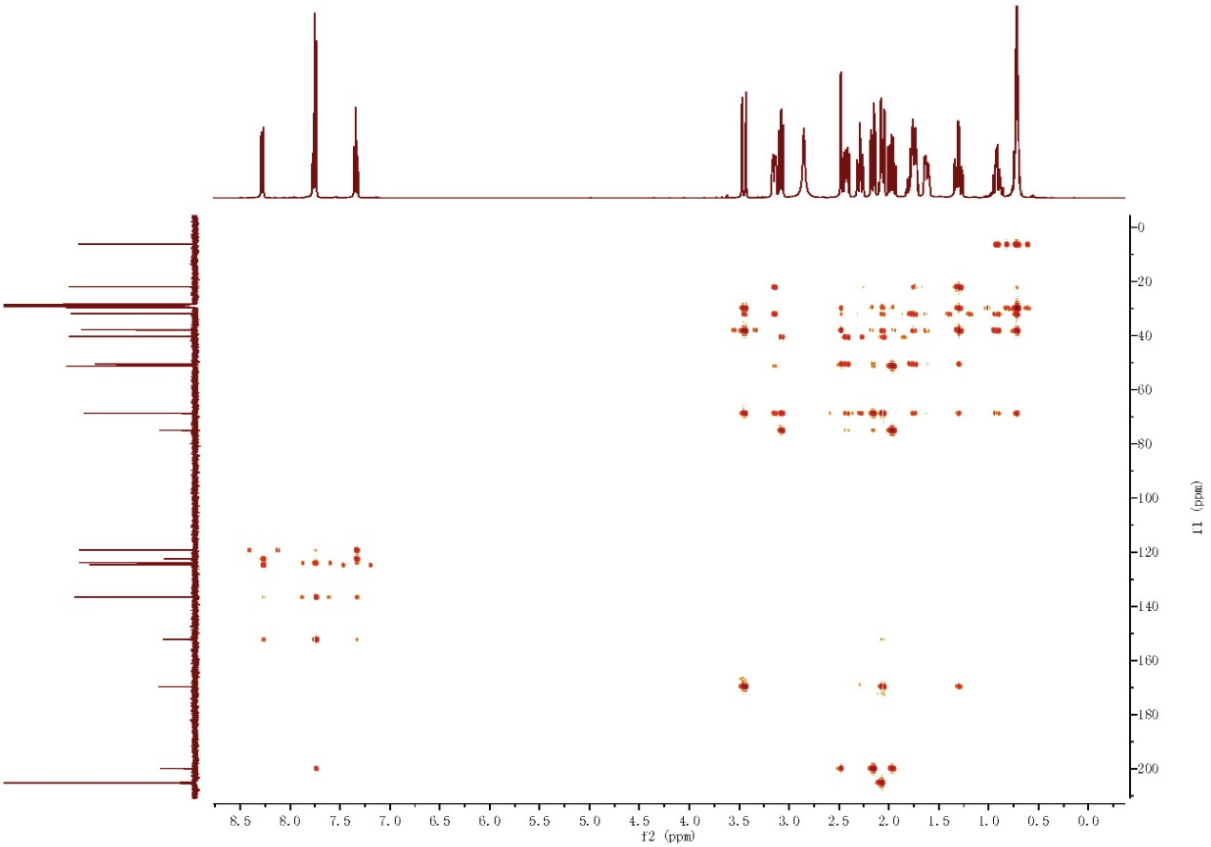


Figure S41. ROESY spectrum of Melokhanine E (**5**) (Acetone-d_6)

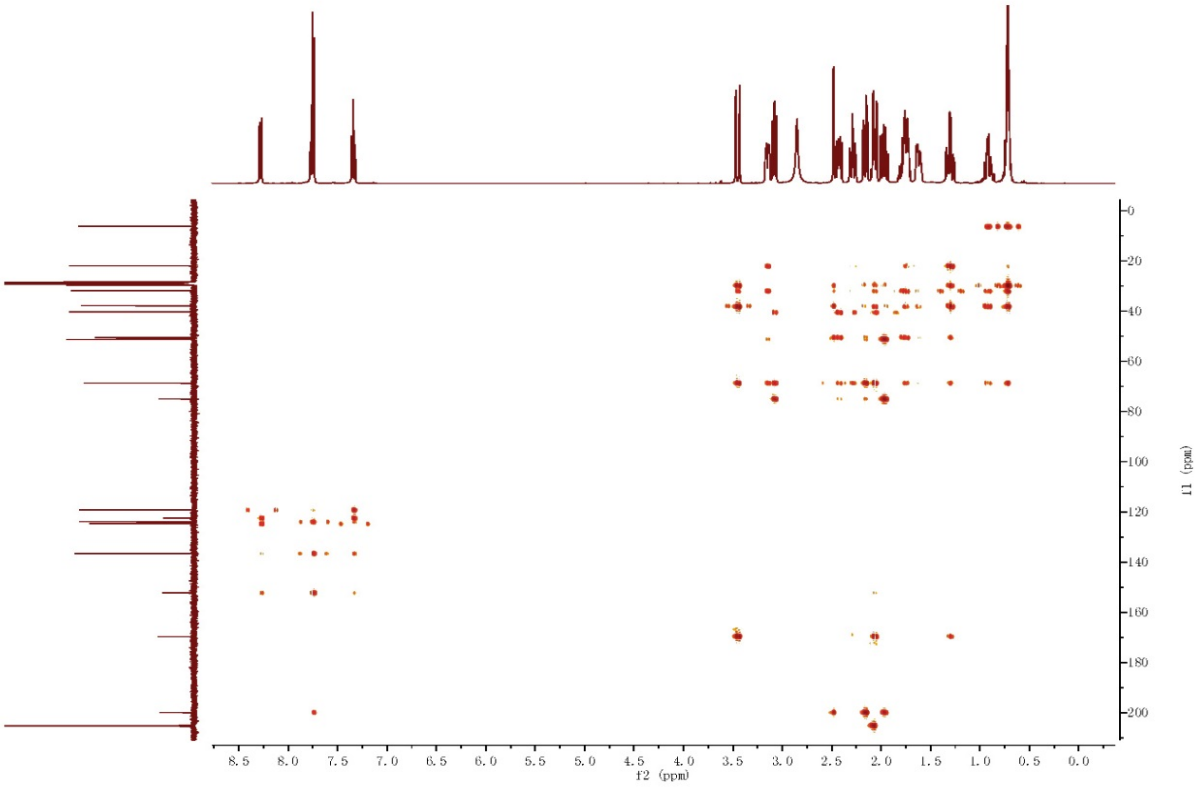


Figure S42. HREIMS spectrum of Melokhanine E (**5**)

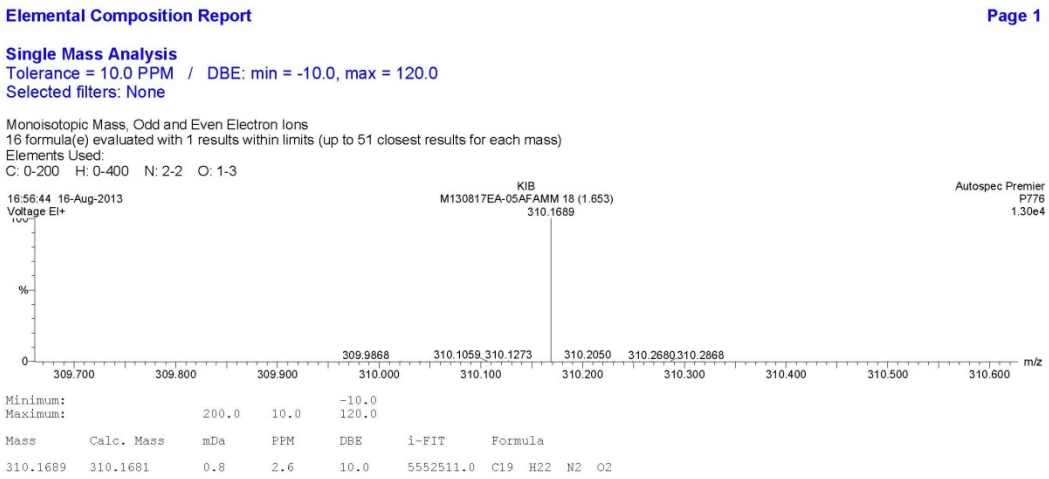
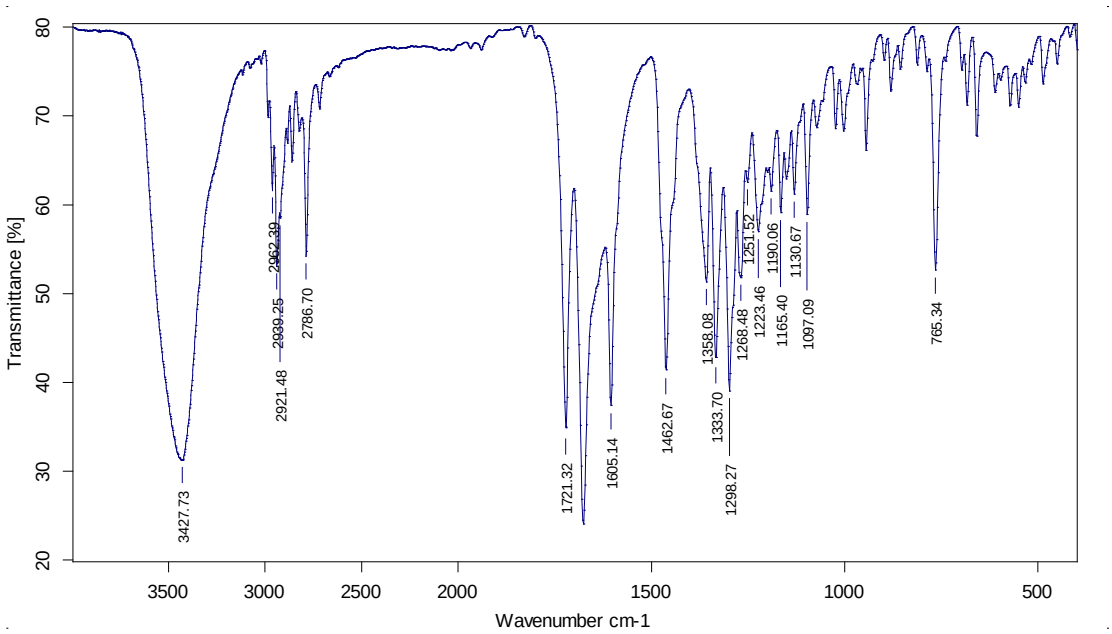


Figure S43. IR spectrum spectrum of Melokhanine E (**5**)



Sample : MHA-6	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2013	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 130925IR14	Zerofilling : 2	Acquisition : Double Sided,Forv	

Figure S44. ^{1}H NMR spectrum of Melokhanine F (**6**) ($CDCl_3$)

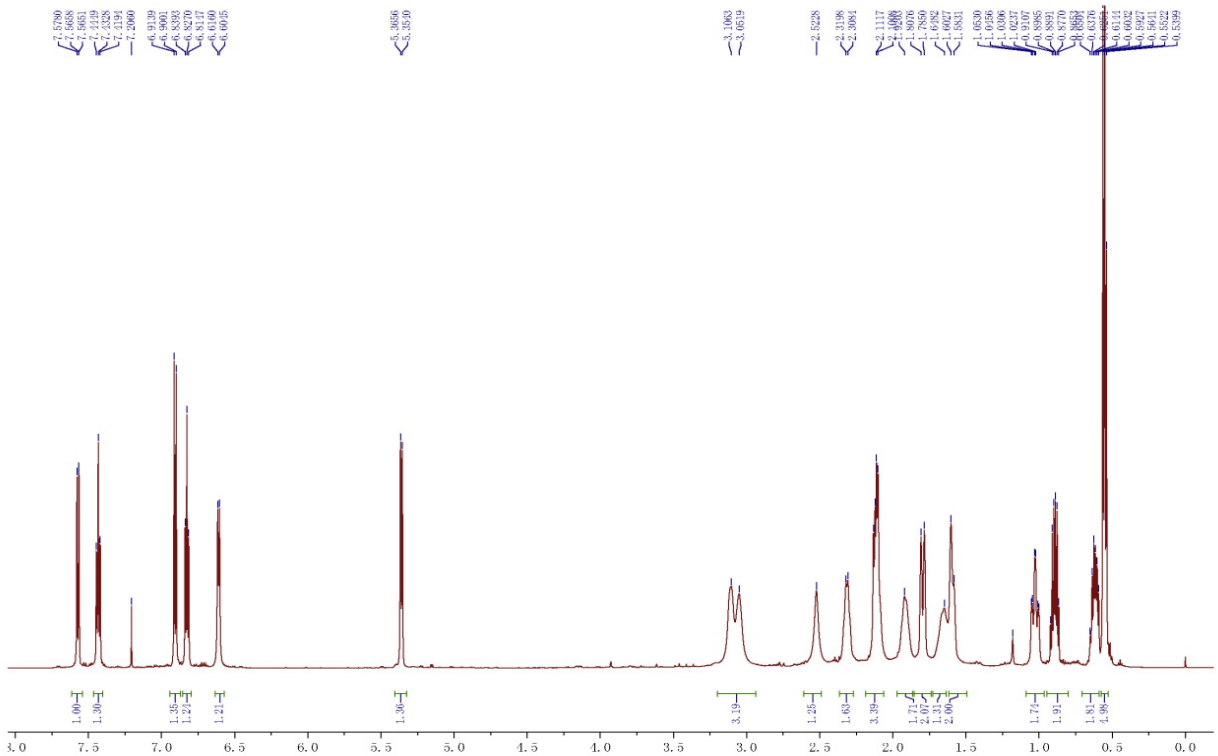


Figure S45. ^{13}C NMR spectrum of F Melokhanine (**6**) ($CDCl_3$)

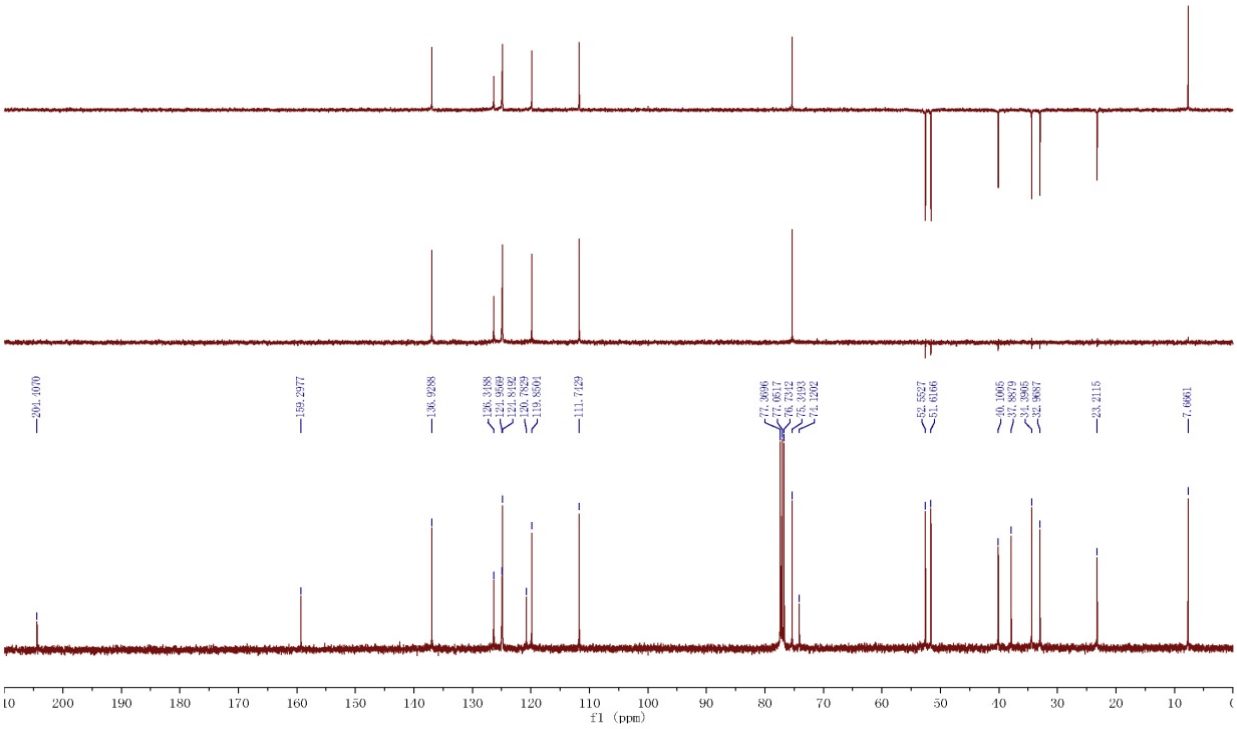


Figure S46. HSQC spectrum of Melokhanine F (**6**) ($CDCl_3$)

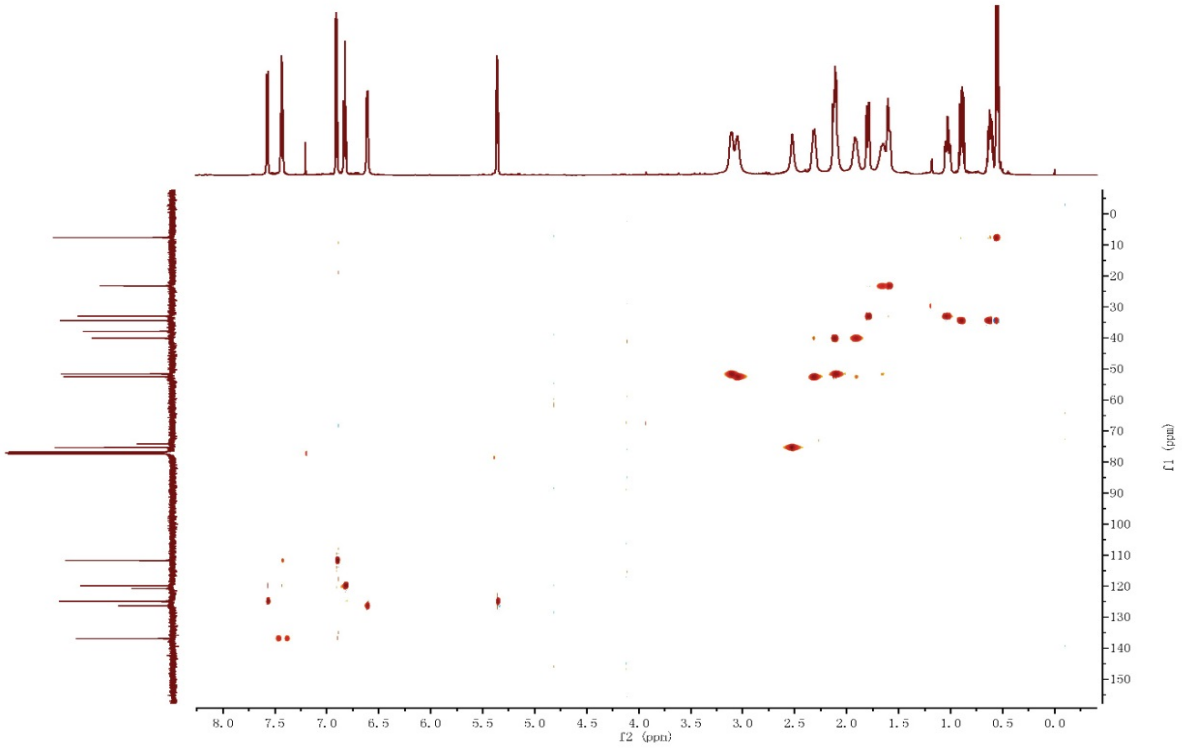


Figure S47. HMBC spectrum of Melokhanine F (**6**) ($CDCl_3$)

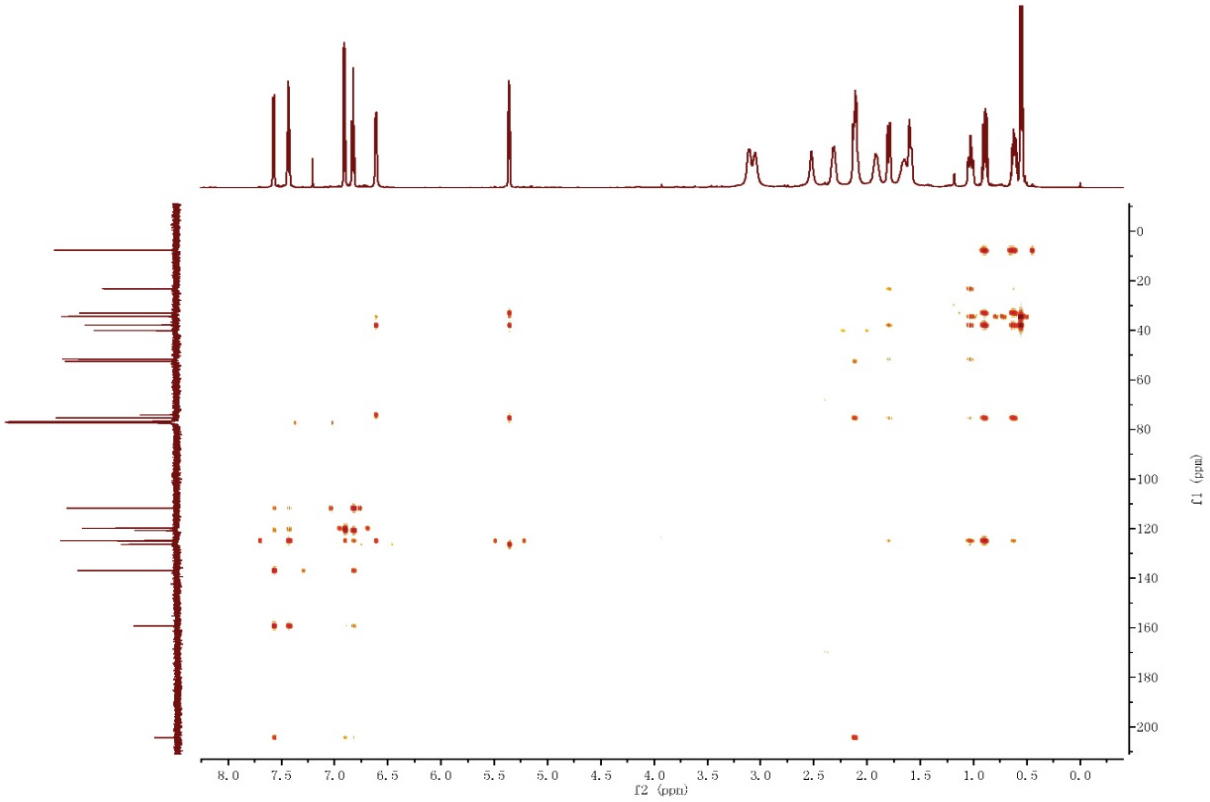


Figure S48. ^{1}H-^{1}H COSY spectrum of Melokhanine F (**6**) ($CDCl_3$)

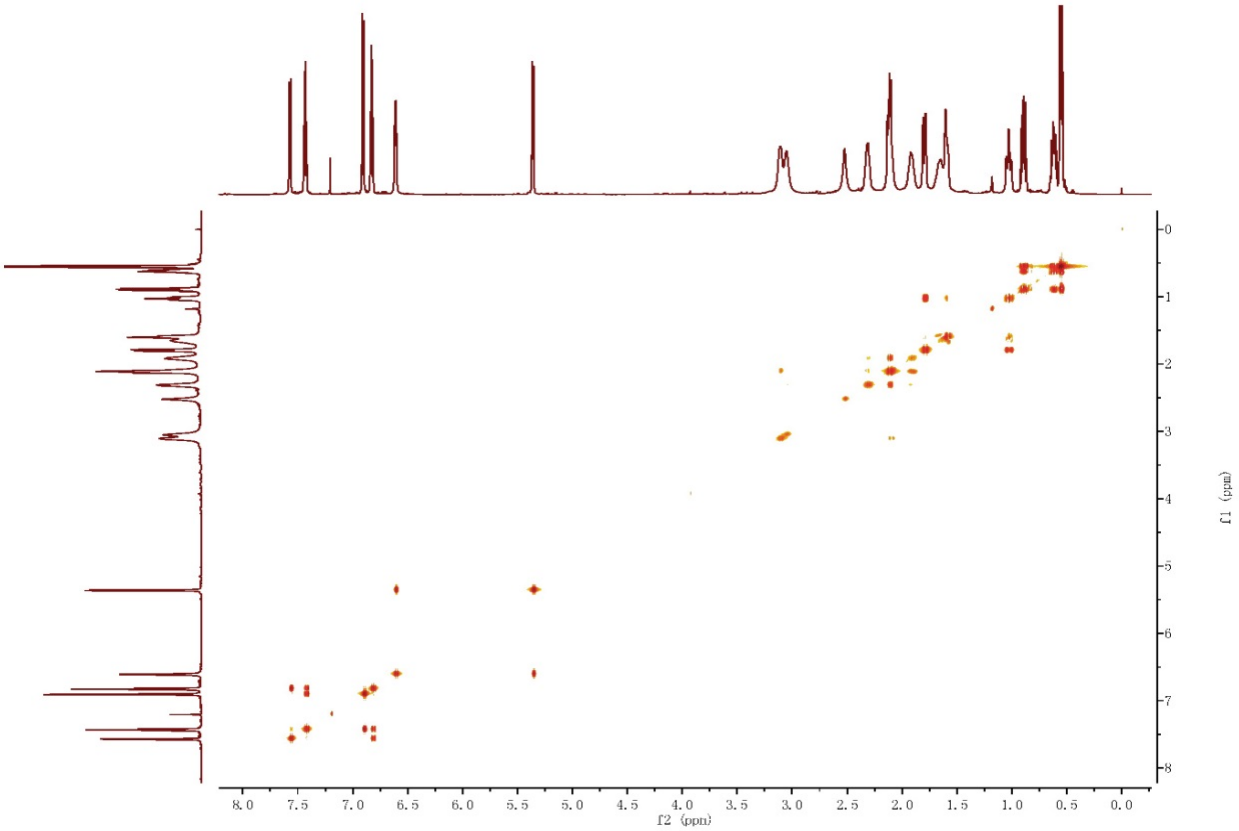


Figure S49. ROESY spectrum of Melokhanine F (**6**) ($CDCl_3$)

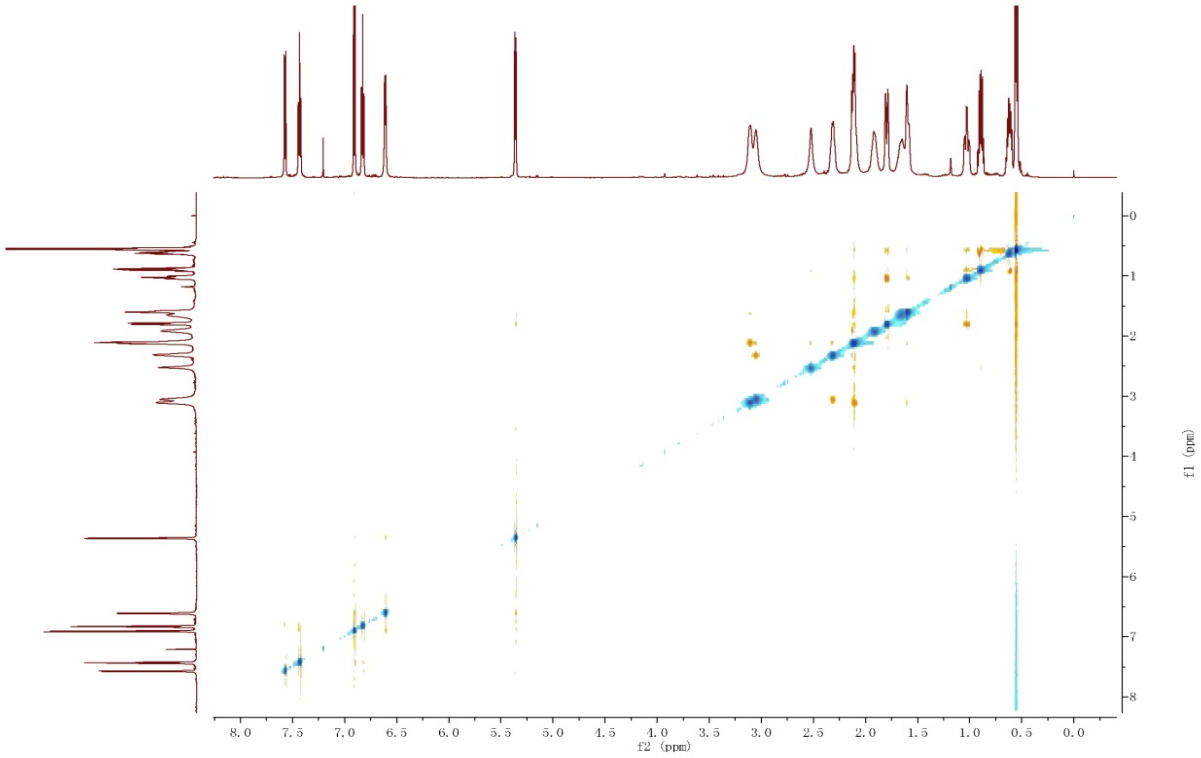


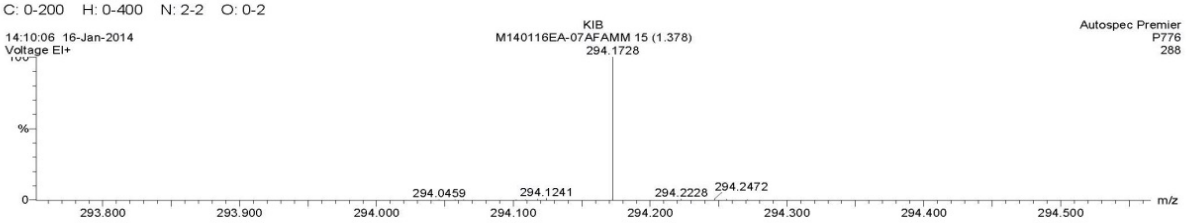
Figure S50. HREIMS spectrum of Melokhanine F (**6**) ($CDCl_3$)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 N: 2-2 O: 0-2

14:10:06 16-Jan-2014
Voltage EI+
KIB
M140116EA-07AFAMM 15 (1.378)
Autospec Premier
P776
288



Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
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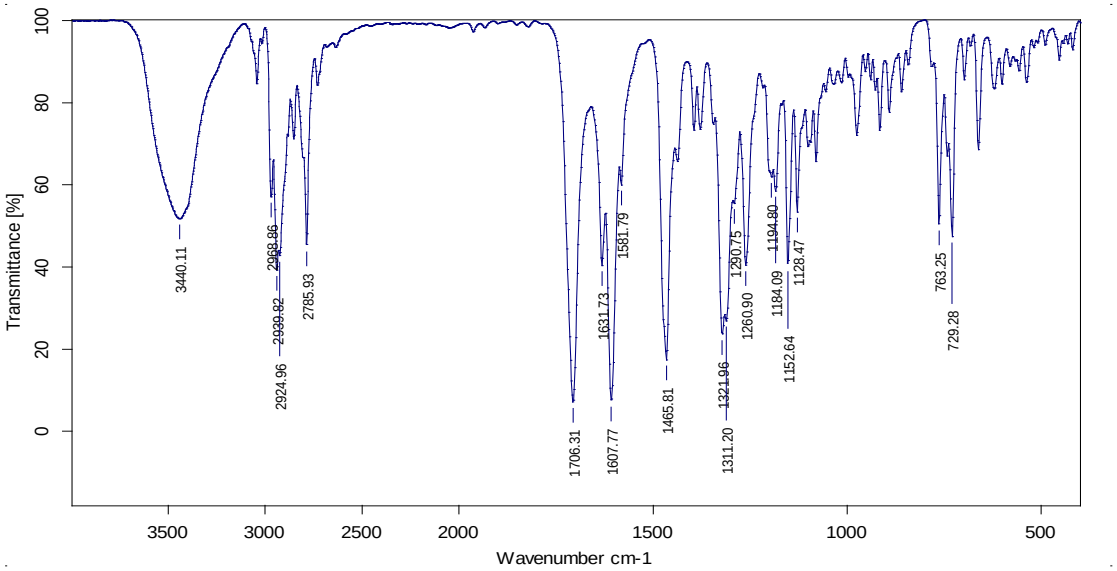
Figure S51. IR spectrum spectrum of Melokhanine F (**6**) ($CDCl_3$)



Sample : MHA-23	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2013	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 130925IR15	Zerofilling : 2	Acquisition : Double Sided,Forw	

Figure S52. ^{1}H NMR spectrum of Melokhanine G (**7**) ($CDCl_3$)

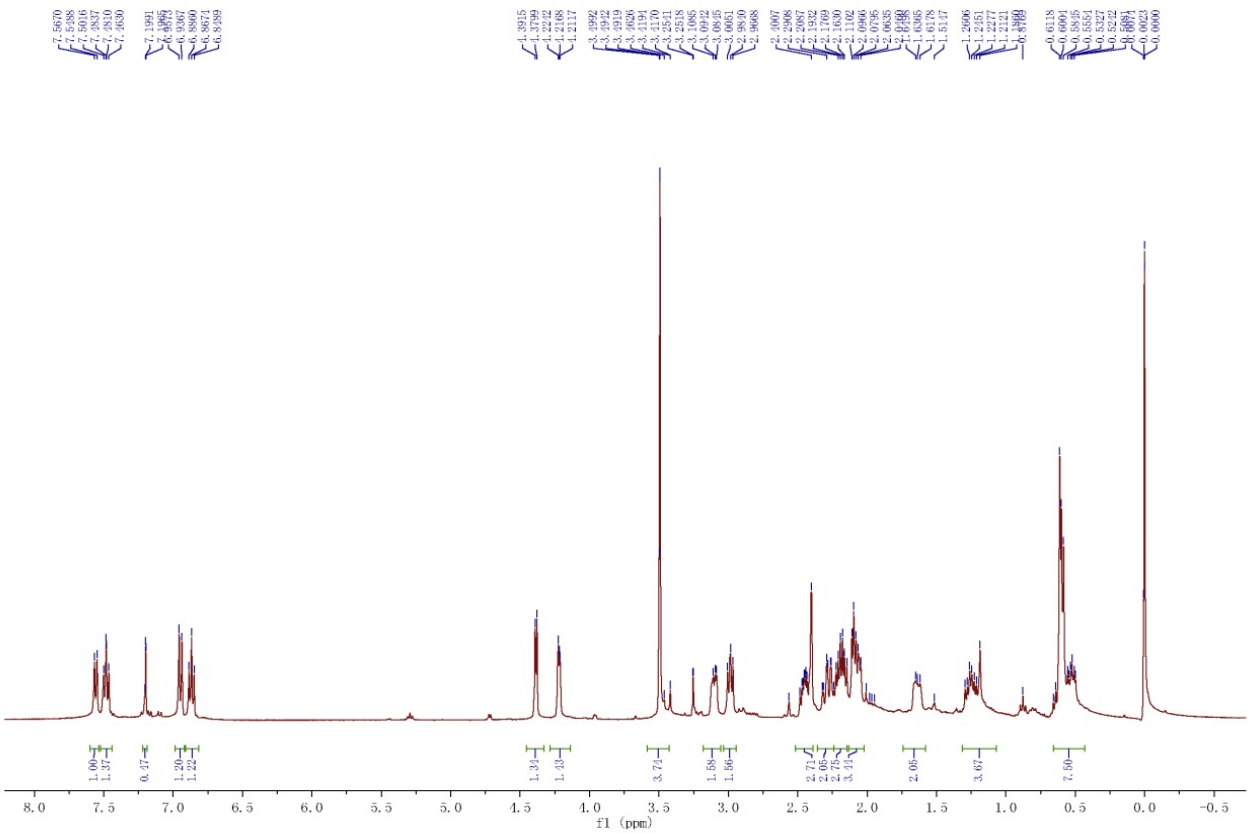


Figure S53. ^{13}C NMR spectrum of G (**7**) ($CDCl_3$)

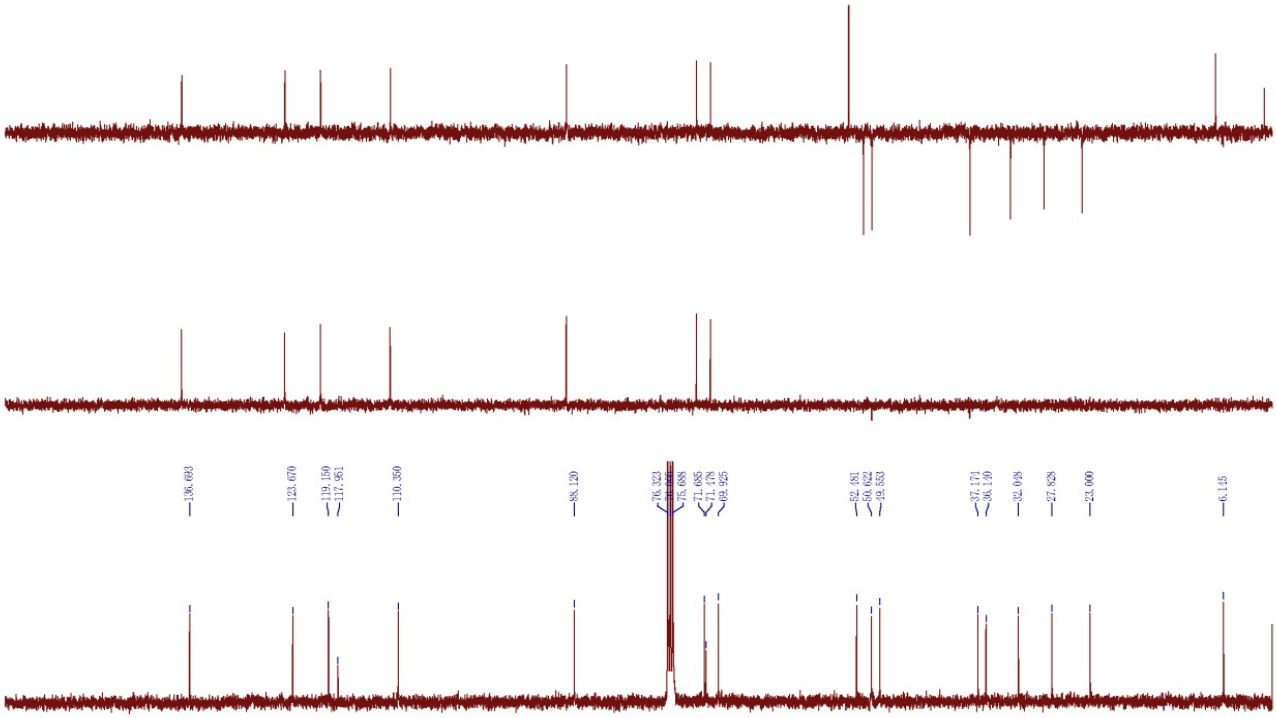


Figure S54. HSQC spectrum of Melokhanine G (**7**) ($CDCl_3$)

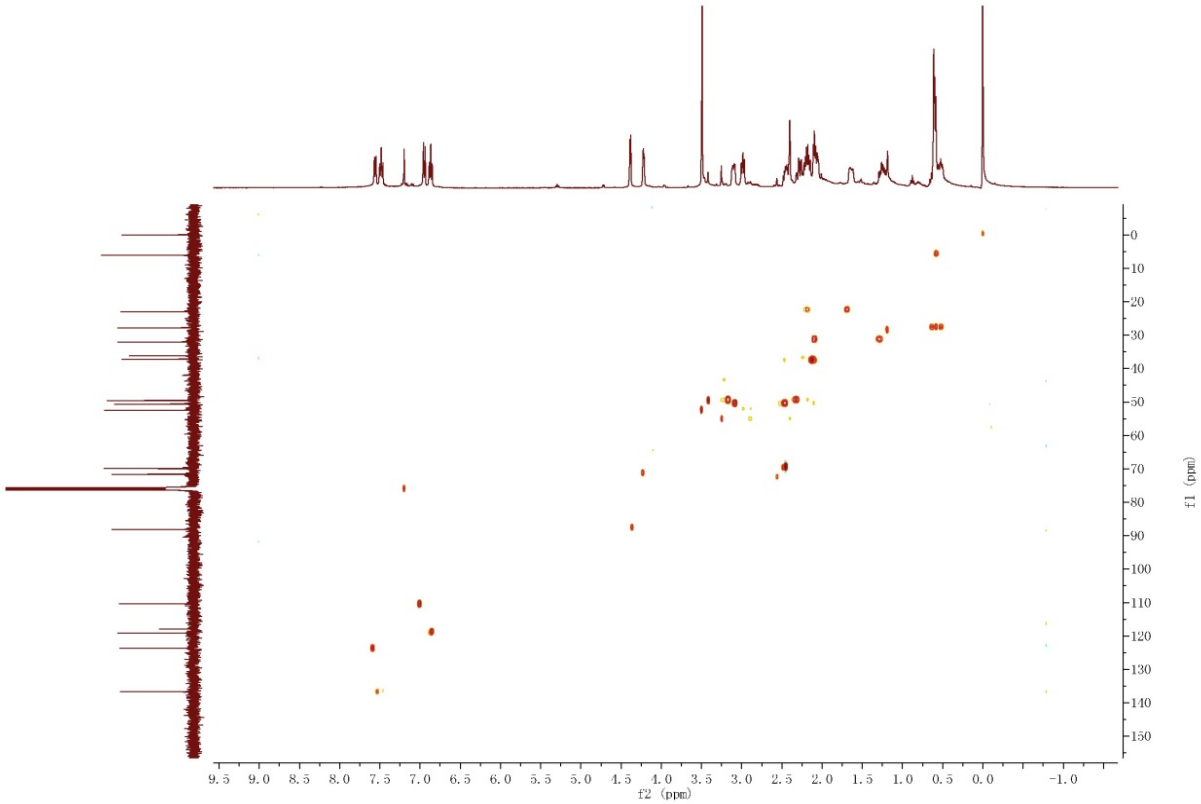


Figure S55. HMBC spectrum of Melokhanine G (**7**) ($CDCl_3$)

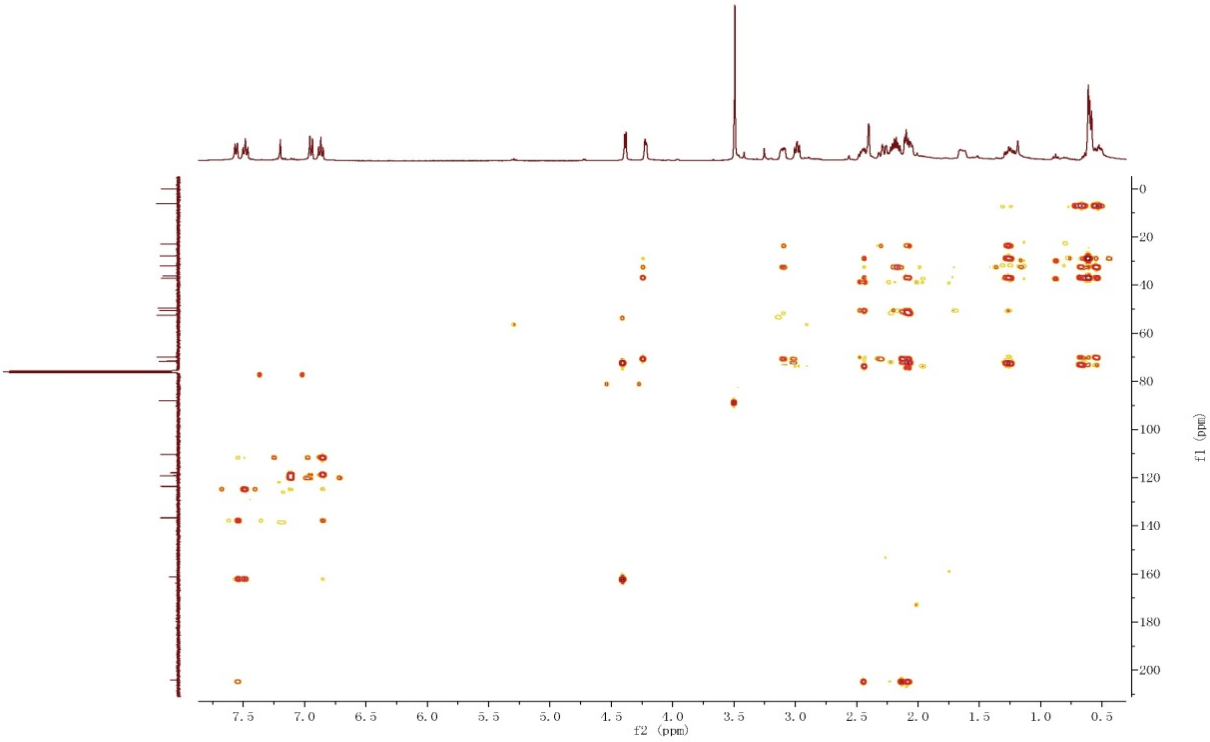


Figure S56. ^{1}H-^{1}H COSY spectrum of Melokhanine G (**7**) ($CDCl_3$)

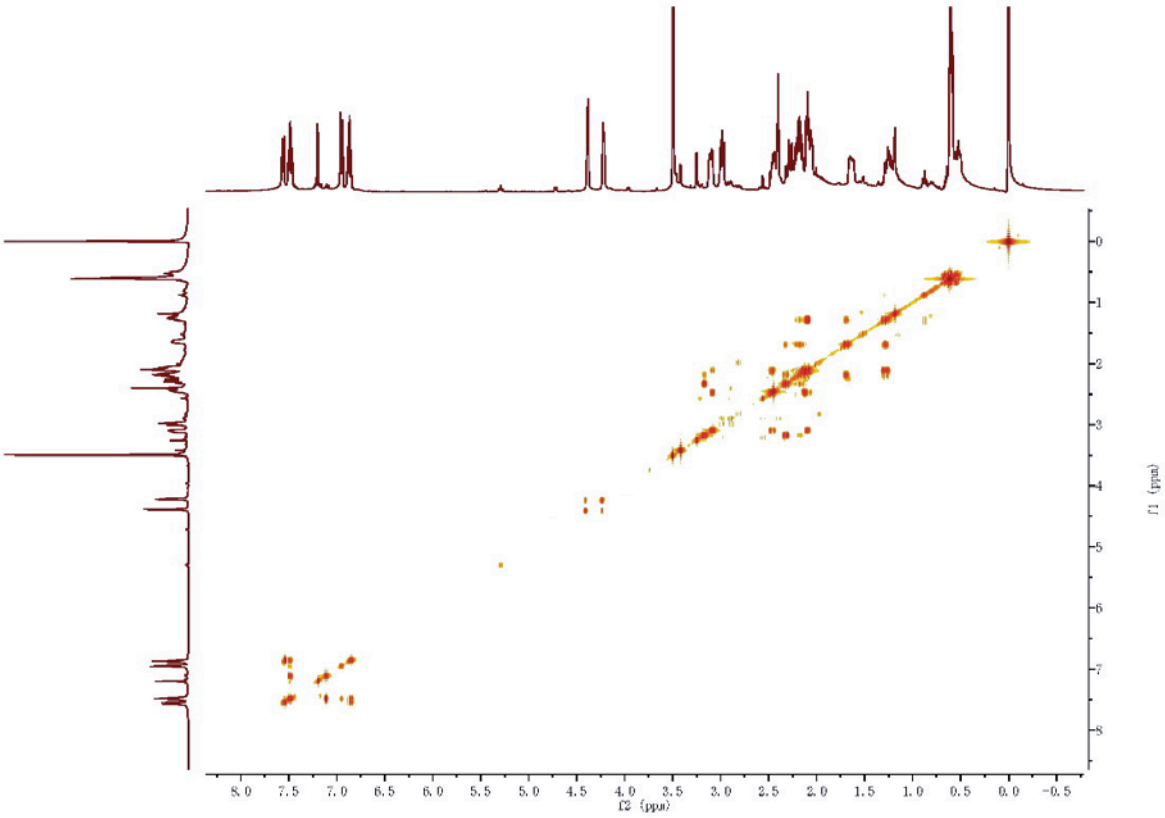


Figure S57. ROESY spectrum of Melokhanine G (**7**) ($CDCl_3$)

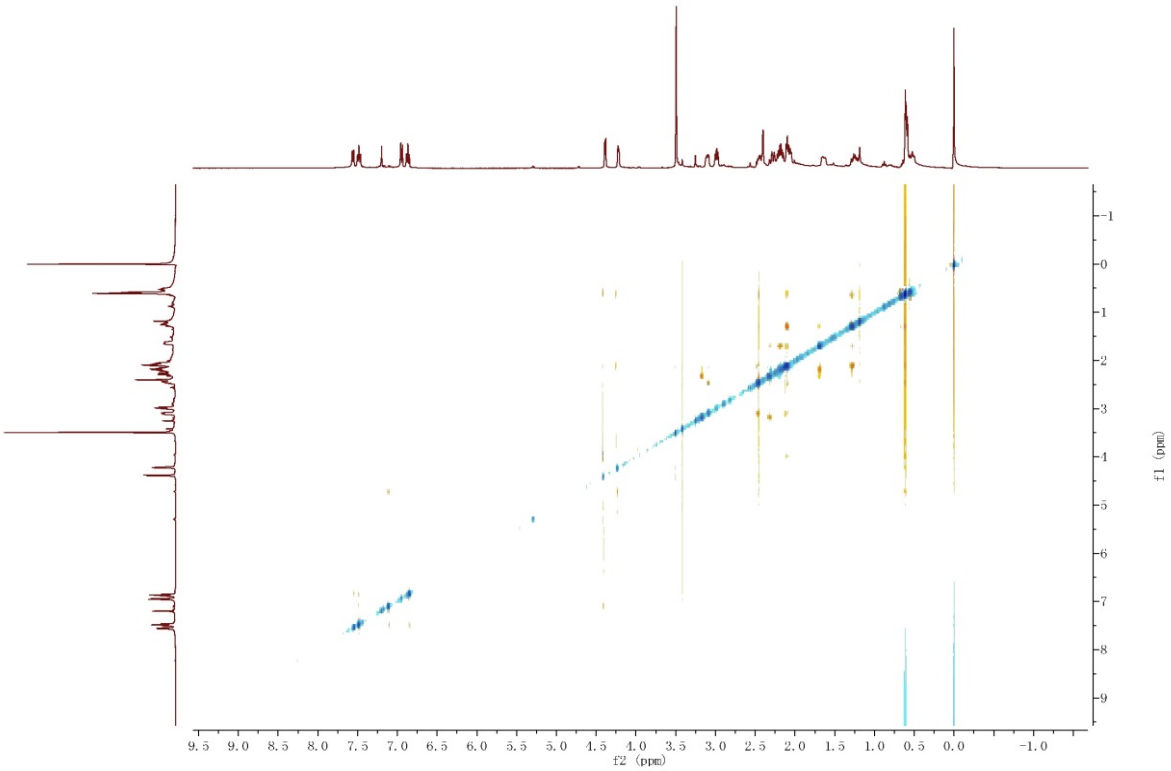


Figure S58. HREIMS spectrum of Melokhanine G (**7**) ($CDCl_3$)

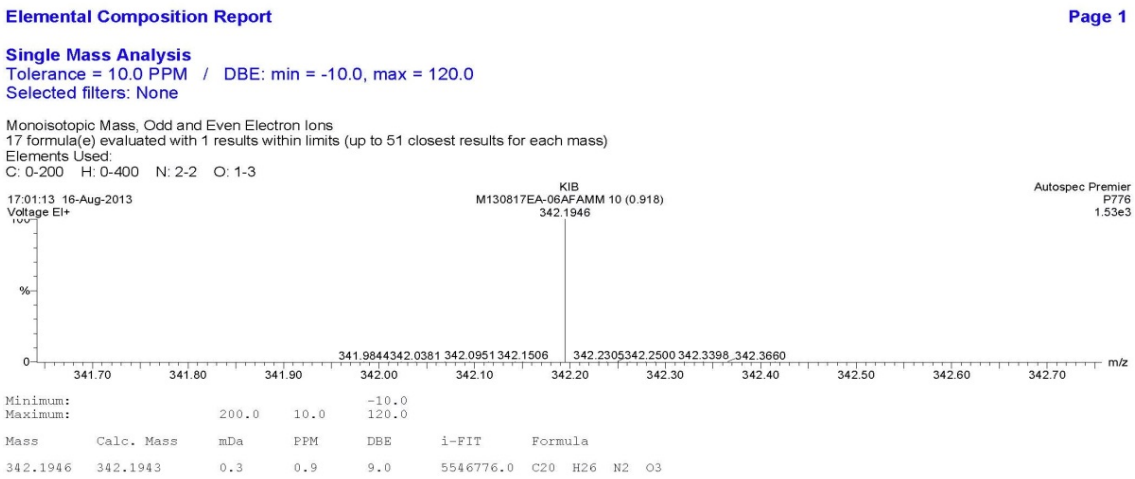
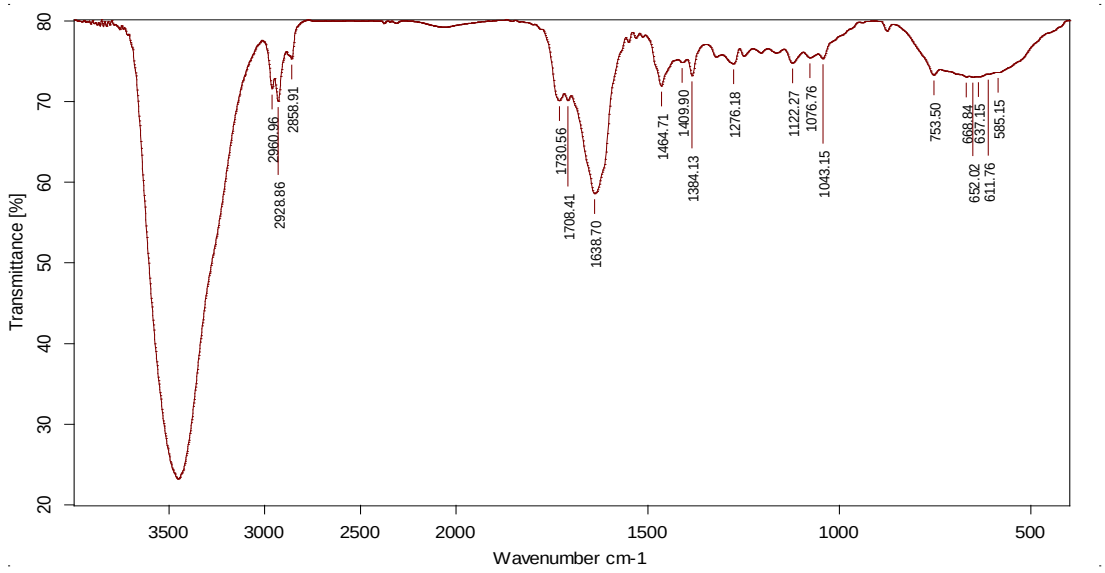


Figure S59. IR spectrum spectrum of Melokhanine G (**7**) ($CDCl_3$)



Sample : wmha-12	Frequency Range : 399.246 - 3996.32	Measured on : 20/01/2014	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 140120IR4	Zerofilling : 2	Acquisition : Double Sided,Forw	

Figure S60. ^{1}H NMR spectrum of Melokhanine H (**8**) ($CDCl_3$)

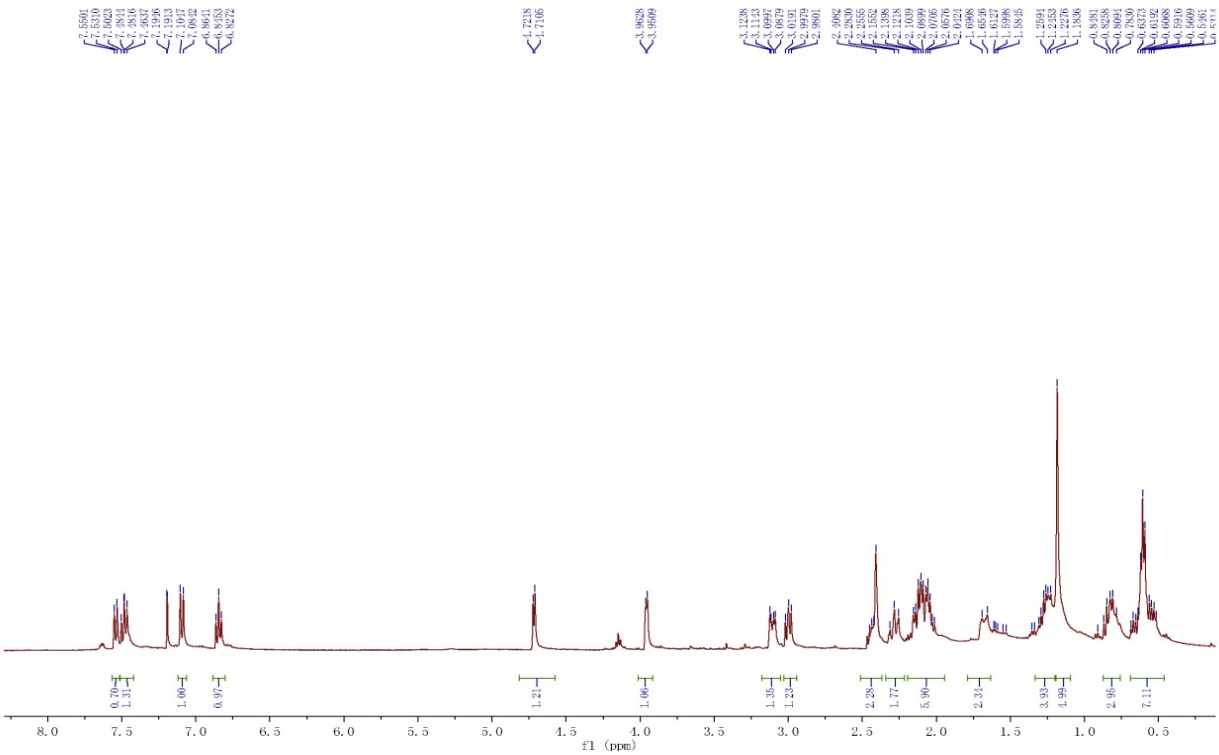


Figure S61. ^{13}C NMR spectrum of Melokhanine H (**8**) ($CDCl_3$)

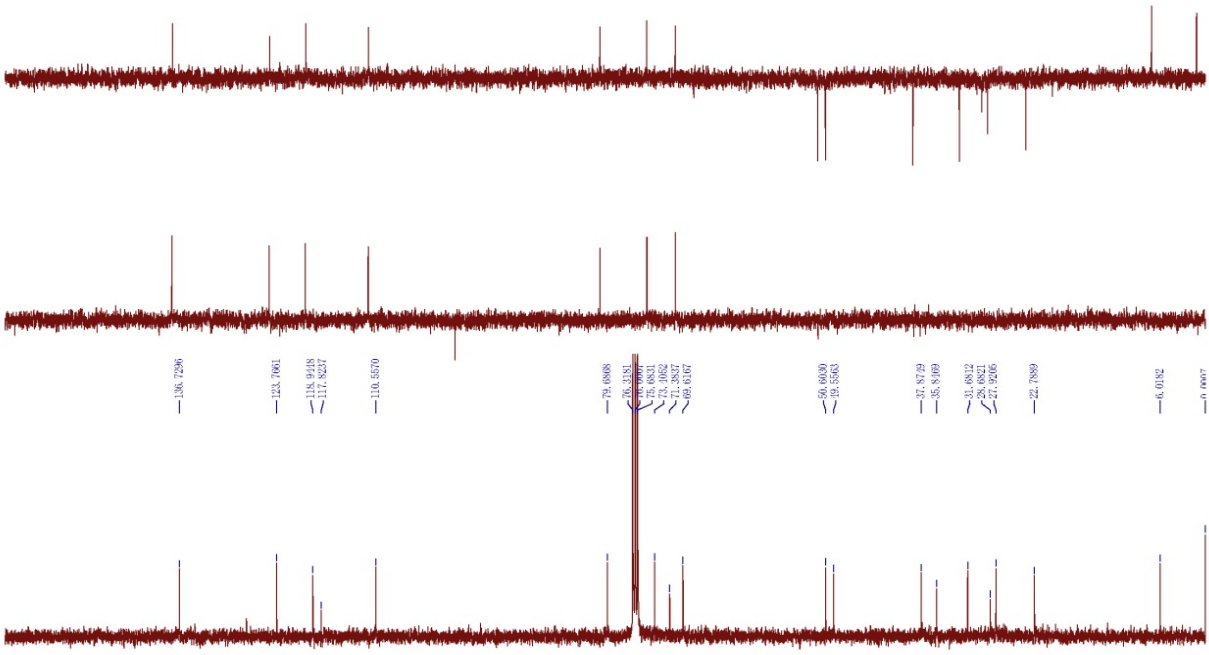


Figure S62. HSQC spectrum of Melokhanine H (**8**) ($CDCl_3$)

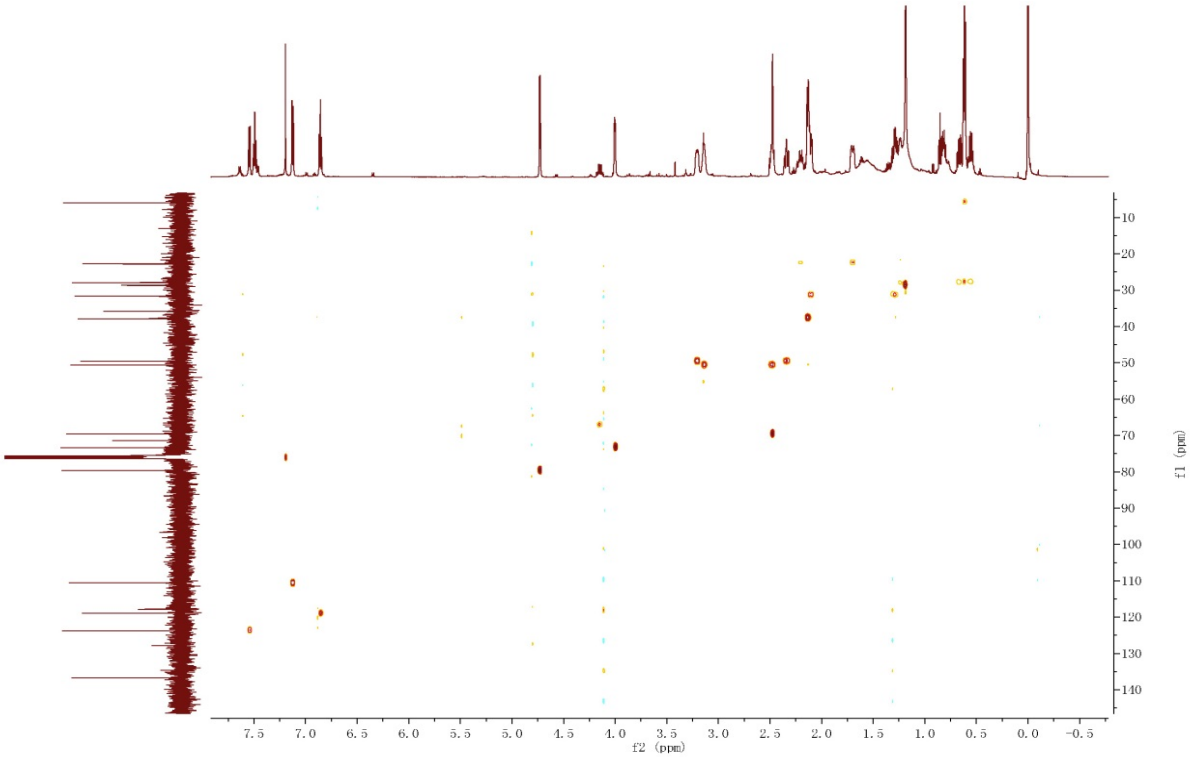


Figure S63. HMBC spectrum of Melokhanine H (**8**) ($CDCl_3$)

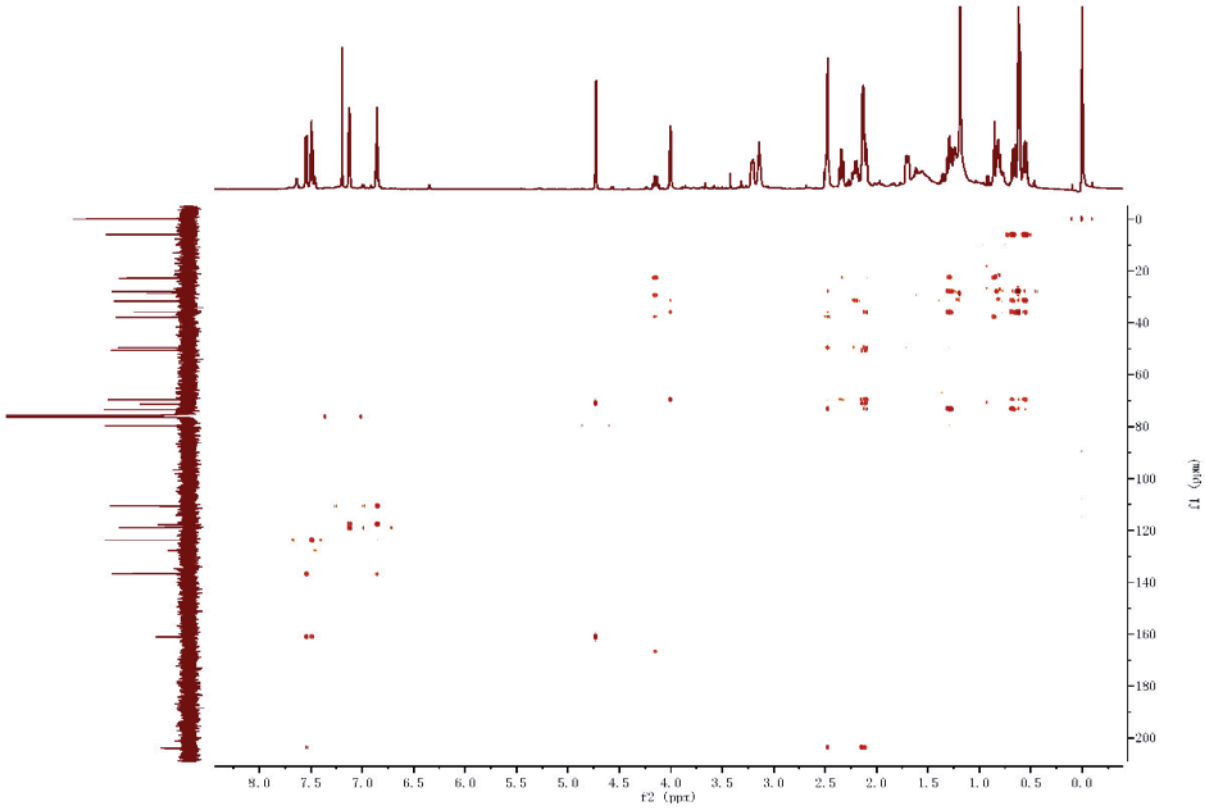


Figure S64. ^{1}H-^{1}H COSY spectrum of Melokhanine H (**8**) ($CDCl_3$)

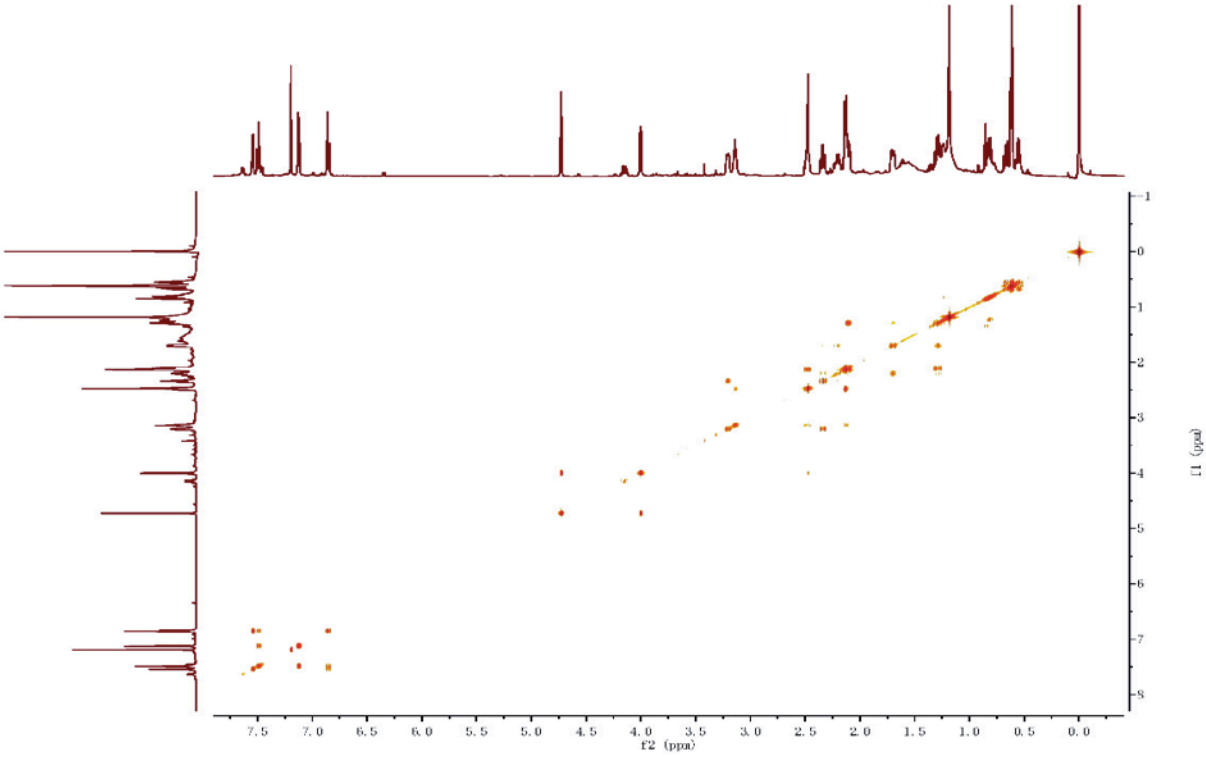


Figure S65. ROESY spectrum of Melokhanine H (**8**) ($CDCl_3$)

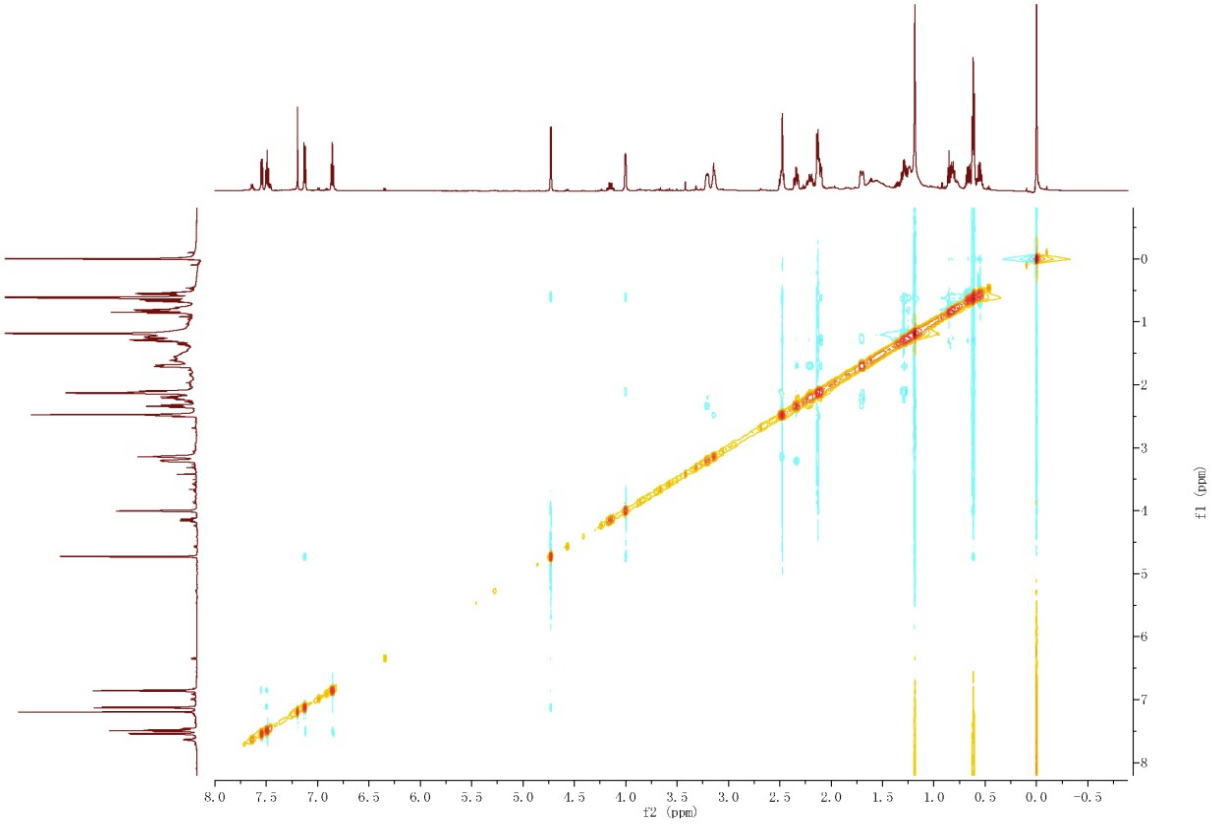
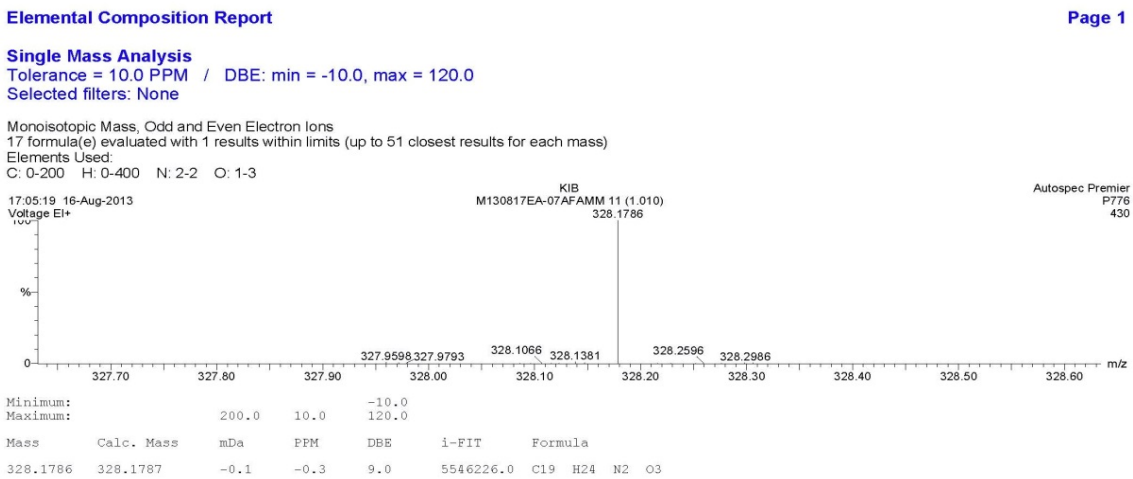


Figure S66. HREIMS spectrum of Melokhanine H (**8**)



Elemental Composition Report **Page 1**

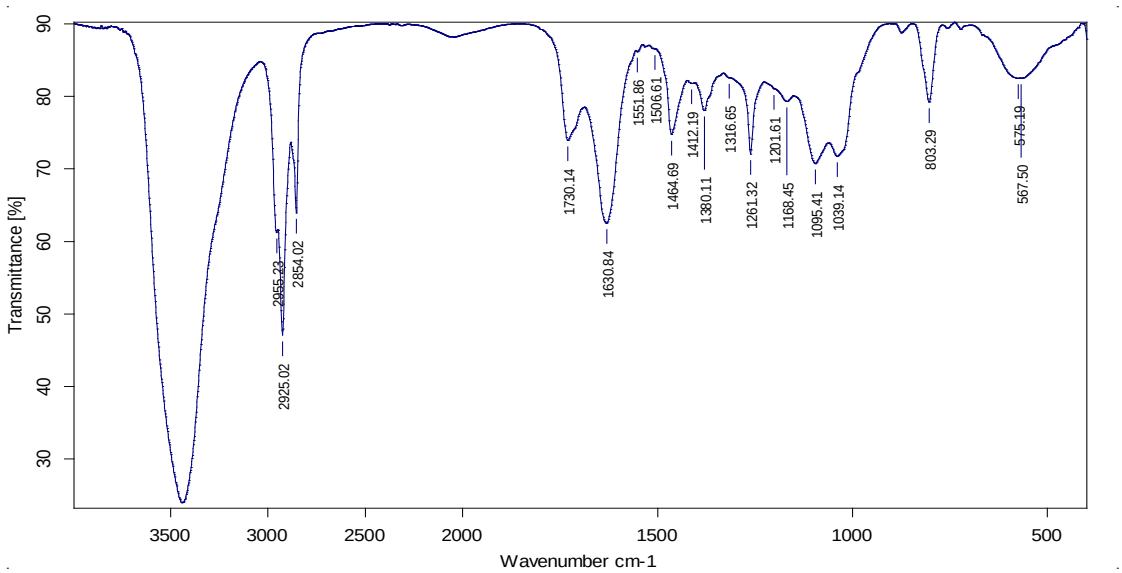
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 N: 2-2 O: 1-3

17:05:19 16-Aug-2013 KIB M130817EA-07AFAMM 11 (1.010) Autospec Premier
Voltage EI+ P776
430

Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.1786	328.1787	-0.1	-0.3	9.0	5546226.0	C19 H24 N2 O3

Figure S67. IR spectrum spectrum of Melokhanine H (**8**)



Sample : wmha14	Frequency Range : 399.246 - 3996.32	Measured on : 20/01/2014	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 140120IR2	Zerofilling : 2	Acquisition : Double Sided,Forv	

Figure S68. ^{1}H NMR spectrum of Melokhanine I (**9**) (DMSO-d_6 and methanol -d_4)

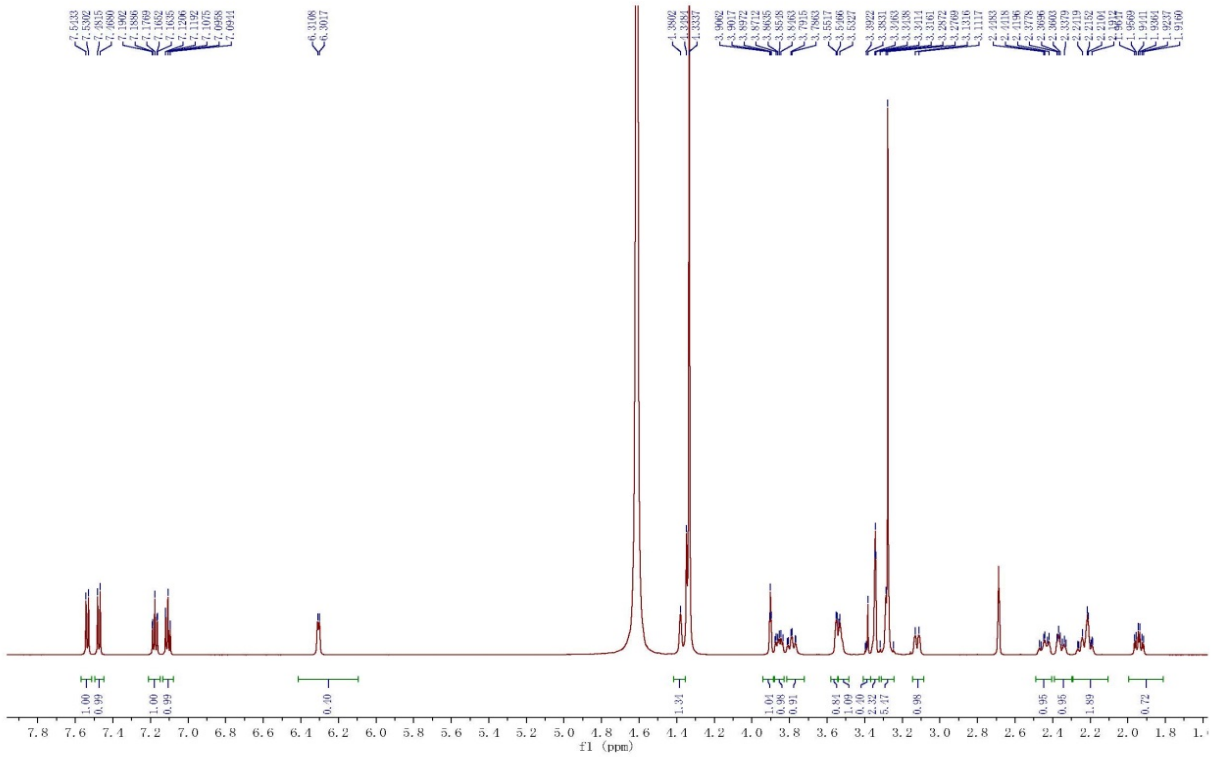


Figure S69. ^{13}C NMR spectrum of Melokhanine I (**9**) (DMSO-d_6 and methanol -d_4)

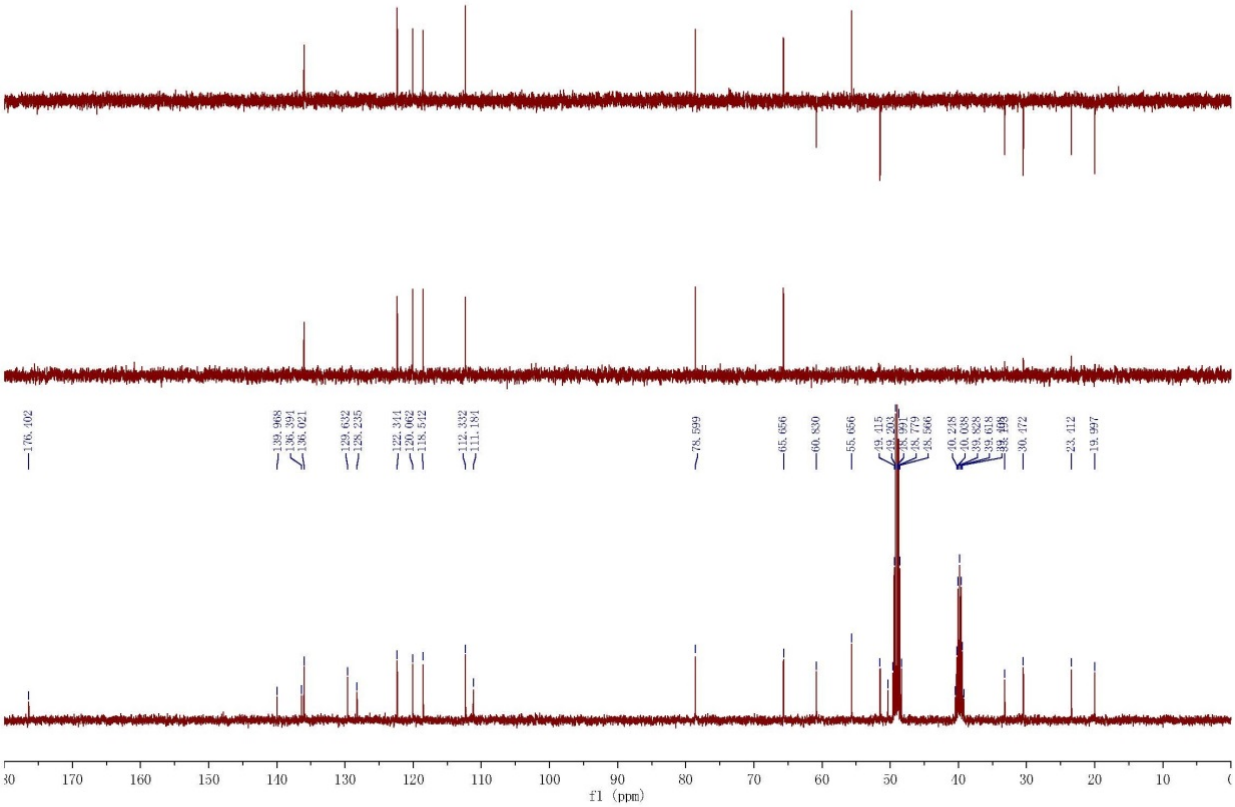


Figure S70. HSQC spectrum of Melokhanine I (**9**) (DMSO-d_6 and methanol -d_4)

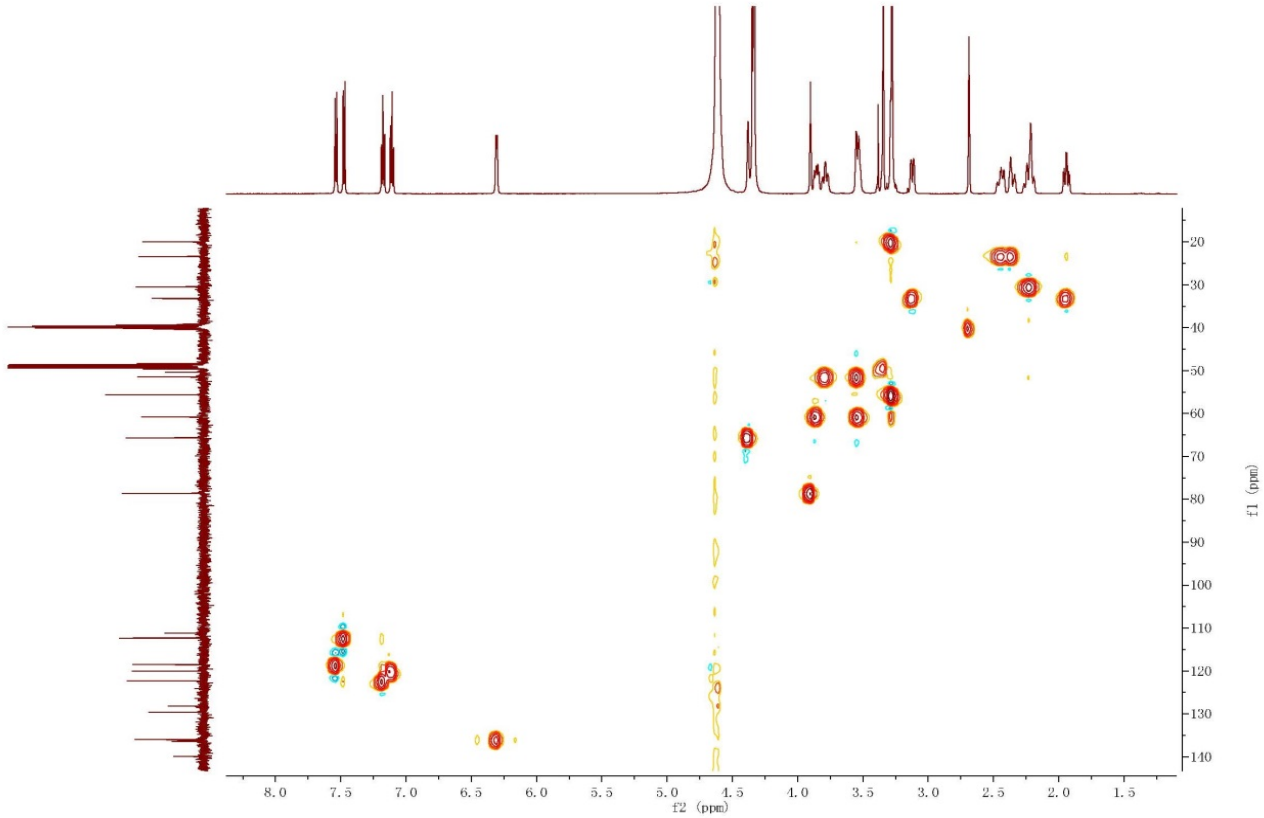


Figure S71. HMBC spectrum of Melokhanine I (**9**) (DMSO-d_6 and methanol -d_4)

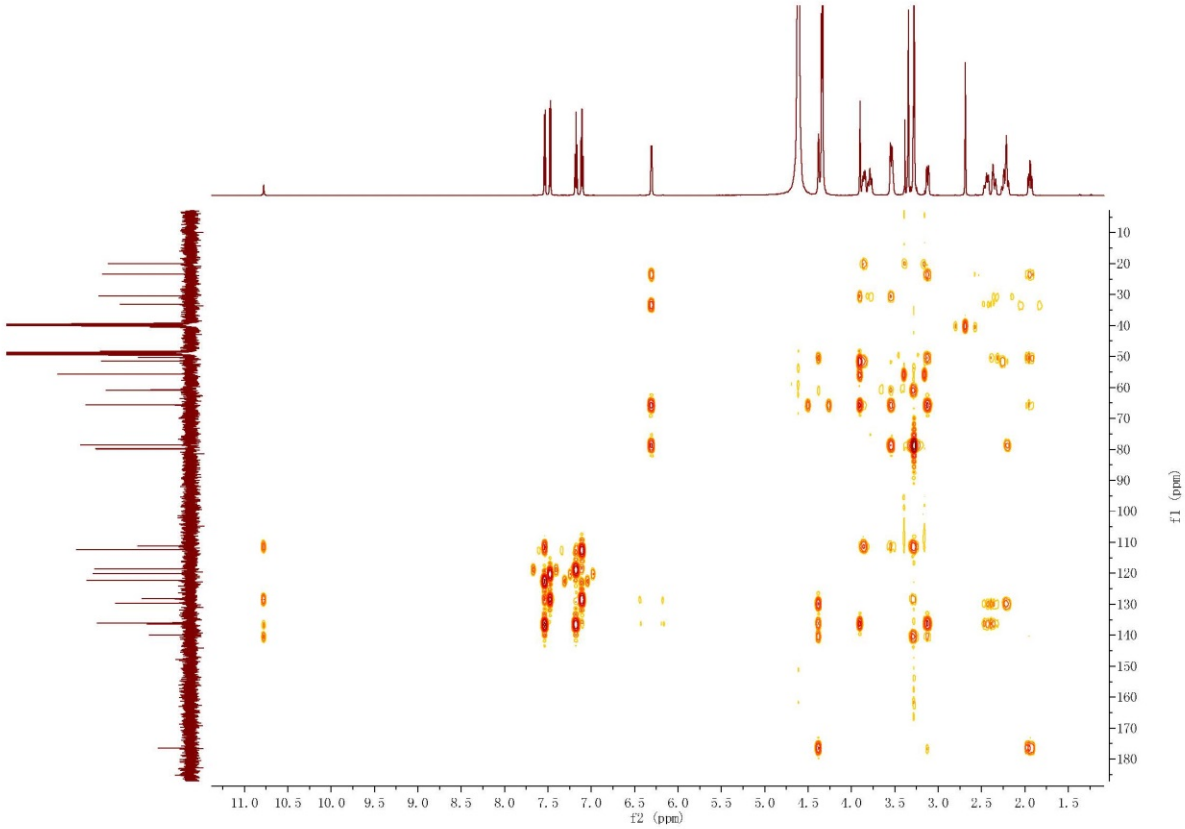


Figure 72. ^{1}H-^{1}H COSY spectrum of Melokhanine I (**9**) (DMSO-d_6 and methanol -d_4)

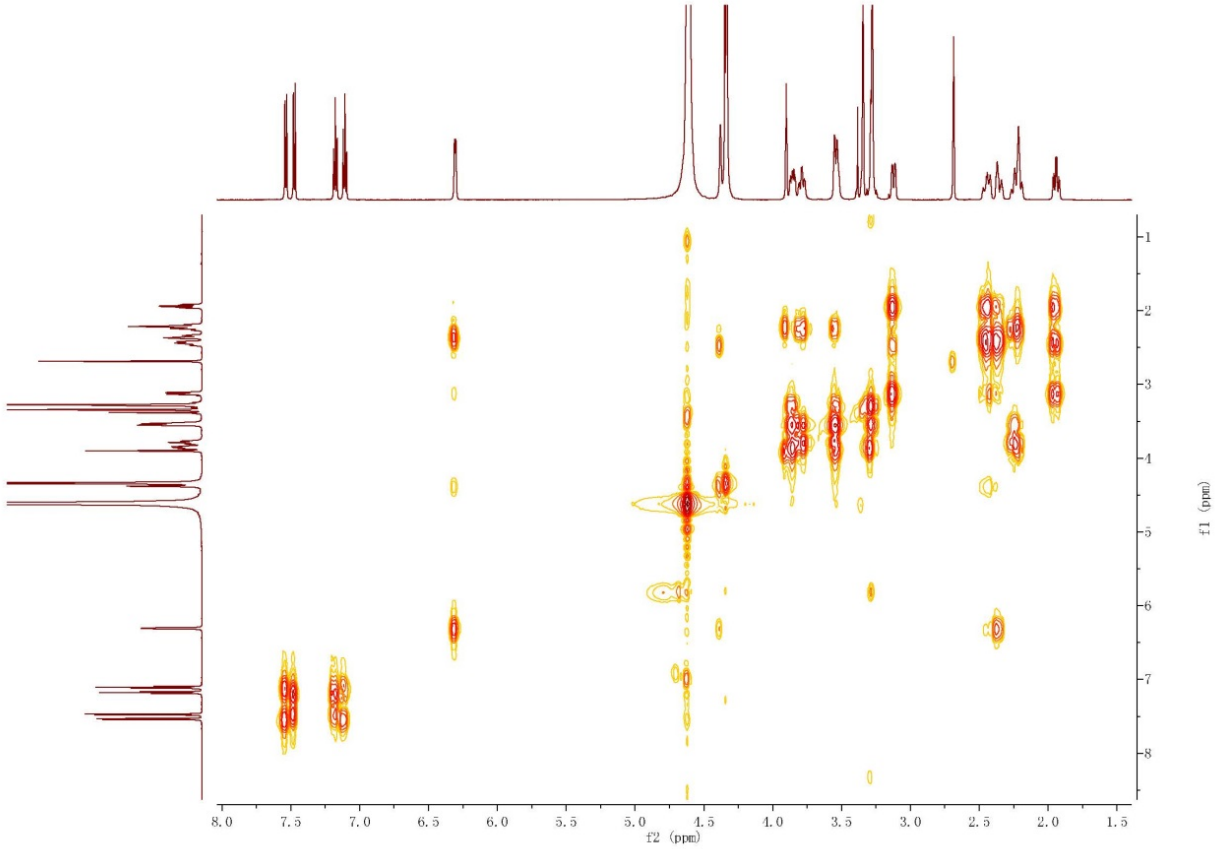


Figure S73. ROESY spectrum of I (**9**) (DMSO-d_6 and methanol -d_4)

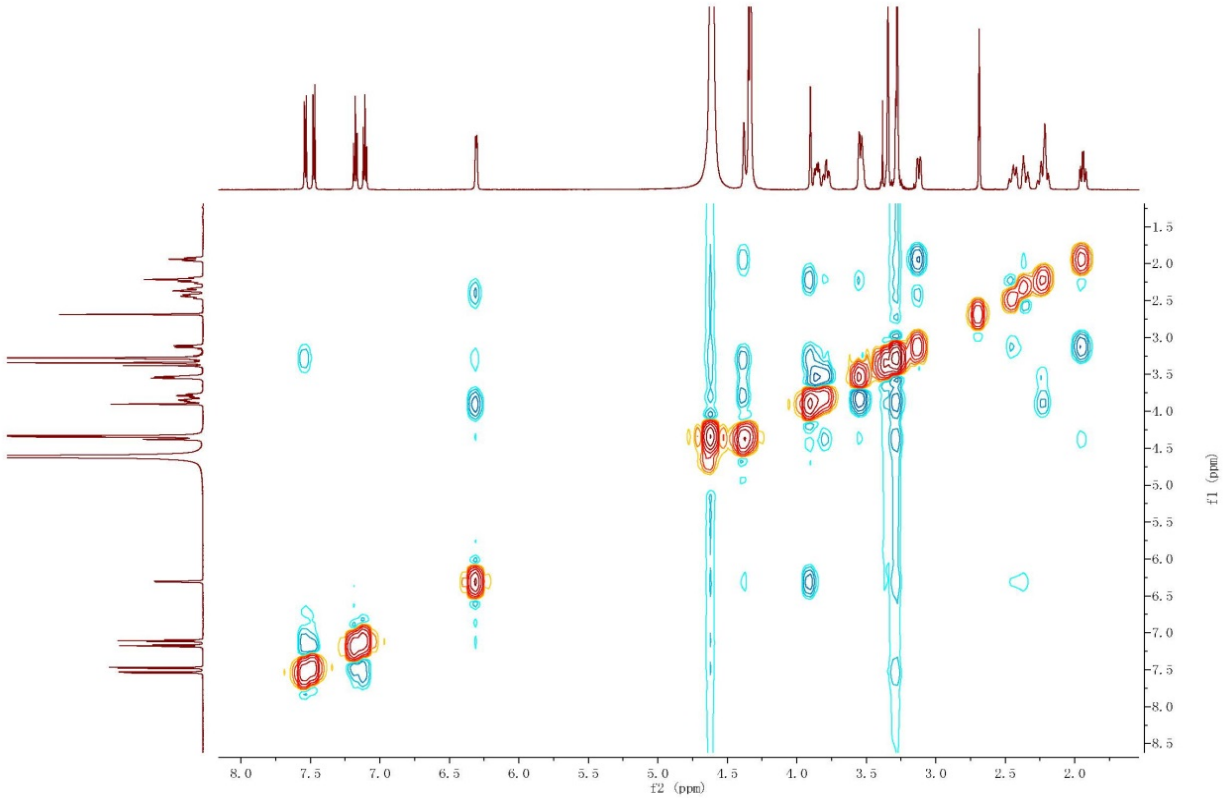


Figure S74. HREIMS spectrum of Melokhanine B (**2**)

Elemental Composition Report **Page 1**

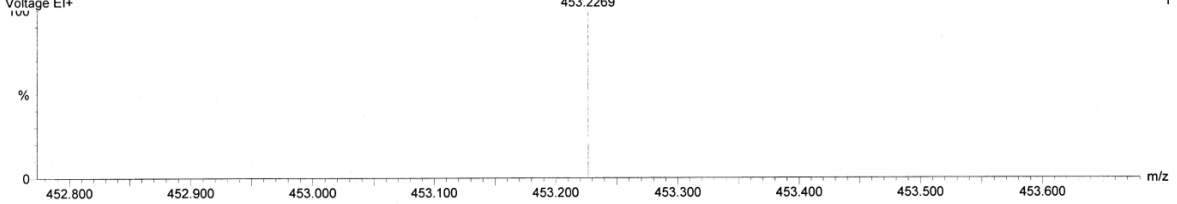
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 N: 3-3 O: 4-6

13:30:10 27-Jun-2013
Voltage EI+

KIB
M130701EA-02AFAMM 26 (2.387)
453.2269

Autospec Premier
P776
1



Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
453.2269	453.2264	0.5	1.1	12.0	5546026.0	C25 H31 N3 O5

Figure S75. ^{1}H NMR spectrum of Melokhanine J (**10**) ($CDCl_3$)

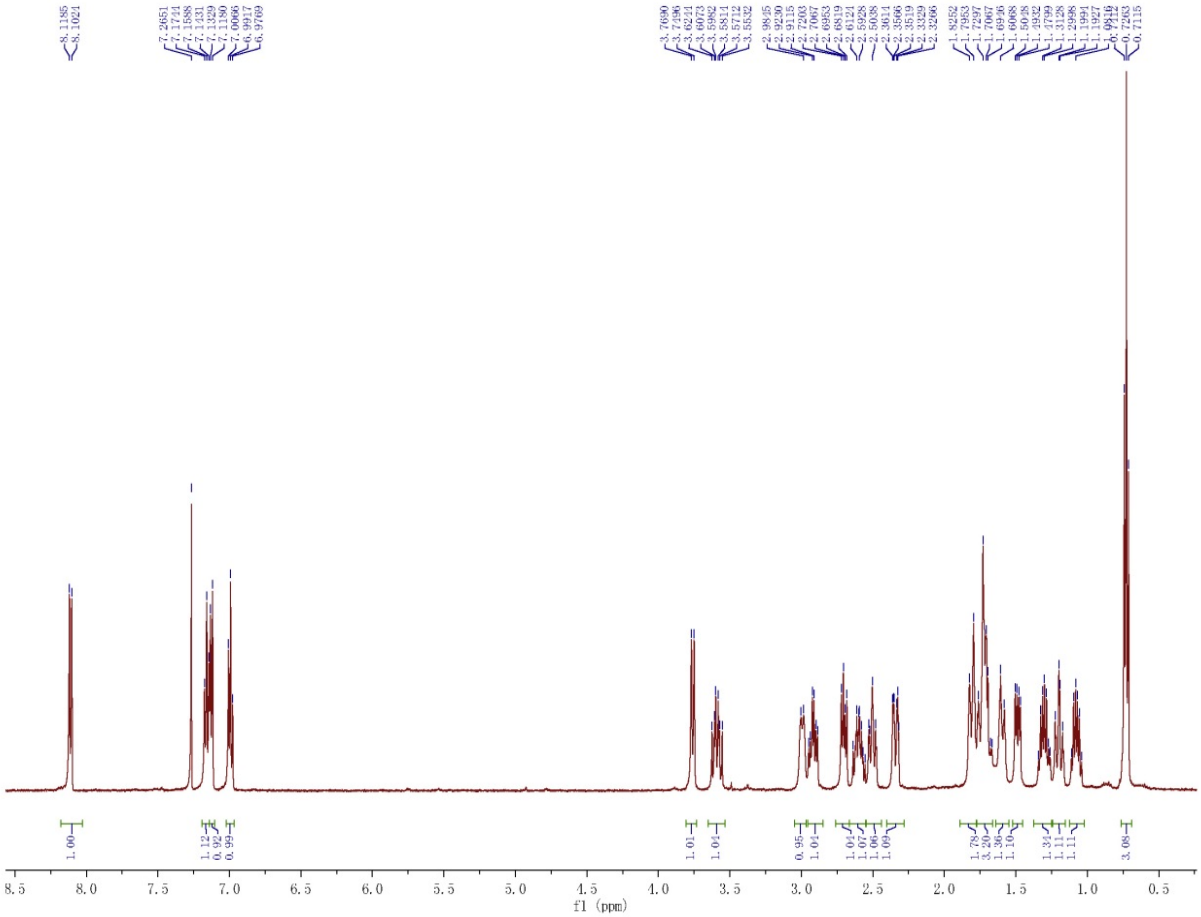


Figure S76. ^{13}C NMR spectrum of Melokhanine J (**10**) ($CDCl_3$)

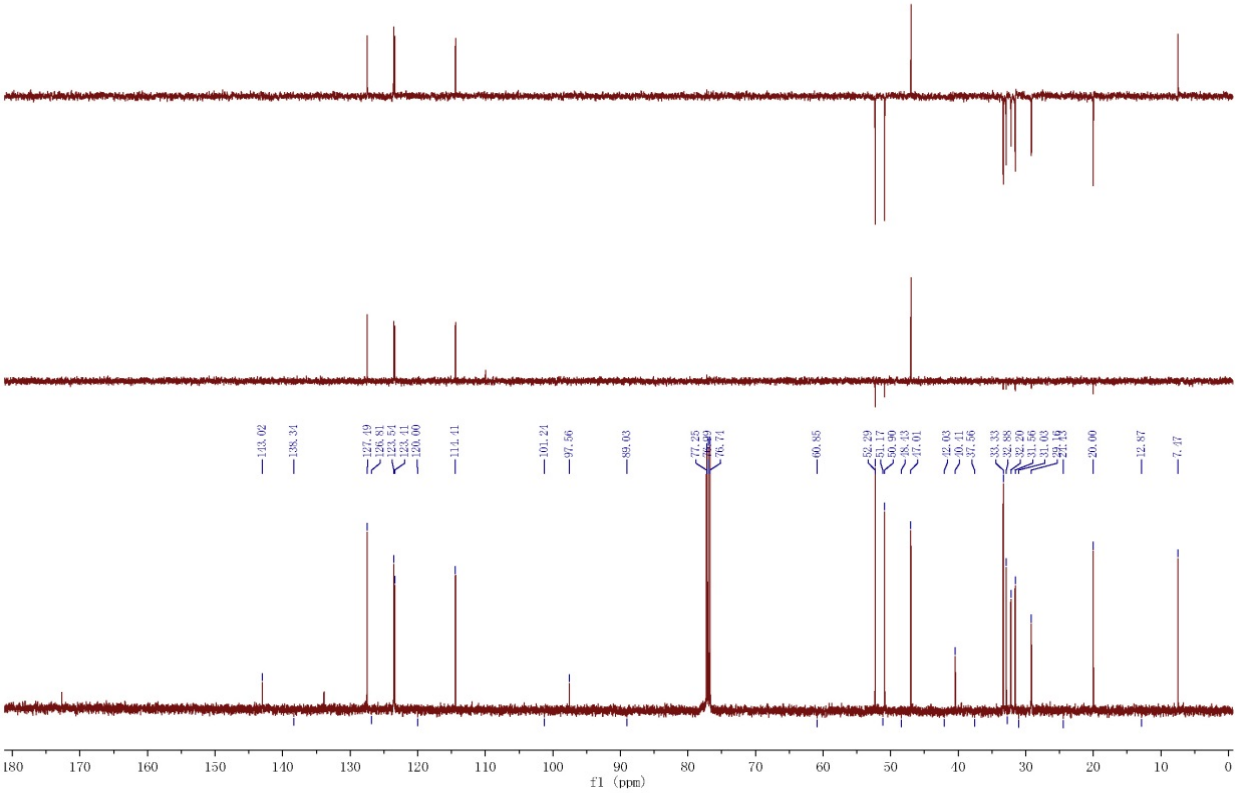


Figure S77. HSQC spectrum of Melokhanine J (**10**) ($CDCl_3$)

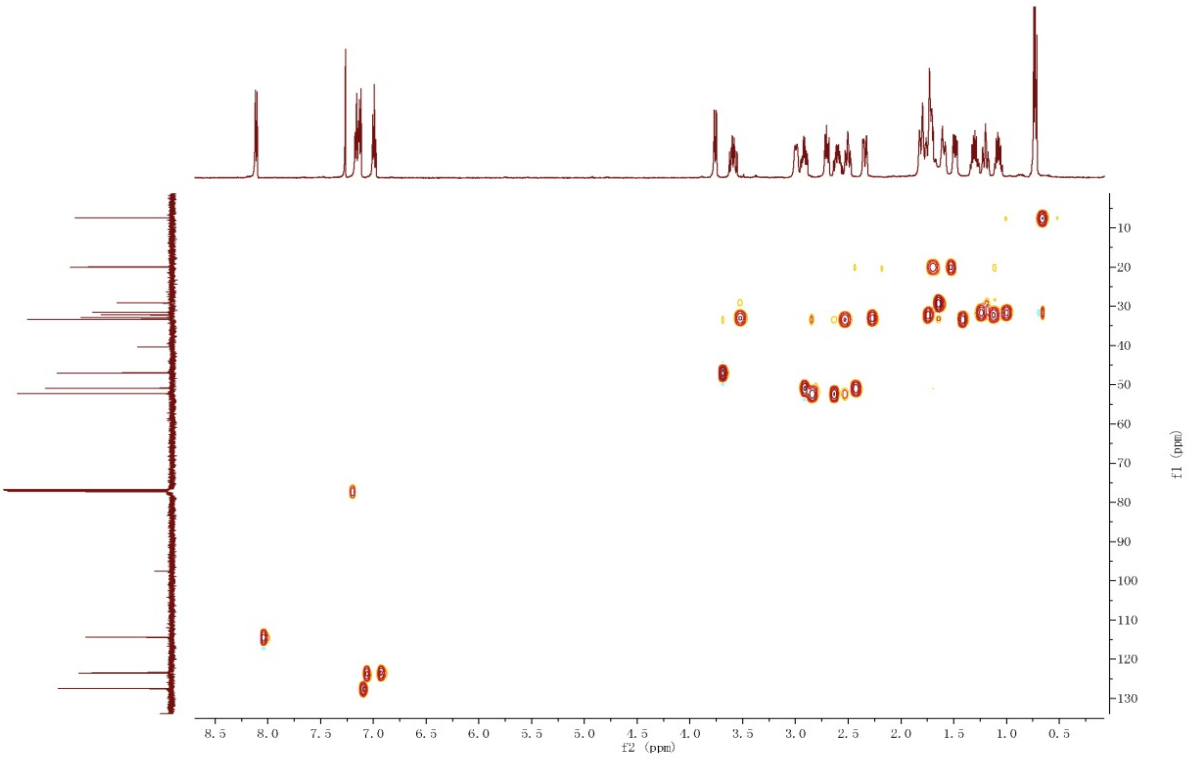


Figure S78. HMBC spectrum of Melokhanine J (**10**) ($CDCl_3$)

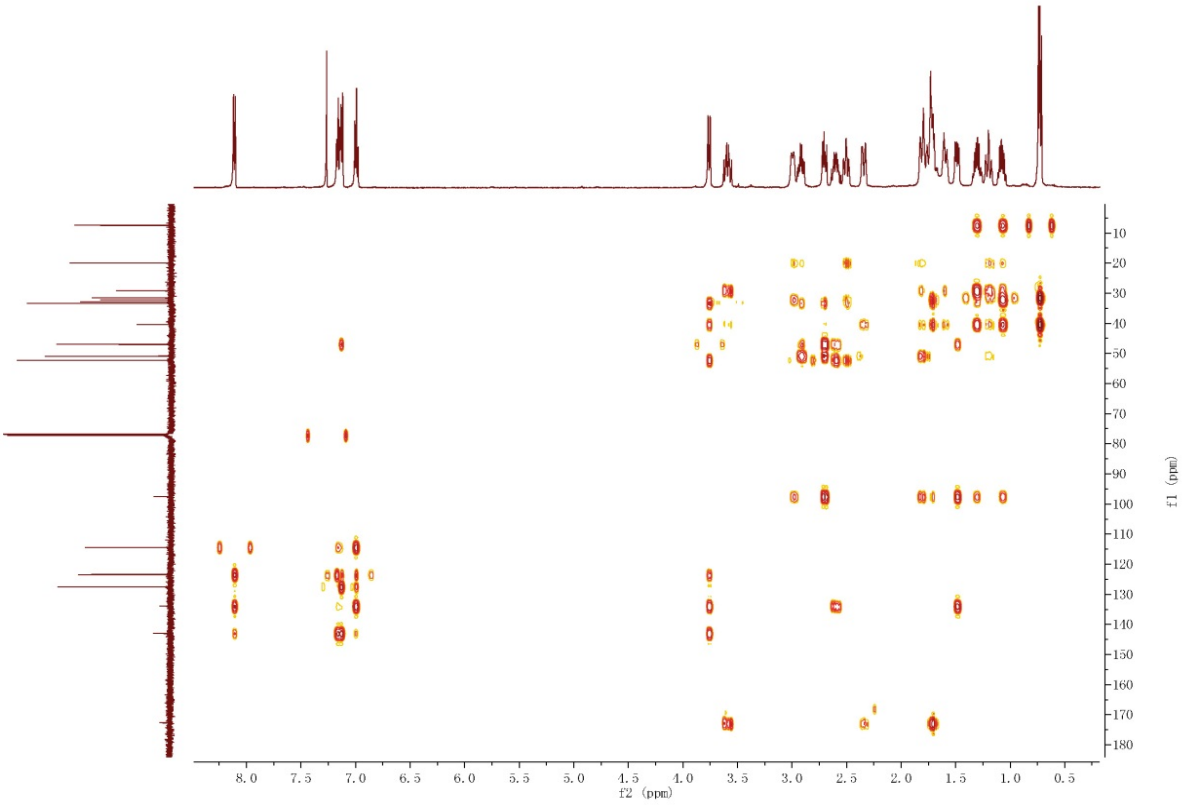


Figure S79. ROESY spectrum of Melokhanine J (**10**) ($CDCl_3$)

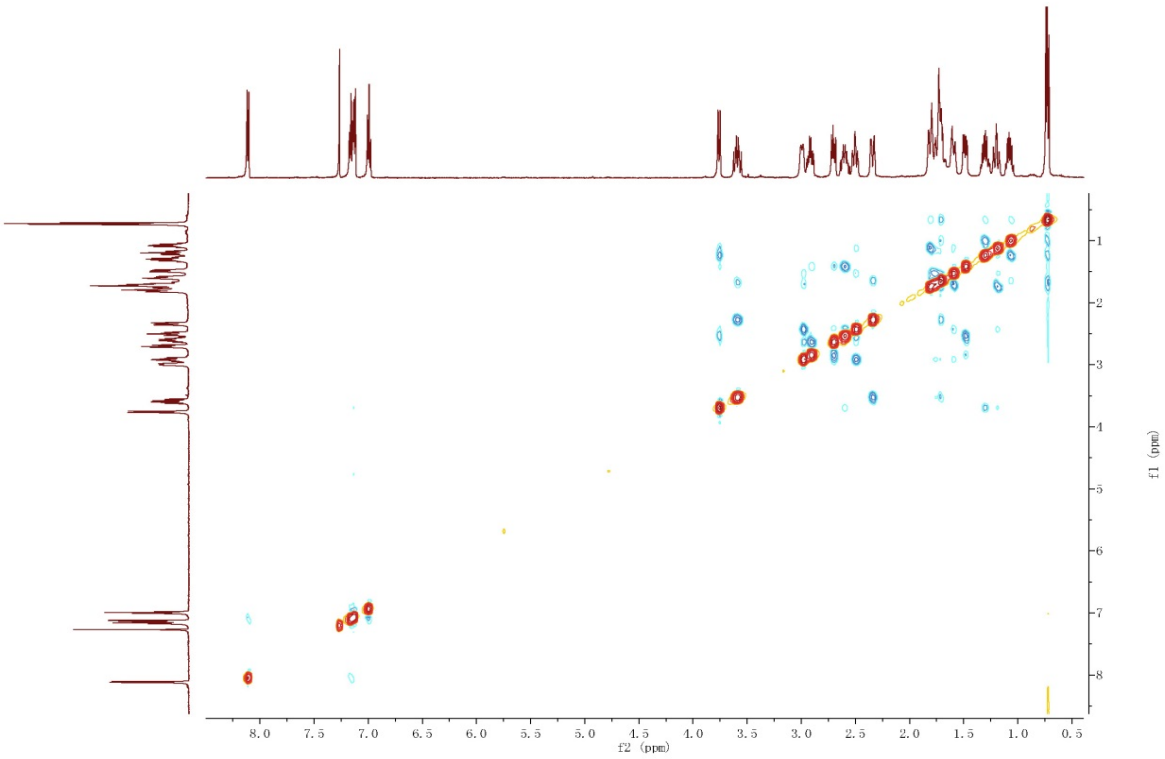


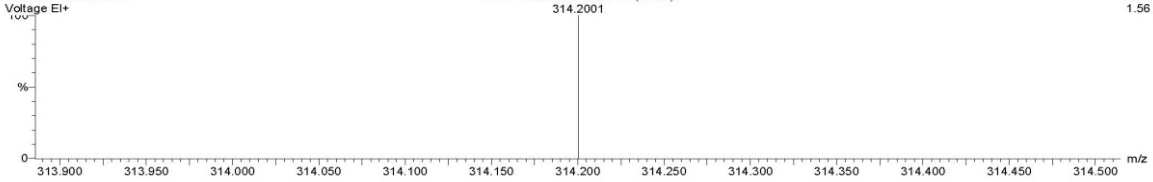
Figure S80. HREIMS spectrum of J (**10**) ($CDCl_3$)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

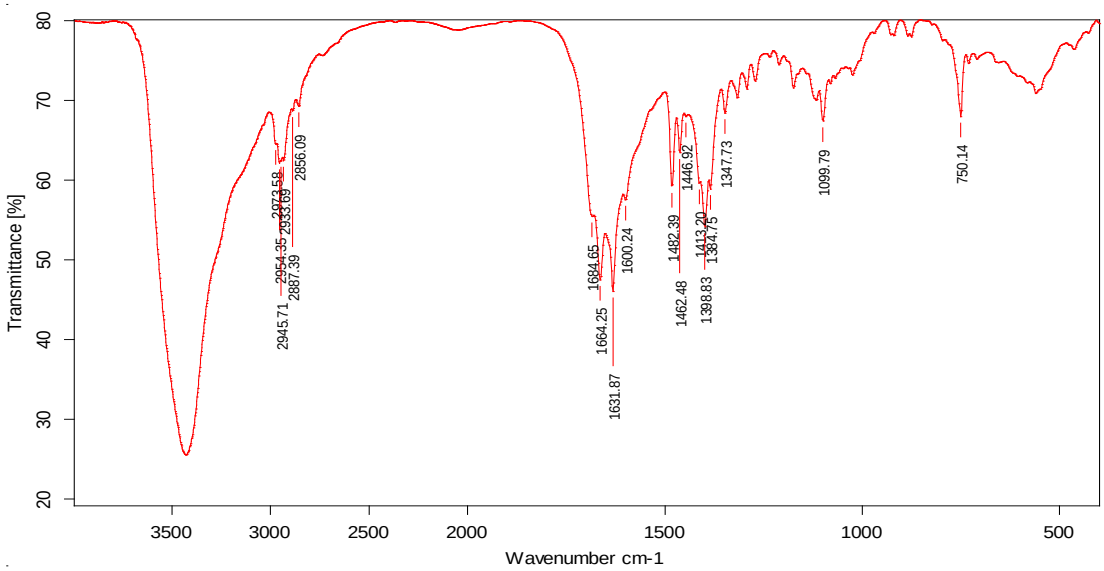
Monoisotopic Mass, Odd and Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 N: 2-2 O: 2-4

14:38:24 16-Jan-2014
Voltage EI+
KIB
M140116EA-06AFAMM 18 (1.653)
314.2001
Autospec Premier
P776
1.56



Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.2001	314.1994	0.7	2.2	8.0	5546025.5	C19 H26 N2 O2

Figure S81. IR spectrum spectrum of J (**10**) ($CDCl_3$)



Sample : wmha-15	Frequency Range : 399.246 - 3996.32	Measured on : 20/01/2014	
Technique : KBr 压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 140120IR5	Zerofilling : 2	Acquisition : Double Sided,Forw	

The UHPLC-ESI-MS Analysis of the Crude Extract and Melokhanines A-J (1-10).

In order to confirm the new alkaloids are isolated from *Melodinus khasianus* instead of artifacts of isolation process, a UHPLC-ESI-MS experiment was carried out. The powdered leaves and twigs of *M. khasianus* were extracted with MeOH at room temperature and then filtered. The obtained crude extract was subjected to UHPLC-ESI-MS analysis with the comparison with the retention time and mass data of reference standards, Melokhanines A-J (**1-10**). The results shown in table S6 and figure S82 implied the fact that the new alkaloids were isolated from the leaves and twigs of title species rather than products of the isolation process.

Chromatographic condition

Instrument: A Thermo Scientific Dionex Ultimate 3000 UHPLC system equipped with a Thermo high resolution Q Exactive focus mass spectrometer; Chromatographic column: Thermo Scientific HYPERSIL GOLD C18 (2.1×100 mm, 1.9 μm); Flow rate: 0.2 mL/min; Column temperature: 25 °C;

Table S5. Mobile phase for the UHPLC (A: H_2O; B: CH_3CN)

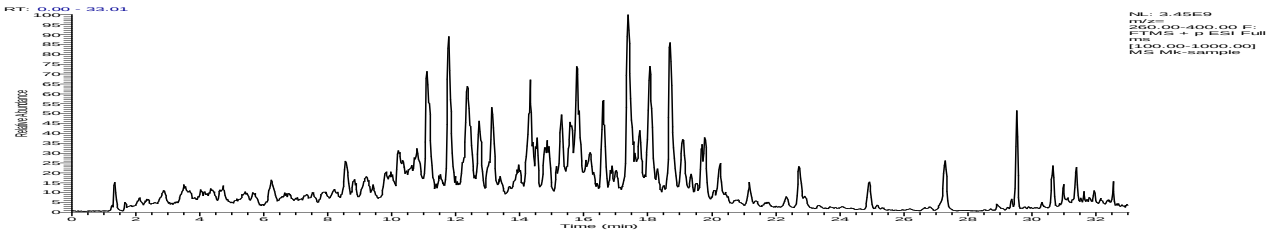
Time (min)	A %	B %
0.0	90	10
2	90	10
5	85	15
10	80	20
25	60	40
27	40	60
30	0	100
31	90	10
33	90	10

Table S6. Identification of new alkaloids in *M. khasianus* by UHPLC-ESI-MS[a]

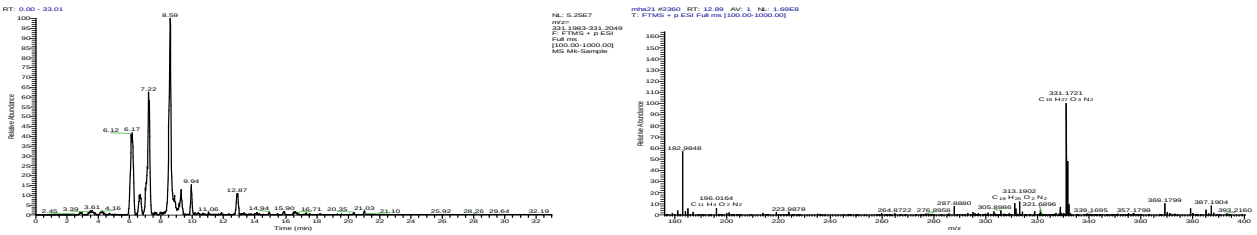
Compound	t_R (min)	Molecular Formula	Measured Mass (*m/z*)	MS/MS fragments (*m/z*)
Melokhanine A	12.89	$C_{19}H_{26}N_2O_3$	331.1721[b]	302, 271, 168
Melokhanine B	20.75	$C_{20}H_{26}N_2O_2$	327.2060[b]	295, 148, 124
Melokhanine C	20.44	$C_{20}H_{26}N_2O_2$	327.2149[b]	295, 148, 124
Melokhanine D	24.22	$C_{21}H_{28}N_2O_2$	341.2320[b]	323, 295, 148, 124
Melokhanine E	14.31	$C_{19}H_{22}N_2O_2$	311.1820[b]	293. 264, 160, 148, 124
Melokhanine F	14.85	$C_{19}H_{22}N_2O$	295.1797[b]	265, 148, 124
Melokhanine G	12.24	$C_{20}H_{26}N_2O_3$	311.1821[b]	293, 172, 148, 134, 124
Melokhanine H	10.25	$C_{19}H_{24}N_2O_3$	329.1942[b]	311, 293, 172, 148, 134, 124
Melokhanine I	15.35	$C_{21}H_{24}N_2O_3$	353.1849[b]	277, 248, 234, 144
Melokhanine J	17.95	$C_{19}H_{26}N_2O_2$	337.1900[c]	315, 299, 270, 195, 167

[a]Compared with a reference standard; [b] $[M+H]^+$; [c] $[M+Na]^+$.

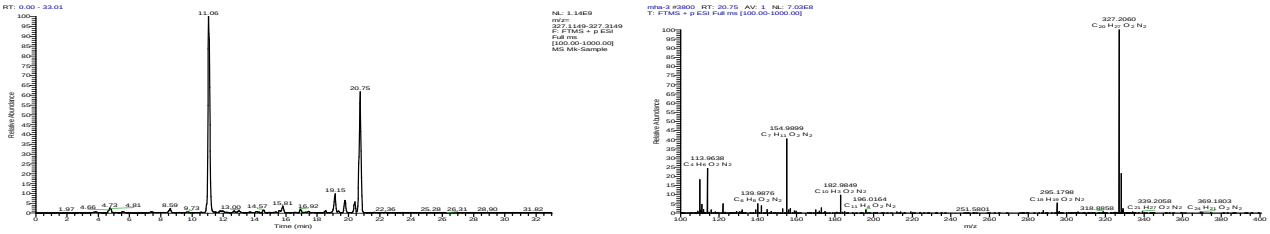
TIC of *Melodinus khasianus*



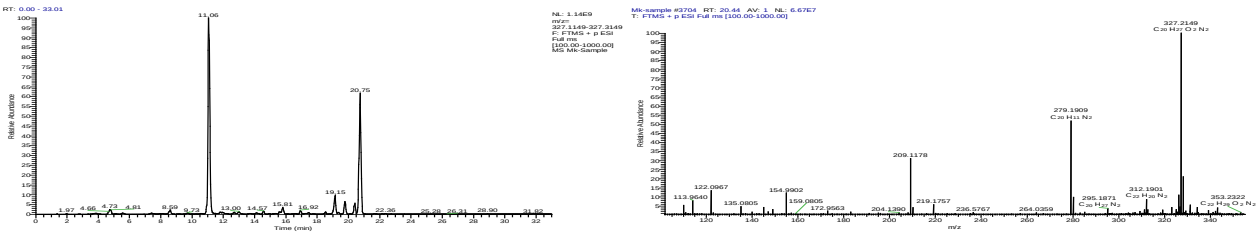
Melokhanine A



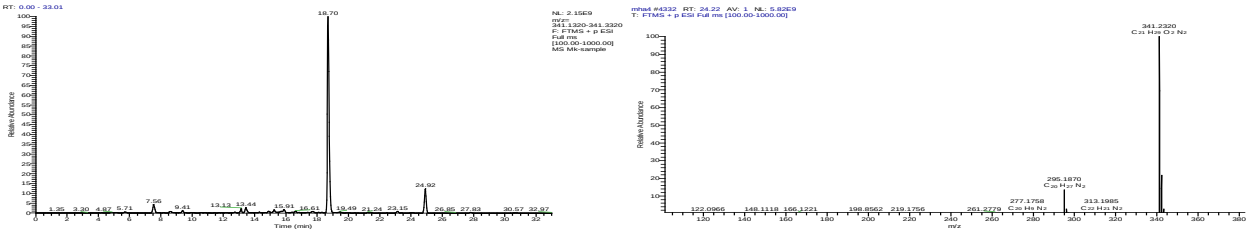
Melokhanine B



Melokhanine C



Melokhanine D



Melokhanine E

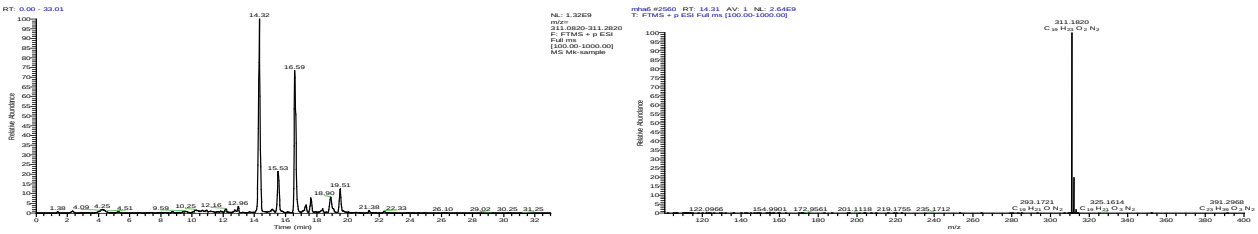
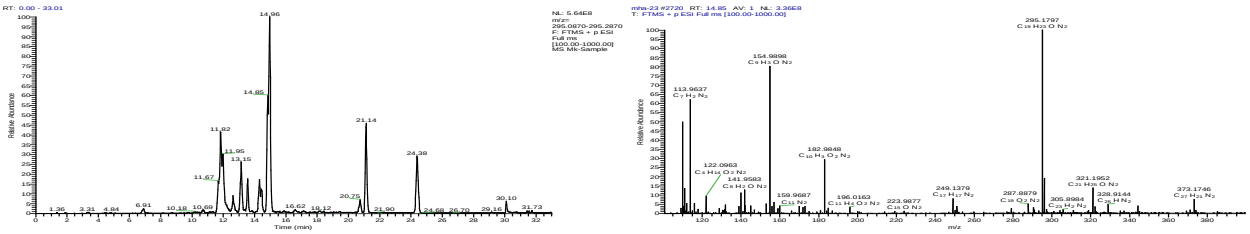
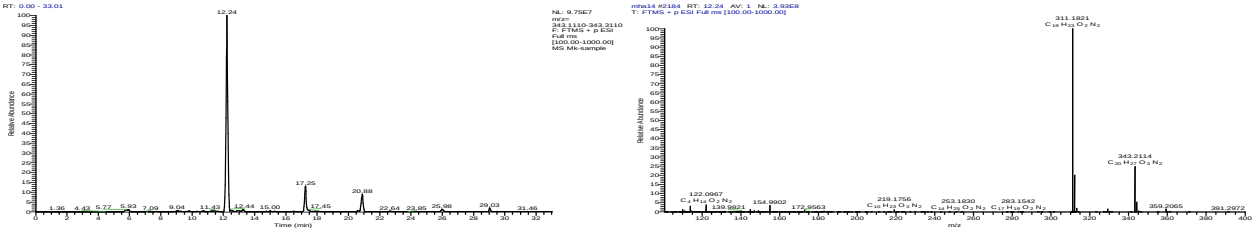


Figure S82. The UHPLC-ESI-MS base peak chromatograms of the crude extract and melokhanines A-J (**1-10**).

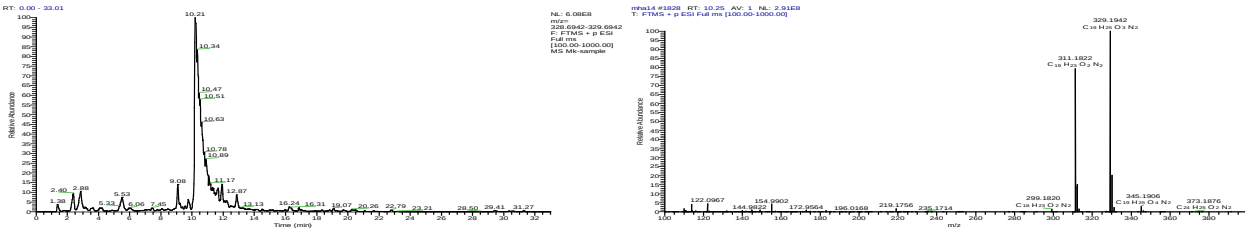
Melokhanine F.



Melokhanine G



Melokhanine H



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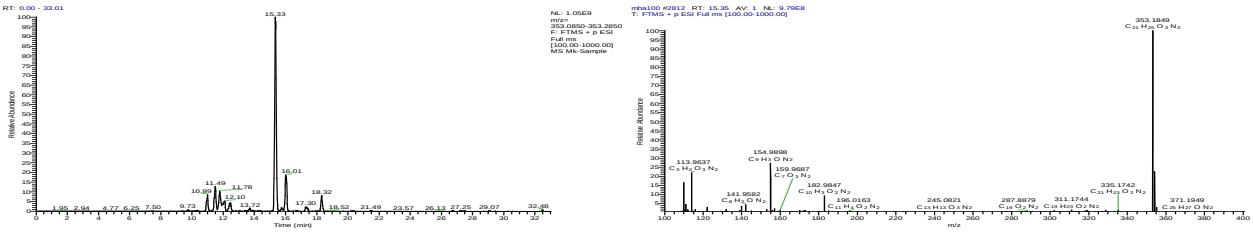

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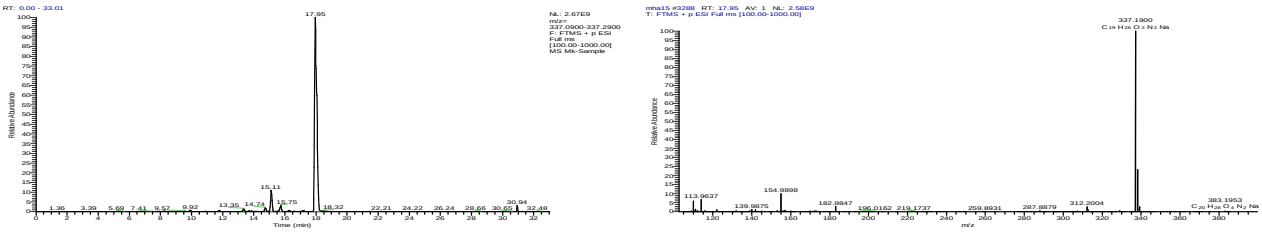

Figure S82. The UHPLC-ESI-MS base peak chromatograms of the crude extract and melokhanines A-J (**1-10**).