

Supporting Information

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Bioassay- guided Isolation of New Urease Inhibitory Constituents from *Monotheca buxifolia* (Falc.) Fruit and Their Molecular Docking Studies

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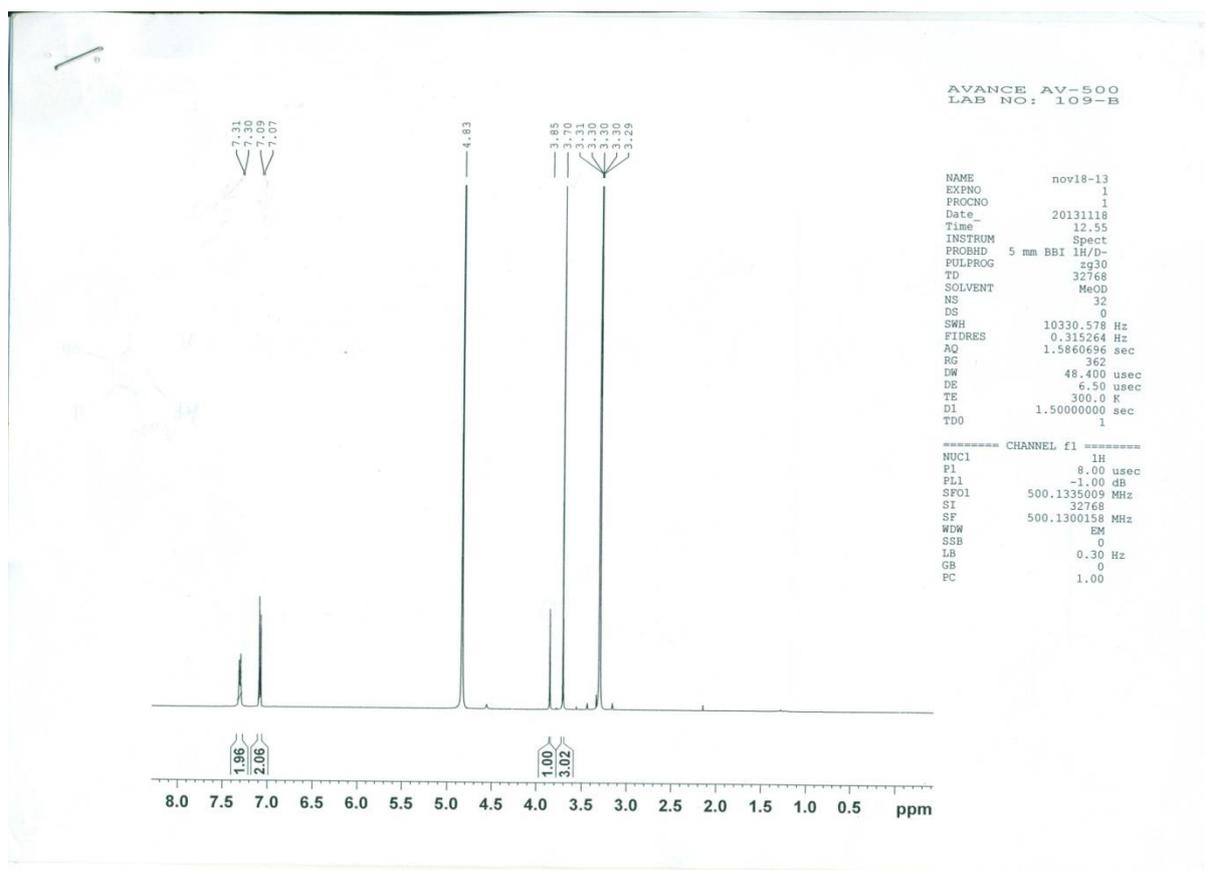
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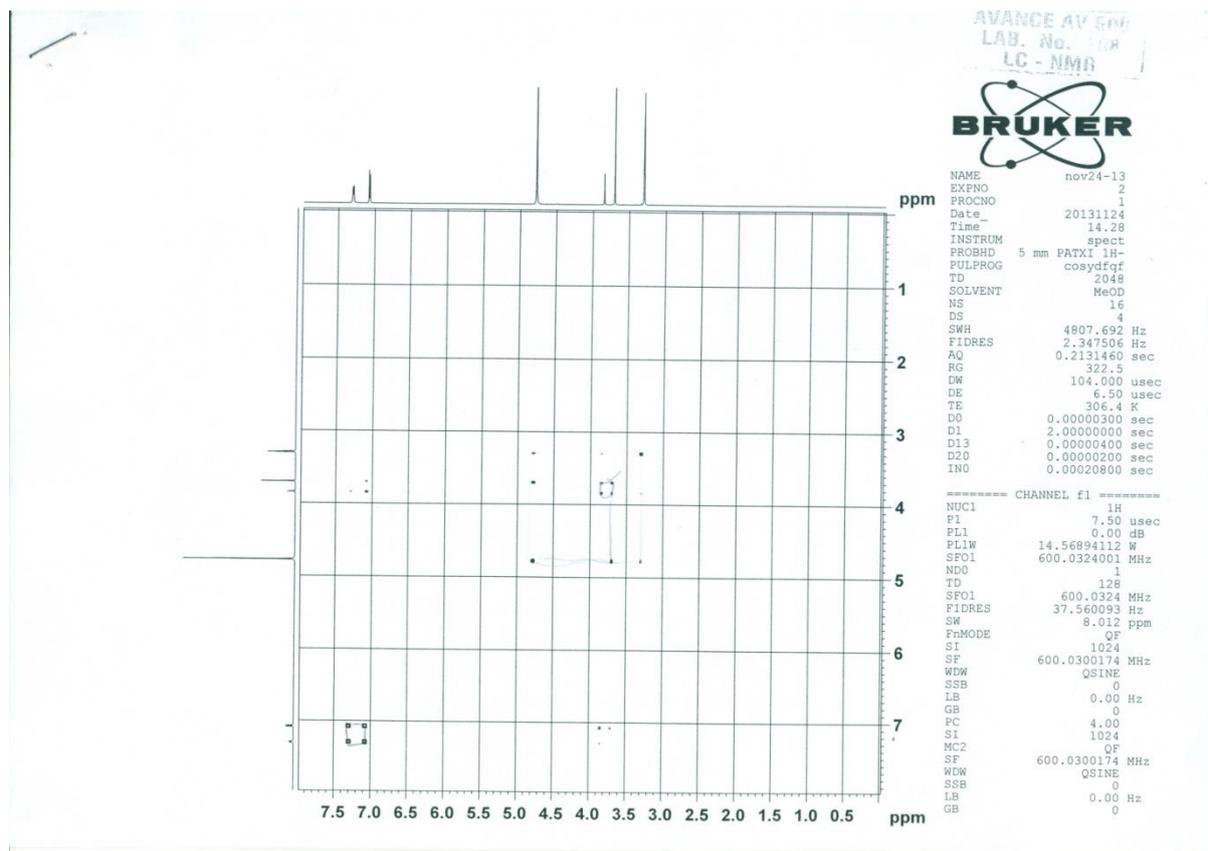
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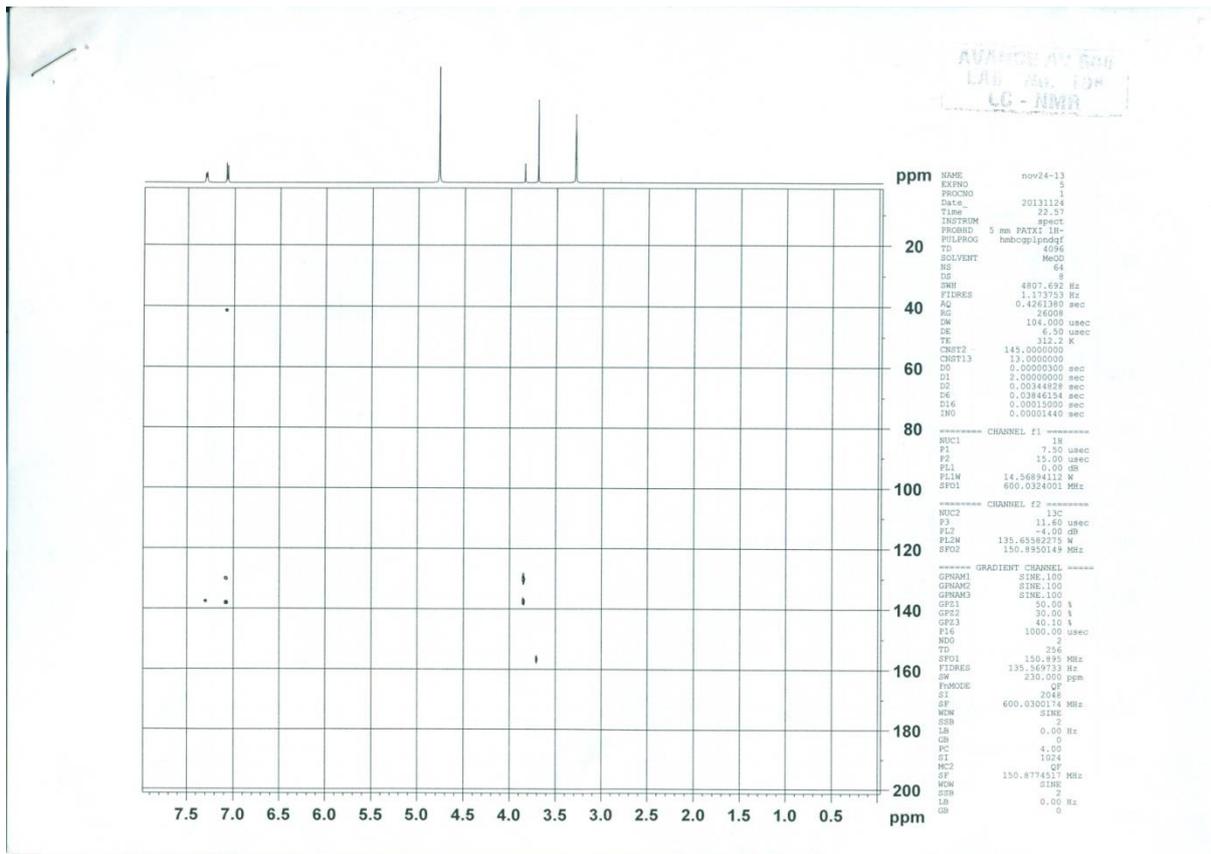
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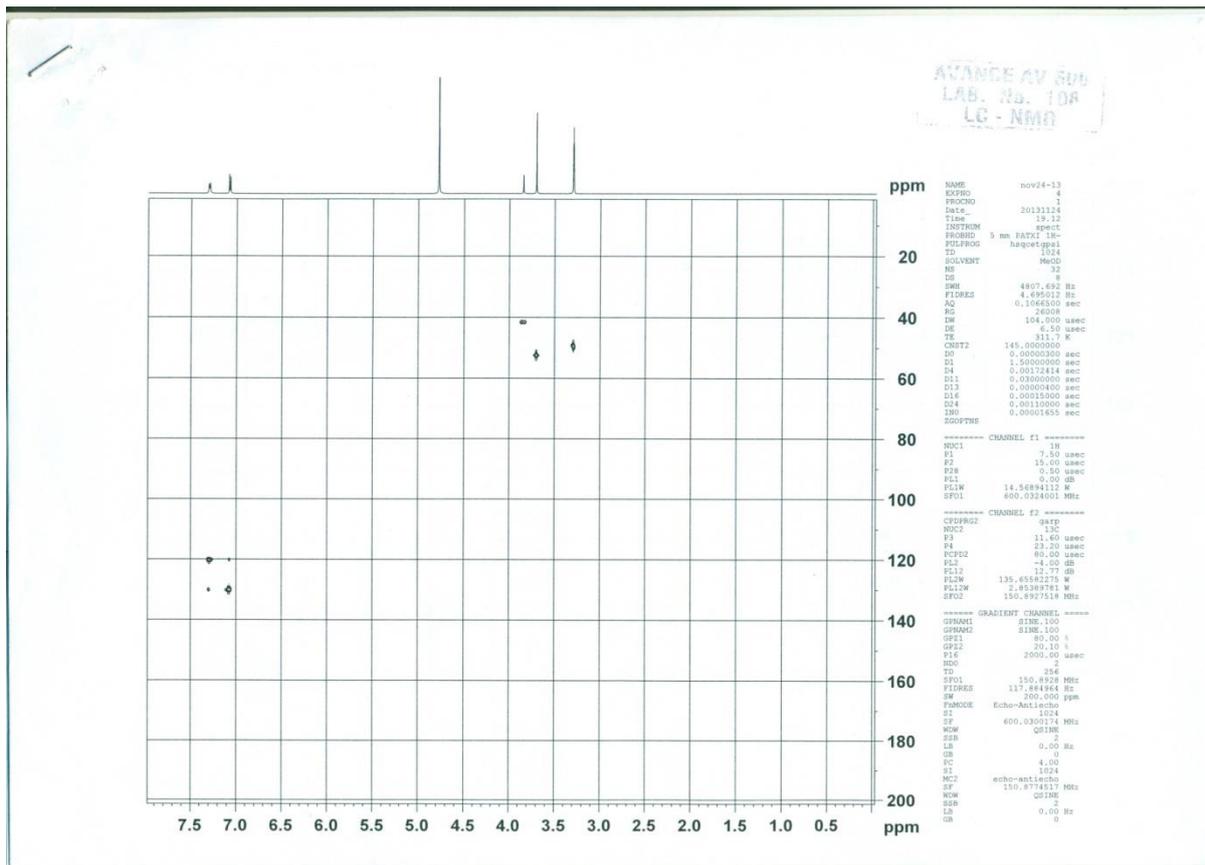
S1: ^1H -NMR of Buxifoline-A (Compound 1)



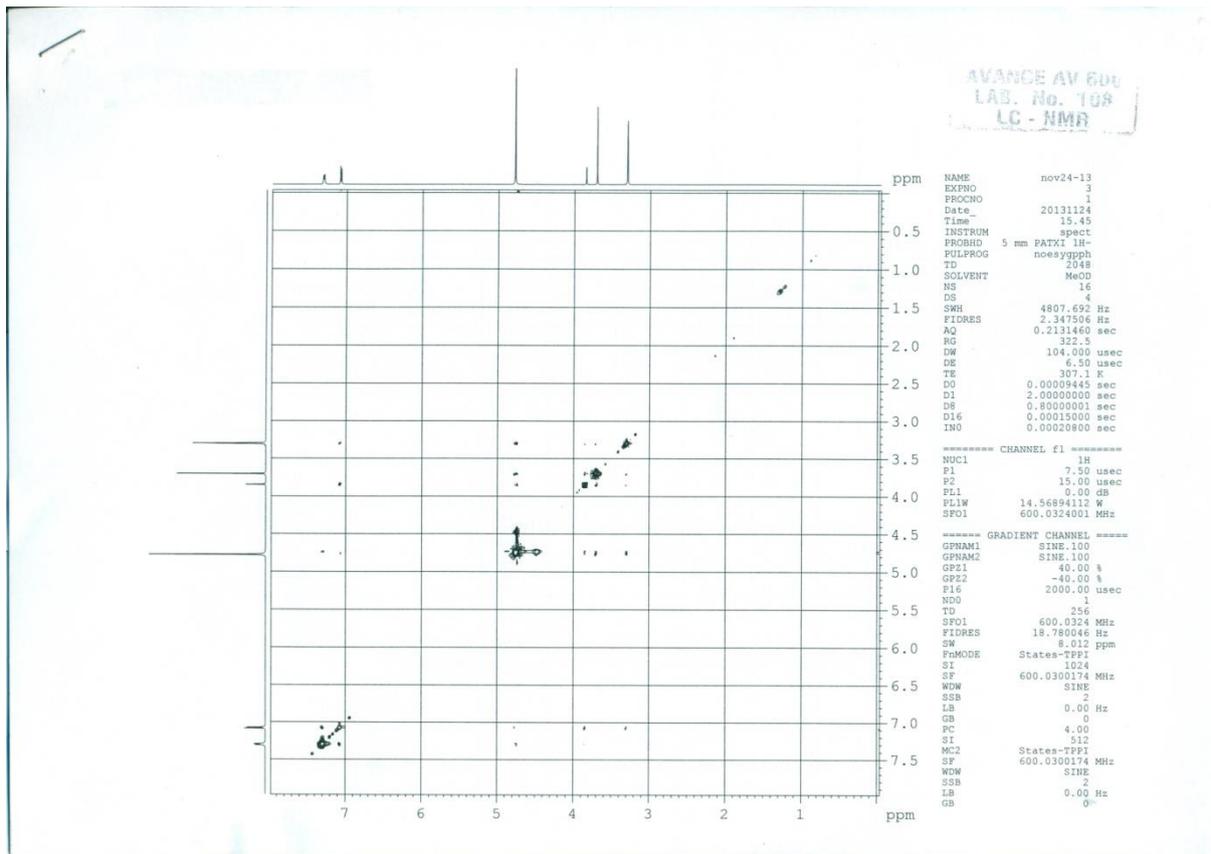
S2: gCOSY spectrum of Buxifolina-A (Compound 1)



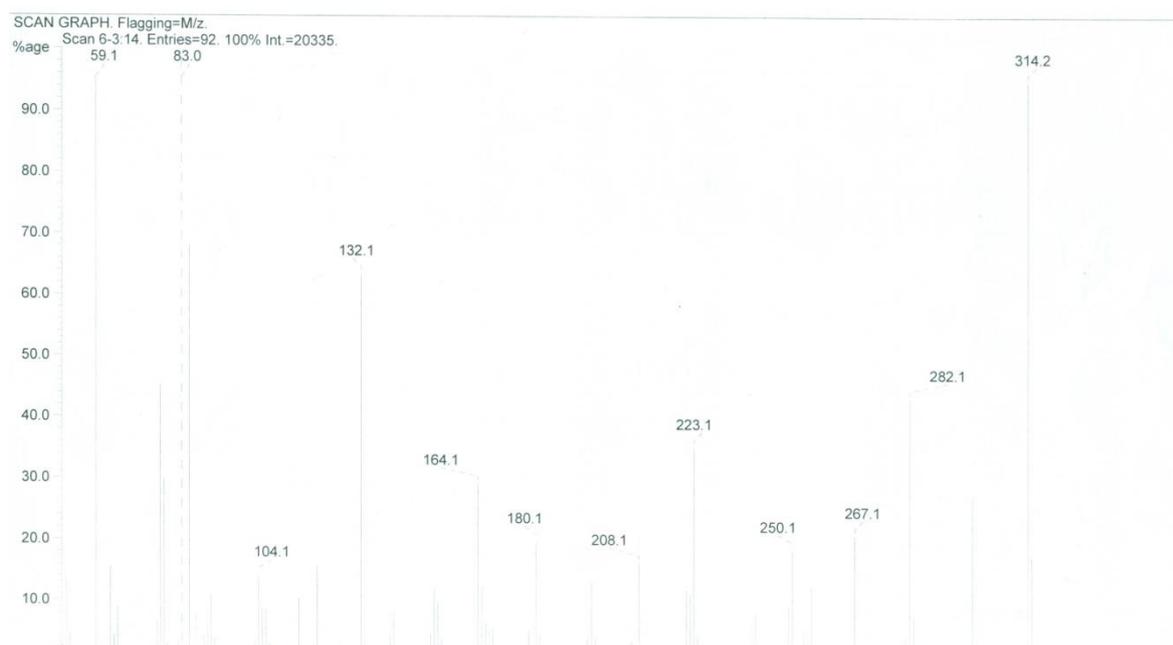
S3: gHMBC spectrum of Buxifolina-A (Compound 1)



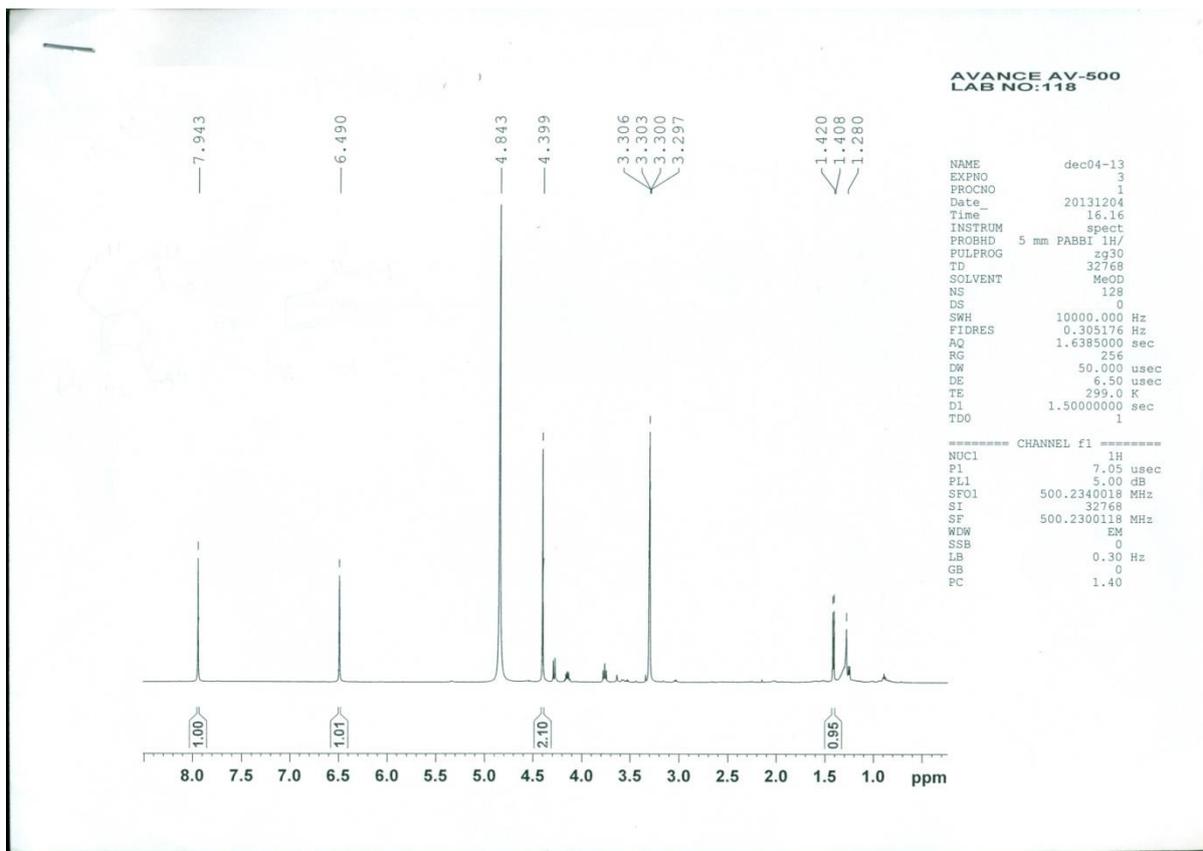
S4: gHSQC spectrum of Buxifolina-A (Compound 1)



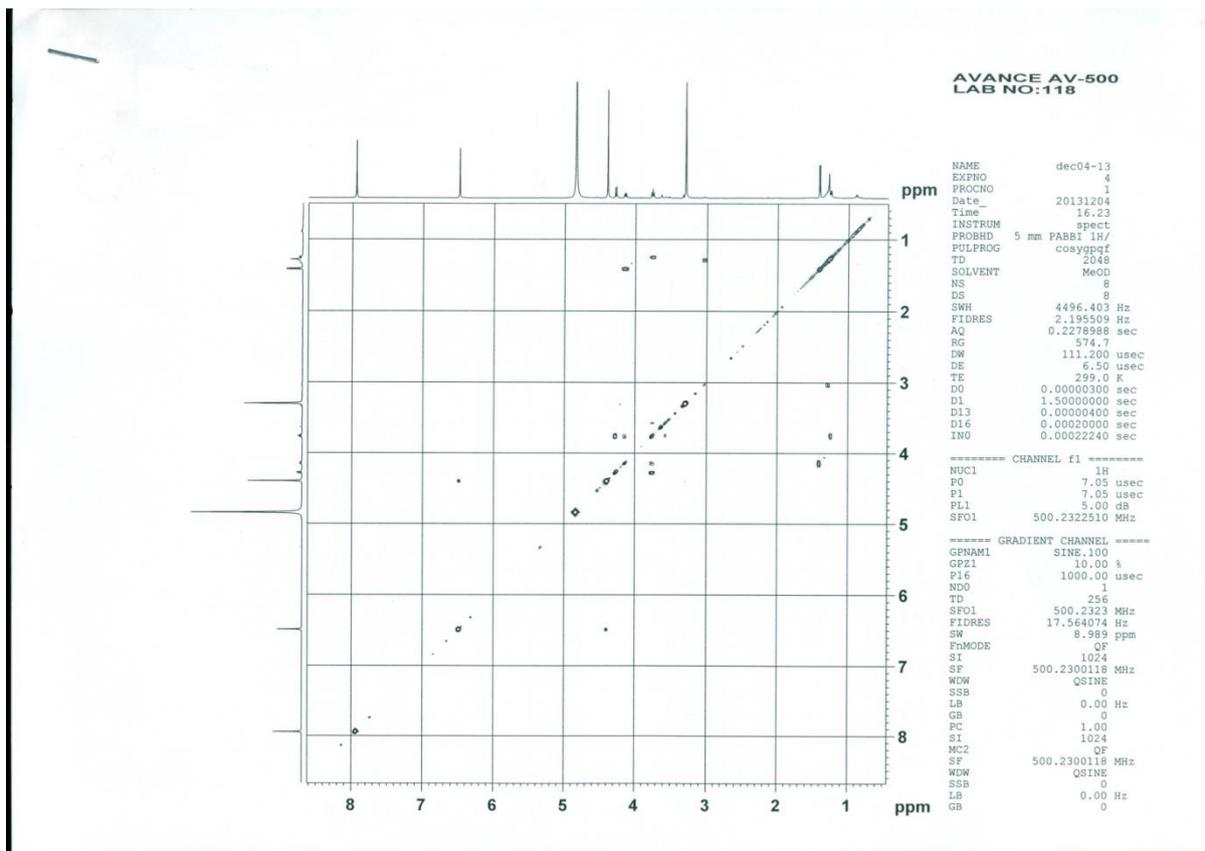
S5: NOESY spectrum of Buxifolina-A (Compound 1)



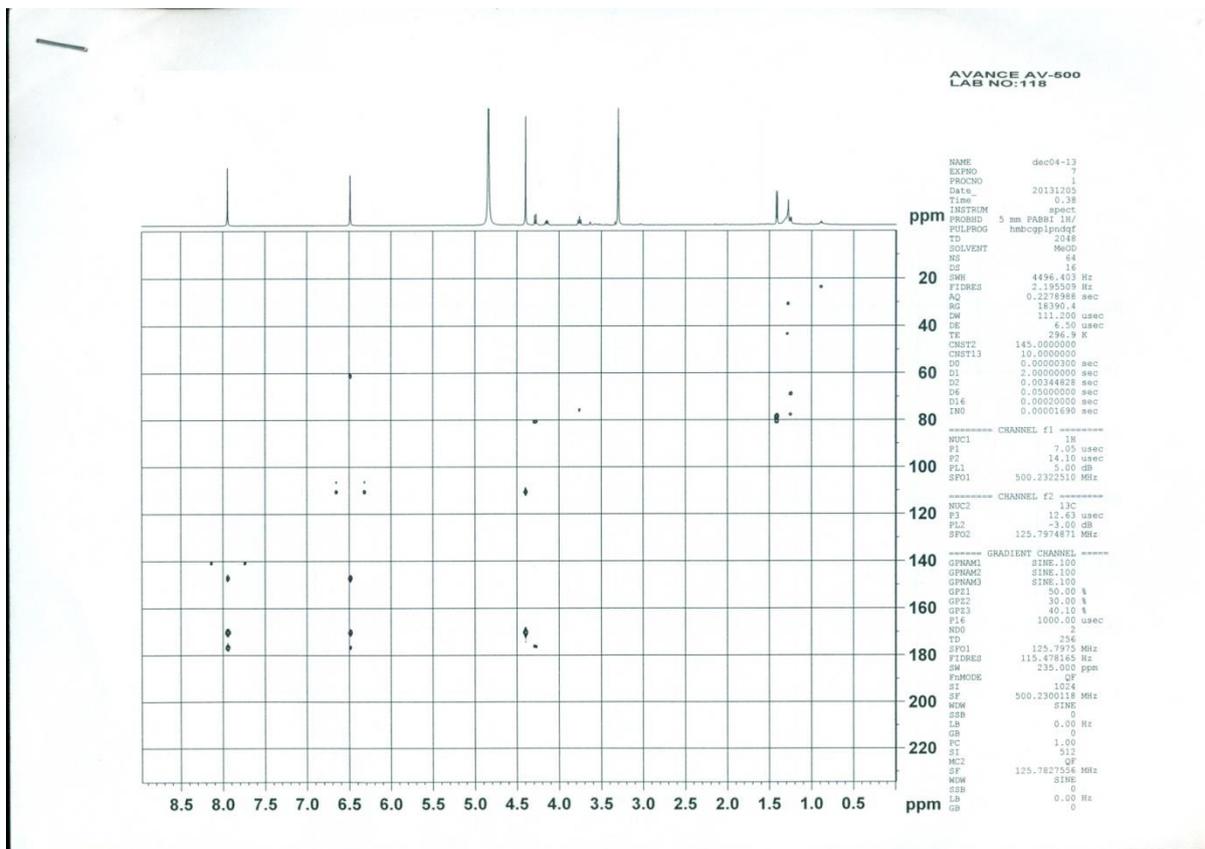
S6: Mass spectrum of Buxifolina-A (Compound **1**)



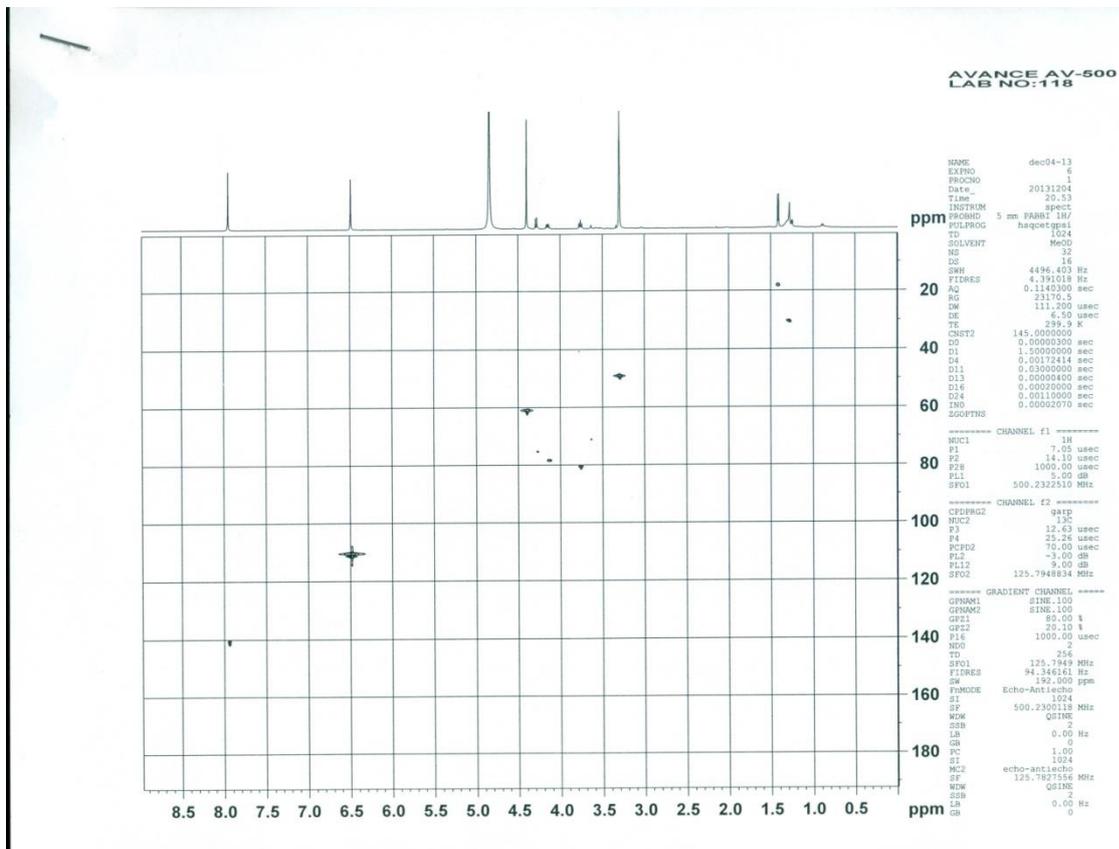
S7: Proton spectrum of Buxilide (Compound 2)



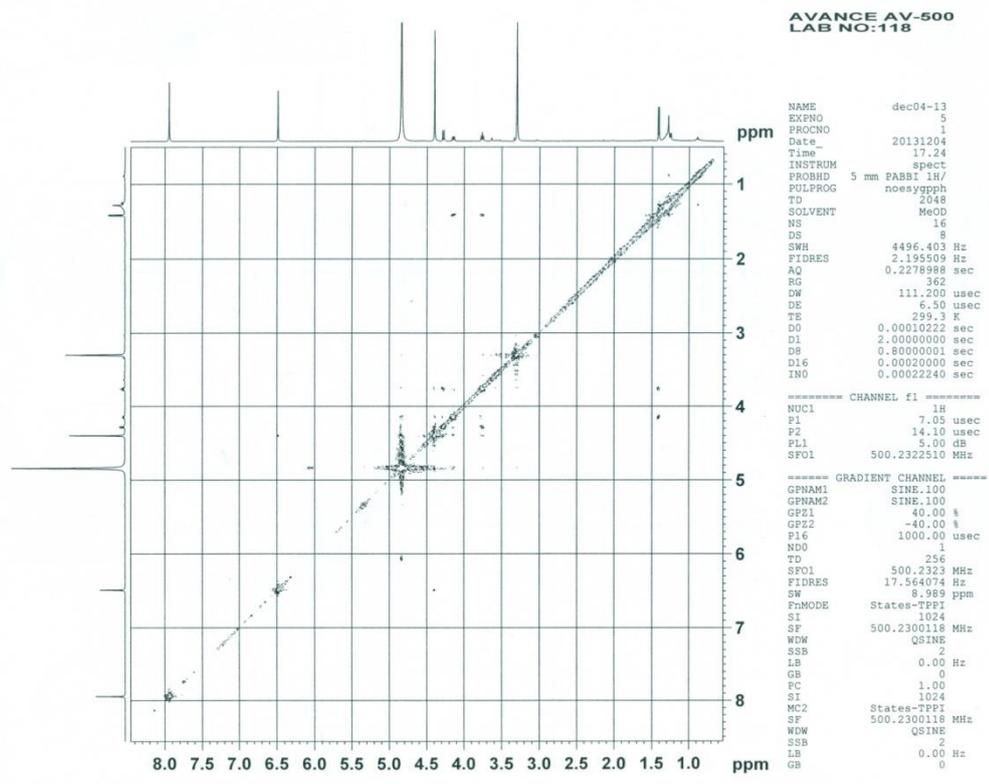
S8: gCOSY spectrum of Buxilide (Compound 2)



S9: gHMBC spectrum of Buxilide (Compound 2)



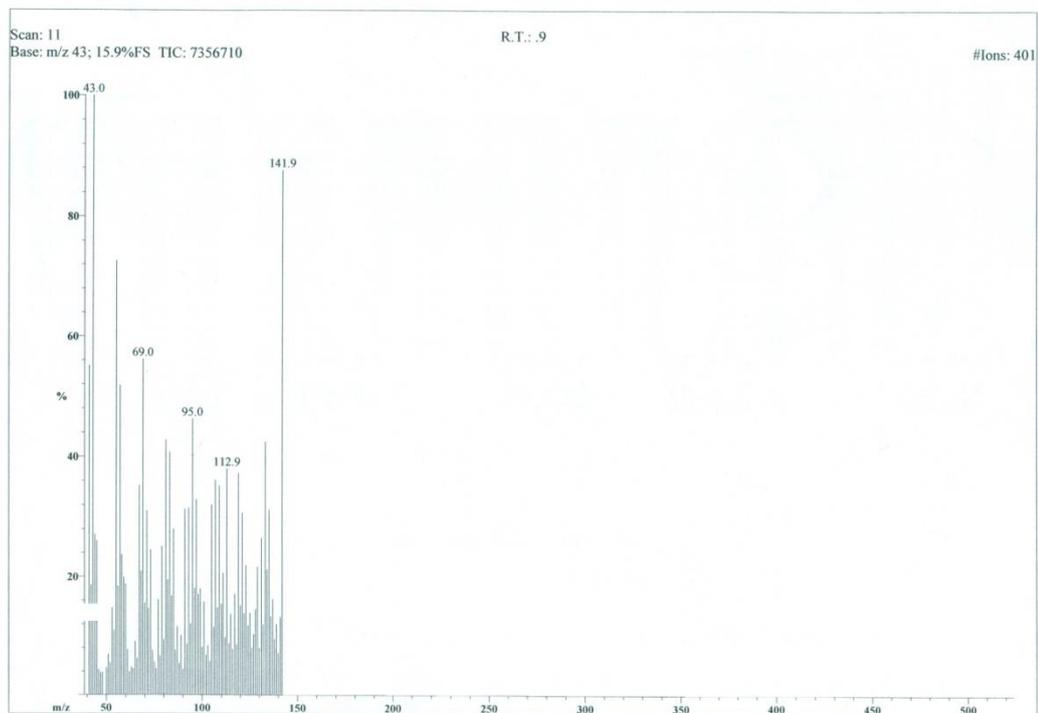
S10: gHSQC spectrum of Buxilide (Compound 2)



S11: NOESY spectrum of Buxilide (Compound 2)

Date Run: 01-06-2014 (Time Run: 16:02:37)

Ionization mode: EI+



S12: Mass spectrum of Buxilide (Compound 2)

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
112.1005	1.1					
112.9797	0.7					
113.0014	26.1	113.0027	-11.9	-1.3	8.5	C ₈ H ₈ O ₁
113.0629	0.5	113.0603	23.0	2.6	2.5	C ₈ H ₈ O ₂
113.1113	1.1					
114.0094	1.6	114.0106	-10.2	-1.2	8.0	C ₈ H ₈ O ₁
114.0737	2.3					
115.0409	0.7	115.0395	11.6	1.3	2.5	C ₈ H ₈ O ₃
115.0863	0.7					
116.9875	1.0					
117.0637	0.9					
118.9920	22.3					
119.0857	1.4	119.0861	-2.8	-0.3	4.5	C ₉ H ₁₁
120.0941	0.6	120.0939	1.4	0.2	4.0	C ₉ H ₁₂
121.1037	1.7	121.1017	16.5	2.0	3.5	C ₉ H ₁₃
122.1064	1.3	122.1096	-25.5	-3.1	3.0	C ₉ H ₁₄
123.1204	2.0	123.1174	24.5	3.0	2.5	C ₉ H ₁₅
123.9982	1.3	124.0008	-21.2	-2.6	1.0	C ₉ H ₁₅ O ₆
		123.9949	26.2	3.2	10.0	C ₉ O ₁
124.1267	1.4	124.1252	12.0	1.5	2.0	C ₉ H ₁₆
125.0275	0.5	125.0239	29.2	3.7	4.5	C ₉ H ₁₆ O ₃
125.1022	0.7					
125.1377	1.4	125.1330	37.3	4.7	1.5	C ₉ H ₁₇
126.0352	1.0	126.0317	27.7	3.5	4.0	C ₉ H ₁₈ O ₃
126.0962	2.8					
126.1440	0.5	126.1409	25.1	3.2	1.0	C ₉ H ₁₈
127.1022	0.6					
128.0652	0.6	128.0626	20.4	2.6	7.0	C ₁₀ H ₈
128.1100	2.1					
129.0709	0.7	129.0704	4.0	0.5	6.5	C ₁₀ H ₉
129.0936	0.5	129.0916	15.5	2.0	1.5	C ₁₀ H ₁₃ O ₂
130.9920	34.6					
131.0860	0.9	131.0861	-0.8	-0.1	5.5	C ₁₀ H ₁₁
131.9953	1.1	132.0000	-35.2	-4.7	12.0	C ₁₁
133.1014	1.3	133.1017	-2.2	-0.3	4.5	C ₁₀ H ₁₃
134.1095	0.6	134.1096	-0.2	-0.0	4.0	C ₁₀ H ₁₄
135.1171	1.6	135.1174	-2.1	-0.3	3.5	C ₁₀ H ₁₅
136.1162	1.1					
137.1335	1.1	137.1330	3.3	0.5	2.5	C ₁₀ H ₁₇
138.1379	0.8	138.1409	-21.7	-3.0	2.0	C ₁₀ H ₁₈
139.1122	0.5	139.1123	-0.5	-0.1	2.5	C ₉ H ₁₅ O ₁
139.1459	0.6	139.1487	-20.0	-2.8	1.5	C ₁₀ H ₁₉
140.0113	1.8	140.0110	2.4	0.3	5.0	C ₉ H ₄ O ₄
140.1080	1.1					
141.0172	0.7	141.0188	-11.0	-1.6	4.5	C ₉ H ₁₆ O ₄
142.0271	59.6	142.0266	3.8	0.5	4.0	C ₉ H ₁₆ O ₄
142.1247	0.7					
142.9920	3.6					
143.0305	4.7	143.0344	-27.5	-3.9	3.5	C ₉ H ₁₆ O ₄
143.0843	0.6	143.0861	-12.6	-1.8	6.5	C ₁₁ H ₁₁
144.0331	0.7					
145.1009	0.7	145.1017	-5.6	-0.8	5.5	C ₁₁ H ₁₃
147.1169	1.0	147.1174	-3.4	-0.5	4.5	C ₁₁ H ₁₅
149.0226	4.9	149.0239	-8.5	-1.3	6.5	C ₉ H ₁₅ O ₃
149.1316	1.0	149.1330	-9.9	-1.5	3.5	C ₁₁ H ₁₇
149.9886	1.1					
150.0272	0.5	150.0317	-30.1	-4.5	6.0	C ₈ H ₆ O ₃
150.1339	0.6					
150.9966	0.8					
151.1478	0.7	151.1487	-6.0	-0.9	2.5	C ₁₁ H ₁₉
152.1519	0.5	152.1565	-30.5	-4.6	2.0	C ₁₁ H ₂₀
154.1225	0.8					
154.9920	2.9	154.9980	-39.0	-6.0	5.5	C ₈ H ₈ O ₅

S13: HR-Mass spectrum of Buxilide (Compound 2)