Supplementary material

Density functional theory of a new derivative of allantoin with antiplasmodial properties, antimycobacterial activities of essential oil from *Cordia batesii* WERNHAM (Boraginaceae)

Eric Robert Tiam[1], **Dominique Serge Ngono Bikobo**[1], **Ibrahim Mbouombouo Ndassa**[2,3], **Norbert Mbabi Nyemeck II**[1], **Auguste Abouem A Zintchem**[1,3*], **Lawrence Ayong**[4], **Patrick Hervé Betote Diboué**[5], **Bruno Lenta Ndjakou**[1,3], **Joséphine Ngo Mbing**[1†], **Dieudonné Emmanuel Pegnyemb**[1†].

Corresponding author:

Dr Auguste Abouem A Zintchem, Higher Teachers Training College, Department of Chemistry, University of Yaoundé I, P.O Box 47, Yaounde, Cameroon. E-mail: augabouem@yahoo.fr Phone: +237 699 73 22 16.

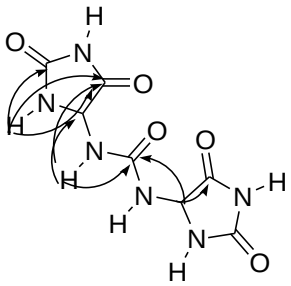

Fig. 1S. Selected HMBC correlations of compound **2**

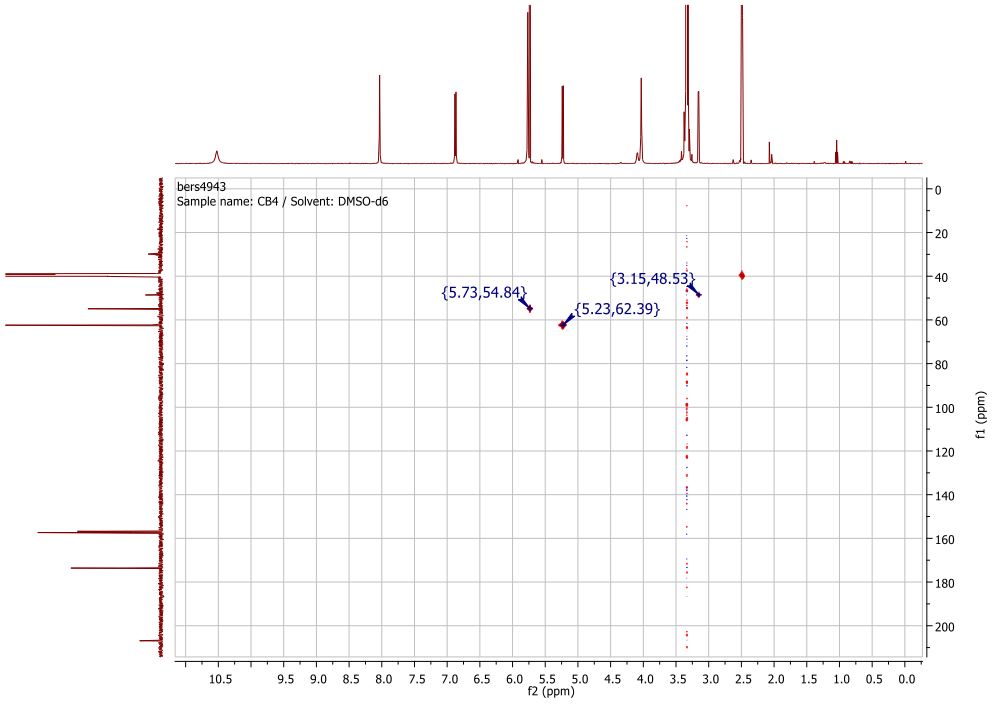

Fig. 2S. HSQC spectrum of compound **2**

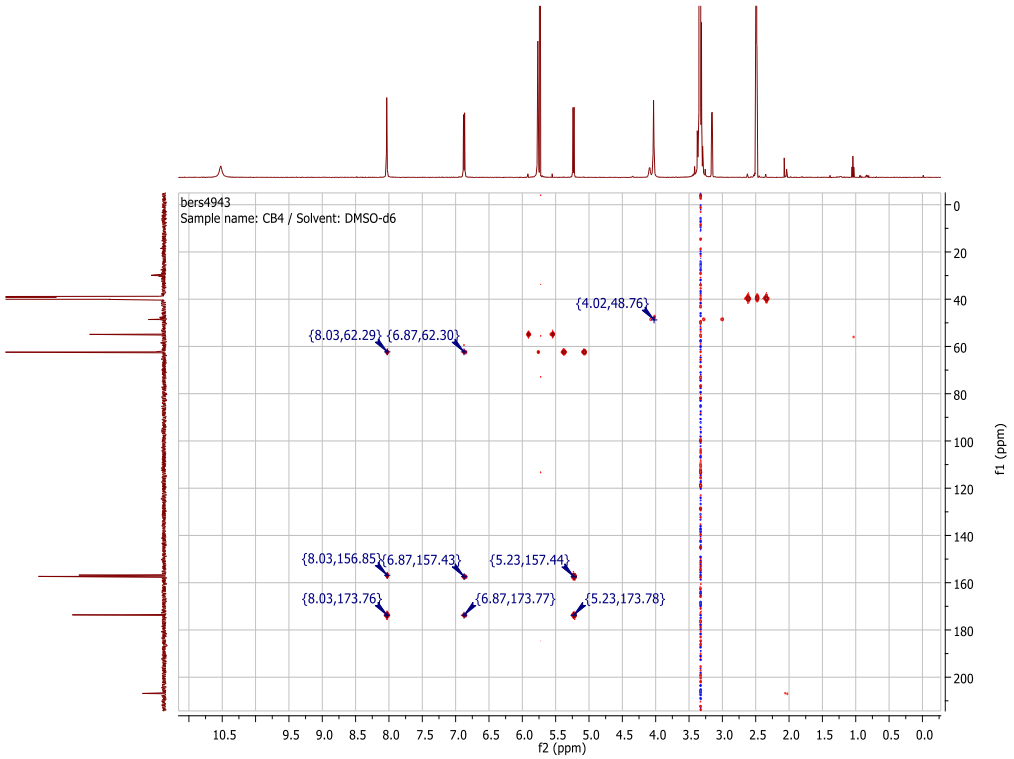

Fig. 3S. HMBC spectrum of compound **2**

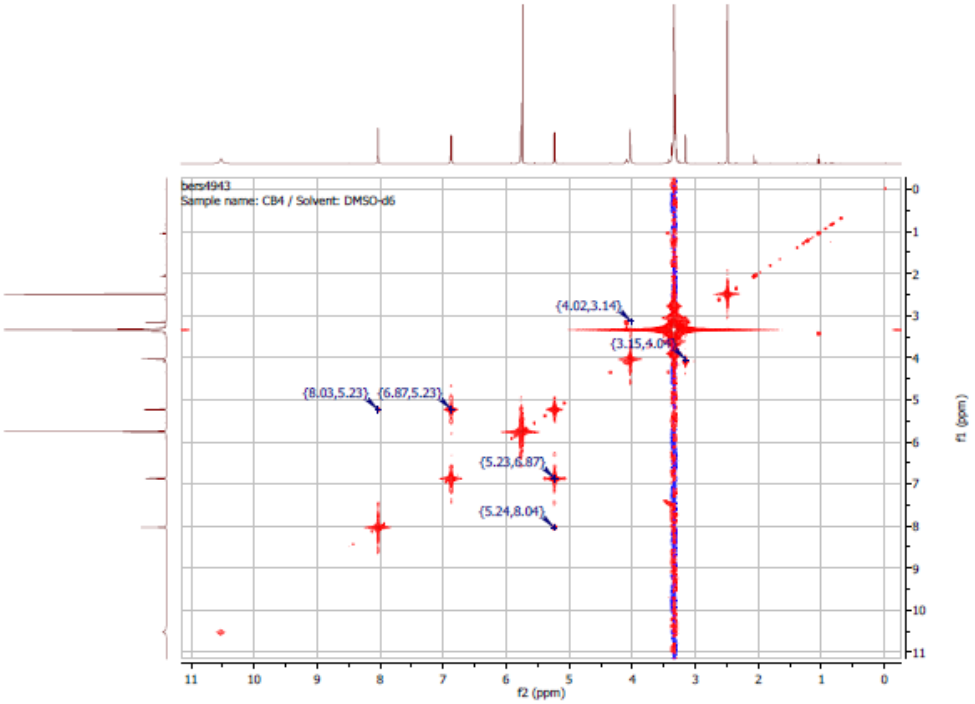

Fig. 4S. ^{1}H - ^{1}H COSY spectrum of compound **2**

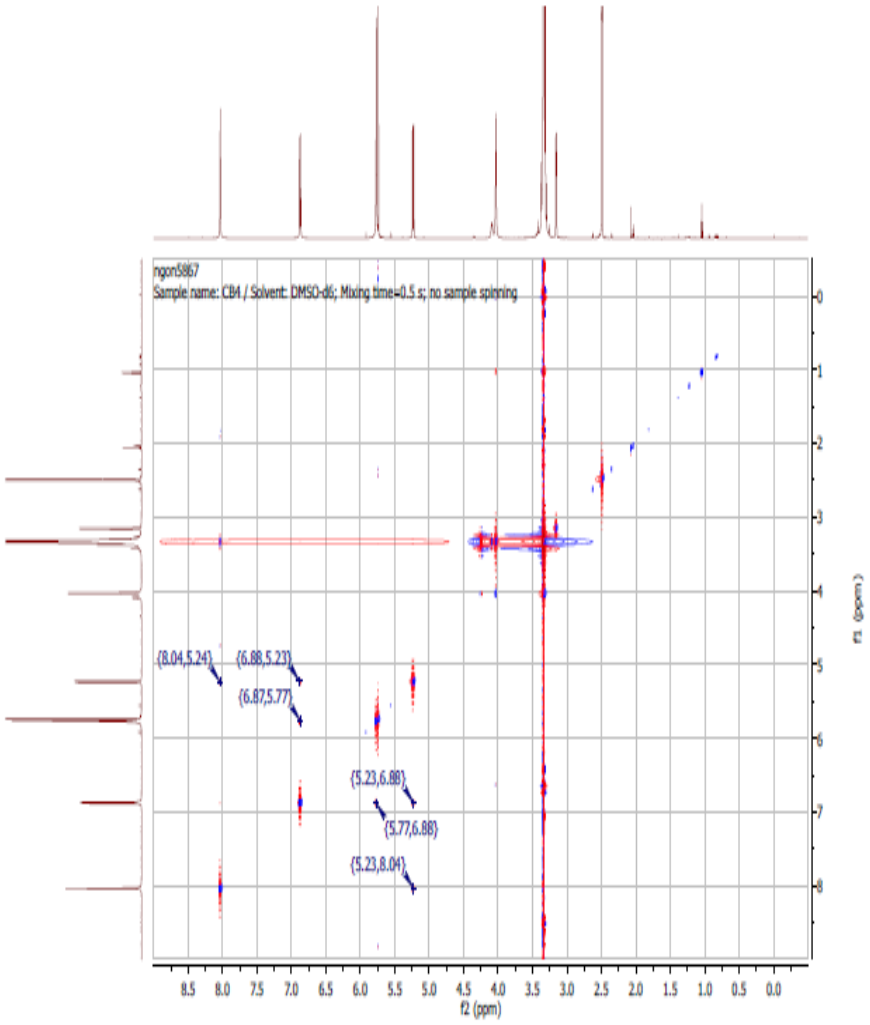

Fig. 5S. NOESY spectrum of compound **2**

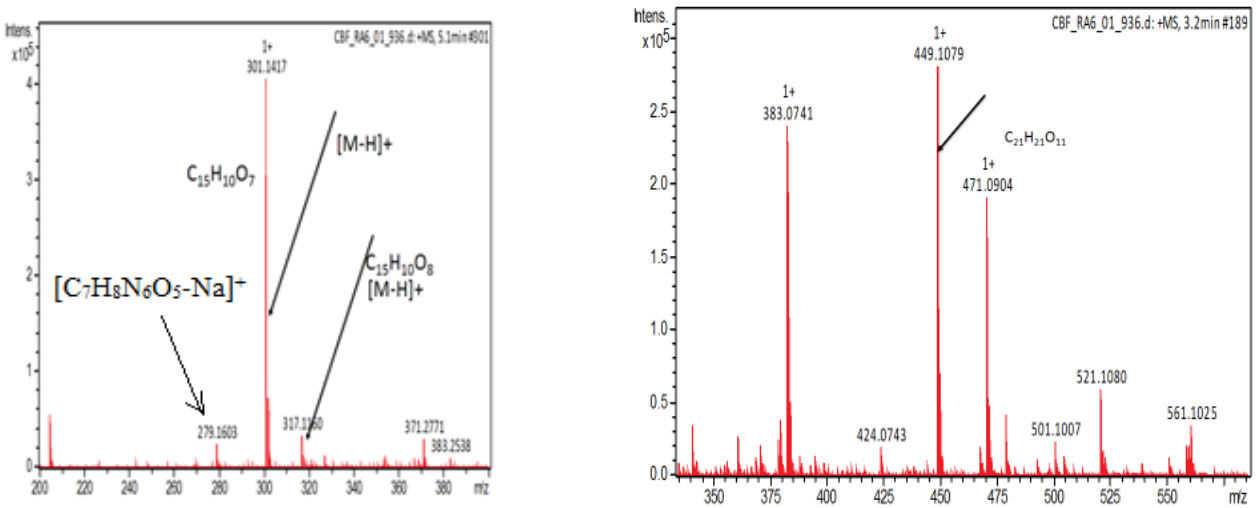

Fig. 6S: LC–MS chromatogram obtained from *C. batesii* (Compounds **6**, **7** and **8**)

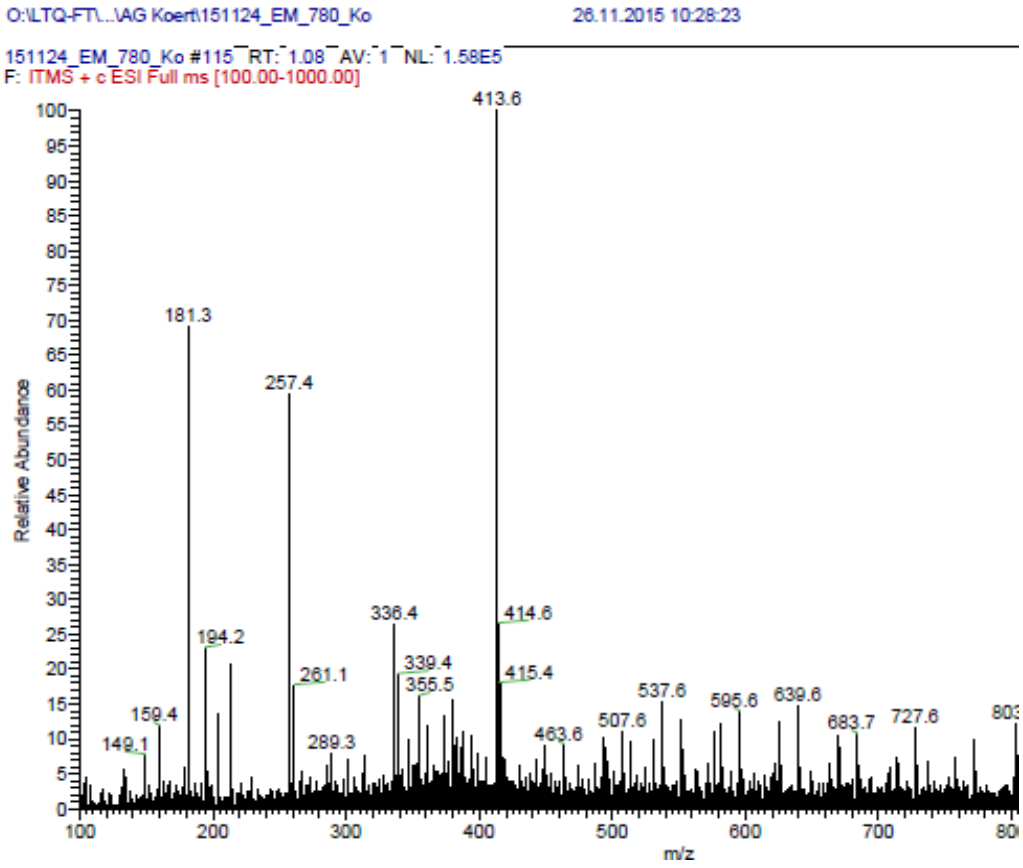

Fig. 7S. ESI-MS spectrum of compound **2**

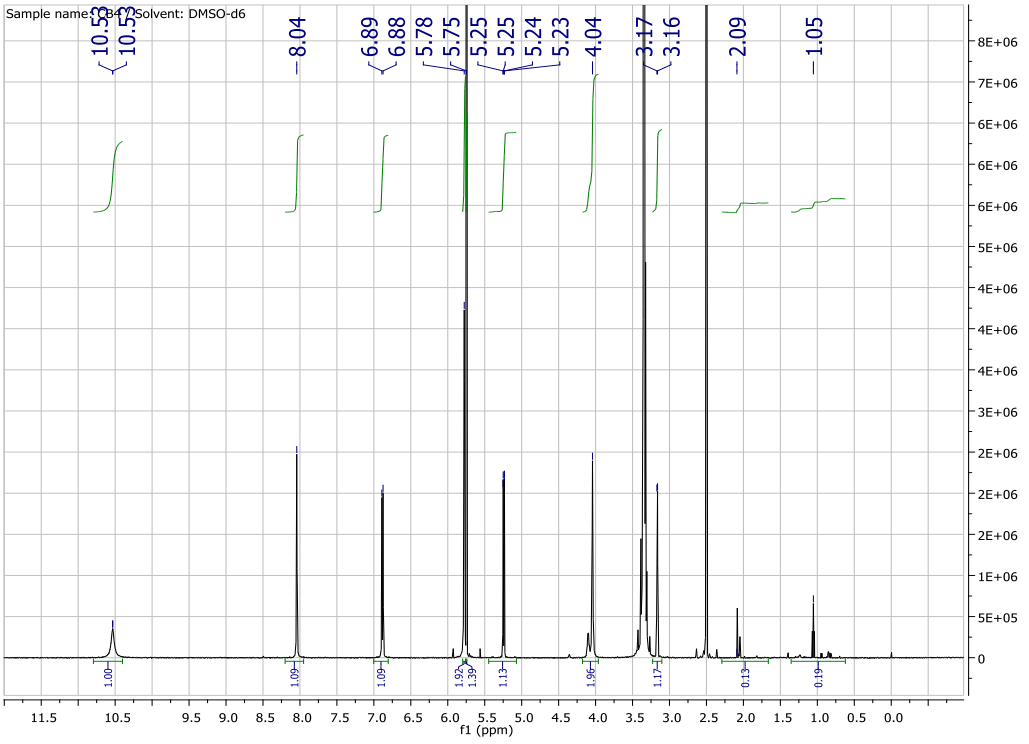

Fig. 8S. ^{1}H–NMR spectrum of compound **2**

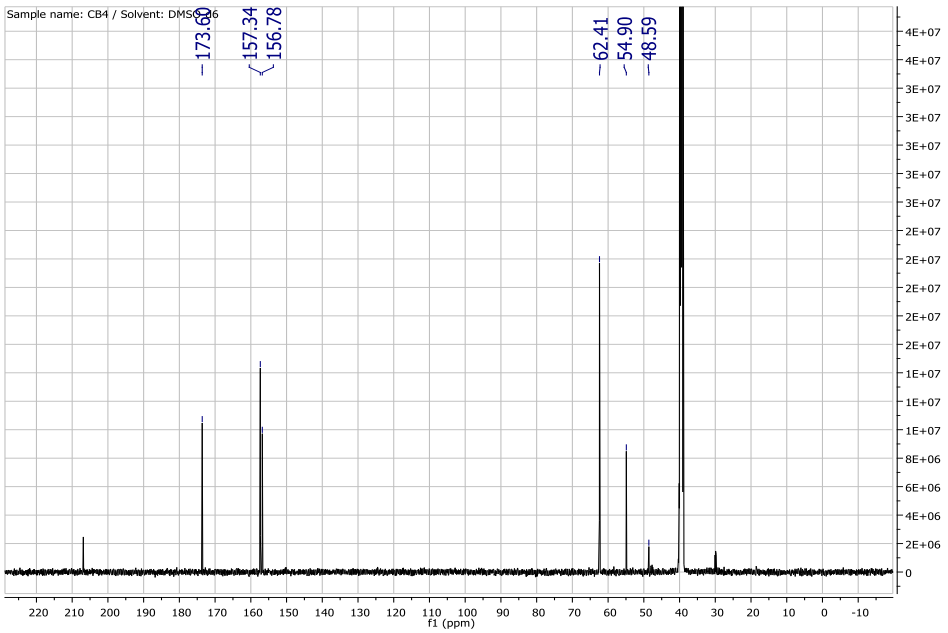

Fig. 9S. ^{13}C–NMR spectrum of compound **2**

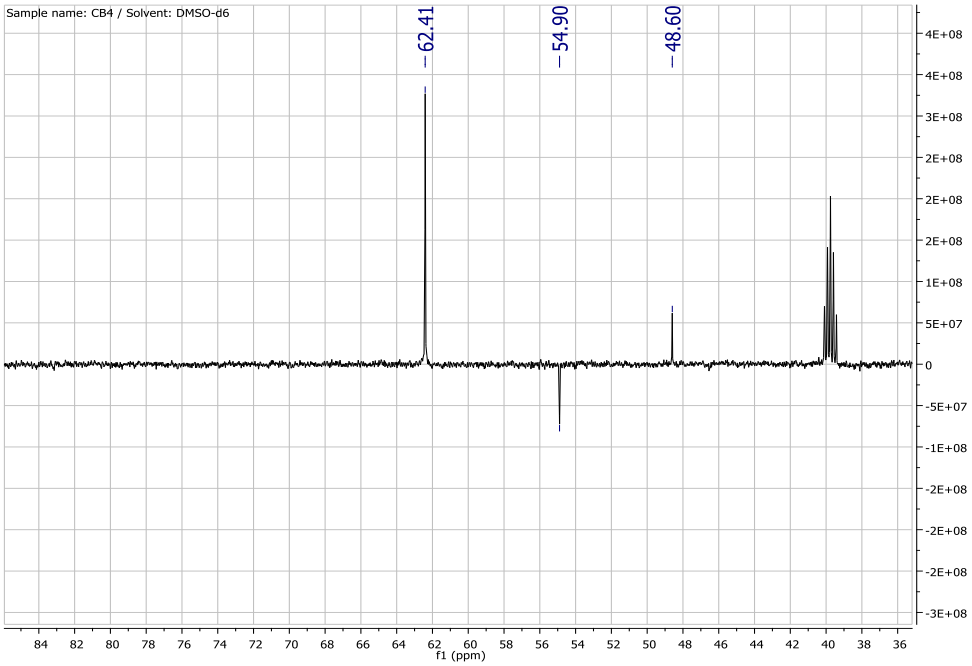

Fig. 10S. DEPT 135 spectrum of compound **2**

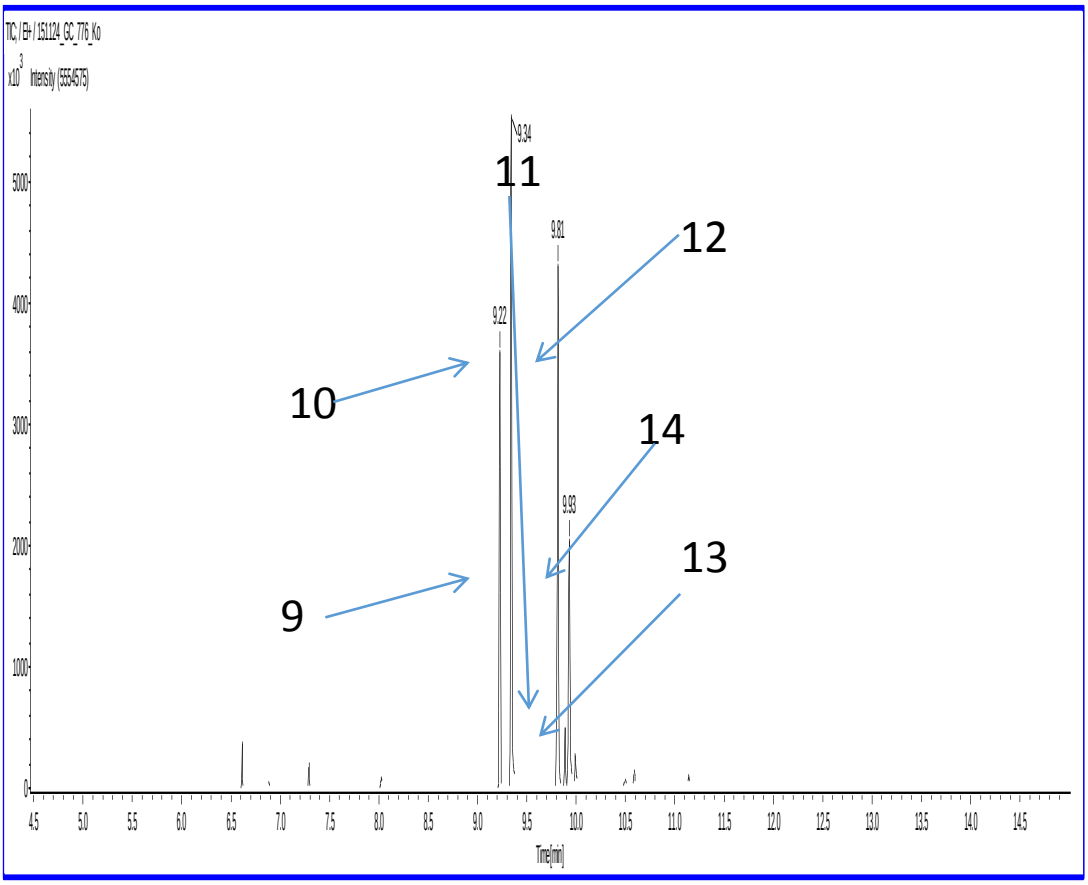

Fig. 11S: GC-MS spectrum of mixture of fatty acids

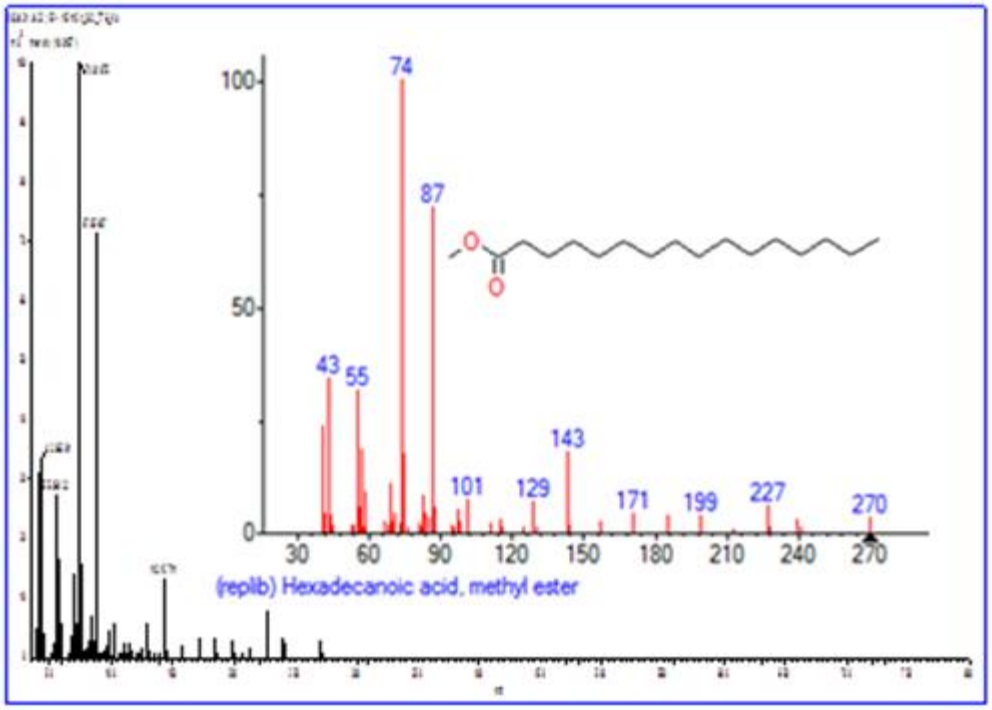

Fig. 12S: identification of compound 9

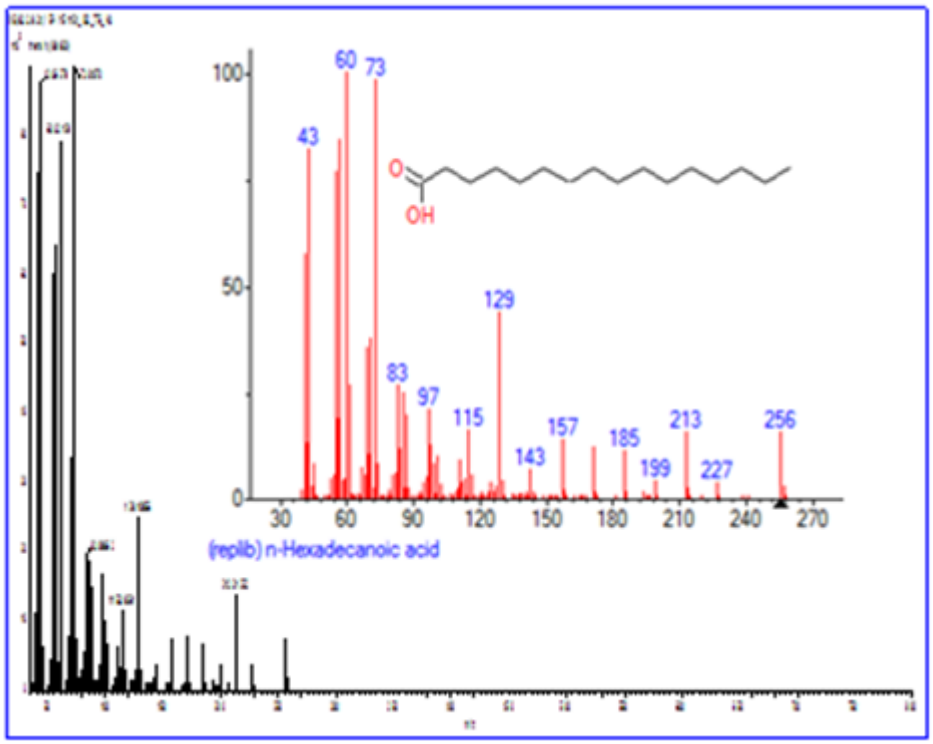

Fig. 13S: identification of compound 10

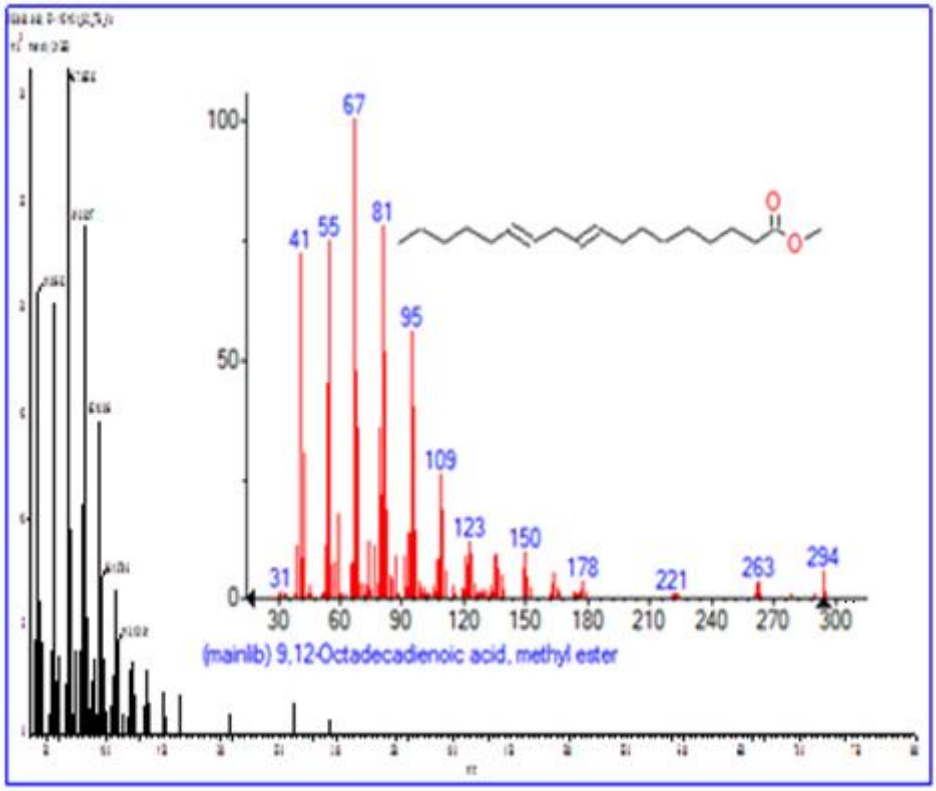

Fig. 14S: identification of compound 11

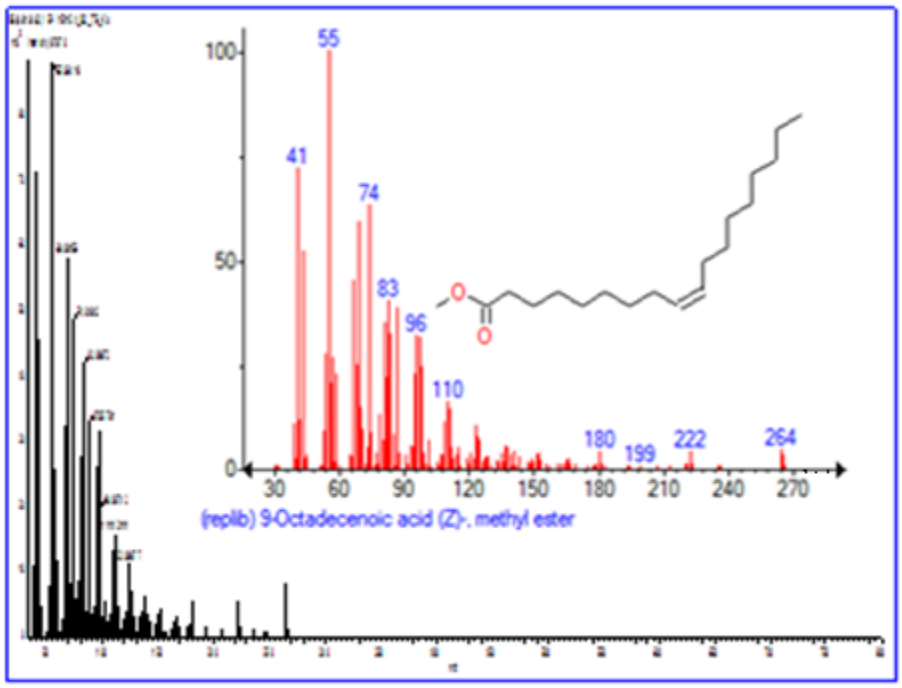

Fig. 15S: identification of compound 12

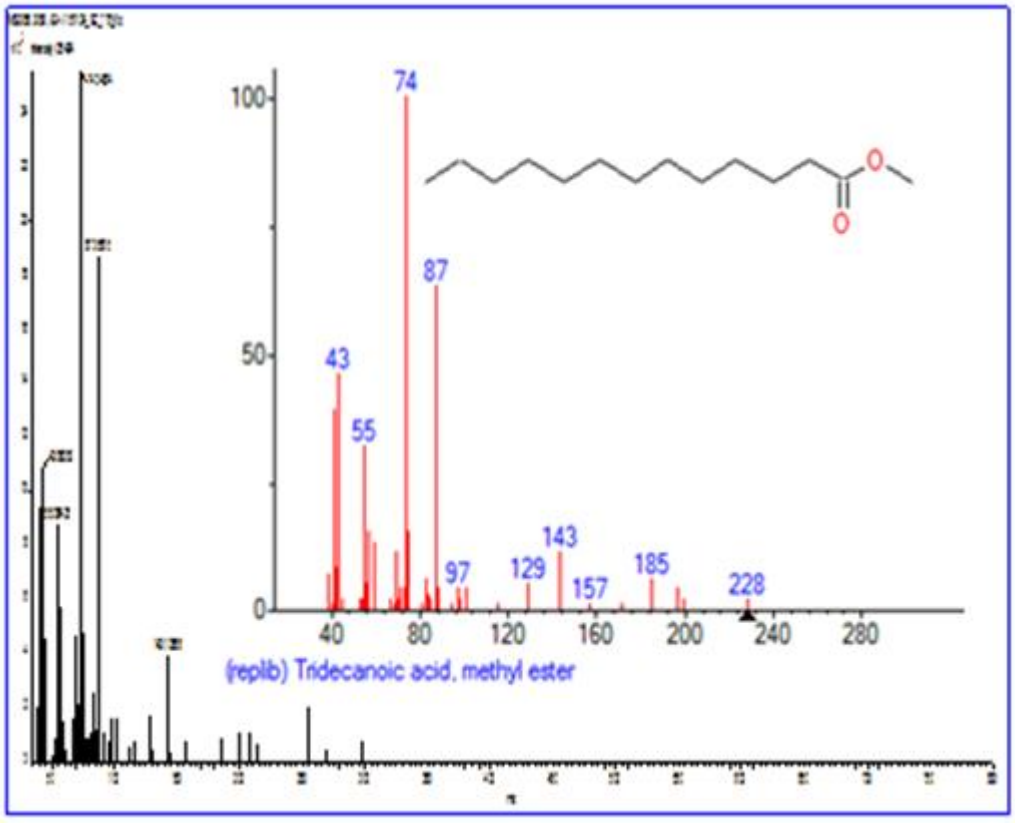

Fig. 16S: identification of compound 13

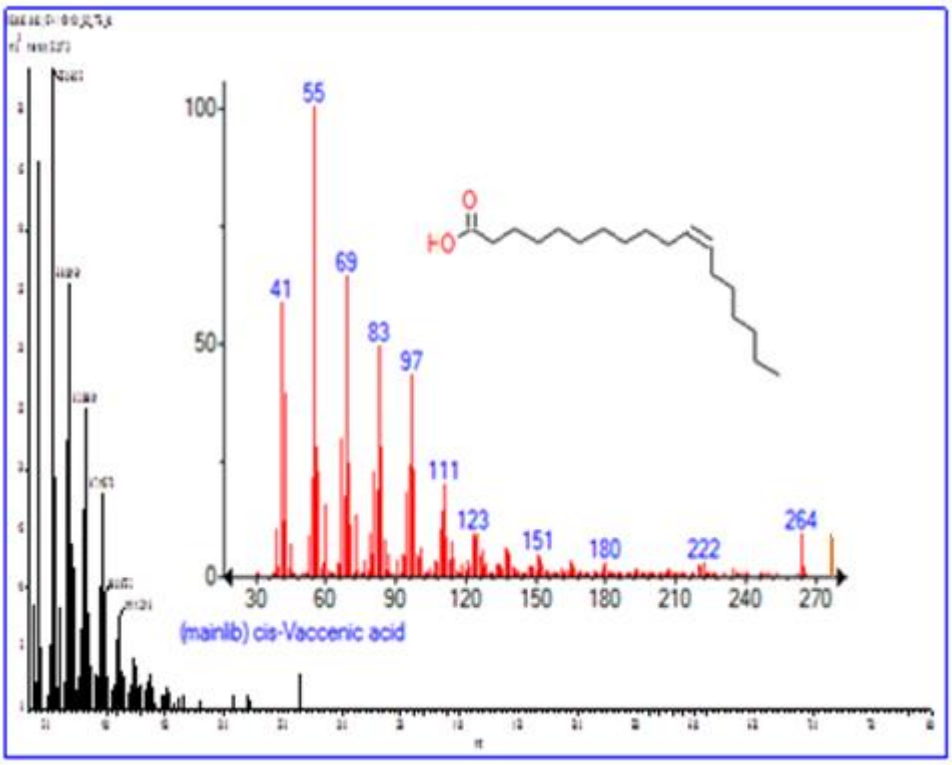

Fig. 17S: identification of compound 14

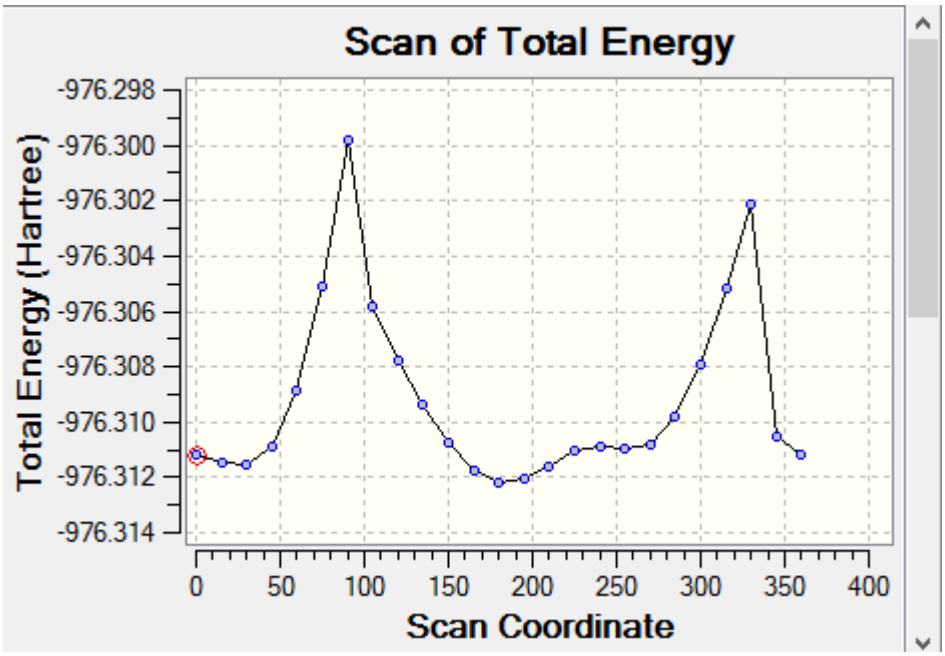

Fig. 18S. Conformational analysis of compound **2**.

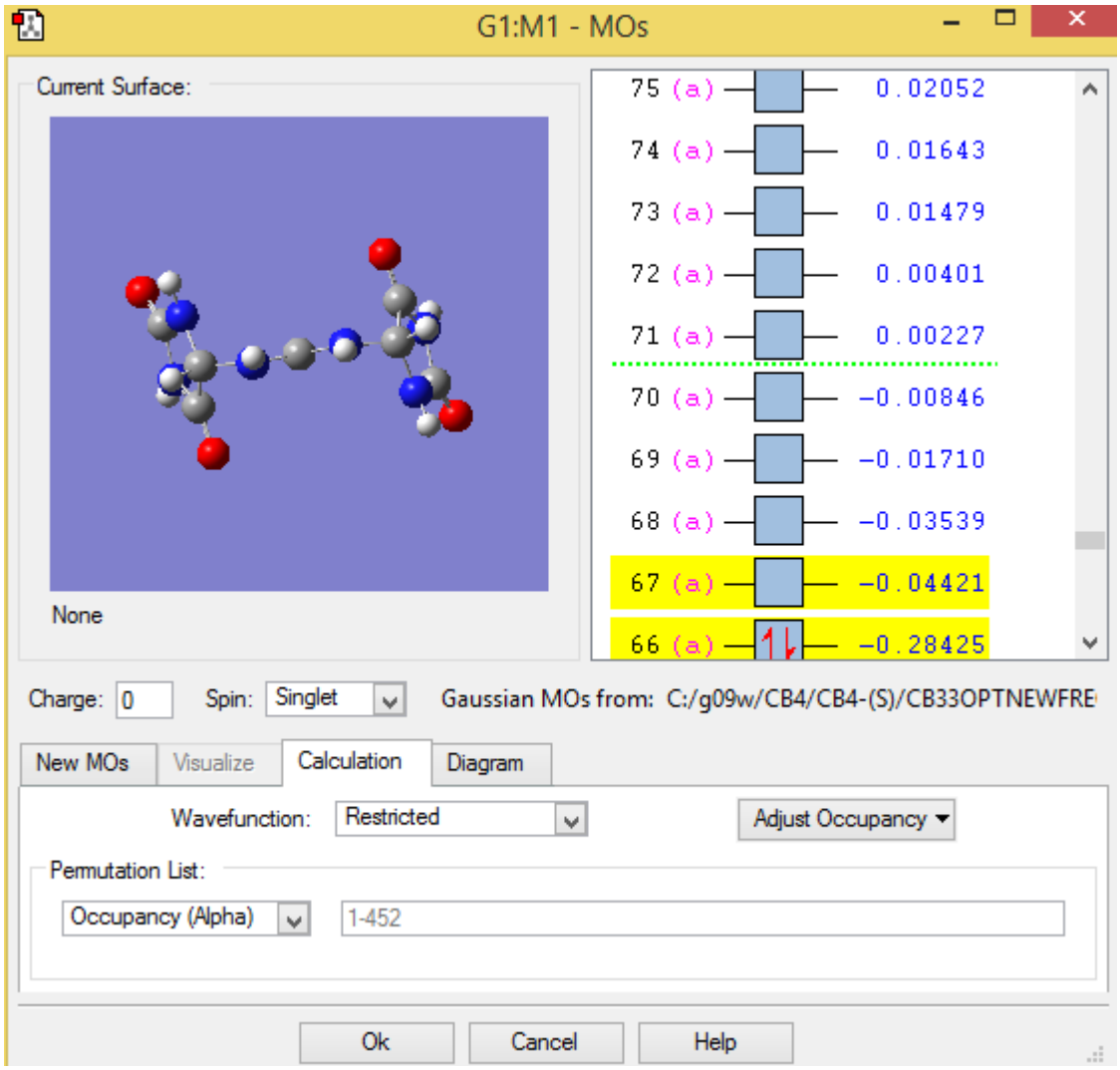

Fig. 19**S**. Graph representing *HOMO*/*LUMO* at B3LYP/6–311++G(d,p) of **2**.

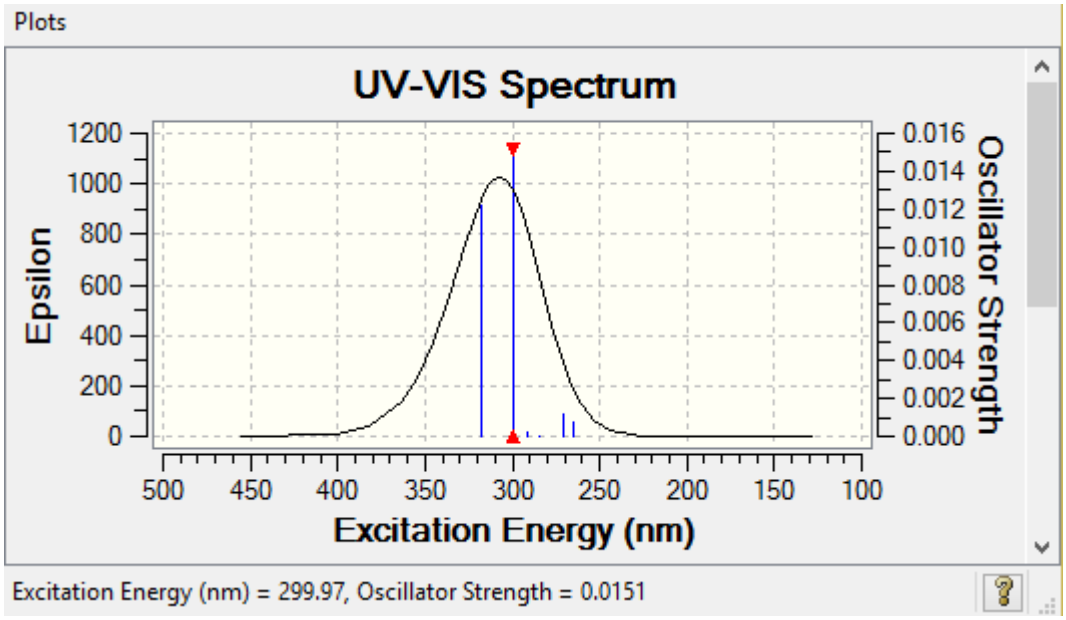

Fig. 20**S**. UV–visible spectrum of **2** in chloroform at B3LYP/6–31+G(d,p).

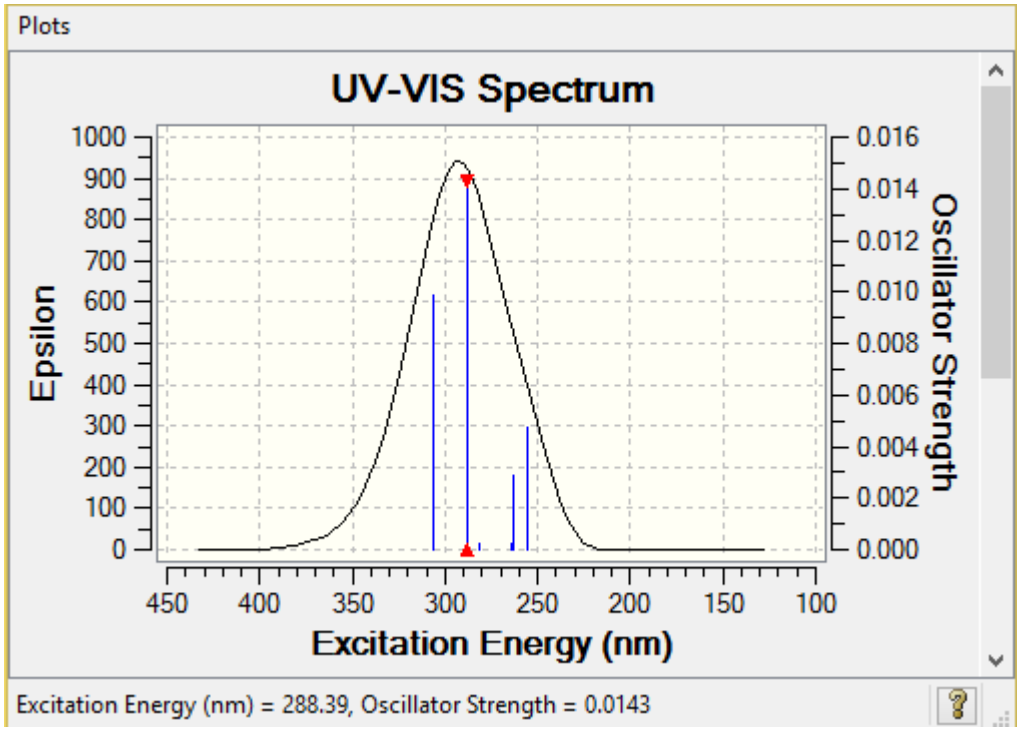

Fig. 21**S**. UV–visible spectrum of **2** in ethanol at B3LYP/6–31+G(d,p).

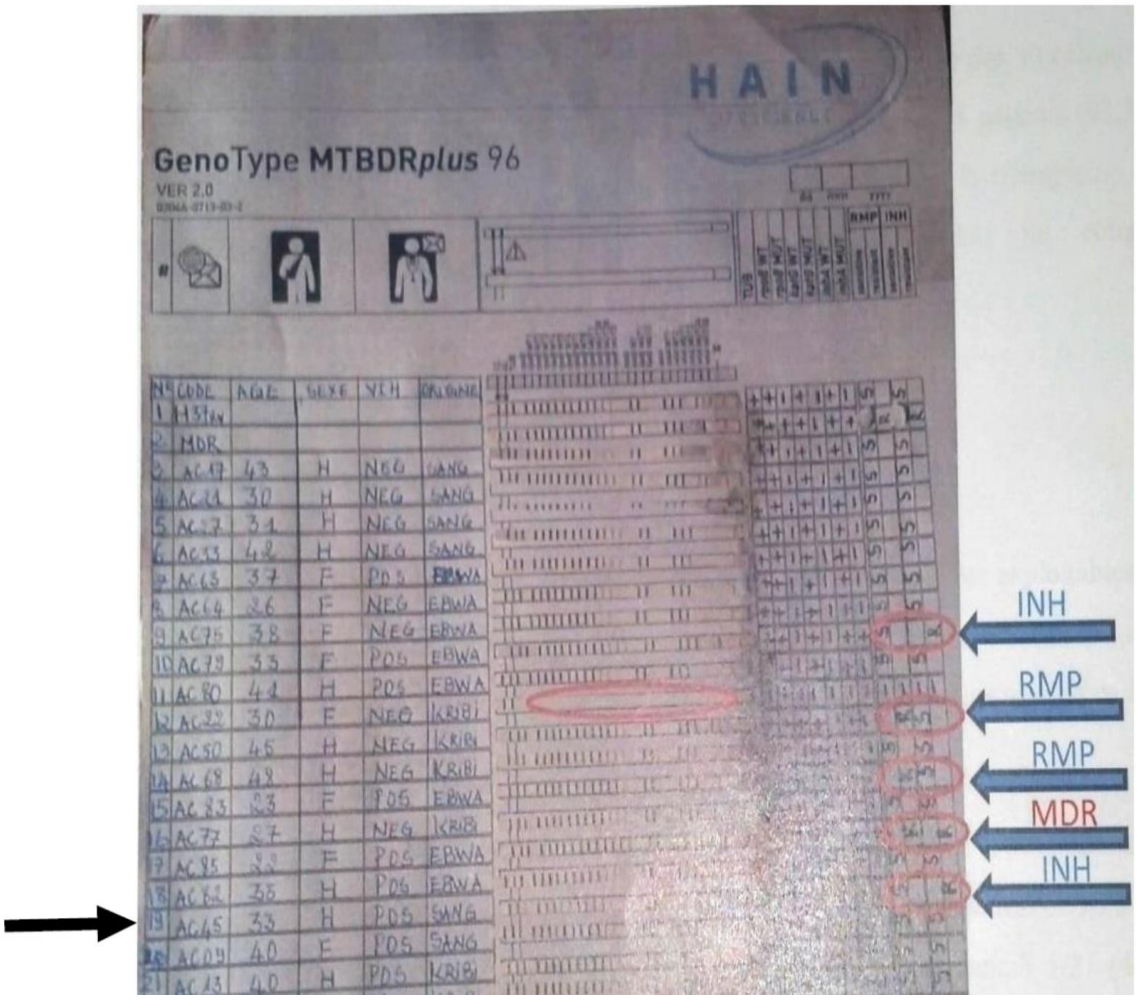

Figure 20S. Genotype profile of *M. tuberculosis* codified AC 45

Table 1S. Cartesian coordinates for the optimized geometry of **2** at B3LYP/6–31G(d,).

1	6	0	1.434569	-1.339099	2.830396
2	6	0	-0.420739	-0.764138	1.342043
3	6	0	-2.222443	-0.003300	-0.128649
4	8	0	-0.760548	-1.942274	1.230162
5	7	0	0.703007	-0.385022	2.041291
6	7	0	-1.137990	0.266074	0.776626
7	1	0	2.352516	-0.837872	3.155243
8	1	0	-0.761893	1.204585	0.775831
9	1	0	-2.719530	0.954607	-0.314930
10	1	0	0.879834	0.593520	2.224157
11	6	0	1.838152	-2.610815	2.035658
12	7	0	0.719707	-1.916040	3.960713
13	6	0	0.813877	-3.281015	4.009860
14	7	0	1.489218	-3.669082	2.837223
15	6	0	-3.276073	-0.985328	0.452073
16	6	0	-2.662800	-1.740049	-1.657449
17	7	0	-1.864519	-0.663834	-1.376486
18	7	0	-3.499042	-1.909805	-0.537783
19	8	0	0.410375	-4.035840	4.876351
20	8	0	2.395270	-2.644256	0.958801
21	8	0	-3.819981	-0.906133	1.533282
22	8	0	-2.675978	-2.429868	-2.661120
23	1	0	-4.120006	-2.703453	-0.444222
24	1	0	1.601137	-4.640421	2.576068
25	1	0	0.507132	-1.392721	4.799269
26	1	0	-1.365858	-0.195343	-2.120851

C	0	-2.427649	-0.291600	1.079701
C	0	0.000001	-0.000012	0.982576
C	0	2.427650	0.291588	1.079708
O	0	0.000001	-0.000008	-0.248680
N	0	-1.141158	-0.225628	1.719012
N	0	1.141160	0.225593	1.719014
H	0	-3.138901	-0.626500	1.842161
H	0	1.132994	0.088874	2.720759
H	0	3.138899	0.626480	1.842173
H	0	-1.132997	-0.088895	2.720755
C	0	-2.475696	-1.302785	-0.097985
N	0	-2.883694	0.931266	0.433073
C	0	-3.335065	0.722771	-0.842558
N	0	-3.073425	-0.629388	-1.134057
C	0	2.475691	1.302788	-0.097968
C	0	3.335070	-0.722756	-0.842566
N	0	2.883707	-0.931267	0.433061
N	0	3.073434	0.629412	-1.134044
O	0	-3.862625	1.519774	-1.597439
O	0	-2.109379	-2.458796	-0.074082
O	0	2.109360	2.458794	-0.074049
O	0	3.862625	-1.519745	-1.597466
H	0	3.218874	1.019888	-2.056325
H	0	-3.218896	-1.019863	-2.056334
H	0	-3.188304	1.744181	0.951347
H	0	3.188301	-1.744196	0.951322

E(RB3LYP/6–31G(d)) = -976.311577711

Table 2S. Shielding tensors (σ) at B3LYP/6-31g(d,p) and experimental chemical shifts (δ_{exp}) of carbons of compound **2**.

Position	σ (ppm)	δ_{exp} (ppm)	δ_{calc} (ppm)
C(2)	44.7895	156.8	156.1
C(4)	28.2611	173.6	174.4
C(5)	126.3013	62.4	61.7
C(7)	45.0912	157.4	157.0

Table 3S. Shielding tensors (σ) at MPW1PW91/6–31+G(d,p) and experimental chemical shifts (δ_{exp}) of carbons of compound **2**.

Position	σ (ppm)	δ_{exp} (ppm)	δ_{calc} (ppm)
C(2)	44.9493	156.8	157.0
C(4)	28.4488	173.6	174.6
C(5)	129.3335	62.4	62.7
C(7)	45.5375	157.4	158.0

Table 4S. Electronic and thermodynamic parameters of **2** at B3LYP/6–311++G(d,p).

		E (Thermal)	C_V	S
		kcal mol	cal mol K^{-1}	cal mol K^{-1}
Total		126.022	58.650	126.868
Electronic		0.000	0.000	0.000
Translational		0.889	2.981	42.521
Rotational		0.889	2.981	33.260
Vibrational		124.245	52.689	51.087
Vibration	1	0.594	1.981	5.206
Vibration	2	0.595	1.979	4.928
Vibration	3	0.596	1.977	4.748
Vibration	4	0.601	1.960	3.772
Vibration	5	0.603	1.952	3.530
Vibration	6	0.615	1.913	2.805
Vibration	7	0.623	1.886	2.498
Vibration	8	0.628	1.870	2.353
Vibration	9	0.628	1.870	2.350
Vibration	10	0.647	1.810	1.956
Vibration	11	0.659	1.774	1.781
Vibration	12	0.696	1.664	1.389
Vibration	13	0.726	1.579	1.174
Vibration	14	0.758	1.492	1.001
Vibration	15	0.762	1.481	0.981
Vibration	16	0.783	1.425	0.889
Vibration	17	0.785	1.422	0.884
Vibration	18	0.798	1.389	0.835
Vibration	19	0.819	1.337	0.764
Vibration	20	0.831	1.308	0.727
Vibration	21	0.883	1.188	0.592
Vibration	22	0.905	1.141	0.546

Vibration	23	0.942	1.063	0.476
Vibration	24	0.949	1.050	0.465

Table 5S. Excitation energies and oscillator strengths of **2** in $CHCl_3$ at B3LYP/6–31+G(d,p).

Excited State 1: Singlet-A 3.8954 eV 318.29 nm f = 0.0122 <S**2>=0.000

H–3 → L 0.14458

H–2 → L 0.18828

H–1 → L 0.63487

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -976.021677358

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.1332 eV 299.97 nm f=0.0151 <S**2>=0.000

H–5 → L -0.12204

H–3 → L 0.26295

H–2 → L 0.55559

H–1 → L -0.22816

H–1 → L+2 -0.17440

Excited State 3: Singlet-A 4.2614 eV 290.95 nm f=0.0002 <S**2>=0.000

H → L 0.15406

H → L 0.67051

H → L 0.10053

Excited State 4: Singlet-A 4.3524 eV 284.86 nm f=0.0000 <S**2>=0.000

H → L 0.68775

H → L -0.14940

Excited State 5: Singlet-A 4.5856 eV 270.38 nm f=0.0012 <S**2>=0.000

H–5 → L 0.50163

H–5 → L+2 0.11853

H–4 → L -0.19248

H–2 → L 0.17979

H–1 → L+2 0.34446

Excited State 6: Singlet-A 4.6727 eV 265.34 nm f=0.0007 <S**2>=0.000

H–6 → L -0.12195

H–5 → L -0.10366

H–4 → L 0.30015

H–3 → L 0.48758

H–2 → L -0.25917

H–1 → L -0.10994

H–1 → L+2 0.21890

Table 6S. Excitation energies and oscillator strengths of **2** in EtOH at B3LYP/6–31+G(d,p).

Excited State 1: Singlet-A 4.0514 eV 306.03 nm f=0.0099 <S**2>=0.000

H–8 → L -0.11109

H–3 → L 0.10020

H–2 → L -0.18726

H → L 0.63954

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -976.030682697

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 4.2992 eV 288.39 nm f = 0.0143 <S**2>=0.000

H–4 → L 0.11974

H–3 → L -0.12646

H–2 → L 0.59334

H → L 0.17578

H → L+2 0.22259

Excited State 3: Singlet-A 4.4026 eV 281.62 nm f=0.0002 <S**2>=0.000

H–1 → L+2 0.68009

Excited State 4: Singlet-A 4.6842 eV 264.68 nm f=0.0002 <S**2>=0.000

H–5 → L 0.14469

H–1 → L 0.67282

Excited State 5: Singlet-A 4.7157 eV 262.92 nm f=0.0029 <S**2>=0.000

H–5 → L 0.25665

H–4 → L 0.29579

H–4 → L+2 0.12092

H–3 → L 0.19842

H–2 → L -0.20075

H–2 → L+2 0.14680

H–1 → L -0.12424

H → L -0.14877

H → L+2 0.38483

Excited State 6: Singlet-A 4.8542 eV 255.42 nm f=0.0047 <S**2>=0.000

H–5 → L 0.45500

H–4 → L 0.29489

H–3 → L -0.15182

H–2 → L+2 -0.12704

H–1 → L -0.10526

H → L 0.12310

H → L+2 -0.33526