

# Supplementary Information

## Correlation between Electrochemical and Theoretical Studies on the Leishmanicidal Activity of Twelve Morita-Baylis-Hillman Adducts

Yen G. de Paiva,<sup>a,b</sup> Antônio A. de Souza,<sup>b,c</sup> Claudio G. Lima-Junior,<sup>a</sup> Fábio P. L. Silva,<sup>a</sup>  
Edilson B. A. Filho,<sup>a,d</sup> Camila C. de Vasconcelos,<sup>b</sup> Fabiane C. de Abreu,<sup>b</sup>  
Marília O. F. Goulart<sup>\*a,b</sup> and Mário L. A. A. Vasconcellos<sup>\*a</sup>

<sup>a</sup>Departamento de Química, Universidade Federal da Paraíba, Campus I, 58059-900 João Pessoa-PB, Brazil

<sup>b</sup>Instituto de Química e Biotecnologia, Universidade Federal de Alagoas, 57072-970 Maceió-AL, Brazil

<sup>c</sup>Departamento de Química, Instituto Federal de Alagoas, 57020-600 Maceió-AL, Brazil

<sup>d</sup>Colegiado de Ciências Farmacêuticas, Universidade Federal do Vale do São Francisco, 56304-917 Petrolina-PE, Brazil

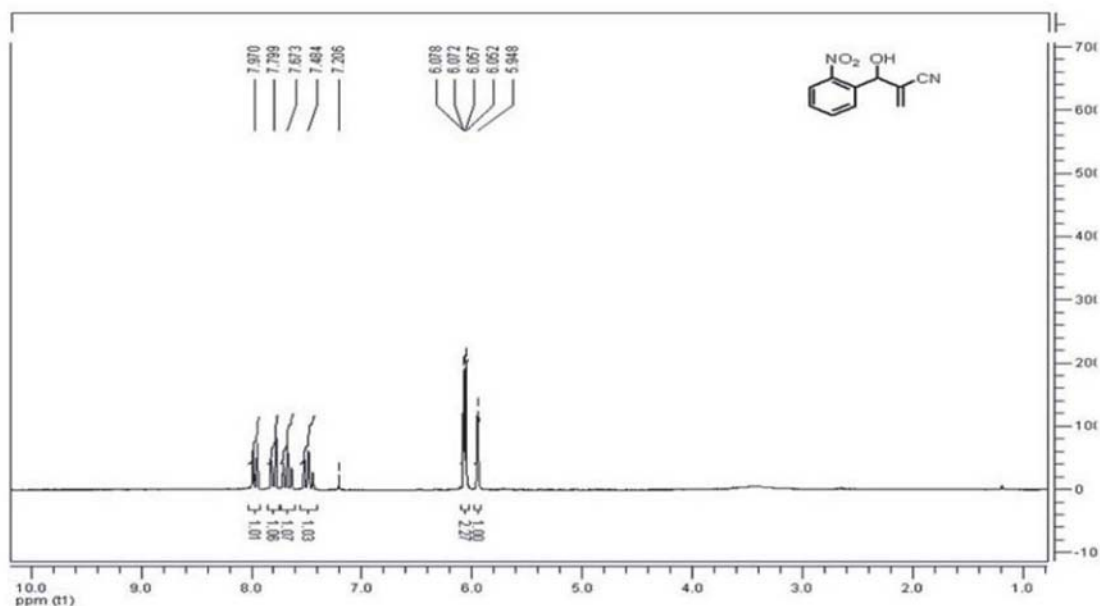
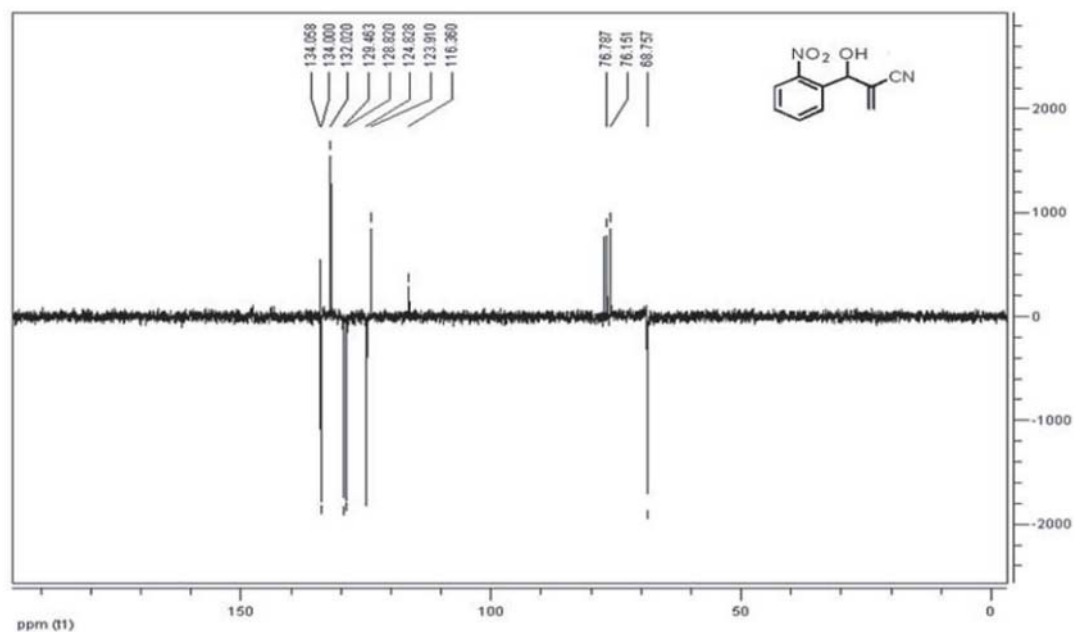
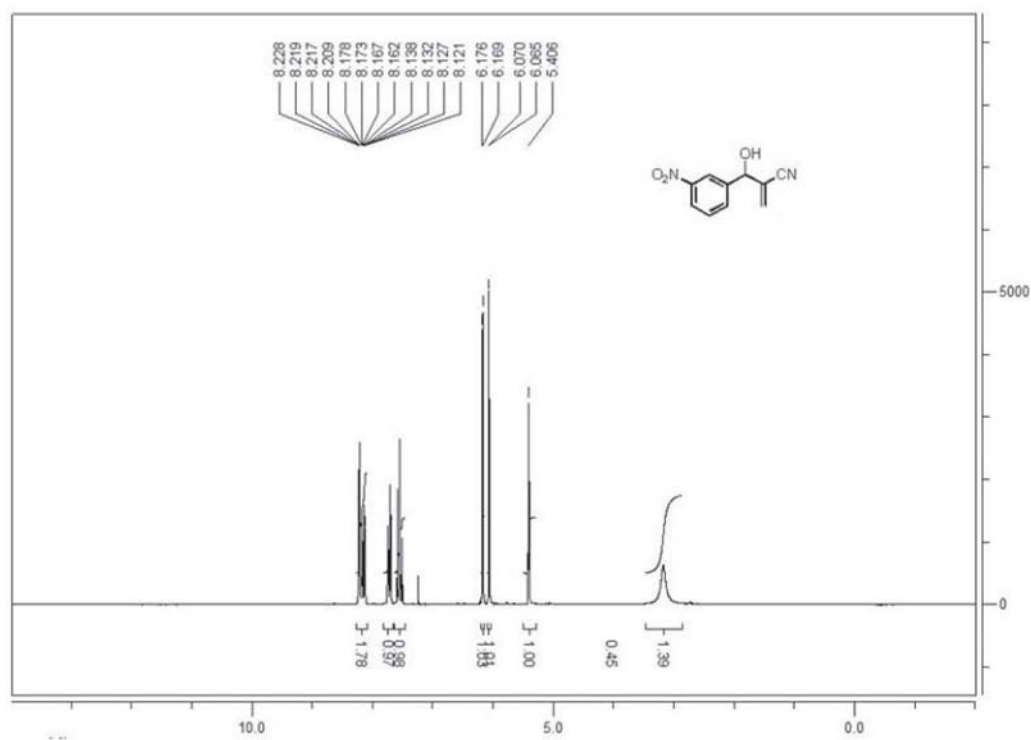


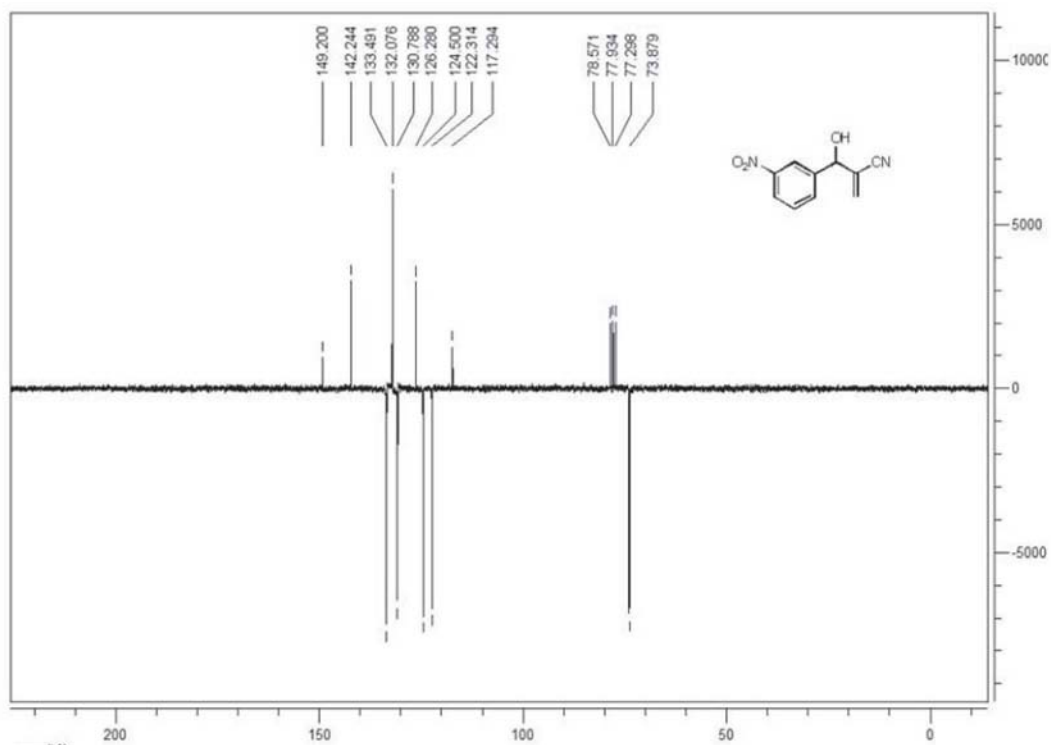
Figure S1. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) spectrum of 2-[hydroxy(2-nitrophenyl)methyl]acrylonitrile (Ia).



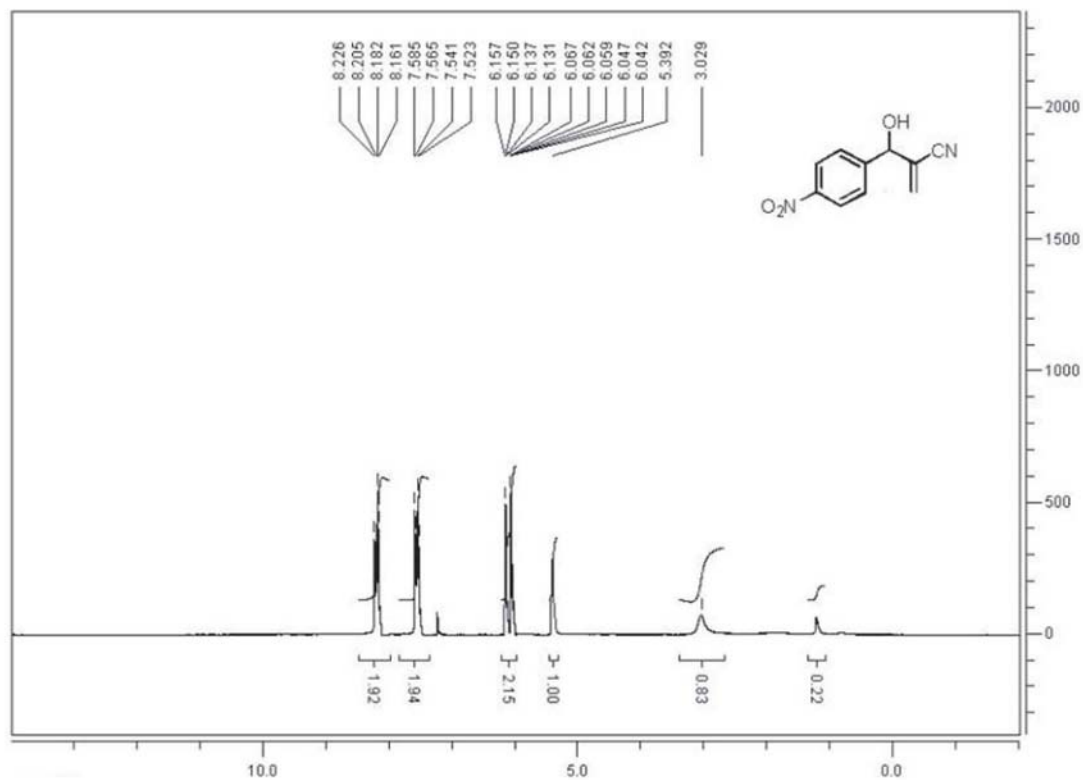
**Figure S2.** <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) spectrum of 2-[hydroxy(2-nitrophenyl)methyl]acrylonitrile (Ia).



**Figure S3.** <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) spectrum of 2-[hydroxy(3-nitrophenyl)methyl]acrylonitrile (Ib).



**Figure S4.** <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) spectrum of 2-[hydroxy(3-nitrophenyl)methyl]acrylonitrile (Ib).



**Figure S5.** <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) spectrum of 2-[hydroxy(4-nitrophenyl)methyl]acrylonitrile (Ic).

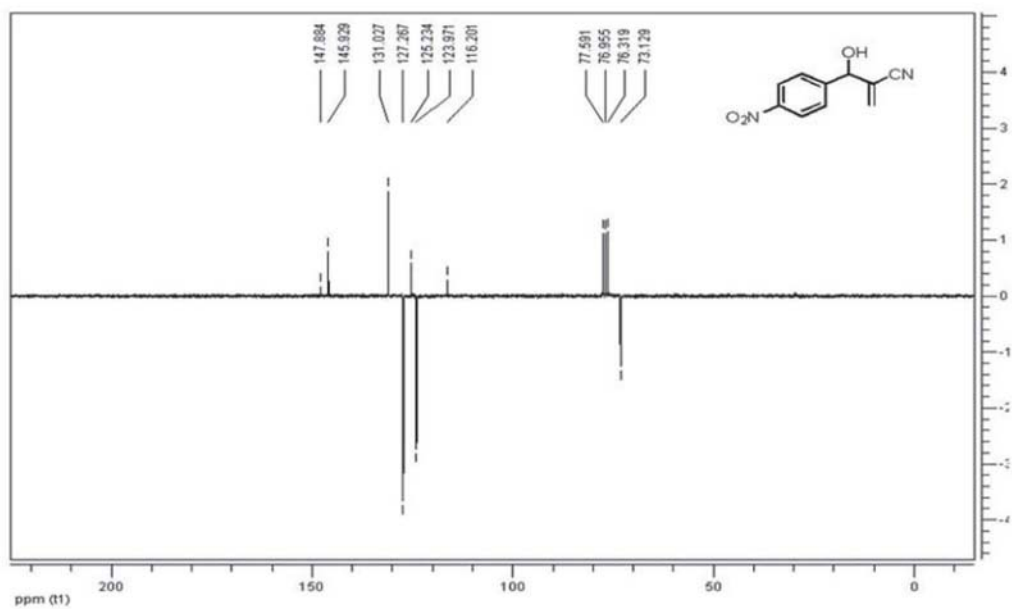


Figure S6. <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) spectrum of 2-[hydroxy(3-nitrophenyl)methyl]acrylonitrile (Ic).

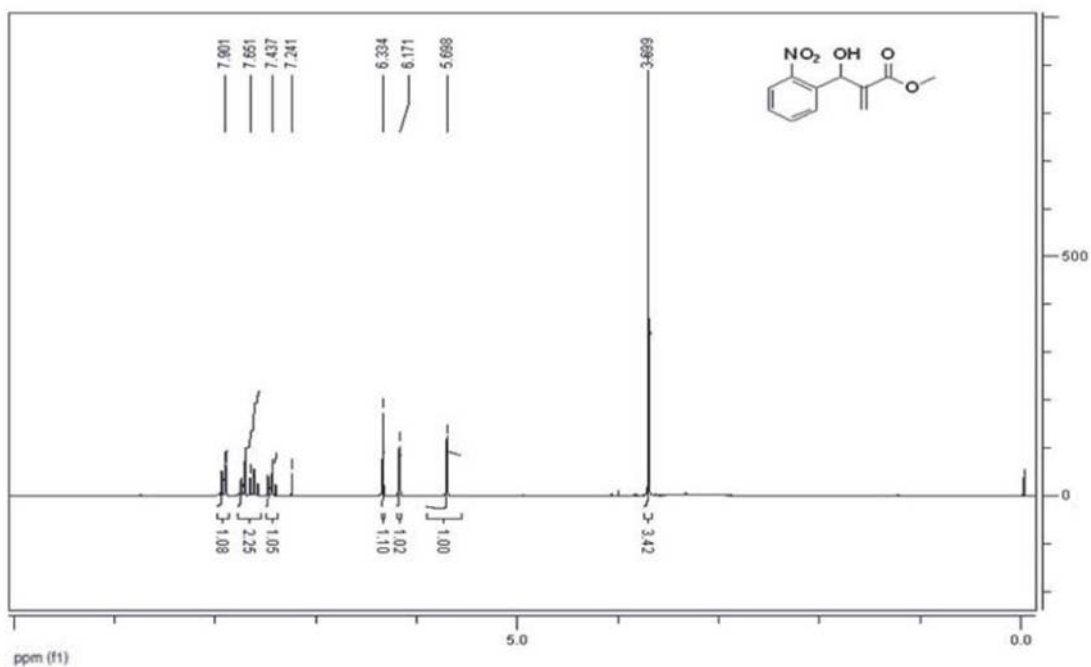
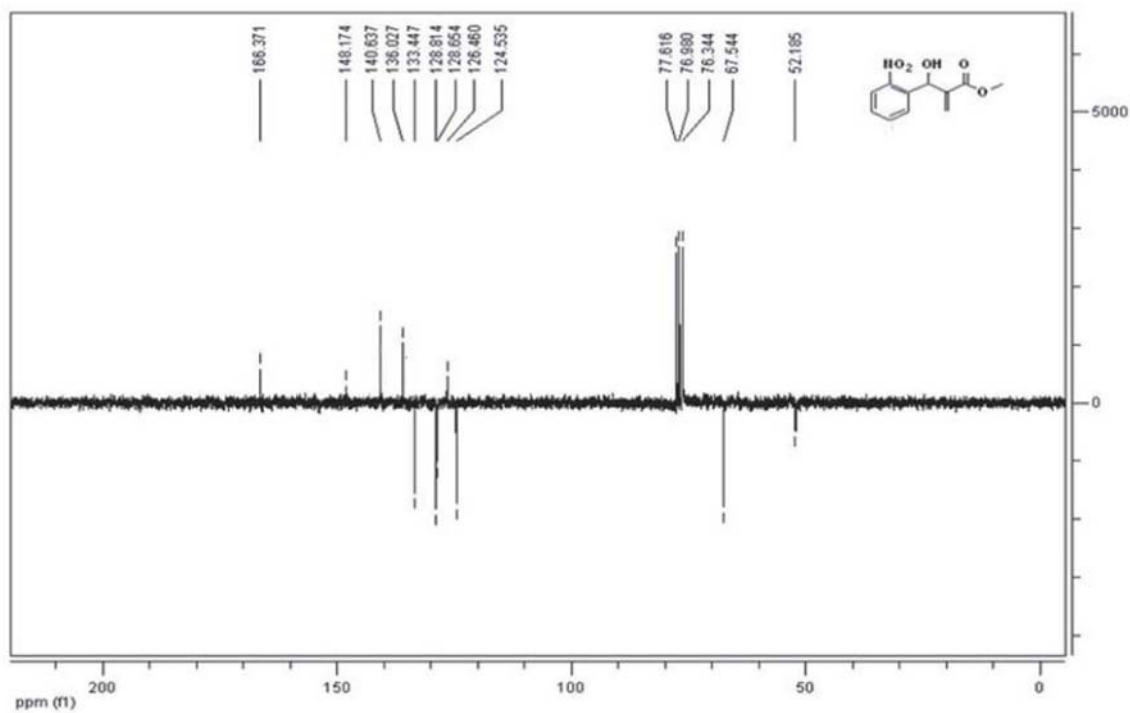
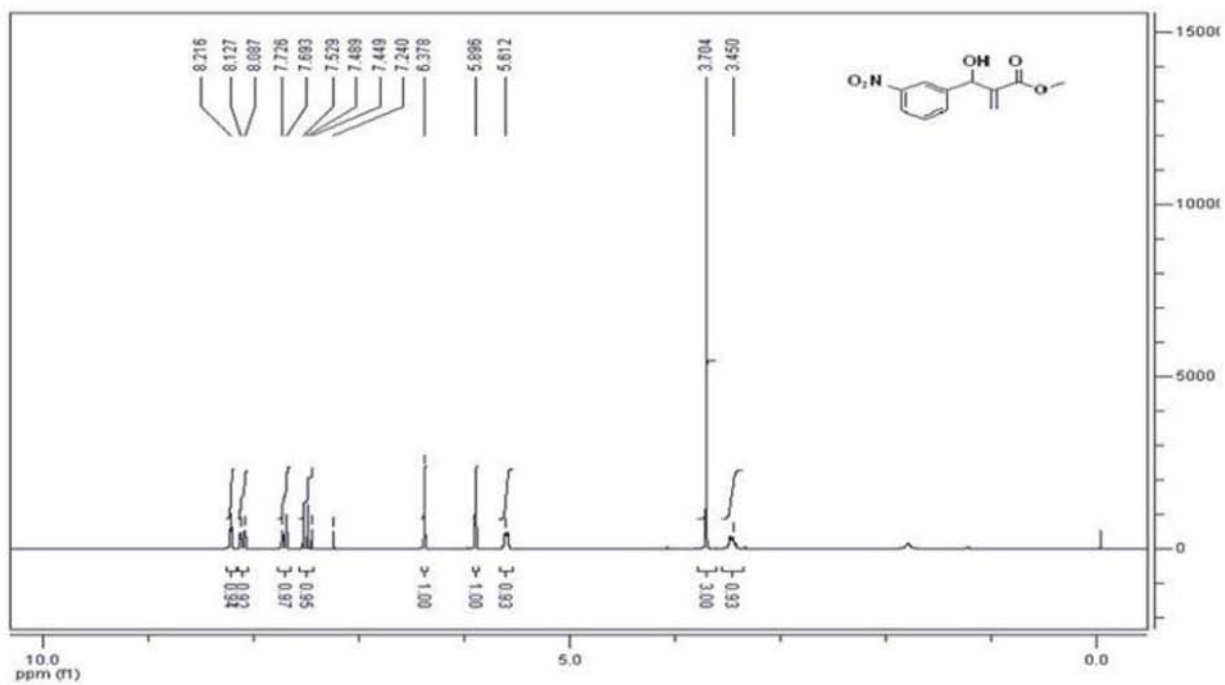


Figure S7. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) spectrum of methyl 2-[hydroxy(2-nitrophenyl)methyl]acrylate (IIa).



**Figure S8.** <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>) spectrum of methyl 2-[hydroxy(2-nitrophenyl)methyl]acrylate (IIa).



**Figure S9.** <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>) spectrum of methyl 2-[hydroxy(3-nitrophenyl)methyl]acrylate (IIb).

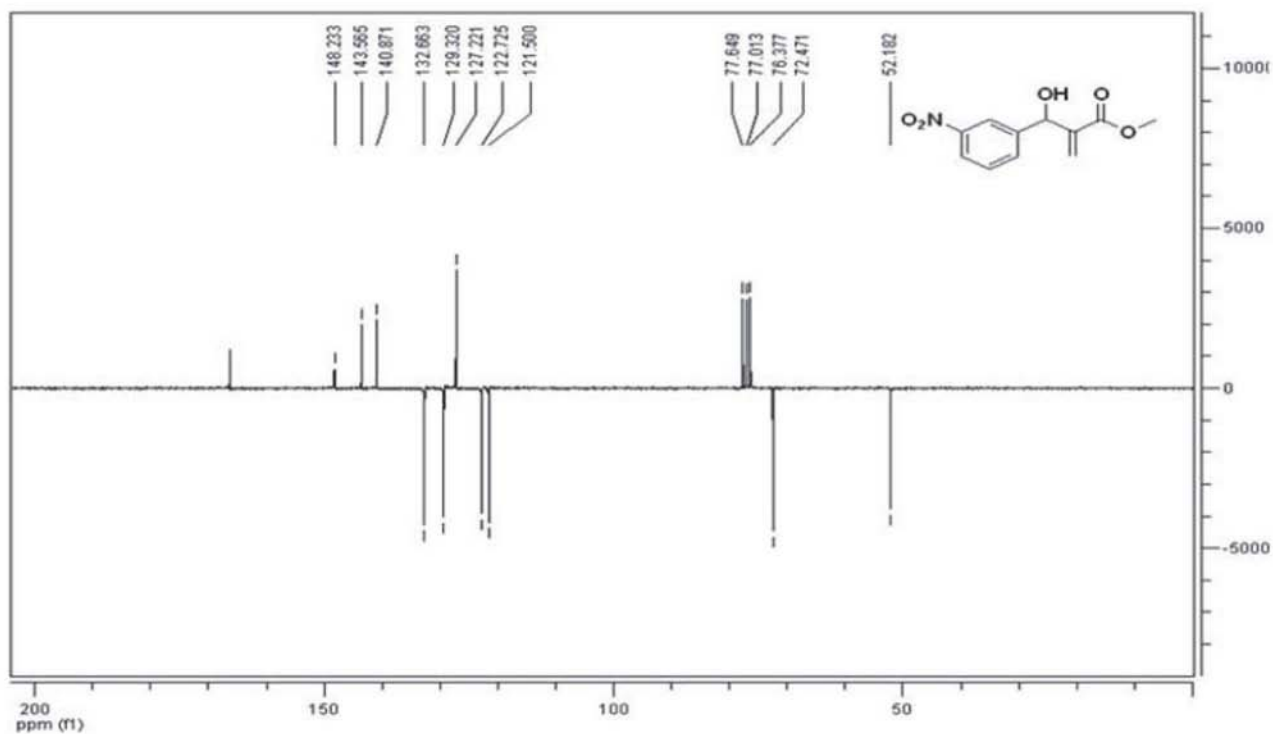


Figure S10.  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) spectrum of methyl 2-[hydroxy(3-nitrophenyl)methyl]acrylate (IIb).

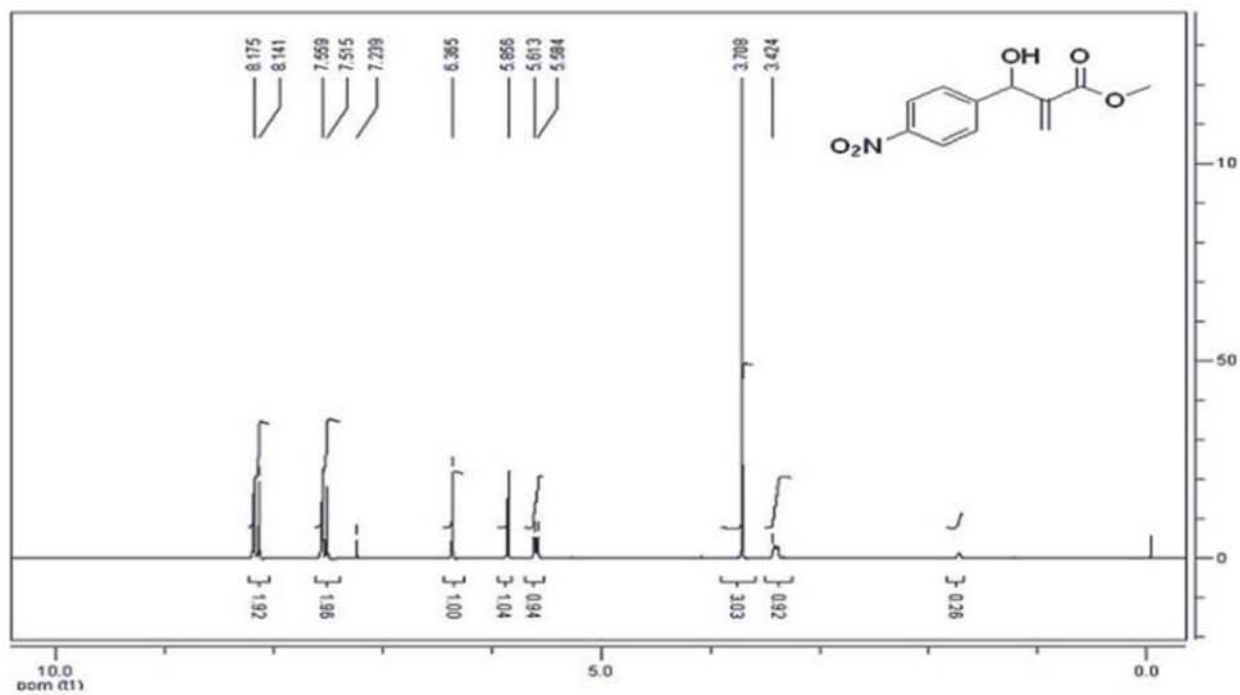
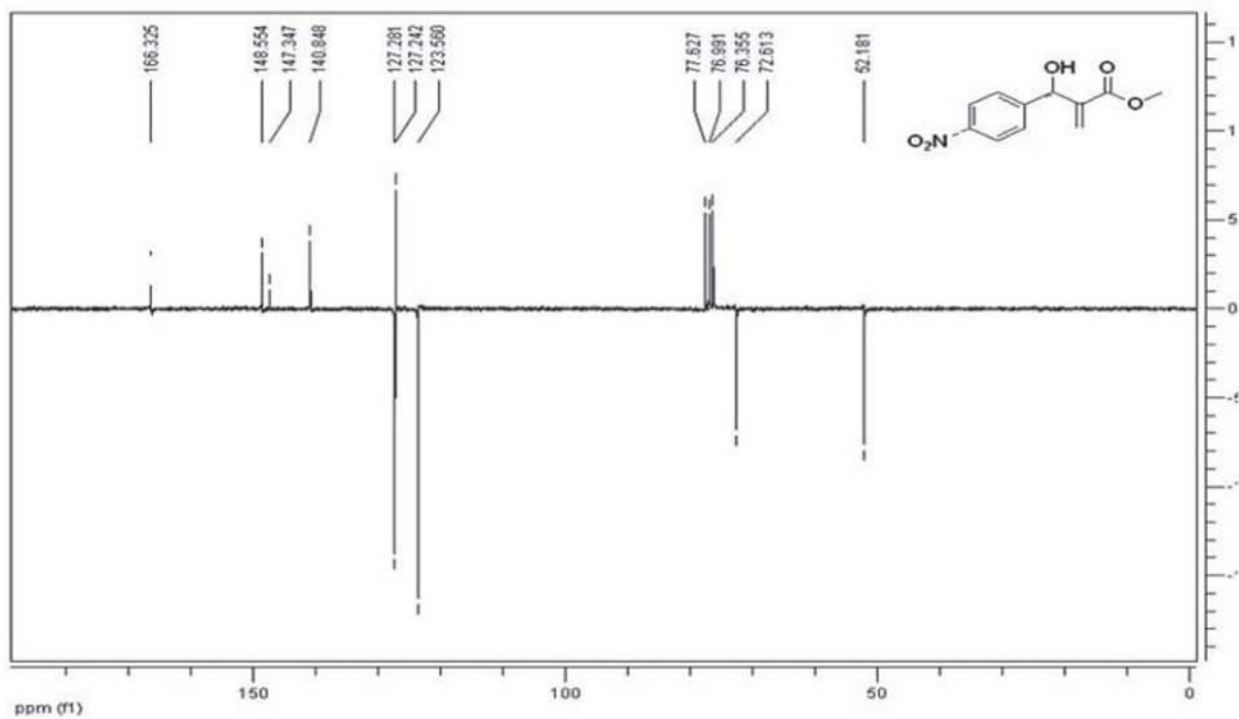
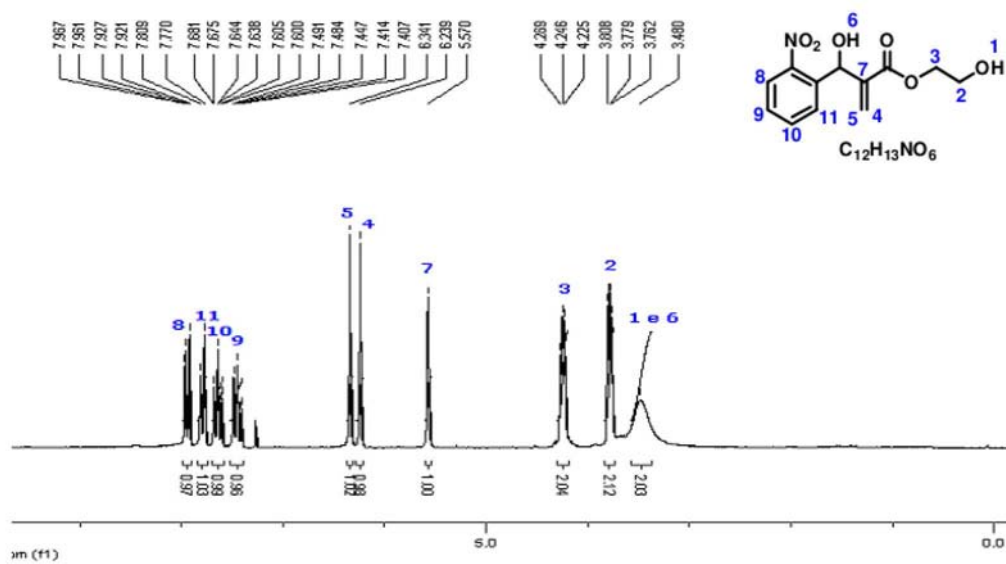


Figure S11.  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) spectrum of methyl 2-[hydroxy(4-nitrophenyl)methyl]acrylate (IIc).



**Figure S12.**  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) spectrum of methyl 2-[hydroxy(4-nitrophenyl)methyl]acrylate (IIc).



**Figure S13.**  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(2-nitrophenyl)hydroxyethyl]propanoate (IIIa).

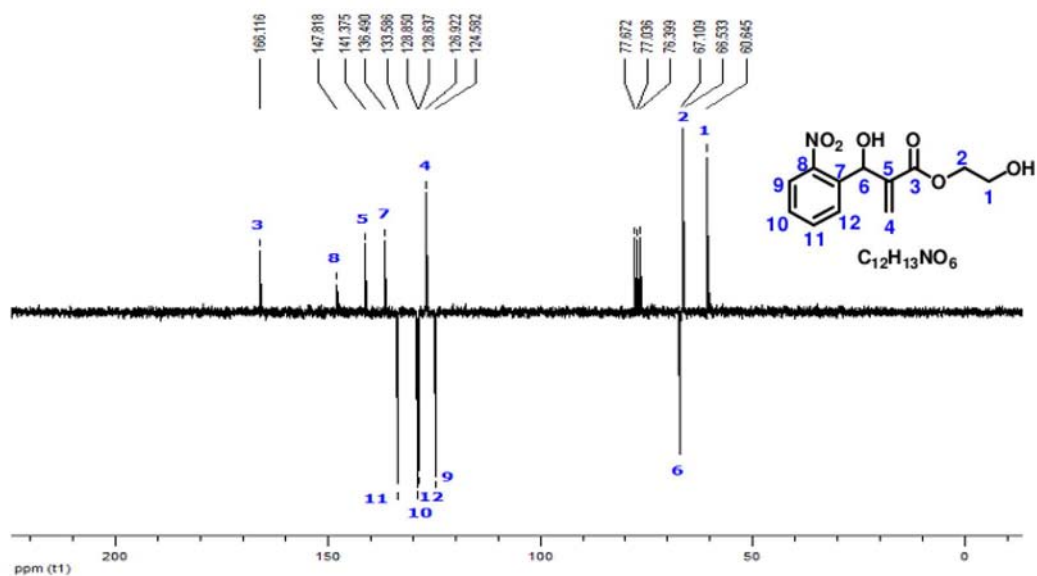


Figure S14.  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(2-nitrophenyl)hydroxyethyl]propanoate (IIIa).

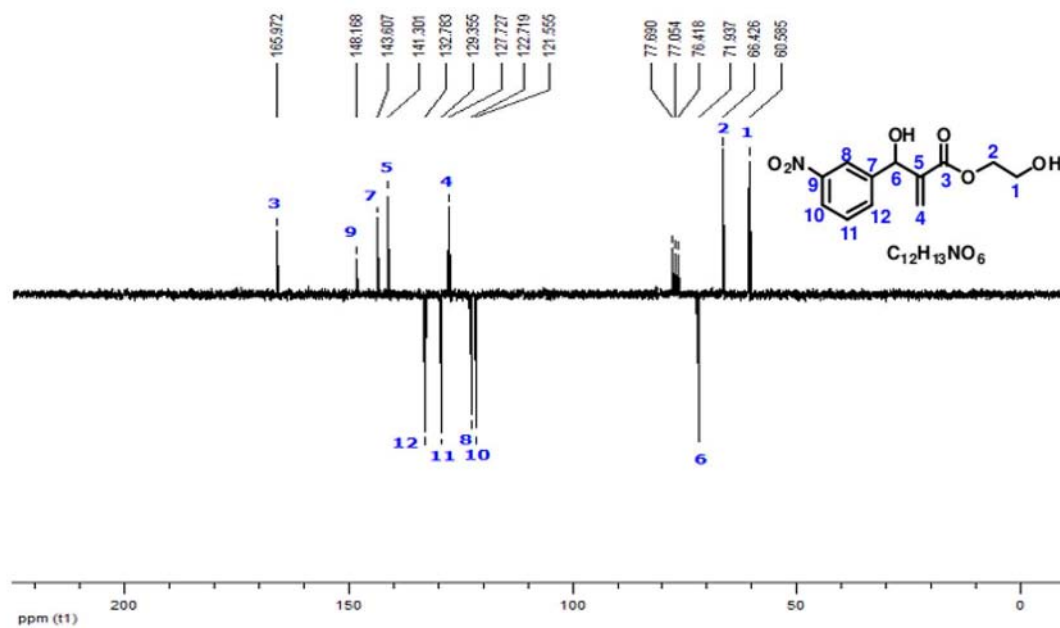
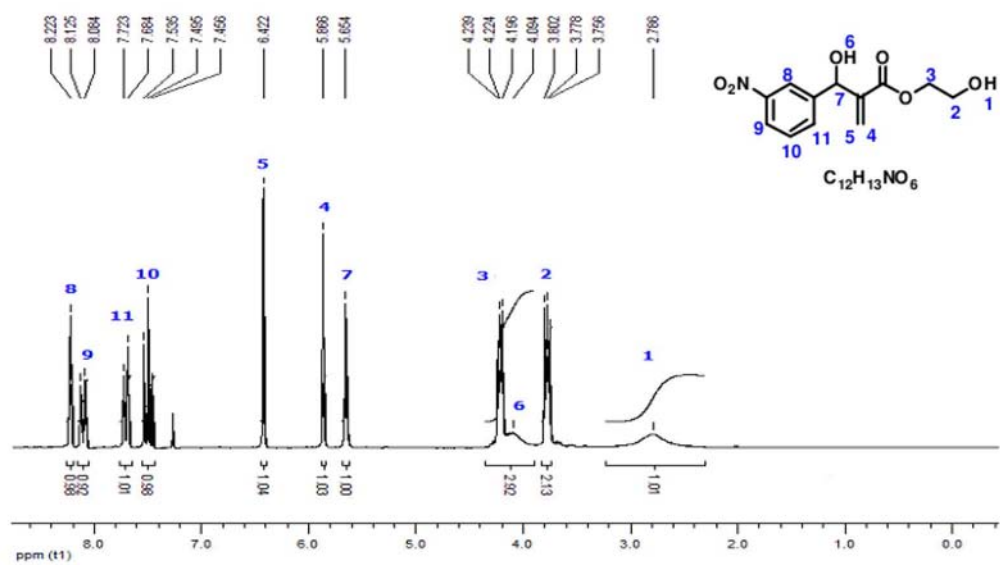
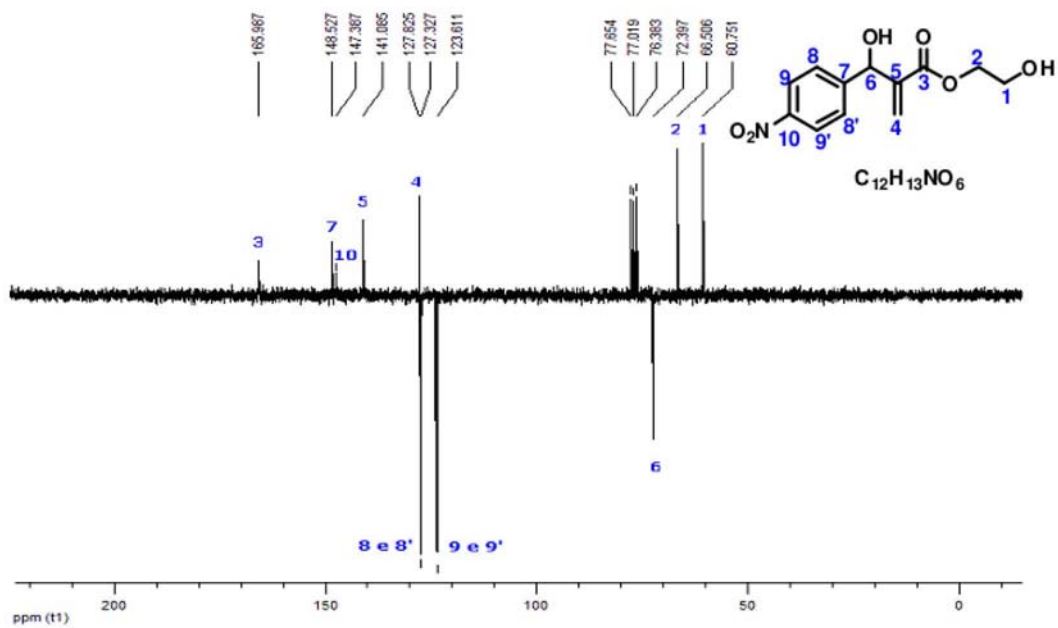


Figure S15.  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(3-nitrophenyl)hydroxyethyl]propanoate (IIIb).





**Figure S16.**  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(3-nitrophenyl)hydroxyethyl]propanoate (IIIb).



**Figure S17.**  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(4-nitrophenyl)hydroxyethyl]propanoate (IIIc).

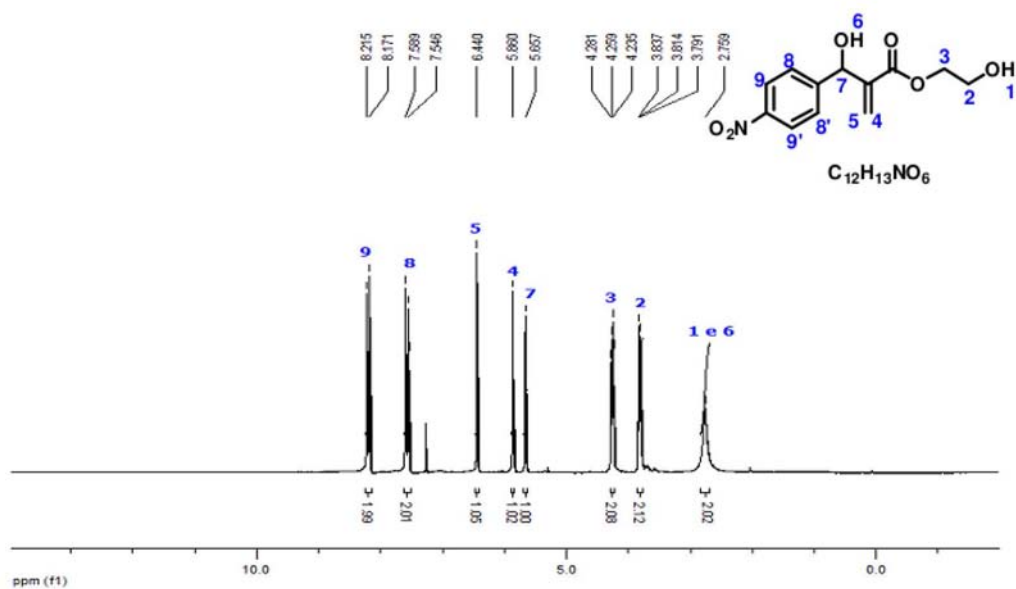


Figure S18.  $^1H$  NMR (200 MHz,  $CDCl_3$ ) spectrum of 2-[hydroxy(4-nitrophenyl)hydroxyethyl]propanoate (IIIc).

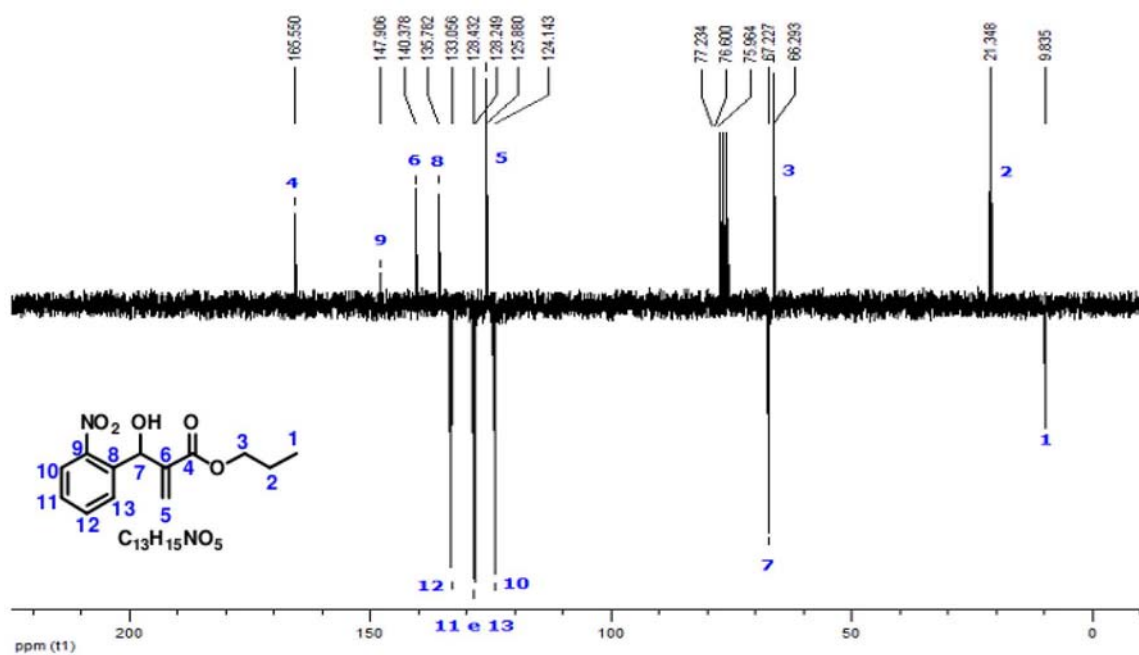
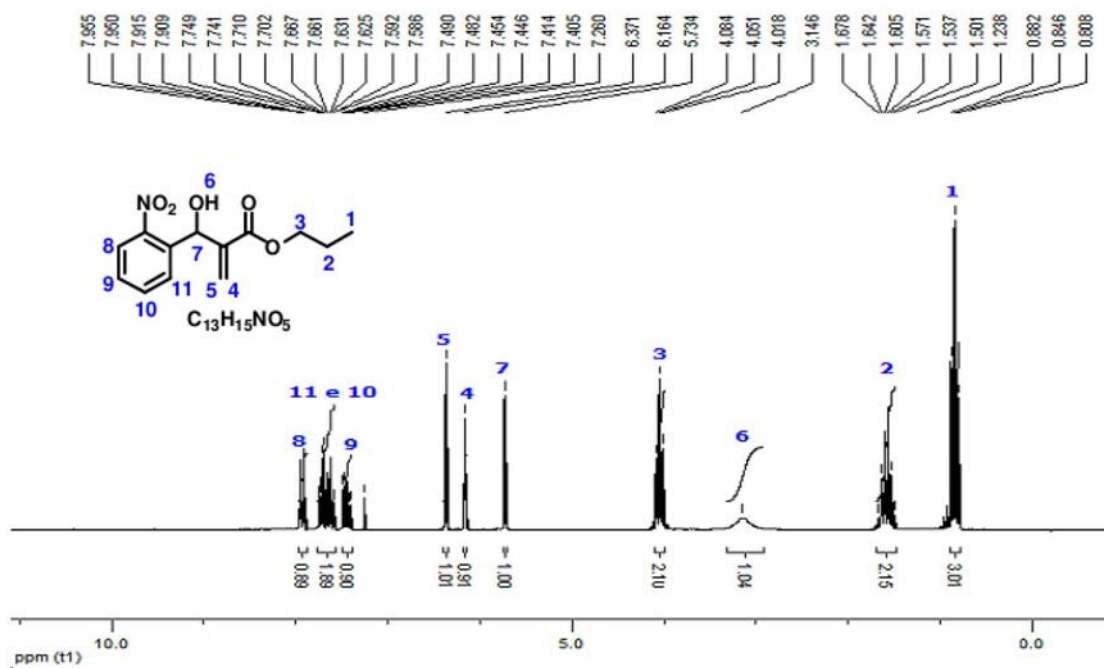
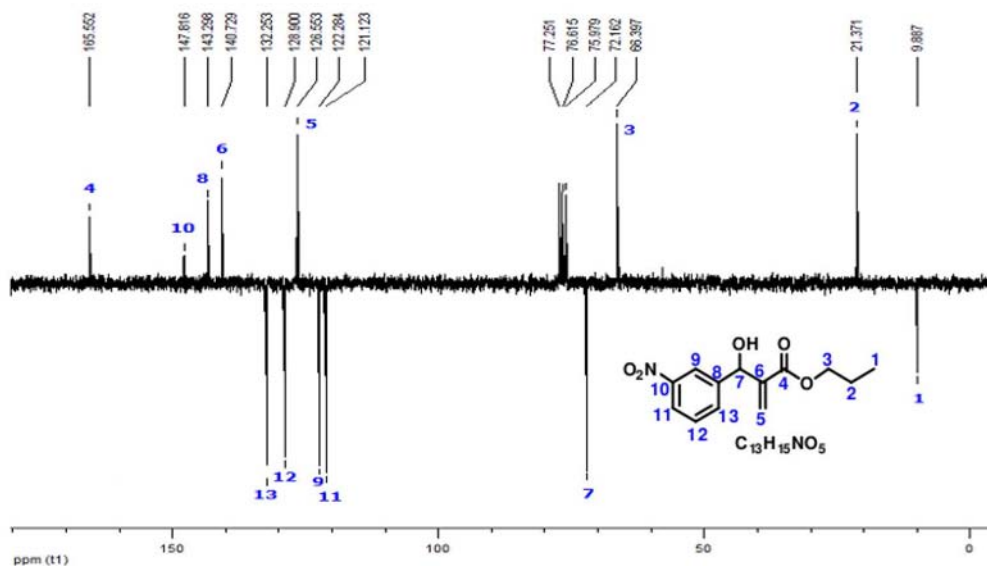


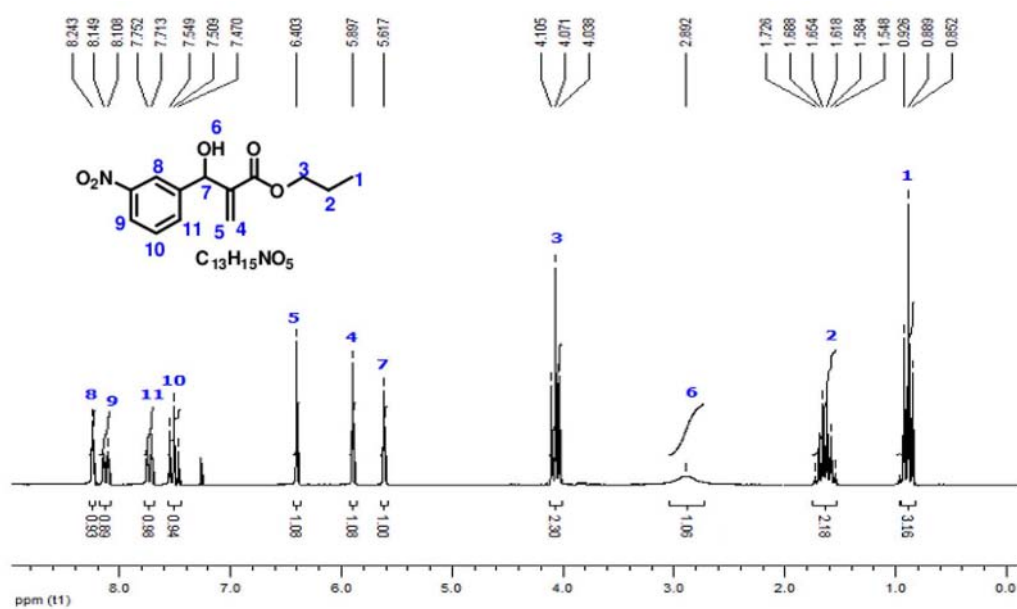
Figure S19.  $^{13}C$  NMR (50 MHz,  $CDCl_3$ ) spectrum of 2-[hydroxy(2-nitrophenyl)propyl]propanoate (IVa).



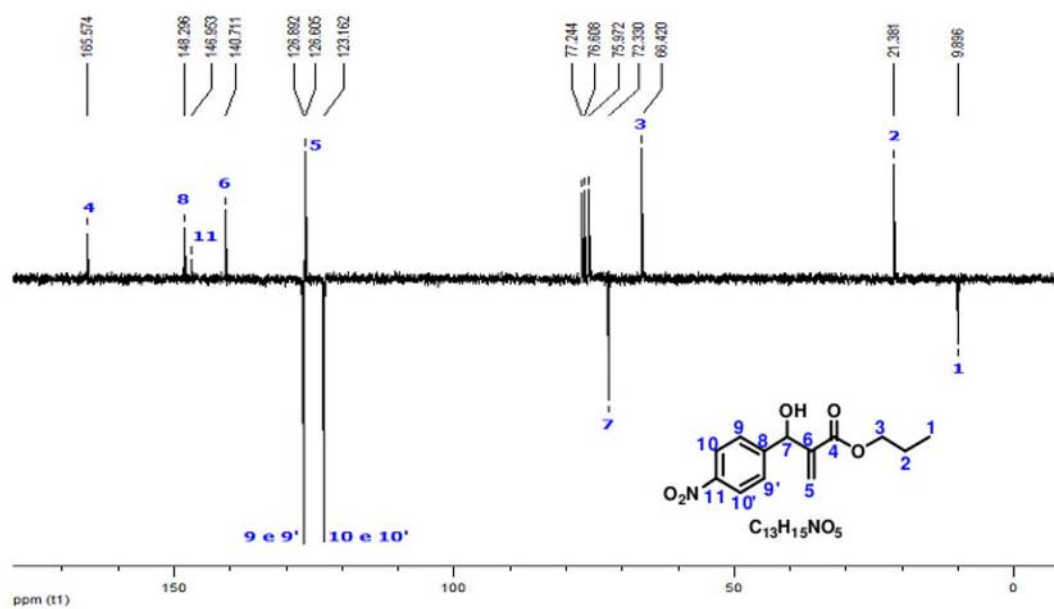
**Figure S20.**  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(2-nitrophenyl)propyl]propanoate (IVa).



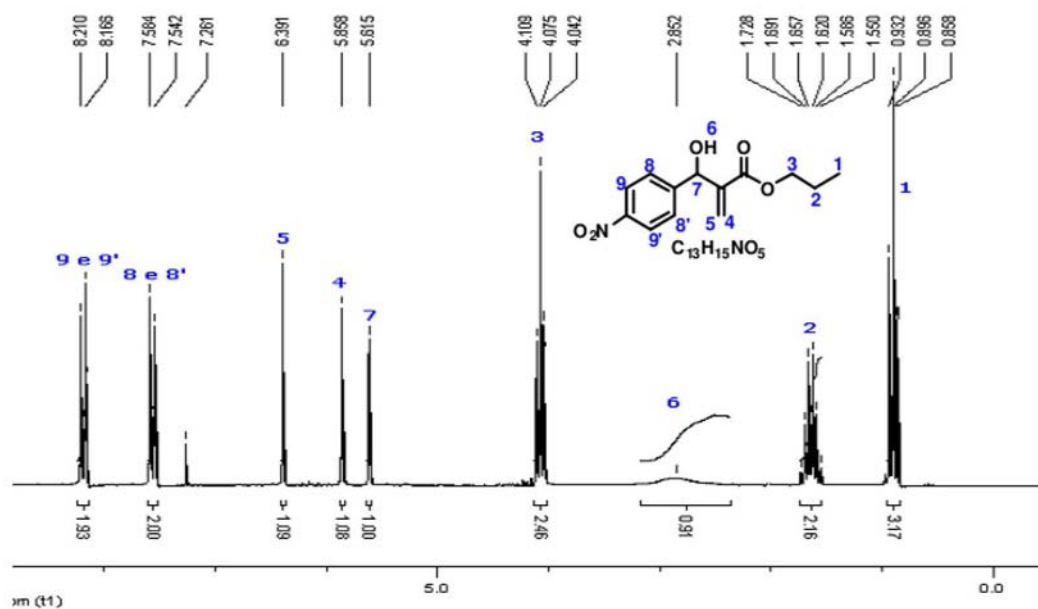
**Figure S21.**  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(3-nitrophenyl)propyl]propanoate (IVb).



**Figure S22.**  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(3-nitrophenyl)propyl]propanoate (IVb).



**Figure S23.**  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(4-nitrophenyl)propyl]propanoate (IVc).



**Figure S24.**  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ) spectrum of 2-[hydroxy(4-nitrophenyl)propyl]propanoate (IVc).

Geometrical parameters for the conformational minima of MBHA Ia to IVc

MBHA Ia

C	1	B1				B3	1.38760511
C	2	B2	1	A1		B4	1.38941486
C	3	B3	2	A2	1	B5	1.38427091
C	4	B4	3	A3	2	B6	1.53437363
C	1	B5	2	A4	3	B7	1.51931471
C	5	B6	4	A5	3	B8	1.32347649
C	7	B7	5	A6	4	B9	1.44937814
C	8	B8	7	A7	5	B10	1.13786359
C	8	B9	7	A8	5	B11	1.39607244
N	10	B10	8	A9	7	B12	1.46101920
O	7	B11	5	A10	4	B13	1.19261989
N	6	B12	1	A11	2	B14	1.20058064
O	13	B13	6	A12	1	B15	1.07205161
O	13	B14	6	A13	1	B16	1.07380089
H	1	B15	2	A14	3	B17	1.07456887
H	2	B16	1	A15	6	B18	1.07316973
H	3	B17	2	A16	1	B19	1.08185592
H	4	B18	3	A17	2	B20	1.07392257
H	7	B19	5	A18	4	B21	1.07212466
H	9	B20	8	A19	7	B22	0.94617233
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H	12	B22	7	A21	5	A2	120.51248895
B1	1.38305662					A3	121.76406589
B2	1.38481561					A4	119.12025080
						A5	120.50334315
						A6	112.76900261
						A7	125.24702616
						A8	115.49375891
						A9	179.07698534
						A10	110.89198169

A11	115.68226307	20					
A12	118.15153232	21					
A13	118.13452172	22					
A14	120.96866246	23					
A15	119.91559372						
A16	120.09664411		MBHA lb				
A17	118.93106332						
A18	108.87139635		C	1	B1		
A19	121.24487099		C	2	B2	1	A1
A20	120.50187770		C	3	B3	2	A2 1 D1
A21	108.62086512		C	4	B4	3	A3 2 D2
D1	-0.55318943		C	1	B5	2	A4 3 D3
D2	0.83865195		C	5	B6	4	A5 3 D4
D3	-0.64089954		C	7	B7	5	A6 4 D5
D4	179.94129180		C	8	B8	7	A7 5 D6
D5	31.48705916		C	8	B9	7	A8 5 D7
D6	-118.88878982		N	10	B10	8	A9 7 D8
D7	64.06845655		O	7	B11	5	A10 4 D9
D8	14.05594387		N	1	B12	6	A11 5 D10
D9	-89.62217134		O	13	B13	1	A12 6 D11
D10	-176.47602408		O	13	B14	1	A13 6 D12
D11	-35.25867635		H	2	B15	1	A14 6 D13
D12	143.29221660		H	3	B16	2	A15 1 D14
D13	-179.46966029		H	4	B17	3	A16 2 D15
D14	179.11830247		H	6	B18	1	A17 2 D16
D15	179.85154761		H	7	B19	5	A18 4 D17
D16	-178.90606532		H	9	B20	8	A19 7 D18
D17	149.25623806		H	9	B21	8	A20 7 D19
D18	-177.69935806		H	12	B22	7	A21 5 D20
D19	2.10292281						
D20	-70.51238570		B1	1.38442332			
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2 3 2.0 17 1.0			B4	1.39149100			
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4 5 1.5 19 1.0			B6	1.52979429			
5 6 1.5 7 1.0			B7	1.52113806			
6 13 1.0			B8	1.32420404			
7 8 1.0 12 1.0 20 1.0			B9	1.45032983			
8 9 2.0 10 1.0			B10	1.13788360			
9 21 1.0 22 1.0			B11	1.40128747			
10 11 3.0			B12	1.45831034			
11			B13	1.19681826			
12 23 1.0			B14	1.19656965			
13 14 2.0 15 2.0			B15	1.07091374			
14			B16	1.07386078			
15			B17	1.07256765			
16			B18	1.07108001			
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B22	0.95076710	9 21 1.0 22 1.0
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A2	120.42838240	11
A3	121.15322885	12 23 1.0
A4	122.68479441	13 14 2.0 15 2.0
A5	120.81598615	14
A6	113.31917535	15
A7	124.02528682	16
A8	116.56513543	17
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A10	112.14330666	19
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A14	120.88554474	23
A15	119.72735521	
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A19	121.94804234	C 2 B2 1 A1
A20	120.75398244	C 3 B3 2 A2 1 D1
A21	111.69409760	C 4 B4 3 A3 2 D2
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D2	-0.34347034	C 5 B6 4 A5 3 D4
D3	0.31346858	C 7 B7 5 A6 4 D5
D4	177.64918800	C 8 B8 7 A7 5 D6
D5	142.50950504	C 8 B9 7 A8 5 D7
D6	117.78416904	N 10 B10 8 A9 7 D8
D7	-63.86539027	O 7 B11 5 A10 4 D9
D8	-14.89471381	N 2 B12 1 A11 6 D10
D9	15.87808588	O 13 B13 2 A12 1 D11
D10	-179.93403207	O 13 B14 2 A13 1 D12
D11	-0.67400553	H 1 B15 2 A14 3 D13
D12	179.35055116	H 3 B16 2 A15 1 D14
D13	-179.80007441	H 4 B17 3 A16 2 D15
D14	179.68458815	H 6 B18 1 A17 2 D16
D15	179.23511518	H 7 B19 5 A18 4 D17
D16	-179.82324025	H 9 B20 8 A19 7 D18
D17	-99.33538992	H 9 B21 8 A20 7 D19
D18	179.01778633	H 12 B22 7 A21 5 D20
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		B2 1.38508485
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3 4 1.5 17 1.0		B5 1.38535839
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6 19 1.0		B8 1.32408637
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H	17	B26	15	A25	10	D24	A22	121.31101194
H	17	B27	15	A26	10	D25	A23	109.88285902
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B1	1.37951972						A25	110.10823453
B2	1.38693653						A26	110.13054161
B3	1.38456832						D1	-0.46509479
B4	1.39467655						D2	-1.18586840
B5	1.38841438						D3	1.60299187
B6	1.53988252						D4	177.86891011
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B8	1.32478058						D6	111.38904873
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B17	1.07171551						D15	-179.02825763
B18	1.07381958						D16	-178.91331571
B19	1.07465197						D17	179.10532630
B20	1.07059044						D18	178.60787814
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B22	1.07271337						D20	178.55472954
B23	1.07275165						D21	-1.33436848
B24	0.95069748						D22	82.09906565
B25	1.07715456						D23	-179.23563925
B26	1.07919068						D24	61.61796914
B27	1.07935758						D25	-60.05418753
A1	118.97656358							
A2	120.58263944						1	2 2.0 6 1.5 18 1.0
A3	122.18793603						2	3 1.5 19 1.0
A4	119.48460303						3	4 2.0 20 1.0
A5	119.41595393						4	5 1.5 21 1.0
A6	113.44755758						5	6 1.5 7 1.0
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A8	117.99042746						7	8 1.0 11 1.0 22 1.0
A9	110.54343824						8	9 2.0 10 1.0
A10	114.86594968						9	23 1.0 24 1.0
A11	117.79229423						10	15 1.5 16 2.0
A12	118.52745352						11	25 1.0
A13	114.38333438						12	13 2.0 14 2.0
A14	122.61428189						13	
A15	118.18142868						14	
A16	120.83481684						15	17 1.0
A17	120.09499205						16	
A18	120.10008079						17	26 1.0 27 1.0 28 1.0







O	10	B14	8	A13	7	D12	A2	120.31777296
O	10	B15	8	A14	7	D13	A3	122.26657990
C	15	B16	10	A15	8	D14	A4	119.36449096
C	17	B17	15	A16	10	D15	A5	117.09664970
O	18	B18	17	A17	15	D16	A6	114.16612116
H	1	B19	2	A18	3	D17	A7	124.11094900
H	2	B20	1	A19	6	D18	A8	115.33458594
H	3	B21	2	A20	1	D19	A9	112.29200015
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H	7	B23	5	A22	4	D21	A11	118.11092718
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H	11	B26	7	A25	5	D24	A14	122.31415046
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B5	1.38547376						A25	109.84883407
B6	1.53681925						A26	103.15389324
B7	1.52647616						A27	109.19695219
B8	1.32381511						A28	109.28704632
B9	1.49126133						A29	107.86079798
B10	1.39772833						A30	109.20878374
B11	1.46154690						D1	0.38002347
B12	1.19187026						D2	-1.10019233
B13	1.20024007						D3	0.89400077
B14	1.31063892						D4	178.77575569
B15	1.20247576						D5	-123.18354627
B16	1.43644495						D6	-123.44645732
B17	1.52124934						D7	62.83086614
B18	1.40379424						D8	106.71747670
B19	1.07217435						D9	176.79388571
B20	1.07378094						D10	39.77275390
B21	1.07450403						D11	-138.46075604
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B23	1.07850053						D13	12.41279726
B24	1.07248993						D14	-170.92030628
B25	1.07246097						D15	-75.98841119
B26	0.94969150						D16	89.43799457
B27	1.07849630						D17	179.65797708
B28	1.08074265						D18	-178.98966238
B29	1.08615082						D19	179.81210314
B30	1.08193271						D20	178.14111093
B31	0.95115391						D21	-6.84502846
A1	119.17775985						D22	-176.89811787

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 D25 165.23776585  
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## MBHA IIIb

C 1 B1  
 C 2 B2 1 A1  
 C 3 B3 2 A2 1 D1  
 C 4 B4 3 A3 2 D2  
 C 1 B5 2 A4 3 D3  
 C 5 B6 4 A5 3 D4  
 C 7 B7 5 A6 4 D5  
 C 8 B8 7 A7 5 D6

C 8 B9 7 A8 5 D7  
 O 7 B10 5 A9 4 D8  
 O 10 B11 8 A10 7 D9  
 O 10 B12 8 A11 7 D10  
 C 12 B13 10 A12 8 D11  
 C 14 B14 12 A13 10 D12  
 O 15 B15 14 A14 12 D13  
 H 2 B16 1 A15 6 D14  
 H 3 B17 2 A16 1 D15  
 H 4 B18 3 A17 2 D16  
 H 7 B19 5 A18 4 D17  
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 H 9 B21 8 A20 7 D19  
 H 11 B22 7 A21 5 D20  
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 H 14 B24 12 A23 10 D22  
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 H 16 B27 15 A26 14 D25  
 H 6 B28 1 A27 2 D26  
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 O 30 B30 1 A29 6 D28  
 O 30 B31 1 A30 6 D29

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A3	121.24906781	D24	-151.32466993
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A5	121.06177776	D26	-179.89320764
A6	113.32028877	D27	-179.84035130
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D2	-0.27949088		23
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D6	112.95808779		27
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D8	12.58372718		29
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D14	-179.80513351		
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D16	179.51123477	C	2 B2 1 A1
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B10	1.40123377						A30	34.20448682
B11	1.30597338						D1	-0.20621366
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B14	1.52166795						D4	177.64721141
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B19	1.07270711						D9	173.50184548
B20	1.07509194						D10	-7.30434482
B21	0.95110618						D11	-175.23923640
B22	1.07814843						D12	-73.49118086



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D18	-0.46852756	C	4	B4	3	A3 2 D2
D19	71.13583798	C	1	B5	2	A4 3 D3
D20	167.60152417	C	5	B6	4	A5 3 D4
D21	51.50896112	C	7	B7	5	A6 4 D5
D22	-34.30634581	C	8	B8	7	A7 5 D6
D23	-151.37332449	C	8	B9	7	A8 5 D7
D24	-47.03051805	O	7	B10	5	A9 4 D8
D25	-179.96046652	N	6	B11	1	A10 2 D9
D26	-179.90933365	O	12	B12	6	A11 1 D10
D27	-179.57525335	O	12	B13	6	A12 1 D11
D28	-0.33776816	O	10	B14	8	A13 7 D12
D29	-0.34240553	O	10	B15	8	A14 7 D13
		C	15	B16	10	A15 8 D14
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B25	1.07278790	D11	34.94453573
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B28	1.08116278	D14	176.16971790
B29	1.08575162	D15	-179.21059846
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B31	1.08471457	D17	-178.99515557
B32	1.08611103	D18	-178.93509208
B33	1.08612044	D19	179.07733782
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D12	170.38295541	31
D13	-10.18291520	32
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D16	-179.80061249	
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D18	179.76593273	
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D21	-103.88594407	C 3 B3 2 A2 1 D1
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O	2	B27	1	A26	6	D25	A11	121.66204627
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N	28	B29	2	A28	1	D27	A13	111.23587443
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