

Supporting Information

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Spectroscopic and Density Functional Theory Studies of a New Rosane Type Diterpenoid from *Stachys parviflora*

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S1: ^1H -NMR data of **1a** (in CDCl_3) and its comparison with the unscaled theoretical values calculated at B3LYP/6-311+(2d,p)

^1H -NMR, δ and multiplicity	^1H NMR, δ calculated at B3LYP/6-311+(2d,p)	^1H NMR, δ calculated at B3LYP/6-311+(2d,p)
5.25, m	6.00	5.99
2.20-2.29, m	3.32-3.03	3.3-3.02
1.25, m		
6.42, br s	7.40	7.42
-		
3.01, d, $J = 7.1$ Hz	3.58	3.56
3.75, m	5.02	5.03
1.76, m	1.42, 1.72	1.47, 1.75
1.82, m	1.69	1.71
-		
-		
1.31, m	1.76	1.74
1.43, m		
1.10, m	1.95, 1.44	1.21
1.47, m		1.77
-		
1.18-1.23, m	1.39, 1.23	1.6-1.01
5.40 dd, $J = 17.4, 10$ Hz	6.26	6.20
5.03, dd, $J = 16.8, 1.3$ Hz	5.06, 5.14	5.02-5.17
4.98, dd, $J = 10.8, 1.3$ Hz		
1.05, s	1.09	1.18
-		
1.07, s	0.86	0.98
-		

S2: Comparison of ^1H -NMR data of **1a** (in CDCl_3) with the scaled theoretical chemical shifts calculated at B3LYP/6-311+(2d,p), B3LYP/6-31G(d) and WP04/6-31G(d)

Position	^1H -NMR (δ) and multiplicity	(δ) ^1H -NMR calculated at B3LYP/6-311+(2d,p)	^1H -NMR calculated at B3LYP/6-31G(d)	^1H -NMR calculated at WP04/6-31G(d)
1	5.25, m	5.55	5.70	5.61
2	2.20-2.29, m	2.96-3.06	2.88-2.98	2.89-2.95
	1.25, m			
3	6.42, m	6.88	7.0	6.99
4	-	-		
5	3.01, d, $J = 7.1$ Hz	3.30	3.4	3.45
6	3.75, m	4.66	4.79	4.79
7	1.76, m	1.36, 1.62	1.49, 1.70	1.66, 1.86
8	1.82, m	1.58	1.84	1.90
9	-	-		
10	-	-		
11	1.31, m	1.61	1.77, 1.87	1.84, 1.88
	1.43, m			
12	1.10, m	1.12, 1.64	1.35, 1.85	1.40, 1.90
	1.47, m			
13	-	-		
14	1.18-1.23, m	1.48-0.93	1.0, 1.79	1.30, 1.81
15	5.40 dd, $J = 17.4, 10$ Hz	5.75	6.01	5.89
16	5.03, dd, $J = 16.8, 1.3$ Hz	4.65-4.79	4.79, 4.96	4.87, 4.91
	4.98, dd, $J = 10.8, 1.3$ Hz			
17	1.05, s	1.09	1.21	1.32
18	-	-		
19	1.07, s	0.91	0.78	1.26

S3: Unscaled and scaled harmonic vibrations for **1a**, simulated in the gas phase at B3LYP/6-31G(d)

Sr. No	Simulated harmonic vibration (Unscaled)	Simulated harmonic vibrations (scaled) cm ⁻¹
1	3243	3117
2	3202	3078
3	3177	3054
4	3170	3047
5	3144	3022
6	3131	3009
7	3129	3008
8	3123	3002
9	3117	2996
10	3106	2986
11	3082	2963
12	3073	2954
13	3072	2953
14	3070	2951
15	3063	2944
16	3055	2937
17	3043	2925
18	3038	2920
19	3037	2919
20	2994	2878
21	2990	2874
22	2980	2867
23	1860	1788
24	1756	1688
25	1724	1657
26	1390	1336
27	1241	1193
28	1220	1173
29	1136	1092
30	1067	1026
31	1056	1015
32	1037	997
33	938	902

Only prominent peaks are listed in this table for vibrations below 1800 cm⁻¹

S4: Cartesian Coordinates

1a (gas phase)

C	2.22954700	-1.04850900	0.45110500
C	0.80417200	-0.69441300	-0.00042000
C	0.42574500	0.78147100	0.33154800
C	1.46261800	1.68554200	-0.38729100
C	2.91441400	1.36531800	0.01406600
C	3.32424400	-0.12674700	-0.17256600
H	0.80464200	-0.76674900	-1.09987500
H	2.29683500	-1.00876600	1.54613100
H	2.44966600	-2.08839400	0.17646100
H	1.33653600	1.57307400	-1.47227200
H	1.25451600	2.73983000	-0.16598900
H	3.60248100	1.99570700	-0.56364900
H	3.06449200	1.64679800	1.06415000
C	-0.28167300	-1.67396700	0.48529000
H	-0.60381800	-1.44543300	1.50735400
H	0.08341100	-2.70742800	0.48849000
C	-3.88010700	1.18521300	-0.13970200
C	-3.09193200	2.45599300	-0.34706700
C	-1.62094300	2.24163800	-0.02630300
C	-1.83209200	-0.06484400	-0.78905600
C	-3.26004800	0.01984100	-0.33063600
H	-4.90222400	1.22318400	0.22849000
H	-3.21551100	2.81138900	-1.38534800
H	-1.08887500	3.09977500	0.37910900
C	-1.00562500	1.05843100	-0.15810100

H	-1.79522100	0.07220500	-1.88092200
H	-3.49757200	3.25901500	0.28029300
C	4.61233100	-0.35498500	0.59788600
H	4.53238200	-0.13307900	1.66466200
C	5.78714300	-0.78307000	0.13369300
H	5.95597900	-1.02754900	-0.91102400
H	6.63872300	-0.90664100	0.79752400
C	3.50510300	-0.44312100	-1.66834200
H	4.29278700	0.18099600	-2.10477900
H	3.78268100	-1.49257200	-1.81900900
H	2.59052500	-0.25882200	-2.23942400
C	0.45737100	1.06114100	1.85806400
H	0.26922400	2.12314200	2.04514600
H	-0.31803800	0.50059900	2.38848800
H	1.41985800	0.81186800	2.31250700
C	-3.73175300	-1.32757500	0.06282200
C	-1.45851900	-1.54177800	-0.47604600
O	-2.65715200	-2.17934100	0.03085600
H	-1.21117000	-2.06673000	-1.40535800
O	-4.83063400	-1.68427000	0.41104200

1a (CHCl₃)

C	2.22899000	-1.04959700	0.45004300
C	0.80412700	-0.69407000	-0.00160400
C	0.42578700	0.78103800	0.33281000
C	1.46121300	1.68530500	-0.38800300
C	2.91343600	1.36534500	0.01200700

C	3.32321400	-0.12710200	-0.17394400
H	0.80394500	-0.76599000	-1.10062200
H	2.29614200	-1.01068300	1.54498000
H	2.44758300	-2.08907800	0.17272000
H	1.33411800	1.57156400	-1.47266800
H	1.25375900	2.73932400	-0.16550000
H	3.59969600	1.99505200	-0.56873400
H	3.06467400	1.64836200	1.06137800
C	-0.28093100	-1.67484200	0.48487600
H	-0.60206200	-1.44509300	1.50698100
H	0.08576900	-2.70756100	0.48540700
C	-3.88087800	1.18600600	-0.14064700
C	-3.09266600	2.45557000	-0.34758400
C	-1.62254200	2.24101900	-0.02278900
C	-1.83111000	-0.06454300	-0.78960600
C	-3.25986500	0.01961000	-0.33153700
H	-4.90329700	1.22924300	0.22614100
H	-3.21458500	2.80617600	-1.38739700
H	-1.09309900	3.09948200	0.38486200
C	-1.00604200	1.05842200	-0.15533800
H	-1.79381000	0.07291900	-1.88072100
H	-3.50152800	3.25919600	0.27594400
C	4.61026400	-0.35404500	0.59886600
H	4.52781200	-0.13222100	1.66547100
C	5.78713100	-0.78076600	0.13640800
H	5.95753500	-1.02483100	-0.90835900
H	6.63786600	-0.90316300	0.80204100

C	3.50508200	-0.44441000	-1.66947100
H	4.29214600	0.18033700	-2.10630400
H	3.78347000	-1.49380900	-1.81931600
H	2.59014500	-0.26124900	-2.24015700
C	0.46015400	1.06034200	1.85938000
H	0.26926000	2.12184200	2.04652300
H	-0.31142300	0.49589200	2.39163400
H	1.42473900	0.81401600	2.31084500
C	-3.72687600	-1.32455100	0.06231800
C	-1.45405600	-1.53926100	-0.47865500
O	-2.66168000	-2.17784800	0.02994400
H	-1.21314100	-2.06713900	-1.40640600
O	-4.82860700	-1.68832800	0.41456600

1a (Methanol)

C	2.22897100	-1.04938600	0.44962200
C	0.80453600	-0.69376300	-0.00313600
C	0.42545200	0.78062200	0.33310900
C	1.46063700	1.68610700	-0.38657100
C	2.91285300	1.36599400	0.01356500
C	3.32297900	-0.12621000	-0.17394100
H	0.80522700	-0.76488000	-1.10187600
H	2.29570800	-1.01045100	1.54456000
H	2.44726900	-2.08863600	0.17110100
H	1.33378600	1.57332300	-1.47128500
H	1.25315600	2.73965800	-0.16204000
H	3.59863200	1.99656800	-0.56697900

H	3.06364400	1.64765800	1.06332000
C	-0.28004300	-1.67607900	0.48209200
H	-0.60050100	-1.44784700	1.50479100
H	0.08778500	-2.70836900	0.47944900
C	-3.88112200	1.18617300	-0.14038100
C	-3.09302000	2.45501300	-0.34938600
C	-1.62318000	2.24085100	-0.02260100
C	-1.83112200	-0.06437500	-0.79038300
C	-3.25970800	0.01936300	-0.33096500
H	-4.90335400	1.23167900	0.22679400
H	-3.21404200	2.80142000	-1.39057900
H	-1.09482200	3.09973800	0.38541300
C	-1.00633100	1.05834500	-0.15502900
H	-1.79463200	0.07412700	-1.88102700
H	-3.50311300	3.26023300	0.27086500
C	4.60978500	-0.35342800	0.59932800
H	4.52736900	-0.13032700	1.66566700
C	5.78650100	-0.78213700	0.13726300
H	5.95648200	-1.02741600	-0.90739000
H	6.63715000	-0.90480000	0.80318400
C	3.50494100	-0.44237500	-1.66969900
H	4.29241300	0.18236300	-2.10595700
H	3.78268300	-1.49184100	-1.82053700
H	2.59001200	-0.25833900	-2.23993800
C	0.45974800	1.05846800	1.85995300
H	0.26798900	2.11971000	2.04768900
H	-0.31095900	0.49216000	2.39171100

H	1.42469700	0.81255500	2.31078500
C	-3.72451700	-1.32358900	0.06343100
C	-1.45230400	-1.53830800	-0.48160500
O	-2.66303500	-2.17763800	0.02856900
H	-1.21457700	-2.06655100	-1.40933200
O	-4.82675900	-1.68979300	0.41938200

1b

C	-2.20055400	-1.20292000	-0.35411900
C	-0.77973900	-0.78837200	0.05479500
C	-0.48367200	0.70835800	-0.26821300
C	-1.54101100	1.54992400	0.49594700
C	-2.98767100	1.16404500	0.13488800
C	-3.31076600	-0.33833200	0.32021400
H	-0.74149400	-0.87282300	1.15273800
H	-2.31435800	-1.15158600	-1.44393000
H	-2.35740900	-2.25653400	-0.08443800
H	-1.37367400	1.43175200	1.57464400
H	-1.39232600	2.61572400	0.28261300
H	-3.68174000	1.76315800	0.73861600
H	-3.17708600	1.44224100	-0.90843800
C	0.33688700	-1.70817500	-0.47606700
H	0.61805800	-1.45156400	-1.50346100
H	0.02223000	-2.75816500	-0.48329200
C	3.81072100	1.31258200	0.07808300
C	2.96960200	2.54184000	0.32376700
C	1.50152200	2.26027100	0.04398100

C	1.84500400	-0.04086100	0.77331400
C	3.25264400	0.11700800	0.27335500
H	4.81846000	1.40313200	-0.31939400
H	3.10702800	2.89141600	1.36230400
H	0.91711200	3.09555600	-0.33585900
C	0.94707000	1.04792600	0.18086100
H	1.83546000	0.08263800	1.86742700
H	3.31753500	3.37015300	-0.30535100
C	-4.63800000	-0.72440200	-0.30807100
H	-4.85215100	-1.79471800	-0.25682000
C	-5.54437900	0.07111900	-0.87763100
H	-5.41618800	1.14646200	-0.96254800
H	-6.46722400	-0.33395300	-1.28433400
C	-3.41796200	-0.68389600	1.82756100
H	-4.22025400	-0.10145400	2.29362400
H	-3.65158500	-1.74619400	1.96834100
H	-2.49262900	-0.47431100	2.37408300
C	-0.57875700	1.00525000	-1.78889600
H	-0.44418000	2.07688200	-1.96767200
H	0.20287600	0.48649700	-2.35173200
H	-1.54393800	0.71936900	-2.21529000
C	3.77649400	-1.20210200	-0.14848700
C	1.53308900	-1.53066700	0.45377800
O	2.74578100	-2.10535200	-0.09305000
H	1.33661200	-2.07636300	1.38329000
O	4.88018600	-1.50200900	-0.53313600