Supplementary Information

X-ray crystal structure, NMR, DFT investigations, pharmaco-kinetic, and toxicity of sarcotrocheliol: A pyrane-based cemranoids of marine origin

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Fig. S1. Comparison of bond lengths in optimized structure (left) and crystal structure (right).

Fig. S2. Correlation between experimental and calculated ^{1}H and ^{13}C chemical shifts in $CDCl_3$, CD_3CN, MeOH-D4 and DMSO-d_6.

Fig. S3. Molecular orbital shapes of sarcotrocheliol using B3LYP/6-311G++(d,p).

Fig. S4. Molecular orbital energies of sarcotrocheliol molecule in gas phase and in different solvents using B3LYP/6-311G++(d,p).

Fig. S5. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in $CDCl_3$.

Fig. S6. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in CD_3CN.

Fig. S7. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in MeOH-D4.

Fig. S8. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in DMSO-d_6.

Table S1. The full structural information determined; bond length, bond angles and torsion angles by single crystal X-ray (experimental) and theoretical calculations (DFT).

Table S2. The calculated harmonic vibrational frequencies (in cm^{-1}) and their assignments and contribution for sarcotrocheliol using DFT computational with B3LYP exchange correlation and 6-311G++(d,p) basis sets.

Table S1. The full structural information determined; bond length, bond angles and torsion angles by single crystal X-ray (experimental) and theoretical calculations (DFT).

Bond length	Exp	DFT	Angles / °	Exp	DFT	Torsion Angles / °	Exp	DFT
O1-C2	1.484(8)	1.4571	C2-O1-C12	120.2(4)	121.5	C12-O1-C2-C1	52.6(5)	48.48
O1-C12	1.461(8)	1.447	H21-O2-C11	117(4)	109.19	C12-O1-C2-H2	167.8	163.53
O2-H21	1.04(8)	0.9611	H16A-C16-H16C	109.5	107.88	C12-O1-C2-C3	-74.6(5)	-79.77
O2-C11	1.438(8)	1.4414	H16A-C16-H16B	109.4	107.5	C2-O1-C12-C11	83.2(5)	83.23
C16-H16A	0.961	1.096	H16A-C16-C15	109.5	111	C2-O1-C12-C14	-42.8(6)	-41.15
C16-H16C	0.96	1.0919	H16C-C16-H16B	109.4	107.23	C2-O1-C12-C20	-158.5(4)	-158.1
C16-H16B	0.959	1.0937	H16C-C16-C15	109.5	112.7	H21-O2-C11-C12	117(4)	79.86
C16-C15	1.56(1)	1.5383	H16B-C16-C15	109.5	110.31	H21-O2-C11-H11	-3	-0.03
C15-H15	0.979	1.0971	C16-C15-H15	107.2	107.67	H21-O2-C11-C10	-121(4)	-156.15
C15-C1	1.56(1)	1.5503	C16-C15-C1	112.2(5)	111.86	H16A-C16-C15-H15	167.8	176.68
C15-C17	1.53(1)	1.5379	C16-C15-C17	110.6(6)	109.27	H16A-C16-C15-C1	50.5	57.93
C1-H1	0.98	1.0999	H15-C15-C1	107.2	108.2	H16A-C16-C15-C17	-75.7	-66.67
C1-C2	1.549(9)	1.5483	H15-C15-C17	107.2	107.65	H16C-C16-C15-H15	47.7	55.55
C1-C13	1.525(9)	1.5374	C1-C15-C17	112.3(5)	112.01	H16C-C16-C15-C1	-69.6	-63.2
C2-H2	0.98	1.0892	C15-C1-H1	107.2	106.87	H16C-C16-C15-C17	164.2	172.19
C2-C3	1.515(8)	1.5113	C15-C1-C2	111.2(5)	113.42	H16B-C16-C15-H15	-72.3	-64.27
C12-C11	1.56(1)	1.5698	C15-C1-C13	115.1(5)	114.52	H16B-C16-C15-C1	170.4	176.98
C12-C14	1.54(1)	1.5426	H1-C1-C2	107.2	105.95	H16B-C16-C15-C17	44.2	52.37
C12-C20	1.532(9)	1.532	H1-C1-C13	107.2	106.86	C16-C15-C1-H1	-69	-61.53
C11-H11	0.98	1.0933	C2-C1-C13	108.6(5)	108.65	C16-C15-C1-C2	174.2(5)	177.91
C11-C10	1.540(9)	1.5302	O1-C2-C1	109.6(4)	111.15	C16-C15-C1-C13	50.2(7)	56.6
C10-H10A	0.97	1.0935	O1-C2-H2	106.8	101.12	H15-C15-C1-H1	173.7	179.97
C10-H10B	0.97	1.0918	O1-C2-C3	114.0(4)	114.25	H15-C15-C1-C2	56.8	63.65
C10-C9	1.56(1)	1.5514	C1-C2-H2	106.7	108.54	H15-C15-C1-C13	-67.1	-61.84
C9-H9A	0.97	1.0958	C1-C2-C3	112.6(4)	112.23	C17-C15-C1-H1	56.3	61.53
C9-H9B	0.97	1.0933	H2-C2-C3	106.8	108.83	C17-C15-C1-C2	-60.6(7)	-54.85
C9-C8	1.53(1)	1.5139	O1-C12-C11	110.2(4)	108.8	C17-C15-C1-C13	175.4(5)	179.66
C8-C18	1.53(1)	1.5094	O1-C12-C14	110.4(4)	110.8	C16-C15-C17-H17A	69.1	66.9
C8-C7	1.34(1)	1.339	O1-C12-C20	103.7(4)	104.85	C16-C15-C17-H17B	-50.7	-52.15
C18-H18C	0.961	1.0963	C11-C12-C14	113.4(5)	112.66	C16-C15-C17-H17	-170.8	-171.91
C18-H18A	0.96	1.0954	C11-C12-C20	110.6(4)	110.88	H15-C15-C17-H17A	-174.4	-176.45
C18-H18B	0.96	1.0896	C14-C12-C20	108.1(5)	108.57	H15-C15-C17-H17B	65.8	64.51
C17-H17A	0.961	1.0958	O2-C11-C12	109.8(4)	111.86	H15-C15-C17-H17	-54.3	-55.25
C17-H17B	0.96	1.0937	O2-C11-H11	108.9	109.07	C1-C15-C17-H17A	-57	-57.62
C17-H17	0.959	1.0915	O2-C11-C10	108.1(4)	105.68	C1-C15-C17-H17B	-176.8	-176.66
C13-H13A	0.969	1.0971	C12-C11-H11	108.8	107.64	C1-C15-C17-H17	63.1	63.58
C13-H13	0.97	1.0921	C12-C11-C10	112.3(5)	113.51	C15-C1-C2-O1	174.4(4)	176.65
C13-C14	1.53(1)	1.5308	H11-C11-C10	108.9	109	C15-C1-C2-H2	59.2	66.3
C14-H14A	0.97	1.0931	C11-C10-H10A	108.9	107.24	C15-C1-C2-C3	-57.6(6)	-54.02
C14-H14B	0.97	1.0951	C11-C10-H10B	109	108.9	H1-C1-C2-O1	57.6	59.73
C3-H3	0.931	1.0872	C11-C10-C9	113.3(5)	113.88	H1-C1-C2-H2	-57.7	-50.62
C3-C4	1.350(9)	1.3405	H10A-C10-H10B	107.7	107.32	H1-C1-C2-C3	-174.5	-170.94
C4-C19	1.49(1)	1.5069	H10A-C10-C9	108.9	109.47	C13-C1-C2-O1	-58.0(5)	-54.78
C4-C5	1.517(9)	1.5163	H10B-C10-C9	108.9	109.8	C13-C1-C2-H2	-173.2	-165.13
C19-H19A	0.959	1.0895	C10-C9-H9A	109.6	108.71	C13-C1-C2-C3	70.0(6)	74.55
C19-H19B	0.959	1.0962	C10-C9-H9B	109.6	109.2	C15-C1-C13-H13A	63.6	63.63
C19-H19C	0.959	1.095	C10-C9-C8	110.5(5)	111.61	C15-C1-C13-H13	-54.9	-53.54
C5-H5B	0.97	1.0972	H9A-C9-H9B	108.1	106.6	C15-C1-C13-C14	-175.7(5)	-173.17
C5-H5A	0.97	1.0945	H9A-C9-C8	109.6	109.56	H1-C1-C13-H13A	-177.3	-178.24
C5-C6	1.56(1)	1.5567	H9B-C9-C8	109.5	111	H1-C1-C13-H13	64.3	64.6
C6-H6A	0.97	1.0969	C9-C8-C18	115.0(6)	114.49	H1-C1-C13-C14	-56.5	-55.04
C6-H6B	0.97	1.0918	C9-C8-C7	121.6(6)	120.83	C2-C1-C13-H13A	-61.8	-64.33
C6-C7	1.50(1)	1.5023	C18-C8-C7	123.4(7)	124.61	C2-C1-C13-H13	179.8	178.51
C7-H7	0.93	1.0903	C8-C18-H18C	109.5	109.76	C2-C1-C13-C14	59.0(6)	58.88
C20-H20B	0.96	1.0899	C8-C18-H18A	109.6	111.35	O1-C2-C3-H3	86.6	92.45
C20-H20A	0.96	1.093	C8-C18-H18B	109.5	113.47	O1-C2-C3-C4	-93.3(7)	-89.13
C20-H20C	0.96	1.0918	H18C-C18-H18A	109.4	106.46	C1-C2-C3-H3	-39	-35.25
			H18C-C18-H18B	109.5	107.58	C1-C2-C3-C4	141.2(6)	143.17
			H18A-C18-H18B	109.4	107.91	H2-C2-C3-H3	-155.8	-155.4

			C15-C17-H17A	109.5	110.95	H2-C2-C3-C4	24.4	23.02
			C15-C17-H17B	109.4	110.39	O1-C12-C11-O2	-177.0(4)	-171.67
			C15-C17-H17	109.5	112.42	O1-C12-C11-H11	-57.9	-51.86
			H17A-C17-H17B	109.4	107.48	O1-C12-C11-C10	62.7(6)	68.85
			H17A-C17-H17	109.6	108.11	C14-C12-C11-O2	-52.7(6)	-48.4
			H17B-C17-H17	109.5	107.29	C14-C12-C11-H11	66.4	71.41
			C1-C13-H13A	109.6	110.46	C14-C12-C11-C10	-173.0(5)	-167.88
			C1-C13-H13	109.6	110.68	C20-C12-C11-O2	68.9(6)	73.52
			C1-C13-C14	110.3(5)	109.55	C20-C12-C11-H11	-172	-166.67
			H13A-C13-H13	108	106.06	C20-C12-C11-C10	-51.4(6)	-45.96
			H13A-C13-C14	109.6	111.5	O1-C12-C14-C13	41.3(6)	43.06
			H13-C13-C14	109.6	108.52	O1-C12-C14-H14A	163.1	169.24
			C12-C14-C13	115.7(5)	114.56	O1-C12-C14-H14B	-80.5	-76.31
			C12-C14-H14A	108.4	109.44	C11-C12-C14-C13	-82.9(6)	-79.09
			C12-C14-H14B	108.4	107.38	C11-C12-C14-H14A	39	47.09
			C13-C14-H14A	108.3	111.59	C11-C12-C14-H14B	155.3	161.54
			C13-C14-H14B	108.3	107.54	C20-C12-C14-C13	154.2(5)	157.69
			H14A-C14-H14B	107.5	105.85	C20-C12-C14-H14A	-84	-76.13
			C2-C3-H3	116.4	115.95	C20-C12-C14-H14B	32.4	38.33
			C2-C3-C4	127.5(5)	127.75	O1-C12-C20-H20B	-52	-54.04
			H3-C3-C4	116.2	116.28	O1-C12-C20-H20A	-172	-174.78
			C3-C4-C19	123.7(5)	124.59	O1-C12-C20-H20C	68	65.31
			C3-C4-C5	119.2(5)	119.75	C11-C12-C20-H20B	66.1	63.21
			C19-C4-C5	117.1(5)	115.63	C11-C12-C20-H20A	-53.9	-57.52
			C4-C19-H19A	109.5	113.13	C11-C12-C20-H20C	-173.9	-177.43
			C4-C19-H19B	109.4	110.58	C14-C12-C20-H20B	-169.3	-172.51
			C4-C19-H19C	109.5	110.55	C14-C12-C20-H20A	70.7	66.76
			H19A-C19-H19B	109.5	108.51	C14-C12-C20-H20C	-49.3	-53.15
			H19A-C19-H19C	109.6	107.18	O2-C11-C10-H10A	-44	-44.6
			H19B-C19-H19C	109.5	106.62	O2-C11-C10-H10B	-161.2	-160.44
			C4-C5-H5B	109	109.77	O2-C11-C10-C9	77.4(6)	76.67
			C4-C5-H5A	109	109.11	C12-C11-C10-H10A	77.3	78.35
			C4-C5-C6	112.8(5)	114.15	C12-C11-C10-H10B	-40	-37.49
			H5B-C5-H5A	107.8	106.75	C12-C11-C10-C9	-161.4(5)	-160.38
			H5B-C5-C6	108.9	108.37	H11-C11-C10-H10A	-162.2	-161.7
			H5A-C5-C6	109.1	108.42	H11-C11-C10-H10B	80.6	82.46
			C5-C6-H6A	109.4	107.49	H11-C11-C10-C9	-40.8	-40.43
			C5-C6-H6B	109.5	109.8	C11-C10-C9-H9A	-149	-149.44
			C5-C6-C7	110.7(6)	111.01	C11-C10-C9-H9B	-30.5	-33.5
			H6A-C6-H6B	108.2	106.31	C11-C10-C9-C8	90.2(6)	89.6
			H6A-C6-C7	109.5	110.51	H10A-C10-C9-H9A	-27.6	-29.42
			H6B-C6-C7	109.5	111.54	H10A-C10-C9-H9B	90.8	86.52
			C8-C7-C6	127.3(7)	128.35	H10A-C10-C9-C8	-148.4	-150.37
			C8-C7-H7	116.4	117	H10B-C10-C9-H9A	89.5	88.16
			C6-C7-H7	116.4	114.37	H10B-C10-C9-H9B	-152	-155.91
			C12-C20-H20B	109.5	111.29	H10B-C10-C9-C8	-31.2	-32.8
			C12-C20-H20A	109.5	110.22	C10-C9-C8-C18	76.7(7)	79.02
			C12-C20-H20C	109.5	109.77	C10-C9-C8-C7	-100.4(8)	-97.91
			H20B-C20-H20A	109.5	108.74	H9A-C9-C8-C18	-44.1	-41.44
			H20B-C20-H20C	109.5	107.88	H9A-C9-C8-C7	138.8	141.62
			H20A-C20-H20C	109.5	108.87	H9B-C9-C8-C18	-162.4	-158.91
						H9B-C9-C8-C7	20	24.16
						C9-C8-C18-H18C	90.3	62.77
						C9-C8-C18-H18A	-29.6	-54.85
						C9-C8-C18-H18B	-149.7	-176.83
						C7-C8-C18-H18C	-92.6	-120.43
						C7-C8-C18-H18A	147.4	121.95
						C7-C8-C18-H18B	27	39.1
						C9-C8-C7-C6	168.0(7)	168.06
						C9-C8-C7-H7	-12	-5.38
						C18-C8-C7-C6	-9(1)	-8.55
						C18-C8-C7-H7	170.9	178.01
						C1-C13-C14-C12	-52.1(7)	-54.56
						C1-C13-C14-H14A	-174	-179.62

						C1-C13-C14-H14B	69.8	64.71
						H13A-C13-C14-C12	68.6	68.03
						H13A-C13-C14-	-53.2	-57.04
						H13A-C13-C14-	-169.5	-172.7
						H13-C13-C14-C12	-172.9	-175.51
						H13-C13-C14-H14A	65.2	59.43
						H13-C13-C14-H14B	-51.1	-56.24
						C2-C3-C4-C19	4.2(9)	2.13
						C2-C3-C4-C5	-176.4(5)	-179.87
						H3-C3-C4-C19	-175.6	-179.46
						H3-C3-C4-C5	3.8	-1.46
						C3-C4-C19-H19A	17.9	-2.53
						C3-C4-C19-H19B	-102.1	-124.48
						C3-C4-C19-H19C	138	117.68
						C5-C4-C19-H19A	-161.5	-179.4
						C5-C4-C19-H19B	78.5	57.45
						C5-C4-C19-H19C	-41.4	-60.4
						C3-C4-C5-H5B	131.1	132.68
						C3-C4-C5-H5A	13.6	16.01
						C3-C4-C5-C6	-107.8(6)	-105.44
						C19-C4-C5-H5B	-49.5	-49.15
						C19-C4-C5-H5A	-167	-165.81
						C19-C4-C5-C6	71.6(7)	72.74
						C4-C5-C6-H6A	178.2	177.63
						C4-C5-C6-H6B	-63.3	-67.13
						C4-C5-C6-C7	57.5(7)	56.66
						H5B-C5-C6-H6A	-60.6	-59.72
						H5B-C5-C6-H6B	57.9	55.52
						H5B-C5-C6-C7	178.7	179.31
						H5A-C5-C6-H6A	56.9	55.79
						H5A-C5-C6-H6B	175.3	171.03
						H5A-C5-C6-C7	-63.9	-65.17
						C5-C6-C7-C8	-108.1(8)	-113.15
						C5-C6-C7-H7	72.1	60.44
						H6A-C6-C7-C8	131.1	127.69
						H6A-C6-C7-H7	-48.6	-58.73
						H6B-C6-C7-C8	13	9.65
						H6B-C6-C7-H7	-167.1	-176.76

Table S2. The calculated harmonic vibrational frequencies (in cm^{-1}) and their assignments and contribution for sarcotrocheliol using DFT computational with B3LYP exchange correlation and 6-311G++(d,p) basis sets.

cm^{-1}	Assign													
3728.6	υOH	21.13	υOH	100										
3028.1	υCH	25.7	βHCH	94										
3025.0	υCH	21.16	υCH	80	υCH	-14								
3022.7	υCH	17.06	υCH	85										
3018.9	υCH	28.84	υCH	85										
3007.6	υCH	26.81	υCH	-42	υCH	55								
3002.7	υCH	32.6	υCH	86										
3001.5	υCH	28.31	βHCH	10	υCH	73								
2996.9	υCH	40.04	υCH	75	υCC	-10								
2995.5	υCH	14.96	υCH	-28	υCH	67								
2988.9	υCH	20.99	βHCH	83										
2980.6	υCH	73.12	υCH	-17	υCC	31	υCH	-17	υCH	28				
2980.1	υCH	11.34	υCH	70	υCH	11								
2972.9	υCH	33.2	υCH	17	υCH	-10	υCH	44	υCH	-13				
2972.4	υCH	3.35	υCH	15	υCC	-30	υCH	-18	υCH	31				
2972.1	υCH	22.47	υCH	-11	υCH	50	υCH	-22						
2971.2	υCH	46.45	υCH	67	υCH	15								
2962.0	υCH	16.24	υCH	-29	υCH	65								
2957.7	υCH	27.42	γCCOC	63										
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2948.8	υCH	26.22	υCH	39	υCH	16	υCH	12	υCH	10				
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2918.4	υCH	22.28	υCH	-23	υCH	10	υCH	39						
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2910.5	υCH	4.77	υCC	73	υCH	-11								
2907.8	υCH	11.85	υCH	53	υCH	14	υCH	-30						
2884.7	υCH	8.68	βHCH	91										
1670.4	υCC	3.06	υCC	69										
1654.7	υCC	24.31	υCC	71										
1468.2	υCC	12.78	βHCH	-11	βHCH	25	βHCH	-13	βHCH	26				
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1459.4	υCC	6.41	βHCH	10	βHCH	52								
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1427.6	υCC	1.79	βHCH	33	γCCOC	-25	γCCOC	12						
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1367.8	βHOC	9.07	βHCO	10	γCCOC	-15	υCH	-12						
1366.4	βHCH	15.38	γCCOC	20	γCCOC	23								

1355.7	βHCH	5.77	βHCH	-12	βHCH	-14	βHCH	-10	βHCH	21	βHCH	18	βHCH	14
1353.3	βHCH	1.66	βHCO	-19	βHCC	18								
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951.7	βCCC	1.89												
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822.8	τHCCH	5.96	υCH	10										
809.5	τHCOH	1.43												
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566.7	τHCCC	0.81	υCH	11										

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518.1	τHCCC	2.17	υCH	-13										
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294.7	τHCCC	9.38												
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173.3	τCCCC	0.28												
157.4	τOCCC	0.2												
155.0	τCCCC	0.15	υCH	29										
144.7	τCOCC	0.19	υCH	-13	υCH	-15	υCH	-15	υCH	-10				
128.8	τCCCC	0.75	υCH	-10	υCH	-13	υCH	-13						
118.8	γOCCC	0.14	υCH	10	υCH	11	υCH	-10						
87.4	γCCOC	0.41	υCH	-17	υCH	14								
72.0	γCCCC	0.02	υCH	-14	υCH	11	υCH	10						
66.6	γCCCC	0.5	υCH	29										
52.7	γCCCC	0.04	υCH	50										
48.0	γCCCC	0.12	υCH	41										
35.5	γCCOC	0.14	υCH	22										

υ – stretching; γ – out-of-plane deformation; τ – torsion; s – symmetric; β – bending.

Fig. S1. Comparison of bond lengths in optimized structure (left) and crystal structure (right).

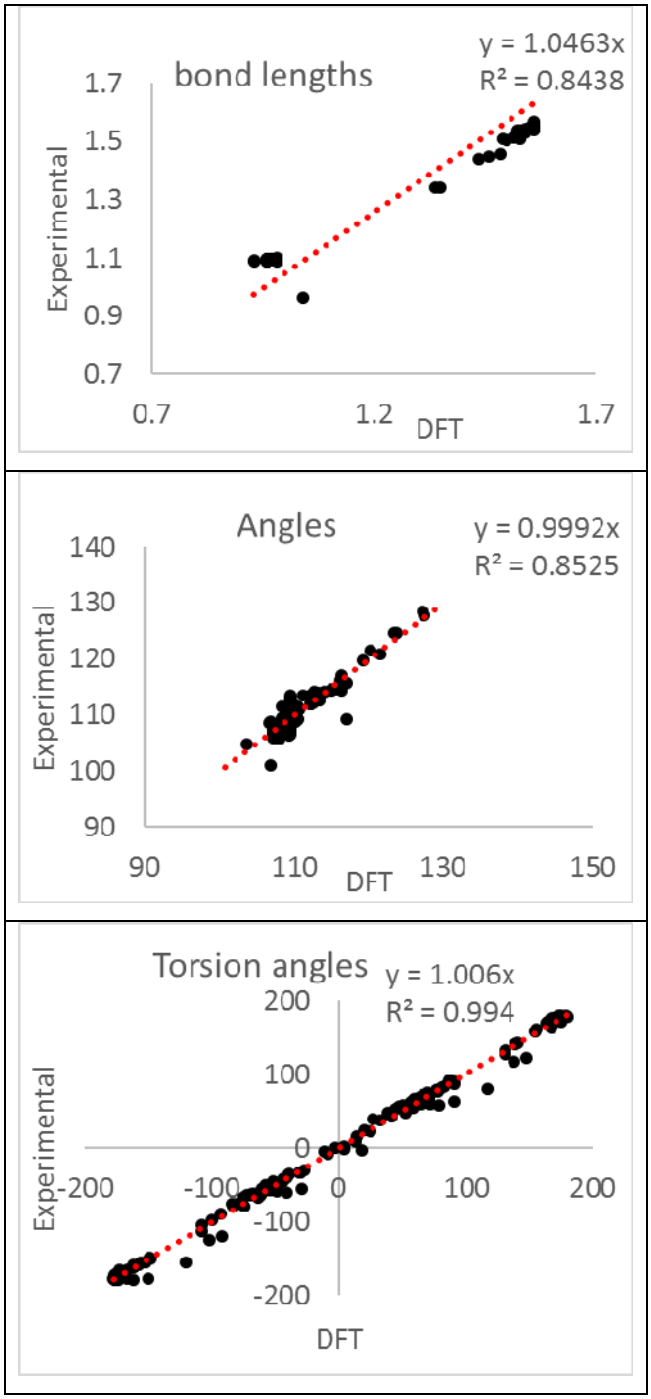


Fig. S2. Correlation between experimental and calculated ^{1}H and ^{13}C chemical shifts in $CDCl_3$, CD_3CN, MeOH-D4 and DMSO-d_6.

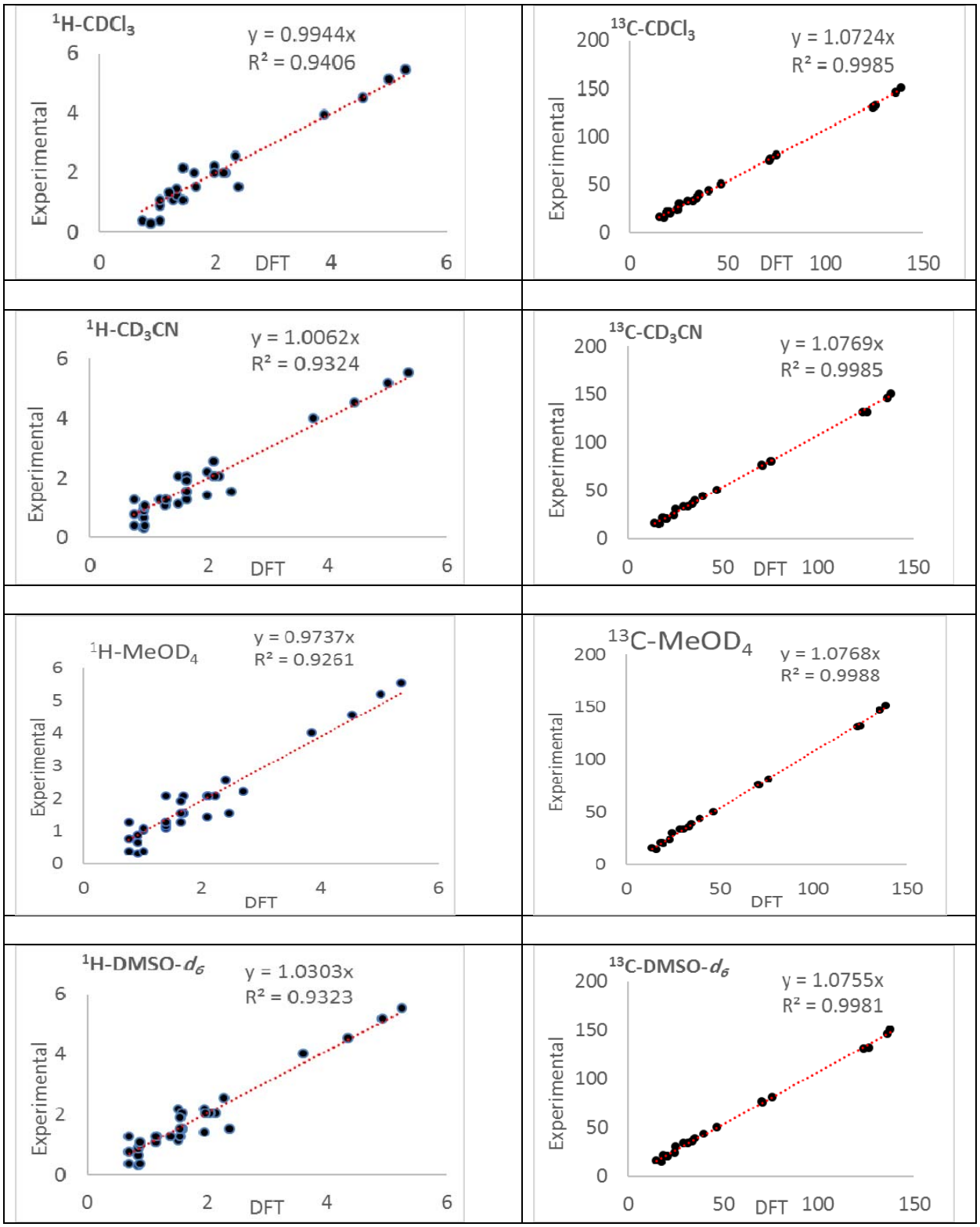
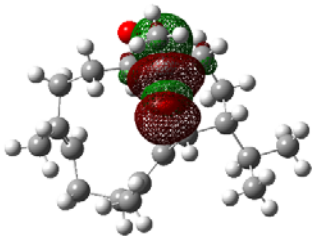
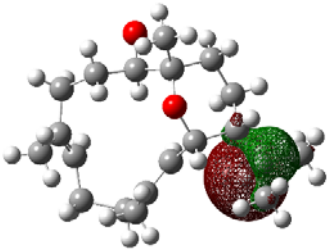


Fig. S3. Molecular orbital shapes of sarcotrocheliol using B3LYP/6-311G++(d,p).

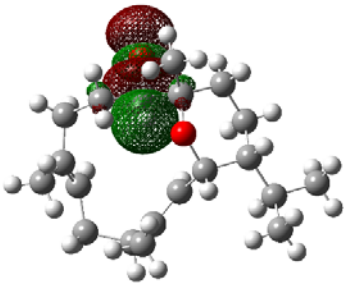
LUMO+4



HOMO-4



LUMO+3



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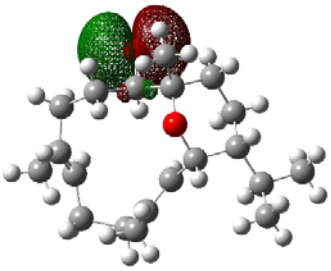

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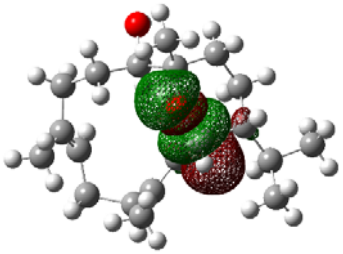

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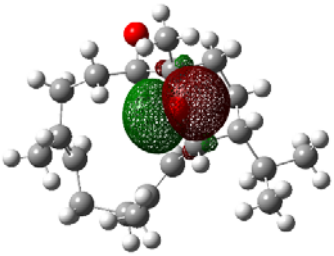

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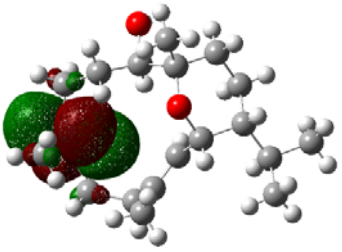

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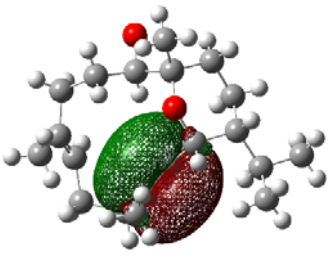


LUMO

HOMO

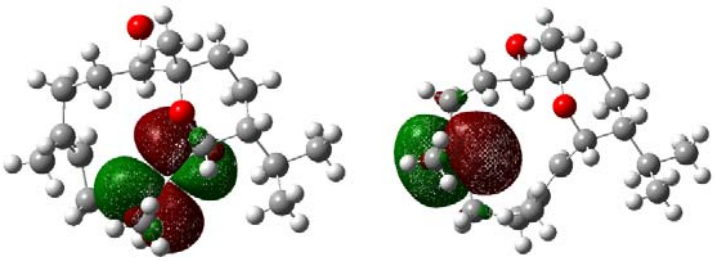


Fig. S4. Molecular orbital energies of sarcotrocheliol molecule in gas phase and in different solvents using B3LYP/6-311G++(d,p).

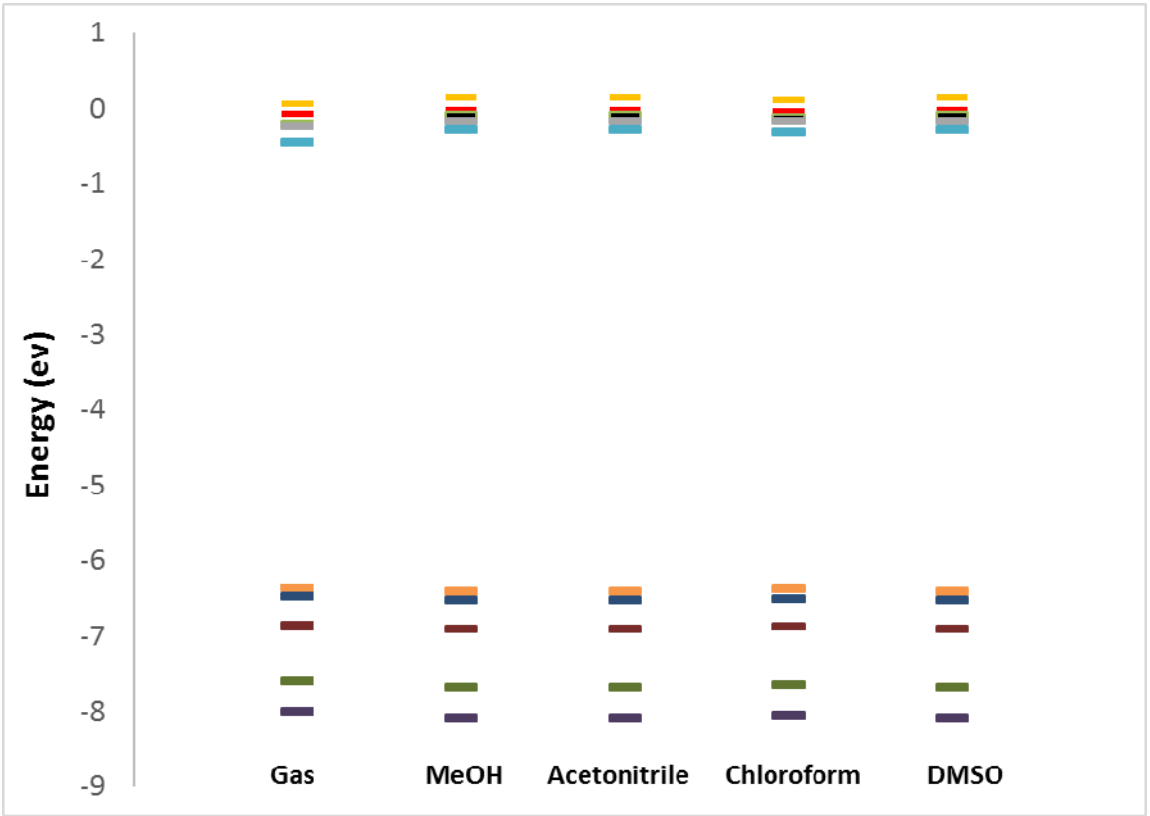
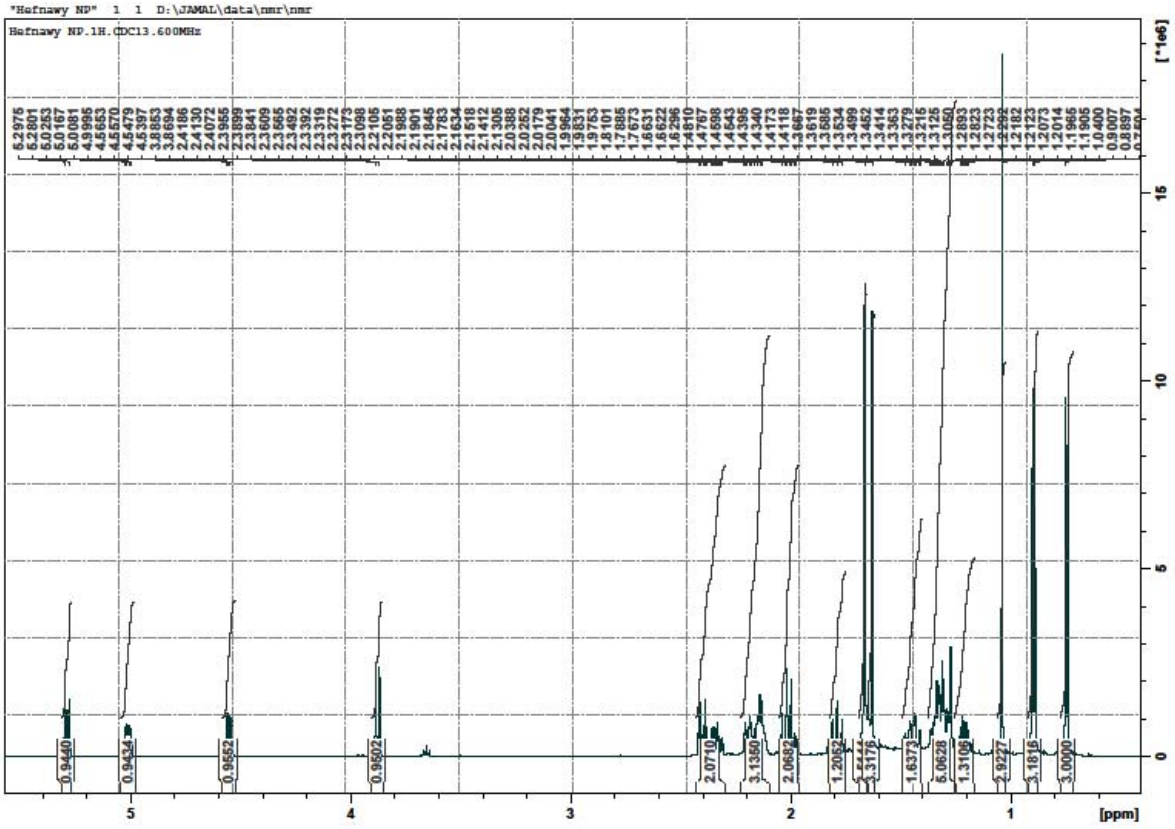
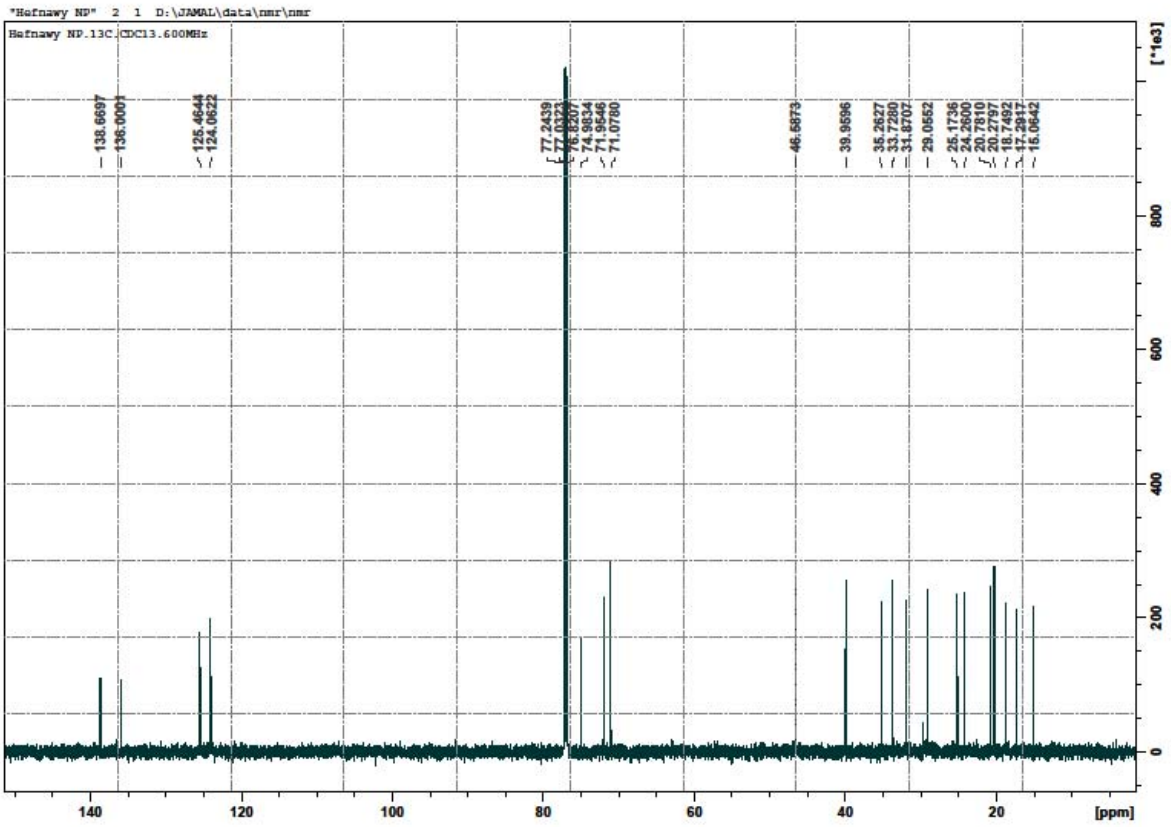


Fig. S5. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in $CDCl_3$.

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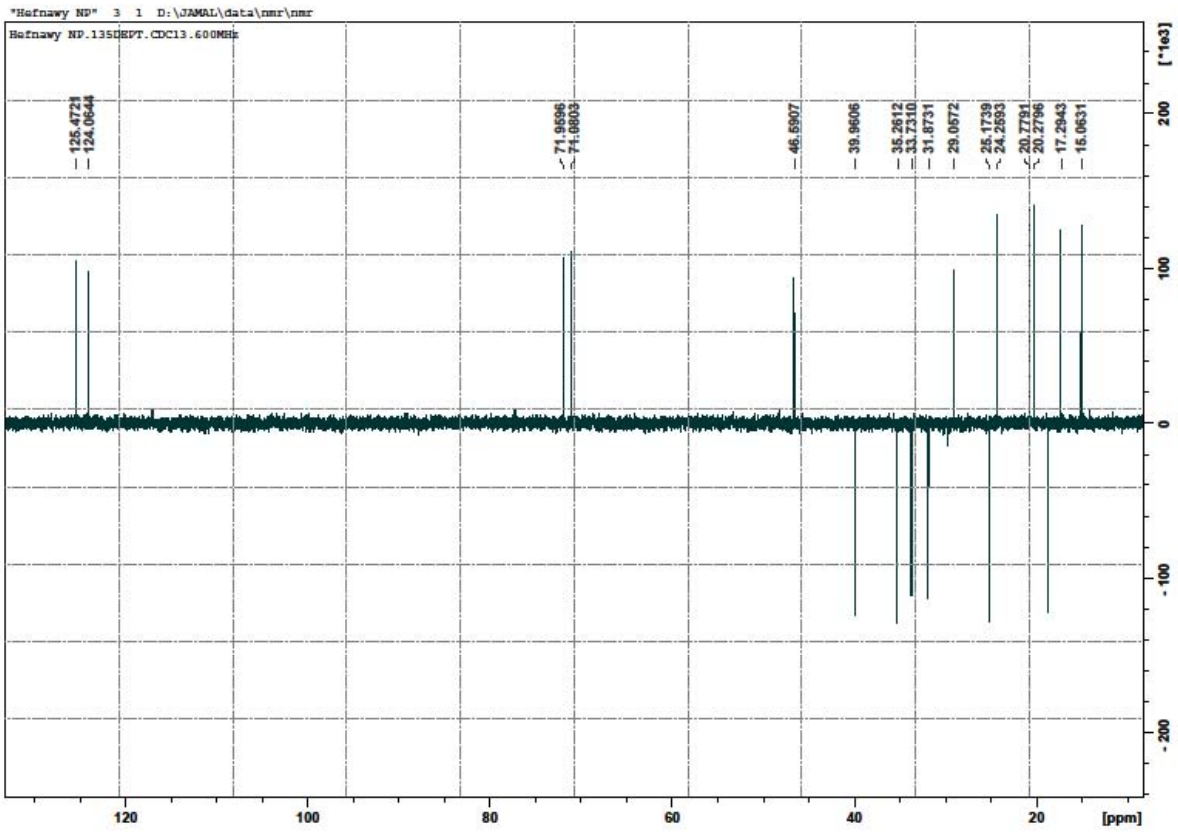
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15.0631
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0
- 100
- 200
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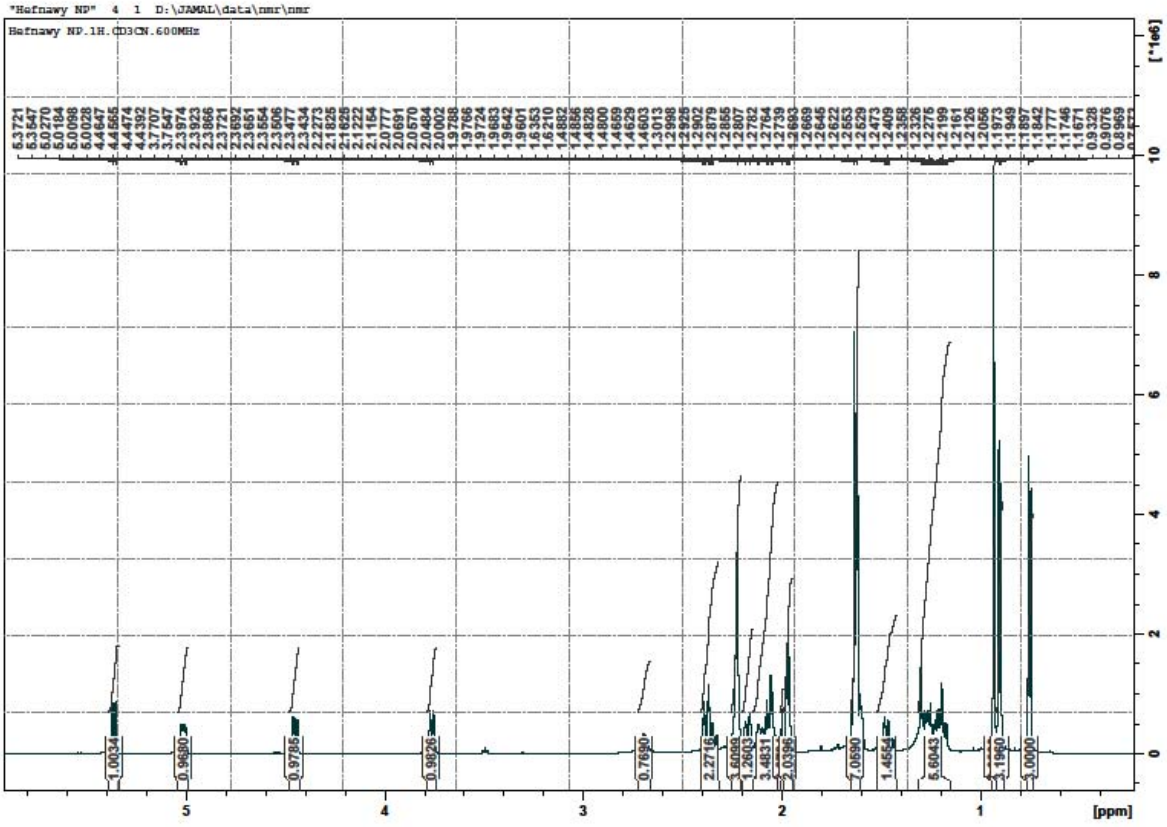
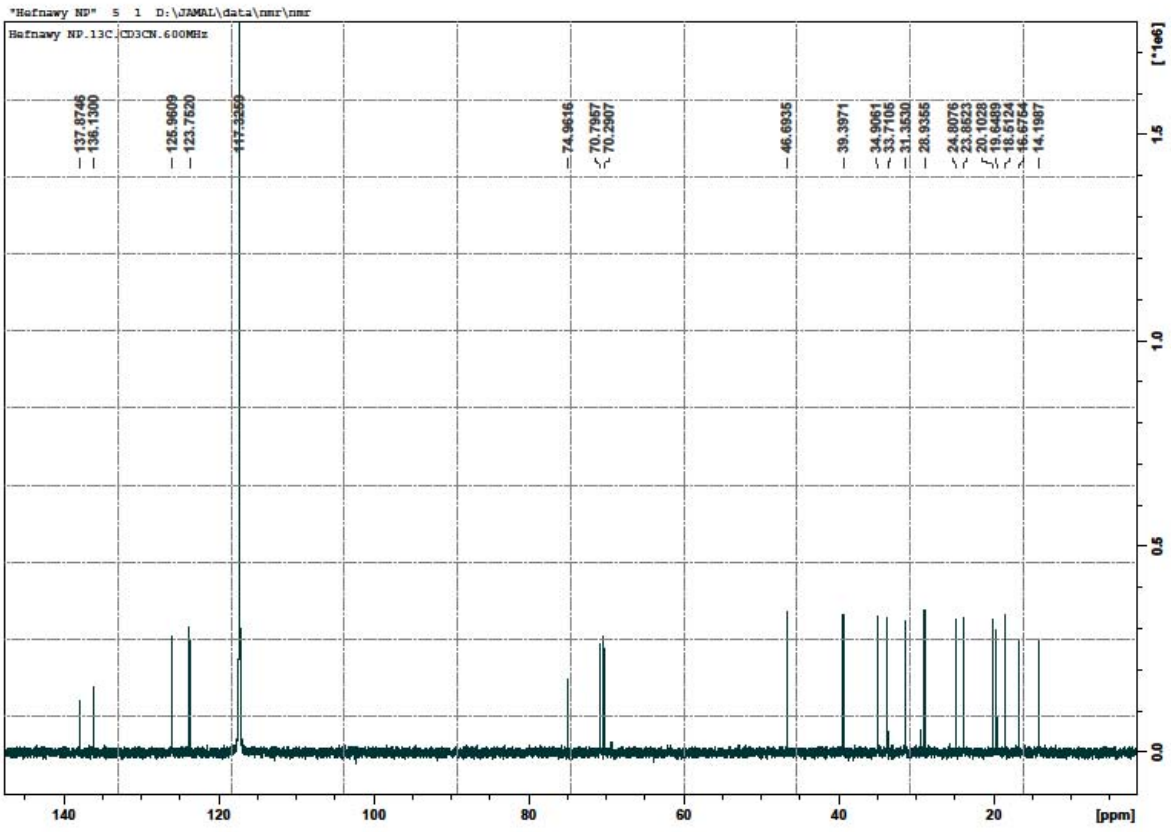
[ppm]

Fig. S6. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in CD_3CN.

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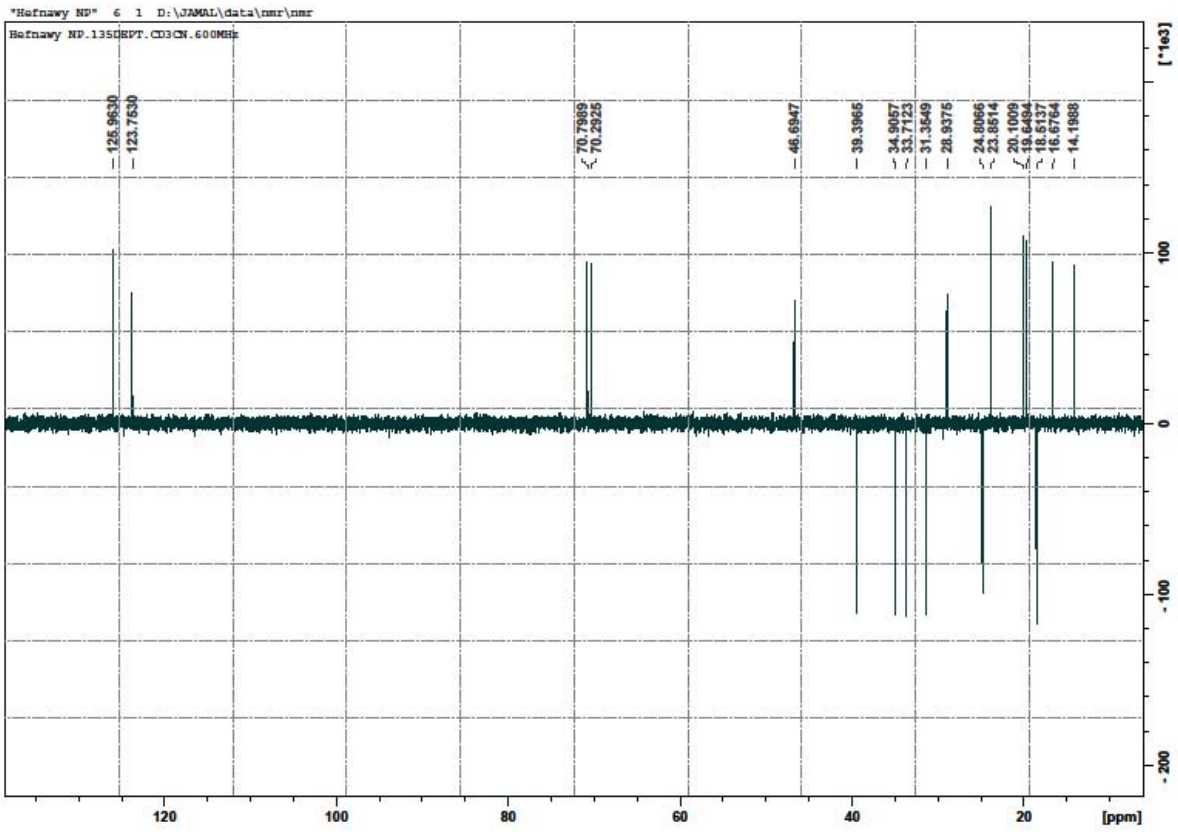
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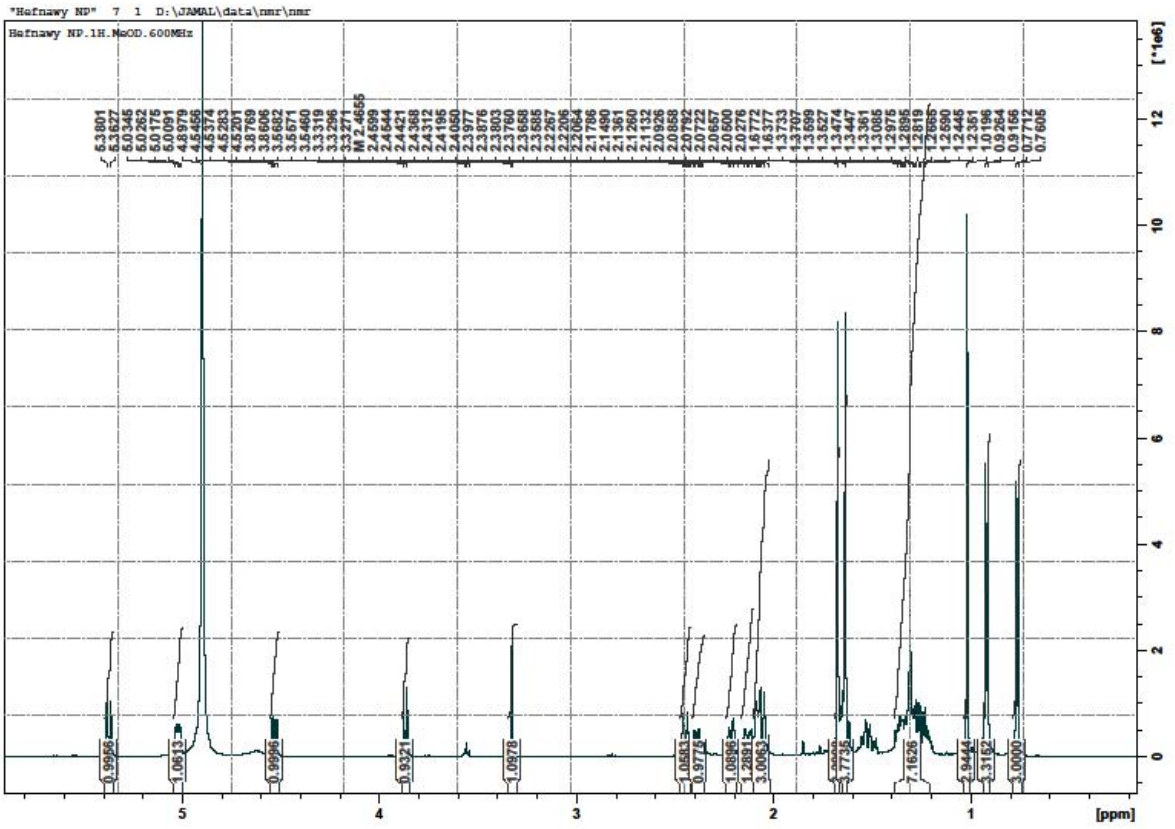
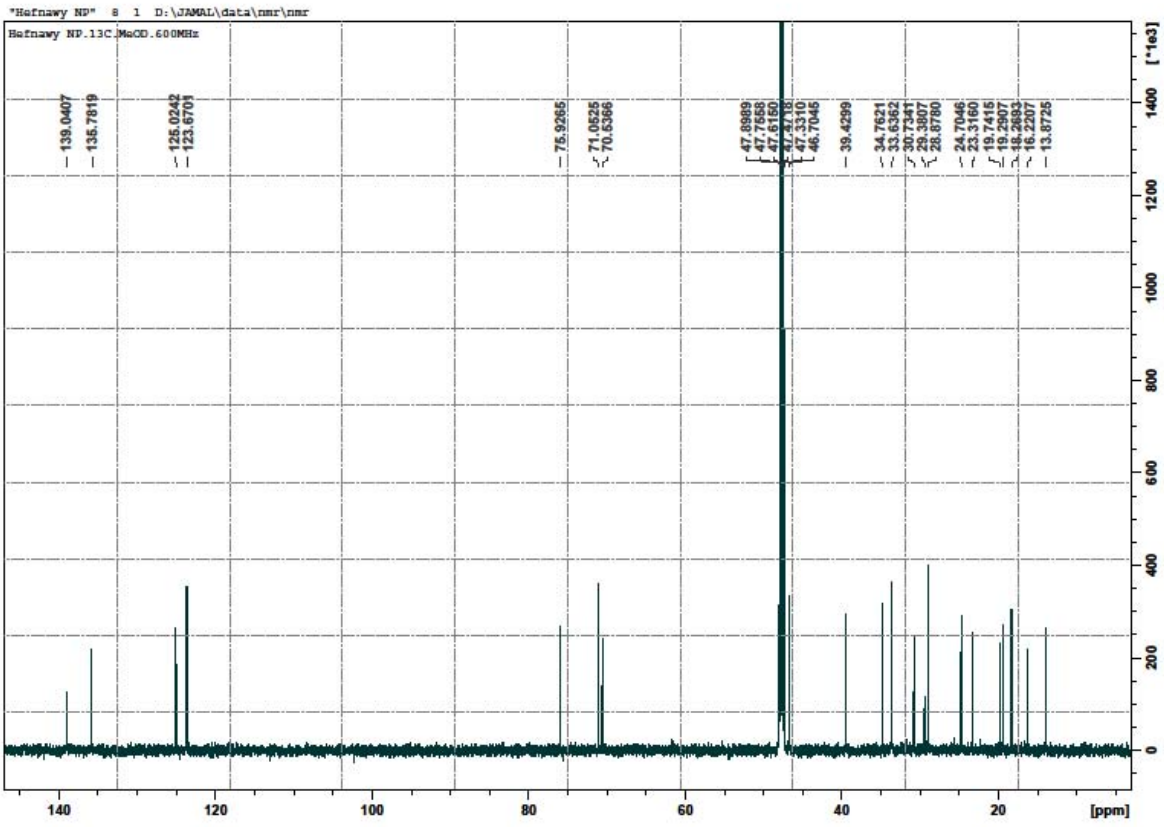
Fig. S7. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in MeOH-D4.

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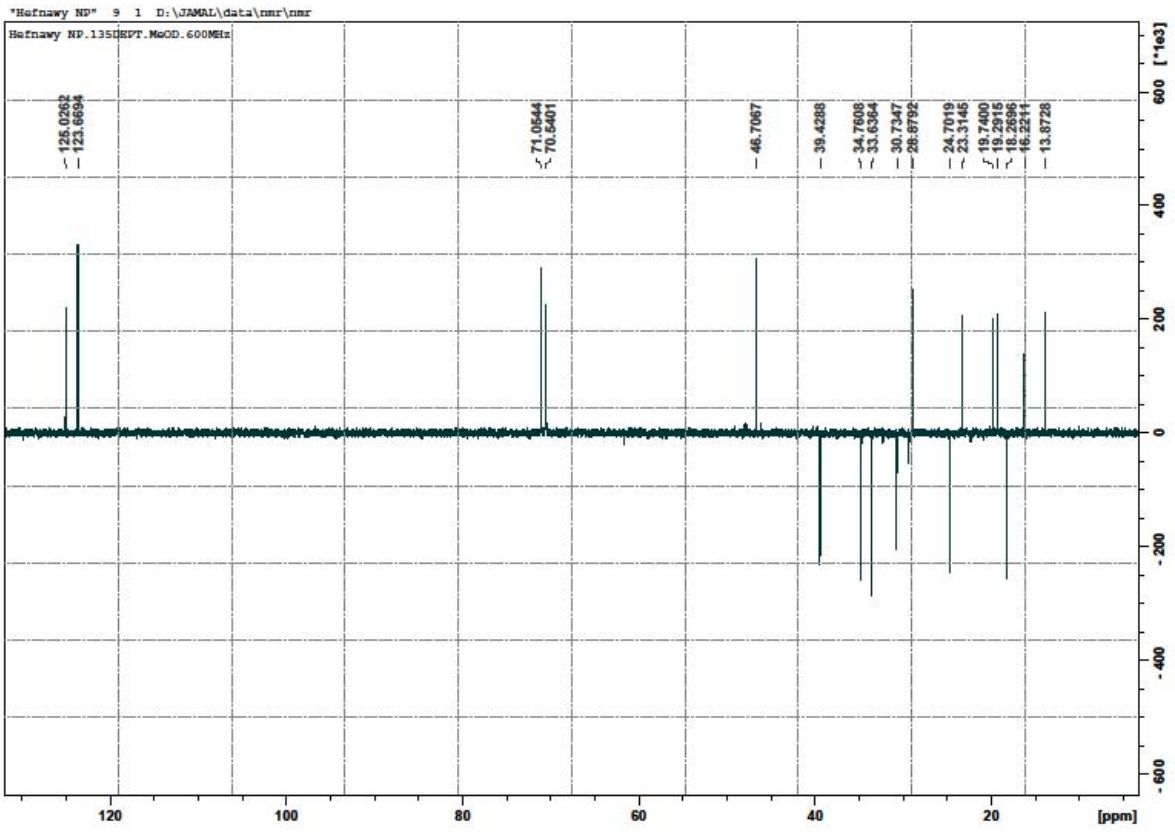
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- 400
- 600
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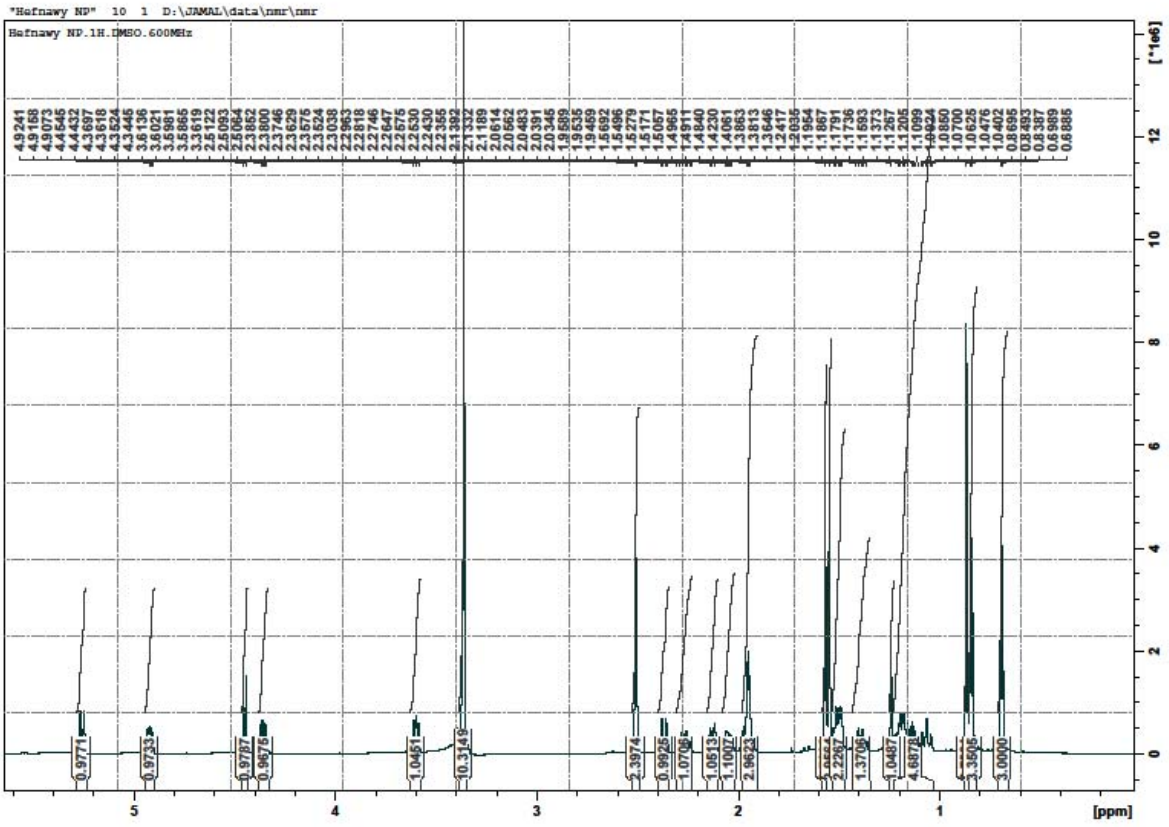
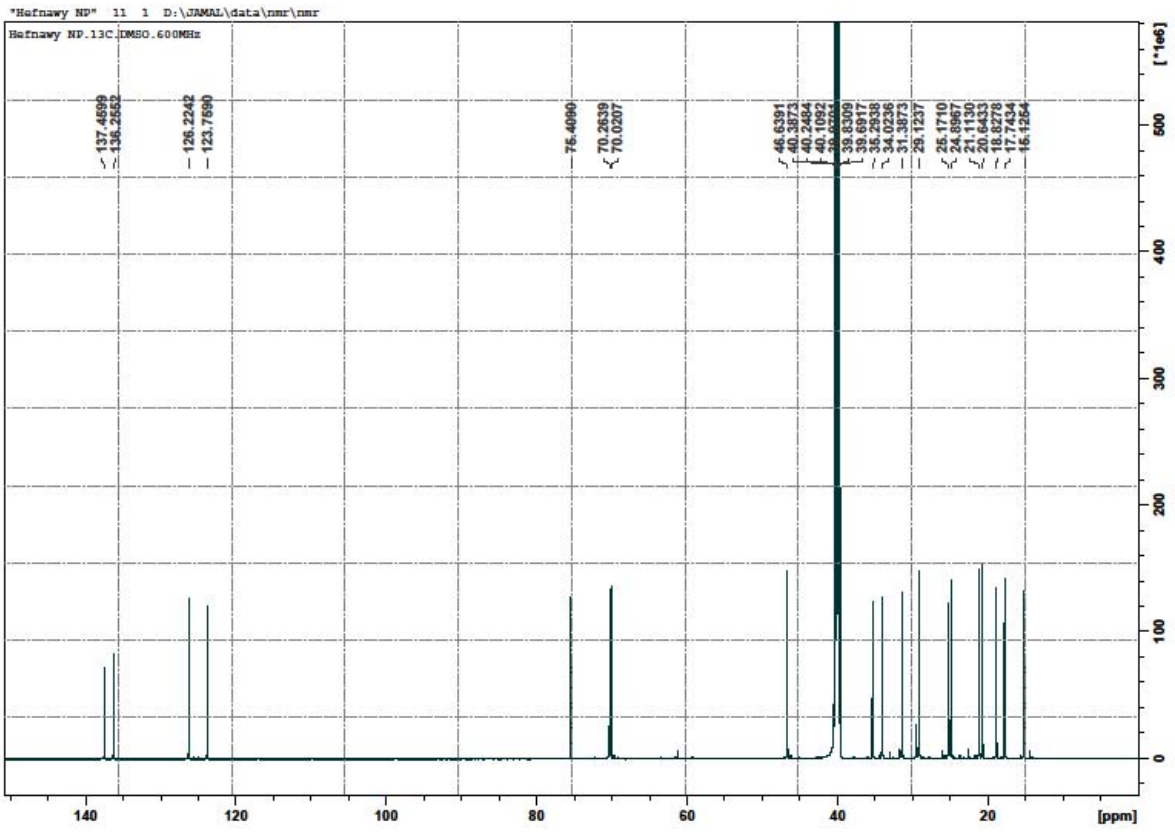
Fig. S8. ^{1}H, ^{13}C and DEPT-135 NMR spectra of sarcotrocheliol in DMSO-d_6.

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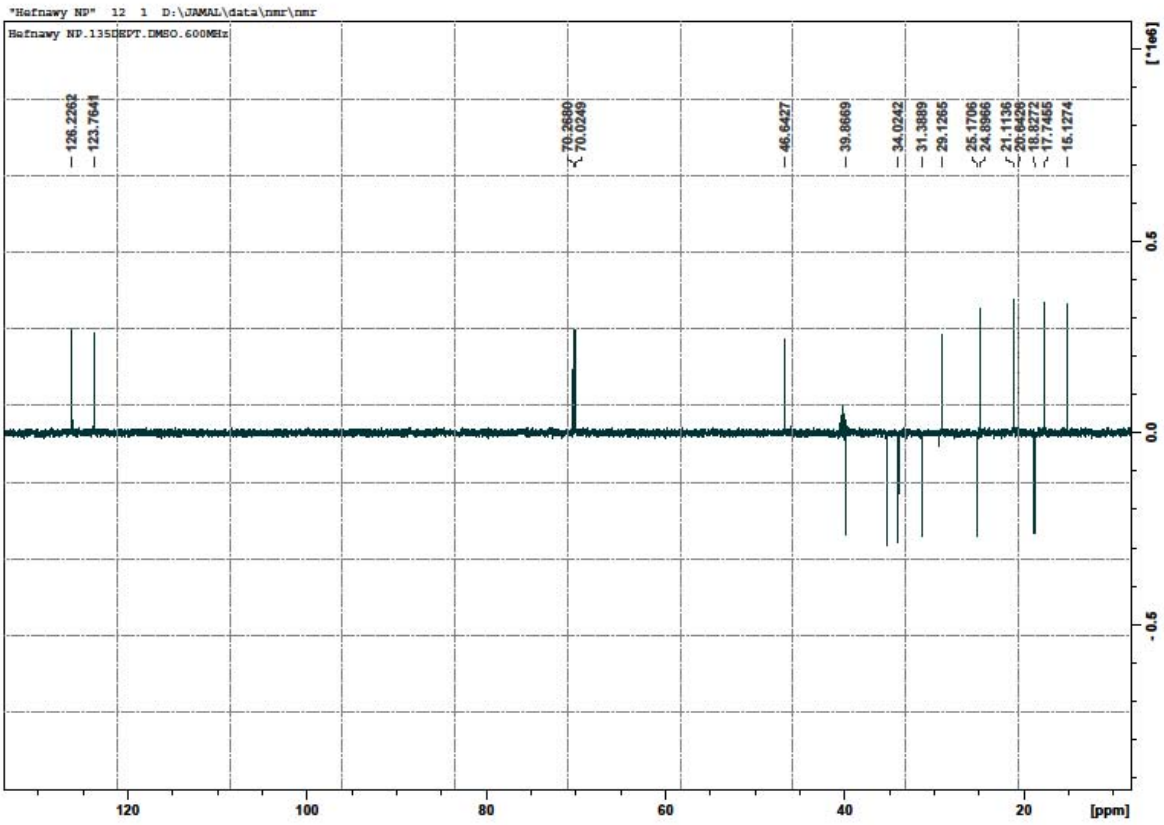
126.2242
123.7690
75.4090
70.2639
70.0207
46.6391
40.3873
40.2484
40.1092
39.8309
39.6917
35.2938
34.0236
31.3873
29.1237
25.1710
24.8967
21.1130
20.6433
18.8278
17.7434
16.1264
[*1e6]
500
400
300
200
100
0
140
120
100
80
60
40
20
[ppm]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Hefnawy NP.135DEPT.DMSO.600MHz
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123.7641
70.2680
70.0249
46.6427
39.8669
34.0242
31.3889
29.1265
25.1706
24.8966
21.1136
20.6426
18.8272
17.7455
15.1274
[*1e6]
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0.0
-0.5
120
100
80
60
40
20
[ppm]