Supplementary Information

Structure of saligenin: Microwave, UV and IR spectroscopy studies in a supersonic jet combined with quantum chemistry calculations

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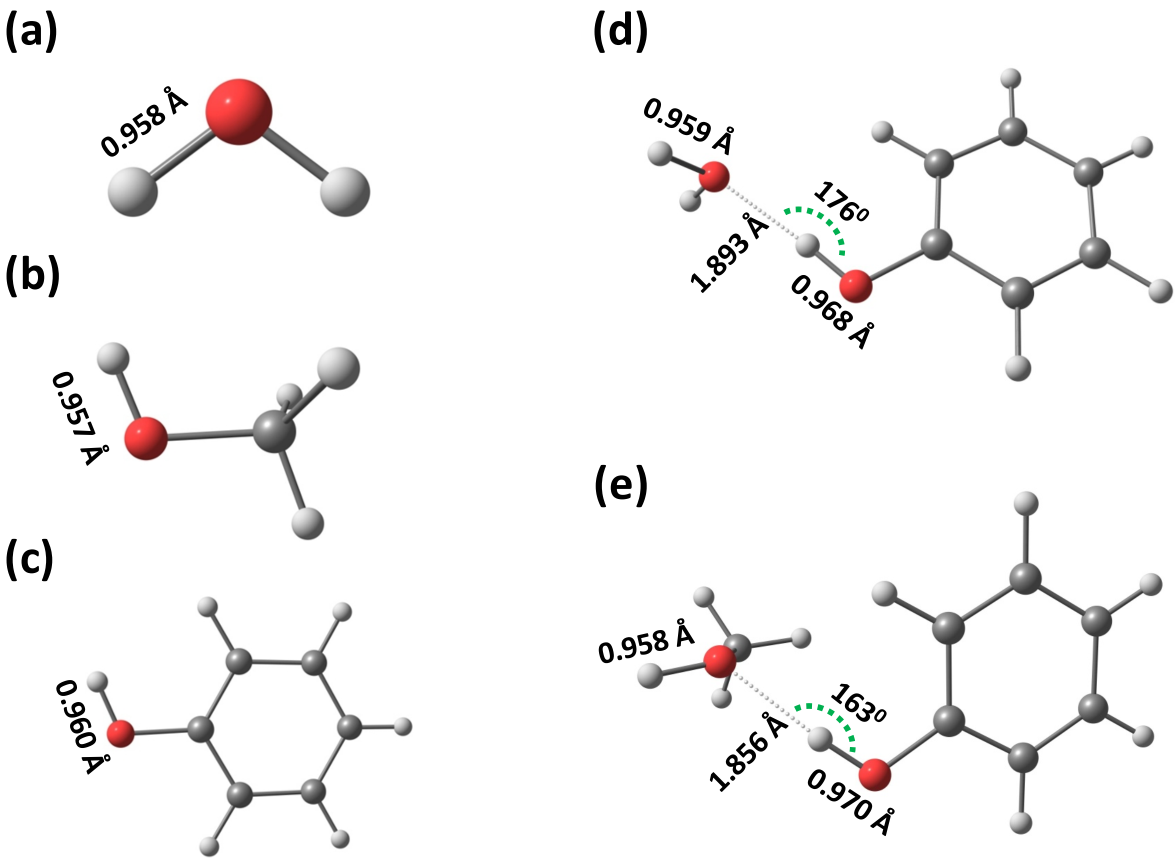
(a)
0.958 Å
(b)
0.957 Å
(c)
0.960 Å
(d)
0.959 Å
176^0
1.893 Å
0.968 Å
(e)
0.958 Å
163^0
1.856 Å
0.970 Å

Figure S1: Optimized structures of (a) water (b) methanol (c) phenol (d) phenol…water complex and (e) phenol…methanol complex obtained at the M05-2X/aug-cc-pVTZ level of theory.

Table S1: Theoretical OH stretch frequencies ($\nu_{OH}^{benzylic}$ *and* $\nu_{OH}^{phenolic}$) of SA1, SA2, and SA3 conformers of saligenin calculated using different basis sets at the M05-2X level of theory. Scaling of the calculated harmonic frequencies has been done with respect to experimental frequency of phenol OH stretch, gauche benzyl alcohol (BA1) O-H stretch, phenolic as well as benzylic O-H stretch of saligenin (SA1) and water O-H stretch

Scaling factor has been obtained by taking the ratio of experimental and calculated frequencies. [a]Experimental OH stretch frequency of phenol,ν_{OH} (phenol): 3657 cm^{-1} (Ref.

Theory	Scaling factor	$\nu_{OH}^{benzylic}$ (cm^{-1})			$\nu_{OH}^{phenolic}$ (cm^{-1})		
		SA1	SA2	SA3	SA1	SA2	SA3
Scaling with respect to ν_{OH} (phenol)[a]							
M05-2X/cc-pVTZ	0.9424	3638	3492	3641	3492	3493	3657
M05-2X/cc-pVQZ	0.9393	3632	3490	3634	3490	3492	3651
M05-2X/aug-cc-pVDZ	0.9393	3636	3498	3642	3498	3500	3659
M05-2X/aug-cc-pVTZ	0.9440	3638	3499	3641	3499	3500	3658
Scaling with respect to ν_{OH} (BA1)[b]							
M05-2X/cc-pVTZ	0.9431	3641	3495	3644	3663	3495	3660
M05-2X/cc-pVQZ	0.9414	3640	3498	3643	3662	3499	3659
M05-2X/aug-cc-pVDZ	0.9401	3639	3501	3645	3662	3503	3662
M05-2X/aug-cc-pVTZ	0.9443	3639	3500	3642	3661	3500	3659
Scaling with respect to $\nu_{OH}^{benzylic}$ (SA1)[c]							
M05-2X/cc-pVTZ	0.9418	3636	3658	3639	3490	3490	3659
M05-2X/cc-pVQZ	0.9403	3636	3658	3638	3494	3495	3655
M05-2X/aug-cc-pVDZ	0.9394	3636	3659	3643	3499	3500	3654
M05-2X/aug-cc-pVTZ	0.9435	3636	3658	3639	3497	3497	3652
Scaling with respect to $\nu_{OH}^{phenolic}$ (SA1)[c]							
M05-2X/cc-pVTZ	0.9430	3640	3662	3643	3494	3495	3659
M05-2X/cc-pVQZ	0.9403	3636	3658	3638	3494	3495	3655
M05-2X/aug-cc-pVDZ	0.9381	3631	3654	3638	3494	3496	3654
M05-2X/aug-cc-pVTZ	0.9426	3633	3654	3636	3494	3494	3652

35); [b]Experimental OH stretch frequency of gauche benzyl alcohol,ν_{OH} (BA1): 3657 cm^{-1} (Ref. 10); [c]Experimental stretch frequencies of benzylic and phenolic OH groups of saligenin, respectively, $\nu_{OH}^{benzylic}$ (SA1): 3636 cm^{-1}, $\nu_{OH}^{phenolic}$ (SA1): 3494 cm^{-1} (This work).

Table S2. Experimental rotational frequencies (MHz) of saligenin and its hydroxyl deuterated species

	Saligenin		Saligenin-CH2OD-OH		Saligenin-CH2OH-OD		Saligenin-CH2OD-OD	
J''(K''$_a$,K''$_c$)-J'(K'$_a$,K'$_c$)	Exp	Exp-calc	Exp	Exp-calc	Exp	Exp-calc	Exp	Exp-calc
18(5,14)- 17(4,14)	64835.69	-0.01975						
17(5,12)- 16(4,13)	71071.83	-0.00056						
16(5,11)- 15(4,12)	64811.45	-0.00973						
14(4,10)- 13(3,11)	60150.15	0.02035						
16(6,10)- 15(5,11)	60520.17	0.0221						
17(6,11)- 16(5,12)	64710.34	-0.01818						
18(6,12)- 17(5,13)	69654.03	0.00171						
18(6,13)- 17(5,13)	64839.4	-0.00712						
25(6,20)- 24(5,19)	60605	-0.00358						
16(7,10)- 15(6, 9)	60837.31	-0.00543						
16(7, 9)- 15(6,10)	61875.83	0.0027						
16(7,10)- 15(6,10)	61687.09	-0.00525						
16(7, 9)- 15(6, 9)	61026.01	-0.03748						
17(7,10)- 16(6,11)	64567.69	-0.01527						
17(7,11)- 16(6,10)	62494.06	-0.00968						
17(7,10)- 16(6,10)	62913.84	0.02185						
17(7,11)- 16(6,11)	64147.96	0.0032						
18(7,12)- 17(6,11)	63749.89	-0.00775						
18(7,11)- 17(6,12)	67562.43	0.04124						
19(7,13)- 18(6,12)	64554.75	-0.00194						
19(7,12)- 18(6,13)	71026.18	0.0052						
20(7,14)- 19(6,13)	64940.35	0.04247						
21(7,15)- 20(6,14)	65012.07	-0.00182						
22(7,16)- 21(6,15)	64920.52	0.02885						
23(7,17)- 22(6,16)	64837.38	-0.01705						
24(7,18)- 23(6,17)	64934.46	-0.02743						
14(8, 7)- 13(7, 6)	60500.56	0.01447			59901.00	-0.03446		
14(8, 6)- 13(7, 7)	60512.34	0.01664			59913.02	-0.05584		
14(8, 7)- 13(7, 7)	60510.89	-0.01048						
14(8, 6)- 13(7, 6)	60501.98	0.01159						
15(8, 8)- 14(7, 7)	62858.17	-0.01256						
15(8, 7)- 14(7, 8)	62892.64	0.00164						
15(8, 7)- 14(7, 7)	62862.72	-0.00297						
15(8, 8)- 14(7, 8)	62888.08	-0.01796						
16(8, 9)- 15(7, 8)	65172.66	0.02192						
16(8, 8)- 15(7, 9)	65264.19	-0.02074						
16(8, 8)- 15(7, 8)	65185.78	0.00361						
16(8, 9)- 15(7, 9)	65251.00	-0.07243						
17(8,10)- 16(7, 9)	67415.08	-0.00082						
17(8, 9)- 16(7,10)	67638.75	0.02174						

17(8, 9)- 16(7, 9)	67449.98	-0.01622						
17(8,10)- 16(7,10)	67603.76	-0.05287						
18(8,10)- 17(7,11)	70042.43	0.01003						
18(8,11)- 17(7,10)	69536.67	0.00097						
13(9, 5)- 12(8, 4)	61696.96	0.04514	60879.16	0.08422	61081.8	0.06065	60272.34	0.05831
13(9, 4)- 12(8, 5)	61696.96	-0.06124	60879.16	0.00414	61081.8	-0.04868	60272.34	-0.02477
13(9, 4)- 12(8, 4)	61696.96	0.03513	60879.16	0.07691	61081.8	0.05031	60272.34	0.05069
13(9, 5)- 12(8, 5)	61696.96	-0.05123	60879.16	0.01144	61081.8	-0.03834	60272.34	-0.01715
14(9, 6)- 13(8, 5)	64106.95	0.04825	63248.19	0.19826	63469.35	-0.00273	62620.19	0.18732
14(9, 5)- 13(8, 5)	64106.95	0.00291	63248.19	-0.13525	63469.35	-0.04952	62620.19	-0.15861
14(9, 5)- 13(8, 6)	64107.36	0.01563	63248.19	0.16515	63469.73	-0.07754	62620.19	0.15279
14(9, 6)- 13(8, 6)	64107.36	0.06097	63248.19	-0.10214	63469.73	-0.03075	62620.19	-0.12408
15(9, 7)- 14(8, 6)	66506.24	0.00899	65607.2	0.02161	65846.37	0.06976	64957.95	-0.01462
15(9, 6)- 14(8, 6)	66506.4	-0.00885	65607.2	-0.10844	65846.37	-0.11375	64958.12	0.01978
15(9, 6)- 14(8, 7)	66507.83	-0.00172	65608.37	-0.0161	65847.94	-0.0048	64959.20	-0.01701
15(9, 7)- 14(8, 7)	66507.83	0.17612	65608.37	0.11395	65847.94	0.17871	64959.20	0.11858
16(9, 8)- 15(8, 7)	68890.94	0.00989	67953.14	-0.00679	68208.6	0.01629	67282.60	-0.04543
16(9, 7)- 15(8, 7)	68891.53	-0.02026						
16(9, 7)- 15(8, 8)	68896.10	0.00934	67957.04	-0.00682	68213.87	-0.01429	67286.71	0.02139
16(9, 8)- 15(8, 8)	68895.47	-0.00051			68213.29	0.04546		
17(9, 9)- 16(8, 8)	71255.15	0.02992						
17(9, 8)- 16(8, 8)	71257.09	0.01207						
17(9, 8)- 16(8, 9)	71270.20	-0.01625						
17(9, 9)- 16(8, 9)	71268.25	-0.0084						
11(10, 2)- 10(9, 1)	60403.91	-0.0123	59638.42	-0.01481	59795.27	-0.08489		
11(10, 1)- 10(9, 2)	60403.91	-0.01233	59638.42	-0.01483	59795.27	-0.08492		
11(10, 1)- 10(9, 1)	60403.91	-0.0123	59638.42	-0.01481	59795.27	-0.08489		
11(10, 2)- 10(9, 2)	60403.91	-0.01233	59638.42	-0.01483	59795.27	-0.08492		
12(10, 3)- 11(9, 2)	62831.17	-0.02222	62023.27	0.01002	62200.23	-0.01299	61398.64	-0.00074
12(10, 2)- 11(9, 3)	62831.17	-0.02251	62023.27	0.00981	62200.23	-0.01329	61398.64	-0.00095
12(10, 2)- 11(9, 2)	62831.17	-0.02224	62023.27	0.01001	62200.23	-0.01301	61398.64	-0.00075
12(10, 3)- 11(9, 3)	62831.17	-0.02249	62023.27	0.00983	62200.23	-0.01326	61398.64	-0.00094
13(10, 4)- 12(9, 3)	65255.73	-0.01722	64405.57	-0.00604	64602.4	-0.01891	63759.81	0.02407
13(10, 3)- 12(9, 4)	65255.73	-0.01923	64405.57	-0.0075	64602.4	-0.02098	63759.81	0.02254
13(10, 3)- 12(9, 3)	65255.73	-0.01738	64405.57	-0.00616	64602.4	-0.01908	63759.81	0.02394
13(10, 4)- 12(9, 4)	65255.73	-0.01906	64405.57	-0.00738	64602.4	-0.02081	63759.81	0.02266
14(10, 5)- 13(9, 4)	67676.21	0.01893	66784.04	-0.05693	67000.54	0.05277	66117.15	0.01882
14(10, 4)- 13(9, 5)	67676.21	0.00794	66784.04	-0.06493	67000.54	0.04141	66117.15	0.01048
14(10, 4)- 13(9, 4)	67676.21	0.01795	66784.04	-0.05763	67000.54	0.05175	66117.15	0.0181
14(10, 5)- 13(9, 5)	67676.21	0.00892	66784.04	-0.06424	67000.54	0.04243	66117.15	0.01121
15(10, 6)- 14(9, 5)	70090.92	0.0354	69157.34	0.02205	69392.84	0.03104	68469.17	0.00147
15(10, 5)- 14(9, 6)	70090.92	-0.01478	69157.34	-0.01448	69392.84	-0.02076	68469.17	-0.03664
15(10, 5)- 14(9, 5)	70090.92	0.03056	69157.34	0.01863	69392.84	0.02603	68469.17	-0.00211

15(10, 6)- 14(9, 6)	70090.92	-0.00994	69157.34	-0.01106	69392.84	-0.01575	68469.17	-0.03306
16(10, 7)- 15(9, 6)	72497.97	0.08037	71523.52	0.04962	71777.6	0.15564	70814.19	0.06622
16(10, 6)- 15(9, 7)	72497.97	-0.11809	71523.52	-0.09498	71777.6	-0.04925	70814.19	-0.08464
16(10, 6)- 15(9, 6)	72497.97	0.05976	71523.52	0.03506	71777.6	0.13426	70814.19	0.05095
16(10, 7)- 15(9, 7)	72497.97	-0.09747	71523.52	-0.08043	71777.6	-0.02787	70814.19	-0.06937
17(10, 8)- 16(9, 7)			73880.49	0.05236	74152.03	-0.01438		
17(10, 7)- 16(9, 7)			73880.49	-0.00274	74152.03	-0.09515		
17(10, 7)- 16(9, 8)			73880.91	-0.03696	74152.76	-0.0049		
17(10, 8)- 16(9, 8)			73880.91	0.01814	74152.76	0.07587		
11(11, 1)- 10(10, 0)	63949.33	0.02238	63152.55	0.02763	63302.69	0.0918	62510.13	0.07111
11(11, 0)- 10(10, 1)	63949.33	0.02238	63152.55	0.02763	63302.69	0.0918	62510.13	0.07111
11(11, 0)- 10(10, 0)	63949.33	0.02238	63152.55	0.02763	63302.69	0.0918	62510.13	0.07111
11(11, 1)- 10(10, 1)	63949.33	0.02238	63152.55	0.02763	63302.69	0.0918	62510.13	0.07111
12(11, 2)- 11(10, 1)	66378.19	-0.02269	65538.86	0.00185	65709.1	-0.01966	64875.22	-0.00809
12(11, 1)- 11(10, 2)	66378.19	-0.02269	65538.86	0.00185	65709.1	-0.01966	64875.22	-0.00809
12(11, 1)- 11(10, 1)	66378.19	-0.02269	65538.86	0.00185	65709.1	-0.01966	64875.22	-0.00809
12(11, 2)- 11(10, 2)	66378.19	-0.02269	65538.86	0.00185	65709.1	-0.01966	64875.22	-0.00809
13(11, 3)- 12(10, 2)	68805.87	-0.02252	67924.03	-0.02986	68114.42	0.00279	67239.26	-0.00212
13(11, 2)- 12(10, 3)	68805.87	-0.02254	67924.03	-0.02988	68114.42	0.00276	67239.26	-0.00214
13(11, 2)- 12(10, 2)	68805.87	-0.02252	67924.03	-0.02986	68114.42	0.00279	67239.26	-0.00212
13(11, 3)- 12(10, 3)	68805.87	-0.02254	67924.03	-0.02988	68114.42	0.00277	67239.26	-0.00213
14(11, 4)- 13(10, 3)	71231.40	-0.01532	70307.29	0.02293	70517.56	0	69601.29	-0.00957
14(11, 3)- 13(10, 4)	71231.40	-0.0155	70307.29	0.0228	70517.56	-0.00019	69601.29	-0.0097
14(11, 3)- 13(10, 3)	71231.40	-0.01534	70307.29	0.02292	70517.56	-0.00001	69601.29	-0.00958
14(11, 4)- 13(10, 4)	71231.40	-0.01549	70307.29	0.02281	70517.56	-0.00017	69601.29	-0.00969
15(11, 5)- 14(10, 4)	73653.69	-0.00961	72687.47	-0.01254	72917.48	0.01266	71960.31	-0.03178
15(11, 4)- 14(10, 5)	73653.69	-0.01068	72687.47	-0.01329	72917.48	0.01155	71960.31	-0.03257
15(11, 4)- 14(10, 4)	73653.69	-0.0097	72687.47	-0.0126	72917.48	0.01257	71960.31	-0.03184
15(11, 5)- 14(10, 5)	73653.69	-0.01059	72687.47	-0.01323	72917.48	0.01164	71960.31	-0.0325
16(11, 6)- 15(10, 5)							74315.23	-0.00959
16(11, 5)- 15(10, 6)							74315.23	-0.01353
16(11, 5)- 15(10, 5)							74315.23	-0.00995
16(11, 6)- 15(10, 6)							74315.23	-0.01317
12(12, 1)- 11(11, 0)	69923.31	0.00436	69052.63	-0.03368	69216.09	0.01925	68350.03	0.00887
12(12, 0)- 11(11, 1)	69923.31	0.00436	69052.63	-0.03368	69216.09	0.01925	68350.03	0.00887
12(12, 1)- 11(11, 1)	69923.31	0.00436	69052.63	-0.03368	69216.09	0.01925	68350.03	0.00887
12(12, 0)- 11(11, 0)	69923.31	0.00436	69052.63	-0.03368	69216.09	0.01925	68350.03	0.00887
13(12, 2)- 12(11, 1)	72352.30	0.02257	71439.10	0.04109	71622.63	-0.02882	70715.27	0.02013
13(12, 1)- 12(11, 2)	72352.30	0.02257	71439.10	0.04109	71622.63	-0.02882	70715.27	0.02013
13(12, 2)- 12(11, 2)	72352.30	0.02257	71439.10	0.04109	71622.63	-0.02882	70715.27	0.02013
13(12, 1)- 12(11, 1)	72352.30	0.02257	71439.10	0.04109	71622.63	-0.02882	70715.27	0.02013
14(12, 3)- 13(11, 2)			73824.52	-0.00324	74028.23	-0.01279	73079.50	-0.04683
14(12, 2)- 13(11, 3)			73824.52	-0.00324	74028.23	-0.01279	73079.50	-0.04683

14(12, 3)- 13(11, 3)			73824.52	-0.00324	74028.23	-0.01279	73079.50	-0.04683
14(12, 2)- 13(11, 2)			73824.52	-0.00324	74028.23	-0.01279	73079.50	-0.04683
13(13, 1)- 12(12, 0)							74189.74	-0.04061
13(13, 0)- 12(12, 1)							74189.74	-0.04061
13(13, 1)- 12(12, 1)							74189.74	-0.04061
13(13, 0)- 12(12, 0)							74189.74	-0.04061
30(0,30)- 29(1,29)	60850.52	0.03859						
30(1,30)- 29(0,29)	60850.52	0.03859						
31(0,31)- 30(1,30)	62848.47	-0.05083						
31(1,31)- 30(0,30)	62848.47	-0.05083						
29(1,28)- 28(2,27)	60655.21	0.01165						
29(2,28)- 28(1,27)	60655.21	0.01154						
30(2,28)- 29(3,27)	64461.17	0.03336						
30(3,28)- 29(2,27)	64461.17	0.03064						
28(2,26)- 27(3,25)	60466.78	0.00501						
28(3,26)- 27(2,25)	60466.78	-0.00959						
29(2,27)- 28(3,26)	62463.90	-0.01304						
29(3,27)- 28(2,26)	62463.90	-0.01935						