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Computational Studies of β-amyrin acetate ($C_{32}H_{52}O_2$) Detected in Methanol Leaf Extract of *Chrysophyllum albidium*

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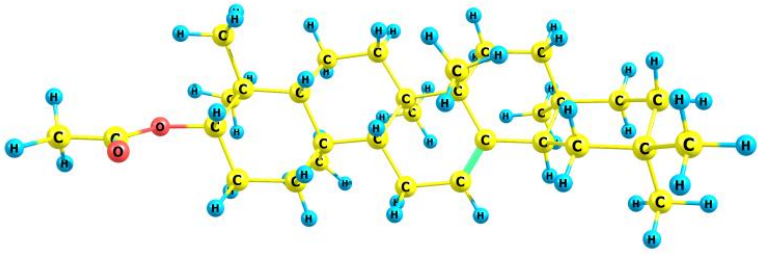
Abstract

In this work, we report the computational studies of β-amyrin acetate which was reported to be present in the leaf of *Chrysophyllum albidium*. Computational calculations are here used to optimized the compound and generate parameters of interest such as, van der waals force field, IR frequencies, bond radius, NMR as well as angles and molecular coordinates of the compound. Given the high accuracy of computational techniques to predict properties of systems, reactants etc. with great consistency, there results are acceptable. The experimental results and the computational results when compared were found to be in good agreement and consistent.

Keywords: β-amyrin acetate, *Chrysophyllum albidium*, characterization, computational.



Introduction

Traditionally, plants have been used as medicine against all kind of illnesses. Plants derived medicines have made large contributions to human health and well-being [1]. According to the World Health Organization (WHO), nearly 20,000 medicinal plants exist in 91 countries including 12 mega biodiversity countries [2]. It is observed that in Nigeria, 70% to 80% of the populations rely on plants for their primary health care needs [3]. The research on medicinal plants is gradually gaining ground due to increasing number of people relying on the use of different parts of these materials for various ailments [4]. Only a small fraction of the world's biodiversity has been explored for bioactivity to date.

Most of the claims are made by traditional medical practitioners themselves and may not have been exhaustively investigated scientifically [5]. For this reasons therefore, it could be argued that further research into this medicinal plant is needed. The leaves of African Star Apple known as Udara in efik**,** Agbalumo in the western and Udala in the eastern part of Nigeria is used by the rural inhabitants and traditional medicine practitioners in Calabar municipality Government of Cross River State for the treatment of malaria, yellow fever, diarrhea, vaginal and dermatological infections. The β-amyrin acetate has been identified for the first time in the leaves of *C. albidum*. The

data here suggest that the leaves of *Chrysophyllum albidum* containing β-amyrin acetate compound which is used as anticancer, cytotoxic [6-9], antiparasitic, antiallergenic, antispasmodic, antihyperglycemic and as herbicide, fungicide and antibiotic in medicines [10-14] pointed out that α,β-amyrin acetate has the potential to combat acute pancreatitis by acting as an anti-inflammatory and antioxidant agent. *C. albidum* was shown to exhibited antioxidant activity [15-18], this could be attributed to the presence of β-amyrin acetate. *C. albidum* may be used for, acquired immunodeficiency syndrome, heart disease, stroke, arteriosclerosis, diabetes and cancer because of the strong antioxidant activity of these extracts of the leaf [19-23]. The present work is designed to probe and validate the reported experimental isolation of compound β-amyrin acetate from the leaves of *C. albidum* through quantum chemical calculations with the view to give insights about the isolated compound.

Quantum Chemical Calculations:

The recent advances in theoretical and computational methods have made it possible to study systems, reactions and predict parameters which would have been either impossible or very difficult to study experimentally. The GAUSSIAN 09 suite of programs was used for all the quantum chemical calculations reported in this work. The molecule was optimized at the M06-2X level of theory with the 6-31g(d,p) 6-31+G* basis set. The M06-2X functional is a high nonlocality function with double the amount of nonlocal exchange (2X). The optimized structure was found to be stable with no imaginary frequency as shown from the frequency calculations [24-32].

Results and Discussion

Optimized Geometry:

Figure 1 displays the optimized geometry of decyl heptadecanoate isolated from *β*-amyrin acetate with the ethyl acetate. Figure 2 shows the Van der Waals sphere of *β*-amyrin acetate obtained from its optimized geometry.

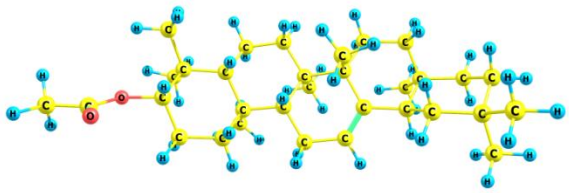


Figure 1. Optimized geometry of *β*-amyrin acetate obtained at the M062x/6-31g(d,p) level of theory.

The Van der Waals sphere is an abstract representation of the molecule illustrating where a surface might reside for the molecule based on the hard cutoffs of Van der Waals radii for the individual atoms making up the molecule.

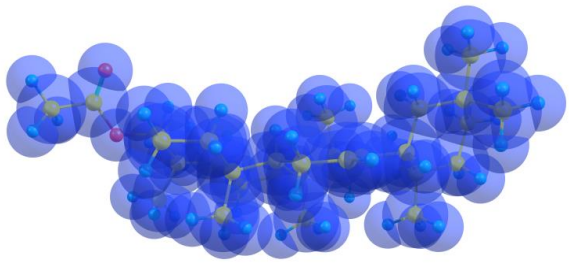


Figure 2. Van der Waals sphere for *β*-amyrin acetate obtained at the M062x/6-31g(d,p) level of theory.

FT-IR Spectra for Isolated Methanol Fraction

The IR spectrum displayed C-H asymmetric stretching in $-CH_3$ at 2964 cm^{-1}, C-H symmetric stretching in $–CH_2$ and =CH at 2915 cm^{-1} and 2843 cm^{-1} respectively. It also showed C-H bending vibration in $–CH_2$ and $–CH_3$ at 1468 and 1413 respectively and C-C stretch in C-C at 997 [53-56]. The FT-IR analysis of isolated methanol component of *C. albidum* leaves extract is presented in Table 1 below.

Table 1: The FT-IR of Isolated methanol component of *C. albidum*

S/N	Freq.	Mode of Vibrations	Mode of Vibrations
1	2964	C-H Asymmetric stretching	$-CH_3$
2	2915	C-H Symmetric stretching	$-CH_2-$
3	2843	C-H Symmetric stretching	=CH-
4	1468	C-H bending vibration	$-CH_2-$
5	1413	C-H bending vibration	$-CH_3$
6	997	C-C Stretch	C-C

All the major peaks obtained experimentally are in good agreement with those obtained computationally at the M062x/6-31g (d,p) level. This further validates both the experimental and computational results. The frequency from 8 cm^{-1} to 3902 cm^{-1} and the corresponding intensity for the IR spectrum of *β*-amyrin acetate obtained at the M062x/6-31g (d,p) level are presented in Table 1A of the supporting information. Additionally, this molecule was found to be microwave active with a dipole moment of 1.9995 Debye obtained at the M062x/6-31g (d, p) level. Thus, its microwave spectrum could be obtained experimentally. As an asymmetric molecule with three different moments of inertia corresponding to the three principal axes, this molecule will be expected to have three different rotational constants. At the M062x/6-31g (d,p) level, the rotational constants obtained for the molecule are 0.31025, 0.05290 and 0.05017 GHz corresponding to the A, B and C rotational constants respectively.

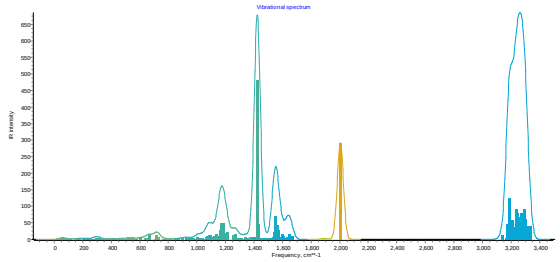


Figure 3. IR spectrum of *β*-amyrin acetate obtained at the M062x/6-31g(d,p) level of theory.

Table 2: The ^{13}CNMR and ^{1}HNMR Spectral Data of Isolated Methanol Component

C positions	Carbon type or Group	Carbon Signal (δ)	Proton Signal (δ)
C-1	CH_2	38.7	1.31,d
C-2	CH_2	28.8	1.67,d
C-3	CH	79.1	3.2t
C-4	C	38.5	-
C-5	CH	55.5	0.86t
C-6	CH_2	18.8	1.58m
C-7	CH_2	33.1	1.28t
C-8	C	38.8	-
C-9	CH	49.2	1.65s
C-10	C	36.7	-
C-11	CH_2	22.7	1.96,m
C-12	CH	116.8	5.5,m
C-13	C	142.7	-
C-14	C	41.3	-
C-15	CH_2	27.4	1.99,m
C-16	CH_2	27.1	1.60,m
C-17	C	49.2	-
C-18	CH	33.3	2.04,m
C-19	CH_2	48.7	1.93, d
C-20	C	29.1	-
C-21	CH_2	35.1	1.31, s
C-22	CH_2	37.5	1.63,s
C-23	CH_3	29.7	0.82,s
C-24	CH_3	15.43	0.84,s
C-25	CH_3	15.4	0.93,s
C-26	CH_3	17.54	0.95,s
C-27	CH_3	21.32	0.97,s
C-28	CH_3	28.0	1.0,s
C-29	CH_3	33.7	1.1,s
C-30	CH_3	25.9	1.2,s
C=O	C	158.1	-
Me	CH_3	29.8	2.07s

NMR methods have indisputably become the single most important spectroscopic techniques for the identification and structure elucidation of amyrins [33]. A large number of pentacyclic triterpenoids have been examined by ^{13}CNMR spectroscopy and considerable ^{13}C chemical shift data have accumulated [34]. The ^{1}H NMR spectrum (400 MHz, $CDCl_3$) showed the presence of eight tertiary methyl group singlets at δ 0.82, 0.84, 0.93, 0.95, 0.97, 1.0, 1.1 and 1.25. The ^{13}C NMR spectrum (400 MHz, CDCl3) showed compound 1 has a total of 32 carbon atoms with eight tertiary methyl groups by exhibiting signals at δ 15.4, 15.4, 17.5, 21.32, 25.9, 28.0, 29.7, and 33.7 ppm. The ^{13}CNMR spectrum displaced seven quaternary carbons at a δ of 29.83, 33.36, 36.77, 38.77, 41.30, 55.53 and 142.70 ppm. A proton is exhibited a signal at δ 3.2 and is placed at C-3 and the presence of an oxycarbon atom exhibited a signal at δ 79.1. Compound 1 has the alkene protons (an unsaturated proton) at δ 5.5 suggesting the presence of a double bond. One of the

carbon atoms is tetrasubstituted and the other carbon is trisubstituted. Also presence of a double bond (carbon 12 and carbon 13) exhibited signals at δ 116.8 and 142.7. The presence of a carbonyl carbon is indicated by exhibiting a signal at δ 158.1. The presence of methyl carbon of the acyl group is exhibited a signal at δ 29.8. The identity of compound 1 as β – amyrin acetate was confirmed by comparison with published values of [35- 38].

Bond Distance and Bond Angle:

In Figure 4, the optimized geometry of Decyl heptadecanoate is shown with the atoms in numbers. The numbers help in determining the distance between two atoms (say atoms 2 and 4) and the angles between atoms. Table A2 of the supporting information contains the complete bonds distances (in Angstrom) and bond angles (in degrees). *β*-Amyrin acetate here is methanol isolated. The methanol extract was separated using equal volume of chloroform and water in a separating funnel. The recovery of the chloroform fraction obtained was 0.104 %. Chloroform fraction was subjected to silica gel column chromatography and final purification with Sephadex LH- 20 to obtain *β*-amyrin acetate.

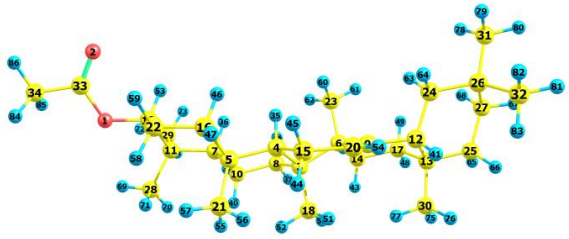


Figure 4. Optimized structure of *β*-amyrin acetate, obtained at the M062x/6-31g(d,p) level of theory, showing the numbering of atoms. The isolated compound was subjected to Thin Layer Chromatography (TLC) monitoring where the silica gel on the TLC plate was impregnated with a fluorescent material (Anisaldehyde- H_2SO_4) reagent followed by warming to glow under ultraviolet (UV) light. The mobile phase was made of chloroform: methanol (4:6 V/V) and chamber saturation time was 30 minutes and the R_f value was 0.894. The structure of

compound 1 (β-amytin acetate was elucidated by comparison with literature values. The β-amytin acetate was isolated as yellowish substance. This compound was found to be a triterpenoid.

Conclusion

It can be concluded that the structural elucidation by spectroscopic methods (IR, ^{1}H-NMR, ^{13}C-NMR) of ethyl acetate extract of *C. albidum* yielded one new compound characterized as β-amytin acetate, using IR, ^{1}H-NMR and ^{13}C-NMR. Quantum chemical calculations have been employed to further gain understanding about the newly characterized molecule, ($C_{32}H_{52}O_2$). The IR frequencies obtained experimentally are in good agreement with those obtained computationally. Bond distances, bond angles, dipole moments, rotational constants and other parameters of interest have been determined computationally for the newly isolated molecule.

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Supporting Information

Table A1. IR frequency and intensity for *β*-amyrin acetate obtained at the M06-2x/6-31g (d,p) level.

Frequencies	Intensities
23.4848	0.114
40.1465	0.4171
55.5563	3.3049
61.1917	0.2822
63.8372	0.5684
75.1173	0.4565
92.4076	0.0835
102.6675	0.2378
103.1713	0.2316
109.7543	0.3358
151.3567	0.9392

156.9219	0.1468
169.2853	0.1459
176.9536	1.6259
201.8341	0.3452
212.6611	0.6953
224.7846	0.0243
229.3578	0.7822
236.4337	0.1927
244.7502	0.208
248.5298	0.2688
253.6254	0.5386
266.8058	0.5638
268.9215	0.2723
274.219	0.045
279.5547	0.5093
294.1856	3.4062
298.275	0.5274
302.7738	2.4845
305.7341	0.2967
315.0424	1.2342
325.284	0.1115
326.5071	0.0943
340.6847	0.7845
345.0242	0.0928
351.695	0.3387
359.5682	0.153
371.9133	0.1448
379.912	0.1871
383.8198	0.0414
400.302	0.1098
413.2941	1.0675
423.8925	0.4339
431.3037	0.0174
438.2346	0.2905
443.1674	0.5188
457.0834	0.1522
465.6236	0.321
474.6447	1.1629
481.3017	0.2263

498.7269	0.2048
502.6898	0.4548
512.6473	1.9703
536.4089	1.0012
543.8544	1.6411
547.5229	1.1254
568.3389	0.2842
576.4201	0.3877
602.9455	4.2763
634.0651	1.4785
641.0731	2.4834
654.7104	0.683
668.1848	12.0248
703.0573	0.2512
712.8352	12.2455
726.5169	6.2033
729.4619	4.204
762.7609	0.4818
773.0577	0.9204
781.0739	0.639
789.6922	0.2984
809.259	0.6259
847.5401	1.0104
868.336	0.9268
892.8031	0.6618
894.6768	2.2139
926.2536	3.2841
938.2722	1.4571
947.4309	1.374
968.4015	1.3449
976.6823	0.1975
986.4318	0.3461
999.4822	0.5811
1000.8421	3.4614
1004.3021	6.163
1013.0951	0.4286
1021.0996	0.996
1023.2208	0.1813
1028.0126	3.5457

1031.2251	1.4572
1034.3265	2.7907
1048.0858	0.5528
1052.0601	0.1581
1061.7382	4.2495
1068.7528	7.9207
1073.625	7.8813
1076.5021	1.8027
1085.817	11.1546
1092.7564	11.72
1101.5774	3.5997
1104.798	6.5401
1105.9609	1.7872
1114.6608	0.9507
1118.6302	1.05
1124.4323	7.1038
1135.0466	15.0914
1145.483	0.9475
1153.3436	8.4089
1159.92	27.6454
1165.7058	47.2375
1172.6698	8.6982
1182.4646	47.4908
1184.9489	23.5629
1186.7778	0.7263
1203.0373	8.236
1207.2993	18.4304
1210.3788	20.3026
1249.878	11.1775
1263.1646	3.0705
1269.5103	13.6506
1270.0126	4.6463
1280.6335	2.9013
1291.8166	0.3419
1297.9145	0.8989
1300.8174	2.9747
1309.194	1.9839
1317.6111	0.5881
1332.6508	1.2253
1333.5853	4.051
1334.5733	0.5976
1340.8413	1.8721
1349.5173	1.7879
1356.299	3.4329
1359.6233	0.7853
1375.3098	4.1245
1390.9109	4.5783
1405.1027	0.7544
1407.5975	5.9402
1420.0097	148.6555
1423.2019	481.0184
1429.7824	44.2405
1445.03	1.0993
1449.623	2.1457
1468.5921	0.9464
1475.0963	0.3823
1477.656	1.182
1482.8552	1.881
1496.4386	1.3717
1498.2872	0.5119
1502.0304	0.3886
1506.5634	0.059
1510.8485	0.7804
1512.6594	1.6153
1516.4903	0.0844
1520.3911	2.6222
1523.0284	1.1429
1531.6328	4.648
1535.7353	6.2135
1537.9412	4.5589
1540.7172	6.1078
1542.4354	19.9765
1544.7858	28.3403
1548.2608	70.4658
1550.2907	1.5443
1557.5142	18.2155
1559.0659	40.1325
1560.6491	4.9259

1568.7148	6.0392
1571.5275	26.8768
1575.1273	4.8893
1595.5948	15.0019
1605.2372	7.3317
1612.2661	0.4819
1616.2977	1.7444
1616.6823	0.0771
1618.2111	0.9321
1618.6893	0.647
1619.1095	0.5544
1622.2792	1.5874
1623.7996	0.4788
1628.1197	2.4838
1628.7171	0.4251
1630.7299	6.6761
1634.2343	3.5472
1635.132	1.9592
1635.7033	2.3435
1637.522	1.5869
1638.2693	4.1545
1643.8632	3.0878
1645.2593	6.4264
1646.4872	15.1406
1647.2045	1.7897
1649.3447	3.216
1650.6516	5.2463
1654.1338	5.6071
1656.0483	1.1055
1662.7531	1.9425
1665.5806	8.4296
1888.0731	2.1583
2004.4421	291.6662
3138.5	13.2473
3167.3167	2.5477
3171.1762	43.8023
3175.9839	6.9036
3176.6861	29.749
3177.6189	25.1509

3182.468	32.9245
3187.3766	123.6193
3188.1243	30.872
3189.4135	26.2967
3193.4504	41.5731
3197.6463	23.4416
3198.9287	16.1242
3201.9179	20.5473
3206.6095	56.3933
3207.4509	9.6085
3209.4542	4.4174
3210.0525	8.3549
3214.7748	11.9875
3216.6215	36.1899
3221.3873	2.05
3225.3164	32.0331
3230.6918	26.6323
3232.0052	2.9777
3232.8786	31.4892
3234.5193	18.2767
3237.7529	2.1275
3238.2164	90.7737
3240.2623	29.352
3241.0265	76.8669
3241.2202	36.6802
3247.64	31.6316
3248.9134	24.0207
3256.1278	67.2098
3259.9805	12.3287
3264.5325	11.4365
3267.7525	77.9678
3269.0767	71.4425
3271.1353	74.4136
3276.6389	30.3741
3276.7414	30.5034
3282.7103	30.7211
3291.1083	58.8526
3291.6964	90.8311
3294.5314	29.7862

3300.5961	61.8523
3301.4371	39.8034
3306.9416	14.3462
3311.175	38.5255
3312.1821	33.6221
3322.3952	14.6928
3330.4755	37.4121

Table A2.Bond distance (Å) and bond angles (□) for *β*-amyrin acetate obtained at the M06-2x/6-31g(d,p).

R(1-19)	1.433
R(1-33)	1.325
R(2-33)	1.189
R(3-4)	1.561
R(3-6)	1.600
R(3-8)	1.548
R(3-18)	1.547
R(4-5)	1.578
R(4-15)	1.540
R(4-35)	1.083
R(5-7)	1.563
R(5-16)	1.549
R(5-21)	1.550
R(6-9)	1.541
R(6-14)	1.555
R(6-23)	1.556
R(7-10)	1.535
R(7-11)	1.566
R(7-36)	1.091
R(8-10)	1.531
R(8-37)	1.086
R(8-38)	1.082
R(9-12)	1.534
R(9-20)	1.322
R(10-39)	1.084
R(10-40)	1.084
R(11-19)	1.543
R(11-28)	1.540
R(11-29)	1.543
R(12-13)	1.550
R(12-24)	1.547
R(12-41)	1.086
R(13-17)	1.539
R(13-25)	1.546
R(13-30)	1.539
R(14-17)	1.533
R(14-42)	1.086
R(14-43)	1.079
R(15-20)	1.504
R(15-44)	1.086
R(15-45)	1.087
R(16-22)	1.529
R(16-46)	1.088
R(16-47)	1.085
R(17-48)	1.088
R(17-49)	1.085
R(18-50)	1.082
R(18-51)	1.081
R(18-52)	1.079
R(19-22)	1.519
R(19-53)	1.082
R(20-54)	1.080
R(21-55)	1.080
R(21-56)	1.081
R(21-57)	1.081
R(22-58)	1.085
R(22-59)	1.085
R(23-60)	1.082
R(23-61)	1.081
R(23-62)	1.082
R(24-26)	1.540
R(24-63)	1.083
R(24-64)	1.087
R(25-27)	1.529
R(25-65)	1.088
R(25-66)	1.087

R(26-27)	1.538
R(26-31)	1.536
R(26-32)	1.538
R(27-67)	1.088
R(27-68)	1.088
R(28-69)	1.083
R(28-70)	1.085
R(28-71)	1.080
R(29-72)	1.084
R(29-73)	1.087
R(29-74)	1.083
R(30-75)	1.087
R(30-76)	1.086
R(30-77)	1.082
R(31-78)	1.086
R(31-79)	1.087
R(31-80)	1.087
R(32-81)	1.087
R(32-82)	1.087
R(32-83)	1.083
R(33-34)	1.505
R(34-84)	1.084
R(34-85)	1.084
R(34-86)	1.080
A(19-1-33)	119.3
A(1-19-11)	108.2
A(1-19-22)	109.4
A(1-19-53)	107.6
A(1-33-2)	124.2
A(1-33-34)	111.2
A(2-33-34)	124.6
A(4-3-6)	107.4
A(4-3-8)	110.1
A(4-3-18)	110.8
A(3-4-5)	117.7
A(3-4-15)	110.4
A(3-4-35)	105.1
A(6-3-8)	110.6
A(6-3-18)	110.8

A(3-6-9)	109.1
A(3-6-14)	110.7
A(3-6-23)	112.3
A(8-3-18)	107.2
A(3-8-10)	114.7
A(3-8-37)	109.4
A(3-8-38)	110.6
A(3-18-50)	111.6
A(3-18-51)	112.7
A(3-18-52)	110.9
A(5-4-15)	113.7
A(5-4-35)	102.6
A(4-5-7)	106.1
A(4-5-16)	107.3
A(4-5-21)	114.0
A(15-4-35)	105.9
A(4-15-20)	114.2
A(4-15-44)	111.6
A(4-15-45)	109.6
A(7-5-16)	108.1
A(7-5-21)	113.5
A(5-7-10)	110.2
A(5-7-11)	117.4
A(5-7-36)	104.2
A(16-5-21)	107.6
A(5-16-22)	113.8
A(5-16-46)	109.3
A(5-16-47)	110.2
A(5-21-55)	113.6
A(5-21-56)	111.6
A(5-21-57)	111.2
A(9-6-14)	111.6
A(9-6-23)	106.9
A(6-9-12)	121.2
A(6-9-20)	120.2
A(14-6-23)	106.2
A(6-14-17)	115.0
A(6-14-42)	108.5
A(6-14-43)	110.9

A(6-23-60)	112.6
A(6-23-61)	110.1
A(6-23-62)	112.5
A(10-7-11)	114.7
A(10-7-36)	105.4
A(7-10-8)	110.7
A(7-10-39)	110.6
A(7-10-40)	111.2
A(11-7-36)	103.4
A(7-11-19)	106.6
A(7-11-28)	114.8
A(7-11-29)	109.2
A(10-8-37)	109.1
A(10-8-38)	106.5
A(8-10-39)	107.5
A(8-10-40)	110.9
A(37-8-38)	106.1
A(12-9-20)	118.5
A(9-12-13)	112.8
A(9-12-24)	110.9
A(9-12-41)	105.9
A(9-20-15)	126.4
A(9-20-54)	118.7
A(39-10-40)	105.8
A(19-11-28)	111.8
A(19-11-29)	107.1
A(11-19-22)	114.4
A(11-19-53)	108.4
A(28-11-29)	107.2
A(11-28-69)	109.9
A(11-28-70)	110.5
A(11-28-71)	113.5
A(11-29-72)	110.1
A(11-29-73)	111.6
A(11-29-74)	111.9
A(13-12-24)	113.3
A(13-12-41)	106.9
A(12-13-17)	109.0
A(12-13-25)	110.6

A(12-13-30)	109.7
A(24-12-41)	106.5
A(12-24-26)	115.3
A(12-24-63)	110.1
A(12-24-64)	107.9
A(17-13-25)	110.6
A(17-13-30)	110.1
A(13-17-14)	113.3
A(13-17-48)	109.2
A(13-17-49)	109.8
A(25-13-30)	106.9
A(13-25-27)	115.5
A(13-25-65)	108.7
A(13-25-66)	108.5
A(13-30-75)	110.7
A(13-30-76)	110.4
A(13-30-77)	112.9
A(17-14-42)	108.5
A(17-14-43)	107.7
A(14-17-48)	108.3
A(14-17-49)	110.1
A(42-14-43)	105.7
A(20-15-44)	107.6
A(20-15-45)	108.2
A(15-20-54)	114.8
A(44-15-45)	105.3
A(22-16-46)	108.1
A(22-16-47)	108.7
A(16-22-19)	111.2
A(16-22-58)	111.6
A(16-22-59)	109.2
A(46-16-47)	106.4
A(48-17-49)	105.8
A(50-18-51)	107.7
A(50-18-52)	106.1
A(51-18-52)	107.5
A(22-19-53)	108.7
A(19-22-58)	109.5
A(19-22-59)	108.5

A(55-21-56)	107.2
A(55-21-57)	106.6
A(56-21-57)	106.2
A(58-22-59)	106.7
A(60-23-61)	106.8
A(60-23-62)	108.4
A(61-23-62)	106.2
A(26-24-63)	107.6
A(26-24-64)	109.7
A(24-26-27)	108.0
A(24-26-31)	108.9
A(24-26-32)	111.4
A(63-24-64)	105.9
A(27-25-65)	109.4
A(27-25-66)	108.7
A(25-27-26)	113.1
A(25-27-67)	109.2
A(25-27-68)	109.8
A(65-25-66)	105.7
A(27-26-31)	109.3
A(27-26-32)	111.3
A(26-27-67)	109.9
A(26-27-68)	108.6
A(31-26-32)	107.9
A(26-31-78)	111.3
A(26-31-79)	111.1
A(26-31-80)	111.0
A(26-32-81)	110.6
A(26-32-82)	110.5
A(26-32-83)	113.1
A(67-27-68)	106.0
A(69-28-70)	107.6
A(69-28-71)	107.4
A(70-28-71)	107.8
A(72-29-73)	108.0
A(72-29-74)	107.1
A(73-29-74)	108.0
A(75-30-76)	107.6
A(75-30-77)	107.9

A(76-30-77)	107.2
A(78-31-79)	107.8
A(78-31-80)	107.7
A(79-31-80)	107.7
A(81-32-82)	107.6
A(81-32-83)	107.4
A(82-32-83)	107.4
A(33-34-84)	109.6
A(33-34-85)	109.7
A(33-34-86)	109.6
A(84-34-85)	107.6
A(84-34-86)	110.2
A(85-34-86)	110.1
W1(A)	23.5
W2(A)	40.1
W3(A)	55.6
W4(A)	61.2
W5(A)	63.8
W6(A)	75.1
W7(A)	92.4
W8(A)	102.7
W9(A)	103.2
W10(A)	109.8
W11(A)	151.4
W12(A)	156.9
W13(A)	169.3
W14(A)	177.0
W15(A)	201.8
W16(A)	212.7
W17(A)	224.8
W18(A)	229.4
W19(A)	236.4
W20(A)	244.8
W21(A)	248.5
W22(A)	253.6
W23(A)	266.8
W24(A)	268.9
W25(A)	274.2
W26(A)	279.6

W27(A)	294.2
W28(A)	298.3
W29(A)	302.8
W30(A)	305.7
W31(A)	315.0
W32(A)	325.3
W33(A)	326.5
W34(A)	340.7
W35(A)	345.0
W36(A)	351.7
W37(A)	359.6
W38(A)	371.9
W39(A)	379.9
W40(A)	383.8
W41(A)	400.3
W42(A)	413.3
W43(A)	423.9
W44(A)	431.3
W45(A)	438.2
W46(A)	443.2
W47(A)	457.1
W48(A)	465.6
W49(A)	474.6
W50(A)	481.3
W51(A)	498.7
W52(A)	502.7
W53(A)	512.6
W54(A)	536.4
W55(A)	543.9
W56(A)	547.5
W57(A)	568.3
W58(A)	576.4
W59(A)	602.9
W60(A)	634.1
W61(A)	641.1
W62(A)	654.7
W63(A)	668.2
W64(A)	703.1
W65(A)	712.8

W66(A)	726.5
W67(A)	729.5
W68(A)	762.8
W69(A)	773.1
W70(A)	781.1
W71(A)	789.7
W72(A)	809.3
W73(A)	847.5
W74(A)	868.3
W75(A)	892.8
W76(A)	894.7
W77(A)	926.3
W78(A)	938.3
W79(A)	947.4
W80(A)	968.4
W81(A)	976.7
W82(A)	986.4
W83(A)	999.5
W84(A)	1000.8
W85(A)	1004.3
W86(A)	1013.1
W87(A)	1021.1
W88(A)	1023.2
W89(A)	1028.0
W90(A)	1031.2
W91(A)	1034.3
W92(A)	1048.1
W93(A)	1052.1
W94(A)	1061.7
W95(A)	1068.8
W96(A)	1073.6
W97(A)	1076.5
W98(A)	1085.8
W99(A)	1092.8
W100(A)	1101.6
W101(A)	1104.8
W102(A)	1106.0
W103(A)	1114.7
W104(A)	1118.6

W105(A)	1124.4
W106(A)	1135.0
W107(A)	1145.5
W108(A)	1153.3
W109(A)	1159.9
W110(A)	1165.7
W111(A)	1172.7
W112(A)	1182.5
W113(A)	1184.9
W114(A)	1186.8
W115(A)	1203.0
W116(A)	1207.3
W117(A)	1210.4
W118(A)	1249.9
W119(A)	1263.2
W120(A)	1269.5
W121(A)	1270.0
W122(A)	1280.6
W123(A)	1291.8
W124(A)	1297.9
W125(A)	1300.8
W126(A)	1309.2
W127(A)	1317.6
W128(A)	1332.7
W129(A)	1333.6
W130(A)	1334.6
W131(A)	1340.8
W132(A)	1349.5
W133(A)	1356.3
W134(A)	1359.6
W135(A)	1375.3
W136(A)	1390.9
W137(A)	1405.1
W138(A)	1407.6
W139(A)	1420.0
W140(A)	1423.2
W141(A)	1429.8
W142(A)	1445.0
W143(A)	1449.6

W144(A)	1468.6
W145(A)	1475.1
W146(A)	1477.7
W147(A)	1482.9
W148(A)	1496.4
W149(A)	1498.3
W150(A)	1502.0
W151(A)	1506.6
W152(A)	1510.8
W153(A)	1512.7
W154(A)	1516.5
W155(A)	1520.4
W156(A)	1523.0
W157(A)	1531.6
W158(A)	1535.7
W159(A)	1537.9
W160(A)	1540.7
W161(A)	1542.4
W162(A)	1544.8
W163(A)	1548.3
W164(A)	1550.3
W165(A)	1557.5
W166(A)	1559.1
W167(A)	1560.6
W168(A)	1568.7
W169(A)	1571.5
W170(A)	1575.1
W171(A)	1595.6
W172(A)	1605.2
W173(A)	1612.3
W174(A)	1616.3
W175(A)	1616.7
W176(A)	1618.2
W177(A)	1618.7
W178(A)	1619.1
W179(A)	1622.3
W180(A)	1623.8
W181(A)	1628.1
W182(A)	1628.7

W183(A)	1630.7
W184(A)	1634.2
W185(A)	1635.1
W186(A)	1635.7
W187(A)	1637.5
W188(A)	1638.3
W189(A)	1643.9
W190(A)	1645.3
W191(A)	1646.5
W192(A)	1647.2
W193(A)	1649.3
W194(A)	1650.7
W195(A)	1654.1
W196(A)	1656.0
W197(A)	1662.8
W198(A)	1665.6
W199(A)	1888.1
W200(A)	2004.4
W201(A)	3138.5
W202(A)	3167.3
W203(A)	3171.2
W204(A)	3176.0
W205(A)	3176.7
W206(A)	3177.6
W207(A)	3182.5
W208(A)	3187.4
W209(A)	3188.1
W210(A)	3189.4
W211(A)	3193.5
W212(A)	3197.6
W213(A)	3198.9
W214(A)	3201.9
W215(A)	3206.6
W216(A)	3207.5
W217(A)	3209.5
W218(A)	3210.1
W219(A)	3214.8
W220(A)	3216.6
W221(A)	3221.4
W222(A)	3225.3
W223(A)	3230.7
W224(A)	3232.0
W225(A)	3232.9
W226(A)	3234.5
W227(A)	3237.8
W228(A)	3238.2
W229(A)	3240.3
W230(A)	3241.0
W231(A)	3241.2
W232(A)	3247.6
W233(A)	3248.9
W234(A)	3256.1
W235(A)	3260.0
W236(A)	3264.5
W237(A)	3267.8
W238(A)	3269.1
W239(A)	3271.1
W240(A)	3276.6
W241(A)	3276.7
W242(A)	3282.7
W243(A)	3291.1
W244(A)	3291.7
W245(A)	3294.5
W246(A)	3300.6
W247(A)	3301.4
W248(A)	3306.9
W249(A)	3311.2
W250(A)	3312.2
W251(A)	3322.4
W252(A)	3330.5

Table A3. Coordinates of *β*-amyrin acetate obtained at the M06-2x/6-31g(d,p) level of theory.

Atomic Number	X (Å)	X (Å)	Z (Å)

8	-6.161733000	0.639258000	-0.129936000
8	-6.280715000	2.758453000	-0.790677000
6	0.280990000	-1.182621000	0.026385000
6	-0.525999000	0.016771000	0.616102000
6	-2.054369000	-0.212783000	0.932912000
6	1.655816000	-0.599457000	-0.546894000
6	-2.689293000	-0.777971000	-0.378722000
6	-0.531928000	-1.868389000	-1.097959000
6	2.413418000	0.112562000	0.590086000
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