Electronic Supplementary Information

Thermodynamic and Kinetic Investigation of Monoketo-Aldehyde-Peroxyhemiacetal-(MKA), a Stereolabile Degradation Product of Dihydroartemisinin.

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Table S1. Results of all the LSER analyses performed through the combination from 1 to 5 among the descriptors of solvent effect discussed in the text.

N.	Descriptor$_i$ / t_i						T-index	F-index	R^2
1	ε 2.53						2.12	2.21E-02	0.287
2	$E_T(30)$ 2.12						2.12	4.97E-02	0.220
3	S_N^{OH} 4.06						2.12	9.07E-04	0.508
4	δ^2 4.69						2.12	2.48E-04	0.578
5	α 2.57						2.12	2.05E-02	0.292
6	β 1.80						2.12	9.07E-02	0.168
7	AN 3.25						2.12	5.00E-03	0.398
8	β_s 5.75	δ^2 8.93					2.13	9.54E-10	0.868
9	ε 3.53	δ^2 5.61					2.13	1.17E-07	0.770
10	$E_T(30)$ 2.87	δ^2 5.29					2.13	5.37E-07	0.728
11	β_s 4.60	α_s 5.24					2.13	1.09E-06	0.706
12	β_s 3.73	ε 4.32					2.13	1.06E-05	0.630
13	β_s 3.59	$E_T(30)$ 3.83					2.13	3.95E-05	0.580
14	β_s	S_N^{OH}					2.13	7.86E-08	0.780

	4.30	**6.45**							
15	$E_T(30)$ **4.29**	S_N^{OH} **6.16**					**2.13**	**8.10E-08**	**0.779**
16	ε **1.04**	S_N^{OH} **2.88**					**2.13**	**1.03E-04**	**0.541**
17	α_s **1.18**	ε **1.13**					**2.13**	**7.31E-03**	**0.348**
18	$E_T(30)$ **0.07**	ε **1.19**					**2.13**	**2.48E-02**	**0.287**
19	α_s **0.75**	δ^2 **3.34**					**2.13**	**2.77E-05**	**0.594**
20	$E_T(30)$ **0.08**	α_s **1.24**					**2.13**	**2.21E-02**	**0.292**
21	ε **3.88**	β_s **6.07**	δ^2 **8.23**				**2.14**	**2.60E-10**	**0.937**
22	ε **5.14**	α_s **2.98**	δ^2 **7.13**				**2.14**	**9.72E-08**	**0.859**
23	ε **3.13**	$E_T(30)$ **2.47**	δ^2 **6.95**				**2.14**	**2.63E-07**	**0.840**
24	ε **2.25**	β_s **5.33**	α_s **3.17**				**2.14**	**2.67E-06**	**0.785**
25	S_N^{OH} **5.36**	β_s **2.92**	$E_T(30)$ **2.90**				**2.14**	**8.10E-08**	**0.863**
26	ε **3.90**	S_N^{OH} **1.52**	δ^2 **4.30**				**2.14**	**1.36E-06**	**0.802**
27	S_N^{OH} **1.14**	β_s **5.84**	δ^2 **3.41**				**2.14**	**2.96E-08**	**0.880**
28	α_s **0.97**	β_s **5.67**	δ^2 **4.40**				**2.14**	**3.54E-08**	**0.877**
29	$E_T(30)$	S_N^{OH}	β_s	δ^2			**2.16**	**7.81E-08**	**0.912**

	4.16	5.49	4.06	2.68					
30	ε 3.81	α_s 1.07	β_s 4.29	δ^2 5.92			2.16	4.70E-09	0.942
31	ε 5.35	S_N^{OH} 2.99	β_s 7.44	δ^2 7.94			2.16	2.58E-10	0.962
32	ε 3.96	$E_T(30)$ 2.44	β_s 5.91	δ^2 9.64			2.16	6.77E-10	0.956
33	δ^2 8.86	$E_T(30)$ 5.05	α_s 4.11	β_s 8.08			2.16	5.06E-10	0.958
34	ε 4.69	$E_T(30)$ 3.56	α_s 5.41	β_s 7.26			2.16	3.25E-07	0.891
35	ε 3.22	$E_T(30)$ 0.34	α_s 1.39	δ^2 6.19			2.16	1.78E-06	0.860
36	ε 3.72	AN 0.75	β_s 5.02	δ^2 5.61			2.16	8.82E-08	0.939
37	$E_T(30)$ 4.29	AN 3.32	β_s 6.85	δ^2 6.61			2.16	3.20E-08	0.948
38	$E_T(30)$ 2.57	ε 1.14	α_s 1.38	β_s 5.71	δ^2 4.78		2.18	3.94E-08	0.9624
39	$E_T(30)$ 2.65	ε 2.06	AN 1.27	β_s 6.13	δ^2 5.49		2.18	4.44E-08	0.9616
40	$E_T(30)$ 0.14	ε 4.15	S_N^{OH} 1.38	β_s 6.16	δ^2 5.64		2.18	3.91E-08	0.9625
41	S_N^{OH} 2.57	ε 4.18	α_s 0.14	β_s 5.65	δ^2 7.28		2.18	3.91E-08	0.9624
42	S_N^{OH} 0.56	$E_T(30)$ 3.90	α_s 3.88	β_s 6.60	δ^2 3.76		2.18	6.23E-08	0.9594
43	ε 2.81	$E_T(30)$ 5.81	α_s 4.34	β_s 5.74	S_N^{OH} 3.54		2.18	3.14E-07	0.9467

Protocol of the performed LSER analyses.

In order to effectively dissect the contribution afforded by each solute-solvent interaction to the ${}^{x}\Delta G^{\circ S}_{\alpha-\beta}$ term, in addition to the limit case of LSER correlations involving each one of the descriptors cited in main text and used as unique parameters, a wide number of linear combinations among the same descriptors (from 2 to 5 of them) were progressively taken into consideration, avoiding the contemporary use of parameters describing the same typology of interaction. All the results obtained by the relevant linear regressions have next been submitted to statistical analysis (F-test and t-test), to quantify the performance of each single relationship (correlation coefficient R^2), to reasonably exclude contributions of casualness (evaluation of F index) and to establish the relevance that each descriptor assumed inside the considered set of parameters (factors t_i related to each D_i descriptor, when compared to index T achieved by t-test). All the obtained results have been collected in Table S1 of the present ESI.

LSER correlations based on the descriptors δ^2, ε, α_s, β_s, and $E_T(30)$.

From inspection of the results reported in Table S1 they can be derived several indications. The first one takes origin from the relevance that each descriptor (and therefore, the related solute-solvent interaction too) has proved to have when used as unique parameter inside to equations of type 1. Thus, the expense of cavitational free energy associated to the differential solvation of **5β** and **5α** (which is monitored by the square of the Hildebrand parameter, δ^2) demonstrated to be the most important among the whole solvent contributions. The correlation coefficient of the relevant regression, in fact, although not high in absolute sense ($R^2 = 0.5785$), is however almost double with respect to those ones coming from the use of α_s or ε ($R^2 = 0.2922$ and 0.2866, respectively), and almost triple with respect to the R^2 values found from $E_T(30)$ or β_s ($R^2 = 0.2197$ and 0.1684, respectively). These preliminary findings appear significantly different from those obtained in the similar thermodynamic study concerning the epimerization of DHA (i.e. compound **2**) [reference 9 of main text]. In that case, in fact, the differential solvation of the epimers **2β** and **2α** proved to have an essentially electrostatic and aspecific origin, while, clearly, this is not the case of MKA. Indeed, this may also be evidenced by the shape of graphs in which values of ${}^x\Delta G°_{\alpha-\beta}$ related to the couple of equilibria **2β⇆2α** or **5β⇆5α** are plotted as a function of permittivity ε of the solvent *x* (Figure S1).

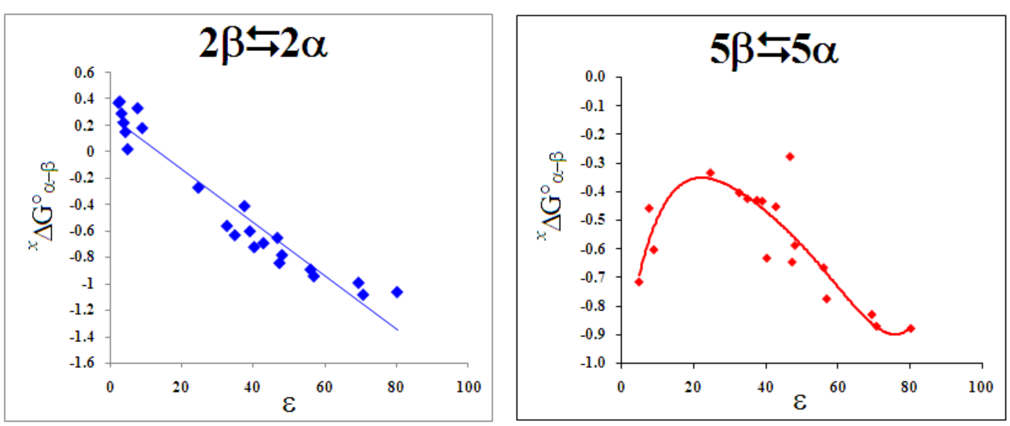


Figure S1. Trend of the ${}^x\Delta G°_{\alpha-\beta}$ values related to the epimerization equilibria of DHA (blue left graph) and MKA (red right graph) on increasing of the solvent permittivity.

In contrast with the quite good linear dependence observed in the case of the equilibrium **2β⇌2α**, the trend found for **5β⇌5α** points, in fact, for a much more complex situation, which evidently arises from the establishment of a wider typology of solute-solvent interactions significantly contributing to the relevant ${}^{x}\Delta G^{\circ S}_{\alpha-\beta}$. A strong support to this interpretation has been indeed suggested by the next LSER analyses performed by means of two-descriptors equations. In particular, a really strong increase of R^2 was observed from correlations again involving δ^2 as one of the two descriptors, with the best performance in absolute sense resulting from the couple δ^2 and β_s ($R^2 = 0.8684$). Interestingly, a really important increase of correlation coefficient was also observed when the regression was based on the equation incorporating α_s and β_s as the couple of solvent descriptors ($R^2 = 0.7064$, to be compared to $R^2 = 0.2922$ and $R^2 = 0.1684$ resulting from the already cited regressions based on α_s and β_s as unique descriptors, respectively). This observation puts in strong evidence the active role played by the HBD and HBA capabilities of the solvent in discriminating the different stability of **5β** and **5α**. On the base of these preliminary results it becomes now easier to face the next LSER analysis founded of three- and four-descriptors equations of type 1. From inspection of correlations coming from three-descriptors equations, in fact, it easily appears that the better results are achieved when the triad of used parameters includes just the couple δ^2/β_s, with a really strong improvement in correlation quality registered by adding the permittivity, ε, as the third descriptor ($R^2 = 0.9366$). However, the addition of α_s instead of ε to the couple δ^2/β_s affords the second better correlation ($R^2 = 0.8768$), although in this case the statistical significance of α_s is assessed to be quite scarce (its t_i value by the Student's t-distribution was computed equal to 0.973, the T index used for comparison being 2.144, see also Experimental Section), when compared to that of δ^2 ($t_i = 4.400$) or β_s ($t_i = 5.670$). Taking into account all these findings, also passing to the use of four-descriptors equations, our attention was initially attracted by results coming from correlations involving the δ^2 and β_s parameters. As expected, among the five possible combinations of descriptors, the three ones containing both δ^2 and β_s afforded the better values of R^2

(from 0.9584 to 0.9418). More in particular, in two among them it was present the triad of descriptors δ^2, β_s and α_s, which, then, give a further and final confirmation of the great importance that differential cavitational free energy and acid-base interactions cover in determining the thermodynamic position assumed by the equilibrium **5β⇌5α**. In addition, as suggested by the favorable role that also ε or $E_T(30)$ can play when present as the fourth descriptor inside the above three equations, it appeared that also the establishment of electrostatic forces must be able to give important contributions to the thermodynamics of the studied epimerization. However, although between the two descriptors $E_T(30)$ demonstrated to be that one allowing the best R^2, the found difference in correlation quality was very modest (the relevant ΔR^2 was just 0.017). Instead, the properties of $E_T(30)$, which is known to be not too specialized and partially interrelated to the behavior of α_s, β_s and ε [C. Reichardt: Solvents and Solvent Effects in Organic Chemistry, Third Edition, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2003], does not play in full support to its selection in performing the final LSER analysis, since this could make more difficult a clear dissection of the single contributions that HBD and aspecific electrostatic solute-solvent interactions may afford to the overall ${}^{x}\Delta G^{\circ S}_{\alpha-\beta}$ amount. Just in agreement with this consideration was, in fact, the result obtained by carrying out the regression with the five-descriptors equation in which, besides δ^2, α_s and β_s, both ε and $E_T(30)$ are also included. In this case, in fact, the quality of the correlation undergoes just a minimal increase (+0.004 of R^2), while the statistical significance of α_s and ε drops down because of their partial mimesis by $E_T(30)$ (for α_s the *ti* value change from 4.11 in equation of entry 33 to 1.38 and for ε from 3.96 in equation of entry 32 to 1.14). Thus, in the limit of the five δ^2, ε, α_s, β_s, and $E_T(30)$ parameters, the equation that most conveniently monitors the thermodynamics of the studied epimerization is the one that includes all of the following four descriptors: δ^2, ε, α_s, β_s (entry 30 in Table S1 of the present ESI), to which is related a really satisfactory correlation coefficient (R^2=0.942).

LSER correlations based on the descriptors δ^2, ε, AN, β_s, and $E_T(30)$.

Even if α_s has widely proved to give an important contribution to the LSER analysis, its statistical relevance in several of the performed correlations in which it was employed was found quite low, lesser than the value of T-index used as the reference (see entries 17, 19, 20, 28, 30, 35 in Table S1 of the present ESI). This unexpected behavior is however understandable in view of the α_s values of water and of the alcoholic solvents, pure or in mixtures, used in the present study (see Figure 6*a*, blue bars, and Table 1 of main text). In fact, among these latter solvents, by moving from the most to the less protic media, α_s undergoes just very small variations (not more than 26%), which, therefore, indicate a quite modest sensitivity of this descriptor to discriminate highly protic solvents. For this reason, we looked for a possible alternative to the α_s descriptor. New regression, again based on a four-descriptors equation, was then performed by substituting α_s with the *acceptor number*, AN[25] (that is to say, the new ensemble of used descriptors was represented by the set δ^2, β_s, ε, AN). Also in this case, however, the achieved quality of the correlation was not characterized by a better value of R^2 (entry 36, R^2=0.939 in Table S1 of ESI) and, instead, by t-test it was pointed out that, similarly to α_s, also the statistical significance of AN was unexpectedly low (t_{AN} = 0.75 in comparison to a T-index of 2.16). Again, this result can be explained in view of the fact that also AN undergoes too modest changes in going from pure water to alcoholic solvents, passing through their mixtures (31% is the maximum change registered for AN within these media, Figure 6*c* of main text, red bars).

Definition of the new descriptor S_N^{OH}.

UV-visible spectral properties of NCEDBU have been tested as a function of polarity and proticity of very different solvents, used as pure species or in suitable mixture. To the purpose we selected 35 media, 17 of which were aprotic, while the proticity of the other 18 was modulated by proper combination of water with either methanol (MeOH) or acetonitrile (ACN), as well as by mixing isopropyl alcohol (IPA) with *n*-hexane (*n*Hex). All the obtained data have been collected in Table S2. Very interestingly, the UV-visible spectra of NCEDBU in *n*-hexane show an absorption band (presumably a $n \rightarrow \pi^*$ transition of an oxygen's lone pair within the NCE^- enolate anion) with the maximum value of absorbance λ_{max} at 321 nm which, in turn, undergoes a systematic bathochromic shift on increasing the permittivity of aprotic solvents, (Table S2 and Figure S2, red trace).

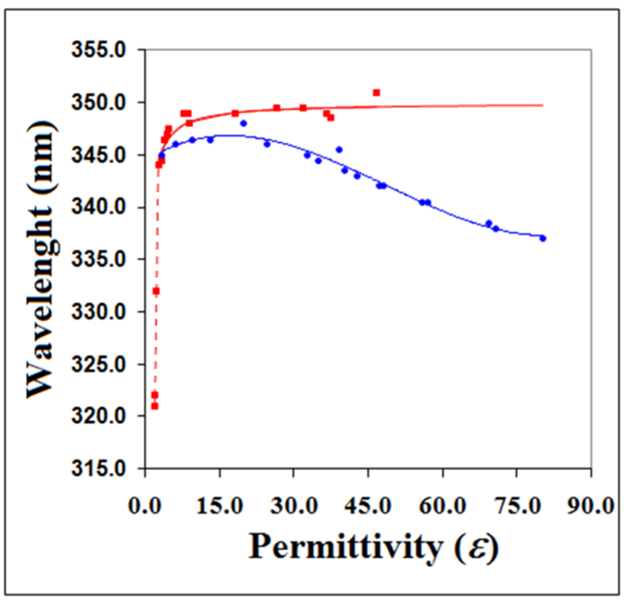


Figure S2. Bathochromic shift of λ_{max} as a function of a change of solvent, looking at λ_{max} in hexane as the reference. Red trace: trend in aprotic solvents (the interpolating solid line was calculated by equation S1). Blue trace: trend in protic solvents.

Table S2. Wavelengths of the maximum of the absorption band of NCEDBU in protic and aprotic solvents and related values of S_N^{OH}.

		Solvent (% composition)	ε	λ_{max}	$^{ap}\lambda_{max}$	S_N^{OH}
Protic solvents	1	H_2O	80.2	337.0	349.7[a]	1.00
	2	MeOH:H_2O (10:90)	70.7	338.0	349.7[a]	0.92
	3	AN:H_2O (10:90)	69.4	338.5	349.7[a]	0.88
	4	MeOH:H_2O (30:70)	56.9	340.5	349.6[a]	0.72
	5	AN:H_2O (30:70)	56.0	340.5	349.6[a]	0.72
	6	AN:H_2O (50:50)	48.0	342.0	349.6[a]	0.60
	7	MeOH:H_2O (50:50)	47.3	342.0	349.6[a]	0.60
	8	AN:H_2O (70:30)	42.8	343.0	349.5[a]	0.51
	9	MeOH:H_2O (70:30)	40.2	343.5	349.5[a]	0.47
	10	AN:H_2O (90:10)	39.0	345.5	349.5[a]	0.31
	11	MeOH:H_2O (90:10)	34.8	344.5	349.5[a]	0.39
	12	MeOH	32.6	345.0	349.4[a]	0.35
	13	EtOH	24.6	346.0	349.3[a]	0.26
	14	IPA	19.9	348.0	349.1[a]	0.09
	15	IPA:nHexane (70:30)	13.2	346.5	348.7[a]	0.17
	16	IPA:nHexane (50:50)	9.4	346.5	348.2[a]	0.13
	17	IPA:nHexane (30:70)	6.1	346.0	347.3[a]	0.11
	18	IPA:nHexane (10:90)	3.2	345.0	345.4[a]	ns
Aprotic and really weacly HBD solvents	19	DMSO	46.7	350.5	349.7[a]	ns
	20	ACN	37.5	348.5	349.5[a]	ns
	21	DMF	36.7	349.0	349.5[a]	ns
	22	CH_2Cl_2:DMF (20:80)	31.7	349.5	349.4[a]	ns
	23	CH_2Cl_2:DMF (40:60)	26.4	349.5	349.3[a]	ns
	24	CH_2Cl_2:DMF (70:30)	18.0	349.0	349.0[a]	ns
	25	CH_2Cl_2	8.9	348.0	348.1[a]	ns
	26	$CHCl_3$:DMSO (90:10)	8.5	349.0	348.0[a]	ns
	27	$CHCl_3$:DMF (90:10)	7.9	349.0	347.9[a]	ns

	28	**$CHCl_3$**	**4.8**	**347.5**	**346.7** [a]	**ns**
	29	**$CHCl_3$:Cyclohexane (90:10)**	**4.4**	**347.0**	**346.5** [a]	**ns**
	30	**$CHCl_3$:Cyclohexane (70:30)**	**3.8**	**346.5**	**345.9** [a]	**ns**
	31	**$CHCl_3$:Cyclohexane (50:50)**	**3.2**	**344.5**	**345.3** [a]	**ns**
	32	**$CHCl_3$:Cyclohexane (30:70)**	**2.7**	**344.0**	**344.6** [b]	**ns**
	33	**$CHCl_3$:Cyclohexane (10:90)**	**2.2**	**332.0**	**329.7** [b]	**ns**
	34	**Cyclohexane**	**2.0**	**322.0**	**323.8** [b]	**ns**
	35	**nHexane**	**1.9**	**321.0**	**320.8** [b]	**ns**

[a]: calculated by equation S1; [b]: calculated by the following equation $^{ap}\lambda_{max} = 0.988\times\varepsilon + 3.881$, which was obtained as the linear best fit on the ε and λ_{max} data of solvents of entries 32 ÷ 35.
ns: non-significant value (for these media S_N^{OH} is assumed equal zero).

More in particular, in this type of solvents such a shift resulted very wide in the range of permittivity from 2 to 5, with an absolute λ_{max} variation of 26.5 nm (equal to 8.3% from the λ_{max} measured in *n*Hex), and much more modest for permittivity values between 5 and 47, the change of λ_{max} being in this latter case of not more than further 4 nm (i.e. a global change of 9.3% with respect to the λ_{max} in *n*-hexane). On the other hand, looking again at λ_{max} in *n*-hexane as reference solvent, at equal permittivity values the monitored bathochromic shift was found progressively much less pronounced in protic solvents, with the difference in shift that quickly increases upon increase in permittivity. In extreme situations, always compared to *n*-hexane, in the protic solvent with the smaller ε value (i.e. 3.2, Table S2) λ_{max} of NCEDBU undergoes a red shift of 24 nm, a value virtually indistinguishable from that observed in aprotic solvent of equal ε, while in pure water (ε = 80) λ_{max} reached the value of 337 nm, the absolute lowest one among those found in protic media, at which corresponds a red shift from λ_{max} in *n*-hexane of 16 nm. Summarizing, the greater the extent of solvent proticity the lesser the bathochromic shift of λ_{max} values from that in *n*-hexane (Table S2 and Figure S2, blue trace). Thus, this behavior is perfectly consistent with a possible use of NCEDBU as probe of HBD interactions. Accordingly, a new descriptor of hydrogen-bond donor capacity, S_N^{OH}, has been defined by means of equations (S1) – (S3):

$$^{ap}\lambda_{max} = e^{(5.858 - 0.049/(\varepsilon + 0.470))} \quad \text{(S1)}$$

$$^{shift}\lambda_{max} = \lambda_{max} - {}^{ap}\lambda_{max} \quad \text{(S2)}$$

$$S_N^{OH} = {}^{shift}\lambda_{max} / ({}^{shift}\lambda_{max})_{H_2O} \quad \text{(S3)}$$

In equation (S1) $^{ap}\lambda_{max}$ represents the hypothetical (and therefore only apparent) λ_{max} value that NCEDBU should assume in a protic solvent just on the base of its relevant permittivity, figuring that HBD interactions between NCEDBU and solvent cannot be established (in other words, if the only effect of solvent would be that modulated by the permittivity). The exponential function used in this equation was empirically chosen to fit with good confidence (R^2=0.983) the experimental values of λ_{max} just measured in aprotic solvents, inside the permittivity range from 3.2 of the [$CHCl_3$:Cyclohexane (50:50)] mixture to 46.7 of DMSO (Figure S2, solid red trace). Instead, $^{shift}\lambda_{max}$ represents the shift that λ_{max} would undergo for the establishment of only NCEDBU-solvent HBD interactions. Therefore, $^{shift}\lambda_{max}$ is a quantity able to measure in a direct way HBD interactions, while descriptor S_N^{OH} (equation S3) is its version normalized with respect to water, the solvent in which $^{shift}\lambda_{max}$ in module achieves the greatest value. By comparing S_N^{OH} with the widely known descriptors α_s and AN (see Figure 6 of main text) it may be clearly inferred that the first one is much more able to discriminate the protic properties of solvents like water and alcohols, especially in the case of water/alcohol mixtures (see Figure S3). In other words, S_N^{OH} may effectively magnify little differences of hydrogen-bond donor capability displayed by solvents strongly protic (typically water-alcohol mixtures), while, by contrast, it strongly compresses those ones relevant to really weakly HBD media, like CH_2Cl_2 or $CHCl_3$, up to assume in these cases non-significant values (lesser than 0.1), virtually indistinguishable from those of aprotic solvents, which fluctuate around zero inside a range of ± 0.04 S_N^{OH} units in average, and that therefore forcedly we assumed equal to zero. Accordingly, the use of S_N^{OH} should be advisable to better monitor the effects of HBD interactions just in the first kind of very strongly protic media.

	α_s	AN	S_N^{OH}
10/90 ACN/H2O	1.072	0.512	0.88
30/70 ACN/H2O	0.876	0.44	0.72
50/50 ACN/H2O	0.68	0.369	0.60
70/30 ACN/H2O	0.484	0.297	0.51
90/10 ACN/H2O	0.288	0.225	0.31
H2O	1.17	0.548	1.00
10/90 MeOH/H2O	1.151	0.535	0.92
30/70 MeOH/ H2O	1.113	0.508	0.72
50/50 MeOH/ H2O	1.075	0.482	0.60
70/30 MeOH/ H2O	1.037	0.455	0.47
90/10 MeOH/ H2O	0.999	0.428	0.39
MeOH	0.98	0.415	0.35
EtOH	0.86	0.379	0.26

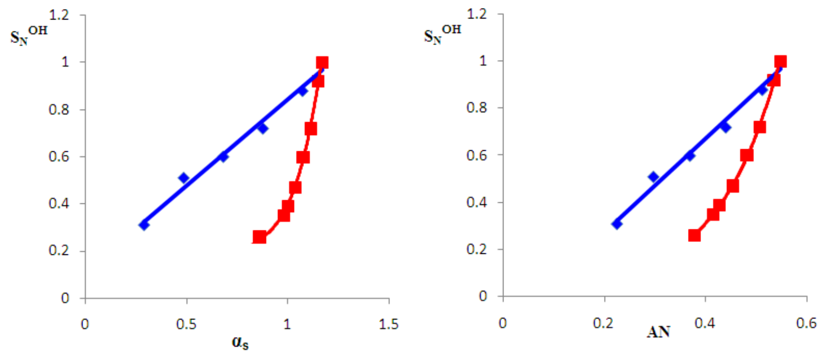


Figure S3. Existing correlation between α_s and S_N^{OH} values (left plot) and between AN and S_N^{OH} values (right plot). ACN/H_2O mixtures show linear correlations (blue traces), while pure alcohols and MeOH/H_2O mixtures exponential trends (red traces).

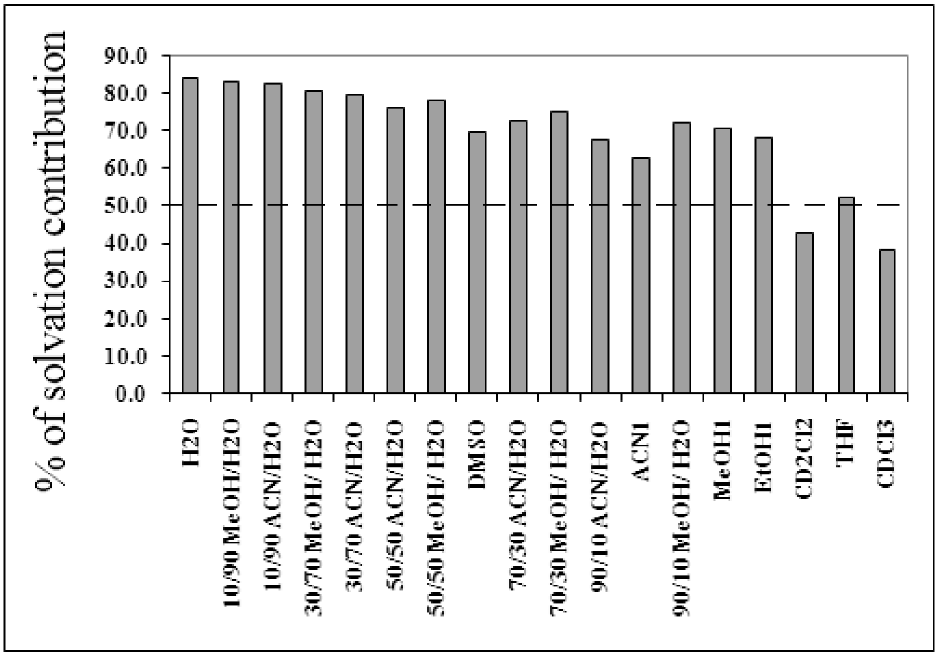


Figure S4. Percentage of solvent effect on ${}^{x}\Delta G°_{\alpha-\beta}$.

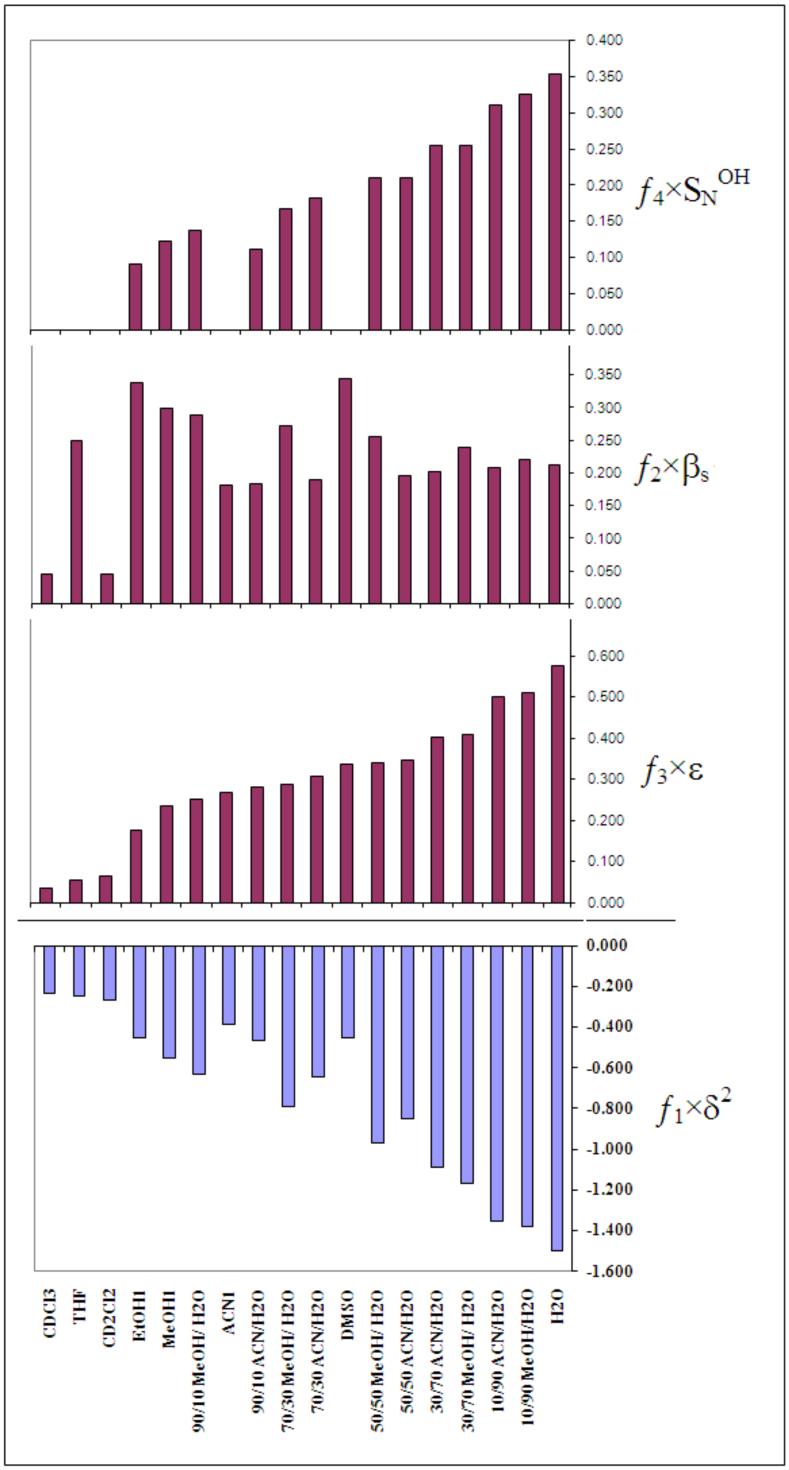


Figure S5. Absolute energy contributions to the overall solvent effect ${}^{x}\Delta G^{\circ S}_{\alpha-\beta}$ monitored by the four descriptors included within the multiparameter equation selected to perform the final LSER analysis.

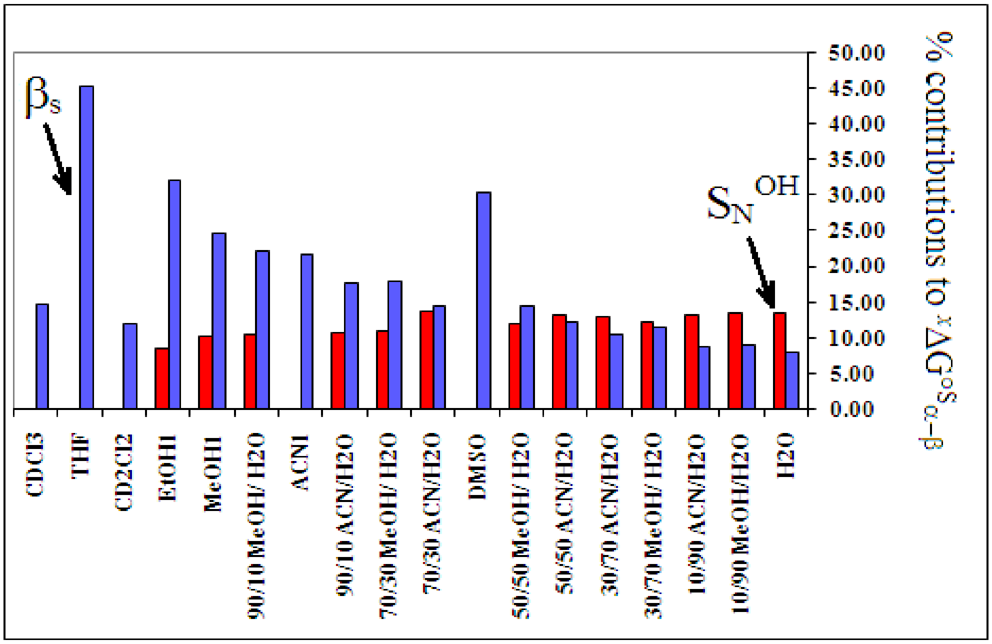


Figure S6. Trend of the energy contribution percentage of the HBD (S_N^{OH} descriptor) and HBA (β_s descriptor) solute-solvent interactions, both favorable to the epimer **5β.**

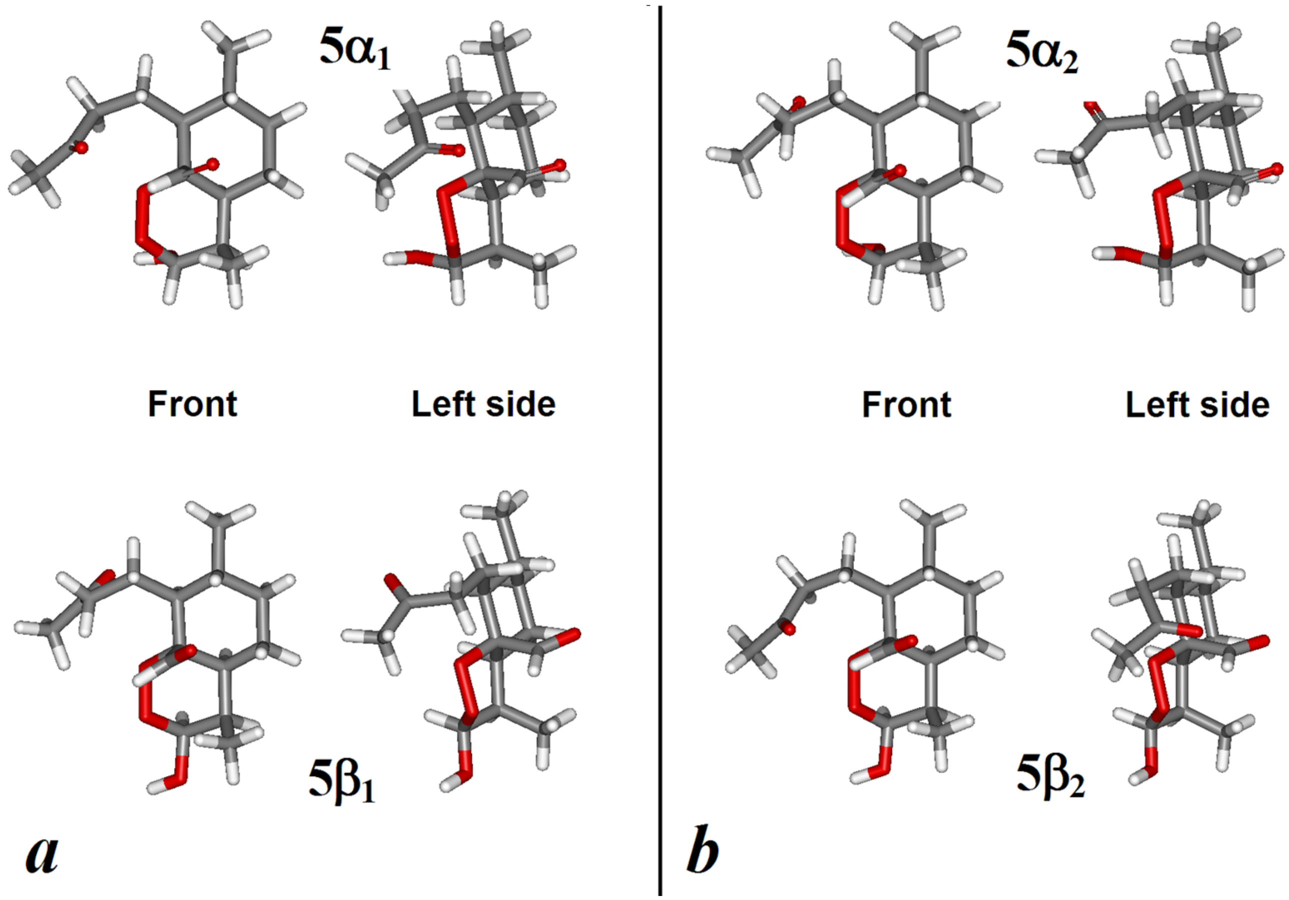


Figure S7. Calculated structures of 5α and 5β (their two most representative conformations). The carbonyl group of the ketonic framework is *anti* with respect to the hemiacetal OH in $5\alpha_1$ and $5\beta_1$ and *syn* in $5\alpha_2$ and $5\beta_2$.

Table S3. Absolute stability energies of the calculated conformations of **5α$_1$**, **5α$_2$**, **5β$_1$**, **5β$_2$**, **5α$_1^–$**, **5α$_2^–$**, **5β$_1^–$** and **5β$_2^–$**.

		Energy (Method[1]) (a.u.)	**Energy (Method[2]) (a.u.)**				
		H_2O	**H_2O**	**CH_3CN**	**CH_2Cl_2**	**$CHCl_3$**	**Vacuum**
5α	5α$_1$	-8.93393635	-8.84699404	-8.84612645	-8.84425285	-8.84262985	-8.83216314
	5α$_2$	-8.93347407	-8.84725977	-8.84636051	-8.84486423	-8.84304456	-8.83266820
5α$^–$	5α$_1^–$	-8.91589026	-8.82676320	-8.82394668	-8.81477230	-8.80497861	–
	5α$_2^–$	-8.91619880	-8.82724670	-8.82446171	-8.81526667	-8.80522929	–
5β	5β$_1$	-8.93287011	-8.84643454	-8.84544237	-8.84417266	-8.84223916	-8.83174280
	5β$_2$	-8.93302063	-8.84607918	-8.84483966	-8.84317500	-8.84119227	-8.83074756
5β$^–$	5β$_1^–$	-8.92105114	-8.83094860	-8.82829483	-8.81911794	-8.80932262	–
	5β$_2^–$	-8.91961293	-8.83026496	-8.82779328	-8.81846056	-8.80850951	–

Method[1]: GGA-BLYP/QZ4P, large core; Method[2]: GGA-BLYP/DZP, medium core.

Table S4. Energy differences and related equilibrium constants (calculated at 25°C) concerning epimers **5α** and **5β** and their conjugate bases **5α⁻** and **5β⁻**, assessed in different solvents.

		^{a} E		^{a} E	$\Delta E^{\alpha^- - \alpha}$	$\Delta E^{\beta^- - \beta}$	$\Delta\Delta E^{\alpha - \beta}$	$\Delta\Delta E^{\alpha^- - \beta^-}$	$\Delta\Delta E_i^{\alpha - \beta}$	$K_{\alpha\beta}$	$K^-_{\alpha\beta}$	K_i^α/K_i^β	$pK_i^\alpha - pK_i^\beta$
		kcal×mol-1		kcal×mol-1	kcal×mol-1	kcal×mol-1	kcal×mol-1	kcal×mol-1	kcal×mol-1				
^{c} $CHCl_3$	5α	0.102	5α⁻	23.80	23.7	20.6	-0.57	2.49	3.05	2.60	0.0151	0.0058	2.24
	5β	0.668	5β⁻	21.31									
^{c} CH_2Cl_2	5α	0.132	5α⁻	18.69	18.6	15.7	-0.46	2.39	2.86	2.19	0.0176	0.0080	2.10
	5β	0.595	5β⁻	16.29									
^{c} AN	5α	0.064	5α⁻	13.86	13.8	10.7	-0.64	2.41	3.05	2.96	0.0172	0.0058	2.24
	5β	0.707	5β⁻	11.45									
^{c} H_2O	5α	0.072	5α⁻	12.67	12.6	9.8	-0.54	2.30	2.83	2.47	0.0207	0.0084	2.08
	5β	0.609	5β⁻	10.38									
^{d} H_2O	5α	0.110	5α⁻	11.21	11.1	7.6	-0.51	2.96	3.47	2.36	0.0067	0.0028	2.55
	5β	0.618	5β⁻	8.25									

		^{b} G		^{b} G	$\Delta G^{\alpha^- - \alpha}$	$\Delta G^{\beta^- - \beta}$	$\Delta\Delta G^{\alpha - \beta}$	$\Delta\Delta G^{\alpha^- - \beta^-}$	$\Delta\Delta G^{\alpha - \beta}$	$K_{\alpha\beta}$	$K^-_{\alpha\beta}$	K_i^α/K_i^β	$pK_i^\alpha - pK_i^\beta$
		kcal×mol-1		kcal×mol-1	kcal×mol-1	kcal×mol-1	kcal×mol-1	kcal×mol-1	kcal×mol-2				
^{c} $CHCl_3$	5α	-0.295	5α⁻	23.39	23.7	20.6	-0.63	2.44	3.07	2.90	0.0163	0.0056	2.25
	5β	0.336	5β⁻	20.95									
^{c} CH_2Cl_2	5α	-0.249	5α⁻	18.30	18.5	15.7	-0.51	2.38	2.89	2.35	0.0180	0.0076	2.12
	5β	0.257	5β⁻	15.92									
^{c} AN	5α	-0.342	5α⁻	13.47	13.8	10.7	-0.67	2.41	3.08	3.08	0.0172	0.0056	2.25
	5β	0.325	5β⁻	11.06									
^{c} H_2O	5α	-0.333	5α⁻	12.28	12.6	9.8	-0.54	2.28	2.82	2.49	0.0213	0.0086	2.07
	5β	0.208	5β⁻	10.00									
^{d} H_2O	5α	-0.283	5α⁻	12.28	12.6	9.8	-0.49	2.28	2.77	2.30	0.0213	0.0093	2.03
	5β	0.209	5β⁻	10.00									

^{a} Average energies coming from the values computed for the couple to conformations **5α₁/5α₂** or **5β₁/5β₂**, weighted on the respective Boltzmann populations.

^{b} Free energies obtained from the respective values *E* integrated with entropy contributions arising from the couple of conformations **5α₁/5α₂** and **5β₁/5β₂**.

^{c}: GGA-BLYP/DZP, medium core; ^{d}: GGA-BLYP/QZ4P, large core.

Table S5. Relative energy stabilities, dipoles, equilibrium constants of epimerization process and differences of acidity of the epimers **5α** and **5β** calculated in different solvents and in vacuum.

		GGA-BLYP/QZ4P, large core calculations in H_2O			GGA-BLYP/DZP, medium core									
		RE (Dipole)	Average Dipole	$K_{\alpha/\beta}$ ($K^-_{\alpha/\beta}$) [$\Delta pK_i^{\alpha-\beta}$]	RE (Dipole)					Average Dipole 5α Average Dipole 5β – $K_{\alpha/\beta}$ ($K^-_{\alpha/\beta}$) [$\Delta pK_i^{\alpha-\beta}$]				
					H_2O	CH_3CN	CH_2Cl_2	$CHCl_3$	Vacuum	H_2O	CH_3CN	CH_2Cl_2	$CHCl_3$	Vacuum
5α	$5\alpha_1$	0.00 (6.25)	5.31	2.30 (0.0213) [2.03]	0.17 (5.90)	0.15 (5.87)	0.38 (5.46)	0.26 (5.34)	0.32 (3.70)	4.49 4.52 – 2.49 (0.0213) [2.07]	4.48 4.08 – 3.08 (0.0172) [2.25]	4.04 3.40 – 2.35 (0.0180) [2.12]	3.99 3.22 – 2.90 (0.0163) [2.25]	2.79 2.35 – 3.18 – –
	$5\alpha_2$	0.29 (3.77)			0.00 (3.43)	0.00 (3.4)	0.00 (3.29)	0.00 (3.12)	0.00 (2.26)					
$5\alpha^-$	$5\alpha_1^-$	11.32	–		12.86	14.06	18.88	23.89	–					
	$5\alpha_2^-$	11.13			12.56	13.74	18.57	23.73	–					
5β	$5\beta_1$	0.67 (2.10)	5.72		0.52 (1.99)	0.58 (1.97)	0.43 (1.92)	0.51 (1.87)	0.58 (1.40)					
	$5\beta_2$	0.57 (8.80)			0.74 (8.21)	0.95 (8.07)	1.06 (7.63)	1.16 (7.31)	1.21 (5.07)					
$5\beta^-$	$5\beta_1^-$	8.09	–		10.24	11.34	16.16	21.16	–					
	$5\beta_2^-$	8.99			10.66	11.65	16.57	21.67	–					

RE=Relative Energies. All energies are expressed in kcal mol^{-1}; Dipoles are in debye. Absolute values of energy stability of all structures are reported in Table S3. Free energy differences used to assess the values of $K_{\alpha/\beta}$, $K^-_{\alpha/\beta}$ and $\Delta pK_i^{\alpha-\beta}$ are reported in Table S4.

[1]H-NMR Analysis of NOE effects and *J*-couplings values involving the hemiacetalic hydrogens of 5α and 5β.

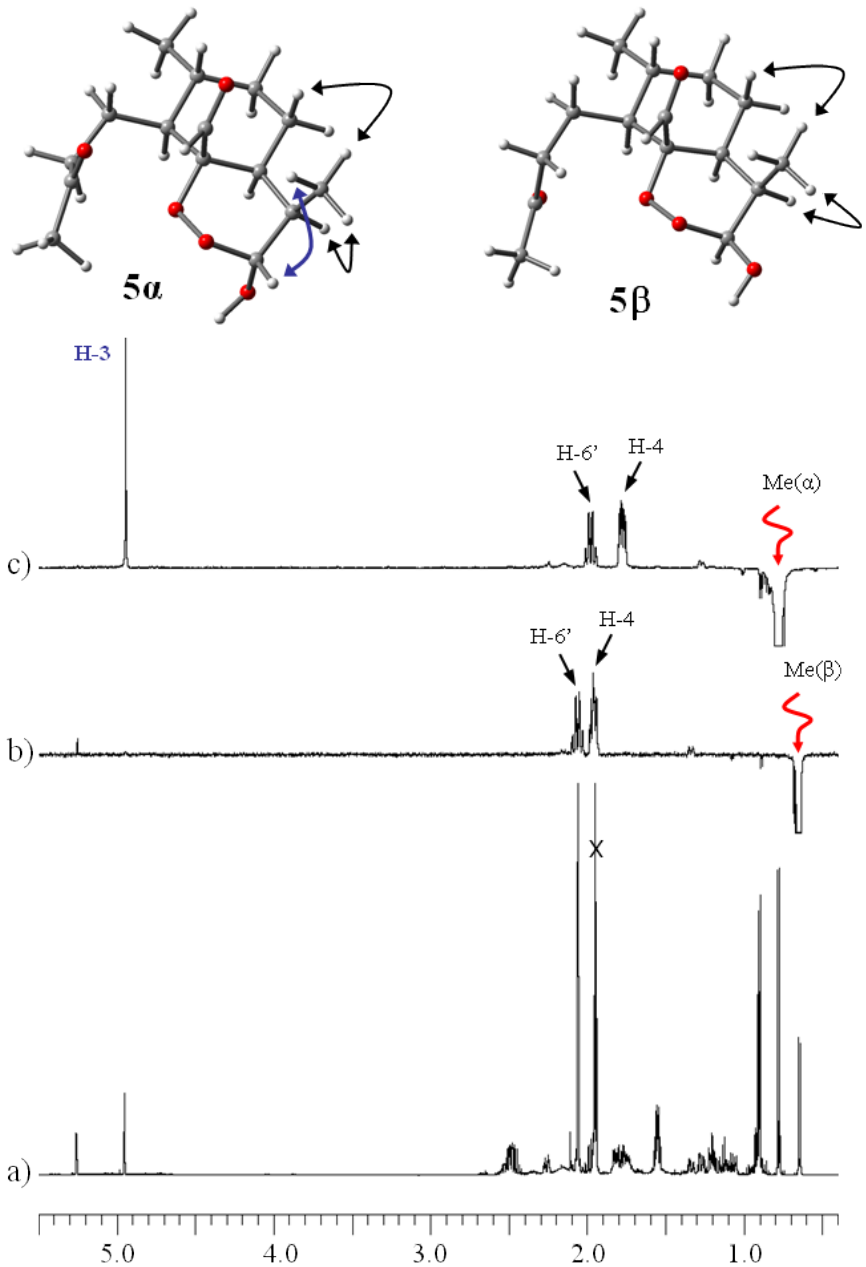


Figure S8. DPFGSE-NOE spectra of the aliphatic region of **5** (600 MHz in CD_3CN at 25 °C). Trace a): [1]H control spectrum. Trace b): NOE spectra obtained on saturation of the Me-16 of the minor epimer. Trace c): NOE spectra obtained on saturation of the Me-16 of the major epimer. The observed NOE are indicated by the arrows in the 3D structures ("control" NOEs in black, diagnostic NOEs in blue).

On selective saturation of the Me-16 signal of the minor isomer (trace b in Figure S8), significant NOE effects were observed only for H-4 and H-6'. These signals act as "control" NOEs, since their spatial relationship with Me-16 is the same in both epimers. When the major signal of Me-16 (trace c in Figure S8) is saturated, NOEs are again observed on H-4 and H-5, and an additional strong NOE is observed on

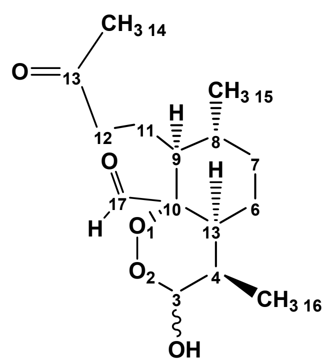
H-3. This indicates that in the major isomer, the hemiacetalic hydrogen H-3 is spatially close to Me-16. The distance ratio derived from the integration of the experimental NOE intensities of H-3 and H-6 (1.01) matches well the ratio calculated from the DFT optimized[22] structure (1.00). Analysis of the *J*-coupling in the two hemiacetalic hydrogens H-3 reveals a $J = 2.3$ Hz in the case of the minor epimer, and a $J < 1$ Hz in the case of the major epimer. Starting from the optimized structure, direct DFT calculation of the *J*-couplings[22] for the two epimers provided *J*-couplings of 0.85 Hz for the α epimer, and 3.14 Hz for the β, in good agreement with the experimental values.

Spectroscopic characterization of compound 5:

1. ^{1}H and ^{13}CNMR data, including COSY, HSQC and HMBC spectra – S25;
2. *J*-coupling calculation for **5α** and **5β** epimers – S35;
3. ESI-MS data (positive mode) – S45;
4. elemental analysis – S46;
5. optical rotation – S46.

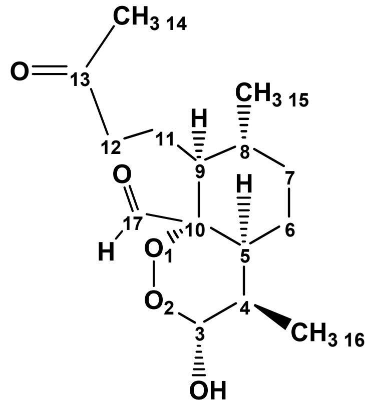
1. ^{1}H and ^{13}CNMR data

NMR Assignment of **5**:



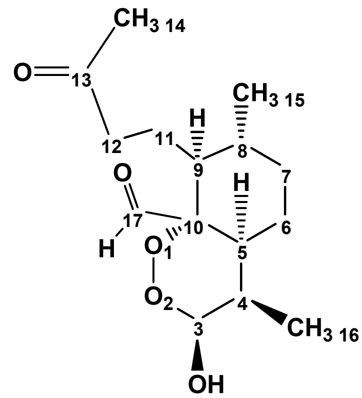
A sample suitable for NMR analysis was prepared in CD_3CN and analyzed at 25°C. Chemical shift references were the residual peaks of CD_3CN (1.95 ppm for ^{1}H, 0.54 ppm for ^{13}C). Standard high resolution ^{13}C-NMR and DEPT-135 spectra were acquired in order to table the exact chemical shifts and multiplicity of the two epimers of **5**. ^{1}H-^{13}C HSQC bi-dimensional spectrum allowed the correlation of each carbon with the corresponding protons. Protons belonging to C-6 and C-4 were assigned from the NOE spectra acquired on saturation of Me-16 (see text), and the ^{13}C chemical shifts of C6 and C4 were derived from HSQC. COSY correlation from Me-16 and Me-15 assigned the chemical shifts of H-4 and H-8, hence the corresponding carbons from HSQC. HMBC correlation (^{3}J) from the protons of Me-16 (doublet) assigned the shift of C-13, and confirmed the assignment of C-3. HMBC correlation (^{3}J) from the protons of Me-15 (doublet) assigned the shift of C-7 and C-9. HMBC correlation (^{3}J) from the protons of Me-14 (singlet) assigned the carbons C-13 and C-12. HMBC correlation (^{3}J) from C-13 assigned the shift of H11 and therefore C-11 was assigned by HSQC. HMBC (^{2}J)correlation of the aldehyde signal allowed the assignment of C-10 and confirmed C-9 and C-13.

Full structural assignment of **5α** and **5β** is reported in the following tables.



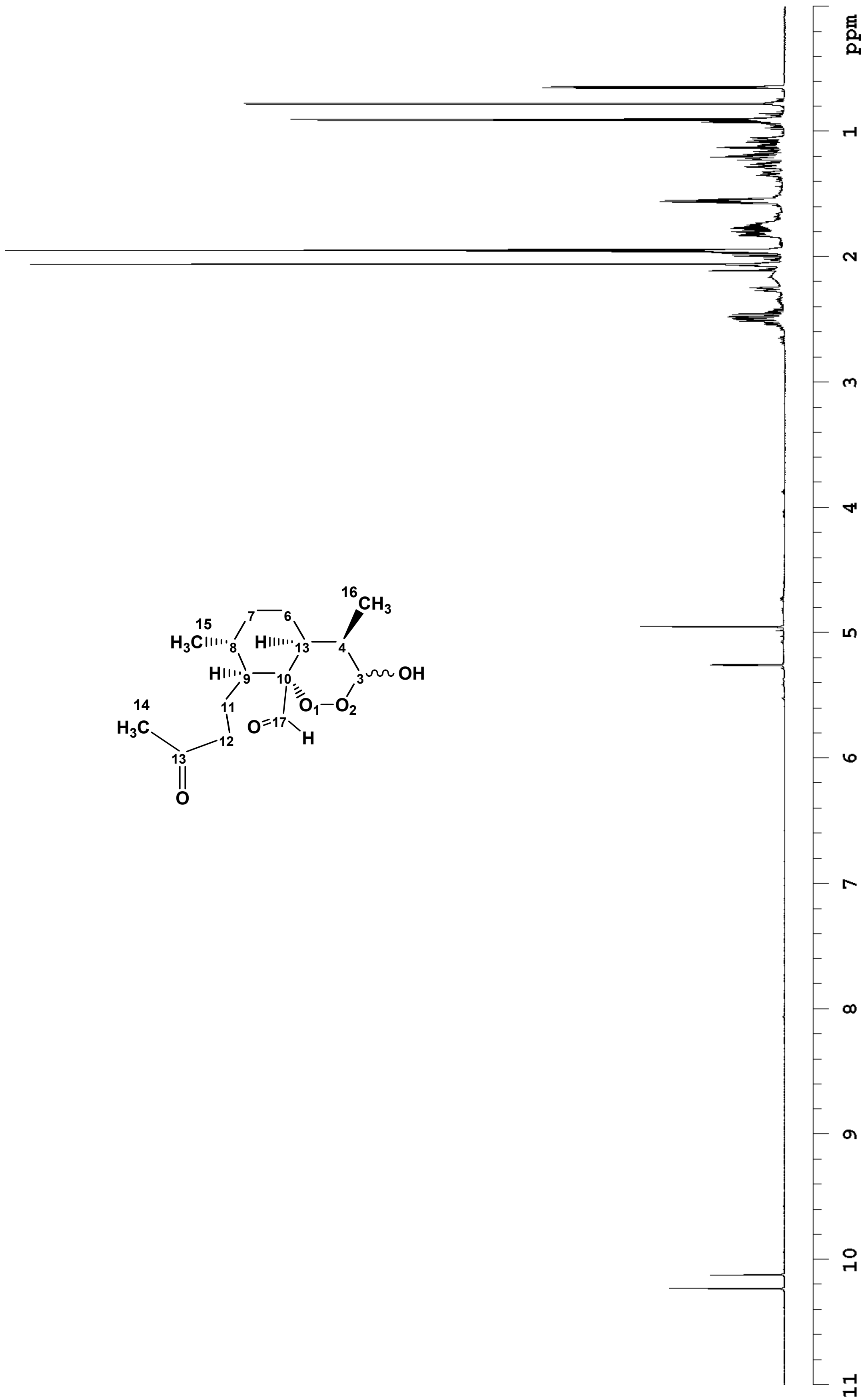
5α

	^{13}C δ	^{1}H δ, multiplicity, *J*
C12	43.32	2.49, m
C11	21.43	1.55, m
C9	50.40	1.21, m
C8	34.19	1.75, m
C7	35.18	1.82, 1.20, m
C6	23.85	1.98, 1.27, m
C5	41.42	2.26, m
C4	35.34	1.78, m
C3	101.31	4.95, s
C10	89.13	-
C15	19.91	0.904, d *J* = 6.5 Hz
C16	13.48	0.78, d, *J* = 7.5 Hz
C14	29.27	2.06, s
CHO	208.07	10.23, dd, *J*= 1.9, 1.5 Hz
C13	208.12	-
OH	-	

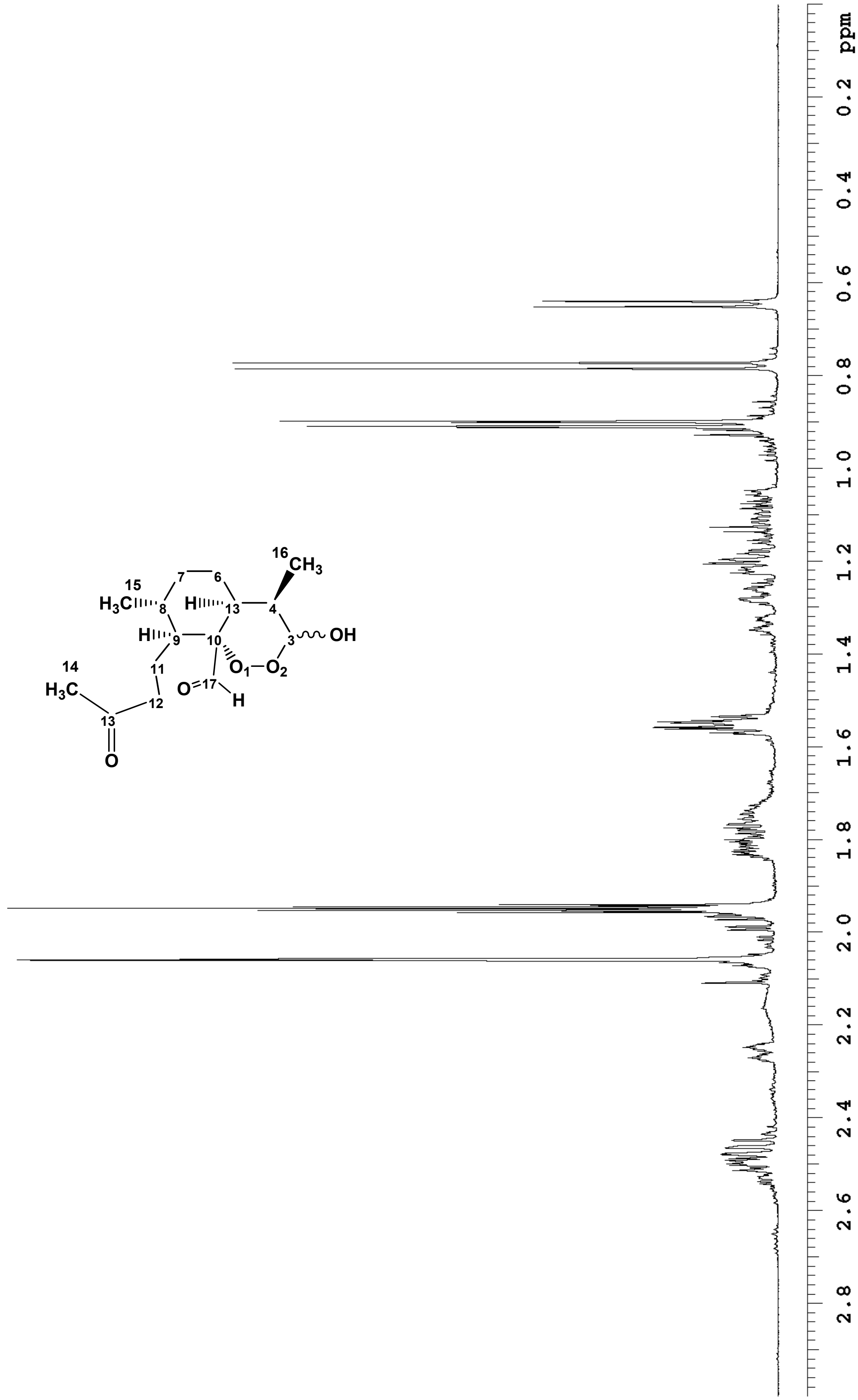


5β

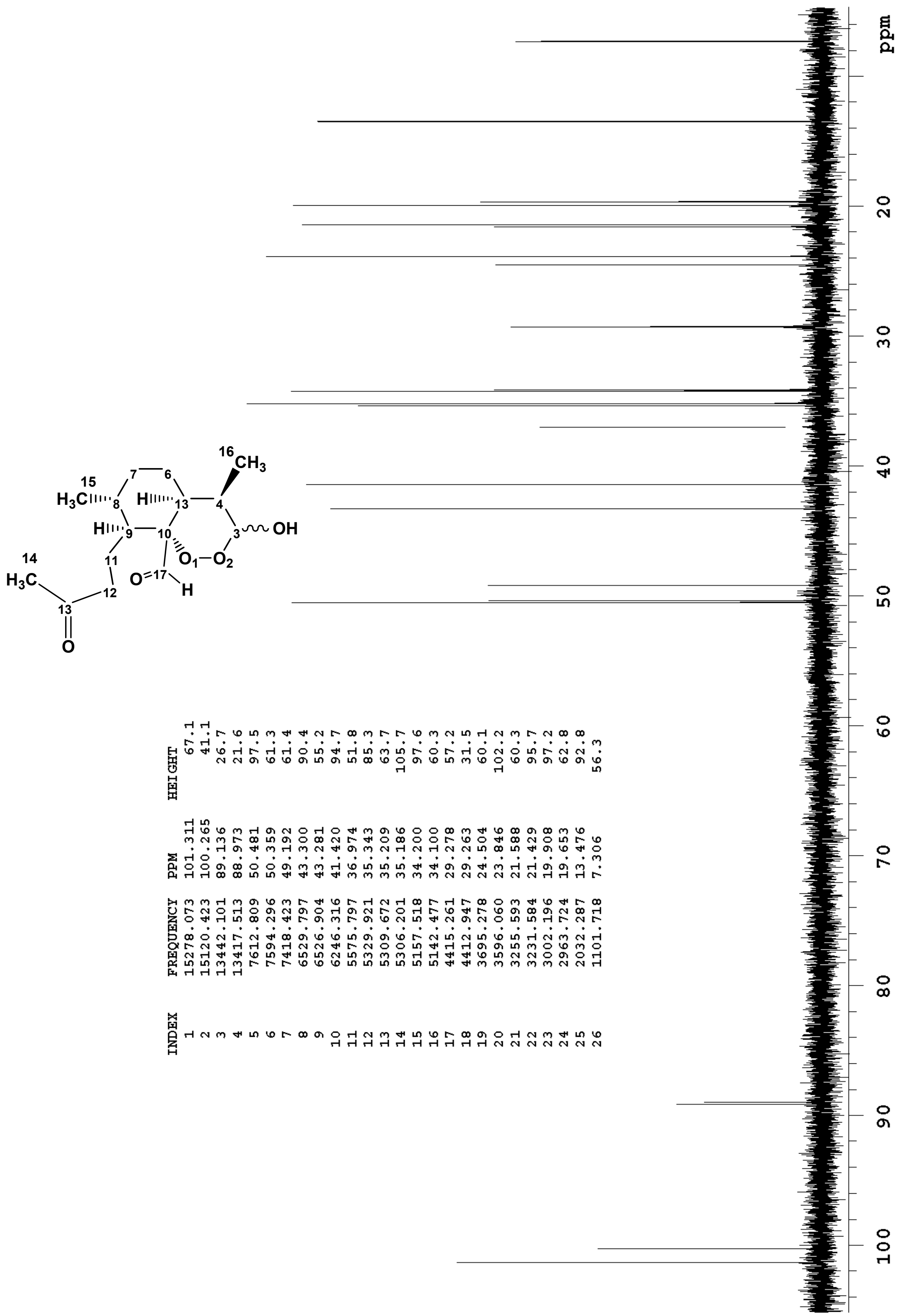
	^{13}C δ	^{1}H δ, multiplicity, *J*
C12	43.28	2.49, m
C11	21.59	1.55, m
C9	50.35	1.11, m
C8	34.10	1.75, m
C7	35.21	1.82, 1.20, m
C6	24.50	2.06, 1.34, m
C5	49.19	1.95, m
C4	36.97	1.96, m
C3	100.26	5.26, d, *J* = 2.4 Hz
C10	88.97	-
C15	19.65	0.906, d, *J* = 6.5 Hz
C16	7.31	0.65, d, *J* = 7.4 Hz
C14	29.26	2.06, s
CHO	207.33	10.12, t, *J* = 1.7 Hz
C13	208.11	-
OH	-	



[1]H spectrum of **5**

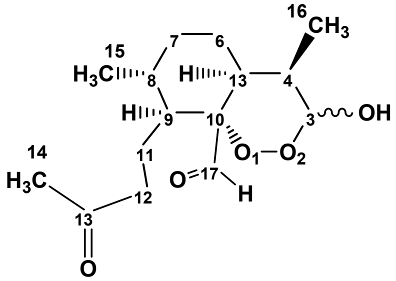


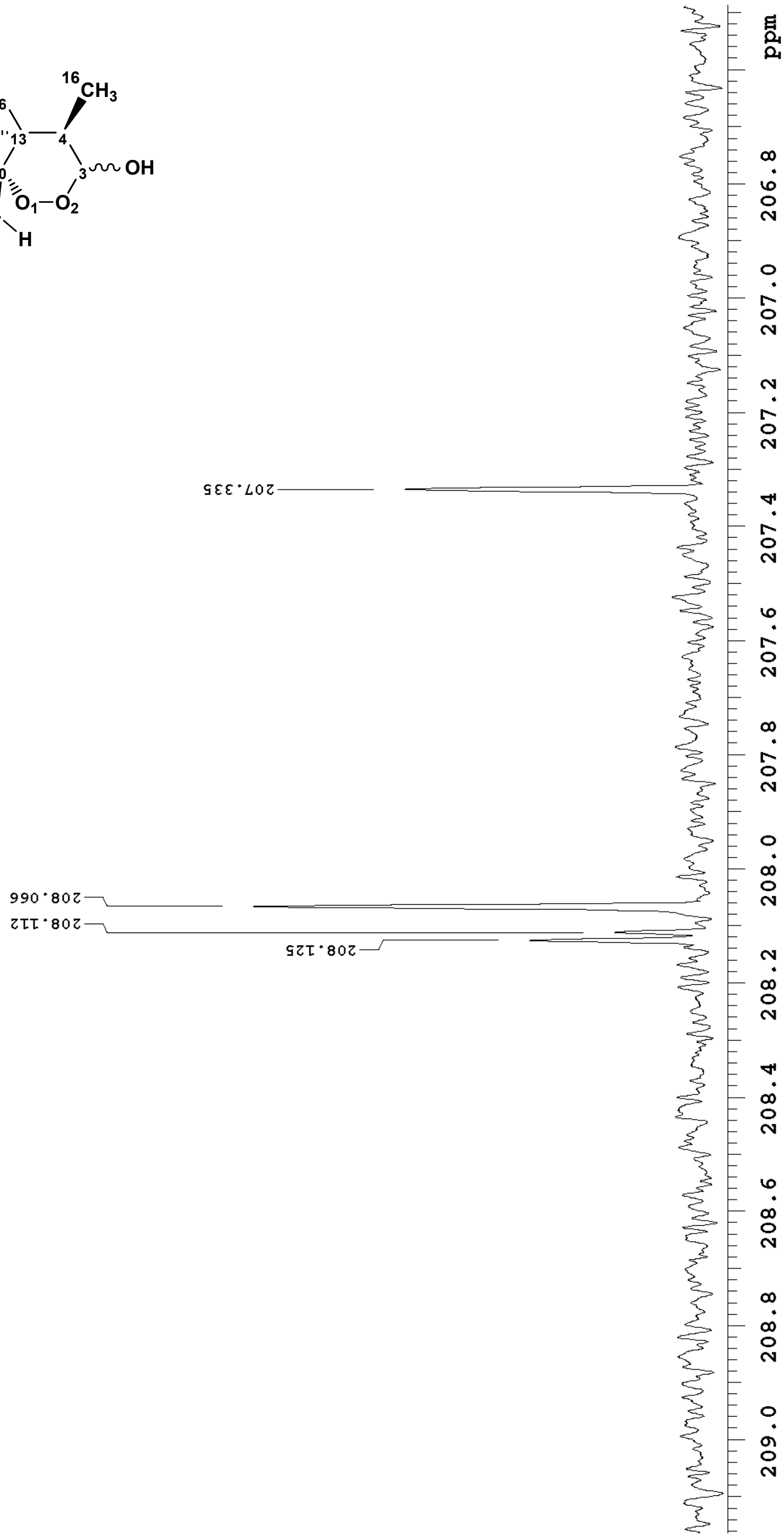
[1]H spectrum of **5**, expansion of the aliphatic region



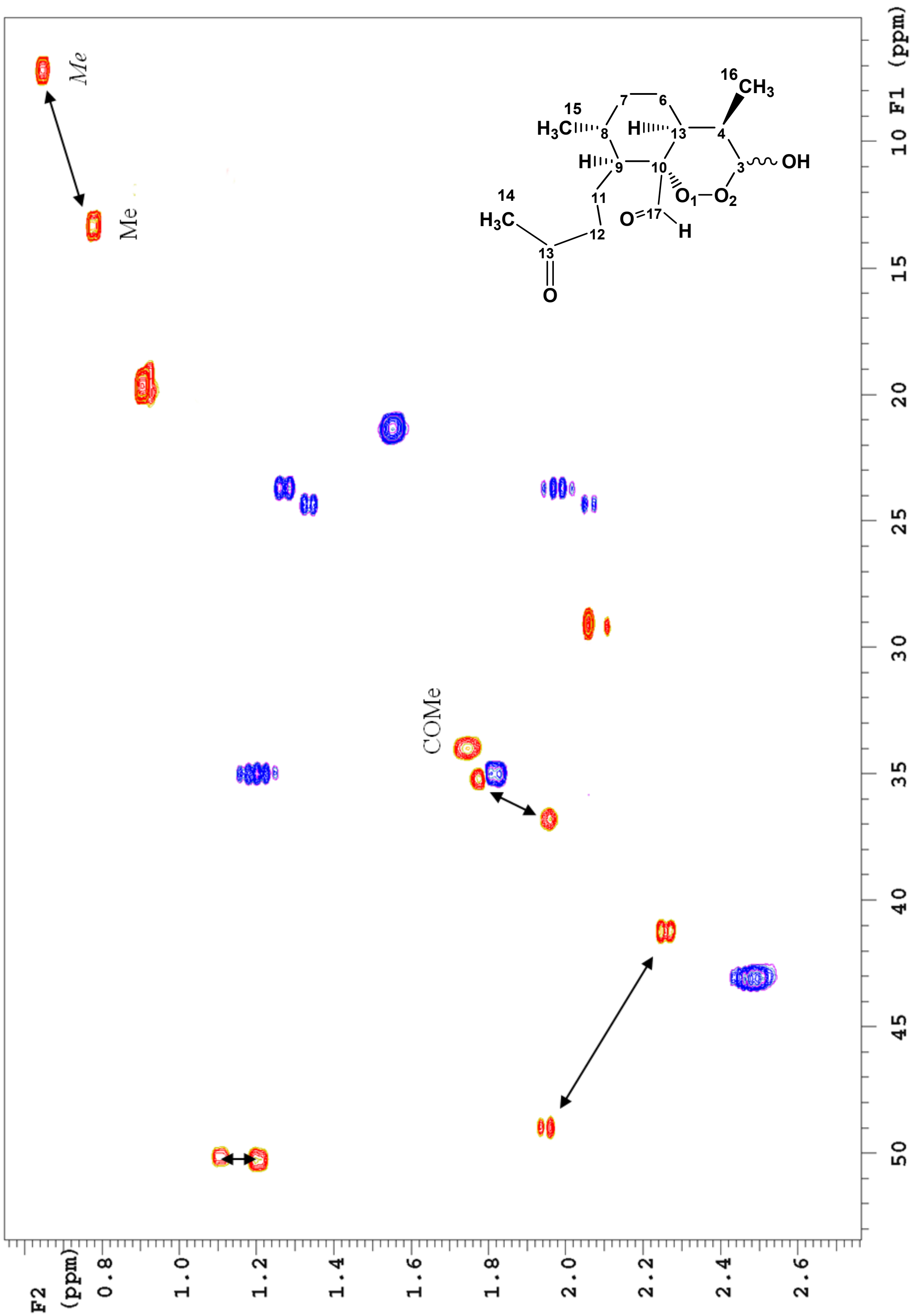
INDEX	FREQUENCY	PPM	HEIGHT
1	15278.073	101.311	67.1
2	15120.423	100.265	41.1
3	13442.101	89.136	26.7
4	13417.513	88.973	21.6
5	7612.809	50.481	97.5
6	7594.296	50.359	61.3
7	7418.423	49.192	61.4
8	6529.797	43.300	90.4
9	6526.904	43.281	55.2
10	6246.316	41.420	94.7
11	5575.797	36.974	51.8
12	5329.921	35.343	85.3
13	5309.672	35.209	63.7
14	5306.201	35.186	105.7
15	5157.518	34.200	97.6
16	5142.477	34.100	60.3
17	4415.261	29.278	57.2
18	4412.947	29.263	31.5
19	3695.278	24.504	60.1
20	3596.060	23.846	102.2
21	3255.593	21.588	60.3
22	3231.584	21.429	95.7
23	3002.196	19.908	97.2
24	2963.724	19.653	62.8
25	2032.287	13.476	92.8
26	1101.718	7.306	56.3

^{13}C spectrum of **5**, expansion of the aliphatic region

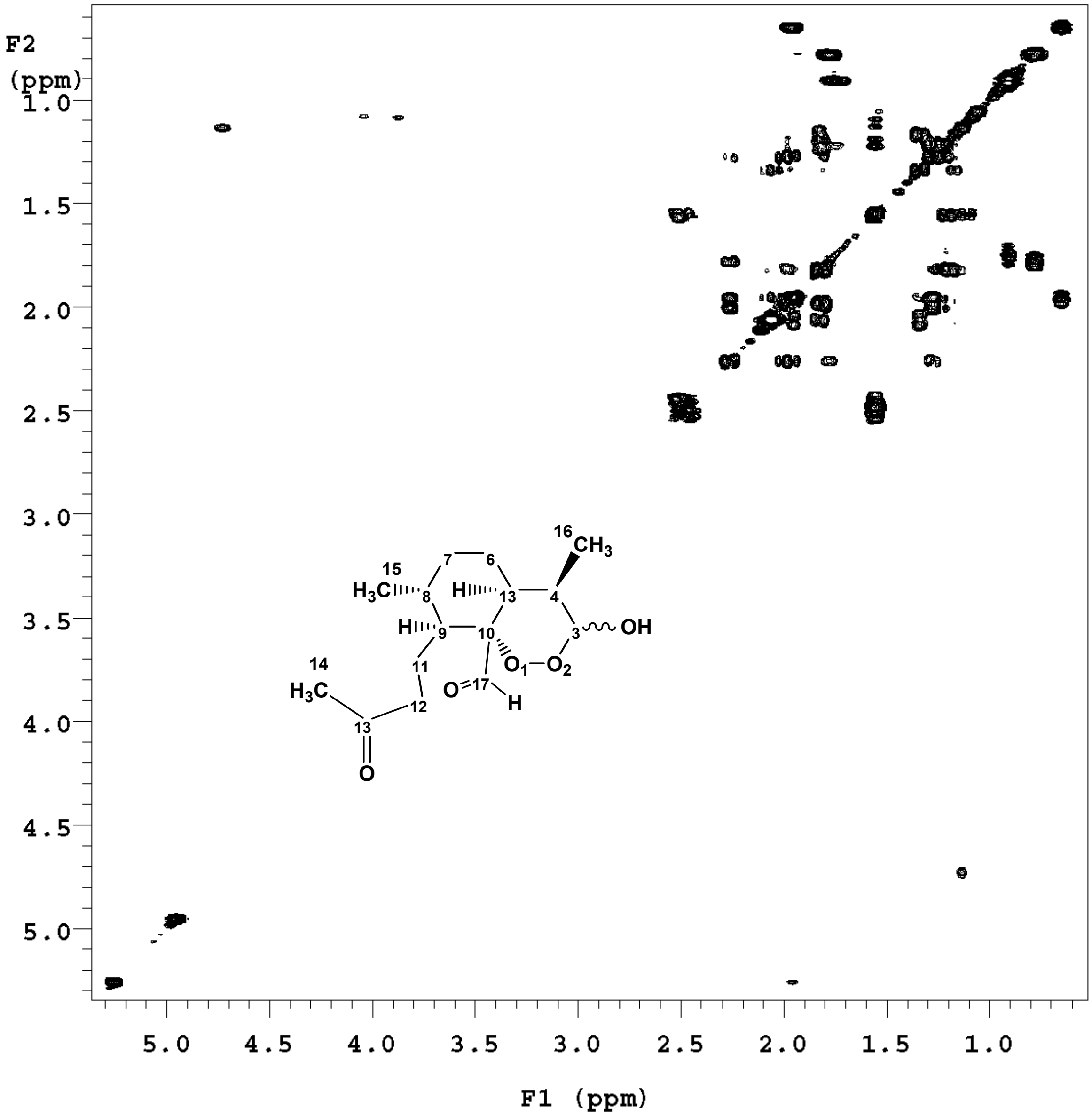




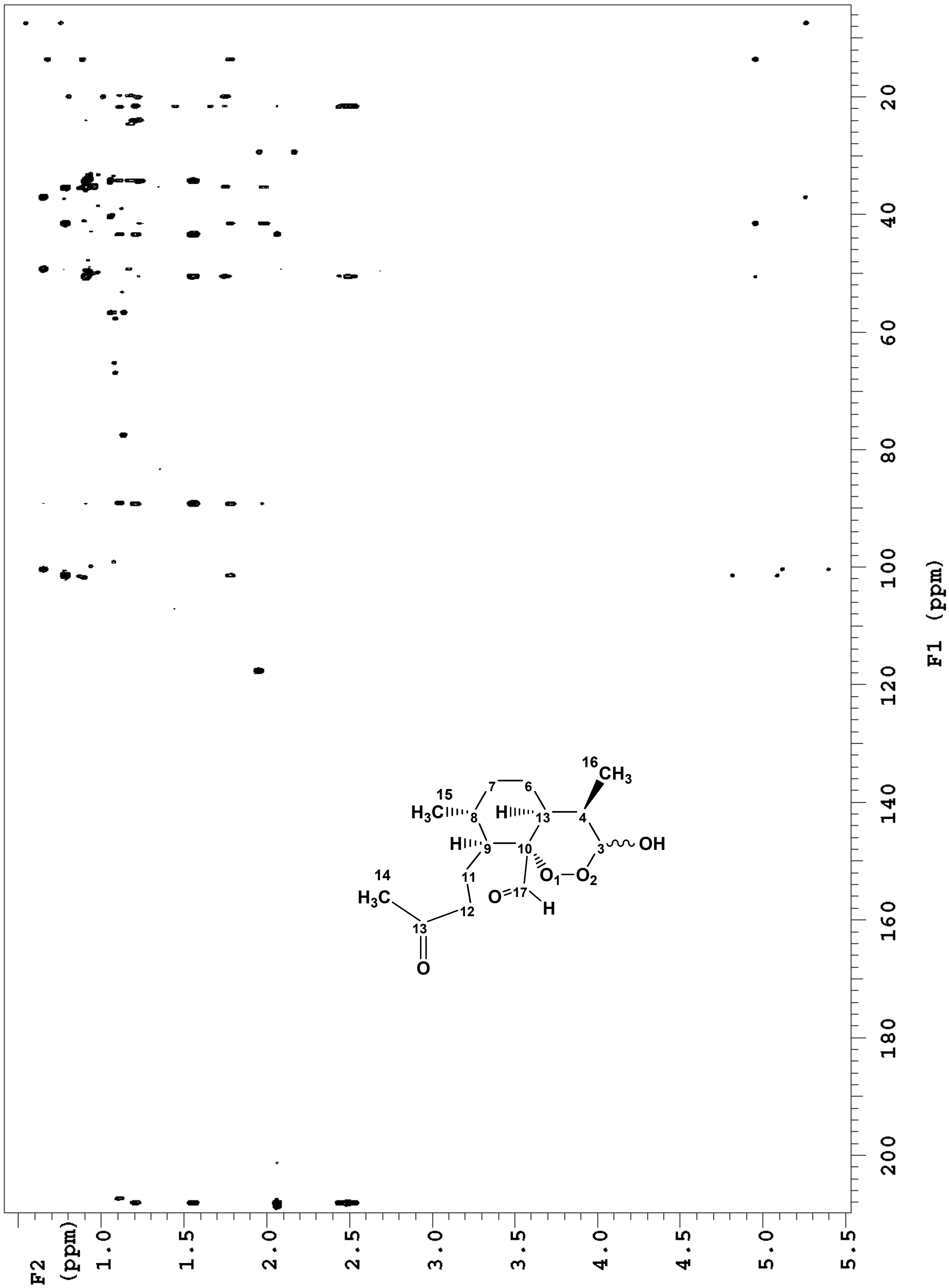
^{13}C spectrum of **5**, expansion of the carbonilic region



Aliphatic region of the edited ^{1}H-^{13}Cgs-HSQC spectrum of **5**. Blue cross peaks indicate the CH_2 signals. Double arrows indicate the pair of signals corresponding to **5α** and **5β**epimers.



Aliphatic region of the ^1H-^1H g-COSYspectrum of **5**.



Full ^{1}H-^{13}C gs-HMBC spectrum of **5**

2. *J*-coupling calculation for 5α and 5β epimers;

MKA – 5α epimer

```
Method: B3LYP/6-31G(d)

SCF Done:  E(RB+HF-LYP) =  -962.068193677     A.U. after    1 cycles
             Convg  =    0.7801D-08             -V/T =  2.0092
             S**2   =   0.0000

 Zero-point correction=                           0.379786 (Hartree/Particle)
 Thermal correction to Energy=                    0.400350
 Thermal correction to Enthalpy=                  0.401295
 Thermal correction to Gibbs Free Energy=         0.332176
 Sum of electronic and zero-point Energies=           -961.688408
 Sum of electronic and thermal Energies=              -961.667843
 Sum of electronic and thermal Enthalpies=            -961.666899
 Sum of electronic and thermal Free Energies=         -961.736018
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.042352	-0.396562	1.473915
2	8	0	-0.007359	-2.266493	-0.017494
3	6	0	-0.349604	1.399132	-0.524439
4	6	0	0.534631	2.630345	-0.147959
5	6	0	2.015105	2.407425	-0.521683
6	6	0	2.598979	1.110560	0.046620
7	6	0	1.732550	-0.072049	-0.392215
8	6	0	0.260455	0.086643	0.076446
9	8	0	-0.494577	-0.982158	-0.534522
10	6	0	-3.189493	-0.523202	0.271312
11	6	0	-2.851153	0.601998	-0.702932
12	6	0	-1.840935	1.636925	-0.177322
13	6	0	2.312203	-1.474263	-0.085419
14	6	0	1.296405	-2.529383	-0.544045
15	6	0	2.740677	-1.734387	1.366486
16	6	0	0.046305	3.931816	-0.807734
17	6	0	-3.759179	-1.792703	-0.330097
18	1	0	-0.278912	1.265514	-1.615556
19	1	0	0.479754	2.754216	0.940557
20	1	0	2.600527	3.267622	-0.173064
21	1	0	2.106450	2.394651	-1.619107
22	1	0	2.646992	1.173471	1.137659
23	1	0	3.624649	0.965404	-0.318935
24	1	0	1.655391	-0.030315	-1.487751
25	1	0	-3.812491	1.103745	-0.899742
26	1	0	-2.538709	0.176888	-1.663202
27	1	0	-2.113973	2.604924	-0.603983
28	1	0	-1.970558	1.730730	0.907468
29	1	0	3.195601	-1.597052	-0.725083
30	1	0	3.430100	-0.963897	1.722610
31	1	0	3.255758	-2.699765	1.438632
32	1	0	1.890332	-1.763749	2.054221
33	1	0	0.771543	4.733813	-0.627693
34	1	0	-0.915125	4.275813	-0.415965
35	1	0	-0.051668	3.815499	-1.895424

36	1	0	-4.481052	-1.575355	-1.126056
37	1	0	-4.225867	-2.400762	0.447850
38	1	0	-2.933183	-2.358534	-0.778751
39	6	0	0.050122	0.022148	1.596333
40	1	0	-0.639531	-0.770769	1.934088
41	8	0	0.569353	0.788371	2.382502
42	1	0	1.496545	-3.509549	-0.080595
43	8	0	1.307963	-2.598317	-1.939727
44	1	0	0.560807	-3.157300	-2.209677

MKA – 5α epimer.

J-coupling calculation, `b3lyp/6-311++g(2d,p)level`

Total nuclear spin-spin coupling J (Hz):

	1	2	3	4	5
1	0.000000D+00				
2	0.251983D-01	0.000000D+00			
3	0.416047D-01	0.880162D+00	0.000000D+00		
4	-0.215157D-02	0.286709D+00	0.319997D+02	0.000000D+00	
5	0.361653D-02	0.971960D-02	-0.830285D+00	0.321132D+02	0.000000D+00
6	-0.511696D-02	-0.558229D+00	0.972062D+00	-0.752527D+00	0.320519D+02
7	0.913773D-02	-0.279380D+01	-0.590280D-01	0.176088D+01	-0.677578D+00
8	-0.204432D+00	-0.671916D+00	0.321426D+02	0.247753D+00	0.975817D+00
9	0.206112D+00	-0.259987D+01	-0.711003D+01	-0.289888D+01	0.233853D+00
10	0.339599D+02	-0.876979D-01	0.951653D-01	-0.789703D-01	-0.138215D-01
11	-0.650889D+00	-0.118393D+00	-0.526822D+00	0.422240D+01	0.332560D+00
12	-0.137126D+01	0.118603D+00	0.349873D+02	0.382292D+00	0.292879D+01
13	-0.143195D-01	-0.145878D+01	0.161422D+01	-0.207923D+00	0.387448D+01
14	-0.250596D-01	0.373471D+02	-0.323106D+00	-0.663279D-01	0.215020D+00
15	-0.109299D-01	-0.341319D-01	-0.512913D-01	-0.869669D-02	-0.635231D-01
16	-0.674280D-02	-0.506017D-01	-0.106440D-01	0.350634D+02	0.436630D+00
17	-0.206509D+01	-0.985071D-01	-0.109359D+00	0.162546D+00	0.326563D-03
18	-0.840881D-01	0.293750D+00	0.132771D+03	-0.431387D+01	0.185599D+01
19	0.637037D-02	0.181282D-01	-0.404358D+01	0.135140D+03	-0.324225D+01
20	0.257980D-02	0.145075D-01	0.760003D+01	-0.241008D+01	0.132835D+03
21	0.120500D-02	0.263878D-01	0.187824D+01	-0.388778D+01	0.127319D+03
22	-0.102971D-01	-0.121609D-01	-0.178851D-02	0.138241D+01	-0.317804D+01
23	0.975840D-02	-0.156184D+00	-0.573518D+00	0.846572D+01	-0.311373D+01
24	-0.103859D-01	0.698638D-01	0.343176D+01	-0.339613D+00	0.335036D+01
25	-0.178863D+01	-0.520918D+00	0.646283D+01	0.191333D+00	0.175518D+00
26	-0.164253D+01	-0.322427D+00	0.482912D+01	-0.199054D+00	-0.280923D-01
27	0.382639D-01	-0.289888D-01	-0.293057D+01	0.249456D+01	-0.248369D+00
28	0.263246D+00	0.292396D-01	-0.381600D+01	0.153477D+01	-0.191424D+00
29	-0.184969D-01	-0.146901D+01	-0.279650D-02	0.172250D+00	-0.233047D+00
30	-0.210774D-01	0.828846D-01	0.103637D+00	-0.132256D-01	0.498822D-01
31	-0.212269D-01	-0.740715D-01	0.315313D-01	-0.187513D-01	-0.566217D-01
32	-0.545579D-01	-0.322787D+00	-0.609859D-01	-0.358447D-02	0.181397D-01
33	0.913467D-02	-0.125873D+00	0.986377D+01	-0.200558D+01	0.430113D+01
34	0.198953D-01	0.189925D-01	0.350340D+00	-0.256663D+01	0.110412D+02
35	0.145649D-01	-0.520543D-02	0.373193D+01	-0.416119D+01	0.163004D+01
36	-0.255796D+01	-0.519765D-01	0.292106D-01	0.334514D-02	-0.155881D-01
37	-0.142094D+01	0.226564D-01	-0.653917D-01	0.210101D-02	-0.195756D-01
38	-0.198811D+01	-0.133633D+00	0.215534D+00	0.836942D-02	0.226912D-02
39	-0.204218D+01	-0.862744D+00	0.235109D+00	0.324747D-01	-0.639785D-01
40	-0.546087D+00	-0.236946D+00	0.467357D+00	-0.193923D+00	-0.456743D-01
41	0.146234D+00	-0.150025D+00	-0.256818D+00	-0.994634D+00	0.126022D+00
42	-0.431353D-01	-0.321613D+02	0.153020D+01	0.117602D+00	0.264906D+00
43	0.436748D-02	-0.790522D-01	0.332136D-01	0.838770D-02	-0.113700D-01

44	-0.387093D-01	0.575058D+00	-0.344583D-01	-0.290523D-01	-0.532255D-02

	6	7	8	9	10
6	0.000000D+00				
7	0.330967D+02	0.000000D+00			
8	-0.294457D+00	0.335980D+02	0.000000D+00		
9	-0.307618D+00	-0.193853D+01	0.333663D+02	0.000000D+00	
10	-0.236736D-02	-0.778548D-02	0.374841D-01	-0.108994D+01	0.000000D+00
11	-0.222845D-01	-0.149714D+00	0.101629D+00	-0.249227D+01	0.386285D+02
12	-0.307754D+00	0.206637D+01	-0.629214D+00	0.163019D+00	-0.167695D+01
13	-0.682646D-01	0.330023D+02	-0.115906D+01	-0.244656D+01	0.165029D-02
14	0.234753D+01	-0.202208D+01	0.132917D+01	-0.147064D+01	0.934049D-02
15	0.158179D+01	-0.758903D+00	0.245044D+00	-0.376426D-01	0.753760D-02
16	0.457384D+01	-0.296400D+00	0.287855D+01	-0.496958D+00	0.152447D+00
17	-0.335671D-02	0.480120D-02	-0.315285D-01	-0.236565D+00	0.404040D+02
18	-0.227279D+00	0.238057D+01	-0.529481D+01	-0.256093D+01	-0.101050D+00
19	0.143171D+01	-0.131032D+00	0.893666D+00	0.329323D+00	0.690626D-02
20	-0.215768D+01	0.976231D+01	-0.692539D+00	-0.275614D+00	-0.215765D-01
21	-0.334166D+01	0.213681D+01	-0.306591D+00	-0.534503D-01	-0.227853D-02
22	0.135208D+03	-0.463361D+01	0.195707D+01	0.132420D+00	-0.134314D-01
23	0.130689D+03	-0.281586D+01	0.851051D+01	-0.195330D+00	-0.247391D-01
24	-0.431586D+01	0.133211D+03	-0.632831D+01	-0.522286D+00	-0.800418D-02
25	-0.451345D-01	0.123532D+00	-0.331560D+00	-0.354012D+01	-0.569079D+01
26	-0.248117D-01	0.497792D-01	-0.178017D+00	-0.215944D+01	-0.354179D+01
27	-0.157518D-01	0.444466D+00	0.908286D+01	0.229757D+00	0.809225D+01
28	0.337237D-01	-0.188097D+00	0.235640D+01	-0.544983D-01	0.535184D+01
29	0.135310D+01	-0.306730D+01	0.596957D+01	-0.748287D+00	-0.134831D-01
30	0.359136D+00	0.174011D+01	-0.139391D+00	0.698068D-02	-0.586596D-02
31	0.335749D+00	0.875937D+01	-0.333281D+00	-0.251144D-01	0.150501D-02
32	-0.178237D+00	0.159491D+01	-0.731513D-01	-0.138216D+00	0.266761D-01
33	0.247078D+00	0.604342D-01	0.113754D+01	-0.101733D+01	0.511111D-01
34	0.175814D+01	-0.876572D-01	-0.317643D+00	0.528145D-01	0.496713D-01
35	-0.248864D+00	0.172074D-01	-0.859933D-01	-0.331081D-01	-0.202864D-01
36	-0.172522D-01	-0.147460D-01	-0.832548D-02	-0.148164D+00	-0.298825D+01
37	-0.169251D-01	-0.205800D-01	-0.267813D-01	0.188023D-01	-0.585546D+01
38	-0.181799D-03	0.306159D-02	0.505924D-01	-0.448435D+00	-0.626807D+01
39	-0.625004D-01	0.189640D+01	0.412388D+02	-0.301843D+01	0.138975D+00
40	-0.192937D+00	0.129567D+01	0.197780D+02	-0.968118D+00	0.301577D+00
41	-0.110462D+01	0.115592D+00	0.239653D+00	0.224329D-01	0.366578D-01
42	0.460667D+00	0.265550D+01	-0.898164D+00	-0.273432D+01	0.481338D-01
43	0.178395D+00	0.149104D+00	0.147703D-01	-0.226831D+00	-0.307632D-02
44	0.406812D-01	-0.370601D+00	-0.350421D-01	-0.233957D+00	0.213945D-01

	11	12	13	14	15
11	0.000000D+00				
12	0.364600D+02	0.000000D+00			
13	-0.135780D-01	0.512030D+00	0.000000D+00		
14	0.193049D-01	0.513238D-01	0.417327D+02	0.000000D+00	
15	-0.510395D-02	-0.251920D-01	0.347072D+02	0.231359D+01	0.000000D+00
16	0.631835D-01	0.205850D+01	0.165527D+00	-0.228031D-01	-0.267149D-02
17	0.158222D+02	0.929902D+00	0.961186D-02	-0.127172D-01	-0.554061D-02
18	0.283593D+01	-0.319918D+01	-0.139471D+00	0.216681D-01	0.451002D-01
19	-0.281163D+00	0.213222D+01	0.515521D-01	-0.284089D-01	0.112280D-01
20	0.467751D+00	0.890138D+00	0.842744D+00	0.246118D+00	-0.634402D-01
21	-0.409080D-01	-0.225183D+00	-0.256767D+00	-0.547237D-02	0.250924D+00
22	-0.191752D-01	0.709797D-01	0.989842D+00	-0.169893D+00	0.208068D+00
23	-0.112325D-02	0.352062D+00	0.263019D+01	0.606998D-01	-0.355478D-01
24	-0.104097D-01	-0.106747D+00	-0.357983D+01	0.112510D+01	0.784643D+01
25	0.123347D+03	-0.328889D+01	-0.620823D-01	-0.223165D-01	-0.296138D-01
26	0.134134D+03	-0.252764D+01	-0.605323D-02	-0.151953D-01	-0.108635D-01
27	-0.344264D+01	0.130465D+03	0.322767D+00	-0.153717D-01	-0.347692D-01
28	-0.392946D+01	0.133710D+03	-0.847741D-01	-0.217631D-01	0.129034D-01
29	-0.499126D-01	0.266732D+00	0.134550D+03	-0.434947D+01	-0.362646D+01

30	-0.221708D-01	-0.136517D-01	-0.254518D+01	0.151208D+02	0.133282D+03
31	-0.184166D-01	0.348653D-01	-0.272869D+01	0.286001D+01	0.128824D+03
32	-0.195925D-01	-0.367111D-02	-0.405816D+01	0.304625D+01	0.131069D+03
33	-0.966791D-01	0.952846D+00	0.290352D-01	-0.409413D-01	-0.186976D-01
34	0.385392D-01	0.828628D+00	0.360206D-01	-0.192103D-01	-0.104190D-01
35	0.430453D-01	-0.147007D+00	-0.161570D-01	-0.212621D-01	-0.223163D-01
36	0.299078D+00	0.774499D+00	-0.102479D-01	-0.235968D-01	-0.162418D-01
37	0.521123D+01	0.124184D+01	-0.160120D-01	0.456631D-02	-0.107556D-01
38	-0.508118D+00	-0.249029D+00	-0.496447D-03	0.345987D-01	-0.343068D-02
39	-0.178645D+00	0.100083D+01	0.349070D+00	-0.153059D+00	0.374234D-01
40	-0.317361D-01	-0.168500D+00	-0.141382D+00	0.172646D-01	0.772120D+00
41	-0.178525D-02	-0.107258D+00	-0.407542D-01	-0.111322D-01	-0.283913D+00
42	0.440009D-01	-0.882779D-01	0.299410D+00	0.168974D+03	0.341627D+01
43	-0.708580D-02	0.853146D-02	-0.112694D+02	0.271972D+02	-0.295001D+01
44	-0.589098D-02	-0.240108D-01	0.855921D+01	-0.407057D+01	0.105799D+01

	16	17	18	19	20
16	0.000000D+00				
17	0.326345D-01	0.000000D+00			
18	0.261743D+01	0.505534D-01	0.000000D+00		
19	-0.280320D+01	-0.267702D-01	0.107071D+02	0.000000D+00	
20	0.220834D+01	-0.460315D-03	-0.464432D+00	0.459990D+01	0.000000D+00
21	0.335512D+01	-0.171251D-01	0.375460D-01	0.123921D+02	-0.141694D+02
22	-0.339235D+00	-0.214119D-01	-0.164173D+00	-0.517451D-02	0.456656D+01
23	0.181587D+00	-0.111956D-01	0.332860D+00	-0.670852D+00	0.278015D+01
24	0.321123D+00	-0.211323D-01	0.139189D+00	-0.112820D+00	-0.173482D+00
25	0.113725D-01	-0.836313D+00	-0.397928D+00	-0.676909D-01	0.109217D-01
26	-0.301607D-01	0.471646D+00	0.166794D-01	-0.546542D-01	-0.350527D-01
27	0.405110D+00	0.519825D+00	0.330848D+01	-0.283850D+00	0.105518D+00
28	-0.268747D+00	-0.309362D+00	0.129419D+02	0.771789D-01	-0.114532D+00
29	-0.193250D-01	-0.200092D-01	-0.505255D-01	-0.116946D+00	-0.318970D-01
30	-0.136735D-01	-0.158020D-01	-0.103244D+00	0.187780D-01	0.514844D-01
31	-0.340117D-01	-0.144332D-01	-0.475283D-01	-0.848910D-01	-0.774171D-02
32	-0.177657D-01	-0.802191D-03	-0.843177D-01	0.411875D-02	-0.740306D-01
33	0.129989D+03	-0.142080D-01	-0.477910D+00	0.240694D+01	0.718461D-01
34	0.131046D+03	-0.106657D-02	-0.270045D+00	0.543183D+01	-0.172851D+00
35	0.127717D+03	-0.913332D-02	0.746655D-01	0.134822D+02	-0.368237D+00
36	-0.172252D-01	0.128560D+03	-0.307757D-01	-0.699385D-01	-0.705122D-01
37	0.886775D-02	0.137996D+03	-0.922513D-01	-0.707807D-01	-0.790982D-01
38	-0.125223D-01	0.129126D+03	0.117888D-01	-0.649236D-01	-0.736055D-01
39	-0.750787D-01	0.190396D-02	0.532201D+01	-0.115484D+00	-0.110582D+00
40	-0.228690D-01	0.586347D-01	0.196374D+01	-0.338234D+00	-0.102700D+00
41	-0.171205D+00	0.973113D-02	-0.745989D-01	-0.428557D+00	-0.192591D-01
42	0.179785D+00	-0.192290D-01	-0.211374D+00	-0.133727D+00	0.142926D+00
43	0.635703D-03	0.306182D-02	-0.962022D-02	0.929358D-02	0.308231D-01
44	-0.143665D-01	0.244048D-01	0.202105D-02	-0.114921D+00	-0.109447D+00

	21	22	23	24	25
21	0.000000D+00				
22	0.135211D+02	0.000000D+00			
23	0.493460D+01	-0.140939D+02	0.000000D+00		
24	0.209725D-01	0.139243D+02	0.354046D+01	0.000000D+00	
25	-0.675741D-01	-0.100628D+00	-0.836876D-01	-0.655211D-01	0.000000D+00
26	0.532219D-01	-0.884590D-01	-0.753371D-01	0.107809D+00	-0.197192D+02
27	0.131816D-01	-0.932683D-01	-0.154953D+00	-0.470648D-01	0.108212D+02
28	0.112939D+00	0.258888D-01	-0.136268D+00	-0.340566D-01	0.773623D+00
29	0.152321D+00	-0.294211D+00	0.505488D-01	0.536074D+01	-0.896628D-01
30	0.103791D-01	0.224068D+00	0.211168D+00	-0.594373D+00	-0.922585D-01
31	0.608838D-01	-0.785443D-01	-0.600224D-01	0.694119D+00	-0.938956D-01
32	-0.116502D+00	0.142817D+00	-0.198150D-01	-0.737375D+00	-0.804563D-01
33	-0.158665D+00	-0.250055D-01	0.123691D-01	-0.692595D-01	0.977974D-01
34	-0.244526D+00	-0.220423D+00	0.158159D+00	-0.797044D-01	0.145341D+00
35	-0.132622D-01	0.852029D-01	-0.113553D+00	0.506294D-01	0.585089D-02

36	-0.436914D-01	-0.802212D-01	-0.777477D-01	-0.377471D-01	0.468537D+00
37	-0.716374D-01	-0.674369D-01	-0.787388D-01	-0.754028D-01	-0.319742D+00
38	-0.319122D-01	-0.598659D-01	-0.590348D-01	0.156879D-01	0.591498D+00
39	-0.600540D-01	-0.186842D+00	-0.282888D+00	0.630378D+01	0.289015D+00
40	-0.138957D+00	-0.309663D+00	-0.319425D+00	0.182994D+01	-0.136106D+00
41	-0.422778D+00	-0.434397D+00	-0.530590D+00	-0.674692D-02	-0.190322D-01
42	-0.113805D+00	-0.108361D+00	-0.119305D-02	-0.762071D+00	0.815391D-01
43	-0.160233D-02	-0.235941D+00	-0.302628D-01	0.768796D-02	0.612774D-02
44	-0.647942D-01	-0.120994D+00	-0.134094D+00	-0.138290D+00	-0.527850D-01

	26	27	28	29	30
26	0.000000D+00				
27	0.526435D+00	0.000000D+00			
28	0.109693D+02	-0.162336D+02	0.000000D+00		
29	-0.561651D-01	0.687623D-01	-0.820722D-01	0.000000D+00	
30	-0.771065D-01	-0.838719D-01	-0.475384D-01	0.318525D+01	0.000000D+00
31	-0.700282D-01	-0.106462D+00	-0.851717D-01	0.542941D+01	-0.144645D+02
32	-0.486996D-01	-0.889124D-01	-0.444174D-02	0.159003D+02	-0.145665D+02
33	-0.680179D-01	-0.289250D+00	-0.855817D-01	-0.663963D-01	-0.274743D-01
34	-0.117634D-01	-0.280146D+00	0.121271D+00	-0.876476D-01	-0.571945D-01
35	0.508494D-01	0.219332D+00	0.366288D-01	-0.457559D-01	-0.568971D-01
36	-0.238005D+00	-0.981519D-01	-0.144351D+00	-0.826914D-01	-0.809438D-01
37	0.137273D+01	0.299937D+00	-0.158992D+00	-0.865951D-01	-0.636777D-01
38	0.576920D+00	-0.499120D-01	-0.661400D-01	-0.575617D-01	-0.588999D-01
39	0.252190D-01	-0.133630D+00	0.341821D-01	-0.206301D+00	0.174130D+00
40	-0.678474D-01	0.117484D+00	0.521663D+00	-0.159433D+00	-0.122172D+00
41	0.524435D-01	-0.101533D+00	-0.619707D+00	-0.151088D+00	-0.262157D+00
42	0.290602D-01	-0.120764D+00	-0.937415D-01	0.859213D+00	0.117289D+00
43	-0.145587D-01	0.139629D-01	0.199260D-01	-0.305950D+01	-0.173065D+01
44	0.805786D-01	-0.825747D-01	-0.911870D-01	0.628667D+00	0.478008D+00

	31	32	33	34	35
31	0.000000D+00				
32	-0.141721D+02	0.000000D+00			
33	-0.743660D-01	-0.573359D-01	0.000000D+00		
34	-0.849297D-01	-0.578782D-01	-0.146854D+02	0.000000D+00	
35	-0.791766D-01	-0.745437D-01	-0.143048D+02	-0.129413D+02	0.000000D+00
36	-0.687052D-01	-0.555588D-01	-0.647256D-01	-0.219064D-01	-0.187196D-01
37	-0.406090D-01	0.149544D-03	-0.676816D-01	-0.470730D-01	-0.652803D-01
38	-0.266978D-01	0.196012D-01	-0.669410D-01	-0.441274D-01	-0.274013D-01
39	-0.984072D-01	0.188101D+00	-0.582140D-01	0.628769D-02	0.260554D-01
40	0.129568D+00	0.326738D+00	-0.135679D+00	-0.782615D-01	-0.119781D+00
41	-0.458087D+00	-0.110738D+01	0.130387D-01	-0.744936D-01	-0.267347D+00
42	0.641179D-01	0.169967D-01	-0.458594D-01	-0.109088D+00	-0.940968D-01
43	-0.114881D-01	0.349510D+00	0.112836D-01	0.110867D-01	0.481231D-02
44	-0.143014D+00	-0.246167D+00	-0.821240D-01	-0.716671D-01	-0.392961D-01

	36	37	38	39	40
36	0.000000D+00				
37	-0.108126D+02	0.000000D+00			
38	-0.193070D+02	-0.157853D+02	0.000000D+00		
39	-0.184611D-01	0.256676D-01	0.130828D+00	0.000000D+00	
40	-0.774986D-01	0.573959D-01	0.108413D+00	0.197070D+03	0.000000D+00
41	0.587146D-01	0.514937D-01	0.101570D+00	0.365198D+02	-0.439396D+01
42	-0.687936D-01	-0.257734D-01	0.215709D-01	0.101576D+00	0.103188D+00
43	0.137385D-02	0.807771D-02	0.100571D-02	-0.271618D+00	-0.928444D-02
44	0.316069D-01	0.922609D-02	0.200748D+00	-0.496857D-01	-0.491206D-01

	41	42	43	44
41	0.000000D+00			
42	-0.733855D-02	0.000000D+00		
43	0.275511D-01	-0.286325D+01	0.000000D+00	
44	0.721006D-01	0.851683D+00	-0.728506D+02	0.000000D+00

MKA – 5β epimer

```
SCF Done:  E(RB+HF-LYP) =  -962.066987698     A.U. after    1 cycles
             Convg  =    0.7806D-08             -V/T =  2.0092

Zero-point correction=                           0.379919 (Hartree/Particle)
 Thermal correction to Energy=                    0.400539
 Thermal correction to Enthalpy=                  0.401483
 Thermal correction to Gibbs Free Energy=         0.331535
 Sum of electronic and zero-point Energies=           -961.687069
 Sum of electronic and thermal Energies=              -961.666449
 Sum of electronic and thermal Enthalpies=            -961.665504
 Sum of electronic and thermal Free Energies=         -961.735453
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.335873	-1.082373	-1.236490
2	8	0	1.286100	-1.924409	0.335684
3	6	0	-1.090718	0.893903	-0.082057
4	6	0	-0.913599	2.444767	-0.130567
5	6	0	0.253696	2.874776	-1.040901
6	6	0	1.574836	2.179899	-0.697577
7	6	0	1.371719	0.664263	-0.743790
8	6	0	0.273164	0.194274	0.248912
9	8	0	0.053209	-1.214351	0.000132
10	6	0	-2.980746	-1.691728	-0.243187
11	6	0	-2.591132	-0.975490	1.045419
12	6	0	-2.259217	0.512878	0.863193
13	6	0	2.664407	-0.189768	-0.670433
14	6	0	2.224447	-1.652602	-0.734683
15	6	0	3.595102	0.081755	0.520418
16	6	0	-2.197975	3.161940	-0.582596
17	6	0	-2.913206	-3.206886	-0.217152
18	1	0	-1.351619	0.547333	-1.090529
19	1	0	-0.675308	2.778712	0.887947
20	1	0	0.371786	3.963483	-0.971600
21	1	0	-0.008876	2.657297	-2.087851
22	1	0	1.917858	2.495400	0.292356
23	1	0	2.352645	2.464337	-1.418988
24	1	0	0.928271	0.437448	-1.726726
25	1	0	-1.784555	-1.529918	1.533040
26	1	0	-3.460364	-1.058786	1.718000
27	1	0	-3.157178	0.990516	0.464007
28	1	0	-2.085197	0.956208	1.852871
29	1	0	3.226900	0.017212	-1.592282
30	1	0	3.844403	1.144888	0.585570
31	1	0	4.524300	-0.481801	0.403233
32	1	0	3.147827	-0.218758	1.471820
33	1	0	-1.998288	4.230615	-0.723375
34	1	0	-3.008636	3.078991	0.146676
35	1	0	-2.561791	2.762337	-1.537782
36	1	0	-3.386977	-3.620433	-1.109965
37	1	0	-3.388783	-3.612512	0.684025
38	1	0	-1.858893	-3.510548	-0.189711

39	8	0	3.299567	-2.505377	-0.521798
40	1	0	1.697161	-1.863860	-1.677604
41	1	0	2.978648	-3.417821	-0.610070
42	6	0	0.605797	0.357880	1.733875
43	1	0	0.530314	-0.581081	2.320057
44	8	0	0.885360	1.410457	2.267927

MKA – 5β epimer.

J-coupling calculation, `b3lyp/6-311++g(2d,p)level`

Total nuclear spin-spin coupling J (Hz):

	1	2	3	4	5
1	0.000000D+00				
2	0.205170D-01	0.000000D+00			
3	-0.516412D+00	0.591721D+00	0.000000D+00		
4	0.530752D-02	0.237788D+00	0.321865D+02	0.000000D+00	
5	-0.113449D-01	0.362927D-01	-0.738427D+00	0.322770D+02	0.000000D+00
6	-0.331198D-02	-0.984275D-01	0.833423D+00	-0.729844D+00	0.319760D+02
7	-0.116071D-01	-0.112312D+01	0.164688D+00	0.169715D+01	-0.731455D+00
8	-0.315676D-02	-0.669068D+00	0.310707D+02	0.187421D+00	0.982428D+00
9	0.802954D-01	-0.126465D+01	-0.693372D+01	-0.279662D+01	0.286560D+00
10	0.345306D+02	-0.352515D-01	0.558413D+00	-0.138859D+00	-0.242092D-01
11	-0.665709D+00	-0.121188D+00	-0.126471D+01	0.394431D+01	0.428837D+00
12	-0.720521D+00	0.140062D+00	0.347864D+02	0.473892D+00	0.299573D+01
13	-0.121019D-01	-0.249490D+01	0.178969D+01	-0.231991D+00	0.375253D+01
14	-0.219711D-01	0.321969D+02	-0.254364D+00	-0.609664D-01	0.358500D+00
15	-0.457375D-02	-0.469546D+00	-0.786496D-01	-0.468268D-02	-0.523208D-01
16	0.139823D-01	-0.102098D+00	0.263454D+00	0.348858D+02	0.432393D+00
17	-0.193787D+01	-0.507884D-02	-0.128038D+00	0.172613D+00	0.657511D-03
18	-0.230270D+00	0.340218D+00	0.138382D+03	-0.415687D+01	0.163388D+01
19	-0.237979D+00	0.214961D-01	-0.426351D+01	0.133277D+03	-0.320701D+01
20	0.113689D-01	0.387509D-01	0.775713D+01	-0.240424D+01	0.132871D+03
21	-0.179081D-01	0.175275D-01	0.176333D+01	-0.389130D+01	0.127764D+03
22	-0.137288D-01	-0.268847D-01	-0.397104D-01	0.146587D+01	-0.303264D+01
23	-0.198490D-01	-0.347605D+00	-0.577769D+00	0.847685D+01	-0.311729D+01
24	-0.864041D-01	-0.304052D-01	0.324841D+01	-0.324069D+00	0.349072D+01
25	-0.177171D+01	-0.272140D+00	0.126805D+01	-0.319987D+00	-0.540665D-01
26	-0.181437D+01	-0.314886D+00	0.771076D+01	0.171403D+00	0.262011D+00
27	0.752408D-01	-0.662603D-01	-0.308219D+01	0.155061D+01	-0.307341D+00
28	0.941702D-01	0.277969D-02	-0.375934D+01	0.277068D+01	-0.155098D+00
29	-0.255546D-01	-0.190248D+01	-0.318971D-01	0.197886D+00	-0.217447D+00
30	-0.945569D-02	-0.131508D+00	0.134701D+00	-0.125008D-01	0.416353D-01
31	-0.678301D-02	0.187907D-01	0.733335D-01	-0.204171D-01	-0.577835D-01
32	-0.153551D-01	-0.304041D+00	-0.607090D-01	-0.139373D-02	0.115810D-01
33	-0.286538D-02	-0.119232D+00	0.995589D+01	-0.210948D+01	0.425919D+01
34	0.219729D-01	0.143902D-01	0.409711D+00	-0.261104D+01	0.111633D+02
35	-0.766419D-01	0.661367D-02	0.368194D+01	-0.418315D+01	0.163456D+01
36	-0.142987D+01	-0.162430D-01	0.120532D-01	0.134414D-01	-0.157959D-01
37	-0.255766D+01	0.851557D-02	0.273766D-01	0.331683D-02	-0.204869D-01
38	-0.208610D+01	-0.583563D-01	0.303171D+00	-0.324378D-03	-0.439149D-02
39	-0.419217D-02	0.162206D+01	-0.180127D+00	0.293910D-01	-0.314496D+00
40	-0.985958D-01	-0.480090D+01	-0.412134D-01	-0.301455D-01	-0.378946D-01
41	-0.353064D-01	0.963196D+00	-0.496789D-01	-0.225311D-01	0.151227D+00
42	-0.124211D+00	-0.118023D+01	-0.604442D-01	0.469332D-01	-0.520523D-01
43	-0.399238D-02	-0.359800D+00	0.124526D+00	-0.184149D+00	-0.426593D-01
44	-0.162687D-01	-0.143354D+00	-0.195385D+00	-0.736523D+00	0.103070D+00

	6	7	8	9	10
6	0.000000D+00				
7	0.327972D+02	0.000000D+00			
8	-0.214125D+00	0.344108D+02	0.000000D+00		
9	-0.294320D+00	-0.132627D+01	0.326905D+02	0.000000D+00	
10	-0.335965D-02	0.160439D-01	-0.411020D-01	-0.546085D+00	0.000000D+00
11	-0.244990D-01	-0.172880D+00	0.365762D+00	-0.264766D+01	0.381601D+02
12	-0.300267D+00	0.203991D+01	-0.703775D+00	0.282782D+00	-0.165481D+01
13	-0.822649D-01	0.330059D+02	-0.132696D+01	-0.909552D+00	0.572369D-03
14	0.346302D+01	-0.468241D+00	0.973260D+00	0.296359D-01	-0.232901D-02
15	0.132867D+01	-0.763377D+00	0.267830D+00	0.580332D-01	-0.357116D-02
16	0.465114D+01	-0.297043D+00	0.299346D+01	-0.451002D+00	-0.289497D-02
17	-0.398873D-02	-0.102309D-01	-0.173017D-01	-0.137477D+00	0.396072D+02
18	-0.178560D+00	0.223681D+01	-0.537161D+01	-0.286731D+01	-0.776571D-01
19	0.150315D+01	-0.119584D+00	0.792532D+00	0.273044D+00	0.382040D-02
20	-0.211079D+01	0.981727D+01	-0.688904D+00	-0.461991D+00	-0.185143D-01
21	-0.329034D+01	0.231225D+01	-0.312783D+00	-0.757363D-01	0.105073D-01
22	0.135338D+03	-0.444604D+01	0.205444D+01	0.197373D+00	-0.168371D-01
23	0.131077D+03	-0.286361D+01	0.862535D+01	-0.170797D+00	-0.134983D-01
24	-0.450603D+01	0.129613D+03	-0.638108D+01	-0.394261D+00	0.380565D-01
25	-0.333769D-01	-0.647200D-03	0.190639D-01	-0.218487D+01	-0.346882D+01
26	-0.395768D-01	0.119734D+00	-0.345265D+00	-0.273580D+01	-0.562739D+01
27	-0.169925D-01	0.544825D+00	0.906789D+01	-0.104750D+00	0.189340D+01
28	0.235381D-01	-0.196992D+00	0.138475D+01	-0.396300D-01	0.102107D+02
29	0.164203D+01	-0.336286D+01	0.614399D+01	-0.120515D+01	-0.122400D-02
30	0.370644D+00	0.199476D+01	-0.157751D+00	0.403670D-01	-0.967616D-02
31	0.357923D+00	0.926133D+01	-0.346364D+00	-0.774942D-02	-0.716382D-02
32	-0.167716D+00	0.142378D+01	-0.698687D-01	-0.105761D+00	0.238830D-02
33	0.196297D+00	0.568353D-01	0.121371D+01	-0.914583D+00	-0.373202D-01
34	0.172016D+01	-0.825181D-01	-0.325604D+00	0.597540D-01	-0.616861D-01
35	-0.266727D+00	0.238387D-01	-0.100022D+00	-0.298883D-01	-0.547964D-01
36	-0.172123D-01	-0.124656D-01	-0.129540D-01	0.581573D-01	-0.578609D+01
37	-0.292485D-01	-0.995312D-02	-0.114185D-01	-0.161053D+00	-0.348896D+01
38	0.464883D-02	-0.780939D-02	0.510527D-01	-0.242880D+00	-0.578940D+01
39	-0.762824D+00	-0.209073D+01	0.191970D+00	-0.199202D+01	-0.209195D-02
40	-0.240637D+00	0.125838D+01	-0.283795D-01	-0.459289D+00	0.458924D-01
41	0.470707D+00	0.862796D+00	-0.502663D-01	0.336507D+00	0.487794D-02
42	-0.119967D+00	0.191802D+01	0.430926D+02	-0.315498D+01	0.180296D-01
43	-0.182388D+00	0.169509D+01	0.188108D+02	-0.107291D+01	0.135174D-02
44	-0.101941D+01	0.105889D+00	0.467408D+00	-0.180775D+00	-0.487137D-02

	11	12	13	14	15
11	0.000000D+00				
12	0.352977D+02	0.000000D+00			
13	-0.118744D-01	0.455887D+00	0.000000D+00		
14	0.898547D-01	0.162441D-01	0.411531D+02	0.000000D+00	
15	-0.786350D-03	-0.275370D-01	0.344887D+02	-0.193644D+01	0.000000D+00
16	0.348497D-01	0.188831D+01	0.195526D+00	0.177823D-01	0.238272D-02
17	0.161242D+02	0.117465D+01	0.219198D-02	-0.802845D-03	-0.451864D-02
18	0.113227D+01	-0.343419D+01	-0.138053D+00	0.255964D-01	0.529642D-01
19	-0.219793D+00	0.251009D+01	0.531624D-01	-0.160213D-01	0.797464D-02
20	0.453057D+00	0.769440D+00	0.871529D+00	0.427788D+00	-0.670248D-01
21	-0.673960D-01	-0.228646D+00	-0.238467D+00	0.147231D-01	0.230736D+00
22	-0.188946D-01	0.778782D-01	0.868517D+00	-0.334680D-01	0.197637D+00
23	0.121551D-02	0.381082D+00	0.273568D+01	0.217973D+00	-0.221789D-01
24	-0.891798D-02	-0.103953D+00	-0.294914D+01	0.225529D+01	0.728131D+01
25	0.135171D+03	-0.240495D+01	-0.302514D-01	0.472930D-01	0.676236D-02
26	0.123759D+03	-0.322294D+01	-0.912309D-02	0.288796D-01	-0.169141D-01
27	-0.545865D+01	0.133513D+03	0.292706D+00	-0.497767D-01	-0.203071D-01
28	-0.135198D+01	0.129387D+03	-0.790100D-01	-0.151908D-01	0.163041D-01
29	-0.567536D-01	0.278404D+00	0.132052D+03	-0.306283D+01	-0.294370D+01
30	-0.225734D-01	-0.227853D-01	-0.247978D+01	0.866356D+01	0.131975D+03

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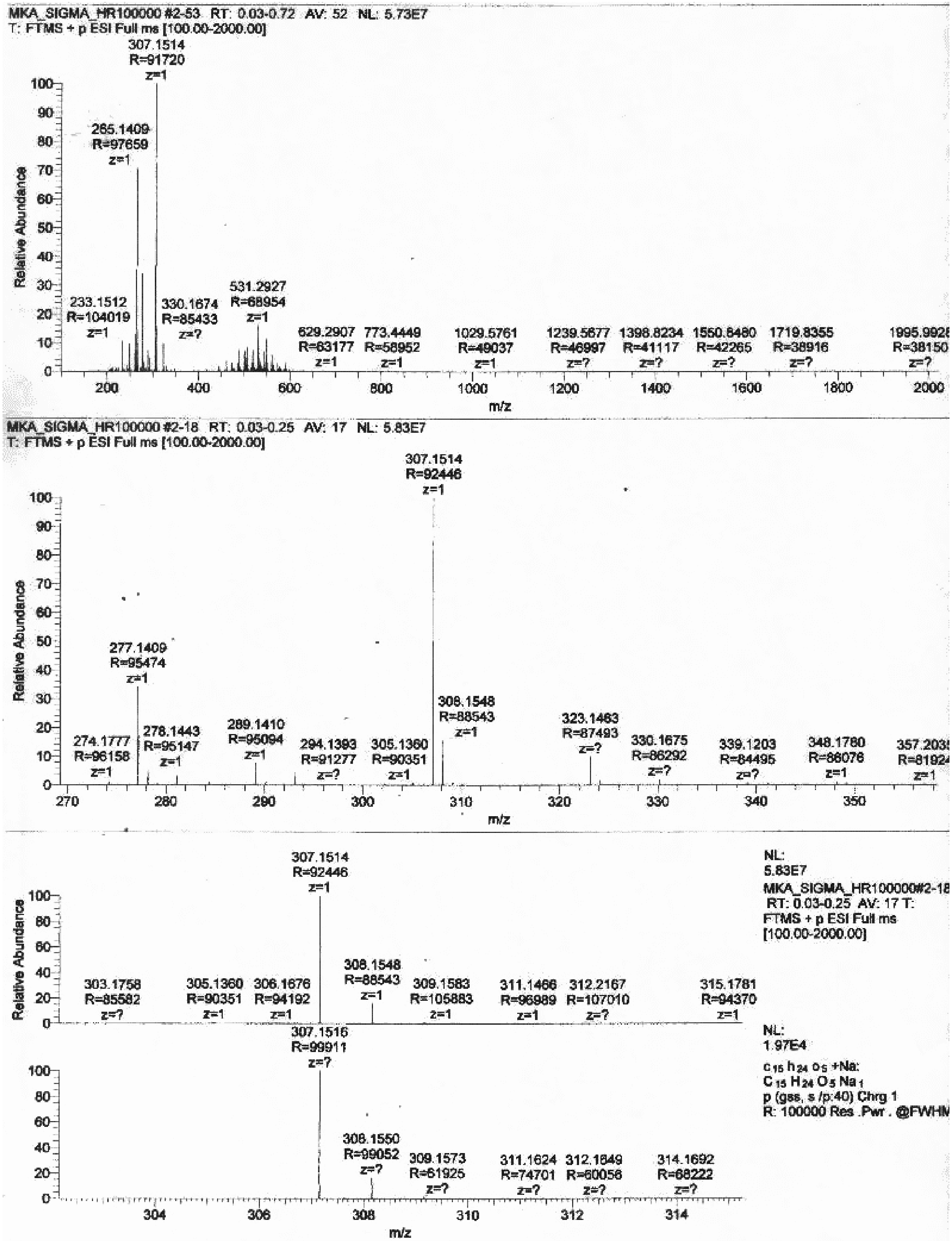
31 -0.166970D-01  0.257555D-01 -0.342013D+01  0.115483D+01  0.133934D+03
32  0.267960D-02 -0.820268D-02 -0.388048D+01  0.290696D+01  0.130934D+03
33 -0.100655D+00  0.850925D+00 -0.415526D-03 -0.350370D-01 -0.201645D-01
34  0.617433D-01  0.759611D+00  0.231861D-01 -0.150428D-01 -0.115561D-01
35 -0.315497D-02 -0.154825D+00 -0.207837D-01 -0.156648D-01 -0.221877D-01
36  0.546460D+01  0.137713D+01 -0.172781D-01 -0.619219D-02 -0.162393D-01
37  0.426557D-01  0.609409D+00 -0.201495D-01 -0.199582D-01 -0.128033D-01
38 -0.362906D+00 -0.202497D+00  0.358097D-02  0.177077D-01 -0.730280D-02
39  0.177308D-03  0.160304D-01 -0.838843D+01  0.239440D+02 -0.291925D+01
40  0.772560D-03 -0.106457D-01  0.438980D+01  0.173198D+03  0.386582D+01
41 -0.124923D-01 -0.337841D-01  0.869176D+01 -0.414027D+01  0.265246D+00
42 -0.238878D+00  0.128606D+01  0.265318D+00 -0.888468D-01  0.118142D-01
43  0.488740D+00 -0.125806D+00 -0.955329D-01  0.376827D-01  0.640495D+00
44 -0.243903D-03 -0.152396D+00 -0.423615D-01 -0.937929D-02 -0.265528D+00
          16            17            18            19            20
16  0.000000D+00
17 -0.377747D-02  0.000000D+00
18  0.269631D+01  0.123346D+00  0.000000D+00
19 -0.306597D+01 -0.276069D-01  0.106820D+02  0.000000D+00
20  0.218747D+01 -0.105775D-01 -0.508564D+00  0.465526D+01  0.000000D+00
21  0.323923D+01 -0.951113D-02  0.281960D-01  0.125527D+02 -0.142628D+02
22 -0.344359D+00 -0.167475D-01 -0.155175D+00  0.540565D-02  0.443677D+01
23  0.194417D+00 -0.146066D-01  0.328054D+00 -0.653530D+00  0.283416D+01
24  0.310305D+00 -0.562353D-02  0.148357D+00 -0.106653D+00 -0.110541D+00
25  0.342839D+00  0.286351D+00 -0.233811D+00  0.408313D-01 -0.127369D+00
26 -0.104071D-01 -0.782882D+00 -0.825380D+00 -0.424133D-01  0.807095D-01
27  0.550613D+00 -0.306977D+00  0.450456D+01 -0.309208D+00  0.486307D-01
28 -0.210419D+00  0.745901D+00  0.125717D+02  0.850630D-01 -0.127704D+00
29 -0.218870D-01 -0.168864D-01 -0.386794D-01 -0.118066D+00 -0.240347D-02
30 -0.688603D-02 -0.135970D-01 -0.102856D+00  0.210545D-01  0.611817D-01
31 -0.291620D-01 -0.115970D-01 -0.394474D-01 -0.837357D-01  0.521943D-02
32 -0.226101D-01 -0.575323D-02 -0.718406D-01  0.442136D-02 -0.768511D-01
33  0.129500D+03 -0.191554D-01 -0.467790D+00  0.243887D+01  0.752025D-01
34  0.130972D+03 -0.331246D-02 -0.258859D+00  0.548896D+01 -0.181853D+00
35  0.129780D+03  0.797689D-02  0.110942D+00  0.136013D+02 -0.368086D+00
36 -0.129670D-01  0.138278D+03 -0.114193D-01 -0.785001D-01 -0.746547D-01
37 -0.277509D-01  0.128284D+03 -0.857873D-01 -0.660618D-01 -0.778558D-01
38  0.102231D-02  0.128815D+03 -0.235074D-02 -0.720363D-01 -0.727081D-01
39 -0.607546D-01  0.209609D-02  0.897420D-01  0.255466D-01 -0.255974D+00
40 -0.224734D-01  0.107421D-01  0.134193D+00 -0.918423D-01 -0.107535D+00
41 -0.967063D-02  0.606278D-02 -0.621450D-01 -0.956700D-01 -0.145383D-01
42 -0.104331D+00  0.504388D-01  0.619255D+01 -0.735023D-01 -0.121330D+00
43 -0.262912D-01 -0.142011D-01  0.171229D+01 -0.331200D+00 -0.110395D+00
44 -0.178861D+00  0.203170D-01 -0.748669D-01 -0.563322D+00 -0.108132D-01
          21            22            23            24            25
21  0.000000D+00
22  0.135737D+02  0.000000D+00
23  0.484730D+01 -0.142300D+02  0.000000D+00
24  0.103273D-01  0.136354D+02  0.341830D+01  0.000000D+00
25 -0.788030D-01 -0.589185D-01 -0.108918D+00 -0.222235D-01  0.000000D+00
26 -0.833896D-01 -0.861842D-01 -0.101076D+00 -0.101616D+00 -0.201210D+02
27  0.301357D-01 -0.865889D-01 -0.146978D+00 -0.572854D-01  0.142268D+02
28  0.503976D-01  0.300970D-01 -0.136286D+00 -0.305448D-01  0.356120D+01
29  0.158282D+00 -0.289300D+00  0.381546D-01  0.486338D+01 -0.937223D-01
30  0.157779D-01  0.250851D+00  0.210097D+00 -0.581556D+00 -0.506948D-01
31  0.724247D-01 -0.656518D-01 -0.538978D-01  0.786470D+00 -0.487174D-01
32 -0.115272D+00  0.138837D+00 -0.285349D-01 -0.720002D+00  0.466828D-01
33 -0.162398D+00 -0.260645D-01  0.121185D-01 -0.686772D-01  0.153365D+00
34 -0.266932D+00 -0.219348D+00  0.171044D+00 -0.816321D-01  0.812732D-01
35 -0.166565D-01  0.867915D-01 -0.114345D+00  0.520265D-01 -0.874838D-01
36 -0.282101D-01 -0.779866D-01 -0.626844D-01 -0.513912D-02  0.120794D+01
```

```
37 -0.643551D-01 -0.705531D-01 -0.797535D-01 -0.580553D-01 -0.396742D+00
38 -0.249377D-01 -0.563049D-01 -0.528180D-01  0.415548D-01  0.101212D+01
39  0.387475D-01  0.596073D-01 -0.510180D-01  0.285948D+00 -0.260959D-01
40  0.413451D-01 -0.216086D-01 -0.188698D-01  0.193426D+00  0.138506D-01
41 -0.920917D-01 -0.149218D+00 -0.117548D+00 -0.225680D+00  0.211764D-02
42 -0.675095D-01 -0.245856D+00 -0.319732D+00  0.643641D+01  0.168738D+00
43 -0.144896D+00 -0.291593D+00 -0.254956D+00  0.204657D+01  0.286955D+00
44 -0.408742D+00 -0.452911D+00 -0.498493D+00 -0.144888D-01  0.487168D-01
          26            27            28            29            30
26  0.000000D+00
27  0.469935D+01  0.000000D+00
28  0.416247D+01 -0.156282D+02  0.000000D+00
29 -0.109531D+00  0.627826D-01 -0.101413D+00  0.000000D+00
30 -0.784911D-01 -0.816325D-01 -0.455128D-01  0.294264D+01  0.000000D+00
31 -0.827723D-01 -0.109151D+00 -0.851496D-01  0.528015D+01 -0.139011D+02
32 -0.471704D-01 -0.880679D-01 -0.959186D-02  0.146100D+02 -0.140458D+02
33 -0.375676D-02 -0.145165D+00 -0.116194D+00 -0.640428D-01 -0.272776D-01
34  0.816031D-01 -0.923576D-01  0.163478D+00 -0.855069D-01 -0.558716D-01
35 -0.529210D-01  0.211635D+00  0.264910D-01 -0.435457D-01 -0.564979D-01
36 -0.481044D+00 -0.173430D+00  0.145776D+00 -0.544767D-01 -0.691053D-01
37  0.823640D+00 -0.741803D-01 -0.547236D-01 -0.784885D-01 -0.643980D-01
38  0.385716D+00  0.687807D-01 -0.956253D-01 -0.354717D-01 -0.505102D-01
39 -0.210797D-01 -0.227259D-01  0.270116D-02  0.995104D-01 -0.923508D+00
40 -0.762174D-01 -0.711480D-01 -0.935832D-01  0.310037D+01  0.487768D+00
41 -0.665600D-01 -0.885683D-01 -0.796241D-01 -0.867261D+00 -0.363366D+00
42  0.520221D-01 -0.102164D+00  0.492600D-01 -0.269741D+00  0.185037D+00
43  0.441853D-01  0.107551D+00  0.596982D+00 -0.111282D+00 -0.132672D+00
44 -0.520405D-01 -0.116707D+00 -0.662734D+00 -0.167001D+00 -0.263986D+00
          31            32            33            34            35
31  0.000000D+00
32 -0.150529D+02  0.000000D+00
33 -0.743819D-01 -0.592305D-01  0.000000D+00
34 -0.837494D-01 -0.571349D-01 -0.145073D+02  0.000000D+00
35 -0.777242D-01 -0.733703D-01 -0.140988D+02 -0.134755D+02  0.000000D+00
36 -0.589050D-01 -0.510333D-01 -0.713309D-01 -0.472858D-01 -0.221722D-01
37 -0.549731D-01 -0.258552D-01 -0.783550D-01 -0.380211D-01 -0.554405D-01
38 -0.292344D-01  0.105880D-01 -0.724958D-01 -0.541453D-01 -0.372975D-01
39 -0.700322D+00  0.151109D+00  0.151412D-01  0.138588D-01  0.197764D-01
40 -0.630234D+00 -0.706455D+00 -0.611759D-01 -0.603843D-01 -0.978011D-03
41 -0.545019D-01 -0.150410D+00 -0.771065D-01 -0.688374D-01 -0.591441D-01
42 -0.113517D+00  0.149065D+00 -0.677750D-01  0.138398D-01  0.105982D-01
43  0.772040D-01  0.310990D+00 -0.137160D+00 -0.723699D-01 -0.112497D+00
44 -0.476396D+00 -0.115595D+01  0.615210D-03 -0.767874D-01 -0.269422D+00
          36            37            38            39            40
36  0.000000D+00
37 -0.114833D+02  0.000000D+00
38 -0.146853D+02 -0.199480D+02  0.000000D+00
39  0.107850D-01  0.205460D-01 -0.450563D-02  0.000000D+00
40  0.273794D-01 -0.311101D-01  0.131485D+00 -0.178456D+01  0.000000D+00
41  0.549142D-02 -0.463408D-02  0.105192D+00 -0.728056D+02  0.328139D+01
42 -0.270410D-01 -0.328703D-02 -0.769581D-02  0.141008D-01  0.199966D+00
43 -0.579287D-01  0.284740D-01  0.751830D-01 -0.267367D-01 -0.121184D+00
44  0.402487D-01  0.421343D-01  0.861916D-01  0.870188D-02  0.287743D-01
          41            42            43            44
41  0.000000D+00
42  0.238919D-03  0.000000D+00
43 -0.517271D-01  0.186100D+03  0.000000D+00
44  0.322436D-01  0.359810D+02 -0.417223D+01  0.000000D+00
```

3. ESI-MS data (positive mode);

High resolution mass spectrum ESI-MS of MKA



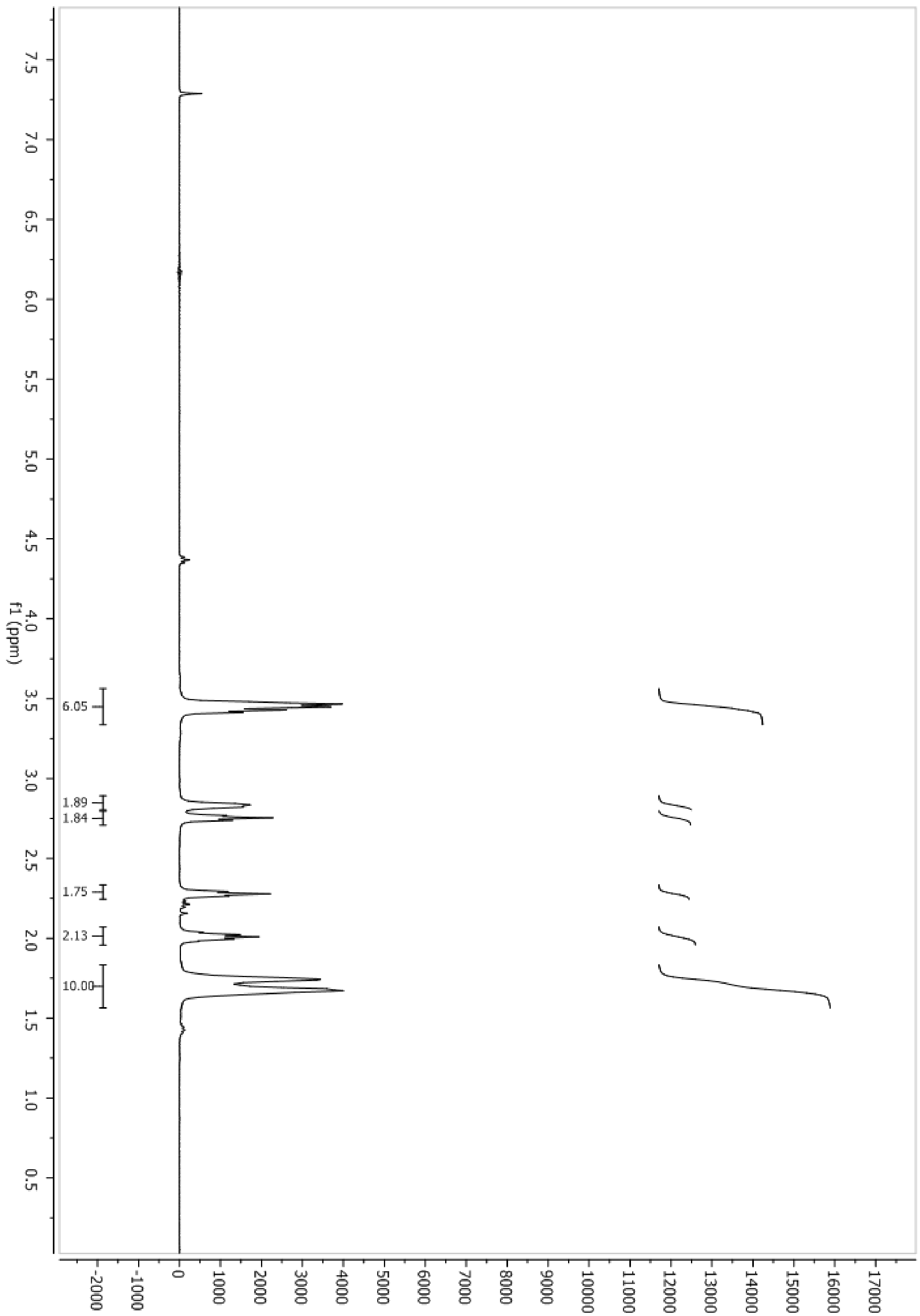
4. elemental analysis

Elemental Anal. Calcd (%) for $C_{15}H_{24}O_5$: C, 63.36; H, 8.51. Found: C, 63.91; H, 8.59.

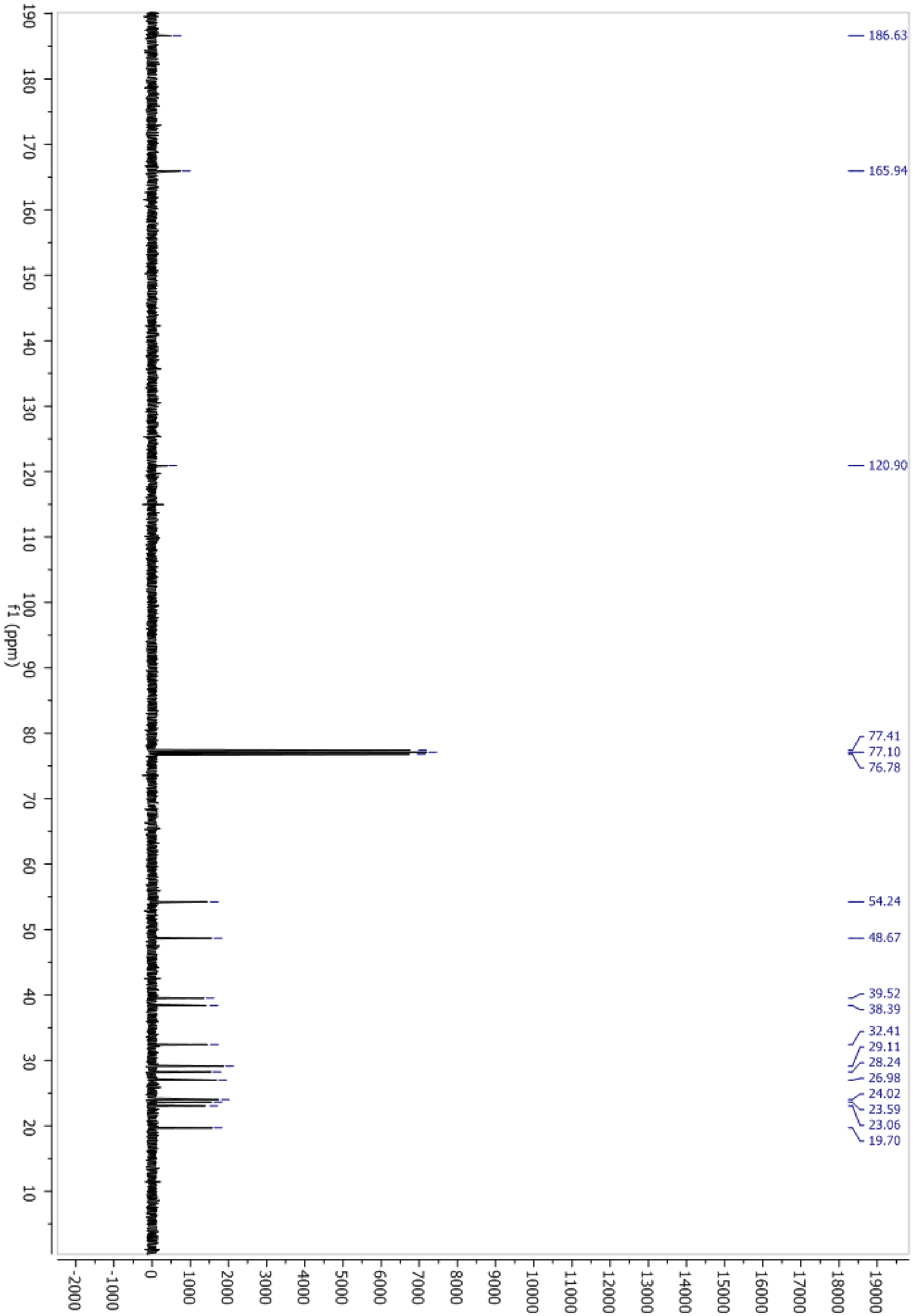
5. optical rotation

$[\alpha]_D^{20} = -166$ (c = 2.0; CH_3CN). Optical rotation of the equilibrated mixture of the two epimers.

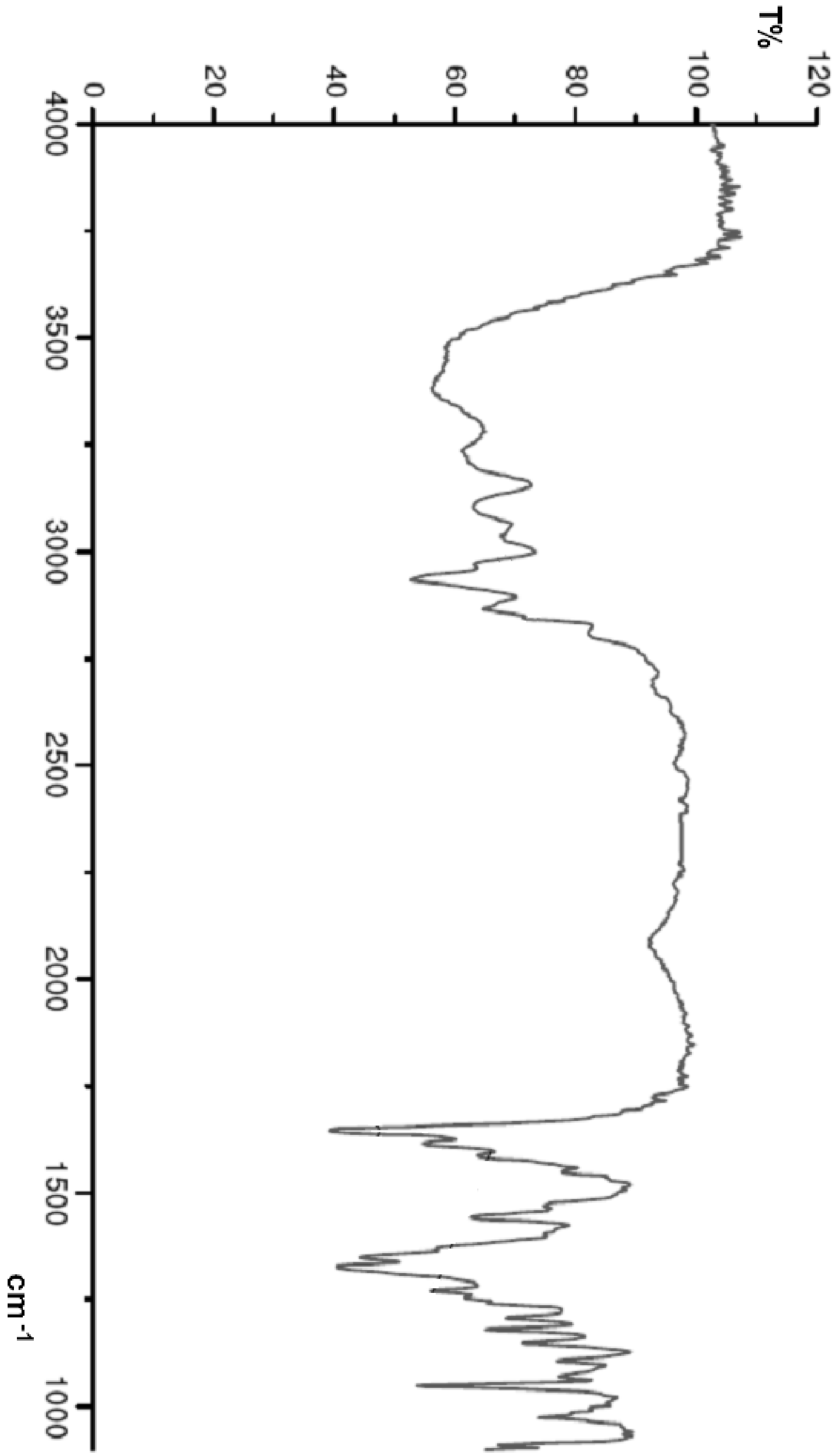
^{1}H-NMR of NCEDBU in $CDCl_3$



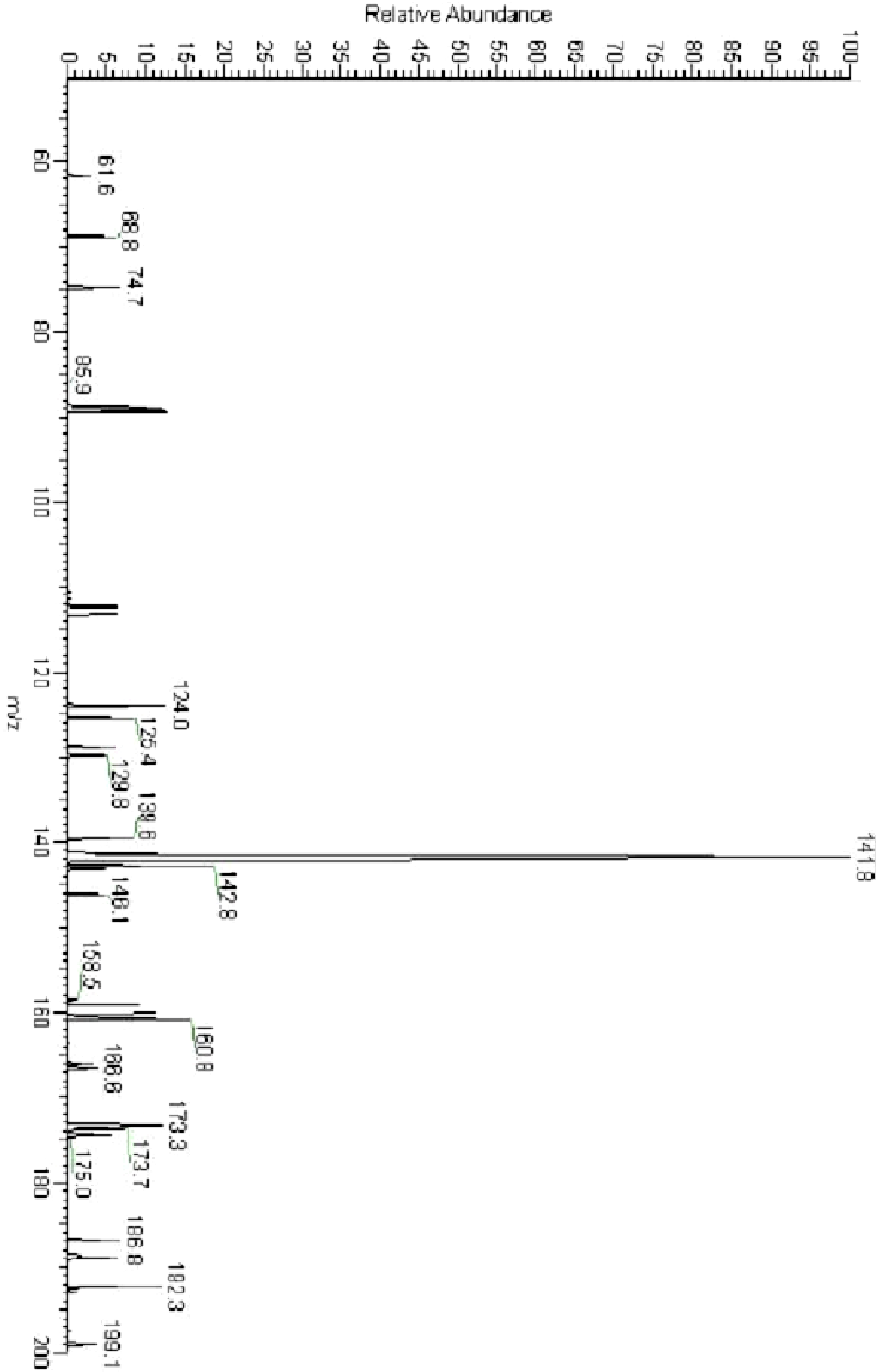
^{13}C-NMR of NCEDBU in $CDCl_3$



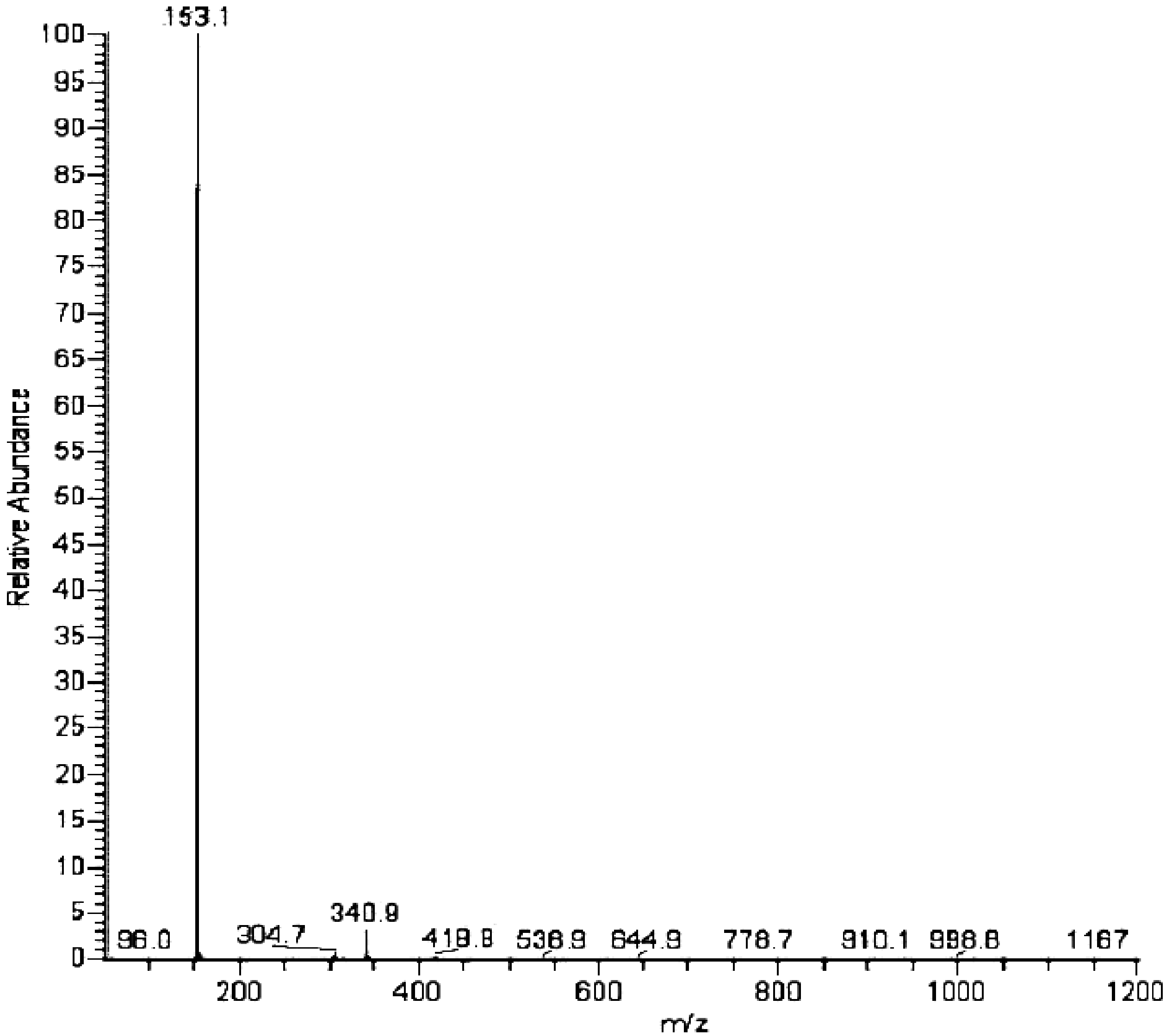
IR spectrum of NCEDBU in KBr



ESI-MS (-) of NCEDBU



ESI-MS (+) of NCEDBU



Structures of conformers $5\alpha_1$, $5\alpha_2$, $5\beta_1$, $5\beta_2$, $5\alpha_1^-$, $5\alpha_2^-$, $5\beta_1^-$ and $5\beta_2^-$ calculated in vacuum and in presence of different solvents simulated by COSMO procedure.

$5\alpha_1$ in water, GGA-BLYP/QZ4P large core
44

O	3.04907068	0.72356610	1.98701323
O	0.07176485	2.53993425	-0.10696551
C	0.46331539	-1.23229944	-0.24220188
C	-0.50140853	-2.43758285	0.07945298
C	-1.91887585	-2.22695319	-0.51284936
C	-2.56574422	-0.89015223	-0.11861285
C	-1.63295235	0.26906496	-0.51658629
C	-0.22400664	0.14250594	0.16503845
O	0.63412501	1.16603444	-0.42827573
C	3.27844790	0.73407773	0.77504067
C	3.00642427	-0.48301384	-0.10550977
C	1.88952600	-1.45015226	0.35604233
C	-2.23633323	1.70323063	-0.39557314
C	-1.17072337	2.73808250	-0.81111724
C	-2.83540400	2.09107090	0.97687374
C	0.05593138	-3.79084897	-0.42644267
C	3.91013332	1.93654738	0.10209095
H	0.56231031	-1.17800368	-1.34107709
H	-0.60210815	-2.49929528	1.17419343
H	-2.56001958	-3.05816005	-0.19276057
H	-1.85683485	-2.28304321	-1.60995843
H	-2.77687523	-0.87974782	0.95796162
H	-3.52855489	-0.77595285	-0.63552910
H	-1.40515896	0.13596126	-1.58743753
H	3.96769339	-1.02353461	-0.09953481
H	2.86360829	-0.16095809	-1.14338920
H	2.20477406	-2.45523840	0.06423220
H	1.84924920	-1.45630415	1.45395043
H	-3.03898382	1.77093008	-1.14375728
H	-3.56956487	1.35410625	1.31464979
H	-3.34394863	3.05942580	0.90190853
H	-2.07025990	2.18606035	1.75515820
H	-0.69461567	-4.57591502	-0.27581761
H	0.96143693	-4.10316515	0.10111910
H	0.28342494	-3.74906128	-1.49979407
H	4.71721318	1.62683719	-0.57168308
H	4.28760259	2.64501572	0.84377539
H	3.14835704	2.42910977	-0.51613405
C	-0.19696917	0.34552709	1.69216551
H	0.41829333	1.20340152	2.02563911
O	-0.75747588	-0.37208560	2.50944899
H	-1.42835044	3.74940458	-0.46261299
O	-1.00354966	2.71274957	-2.22137609
H	-0.38292337	3.42262818	-2.46571183

5α_2 in water, GGA-BLYP/QZ4P large core
44

O	3.53505691	0.35813289	-1.43767568
O	-0.63454969	2.53293127	0.27222199
C	0.73838380	-0.98910609	-0.08031944
C	0.08681292	-2.42408511	-0.02546173
C	-1.26167361	-2.49932616	-0.78430082
C	-2.27164304	-1.42647042	-0.35045193
C	-1.63646149	-0.03330132	-0.51663313
C	-0.32389938	0.12359109	0.33182837
O	0.29386360	1.38438017	-0.07688173
C	3.31855443	1.01963966	-0.41935154
C	2.84776546	0.36601503	0.87582418
C	2.07539173	-0.96515941	0.73064551
C	-2.60499227	1.18046975	-0.36427035
C	-1.81145799	2.48880395	-0.55959552
C	-3.42954957	1.25335300	0.94293100
C	1.03765909	-3.51723364	-0.57356255
C	3.53798068	2.51890775	-0.38107380
H	0.96679032	-0.76683217	-1.13604695
H	-0.11498345	-2.65049402	1.03390986
H	-1.69176685	-3.49834382	-0.63720508
H	-1.07191790	-2.39539032	-1.86322379
H	-2.58444998	-1.60285859	0.68655352
H	-3.17448088	-1.49107236	-0.97347045
H	-1.26576548	0.01853369	-1.55398080
H	2.30275950	1.10542383	1.47068422
H	3.77412850	0.16076279	1.43772368
H	2.75031211	-1.68435370	0.25609578
H	1.89060388	-1.34971537	1.74386068
H	-3.31309943	1.12247141	-1.20341949
H	-3.97249333	0.32143701	1.12522818
H	-4.16789771	2.06083939	0.87337662
H	-2.80702655	1.45813452	1.82092713
H	0.51726658	-4.48229993	-0.59233976
H	1.93637326	-3.64438691	0.03615038
H	1.35201838	-3.28892024	-1.60052732
H	4.14942600	2.79366444	0.48725216
H	2.56648904	3.01338977	-0.25151282
H	4.01004947	2.87149692	-1.30137037
C	-0.49707289	0.16413777	1.85892798
H	-0.12752642	1.09614465	2.33484332
O	-0.94766328	-0.74372979	2.54326145
H	-2.35707387	3.35898648	-0.16433821
O	-1.50636460	2.66268047	-1.93677827

H	-1.06244762	3.52405812	-2.03959853

5α_1^- in water, GGA-BLYP/QZ4P large core
43

O	3.19382848	0.28125627	1.94157468
O	0.50044204	2.50932467	-0.42842788
C	0.26846496	-1.26585219	-0.24322415
C	-0.86628281	-2.27205229	0.18393412
C	-2.24367511	-1.87496128	-0.40392276
C	-2.64964001	-0.42637977	-0.09345664
C	-1.56342227	0.54655405	-0.59299249
C	-0.16342968	0.23507195	0.05493636
O	0.83509958	1.05071272	-0.63341641
C	3.36907332	0.26203579	0.71964544
C	2.90567434	-0.91402894	-0.13615681
C	1.65245674	-1.68283142	0.35265331
C	-1.94324899	2.05805655	-0.56170322
C	-0.80485211	2.88754868	-1.23887333
C	-2.33744978	2.64915845	0.81128358
C	-0.55072825	-3.73571587	-0.21350646
C	4.10750062	1.38365703	0.01619364
H	0.34993418	-1.31319138	-1.34449120
H	-0.94866362	-2.23025495	1.28161912
H	-3.00444315	-2.56776130	-0.01973723
H	-2.21711146	-2.01309261	-1.49584325
H	-2.81969916	-0.31304474	0.98531382
H	-3.60137243	-0.19157489	-0.59109310
H	-1.39686036	0.31948790	-1.66093713
H	3.77038270	-1.59897680	-0.11611497
H	2.80835505	-0.59609210	-1.17936647
H	1.80588018	-2.73323620	0.08901163
H	1.62112371	-1.65262117	1.45072547
H	-2.81395461	2.16379337	-1.23000365
H	-3.12036337	2.06419528	1.30672363
H	-2.72045737	3.66971453	0.68108674
H	-1.48324617	2.71497559	1.49485113
H	-1.41470977	-4.37302788	0.01083456
H	0.30488681	-4.14983427	0.32751300
H	-0.34604259	-3.82091459	-1.28918289
H	4.74930392	1.00170269	-0.78528467
H	4.69125939	1.97275672	0.72841113
H	3.35516067	2.03218703	-0.45313016
C	-0.06345696	0.55737694	1.55482947
H	0.65161453	1.36747317	1.79644720
O	-0.66989753	-0.02087317	2.45038509
H	-0.81403441	3.93433165	-0.83942456
O	-0.68379667	2.77554733	-2.54294959

5α_2^- in water, GGA-BLYP/QZ4P large core
43

O	3.63927199	0.32986131	-1.36528034
O	-0.44437103	2.59457596	-0.14046558
C	0.70192825	-1.00952588	-0.10767625
C	-0.02543913	-2.39538615	0.06875024
C	-1.38342730	-2.45862725	-0.67139270
C	-2.32021835	-1.29471792	-0.31701015
C	-1.62485269	0.04620114	-0.62288221
C	-0.28000365	0.20935378	0.18012385
O	0.40938681	1.37652238	-0.36934457
C	3.35263726	0.98397401	-0.35903149
C	2.81102674	0.32222092	0.90343109
C	2.03392894	-1.00033308	0.71766397
C	-2.53950336	1.30812032	-0.57498139
C	-1.73694209	2.54945020	-1.07884758
C	-3.25862655	1.59570906	0.76322691
C	0.86120242	-3.58354243	-0.38087202
C	3.56339928	2.48381991	-0.29611510
H	0.95504454	-0.89918365	-1.17589962
H	-0.23118615	-2.51713655	1.14485356
H	-1.86732223	-3.41664880	-0.43789994
H	-1.20307121	-2.45471724	-1.75739387
H	-2.61309353	-1.36158448	0.73953165
H	-3.24415565	-1.36565760	-0.90840502
H	-1.27687539	-0.00855129	-1.66954259
H	2.24275252	1.06298189	1.47464904
H	3.70545976	0.10647223	1.51196963
H	2.71284262	-1.71953373	0.24665311
H	1.82900009	-1.39425497	1.72377467
H	-3.31713884	1.14189925	-1.33909271
H	-3.80289458	0.72153075	1.13796872
H	-3.98734486	2.40571954	0.62895964
H	-2.56263691	1.91950739	1.54593577
H	0.29689982	-4.52039678	-0.29847530
H	1.76361436	-3.69247755	0.22732446
H	1.16947228	-3.47234769	-1.42896056
H	4.11326480	2.75395027	0.61393476
H	2.58158001	2.96974282	-0.23076600
H	4.09643270	2.84520301	-1.17898697
C	-0.44419022	0.43332548	1.68902178
H	-0.10338335	1.42781421	2.04213683
O	-0.86605458	-0.39501543	2.48931490
H	-2.15713658	3.48357036	-0.62645339
O	-1.47068909	2.60352238	-2.36206972

5α_1 in water, GGA-BLYP/DZP medium core
44

O	2.99096564	0.71598832	1.97287263
O	0.07388820	2.54791609	-0.09070512
C	0.46164914	-1.22565253	-0.24503058
C	-0.49589900	-2.42118698	0.09046424
C	-1.91166489	-2.21605446	-0.49748807
C	-2.54674907	-0.87373445	-0.10869012
C	-1.60983674	0.27124345	-0.51470202
C	-0.20997487	0.14739565	0.16579660
O	0.65001242	1.16090176	-0.42609861
C	3.24577021	0.73031951	0.76460526
C	2.99333358	-0.48078877	-0.12325679
C	1.88546240	-1.45081173	0.34071031
C	-2.21802237	1.69504410	-0.39621996
C	-1.16103643	2.73349077	-0.81062565
C	-2.82049510	2.06684030	0.97302508
C	0.05864523	-3.77298855	-0.40996935
C	3.87941578	1.93084710	0.10234406
H	0.55171274	-1.17293624	-1.34605731
H	-0.58850607	-2.47017025	1.18734319
H	-2.55379616	-3.04620051	-0.16490404
H	-1.84922169	-2.27856985	-1.59887152
H	-2.74485739	-0.85219127	0.97201519
H	-3.51201846	-0.74825930	-0.62472982
H	-1.37868385	0.13810423	-1.58633130
H	3.96115433	-1.01808167	-0.11554508
H	2.84521424	-0.15725668	-1.16340974
H	2.19581940	-2.45637462	0.03794924
H	1.85163569	-1.45606856	1.44123287
H	-3.02343739	1.75315515	-1.14604559
H	-3.54936062	1.31566156	1.30329997
H	-3.34061198	3.03364737	0.89869803
H	-2.05077177	2.16444740	1.75171961
H	-0.69633298	-4.55705985	-0.25112875
H	0.96997788	-4.08136476	0.11608650
H	0.27806804	-3.72972938	-1.48864764
H	4.68852629	1.62333080	-0.57553672
H	4.25493387	2.63559664	0.85307099
H	3.11310054	2.42758629	-0.51352634
C	-0.18615623	0.34101035	1.69080246
H	0.44288014	1.19256164	2.02345929
O	-0.76439622	-0.37991719	2.49621243
H	-1.43285495	3.74442753	-0.45983181
O	-0.99354375	2.70377247	-2.21831992
H	-0.35240491	3.41403578	-2.45662432

5α_2 in water, GGA-BLYP/DZP medium core
44

O	3.44360628	0.36643224	-1.47219685
O	-0.63597145	2.54014315	0.29723967
C	0.73850151	-0.98274744	-0.07072205
C	0.08970511	-2.40875719	-0.00989470
C	-1.24974892	-2.48815735	-0.77535328
C	-2.25279381	-1.40609133	-0.35170515
C	-1.60532643	-0.02502369	-0.51650064
C	-0.31282706	0.12842288	0.34787113
O	0.31685098	1.37995254	-0.04206150
C	3.27324440	1.02071698	-0.43838574
C	2.83744373	0.36719355	0.86576376
C	2.07644321	-0.96525444	0.72573893
C	-2.57487062	1.17908825	-0.37817980
C	-1.78569120	2.48634479	-0.56698740
C	-3.40431540	1.23939573	0.91970551
C	1.04170451	-3.49975980	-0.54905174
C	3.50494023	2.51307864	-0.39076125
H	0.96282469	-0.75613352	-1.12779024
H	-0.11615565	-2.62586488	1.05140600
H	-1.68394976	-3.48773372	-0.62063625
H	-1.04841368	-2.38785542	-1.85688989
H	-2.56712499	-1.57145717	0.68830966
H	-3.15420652	-1.45740266	-0.98281390
H	-1.21762350	0.02832773	-1.54906818
H	2.29002773	1.10110338	1.47060802
H	3.77645315	0.16834170	1.41686745
H	2.74897691	-1.67367318	0.22786696
H	1.90105450	-1.36208519	1.73886373
H	-3.27637721	1.11219899	-1.22528450
H	-3.93326616	0.29430631	1.09694225
H	-4.15604396	2.03908075	0.84290913
H	-2.78054458	1.45448594	1.79877232
H	0.51399118	-4.46444345	-0.57489798
H	1.93671389	-3.62756337	0.07141247
H	1.36237680	-3.26336042	-1.57610896
H	4.13746452	2.77733344	0.46934657
H	2.53444510	3.01046289	-0.23783604
H	3.95923203	2.86830237	-1.32245920
C	-0.51031809	0.14559803	1.86930331
H	-0.14321183	1.07534563	2.35907170
O	-0.98262883	-0.77489268	2.52569792
H	-2.34951709	3.35577568	-0.18443557
O	-1.46249363	2.64759838	-1.93880678
H	-0.94194962	3.47956130	-2.02429537

5α$_1^-$ in water, GGA-BLYP/DZP medium core
43

O	3.13644547	0.27505481	1.91304427
O	0.52676615	2.50605502	-0.37565894
C	0.26557848	-1.26383400	-0.24326546
C	-0.85901500	-2.25733004	0.20217998
C	-2.23353080	-1.86543032	-0.38614297
C	-2.62217564	-0.40939484	-0.09451342
C	-1.52874644	0.54642225	-0.59551241
C	-0.14366560	0.23357633	0.06365525
O	0.86723212	1.03437675	-0.59909408
C	3.31875464	0.27098269	0.69028472
C	2.88772896	-0.90545563	-0.17477113
C	1.65240948	-1.69056880	0.32195451
C	-1.91779105	2.04754816	-0.56945409
C	-0.79875809	2.88676216	-1.25972386
C	-2.31370428	2.62943739	0.79986126
C	-0.54778137	-3.72080456	-0.18172777
C	4.02334412	1.41704229	0.00282252
H	0.32722320	-1.30825366	-1.34721860
H	-0.93343958	-2.19759150	1.30008005
H	-2.99812436	-2.54934289	0.01544105
H	-2.20651458	-2.02051321	-1.48029383
H	-2.78241382	-0.28000298	0.98613266
H	-3.57165980	-0.16251226	-0.59760720
H	-1.35086918	0.32234250	-1.66390072
H	3.76647501	-1.57933549	-0.16057422
H	2.77340427	-0.58219323	-1.21814749
H	1.80174889	-2.73773437	0.03524405
H	1.63859581	-1.67137051	1.42318164
H	-2.79621543	2.13239053	-1.23483712
H	-3.06620132	2.01423991	1.31320434
H	-2.73860187	3.63737937	0.66588344
H	-1.44164552	2.73036174	1.46158741
H	-1.41890546	-4.35278076	0.04693810
H	0.30999388	-4.13146548	0.36545691
H	-0.34268159	-3.80821210	-1.26081275
H	4.63475129	1.07302663	-0.84202857
H	4.63034775	1.98193277	0.72075255
H	3.24084151	2.07911877	-0.40276766
C	-0.06386452	0.54296792	1.56423811
H	0.66193230	1.34575673	1.80853769
O	-0.69775554	-0.03376672	2.44499477
H	-0.80207907	3.93107179	-0.83558524
O	-0.65388945	2.76222390	-2.54068345

5α_2^- in water, GGA-BLYP/DZP medium core
43

O	3.59504553	0.32417124	-1.37419167
O	-0.43996356	2.59902752	-0.10643560
C	0.69877206	-1.00424877	-0.11048379
C	-0.02532305	-2.37939823	0.07680686
C	-1.37809399	-2.44874469	-0.66214754
C	-2.30204441	-1.27452473	-0.31527011
C	-1.59826305	0.05411321	-0.62731126
C	-0.26640877	0.21522384	0.18158322
O	0.43468241	1.36957613	-0.34795014
C	3.32188384	0.98118220	-0.36382439
C	2.78937567	0.32450346	0.90042017
C	2.03050906	-1.00221373	0.70410000
C	-2.51904079	1.30113341	-0.58293845
C	-1.73675207	2.54789081	-1.10151482
C	-3.23327894	1.57494671	0.75363313
C	0.85809207	-3.56790929	-0.36167806
C	3.53145034	2.47623658	-0.30179783
H	0.94707550	-0.89215060	-1.18127156
H	-0.23182268	-2.48487777	1.15509179
H	-1.86555801	-3.40520727	-0.41381124
H	-1.19353685	-2.45494263	-1.75173268
H	-2.58384580	-1.32584930	0.74723019
H	-3.23207273	-1.33500429	-0.90389858
H	-1.24419557	0.00527053	-1.67370939
H	2.20526480	1.06070036	1.46648199
H	3.68498199	0.11514759	1.51662680
H	2.71514143	-1.70131023	0.20705276
H	1.83267389	-1.41823855	1.70498926
H	-3.29864123	1.11338166	-1.34310877
H	-3.75290007	0.68592114	1.13675131
H	-3.98420071	2.36976274	0.61823414
H	-2.53099077	1.92113529	1.52483692
H	0.28595798	-4.50383911	-0.27528928
H	1.76184340	-3.67248941	0.25122817
H	1.16544664	-3.45723138	-1.41401408
H	4.08927645	2.74713445	0.60681890
H	2.54471790	2.95881301	-0.23108045
H	4.05897965	2.83484345	-1.19290382
C	-0.44578615	0.42624126	1.68666561
H	-0.11169418	1.42778780	2.03556657
O	-0.87406862	-0.41348496	2.47503855
H	-2.15810815	3.47668338	-0.62168523
O	-1.45901541	2.60125458	-2.36532582

5α_1 in acetonitrile, GGA-BLYP/DZP medium core
44

O	2.98874552	0.71644531	1.97171463
O	0.07378302	2.54655245	-0.08965298
C	0.46154264	-1.22494847	-0.24482789
C	-0.49575101	-2.42053783	0.09074299
C	-1.91141221	-2.21553780	-0.49739090
C	-2.54655242	-0.87334645	-0.10866960
C	-1.60971172	0.27154062	-0.51488254
C	-0.20991886	0.14823030	0.16600375
O	0.65080612	1.16053212	-0.42608440
C	3.24532228	0.73083135	0.76408832
C	2.99332529	-0.48038114	-0.12409739
C	1.88547603	-1.45031208	0.34060114
C	-2.21822975	1.69501400	-0.39667473
C	-1.16037614	2.73272803	-0.81000355
C	-2.82100627	2.06708702	0.97225359
C	0.05880657	-3.77230955	-0.40997860
C	3.88132822	1.93027540	0.10192971
H	0.55119682	-1.17159815	-1.34598917
H	-0.58835692	-2.46946188	1.18757184
H	-2.55353645	-3.04568559	-0.16485949
H	-1.84911595	-2.27831315	-1.59880727
H	-2.74412999	-0.85194097	0.97220030
H	-3.51198320	-0.74853864	-0.62471546
H	-1.37797477	0.13862262	-1.58644848
H	3.96137387	-1.01776335	-0.11703269
H	2.84415765	-0.15666069	-1.16408453
H	2.19493787	-2.45667361	0.03879345
H	1.85229284	-1.45424651	1.44112022
H	-3.02323573	1.75347302	-1.14706831
H	-3.55046124	1.31666034	1.30257731
H	-3.34038354	3.03427604	0.89801145
H	-2.05108036	2.16406883	1.75065037
H	-0.69615959	-4.55651682	-0.25182426
H	0.97009459	-4.08139922	0.11570190
H	0.27843455	-3.72838309	-1.48851325
H	4.69123974	1.62201832	-0.57473098
H	4.25771853	2.63419357	0.85300875
H	3.11619264	2.42717771	-0.51494897
C	-0.18679489	0.34092760	1.69130152
H	0.44160565	1.19277392	2.02406320
O	-0.76458623	-0.38061745	2.49639706
H	-1.43215906	3.74413048	-0.46005040
O	-0.99350820	2.70218936	-2.21722685
H	-0.35286760	3.41352501	-2.45345602

5α_2 in acetonitrile, GGA-BLYP/DZP medium core
44

O	3.44501037	0.36576508	-1.47113789
O	-0.63537338	2.53910533	0.29637736
C	0.73850775	-0.98257627	-0.07106578
C	0.08970045	-2.40864237	-0.00931461
C	-1.24977671	-2.48790196	-0.77494051
C	-2.25281394	-1.40623879	-0.35128797
C	-1.60541717	-0.02528664	-0.51664773
C	-0.31259197	0.12864203	0.34725135
O	0.31738230	1.37953158	-0.04369315
C	3.27409582	1.02022262	-0.43775202
C	2.83687097	0.36719725	0.86628761
C	2.07633246	-0.96556195	0.72568000
C	-2.57527228	1.17853938	-0.37828865
C	-1.78606036	2.48581482	-0.56691162
C	-3.40530825	1.23835835	0.91918539
C	1.04156797	-3.49996745	-0.54792757
C	3.50715980	2.51247826	-0.39038954
H	0.96303152	-0.75574575	-1.12772718
H	-0.11676805	-2.62497446	1.05193583
H	-1.68386205	-3.48774845	-0.62007263
H	-1.04873898	-2.38782010	-1.85664838
H	-2.56683513	-1.57160045	0.68899572
H	-3.15453417	-1.45817247	-0.98221622
H	-1.21777138	0.02851935	-1.54896262
H	2.28812627	1.10116735	1.46986218
H	3.77527306	0.16776660	1.41884173
H	2.74933735	-1.67344396	0.22766529
H	1.90085528	-1.36258035	1.73861147
H	-3.27692042	1.11176788	-1.22557051
H	-3.93552407	0.29385497	1.09581601
H	-4.15630208	2.03894038	0.84292862
H	-2.78208996	1.45252908	1.79894977
H	0.51353980	-4.46462608	-0.57355914
H	1.93658533	-3.62792505	0.07255527
H	1.36266553	-3.26407000	-1.57492818
H	4.13909898	2.77787316	0.47005751
H	2.53677495	3.01051367	-0.23875002
H	3.96424756	2.86609950	-1.32150151
C	-0.50971973	0.14584605	1.86892727
H	-0.14229790	1.07562246	2.35857999
O	-0.98112223	-0.77502194	2.52534935
H	-2.35005490	3.35401708	-0.18151455
O	-1.46706014	2.65224061	-1.93912516
H	-0.94839931	3.48640516	-2.02352239

$5\alpha_1^-$ in acetonitrile, GGA-BLYP/DZP medium core
43

O	3.13503858	0.27673825	1.91314745
O	0.52798984	2.50570148	-0.37572282
C	0.26530821	-1.26322873	-0.24232210
C	-0.85920846	-2.25731021	0.20213007
C	-2.23342170	-1.86533395	-0.38660352
C	-2.62175434	-0.40932582	-0.09503953
C	-1.52803071	0.54656725	-0.59559810
C	-0.14289446	0.23463310	0.06382817
O	0.86790681	1.03457315	-0.59972893
C	3.31807532	0.27137023	0.69074826
C	2.88722110	-0.90586759	-0.17362060
C	1.65174955	-1.69027522	0.32362071
C	-1.91731701	2.04734281	-0.56994088
C	-0.79752508	2.88649557	-1.26044589
C	-2.31518987	2.62846349	0.79957040
C	-0.54799953	-3.72088288	-0.18165890
C	4.02481110	1.41491248	0.00154283
H	0.32742779	-1.30705551	-1.34633815
H	-0.93394056	-2.19801057	1.30006710
H	-2.99815907	-2.54954976	0.01461840
H	-2.20611440	-2.02014622	-1.48079629
H	-2.78235189	-0.28040023	0.98545453
H	-3.57113366	-0.16289863	-0.59852906
H	-1.34896031	0.32380894	-1.66385274
H	3.76632186	-1.57945595	-0.15929150
H	2.77191366	-0.58278143	-1.21682960
H	1.80039852	-2.73781987	0.03759175
H	1.63837211	-1.66895507	1.42481382
H	-2.79552380	2.13199987	-1.23606799
H	-3.07034195	2.01457988	1.31091235
H	-2.73825752	3.63714417	0.66509193
H	-1.44423475	2.72762109	1.46339066
H	-1.41929157	-4.35300160	0.04632070
H	0.30930772	-4.13164612	0.36586070
H	-0.34270356	-3.80854459	-1.26075308
H	4.63872243	1.06761481	-0.84009374
H	4.63111825	1.98096586	0.71882020
H	3.24348445	2.07537987	-0.40853989
C	-0.06380579	0.54289805	1.56479702
H	0.66180087	1.34581969	1.80945394
O	-0.69569929	-0.03648821	2.44556270
H	-0.80083837	3.93027930	-0.83343976
O	-0.65743049	2.76523232	-2.54144756

5α_2^- in acetonitrile, GGA-BLYP/DZP medium core

43

O	3.59387227	0.32156723	-1.37432279
O	-0.44120337	2.59684620	-0.10311286
C	0.69894448	-1.00355316	-0.10946677
C	-0.02532738	-2.37890189	0.07687346
C	-1.37702078	-2.44871193	-0.66319517
C	-2.29969519	-1.27417533	-0.31485136
C	-1.59692072	0.05458069	-0.62816585
C	-0.26577777	0.21626056	0.18168683
O	0.43517712	1.37014468	-0.34800693
C	3.32134667	0.98026504	-0.36546701
C	2.78934275	0.32530408	0.90017268
C	2.03042711	-1.00151528	0.70537635
C	-2.51877310	1.30083974	-0.58413671
C	-1.73607326	2.54833591	-1.10115359
C	-3.23454979	1.57410363	0.75195428
C	0.85881018	-3.56733685	-0.36038267
C	3.53374005	2.47534107	-0.30413793
H	0.94839969	-0.89052944	-1.17968680
H	-0.23716050	-2.48444253	1.15399373
H	-1.86451212	-3.40511731	-0.41410453
H	-1.19234408	-2.45529408	-1.75272886
H	-2.57585401	-1.32500280	0.74946597
H	-3.23102244	-1.33519131	-0.90159853
H	-1.24193026	0.00669641	-1.67427556
H	2.20548396	1.06226698	1.46552512
H	3.68508325	0.11543404	1.51661955
H	2.71513196	-1.70079520	0.20857895
H	1.83273548	-1.41623072	1.70687186
H	-3.29785553	1.11309975	-1.34555335
H	-3.75685924	0.68545057	1.13370726
H	-3.98390950	2.37047327	0.61558873
H	-2.53232170	1.91881948	1.52469701
H	0.28727068	-4.50371621	-0.27444615
H	1.76256732	-3.67158312	0.25263717
H	1.16678169	-3.45649619	-1.41254951
H	4.09128049	2.74726377	0.60463803
H	2.54766628	2.95985522	-0.23463407
H	4.06351191	2.83263850	-1.19460326
C	-0.44675470	0.42581612	1.68707470
H	-0.11238828	1.42728661	2.03660614
O	-0.87559940	-0.41421805	2.47485948
H	-2.15940995	3.47637584	-0.61968553
O	-1.46158082	2.60417191	-2.36502401

$5\alpha_1$ in dichloromethane, GGA-BLYP/DZP medium core
44

O	2.97846816	0.72229178	1.96381234
O	0.07298373	2.54548778	-0.08903775
C	0.46135042	-1.22497913	-0.24739297
C	-0.49393663	-2.42043106	0.09248181
C	-1.91029821	-2.21723666	-0.49490188
C	-2.54615782	-0.87552490	-0.10519472
C	-1.61218204	0.27053637	-0.51503082
C	-0.21113984	0.14779451	0.16233103
O	0.64932873	1.15829558	-0.42962226
C	3.25188525	0.73228144	0.76100390
C	2.99159870	-0.47447310	-0.13337413
C	1.88619719	-1.44387547	0.33874355
C	-2.22124103	1.69415405	-0.39373729
C	-1.16064087	2.73153699	-0.80298096
C	-2.82761952	2.06292395	0.97443417
C	0.06219307	-3.77299696	-0.40451868
C	3.91568775	1.92330711	0.10848548
H	0.54950731	-1.17438779	-1.34893704
H	-0.58612074	-2.46643091	1.18953403
H	-2.55130900	-3.04780502	-0.16121970
H	-1.84901994	-2.28023759	-1.59640495
H	-2.73769013	-0.85384611	0.97663242
H	-3.51411274	-0.75291468	-0.61706817
H	-1.38457419	0.13955574	-1.58768656
H	3.95924251	-1.01222541	-0.14089213
H	2.83204244	-0.14215463	-1.16927714
H	2.19692063	-2.45321166	0.04787518
H	1.85331981	-1.43543465	1.43923510
H	-3.02367910	1.75576892	-1.14665524
H	-3.56119565	1.31394499	1.29889869
H	-3.34306725	3.03243464	0.90250466
H	-2.06022554	2.15247017	1.75541091
H	-0.69648863	-4.55553170	-0.25624002
H	0.96632906	-4.08542679	0.13165584
H	0.29466185	-3.72902422	-1.48042793
H	4.73070737	1.60476833	-0.55709905
H	4.29214250	2.61876155	0.86744900
H	3.16656121	2.43425283	-0.51676067
C	-0.18647221	0.33610448	1.68970094
H	0.46368097	1.16994234	2.02635987
O	-0.78442975	-0.37324230	2.49038944
H	-1.43228821	3.74255637	-0.44907328
O	-0.99766450	2.70557472	-2.21257736
H	-0.29243463	3.35746911	-2.43823410

5α_2 in dichloromethane, GGA-BLYP/DZP medium core
44

O	3.48132216	0.34014277	-1.45431554
O	-0.64826957	2.54313618	0.29420130
C	0.73873238	-0.97767251	-0.07883911
C	0.09013892	-2.40436619	-0.01342821
C	-1.24831518	-2.48771224	-0.77959342
C	-2.25196905	-1.40866039	-0.35239130
C	-1.61025109	-0.02546442	-0.52153815
C	-0.31405895	0.13417630	0.33645083
O	0.30757255	1.38781983	-0.05961971
C	3.30002542	1.00616996	-0.43125605
C	2.83003942	0.37134004	0.87089810
C	2.07211856	-0.96152469	0.72507688
C	-2.58644856	1.17273200	-0.37510700
C	-1.80797905	2.48779809	-0.55478431
C	-3.41746129	1.21780118	0.92216572
C	1.04344745	-3.49922543	-0.54223842
C	3.55061102	2.49619233	-0.39388449
H	0.96874424	-0.75332402	-1.13492469
H	-0.11953551	-2.61457877	1.04844786
H	-1.68026366	-3.48848735	-0.62392799
H	-1.04907741	-2.38765909	-1.86165192
H	-2.55814745	-1.57417057	0.69028591
H	-3.15771159	-1.46439770	-0.97736953
H	-1.22887269	0.03111467	-1.55618081
H	2.26622446	1.11347426	1.45024333
H	3.75322094	0.17795712	1.45055657
H	2.74934556	-1.66692488	0.22919138
H	1.89012609	-1.36121421	1.73575409
H	-3.28683595	1.10748738	-1.22361869
H	-3.94824823	0.27167832	1.08745533
H	-4.16806524	2.01962463	0.85457633
H	-2.79514423	1.42056061	1.80515303
H	0.51453596	-4.46356499	-0.56521822
H	1.93484490	-3.62546985	0.08383826
H	1.37087877	-3.26991920	-1.56865367
H	4.16571539	2.76459278	0.47789509
H	2.58315791	3.00830225	-0.27174536
H	4.03378432	2.83215899	-1.31828949
C	-0.50256471	0.15649905	1.85940563
H	-0.13358895	1.08991589	2.34142521
O	-0.96643808	-0.76247744	2.52280607
H	-2.37452624	3.34634369	-0.15046095
O	-1.50792429	2.67356336	-1.92858916
H	-1.00529825	3.51845804	-2.00816525

5α_1^- in dichloromethane, GGA-BLYP/DZP medium core
43

O	3.13920907	0.27870786	1.91174871
O	0.53334381	2.50307000	-0.37338078
C	0.26437182	-1.26274630	-0.23962577
C	-0.86029260	-2.25676290	0.20209995
C	-2.23284048	-1.86383368	-0.38964552
C	-2.61959890	-0.40743921	-0.09832391
C	-1.52519731	0.54904060	-0.59683067
C	-0.14135468	0.23531092	0.06623141
O	0.87250937	1.03127649	-0.59294520
C	3.31735058	0.27354321	0.69010091
C	2.88454138	-0.90580828	-0.17363390
C	1.65005839	-1.68816823	0.32931721
C	-1.91805172	2.04855097	-0.57145787
C	-0.79901421	2.89039643	-1.26697160
C	-2.32067895	2.62843304	0.79704049
C	-0.54892180	-3.72041899	-0.18123000
C	4.02513627	1.41386794	-0.00519660
H	0.32931409	-1.30534034	-1.34359707
H	-0.93769147	-2.19636710	1.29974988
H	-2.99922437	-2.54749476	0.01013848
H	-2.20329352	-2.01860001	-1.48391781
H	-2.78021267	-0.27974760	0.98236911
H	-3.56888338	-0.15990103	-0.60167065
H	-1.34299190	0.32972675	-1.66537460
H	3.76371937	-1.57935730	-0.16094661
H	2.76356698	-0.58186778	-1.21587008
H	1.79892618	-2.73793808	0.05099681
H	1.63728225	-1.65745360	1.43032806
H	-2.79478197	2.13061122	-1.24013307
H	-3.08261862	2.01718148	1.30186564
H	-2.73757423	3.63992850	0.66268977
H	-1.45316209	2.72105914	1.46622744
H	-1.42079748	-4.35254838	0.04511679
H	0.30751511	-4.13174070	0.36738973
H	-0.34199633	-3.80803795	-1.26019121
H	4.64620811	1.05774506	-0.83826362
H	4.62588113	1.98675886	0.71140004
H	3.24587754	2.06887569	-0.42767604
C	-0.06594272	0.54034167	1.56914320
H	0.65422008	1.34796313	1.81499957
O	-0.69432232	-0.04628622	2.44763869
H	-0.79298929	3.93303300	-0.83292224
O	-0.66378632	2.76724188	-2.54217020

$5\alpha_2^-$ in dichloromethane, GGA-BLYP/DZP medium core
43

O	3.61379679	0.27401640	-1.37027383
O	-0.44179786	2.60080550	-0.06718808
C	0.70114446	-0.99352367	-0.10077063
C	-0.01682490	-2.37165537	0.07808374
C	-1.36139373	-2.44366067	-0.67545677
C	-2.29183108	-1.27263241	-0.33515281
C	-1.59227524	0.06200329	-0.63392030
C	-0.26800260	0.22361826	0.19062430
O	0.43417249	1.38237724	-0.31874340
C	3.33318555	0.95976852	-0.38362902
C	2.78925810	0.33954247	0.89670500
C	2.02747777	-0.98783085	0.72147163
C	-2.52666892	1.29906025	-0.59227091
C	-1.76072103	2.56043520	-1.10501656
C	-3.25589548	1.55938520	0.73818059
C	0.87494455	-3.55675187	-0.35334958
C	3.54631859	2.45682545	-0.36016364
H	0.95747323	-0.87614394	-1.16889194
H	-0.23474236	-2.47870894	1.15407906
H	-1.84918045	-3.40229165	-0.43453476
H	-1.16483791	-2.44678579	-1.76306666
H	-2.58252407	-1.32882857	0.72476545
H	-3.21664152	-1.33534439	-0.93207512
H	-1.22673967	0.02412259	-1.67705356
H	2.20058463	1.09152955	1.43591598
H	3.67954095	0.14119917	1.52491121
H	2.71324577	-1.69550804	0.23810816
H	1.82192959	-1.38783098	1.72756915
H	-3.29767295	1.10409657	-1.36095345
H	-3.78727433	0.66861937	1.10304848
H	-3.99953264	2.36149493	0.60253496
H	-2.56027976	1.89094298	1.52228962
H	0.30522046	-4.49522804	-0.27641233
H	1.77224687	-3.66095217	0.26930093
H	1.19495950	-3.44231626	-1.40155484
H	4.08654586	2.75374419	0.55142098
H	2.55896529	2.94264623	-0.32476588
H	4.09444221	2.78668009	-1.25009607
C	-0.46454850	0.42141671	1.69677526
H	-0.14834412	1.42735875	2.05045019
O	-0.88491732	-0.42835907	2.47926453
H	-2.17462603	3.48310337	-0.60490382
O	-1.47383788	2.62423007	-2.35502572

5α$_1$ in chloroform, GGA-BLYP/DZP medium core

44

O	2.98658279	0.71716242	1.97027588
O	0.07522964	2.54608799	-0.08988820
C	0.46161575	-1.22433212	-0.24450701
C	-0.49527253	-2.41998117	0.09176926
C	-1.91076930	-2.21543118	-0.49672883
C	-2.54560514	-0.87319620	-0.10781037
C	-1.60876893	0.27153745	-0.51477259
C	-0.20919730	0.14888783	0.16656107
O	0.65045971	1.16028941	-0.42797283
C	3.24502903	0.73101880	0.76450335
C	2.99339274	-0.48059804	-0.12482741
C	1.88544907	-1.44984141	0.34107980
C	-2.21785481	1.69477111	-0.39667851
C	-1.15917626	2.73200568	-0.80906270
C	-2.82117659	2.06703332	0.97202110
C	0.05895228	-3.77178339	-0.40951138
C	3.88358249	1.92967878	0.10176435
H	0.55091295	-1.17103139	-1.34587944
H	-0.58813534	-2.46792032	1.18861085
H	-2.55293045	-3.04561301	-0.16415598
H	-1.84865569	-2.27859379	-1.59825665
H	-2.74175295	-0.85221636	0.97334329
H	-3.51147777	-0.74885892	-0.62354470
H	-1.37717152	0.13952707	-1.58652849
H	3.96112694	-1.01871047	-0.11840767
H	2.84251490	-0.15651931	-1.16464395
H	2.19406675	-2.45686896	0.04000701
H	1.85298262	-1.45191734	1.44161568
H	-3.02190685	1.75335967	-1.14837965
H	-3.55089739	1.31715679	1.30265667
H	-3.34038068	3.03448613	0.89778844
H	-2.05181391	2.16297161	1.75077145
H	-0.69570502	-4.55638483	-0.25213734
H	0.96982210	-4.08179069	0.11631454
H	0.27875045	-3.72794143	-1.48812016
H	4.69451400	1.62081200	-0.57376866
H	4.25972418	2.63261651	0.85374031
H	3.11923225	2.42753949	-0.51522804
C	-0.18684949	0.34033692	1.69292443
H	0.44192495	1.19142998	2.02749558
O	-0.76758075	-0.38210689	2.49394275
H	-1.43109244	3.74289659	-0.45638517
O	-0.99591427	2.70342475	-2.21670559
H	-0.35023643	3.40911706	-2.45387678

5α_2 in chloroform, GGA-BLYP/DZP medium core
44

O	3.44709185	0.36168312	-1.46750067
O	-0.63512833	2.53952517	0.29640236
C	0.73902823	-0.98181884	-0.07214246
C	0.09013443	-2.40807897	-0.00912733
C	-1.24934019	-2.48784744	-0.77472673
C	-2.25200064	-1.40611425	-0.35073627
C	-1.60489397	-0.02512624	-0.51742177
C	-0.31198707	0.12935184	0.34608620
O	0.31683165	1.38034133	-0.04611341
C	3.27535215	1.01859009	-0.43756845
C	2.83653385	0.36760887	0.86767231
C	2.07626358	-0.96518374	0.72553838
C	-2.57534775	1.17825446	-0.37846808
C	-1.78701669	2.48633074	-0.56532273
C	-3.40590110	1.23747775	0.91868954
C	1.04161491	-3.49991936	-0.54735504
C	3.50910750	2.51174077	-0.39109603
H	0.96562656	-0.75473104	-1.12824716
H	-0.11751257	-2.62347350	1.05215772
H	-1.68341740	-3.48776214	-0.61949733
H	-1.04866754	-2.38855892	-1.85659845
H	-2.56434618	-1.57114951	0.69015432
H	-3.15439567	-1.45883526	-0.98095538
H	-1.21799640	0.02942349	-1.54998217
H	2.28587243	1.10154633	1.46965853
H	3.77418006	0.16783097	1.42156813
H	2.75015611	-1.67089168	0.22554035
H	1.89994529	-1.36379963	1.73776221
H	-3.27592394	1.11173526	-1.22687765
H	-3.93655178	0.29325886	1.09495254
H	-4.15673544	2.03848873	0.84307740
H	-2.78309896	1.45004626	1.79897984
H	0.51381333	-4.46473072	-0.57269135
H	1.93640339	-3.62823153	0.07328880
H	1.36353850	-3.26479428	-1.57420787
H	4.14044876	2.77866253	0.46965028
H	2.53880925	3.01087712	-0.24191454
H	3.96783014	2.86318385	-1.32212535
C	-0.50895886	0.14574154	1.86817725
H	-0.14117442	1.07601094	2.35779376
O	-0.98009862	-0.77503211	2.52358431
H	-2.35129128	3.35305197	-0.17598811
O	-1.47402362	2.65515279	-1.93828781
H	-0.95325736	3.48742463	-2.02343450

5α_1^- in chloroform, GGA-BLYP/DZP medium core
43

O	3.14076534	0.27706986	1.91182808
O	0.53073175	2.50320439	-0.37071884
C	0.26398997	-1.26141799	-0.24050488
C	-0.85974006	-2.25617287	0.20217418
C	-2.23269133	-1.86378518	-0.38879552
C	-2.61863905	-0.40704708	-0.09773562
C	-1.52477364	0.54967788	-0.59750178
C	-0.14115758	0.23646364	0.06606754
O	0.87482994	1.03210340	-0.58990324
C	3.31678751	0.27369048	0.69040480
C	2.88448492	-0.90545836	-0.17431622
C	1.64975773	-1.68815538	0.32738820
C	-1.91738338	2.04898316	-0.57195582
C	-0.79724614	2.88915488	-1.26881897
C	-2.31933546	2.62809347	0.79743007
C	-0.54925882	-3.72022166	-0.18114189
C	4.02455729	1.41428219	-0.00479616
H	0.32810944	-1.30356457	-1.34462608
H	-0.93638655	-2.19491401	1.29988271
H	-2.99853073	-2.54813048	0.01178820
H	-2.20383222	-2.01890955	-1.48314605
H	-2.77740245	-0.27949481	0.98333740
H	-3.56846382	-0.15998659	-0.60069872
H	-1.34302186	0.33252832	-1.66672292
H	3.76345748	-1.57972811	-0.16046537
H	2.76350244	-0.58105426	-1.21654670
H	1.79829412	-2.73764599	0.04678986
H	1.63745257	-1.65837833	1.42847519
H	-2.79381481	2.13180597	-1.24094725
H	-3.07934226	2.01649381	1.30543895
H	-2.73722636	3.63918769	0.66214911
H	-1.45056916	2.72243342	1.46466740
H	-1.42093907	-4.35280208	0.04541553
H	0.30751760	-4.13180363	0.36691884
H	-0.34301461	-3.80796948	-1.26034519
H	4.64408665	1.05953813	-0.83990567
H	4.62721122	1.98426123	0.71259985
H	3.24486613	2.07091707	-0.42458933
C	-0.06673394	0.54091071	1.56910875
H	0.65489191	1.34748516	1.81420632
O	-0.69626925	-0.04621646	2.44630629
H	-0.79062691	3.93266447	-0.83491489
O	-0.66602000	2.76392357	-2.54336343

5α$_2^-$ in chloroform, GGA-BLYP/DZP medium core
43

O	3.61379054	0.27375525	-1.36836421
O	-0.44092715	2.59950238	-0.06580727
C	0.70067574	-0.99374796	-0.10163342
C	-0.01696452	-2.37183279	0.07836961
C	-1.36177063	-2.44384769	-0.67462274
C	-2.29149464	-1.27218881	-0.33434680
C	-1.59229112	0.06264870	-0.63454988
C	-0.26746990	0.22405899	0.18965156
O	0.43586344	1.38165964	-0.31876308
C	3.33186983	0.96043408	-0.38354744
C	2.78838964	0.33950643	0.89698232
C	2.02727224	-0.98802048	0.72020170
C	-2.52610574	1.30000658	-0.59246641
C	-1.75936958	2.56153427	-1.10673756
C	-3.25483376	1.55980837	0.73832971
C	0.87433888	-3.55729031	-0.35336783
C	3.54447527	2.45808652	-0.35869995
H	0.95708363	-0.87609987	-1.16964085
H	-0.23521672	-2.47853296	1.15442672
H	-1.84952806	-3.40265020	-0.43317750
H	-1.16553035	-2.44730716	-1.76229280
H	-2.58114854	-1.32847321	0.72601550
H	-3.21685741	-1.33551304	-0.93043604
H	-1.22767946	0.02579130	-1.67810012
H	2.19864833	1.09097929	1.43552247
H	3.67922827	0.14081076	1.52455934
H	2.71376351	-1.69388669	0.23501894
H	1.82210855	-1.38909159	1.72607327
H	-3.29698241	1.10589813	-1.36144630
H	-3.78580836	0.66907167	1.10451109
H	-3.99854914	2.36185702	0.60219441
H	-2.55902041	1.89251142	1.52177854
H	0.30508994	-4.49617133	-0.27614078
H	1.77230529	-3.66128771	0.26844991
H	1.19367334	-3.44244808	-1.40177853
H	4.08624165	2.75370495	0.55265717
H	2.55701297	2.94403798	-0.32256778
H	4.09164895	2.78871955	-1.24892758
C	-0.46454349	0.42123425	1.69588902
H	-0.14980563	1.42828226	2.04814599
O	-0.88296402	-0.42890740	2.47918461
H	-2.17166485	3.48465328	-0.60475408
O	-1.47661813	2.62318374	-2.35622246

$5\alpha_1$ in vacuum, GGA-BLYP/DZP medium core
44

O	2.95798072	0.72440543	1.95728667
O	0.08583416	2.54224861	-0.09722857
C	0.46484545	-1.22501534	-0.24737259
C	-0.49057703	-2.41935575	0.09647530
C	-1.90717628	-2.21639170	-0.49061116
C	-2.54016343	-0.87350315	-0.09914970
C	-1.60562814	0.27103874	-0.51349793
C	-0.20388348	0.14818068	0.16086347
O	0.65275266	1.15424771	-0.44350740
C	3.24480320	0.73262476	0.76528985
C	2.99589535	-0.47960920	-0.13618857
C	1.88924689	-1.44556440	0.33990512
C	-2.21528392	1.69523883	-0.38857510
C	-1.15278955	2.73164972	-0.79836291
C	-2.82142098	2.06204709	0.98066045
C	0.06261410	-3.77334461	-0.40028030
C	3.91212079	1.92750715	0.11047623
H	0.55287983	-1.17787577	-1.34974403
H	-0.58333240	-2.45929543	1.19368928
H	-2.54872760	-3.04646300	-0.15573455
H	-1.84845039	-2.28316047	-1.59243035
H	-2.72050144	-0.85332195	0.98437829
H	-3.51199948	-0.75159509	-0.60521321
H	-1.38203111	0.14688423	-1.58818043
H	3.96310178	-1.01831971	-0.14227503
H	2.83245462	-0.14706787	-1.17198270
H	2.19672412	-2.45812325	0.05510305
H	1.85840736	-1.42620333	1.44046092
H	-3.01470023	1.75859649	-1.14548698
H	-3.55325743	1.31220388	1.30657538
H	-3.33963296	3.03087449	0.91227939
H	-2.05560959	2.14857520	1.76315197
H	-0.69556696	-4.55658530	-0.25411803
H	0.96486253	-4.08913819	0.13698865
H	0.29610263	-3.73182466	-1.47625921
H	4.73074942	1.61457881	-0.55420703
H	4.28376144	2.61887445	0.87520095
H	3.15972007	2.43947073	-0.50978355
C	-0.18387866	0.33129907	1.69518107
H	0.47995163	1.15159176	2.04154636
O	-0.80550064	-0.37391192	2.47483896
H	-1.41986481	3.74088697	-0.42929840
O	-1.01557852	2.71600147	-2.21005351
H	-0.27593657	3.32460397	-2.43740531

$5\alpha_2$ in vacuum, GGA-BLYP/DZP medium core
44

O	3.45964514	0.34236062	-1.45137464
O	-0.63495298	2.54228789	0.29300335
C	0.74237182	-0.97677799	-0.07838817
C	0.09283730	-2.40306319	-0.01038494
C	-1.24663617	-2.48581958	-0.77555898
C	-2.24824030	-1.40414787	-0.34867239
C	-1.60368885	-0.02224881	-0.52111173
C	-0.30843473	0.13459225	0.33728607
O	0.31591480	1.38542625	-0.06005466
C	3.28478317	1.00682570	-0.43646096
C	2.83198668	0.36930846	0.87940143
C	2.07518798	-0.96446495	0.72762148
C	-2.57958178	1.17745744	-0.37542019
C	-1.79405995	2.48923003	-0.55638119
C	-3.41217979	1.22705259	0.92064350
C	1.04348822	-3.49853491	-0.54206105
C	3.52198271	2.50632352	-0.39746981
H	0.98008266	-0.75135088	-1.13236005
H	-0.11873434	-2.61068427	1.05173690
H	-1.68012771	-3.48592438	-0.61732753
H	-1.04833173	-2.39140584	-1.85835471
H	-2.54915713	-1.56795557	0.69583962
H	-3.15599255	-1.46101283	-0.97186964
H	-1.22282229	0.03886263	-1.55578057
H	2.26927895	1.10597631	1.46750511
H	3.76172853	0.17204653	1.44782738
H	2.75391503	-1.65943677	0.21871470
H	1.89262905	-1.37497279	1.73430341
H	-3.27505397	1.11473946	-1.22883877
H	-3.94245258	0.28208059	1.09328700
H	-4.16478011	2.02755734	0.85084497
H	-2.79077557	1.43235491	1.80307504
H	0.51520206	-4.46312488	-0.56664570
H	1.93499755	-3.62863018	0.08288042
H	1.37248490	-3.26807419	-1.56733803
H	4.15051811	2.78166496	0.46327352
H	2.55093493	3.00772429	-0.26230841
H	3.98821529	2.84226661	-1.33052448
C	-0.50559311	0.14596056	1.86305110
H	-0.13521197	1.07910984	2.35203322
O	-0.97591227	-0.77396974	2.51195958
H	-2.35751729	3.34970235	-0.14568910
O	-1.50924663	2.66838732	-1.93137253
H	-0.92926392	3.46011313	-2.01458894

5β_1 in water, GGA-BLYP/QZ4P large core
44

O	3.53416381	0.71513936	-1.44948940
O	-0.97049849	2.39349741	0.22149401
C	0.89201431	-0.89116412	-0.07258276
C	0.43765266	-2.39980151	0.00892302
C	-0.86776551	-2.67166135	-0.77889902
C	-2.02401075	-1.73677958	-0.39424055
C	-1.58029598	-0.27313238	-0.57160229
C	-0.32072868	0.07371583	0.29773956
O	0.12278116	1.40917540	-0.11261231
C	3.21565080	1.39407977	-0.46997254
C	2.80075871	0.75214192	0.85015245
C	2.19743517	-0.66812873	0.75921343
C	-2.71683823	0.79944362	-0.46896843
C	-2.06641532	2.16324662	-0.73801837
C	-3.56843856	0.78416388	0.82307198
C	1.53822126	-3.37282344	-0.48368263
C	3.24914582	2.90867376	-0.50699316
H	1.10889669	-0.66505456	-1.12983083
H	0.23932537	-2.62484633	1.06939103
H	-1.16482010	-3.71568963	-0.61654871
H	-0.66509272	-2.56636162	-1.85540817
H	-2.33881510	-1.93523171	0.63746722
H	-2.89185137	-1.93272318	-1.03844875
H	-1.19746975	-0.18723958	-1.60360605
H	2.15826981	1.44684572	1.39946996
H	3.73392189	0.68741923	1.43451632
H	2.96463502	-1.32067716	0.33123037
H	2.03877699	-1.02526626	1.78673112
H	-3.38815906	0.60988729	-1.32148027
H	-3.97222390	-0.21614033	1.00866710
H	-4.41497813	1.47221559	0.72818977
H	-2.99825618	1.08620525	1.70846240
H	1.14856695	-4.39783860	-0.48542298
H	2.42803119	-3.36527598	0.15183249
H	1.84917780	-3.13369229	-1.50915540
H	3.67668269	3.26959200	-1.44568069
H	3.82292183	3.29788223	0.34330660
H	2.22508313	3.28829718	-0.39640121
O	-2.96336896	3.22546368	-0.50942241
H	-1.62864799	2.21201081	-1.74127043
H	-2.60891368	4.02610021	-0.93606605
C	-0.52502789	0.10968285	1.82157581
H	-0.24449967	1.07356227	2.29402899
O	-0.90763898	-0.82847260	2.50630397

$5\beta_2$ in water, GGA-BLYP/QZ4P large core

44

O	2.89897414	1.33203496	1.87130151
O	-0.40807075	2.45664501	-0.16095506
C	0.71144423	-1.15385163	-0.25418210
C	0.00248490	-2.51346324	0.11447636
C	-1.42949473	-2.59864432	-0.47351348
C	-2.32325345	-1.40120016	-0.11377578
C	-1.63459934	-0.09148824	-0.54161098
C	-0.22684381	0.07027806	0.13039394
O	0.41520400	1.23515295	-0.48418169
C	3.10496423	1.34956269	0.65529903
C	3.06070498	0.07683120	-0.18625911
C	2.15946630	-1.07277001	0.32467617
C	-2.51250137	1.20309721	-0.45190008
C	-1.64456929	2.36542794	-0.95712305
C	-3.17280612	1.49516854	0.91650197
C	0.81117162	-3.75005680	-0.35017003
C	3.48037782	2.63020257	-0.06391130
H	0.78568940	-1.11192049	-1.35564786
H	-0.08277896	-2.55831997	1.21154689
H	-1.89843728	-3.52693696	-0.12332825
H	-1.35888745	-2.67666785	-1.56871013
H	-2.53433287	-1.40438301	0.96219878
H	-3.28823913	-1.48951292	-0.63077162
H	-1.38895520	-0.20067531	-1.61251772
H	4.10841724	-0.26719220	-0.18745526
H	2.84132761	0.33366947	-1.22893806
H	2.65935183	-2.00695110	0.05612616
H	2.13561391	-1.05170464	1.42287953
H	-3.31378785	1.07709828	-1.19704653
H	-3.73685657	0.62520595	1.26741321
H	-3.87255462	2.33270705	0.83006251
H	-2.44314276	1.75715557	1.69065682
H	0.23154659	-4.66076481	-0.15730717
H	1.76491049	-3.85770150	0.17391492
H	1.01703963	-3.70859162	-1.42790120
H	2.62101568	2.95499224	-0.66506070
H	4.30974379	2.45889099	-0.75958051
H	3.74004468	3.41700262	0.64888115
O	-2.27353417	3.61171816	-0.76437504
H	-1.34581210	2.21751954	-2.00177256
H	-1.81514201	4.27580569	-1.31004962
C	-0.23074219	0.30368045	1.65395516
H	0.24920080	1.24990213	1.96855729
O	-0.67482635	-0.47537067	2.48628470

5β_1^- in water, GGA-BLYP/QZ4P large core

43

O	3.56804025	0.46404983	-1.39507450
O	-0.50487609	2.59639892	-0.19120091
C	0.72300670	-0.99401644	-0.11997487
C	0.03374337	-2.39853790	0.05598966
C	-1.33534884	-2.49266540	-0.65950332
C	-2.29299793	-1.34866281	-0.29323100
C	-1.63339410	0.00626482	-0.61610753
C	-0.28513934	0.20206684	0.17266667
O	0.38059345	1.37239778	-0.39037335
C	3.29129890	1.09089618	-0.36878071
C	2.79687239	0.39078262	0.89229474
C	2.05844179	-0.95261192	0.69896210
C	-2.57348974	1.25437830	-0.57169387
C	-1.79018458	2.50356464	-1.07701641
C	-3.31053657	1.51403827	0.75964990
C	0.94637396	-3.55490081	-0.42537415
C	3.47142419	2.59370767	-0.27898908
H	0.96900785	-0.87599382	-1.18862744
H	-0.14747294	-2.53736010	1.13416859
H	-1.79377982	-3.46026243	-0.41475243
H	-1.17446445	-2.48851446	-1.74862854
H	-2.56490375	-1.41577065	0.76864244
H	-3.22544995	-1.44396886	-0.86705425
H	-1.29073428	-0.05775845	-1.66559801
H	2.21624173	1.10314424	1.48725214
H	3.70886047	0.19413986	1.48069828
H	2.75532483	-1.64729693	0.21744073
H	1.87100936	-1.36107815	1.70259917
H	-3.34228669	1.06965347	-1.34371962
H	-3.88814429	0.63801717	1.07644416
H	-4.00437010	2.35383347	0.64221774
H	-2.62543677	1.77587792	1.57500230
H	0.41030971	-4.50880617	-0.35157552
H	1.86040533	-3.64753760	0.16817730
H	1.23630014	-3.41656615	-1.47550550
H	3.94618566	2.98868472	-1.18053896
H	4.06892801	2.85216242	0.60434062
H	2.48716967	3.05913550	-0.14401649
O	-2.36006271	3.69295552	-0.96133774
H	-1.36914317	2.26547050	-2.08111237
C	-0.44857746	0.42997811	1.68207751
H	-0.16536351	1.44701853	2.02209333
O	-0.81333278	-0.41511222	2.49264463

5β_2^- in water, GGA-BLYP/QZ4P large core

43

O	3.14914389	0.36652734	1.93610863
O	0.44038597	2.52822026	-0.47842050
C	0.30488632	-1.25919922	-0.26415642
C	-0.79389108	-2.30253369	0.16856553
C	-2.19539878	-1.93448637	-0.38066803
C	-2.63017066	-0.49553699	-0.05977940
C	-1.57852062	0.50495297	-0.58073655
C	-0.16537035	0.22818874	0.05111373
O	0.81081562	1.05993378	-0.64338181
C	3.31922873	0.38215067	0.71399245
C	2.92644754	-0.80117539	-0.16288593
C	1.70837681	-1.63860458	0.30836472
C	-1.99427926	2.01181885	-0.55301216
C	-0.88215259	2.85740851	-1.24324780
C	-2.40656406	2.59089016	0.81738419
C	-0.44261584	-3.74651039	-0.26923205
C	3.98114434	1.57038456	0.03598862
H	0.37191466	-1.29470978	-1.36640867
H	-0.85118372	-2.28575451	1.26814695
H	-2.92909977	-2.64458580	0.02384675
H	-2.19624116	-2.07197040	-1.47297817
H	-2.77822965	-0.38470151	1.02217274
H	-3.59774771	-0.28486836	-0.53626909
H	-1.42109172	0.26804523	-1.64929678
H	3.82243533	-1.44473297	-0.14862163
H	2.81461025	-0.47423801	-1.20161752
H	1.90293761	-2.67211044	0.00896217
H	1.68483033	-1.64287861	1.40682497
H	-2.86979413	2.08771322	-1.22270837
H	-3.21088568	2.00601155	1.27770986
H	-2.76286674	3.61947581	0.69259035
H	-1.56991622	2.62604615	1.52526896
H	-1.28317669	-4.41569018	-0.04859368
H	0.43400552	-4.14662178	0.24835567
H	-0.25218116	-3.79813972	-1.34963677
H	3.18054574	2.20723941	-0.36334296
H	4.60272819	1.26034981	-0.80995893
H	4.56674597	2.14845436	0.75443803
O	-0.97365018	4.17771789	-1.19449813
H	-0.69077389	2.42384468	-2.25179220
C	-0.06748735	0.55068783	1.54609189
H	0.58661127	1.40387063	1.79247783
O	-0.63080347	-0.08105875	2.45246541

5β$_1$ in water, GGA-BLYP/DZP medium core

44

O	3.40800660	0.71618705	-1.50041202
O	-0.96973361	2.39299379	0.27153268
C	0.89530723	-0.88633785	-0.05895059
C	0.43858833	-2.38475719	0.03104200
C	-0.85530814	-2.65911811	-0.76660742
C	-2.00442294	-1.71130348	-0.39937113
C	-1.54064078	-0.25973425	-0.57345346
C	-0.30498763	0.07908833	0.31966406
O	0.15204279	1.41038317	-0.06174696
C	3.16160369	1.39090810	-0.49528741
C	2.80029451	0.74799186	0.83618995
C	2.20596966	-0.67160751	0.75342383
C	-2.67307615	0.80567804	-0.49800742
C	-2.02122667	2.16904172	-0.73378242
C	-3.55492920	0.77460511	0.76625107
C	1.53815052	-3.35861280	-0.44789344
C	3.22266624	2.89995194	-0.51284208
H	1.10470444	-0.65885139	-1.11846189
H	0.23090111	-2.59802701	1.09262853
H	-1.15884481	-3.70333428	-0.59494713
H	-0.63640745	-2.55994603	-1.84494750
H	-2.33000826	-1.89677688	0.63358754
H	-2.86913096	-1.89129756	-1.05757364
H	-1.13258886	-0.17588683	-1.59757533
H	2.16625326	1.43545243	1.40962434
H	3.75490413	0.68698060	1.39315534
H	2.96683510	-1.31598404	0.29777834
H	2.06345360	-1.03997761	1.78219293
H	-3.32190959	0.61520378	-1.37052524
H	-3.96110828	-0.23219376	0.92817133
H	-4.39993793	1.46635068	0.65058851
H	-3.00216332	1.07232493	1.66786107
H	1.13782726	-4.38313448	-0.45590358
H	2.42278794	-3.35365155	0.19988512
H	1.85671264	-3.11351968	-1.47345251
H	3.62978428	3.26282398	-1.46336115
H	3.82505150	3.26970725	0.33023020
H	2.20373359	3.29277519	-0.37250405
O	-2.94063887	3.21467682	-0.52752036
H	-1.54508771	2.22294668	-1.72281550
H	-2.55569701	4.03655013	-0.91024362
C	-0.53480701	0.08773847	1.83735157
H	-0.25705663	1.04927420	2.32375644
O	-0.93781986	-0.86489850	2.49338764

5β_2 in water, GGA-BLYP/DZP medium core

44

O	2.84906705	1.31792150	1.85357001
O	-0.40509530	2.46001816	-0.12951315
C	0.70823153	-1.14904924	-0.25519198
C	0.00403543	-2.49668806	0.12767852
C	-1.42513156	-2.58705035	-0.45603516
C	-2.30945293	-1.38135583	-0.10560126
C	-1.61024404	-0.08639617	-0.54127525
C	-0.21409453	0.07516254	0.13466343
O	0.43469295	1.23216792	-0.47232444
C	3.07347750	1.34345992	0.63965269
C	3.04509154	0.07937792	-0.20918996
C	2.15703336	-1.07351969	0.30695383
C	-2.48708391	1.19976799	-0.46248756
C	-1.62121466	2.36433277	-0.95146342
C	-3.15720762	1.48310924	0.89697722
C	0.80928527	-3.73178891	-0.33233991
C	3.45149200	2.62262827	-0.06977849
H	0.77116332	-1.11155405	-1.35887371
H	-0.07545603	-2.52722828	1.22635458
H	-1.89572354	-3.51385926	-0.09341405
H	-1.35163895	-2.67221854	-1.55523882
H	-2.51370135	-1.36830237	0.97397274
H	-3.27736051	-1.45910926	-0.62572904
H	-1.35836277	-0.20109431	-1.61194727
H	4.09925748	-0.25831924	-0.21208905
H	2.81632600	0.33568431	-1.25351424
H	2.65308332	-2.00809245	0.02460287
H	2.14317041	-1.05079375	1.40778662
H	-3.28398407	1.06694915	-1.21460604
H	-3.71997201	0.60524724	1.23947738
H	-3.86100616	2.32064431	0.80202248
H	-2.42709571	1.74830363	1.67409320
H	0.22512482	-4.64201700	-0.13179497
H	1.76828974	-3.83378621	0.18951998
H	1.00639666	-3.68893636	-1.41529484
H	2.58655582	2.95302262	-0.66632859
H	4.28110219	2.45271956	-0.77072679
H	3.71442219	3.40408796	0.65250105
O	-2.27037740	3.59820784	-0.75938393
H	-1.30321798	2.21943338	-1.99362444
H	-1.78782186	4.27980392	-1.28457948
C	-0.22488170	0.29610263	1.65674978
H	0.26854947	1.23789073	1.97327906
O	-0.68906748	-0.48905637	2.47529901

$5\beta_1^-$ in water, GGA-BLYP/DZP medium core

43

O	3.50902749	0.45779906	-1.40894709
O	-0.50755202	2.60414688	-0.17390427
C	0.72207307	-0.99040159	-0.11803444
C	0.03588642	-2.38490703	0.06739731
C	-1.32780152	-2.48396554	-0.64841205
C	-2.27507980	-1.33044179	-0.29058231
C	-1.60459035	0.01109512	-0.62061867
C	-0.26996773	0.20793447	0.17542955
O	0.40824552	1.36531857	-0.37084540
C	3.25827307	1.08701438	-0.37557170
C	2.77894650	0.39246184	0.89026043
C	2.05660103	-0.95394714	0.69130905
C	-2.54622154	1.24723375	-0.58805853
C	-1.78007628	2.50947685	-1.07999644
C	-3.28978966	1.50383241	0.73406252
C	0.94705963	-3.53856194	-0.40768761
C	3.45127800	2.58356705	-0.28430045
H	0.96473510	-0.87199185	-1.18888063
H	-0.14639728	-2.51125009	1.14772606
H	-1.78890897	-3.45132459	-0.39249344
H	-1.16077448	-2.48615662	-1.74087072
H	-2.54118573	-1.38165044	0.77581085
H	-3.21072662	-1.41542126	-0.86620991
H	-1.25137634	-0.05861034	-1.66786738
H	2.18629955	1.10039265	1.48416893
H	3.69504360	0.20247215	1.48243971
H	2.75690503	-1.63337459	0.18938155
H	1.87450215	-1.37729479	1.69229388
H	-3.31258003	1.04773876	-1.36227510
H	-3.87460069	0.62715880	1.04828613
H	-3.97325610	2.35437234	0.60125632
H	-2.60120325	1.76722291	1.55023584
H	0.40430230	-4.49300091	-0.33744492
H	1.86113913	-3.63010688	0.19185770
H	1.23856108	-3.39361889	-1.46045032
H	3.92164922	2.97289744	-1.19476894
H	4.06202716	2.83531035	0.59576809
H	2.46737834	3.05547912	-0.14020771
O	-2.35858481	3.68188930	-0.94474174
H	-1.34150736	2.26930167	-2.08371674
C	-0.45237725	0.42310080	1.67999997
H	-0.17667489	1.44584164	2.01920598
O	-0.82758326	-0.43343548	2.47713942

5β_2^- in water, GGA-BLYP/DZP medium core

43

O	3.09713967	0.35963090	1.91891822
O	0.43718363	2.53881006	-0.45700050
C	0.30179020	-1.25406087	-0.26230888
C	-0.78620663	-2.28859222	0.17972200
C	-2.18503043	-1.92602418	-0.36993882
C	-2.60977190	-0.48405168	-0.05525861
C	-1.55357868	0.50156840	-0.57779863
C	-0.14936078	0.22924672	0.05664440
O	0.83335258	1.04645790	-0.62196162
C	3.29086638	0.38250415	0.69816492
C	2.91098491	-0.79661295	-0.18858499
C	1.70613137	-1.63849936	0.29136757
C	-1.97675334	1.99729601	-0.56031826
C	-0.87655058	2.85739268	-1.24670024
C	-2.38861767	2.58071880	0.80276974
C	-0.43475608	-3.72868878	-0.25599773
C	3.95722562	1.56696337	0.03599943
H	0.35767175	-1.28688692	-1.36668860
H	-0.83818063	-2.26207542	1.28017028
H	-2.92017047	-2.63649742	0.04011479
H	-2.18002014	-2.06680438	-1.46637051
H	-2.74990672	-0.36391117	1.02891638
H	-3.57554451	-0.26203506	-0.53720727
H	-1.39043182	0.25960365	-1.64618206
H	3.81546764	-1.43577915	-0.18054579
H	2.78749537	-0.46176936	-1.22704168
H	1.89502303	-2.67270882	-0.01824247
H	1.69346111	-1.64069040	1.39258910
H	-2.86012167	2.05740277	-1.22559355
H	-3.19591011	1.99828991	1.26970116
H	-2.73692968	3.61338512	0.65832967
H	-1.54265421	2.62111018	1.50431147
H	-1.28160376	-4.39664657	-0.03945906
H	0.44357936	-4.12777122	0.26597605
H	-0.24134443	-3.77142953	-1.34001050
H	3.15418815	2.22125883	-0.34129615
H	4.56918519	1.26719902	-0.82530126
H	4.55744482	2.12693119	0.76310237
O	-0.98113955	4.16628056	-1.19081273
H	-0.66822287	2.40383959	-2.25101188
C	-0.06399950	0.53920743	1.55656081
H	0.61356202	1.38645797	1.79285235
O	-0.64428196	-0.07986001	2.44504429

5β$_1$ in acetonitrile, GGA-BLYP/DZP medium core
44

O	3.40747258	0.71334741	-1.49766041
O	-0.96822940	2.39327955	0.27061180
C	0.89507588	-0.88566572	-0.05970239
C	0.43885157	-2.38408405	0.03080018
C	-0.85512954	-2.65902613	-0.76644702
C	-2.00458461	-1.71163201	-0.39880579
C	-1.54105762	-0.26005699	-0.57371085
C	-0.30522213	0.07946787	0.31865064
O	0.15201325	1.41028614	-0.06406451
C	3.16171673	1.39066653	-0.49457422
C	2.79893135	0.74933898	0.83709675
C	2.20553201	-0.67047545	0.75291580
C	-2.67363571	0.80544512	-0.49781681
C	-2.02094946	2.16897879	-0.73255644
C	-3.55543359	0.77415287	0.76636716
C	1.53872812	-3.35762622	-0.44803322
C	3.22400442	2.90015100	-0.51410149
H	1.10549838	-0.65817624	-1.11907794
H	0.23105446	-2.59668262	1.09252966
H	-1.15842629	-3.70329473	-0.59477182
H	-0.63664369	-2.56003257	-1.84488891
H	-2.32882820	-1.89644810	0.63473771
H	-2.86968590	-1.89248556	-1.05636039
H	-1.13361857	-0.17696652	-1.59833967
H	2.16330794	1.43716747	1.40860495
H	3.75243545	0.68770160	1.39622986
H	2.96726503	-1.31332647	0.29642180
H	2.06305879	-1.03992537	1.78123341
H	-3.32324411	0.61449165	-1.37015037
H	-3.96109985	-0.23279104	0.92846369
H	-4.40079918	1.46562765	0.65131419
H	-3.00179804	1.07188729	1.66746504
H	1.13898766	-4.38237352	-0.45589890
H	2.42343039	-3.35225430	0.19967394
H	1.85745436	-3.11256640	-1.47358446
H	3.63379749	3.26281338	-1.46354031
H	3.82610087	3.27192622	0.32829266
H	2.20480096	3.29319847	-0.37442316
O	-2.94033378	3.21411301	-0.52466975
H	-1.54595328	2.22354252	-1.72244826
H	-2.55975567	4.03598641	-0.91446048
C	-0.53496575	0.08768762	1.83653482
H	-0.25649559	1.04913792	2.32280303
O	-0.93793891	-0.86505306	2.49231802

5β_2 in acetonitrile, GGA-BLYP/DZP medium core
44

O	2.84699671	1.31727702	1.85356748
O	-0.40426295	2.45990557	-0.13036737
C	0.70826967	-1.14864788	-0.25507549
C	0.00402128	-2.49624725	0.12771281
C	-1.42508594	-2.58666895	-0.45605692
C	-2.30937051	-1.38131713	-0.10470435
C	-1.61045822	-0.08645558	-0.54112696
C	-0.21384834	0.07599746	0.13402457
O	0.43475776	1.23210327	-0.47440477
C	3.07346936	1.34334601	0.64027029
C	3.04520133	0.07935233	-0.20905944
C	2.15700124	-1.07335489	0.30756995
C	-2.48736327	1.19947576	-0.46184579
C	-1.62087381	2.36389750	-0.95044655
C	-3.15758963	1.48294493	0.89743988
C	0.80914302	-3.73130427	-0.33276776
C	3.45329340	2.62216957	-0.06904540
H	0.77150062	-1.11070441	-1.35879553
H	-0.07556908	-2.52705524	1.22632734
H	-1.89548081	-3.51361876	-0.09358408
H	-1.35217528	-2.67173632	-1.55528711
H	-2.51268781	-1.36868674	0.97496782
H	-3.27771119	-1.45976618	-0.62398273
H	-1.35860093	-0.20164476	-1.61178318
H	4.09957109	-0.25841412	-0.21295259
H	2.81495669	0.33582724	-1.25308526
H	2.65256754	-2.00871250	0.02617974
H	2.14316491	-1.04955074	1.40842188
H	-3.28523554	1.06655141	-1.21352065
H	-3.72067906	0.60522350	1.23991038
H	-3.86077933	2.32097066	0.80257898
H	-2.42708049	1.74766776	1.67432617
H	0.22502499	-4.64169469	-0.13307258
H	1.76777243	-3.83408085	0.18955835
H	1.00676764	-3.68819685	-1.41565771
H	2.58929796	2.95280648	-0.66678625
H	4.28380818	2.45239206	-0.76907906
H	3.71594604	3.40356321	0.65338106
O	-2.27113101	3.59731397	-0.75891849
H	-1.30307065	2.21857167	-1.99292749
H	-1.79188268	4.27819878	-1.28706350
C	-0.22461654	0.29686531	1.65629088
H	0.26888185	1.23861347	1.97274027
O	-0.68854719	-0.48868818	2.47455640

5β_1^- in acetonitrile, GGA-BLYP/DZP medium core

43

O	3.51201058	0.45773427	-1.40933570
O	-0.50853253	2.60260790	-0.17174664
C	0.72157000	-0.99002274	-0.11798089
C	0.03568975	-2.38458296	0.06760057
C	-1.32787816	-2.48377586	-0.64841671
C	-2.27508982	-1.33024783	-0.29055110
C	-1.60446443	0.01130086	-0.62049162
C	-0.26966721	0.20870346	0.17524999
O	0.40891811	1.36533893	-0.37140179
C	3.25884686	1.08670000	-0.37666273
C	2.77878200	0.39247136	0.88931897
C	2.05626963	-0.95389293	0.69087603
C	-2.54611193	1.24733769	-0.58792768
C	-1.77974292	2.51013781	-1.07884317
C	-3.29040708	1.50402690	0.73375551
C	0.94680502	-3.53846827	-0.40714087
C	3.45276151	2.58323520	-0.28423703
H	0.96440481	-0.87064122	-1.18852603
H	-0.14712447	-2.51051781	1.14791648
H	-1.78901861	-3.45130699	-0.39280202
H	-1.16060247	-2.48558636	-1.74087894
H	-2.54094703	-1.38166444	0.77596107
H	-3.21070398	-1.41541767	-0.86637616
H	-1.25104812	-0.05802467	-1.66764706
H	2.18586950	1.10072478	1.48253840
H	3.69430250	0.20142798	1.48241837
H	2.75651024	-1.63317763	0.18864178
H	1.87424887	-1.37692141	1.69210153
H	-3.31256451	1.04802303	-1.36231514
H	-3.87649442	0.62809054	1.04737392
H	-3.97172513	2.35615836	0.60058488
H	-2.60191402	1.76577532	1.55012293
H	0.40444932	-4.49316216	-0.33681953
H	1.86109433	-3.62979234	0.19218314
H	1.23830766	-3.39367348	-1.45993173
H	3.92552554	2.97198503	-1.19345933
H	4.06231284	2.83582488	0.59657522
H	2.46883801	3.05538146	-0.14193777
O	-2.36089016	3.68102578	-0.94537303
H	-1.33965624	2.26875754	-2.08174806
C	-0.45303446	0.42320579	1.67984409
H	-0.17721712	1.44627200	2.01854048
O	-0.82825980	-0.43322819	2.47720666

5β$_2^-$ in acetonitrile, GGA-BLYP/DZP medium core
43

O	3.09783693	0.36010770	1.91947257
O	0.43810779	2.53865622	-0.45764195
C	0.30138495	-1.25366003	-0.26174561
C	-0.78676470	-2.28837027	0.17976404
C	-2.18543727	-1.92584814	-0.37016626
C	-2.60958519	-0.48378283	-0.05558366
C	-1.55320068	0.50157653	-0.57811981
C	-0.14867174	0.23007429	0.05599553
O	0.83366198	1.04630446	-0.62424243
C	3.29069798	0.38264643	0.69889458
C	2.91075845	-0.79699203	-0.18735041
C	1.70538275	-1.63818631	0.29286055
C	-1.97657173	1.99696978	-0.56070454
C	-0.87652231	2.85842676	-1.24567081
C	-2.39003991	2.58007631	0.80180195
C	-0.43551886	-3.72856147	-0.25591173
C	3.95867075	1.56535749	0.03573351
H	0.35786751	-1.28634321	-1.36617927
H	-0.83948852	-2.26133121	1.28018918
H	-2.92083365	-2.63626522	0.03973201
H	-2.18037698	-2.06648636	-1.46664430
H	-2.74958319	-0.36380411	1.02869711
H	-3.57532711	-0.26166368	-0.53768901
H	-1.38973001	0.25962224	-1.64638094
H	3.81568581	-1.43545286	-0.17891800
H	2.78750372	-0.46227927	-1.22577791
H	1.89349684	-2.67327103	-0.01501099
H	1.69254723	-1.63860222	1.39408453
H	-2.85960575	2.05688237	-1.22664861
H	-3.19937110	1.99916498	1.26697690
H	-2.73495792	3.61356705	0.65638156
H	-1.54557233	2.61881707	1.50485626
H	-1.28220123	-4.39678126	-0.03935524
H	0.44300422	-4.12798129	0.26546946
H	-0.24239611	-3.77166012	-1.34003482
H	3.15694282	2.21825891	-0.34620216
H	4.57292564	1.26215329	-0.82241522
H	4.55637993	2.12692639	0.76379953
O	-0.98408700	4.16640845	-1.18905476
H	-0.66855090	2.40506044	-2.25038831
C	-0.06462949	0.54079769	1.55594178
H	0.60855742	1.39129090	1.79193750
O	-0.64087510	-0.08173441	2.44463148

5β$_1$ in dichloromethane, GGA-BLYP/DZP medium core
44

O	3.40672760	0.70705184	-1.49426253
O	-0.97262616	2.39186455	0.27235715
C	0.89345198	-0.88315645	-0.06123926
C	0.44042863	-2.38234000	0.02908859
C	-0.85433646	-2.65937481	-0.76648806
C	-2.00465272	-1.71386006	-0.39476519
C	-1.54419821	-0.26155318	-0.57468230
C	-0.30785963	0.07933916	0.31582961
O	0.14701113	1.41067086	-0.06650743
C	3.16856707	1.38921882	-0.49450339
C	2.78830558	0.75818110	0.83947966
C	2.20143056	-0.66425943	0.75481469
C	-2.67637218	0.80482902	-0.49653092
C	-2.02316135	2.16939904	-0.72973673
C	-3.55413327	0.77248877	0.77024628
C	1.54329842	-3.35260333	-0.44926785
C	3.25491666	2.89909072	-0.52120680
H	1.10780560	-0.65528914	-1.11972056
H	0.23286819	-2.59514865	1.09078111
H	-1.15535508	-3.70442414	-0.59511064
H	-0.63880445	-2.55907043	-1.84545361
H	-2.32099809	-1.89689135	0.64153099
H	-2.87370765	-1.89883398	-1.04607392
H	-1.13933427	-0.17999687	-1.60058627
H	2.13917587	1.44832816	1.39307301
H	3.73119262	0.70547007	1.41713163
H	2.96703076	-1.30196738	0.29759206
H	2.05766580	-1.03672266	1.78196987
H	-3.32798327	0.61643171	-1.36808837
H	-3.96415345	-0.23309247	0.92972340
H	-4.39528782	1.46991858	0.66192883
H	-2.99517029	1.06270997	1.67043544
H	1.14672527	-4.37854731	-0.46145569
H	2.42562248	-3.34679664	0.20179671
H	1.86618510	-3.10390329	-1.47256570
H	3.66659952	3.24519686	-1.47607505
H	3.86902964	3.26756524	0.31389344
H	2.24333725	3.31090529	-0.38027059
O	-2.94469530	3.21322581	-0.52307449
H	-1.54798253	2.22416114	-1.71990889
H	-2.55470377	4.03858894	-0.89554121
C	-0.53850403	0.08466341	1.83457215
H	-0.26152129	1.04636835	2.32226677
O	-0.94043322	-0.86947350	2.48742629

5β$_2$ in dichloromethane, GGA-BLYP/DZP medium core

44

O	2.83666753	1.31149272	1.85620840
O	-0.40499171	2.46034302	-0.13959488
C	0.70649390	-1.14828287	-0.25875610
C	0.00422367	-2.49625593	0.12598798
C	-1.42795891	-2.58748233	-0.45028913
C	-2.31006347	-1.38238399	-0.09218192
C	-1.61481030	-0.08846550	-0.53809121
C	-0.21501973	0.07652719	0.13035440
O	0.43179389	1.23016097	-0.48310194
C	3.07449835	1.34334603	0.64614961
C	3.04032502	0.08518325	-0.21331736
C	2.15453031	-1.06879162	0.30548255
C	-2.48997732	1.19843220	-0.45921583
C	-1.62233540	2.36058440	-0.95412116
C	-3.15475025	1.48558513	0.90176935
C	0.80886703	-3.73030250	-0.33829725
C	3.47080244	2.62482697	-0.05060123
H	0.76967480	-1.11160188	-1.36267998
H	-0.07099879	-2.52705074	1.22483146
H	-1.89552868	-3.51509690	-0.08571116
H	-1.36188184	-2.67196138	-1.55014340
H	-2.50072798	-1.36784540	0.98977572
H	-3.28414534	-1.46267136	-0.60060595
H	-1.36889858	-0.20826807	-1.60982618
H	4.09425985	-0.25307419	-0.23059571
H	2.80004022	0.35110170	-1.25281452
H	2.65268262	-2.00529745	0.03200941
H	2.13774534	-1.03733953	1.40597425
H	-3.29093792	1.06538354	-1.20780111
H	-3.72581540	0.61254626	1.24325358
H	-3.84907567	2.33130043	0.81011012
H	-2.42054189	1.74055455	1.67821298
H	0.22200493	-4.64089444	-0.14791877
H	1.76413889	-3.83858797	0.18912907
H	1.01330362	-3.68157345	-1.41974617
H	2.61629146	2.96557266	-0.65629852
H	4.30969882	2.45617304	-0.74090984
H	3.72835022	3.39887402	0.68145266
O	-2.27381433	3.59455223	-0.76741762
H	-1.30858320	2.20999875	-1.99751818
H	-1.77391411	4.27825863	-1.27312630
C	-0.22035298	0.29856958	1.65362879
H	0.27104315	1.24222149	1.96780305
O	-0.67744506	-0.48970261	2.47266028

5β$_1^-$ in dichloromethane, GGA-BLYP/DZP medium core

43

O	3.52406846	0.45062849	-1.40497639
O	-0.50865461	2.60431462	-0.16600198
C	0.72010734	-0.98885879	-0.11902276
C	0.03579292	-2.38349955	0.06736333
C	-1.32763998	-2.48380849	-0.64890217
C	-2.27450600	-1.32997919	-0.29082736
C	-1.60523186	0.01221495	-0.62190551
C	-0.26977678	0.21019945	0.17396017
O	0.40921023	1.36488197	-0.36957728
C	3.26133230	1.08423012	-0.37936342
C	2.77555691	0.39477701	0.88863308
C	2.05470100	-0.95253617	0.68999007
C	-2.54739870	1.24701300	-0.58914535
C	-1.78234944	2.51532278	-1.07827682
C	-3.29358371	1.50452544	0.73133287
C	0.94728099	-3.53815421	-0.40477035
C	3.45058423	2.58281889	-0.29058418
H	0.96478565	-0.86831839	-1.18914567
H	-0.14848180	-2.50687485	1.14775684
H	-1.78835224	-3.45186189	-0.39327062
H	-1.16001281	-2.48576955	-1.74147894
H	-2.53852343	-1.38080440	0.77622754
H	-3.21122983	-1.41589971	-0.86496671
H	-1.25215910	-0.05666366	-1.66946652
H	2.17884836	1.10463259	1.47565141
H	3.68914669	0.20542684	1.48546148
H	2.75631669	-1.62988545	0.18671315
H	1.87228753	-1.37601945	1.69093771
H	-3.31357981	1.04839948	-1.36446971
H	-3.88717453	0.63258625	1.04257909
H	-3.96564205	2.36356016	0.59559696
H	-2.60530420	1.76101902	1.54944377
H	0.40554108	-4.49321029	-0.33330138
H	1.86172328	-3.62806028	0.19475513
H	1.23992377	-3.39491468	-1.45756371
H	3.93093595	2.96891991	-1.19704494
H	4.05260882	2.83883362	0.59458798
H	2.46430488	3.05325539	-0.15909609
O	-2.36465623	3.67975514	-0.94206979
H	-1.33674308	2.27401501	-2.08023907
C	-0.45692950	0.42316412	1.67885239
H	-0.19448287	1.45121472	2.01430431
O	-0.82177262	-0.43678811	2.47720218

5β$_2^-$ in dichloromethane, GGA-BLYP/DZP medium core

43

O	3.10328973	0.35636188	1.91983477
O	0.43962810	2.53867427	-0.45704043
C	0.30086666	-1.25316763	-0.26039689
C	-0.78589778	-2.28813439	0.18170999
C	-2.18441434	-1.92609195	-0.36831772
C	-2.60609835	-0.48317209	-0.05487573
C	-1.55113867	0.50260234	-0.58030048
C	-0.14567124	0.23123694	0.05347425
O	0.83700521	1.04325920	-0.62615941
C	3.28958614	0.38269786	0.70025018
C	2.90908667	-0.79786984	-0.18778603
C	1.70425322	-1.63752893	0.29611541
C	-1.97622399	1.99653409	-0.56283361
C	-0.87738539	2.86552246	-1.24711569
C	-2.39202220	2.57945792	0.79881398
C	-0.43605924	-3.72916907	-0.25266741
C	3.95686734	1.56473552	0.03310953
H	0.35893321	-1.28740249	-1.36504154
H	-0.83894392	-2.25803964	1.28203914
H	-2.91985509	-2.63673205	0.04266294
H	-2.17975467	-2.06853754	-1.46494684
H	-2.74204646	-0.36285842	1.02994709
H	-3.57383759	-0.26093194	-0.53377684
H	-1.38731167	0.26151735	-1.64926382
H	3.81403045	-1.43683067	-0.18001293
H	2.78073271	-0.46084322	-1.22490821
H	1.89267960	-2.67474104	-0.00589260
H	1.69177288	-1.62992753	1.39741032
H	-2.85892088	2.05674880	-1.22983555
H	-3.20720722	2.00370684	1.26142327
H	-2.72492952	3.61612075	0.64816733
H	-1.54975038	2.61332599	1.50434767
H	-1.28221766	-4.39810691	-0.03497668
H	0.44342469	-4.12896424	0.26719833
H	-0.24481806	-3.77325204	-1.33744506
H	3.15574348	2.21276773	-0.35890051
H	4.57877807	1.25656270	-0.81839093
H	4.54819676	2.13119238	0.76269194
O	-0.98961572	4.16639901	-1.18080892
H	-0.66765581	2.41199802	-2.25378150
C	-0.06815123	0.54415828	1.55431850
H	0.59550241	1.40248994	1.78913903
O	-0.64299008	-0.08464508	2.43918550

$5\beta_1$ in chloroform, GGA-BLYP/DZP medium core
44

O	3.40211160	0.71127449	-1.49585019
O	-0.96775796	2.39345796	0.27054193
C	0.89553775	-0.88495702	-0.06046493
C	0.43946793	-2.38342886	0.03086001
C	-0.85454173	-2.65879025	-0.76617124
C	-2.00395456	-1.71148216	-0.39782547
C	-1.54055487	-0.25991781	-0.57383367
C	-0.30454615	0.08012577	0.31768253
O	0.15188417	1.41075859	-0.06619025
C	3.16126259	1.38976059	-0.49424223
C	2.79790862	0.75000775	0.83894623
C	2.20527748	-0.67008063	0.75322695
C	-2.67328945	0.80566932	-0.49736166
C	-2.02041743	2.16949006	-0.73157065
C	-3.55504823	0.77419022	0.76686911
C	1.53921247	-3.35709152	-0.44808329
C	3.22621581	2.90006641	-0.51428792
H	1.10867489	-0.65717225	-1.11925272
H	0.23080331	-2.59547550	1.09257976
H	-1.15771024	-3.70317004	-0.59454564
H	-0.63650900	-2.56004179	-1.84479422
H	-2.32662928	-1.89581567	0.63627311
H	-2.86982450	-1.89314066	-1.05447711
H	-1.13340541	-0.17736444	-1.59880483
H	2.16017604	1.43750025	1.40861161
H	3.75003032	0.68823967	1.40058623
H	2.96761154	-1.31058631	0.29439236
H	2.06201162	-1.04167456	1.78078970
H	-3.32326846	0.61527742	-1.36984457
H	-3.96025503	-0.23288038	0.92933823
H	-4.39975838	1.46644395	0.65217910
H	-3.00130084	1.07148631	1.66778164
H	1.14019868	-4.38212267	-0.45604366
H	2.42391394	-3.35175560	0.19950348
H	1.85871504	-3.11199937	-1.47331948
H	3.63792154	3.26015783	-1.46384537
H	3.82842514	3.27303182	0.32779128
H	2.20717150	3.29416394	-0.37631049
O	-2.94109164	3.21340674	-0.52464985
H	-1.54487991	2.22357727	-1.72159973
H	-2.56023065	4.03469098	-0.91384157
C	-0.53480942	0.08729406	1.83594453
H	-0.25611915	1.04894409	2.32270725
O	-0.93749824	-0.86583782	2.48999951

$5\beta_2$ in chloroform, GGA-BLYP/DZP medium core
44

O	2.84520854	1.31640816	1.85340688
O	-0.40335981	2.46066690	-0.13229527
C	0.70809822	-1.14779968	-0.25488552
C	0.00400828	-2.49538101	0.12815040
C	-1.42500124	-2.58612448	-0.45558679
C	-2.30881456	-1.38084320	-0.10311916
C	-1.61010261	-0.08615615	-0.54020297
C	-0.21317289	0.07725340	0.13404892
O	0.43370861	1.23218371	-0.47800298
C	3.07319648	1.34312641	0.64190730
C	3.04531566	0.07897243	-0.20899322
C	2.15666637	-1.07305806	0.30827294
C	-2.48718941	1.19949074	-0.46073870
C	-1.62038809	2.36363183	-0.94976200
C	-3.15737775	1.48341543	0.89856286
C	0.80867154	-3.73064638	-0.33290008
C	3.45518480	2.62192730	-0.06776102
H	0.77178092	-1.11051724	-1.35883541
H	-0.07642268	-2.52531135	1.22671293
H	-1.89529763	-3.51329039	-0.09334180
H	-1.35242715	-2.67128793	-1.55498939
H	-2.50975770	-1.36837493	0.97696446
H	-3.27785846	-1.45968738	-0.62157805
H	-1.35919534	-0.20166344	-1.61128585
H	4.09939445	-0.25984200	-0.21364511
H	2.81352127	0.33581762	-1.25277273
H	2.65132846	-2.00941305	0.02817476
H	2.14285708	-1.04686528	1.40904080
H	-3.28531757	1.06664219	-1.21254842
H	-3.72081011	0.60595609	1.24117356
H	-3.85931805	2.32242656	0.80355937
H	-2.42710456	1.74716185	1.67559772
H	0.22462864	-4.64128916	-0.13440192
H	1.76698978	-3.83458911	0.18973383
H	1.00675145	-3.68751324	-1.41582753
H	2.59145566	2.95330389	-0.66546249
H	4.28687679	2.45238294	-0.76686202
H	3.71727804	3.40245183	0.65563298
O	-2.27333422	3.59594645	-0.76005605
H	-1.30284840	2.21649877	-1.99264956
H	-1.79321557	4.27816980	-1.28433893
C	-0.22353195	0.29717281	1.65739836
H	0.26996216	1.23855478	1.97540356
O	-0.68799973	-0.49119260	2.47154273

5β$_1^-$ in chloroform, GGA-BLYP/DZP medium core

43

O	3.52243712	0.45077634	-1.40540413
O	-0.51079552	2.60418453	-0.16556746
C	0.72004195	-0.98903599	-0.11844406
C	0.03585670	-2.38370794	0.06816089
C	-1.32742239	-2.48386256	-0.64839944
C	-2.27373062	-1.32941770	-0.29077590
C	-1.60430901	0.01276647	-0.62204707
C	-0.26886379	0.21071265	0.17358109
O	0.41066359	1.36505204	-0.36972589
C	3.25990347	1.08395697	-0.38000575
C	2.77565591	0.39403935	0.88854858
C	2.05454562	-0.95320183	0.69056162
C	-2.54640082	1.24762501	-0.58982069
C	-1.78224148	2.51641371	-1.07945318
C	-3.29221745	1.50499854	0.73081319
C	0.94679169	-3.53862010	-0.40471086
C	3.45055851	2.58245757	-0.28895038
H	0.96593410	-0.86807674	-1.18818731
H	-0.14917610	-2.50683892	1.14857392
H	-1.78827429	-3.45224012	-0.39306275
H	-1.15932038	-2.48582772	-1.74099774
H	-2.53774498	-1.38015311	0.77631452
H	-3.21039690	-1.41504227	-0.86542531
H	-1.25125323	-0.05535921	-1.66973363
H	2.17878011	1.10320894	1.47635545
H	3.69007388	0.20394413	1.48437488
H	2.75669723	-1.62985521	0.18685520
H	1.87157493	-1.37623976	1.69185409
H	-3.31286445	1.04907257	-1.36492427
H	-3.88404320	0.63197197	1.04362102
H	-3.96415096	2.36387739	0.59334663
H	-2.60378237	1.76418053	1.54791202
H	0.40532594	-4.49406802	-0.33404169
H	1.86152885	-3.62886017	0.19441717
H	1.23946126	-3.39434540	-1.45740096
H	3.92984598	2.96846193	-1.19599417
H	4.05478996	2.83738331	0.59542103
H	2.46463103	3.05372026	-0.15578057
O	-2.36664819	3.67851894	-0.94134023
H	-1.33610163	2.27493843	-2.08170720
C	-0.45644907	0.42348387	1.67832475
H	-0.19112756	1.45128076	2.01318354
O	-0.82128467	-0.43672185	2.47651472

5β$_2^-$ in chloroform, GGA-BLYP/DZP medium core

43

O	3.10328973	0.35636188	1.91983477
O	0.43962810	2.53867427	-0.45704043
C	0.30086666	-1.25316763	-0.26039689
C	-0.78589778	-2.28813439	0.18170999
C	-2.18441434	-1.92609195	-0.36831772
C	-2.60609835	-0.48317209	-0.05487573
C	-1.55113867	0.50260234	-0.58030048
C	-0.14567124	0.23123694	0.05347425
O	0.83700521	1.04325920	-0.62615941
C	3.28958614	0.38269786	0.70025018
C	2.90908667	-0.79786984	-0.18778603
C	1.70425322	-1.63752893	0.29611541
C	-1.97622399	1.99653409	-0.56283361
C	-0.87738539	2.86552246	-1.24711569
C	-2.39202220	2.57945792	0.79881398
C	-0.43605924	-3.72916907	-0.25266741
C	3.95686734	1.56473552	0.03310953
H	0.35893321	-1.28740249	-1.36504154
H	-0.83894392	-2.25803964	1.28203914
H	-2.91985509	-2.63673205	0.04266294
H	-2.17975467	-2.06853754	-1.46494684
H	-2.74204646	-0.36285842	1.02994709
H	-3.57383759	-0.26093194	-0.53377684
H	-1.38731167	0.26151735	-1.64926382
H	3.81403045	-1.43683067	-0.18001293
H	2.78073271	-0.46084322	-1.22490821
H	1.89267960	-2.67474104	-0.00589260
H	1.69177288	-1.62992753	1.39741032
H	-2.85892088	2.05674880	-1.22983555
H	-3.20720722	2.00370684	1.26142327
H	-2.72492952	3.61612075	0.64816733
H	-1.54975038	2.61332599	1.50434767
H	-1.28221766	-4.39810691	-0.03497668
H	0.44342469	-4.12896424	0.26719833
H	-0.24481806	-3.77325204	-1.33744506
H	3.15574348	2.21276773	-0.35890051
H	4.57877807	1.25656270	-0.81839093
H	4.54819676	2.13119238	0.76269194
O	-0.98961572	4.16639901	-1.18080892
H	-0.66765581	2.41199802	-2.25378150
C	-0.06815123	0.54415828	1.55431850
H	0.59550241	1.40248994	1.78913903
O	-0.64299008	-0.08464508	2.43918550

5β$_1$ in vacuum, GGA-BLYP/DZP medium core
44

O	3.38259499	0.70617916	-1.49574735
O	-0.97116028	2.39422512	0.27845068
C	0.89679341	-0.88029091	-0.06240411
C	0.44199047	-2.37926683	0.03004503
C	-0.85214972	-2.65697746	-0.76607916
C	-2.00070810	-1.71049925	-0.39191969
C	-1.53901753	-0.25913803	-0.57451416
C	-0.30279245	0.08301573	0.31450380
O	0.14920994	1.41487165	-0.06766716
C	3.15906585	1.38381173	-0.49855362
C	2.78937573	0.75360974	0.84723880
C	2.20361508	-0.66868027	0.75709340
C	-2.67105725	0.80705057	-0.49564976
C	-2.01304052	2.16999377	-0.72577245
C	-3.55000849	0.78016723	0.77077201
C	1.54318232	-3.35226997	-0.44603069
C	3.24329133	2.89959105	-0.51932688
H	1.12222180	-0.65120572	-1.11830338
H	0.22903834	-2.58763837	1.09163637
H	-1.15352659	-3.70206975	-0.59403112
H	-0.63643389	-2.56051673	-1.84565429
H	-2.30985951	-1.89090627	0.64689255
H	-2.87345464	-1.89645852	-1.03906166
H	-1.13377844	-0.17782576	-1.60109414
H	2.13774000	1.44043460	1.40298913
H	3.73381175	0.69957301	1.42280278
H	2.96956097	-1.29840076	0.28925594
H	2.05784801	-1.05214163	1.78035991
H	-3.32377352	0.62271403	-1.36814020
H	-3.96230226	-0.22366677	0.93458230
H	-4.38596905	1.48304127	0.65979386
H	-2.99028390	1.07095764	1.66942673
H	1.14613546	-4.37796092	-0.45862980
H	2.42385892	-3.34945582	0.20713806
H	1.87137174	-3.10535118	-1.46783338
H	3.66532644	3.24220169	-1.47084656
H	3.84635686	3.27224578	0.32237804
H	2.22669647	3.30451988	-0.39453708
O	-2.94680857	3.20606756	-0.53789937
H	-1.52745088	2.21615928	-1.71388351
H	-2.53699097	4.04341596	-0.85423512
C	-0.53873675	0.08001847	1.83621637
H	-0.26545003	1.04503292	2.32534208
O	-0.93812947	-0.87693062	2.47843065

$5\beta_2$ in vacuum, GGA-BLYP/DZP medium core

44

O	2.82329903	1.30755858	1.84923112
O	-0.40144461	2.46095186	-0.13838936
C	0.70902320	-1.14508114	-0.25971910
C	0.00664778	-2.49234403	0.12899215
C	-1.42579754	-2.58458950	-0.44642340
C	-2.30582571	-1.37946965	-0.08457661
C	-1.61077269	-0.08740399	-0.53466266
C	-0.20944113	0.07967609	0.12860904
O	0.43102179	1.23109596	-0.49482367
C	3.07024479	1.34315284	0.64930747
C	3.04538263	0.08109825	-0.21904641
C	2.15684472	-1.06772778	0.30537510
C	-2.48594093	1.19929885	-0.45426949
C	-1.61521624	2.35987841	-0.94817419
C	-3.14822451	1.49123116	0.90715948
C	0.80797753	-3.72869281	-0.33373706
C	3.46827400	2.62937975	-0.05079634
H	0.77367415	-1.11269091	-1.36461704
H	-0.07060614	-2.51616264	1.22773633
H	-1.89266455	-3.51310489	-0.08248689
H	-1.36162422	-2.67108969	-1.54685064
H	-2.48440234	-1.36341085	0.99907615
H	-3.28405140	-1.46023548	-0.58637109
H	-1.36851875	-0.20826526	-1.60823343
H	4.09848114	-0.25996243	-0.23445572
H	2.80144452	0.34672864	-1.25832809
H	2.65108258	-2.00920357	0.04082344
H	2.13970547	-1.02143494	1.40552793
H	-3.28874730	1.06974614	-1.20278837
H	-3.72034112	0.62060521	1.25284038
H	-3.83627208	2.34128685	0.81287731
H	-2.41156909	1.74463631	1.68045643
H	0.22146038	-4.63926912	-0.14281267
H	1.76299821	-3.84058430	0.19316495
H	1.01182967	-3.68419194	-1.41573164
H	2.60803506	2.97219616	-0.64675613
H	4.30637026	2.46519581	-0.74403503
H	3.72689749	3.39710950	0.68732487
O	-2.28003820	3.58772105	-0.77248179
H	-1.29869741	2.19977475	-1.99220572
H	-1.74718166	4.28590356	-1.21687675
C	-0.21739082	0.29336855	1.66041182
H	0.29043115	1.22554248	1.98559756
O	-0.69789460	-0.49841919	2.45541654