Supplementary Information

Old Drawback on Azlactone Formation Revealed by a Combination of Theoretical and Experimental Studies

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Experimental IR and ESI(+)-MS data

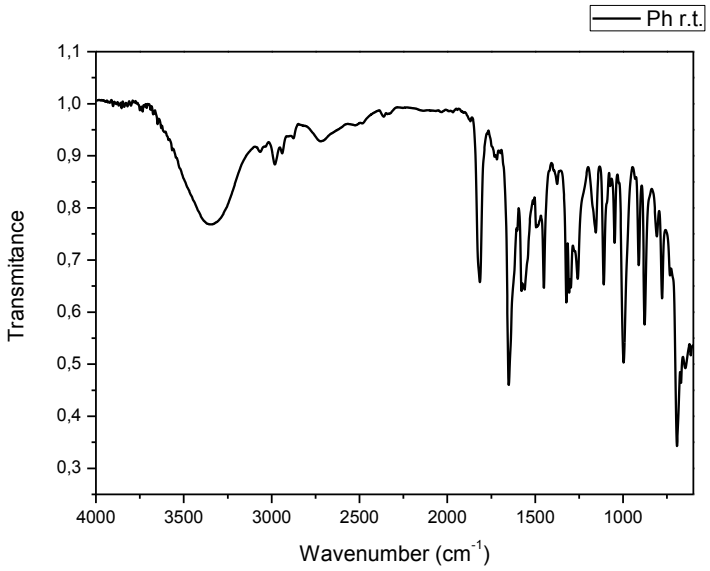

Figure S1. IR (SeZn) of the crude reaction mixture for the formation of a 2-aryl azlactone (R = Ph).

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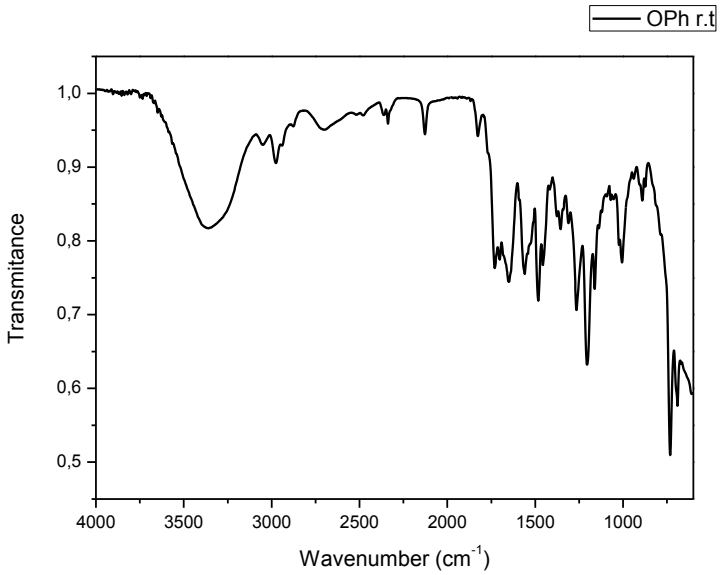


Figure S2. IR (SeZn) of the crude reaction mixture for the formation of a 2-alcoxy azlactone (R = OPh).

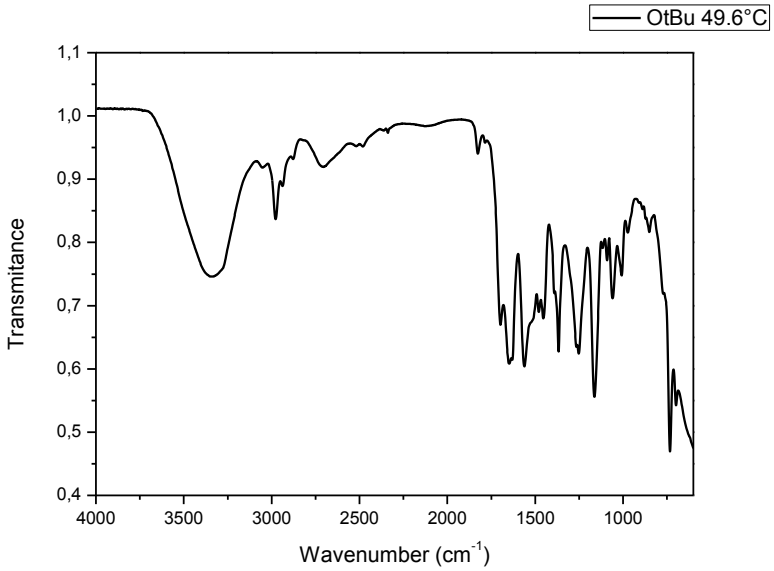


Figure S3. IR (SeZn) of the crude reaction mixture for the formation of a 2-alcoxy azlactone, temperature = 49.6 °C (R = OPh).

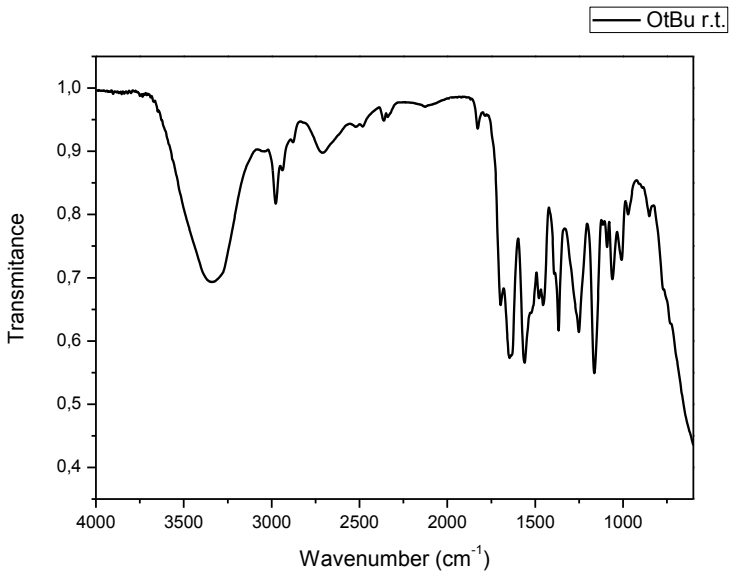


Figure S4. IR (SeZn) of the crude reaction mixture for the formation of a 2-alcoxy (R = O*t*Bu).

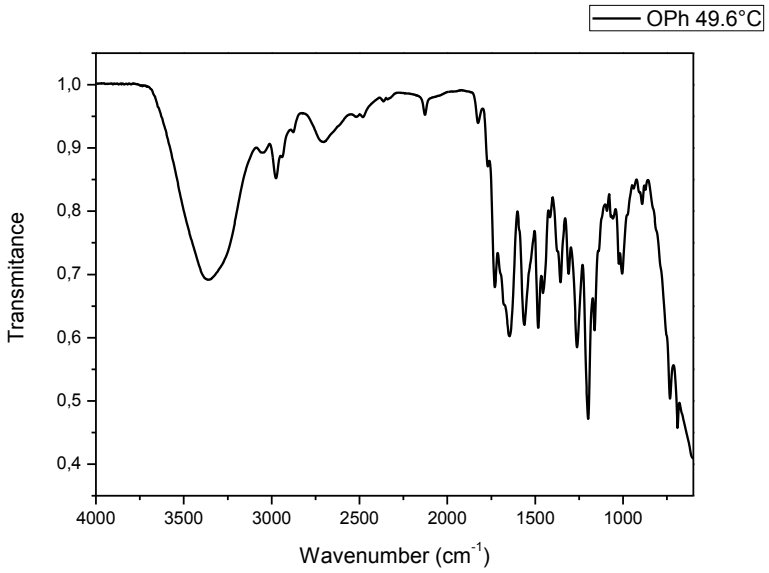


Figure S5. IR (SeZn) of the crude reaction mixture for the formation of a 2-alcoxy azlactone, temperature = 49.6 °C (R = O*t*Bu).

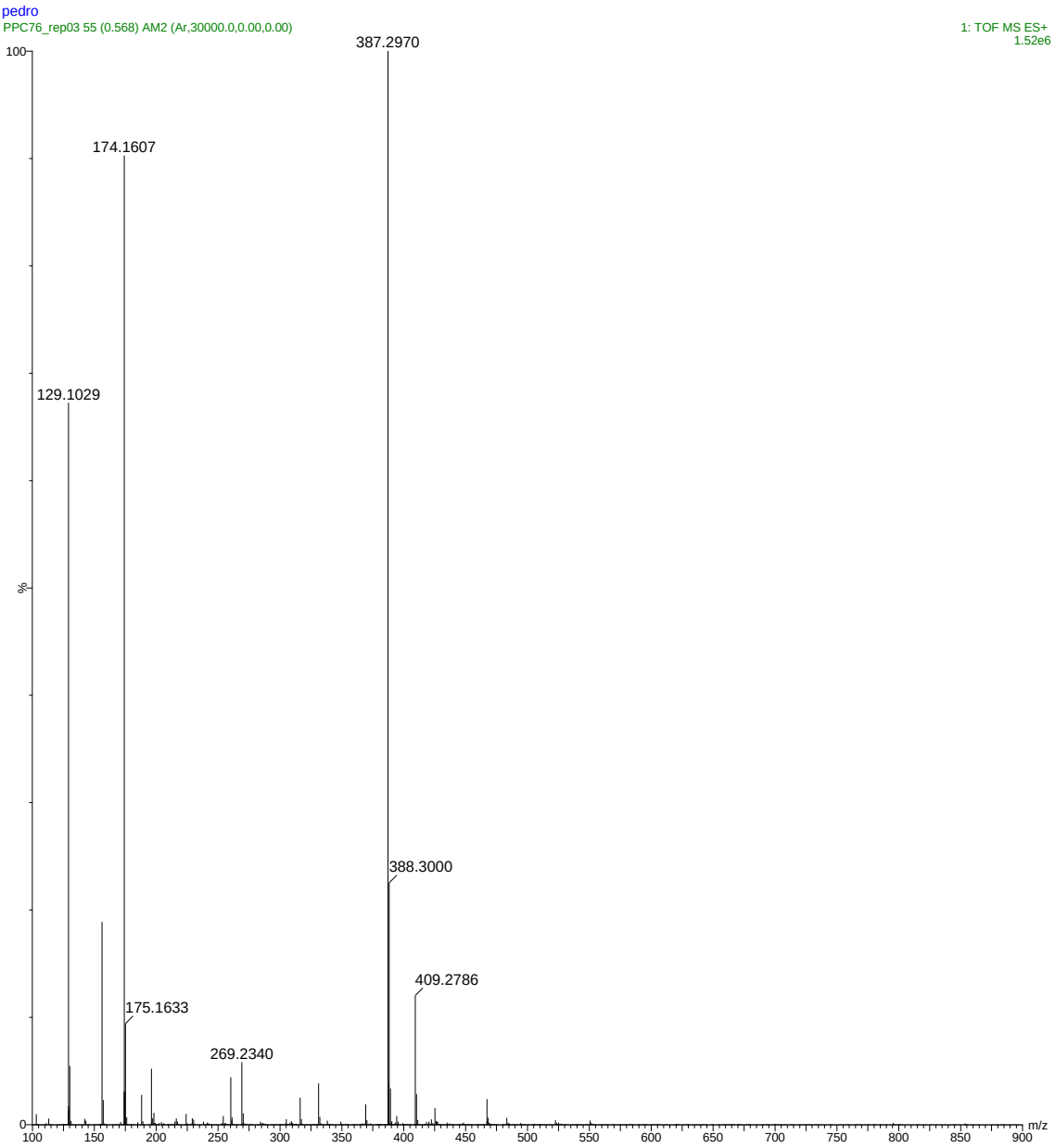


Figure S6. ESI(+)-MS of the crude reaction mixture between EDC and *N*-Boc isoleucine (R = O*t*Bu).

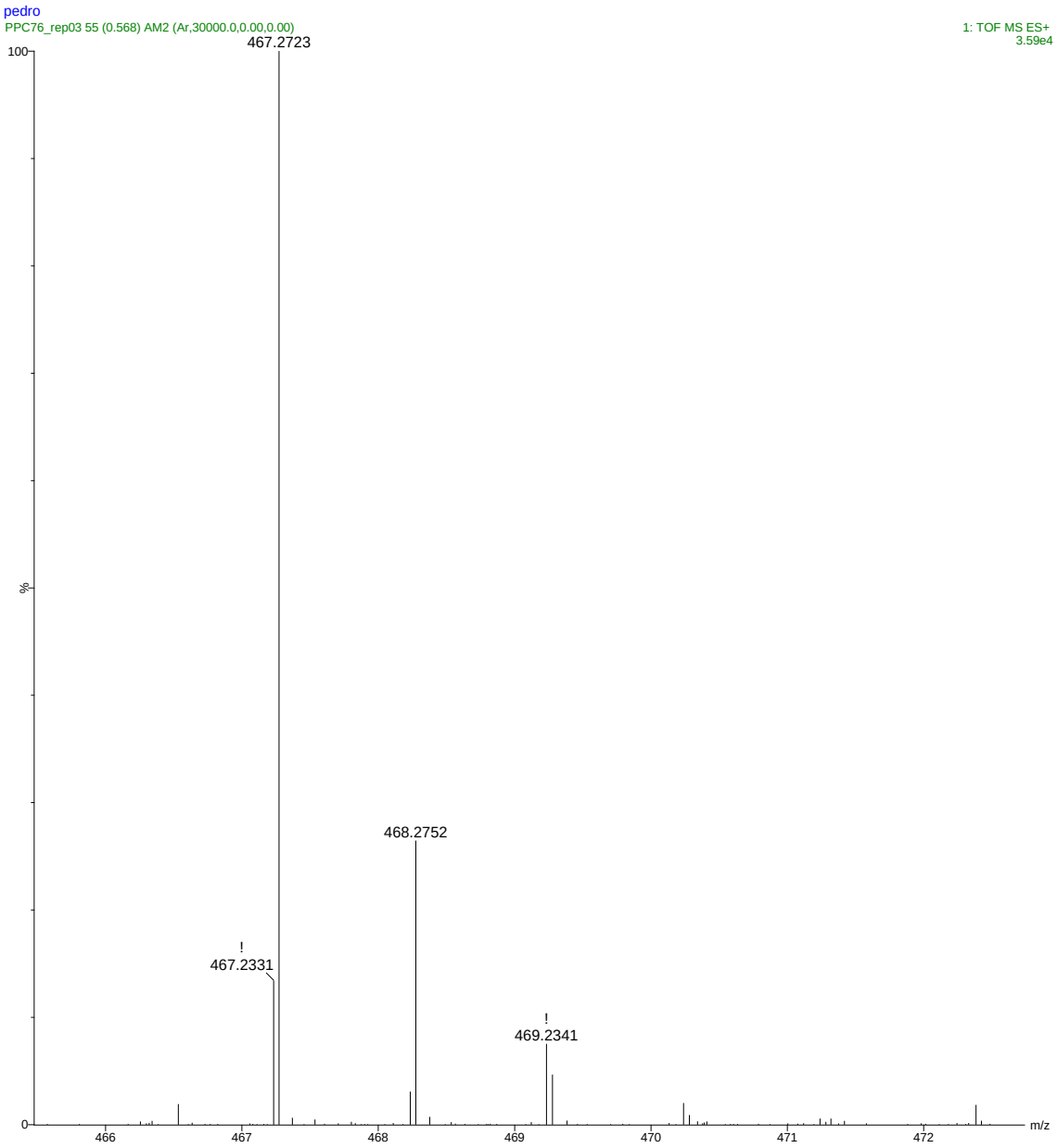


Figure S7. Expansion of ESI(+)-MS of the crude reaction mixture between EDC and *N*-Boc isoleucine (R = O*t*Bu).

ΔE, ΔH and ΔG for azlactone formation

PBE0/6-31++G(d,p)//B3LYP/6-31G(d)

Table S1. ΔE, ΔH and ΔG for R = Ph in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–10.69	–9.32	1.91
TS1	4.03	3.85	17.18
C1	–10.73	–8.74	4.97
C2	–13.90	–11.39	4.81
C3	–9.54	–7.43	7.93
TS2	5.88	5.74	23.11
MC2	–28.75	–26.69	–14.05
Products	–17.42	–16.41	–13.10

Table S2. ΔE, ΔH and ΔG for R = Ph in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–8.14	–6.77	4.46
TS1	4.56	4.38	17.72
C1	–10.17	–8.18	5.52
C2	–12.16	–9.65	6.55
C3	–8.14	–6.03	9.32
TS2	4.65	4.50	21.88
MC2	–27.11	–25.05	–12.41
Products	–18.58	–17.57	–14.26

Table S3. ΔE, ΔH and ΔG for R = Me in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–10.56	–9.19	2.06
TS1	4.31	4.09	17.43
C1	–10.64	–8.77	4.18
C2	–15.94	–13.59	2.83
C3	–8.96	–6.97	7.83
TS2	9.09	8.23	25.41
MC2	–27.82	–25.66	–11.96
Products	–16.40	–15.39	–11.34

Table S4. ΔE, ΔH and ΔG for R = Me in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–7.97	–6.61	4.65
TS1	4.88	4.67	18.00
C1	–10.04	–8.17	4.78
C2	–14.32	–11.96	4.46
C3	–8.06	–6.07	8.73
TS2	7.31	6.45	23.64
MC2	–25.69	–23.54	–9.84
Products	–17.69	–16.68	–12.63

Table S5. ΔE, ΔH and ΔG for R = O*t*Bu in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–10.54	–9.20	1.57
TS1	4.08	3.87	17.16
C1	–10.63	–8.74	4.33
C2	–18.11	–15.59	0.78
C3	–9.46	–7.35	7.73
TS2	12.24	12.15	28.54
MC2	–16.93	–15.03	–2.37
Products	–8.72	–7.78	–4.40

Table S6. ΔE, ΔH and ΔG for R = O*t*Bu in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–7.92	–6.58	4.19
TS1	4.86	4.64	17.93
C1	–10.06	–8.17	4.91
C2	–16.70	–14.18	2.19
C3	–8.00	–5.89	9.19
TS2	10.48	10.38	26.77
MC2	–16.04	–14.14	–1.48
Products	–11.12	–10.18	–6.80

Table S7. ΔE, ΔH and ΔG for R = OBn in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–10.17	–9.02	1.46
TS1	4.18	3.84	16.31
C1	–10.66	–8.78	3.98
C2	–18.16	–15.68	0.84
C3	–9.46	–7.49	7.19
TS2	11.63	11.64	28.91
MC2	–16.44	–14.61	–2.21
Products	–7.69	–6.87	–4.12

Table S8. ΔE, ΔH and ΔG for R = OBn in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	-8.03	-6.88	3.60
TS1	4.61	4.27	16.74
C1	-10.06	-8.18	4.58
C2	-16.63	-14.14	2.37
C3	-8.52	-6.55	8.13
TS2	10.89	10.91	28.18
MC2	-16.15	-14.32	-1.91
Products	-10.48	-9.67	-6.92

Table S9. ΔE, ΔH and ΔG for R = OFm in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–10.69	–9.32	1.41
TS1	3.67	3.50	17.05
C1	–10.77	–8.83	4.60
C2	–18.06	–15.53	1.87
C3	–9.90	–7.75	7.75
TS2	11.21	11.35	28.09
MC2	–17.42	–15.32	–1.58
Products	–8.50	–7.48	–3.67

Table S10. ΔE, ΔH and ΔG for R = OFm in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–8.01	–6.64	4.10
TS1	4.48	4.32	17.87
C1	–10.10	–8.16	5.27
C2	–16.64	–14.12	3.29
C3	–8.46	–6.31	9.19
TS2	9.78	9.91	26.65
MC2	–15.04	–12.94	0.80
Products	–10.28	–9.26	–5.44

Table S11. ΔE, ΔH and ΔG for R = OPh in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–10.93	–9.61	1.33
TS1	3.26	3.09	16.70
C1	–10.75	–8.80	4.54
C2	–18.54	–16.06	0.26
C3	–10.20	–8.08	7.26
TS2	10.85	11.08	27.54
MC2	–16.80	–14.86	–2.46
Products	–7.13	–6.09	–2.52

Table S12. ΔE, ΔH and ΔG for R = OPh in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–8.15	–6.83	4.11
TS1	4.15	3.99	17.60
C1	–10.12	–8.17	5.17
C2	–16.88	–14.40	1.92
C3	–8.44	–6.33	9.02
TS2	9.29	9.53	25.98
MC2	–15.37	–13.43	–1.03
Products	–8.38	–7.34	–3.77

PBE0-D3/6-31++G(d,p)//B3LYP/6-31G(d)

Table S13. ΔE, ΔH and ΔG for R = Ph in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–14.07	–12.70	–1.47
TS1	–0.12	–0.30	13.04
C1	–14.24	–12.25	1.45
C2	–21.68	–19.17	–2.97
C3	–17.40	–15.29	0.07
TS2	–1.59	–1.73	15.64
MC2	–33.29	–31.24	–18.59
Products	–18.12	–17.11	–13.80

Table S14. ΔE, ΔH and ΔG for R = Ph in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–11.52	–10.16	1.08
TS1	0.41	0.24	13.57
C1	–13.68	–11.70	2.01
C2	–19.94	–17.42	–1.23
C3	–16.00	–13.89	1.47
TS2	–2.82	–2.97	14.41
MC2	–31.65	–29.60	–16.95
Products	–19.28	–18.27	–14.96

Table S15. ΔE, ΔH and ΔG for R = Me in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–13.90	–12.53	–1.28
TS1	0.38	0.16	13.50
C1	–14.11	–12.24	0.71
C2	–23.21	–20.86	–4.44
C3	–15.64	–13.65	1.15
TS2	3.29	2.43	19.62
MC2	–31.29	–29.14	–15.43
Products	–17.25	–16.24	–12.19

Table S16. ΔE, ΔH and ΔG for R = Me in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–11.31	–9.95	1.30
TS1	0.95	0.74	14.08
C1	–13.52	–11.64	1.30
C2	–21.59	–19.23	–2.81
C3	–14.74	–12.75	2.05
TS2	1.51	0.65	17.84
MC2	–29.17	–27.01	–13.31
Products	–18.54	–17.52	–13.48

Table S17. ΔE, ΔH and ΔG for R = O*t*Bu in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–13.96	–12.62	–1.85
TS1	0.10	–0.12	13.17
C1	–14.13	–12.25	0.83
C2	–26.77	–24.26	–7.89
C3	–16.00	–13.89	1.19
TS2	5.50	5.40	21.79
MC2	–21.85	–19.95	–7.28
Products	–9.58	–8.64	–5.26

Table S18. ΔE, ΔH and ΔG for R = O*t*Bu in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–11.34	–10.00	0.77
TS1	0.87	0.65	13.94
C1	–13.56	–11.67	1.41
C2	–25.36	–22.85	–6.47
C3	–14.54	–12.43	2.65
TS2	3.73	3.64	20.03
MC2	–20.96	–19.06	–6.40
Products	–11.98	–11.04	–7.66

Table S19. ΔE, ΔH and ΔG for R = OBn in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–13.08	–11.93	–1.45
TS1	0.66	0.32	12.79
C1	–14.12	–12.24	0.52
C2	–26.20	–23.72	–7.20
C3	–16.28	–14.32	0.36
TS2	3.83	3.84	21.11
MC2	–21.07	–19.24	–6.83
Products	–8.01	–7.20	–4.45

Table S20. ΔE, ΔH and ΔG for R = OBn in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–10.94	–9.79	0.69
TS1	1.09	0.75	13.22
C1	–13.52	–11.64	1.12
C2	–24.67	–22.19	–5.67
C3	–15.34	–13.38	1.31
TS2	3.09	3.11	20.38
MC2	–20.78	–18.95	–6.54
Products	–10.81	–10.00	–7.25

Table S21. ΔE, ΔH and ΔG for R = OFm in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–14.10	–12.73	–2.00
TS1	–0.35	–0.51	13.04
C1	–14.28	–12.34	1.09
C2	–28.44	–25.92	–8.51
C3	–17.50	–15.36	0.15
TS2	5.16	5.30	22.04
MC2	–23.10	–21.01	–7.27
Products	–9.28	–8.26	–4.44

Table S22. ΔE, ΔH and ΔG for R = OFm in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–11.42	–10.05	0.68
TS1	0.47	0.31	13.86
C1	–13.60	–11.67	1.77
C2	–27.03	–24.51	–7.10
C3	–16.06	–13.92	1.59
TS2	3.73	3.87	20.61
MC2	–20.72	–18.63	–4.89
Products	–11.06	–10.04	–6.22

Table S23. ΔE, ΔH and ΔG for R = OPh in gas phase

	Gas phase / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–14.29	–12.97	–2.03
TS1	–0.58	–0.75	12.87
C1	–14.24	–12.29	1.05
C2	–27.30	–24.82	–8.50
C3	–17.65	–15.54	–0.19
TS2	4.68	4.92	21.37
MC2	–20.37	–18.44	–6.04
Products	–7.91	–6.87	–3.30

Table S24. ΔE, ΔH and ΔG for R = OPh in dichloromethane

	Dichloromethane / (kcal mol^{-1})		
	ΔE	ΔH	ΔG
Reagents	0.00	0.00	0.00
MC1	–11.51	–10.19	0.75
TS1	0.32	0.15	13.76
C1	–13.60	–11.66	1.69
C2	–25.64	–23.16	–6.84
C3	–15.90	–13.78	1.57
TS2	3.12	3.36	19.81
MC2	–18.94	–17.01	–4.61
Products	–9.17	–8.12	–4.56

Total energy for all calculations

PBE0/6-31++G(d,p)//B3LYP/6-31G(d)

Table S25. Total energy calculations for R = Ph in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1146.200561	–1145.720824	–1145.834337
MC1	–1146.217589	–1145.735679	–1145.831295
TS1	–1146.194145	–1145.714688	–1145.806954
C1	–1146.217659	–1145.734754	–1145.826425
C2	–1146.222716	–1145.738971	–1145.826669
C3	–1146.215769	–1145.73267	–1145.821707
TS2	–1146.191192	–1145.711684	–1145.797506
MC2	–1146.246376	–1145.763361	–1145.85672
Products	–1146.228323	–1145.746975	–1145.85521

Table S26. Total energy calculations for R = Ph in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1146.217834	–1145.738097	–1145.85161
MC1	–1146.230802	–1145.748892	–1145.844508
TS1	–1146.210569	–1145.731111	–1145.823377
C1	–1146.234042	–1145.751137	–1145.842808
C2	–1146.237213	–1145.753468	–1145.841166
C3	–1146.230811	–1145.747713	–1145.83675
TS2	–1146.210431	–1145.730923	–1145.816745
MC2	–1146.261036	–1145.778021	–1145.87138
Products	–1146.247447	–1145.766099	–1145.874334

Table S27. Total energy calculations for R = Me in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–954.6774998	–954.2540944	–954.3606844
MC1	–954.6943203	–954.2687429	–954.3573989
TS1	–954.6706382	–954.247571	–954.332909
C1	–954.6944524	–954.2680648	–954.3540218
C2	–954.702902	–954.2757449	–954.3561689
C3	–954.691778	–954.2652009	–954.3482009
TS2	–954.6630201	–954.2409792	–954.3201832
MC2	–954.7218309	–954.2949885	–954.3797435
Products	–954.7036406	–954.2786183	–954.3787593

Table S28. Total energy calculations for R = Me in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–954.6947097	–954.2713043	–954.3778943
MC1	–954.7074112	–954.2818338	–954.3704898
TS1	–954.6869308	–954.2638636	–954.3492016
C1	–954.7107113	–954.2843237	–954.3702807
C2	–954.7175271	–954.29037	–954.370794
C3	–954.7075522	–954.2809751	–954.3639751
TS2	–954.6830655	–954.2610246	–954.3402286
MC2	–954.7356556	–954.3088132	–954.3935682
Products	–954.7229003	–954.297878	–954.398019

Table S29. Total energy calculations for R = O*t*Bu in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1147.64279	–1147.12485	–1147.241893
MC1	–1147.659586	–1147.139512	–1147.239389
TS1	–1147.63628	–1147.118691	–1147.214555
C1	–1147.659732	–1147.138786	–1147.234987
C2	–1147.67165	–1147.149702	–1147.240654
C3	–1147.657872	–1147.136568	–1147.22958
TS2	–1147.623279	–1147.105488	–1147.196412
MC2	–1147.669766	–1147.148796	–1147.245663
Products	–1147.656688	–1147.137254	–1147.248904

Table S30. Total energy calculations for R = O*t*Bu in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1147.657731	–1147.139791	–1147.256834
MC1	–1147.670349	–1147.150275	–1147.250152
TS1	–1147.649988	–1147.132398	–1147.228262
C1	–1147.673758	–1147.152811	–1147.249012
C2	–1147.684338	–1147.16239	–1147.253342
C3	–1147.670485	–1147.149182	–1147.242194
TS2	–1147.641036	–1147.123244	–1147.214168
MC2	–1147.683298	–1147.162328	–1147.259195
Products	–1147.675452	–1147.156019	–1147.267669

Table S31. Total energy calculations for R = OBn in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1260.622085	–1260.106392	–1260.226933
MC1	–1260.63829	–1260.120762	–1260.224613
TS1	–1260.615419	–1260.100274	–1260.200939
C1	–1260.63908	–1260.120388	–1260.220588
C2	–1260.651028	–1260.131375	–1260.225599
C3	–1260.637157	–1260.11833	–1260.215473
TS2	–1260.603554	–1260.087836	–1260.180855
MC2	–1260.648289	–1260.129678	–1260.230449
Products	–1260.634334	–1260.117345	–1260.233505

Table S32. Total energy calculations for R = OBn in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1260.638987	–1260.123295	–1260.243836
MC1	–1260.65178	–1260.134252	–1260.238103
TS1	–1260.631643	–1260.116498	–1260.217163
C1	–1260.655026	–1260.136334	–1260.236534
C2	–1260.665488	–1260.145835	–1260.240059
C3	–1260.652561	–1260.133734	–1260.230877
TS2	–1260.621628	–1260.10591	–1260.198929
MC2	–1260.664722	–1260.146111	–1260.246882
Products	–1260.655695	–1260.138706	–1260.254866

Table S33. Total energy calculations for R = OFm in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1529.498091	–1528.890044	–1529.021676
MC1	–1529.515129	–1528.904899	–1529.019428
TS1	–1529.492249	–1528.884463	–1528.994501
C1	–1529.515254	–1528.904119	–1529.014347
C2	–1529.526865	–1528.914793	–1529.018689
C3	–1529.513867	–1528.902401	–1529.009327
TS2	–1529.480224	–1528.871962	–1528.976918
MC2	–1529.525848	–1528.914461	–1529.024198
Products	–1529.511639	–1528.901972	–1529.02752

Table S34. Total energy calculations for R = OFm in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1529.517351	–1528.909305	–1529.040937
MC1	–1529.530111	–1528.919881	–1529.03441
TS1	–1529.510204	–1528.902419	–1529.012457
C1	–1529.533442	–1528.922307	–1529.032535
C2	–1529.543876	–1528.931804	–1529.0357
C3	–1529.530833	–1528.919367	–1529.026293
TS2	–1529.501766	–1528.893505	–1528.998461
MC2	–1529.541314	–1528.929927	–1529.039664
Products	–1529.533732	–1528.924065	–1529.049613

Table S35. Total energy calculations for R = OPh in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1221.351604	–1220.866714	–1220.983843
MC1	–1221.369019	–1220.882022	–1220.981719
TS1	–1221.346412	–1220.86179	–1220.957226
C1	–1221.368741	–1220.880744	–1220.976611
C2	–1221.381149	–1220.892307	–1220.983427
C3	–1221.367854	–1220.879598	–1220.972266
TS2	–1221.334318	–1220.849049	–1220.939956
MC2	–1221.378382	–1220.890402	–1220.98777
Products	–1221.362968	–1220.876416	–1220.987858

Table S36. Total energy calculations for R = OPh in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1221.36864	–1220.883749	–1221.000878
MC1	–1221.381624	–1220.894627	–1220.994324
TS1	–1221.36202	–1220.877398	–1220.972834
C1	–1221.384768	–1220.896771	–1220.992638
C2	–1221.395538	–1220.906696	–1220.997816
C3	–1221.382088	–1220.893831	–1220.986499
TS2	–1221.353833	–1220.868564	–1220.959471
MC2	–1221.393138	–1220.905158	–1221.002526
Products	–1221.381999	–1220.895448	–1221.00689

PBE0-D3/6-31++G(d,p)//B3LYP/6-31G(d)

Table S37. Total energy calculations for R = Ph in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1146.225384	–1145.745647	–1145.85916
MC1	–1146.2478	–1145.76589	–1145.861506
TS1	–1146.225576	–1145.746119	–1145.838385
C1	–1146.24808	–1145.765175	–1145.856846
C2	–1146.259935	–1145.77619	–1145.863888
C3	–1146.253108	–1145.77001	–1145.859047
TS2	–1146.227915	–1145.748407	–1145.834229
MC2	–1146.278439	–1145.795424	–1145.888783
Products	–1146.254263	–1145.772915	–1145.88115

Table S38. Total energy calculations for R = Ph in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1146.242656	–1145.762919	–1145.876432
MC1	–1146.261012	–1145.779102	–1145.874718
TS1	–1146.242	–1145.762543	–1145.854809
C1	–1146.264463	–1145.781558	–1145.873229
C2	–1146.274432	–1145.790687	–1145.878385
C3	–1146.268151	–1145.785052	–1145.874089
TS2	–1146.247154	–1145.767646	–1145.853468
MC2	–1146.293099	–1145.810084	–1145.903443
Products	–1146.273387	–1145.792039	–1145.900274

Table S39. Total energy calculations for R = Me in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–954.697728	–954.2743226	–954.3809126
MC1	–954.7198755	–954.2942981	–954.3829541
TS1	–954.6971272	–954.27406	–954.359398
C1	–954.7202168	–954.2938292	–954.3797862
C2	–954.7347157	–954.3075586	–954.3879826
C3	–954.7226526	–954.2960755	–954.3790755
TS2	–954.6924874	–954.2704465	–954.3496505
MC2	–954.747595	–954.3207526	–954.4055076
Products	–954.7252221	–954.3001998	–954.4003408

Table S40. Total energy calculations for R = Me in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–954.7149379	–954.2915325	–954.3981225
MC1	–954.7329664	–954.307389	–954.396045
TS1	–954.7134198	–954.2903526	–954.3756906
C1	–954.7364758	–954.3100882	–954.3960452
C2	–954.7493408	–954.3221837	–954.4026077
C3	–954.7384268	–954.3118497	–954.3948497
TS2	–954.7125328	–954.2904919	–954.3696959
MC2	–954.7614198	–954.3345774	–954.4193324
Products	–954.7444818	–954.3194595	–954.4196005

Table S41. Total energy calculations for R = O*t*Bu in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1147.670979	–1147.153039	–1147.270082
MC1	–1147.69323	–1147.173155	–1147.273032
TS1	–1147.670823	–1147.153234	–1147.249098
C1	–1147.693501	–1147.172554	–1147.268755
C2	–1147.713646	–1147.191698	–1147.28265
C3	–1147.696473	–1147.175169	–1147.268181
TS2	–1147.662221	–1147.14443	–1147.235354
MC2	–1147.705793	–1147.184824	–1147.281691
Products	–1147.686246	–1147.166813	–1147.278463

Table S42. Total energy calculations for R = O*t*Bu in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1147.685919	–1147.16798	–1147.285023
MC1	–1147.703993	–1147.183919	–1147.283796
TS1	–1147.684531	–1147.166941	–1147.262805
C1	–1147.707526	–1147.18658	–1147.282781
C2	–1147.726334	–1147.204386	–1147.295338
C3	–1147.709086	–1147.187783	–1147.280795
TS2	–1147.679978	–1147.162187	–1147.253111
MC2	–1147.719325	–1147.198356	–1147.295223
Products	–1147.705011	–1147.185577	–1147.297227

Table S43. Total energy calculations for R = OBn in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1260.649428	–1260.133735	–1260.254276
MC1	–1260.670271	–1260.152743	–1260.256594
TS1	–1260.648368	–1260.133223	–1260.233888
C1	–1260.671932	–1260.153241	–1260.253441
C2	–1260.691186	–1260.171532	–1260.265756
C3	–1260.675379	–1260.156552	–1260.253695
TS2	–1260.643328	–1260.127609	–1260.220628
MC2	–1260.683008	–1260.164397	–1260.265168
Products	–1260.662199	–1260.14521	–1260.26137

Table S44. Total energy calculations for R = OBn in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1260.66633	–1260.150638	–1260.271179
MC1	–1260.683761	–1260.166233	–1260.270084
TS1	–1260.664591	–1260.149446	–1260.250111
C1	–1260.687878	–1260.169187	–1260.269387
C2	–1260.705646	–1260.185992	–1260.280216
C3	–1260.690783	–1260.171956	–1260.269099
TS2	–1260.661402	–1260.145683	–1260.238702
MC2	–1260.699441	–1260.18083	–1260.281601
Products	–1260.683559	–1260.16657	–1260.28273

Table S45. Total energy calculations for R = OFm in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	-1529.533776	-1528.925729	-1529.057361
MC1	-1529.556251	-1528.946021	-1529.06055
TS1	-1529.534332	-1528.926546	-1529.036584
C1	-1529.556528	-1528.945392	-1529.05562
C2	-1529.579103	-1528.96703	-1529.070926
C3	-1529.561666	-1528.9502	-1529.057126
TS2	-1529.525546	-1528.917284	-1529.02224
MC2	-1529.570593	-1528.959206	-1529.068943
Products	-1529.548561	-1528.938893	-1529.064441

Table S46. Total energy calculations for R = OFm in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1529.553036	–1528.944989	–1529.076621
MC1	–1529.571233	–1528.961002	–1529.075531
TS1	–1529.552287	–1528.944502	–1529.05454
C1	–1529.574715	–1528.96358	–1529.073808
C2	–1529.596114	–1528.984041	–1529.087937
C3	–1529.578632	–1528.967166	–1529.074092
TS2	–1529.547089	–1528.938827	–1529.043783
MC2	–1529.586059	–1528.974672	–1529.084409
Products	–1529.570654	–1528.960986	–1529.086534

Table S47. Total energy calculations for R = OPh in gas phase

	Gas phase / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1221.376742	–1220.891851	–1221.00898
MC1	–1221.399513	–1220.912516	–1221.012213
TS1	–1221.377662	–1220.89304	–1220.988476
C1	–1221.399431	–1220.911434	–1221.007301
C2	–1221.420245	–1220.931403	–1221.022523
C3	–1221.404876	–1220.916619	–1221.009287
TS2	–1221.369287	–1220.884018	–1220.974925
MC2	–1221.409212	–1220.921232	–1221.0186
Products	–1221.389354	–1220.902803	–1221.014245

Table S48. Total energy calculations for R = OPh in dichloromethane

	Dichloromethane / Hartree		
	Electronic energy	Enthalpy	Gibbs free energy
Reagents	–1221.393778	–1220.908887	–1221.026016
MC1	–1221.412118	–1220.925121	–1221.024818
TS1	–1221.39327	–1220.908648	–1221.004084
C1	–1221.415458	–1220.927461	–1221.023328
C2	–1221.434634	–1220.945792	–1221.036912
C3	–1221.419109	–1220.930853	–1221.023521
TS2	–1221.388801	–1220.903533	–1220.99444
MC2	–1221.423967	–1220.935987	–1221.033355
Products	–1221.408385	–1220.921834	–1221.033276

Z-Matrix or cartesian

R = Ph

N-protected alanine

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.87599	0.53419	-0.6211
N	-2.70334	0.74478	0.0514
C	-1.72773	1.7001	-0.44533
C	-0.37203	1.2985	0.12098
O	0.59907	2.14272	-0.32459
O	-0.19018	0.38354	0.88833
H	-2.33423	0.0383	0.67607
O	-4.19229	1.21151	-1.59854
C	-4.75937	-0.56397	-0.09834
C	-5.75758	-1.04576	-0.95554
C	-4.64267	-1.10567	1.1896
C	-6.60967	-2.06679	-0.54207
H	-5.84518	-0.60141	-1.94145
C	-5.50072	-2.12386	1.60524
H	-3.9055	-0.71744	1.88713
C	-6.48156	-2.61001	0.73885
H	-7.37578	-2.43864	-1.21713
H	-5.40677	-2.53225	2.60779
H	-7.14799	-3.40486	1.06326
C	-2.09834	3.15216	-0.09008
H	-2.14786	3.28449	0.99611
H	-1.36546	3.84979	-0.50457
H	-3.07897	3.37125	-0.51791
H	-1.67043	1.62211	-1.53931
H	1.51516	1.89156	-0.18567

EDC

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.05988	1.63028	-0.12462
N	0.8298	0.79877	-0.6776
C	2.26814	0.79569	-0.45951
C	2.76104	-0.65439	-0.3617
C	4.26967	-0.73222	-0.10902
N	4.81431	-2.08636	-0.21443
C	6.26995	-2.06566	-0.24295
H	6.65009	-3.08278	-0.38984
H	6.72367	-1.66499	0.68655
H	6.61644	-1.44993	-1.08042
C	4.33217	-2.97299	0.83674
H	4.60719	-2.62907	1.85495
H	3.24374	-3.06519	0.792
H	4.75734	-3.97209	0.69203
H	4.78281	-0.12059	-0.86367
H	4.50791	-0.27549	0.87606
H	2.19714	-1.14645	0.43868
H	2.52076	-1.18025	-1.29265
H	2.77243	1.2873	-1.30515
H	2.55944	1.34259	0.45124
N	-0.70946	2.46117	0.42795
C	0.37663	3.41118	0.17324
H	1.11392	3.3772	0.98605
H	0.88956	3.10825	-0.74311
C	-0.16201	4.83393	0.02077
H	0.66209	5.53814	-0.1351
H	-0.70025	5.15148	0.92258
H	-0.84552	4.90795	-0.83187

Molecular complex 1 (MC1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.1379	-1.66928	-0.1025
N	1.81345	-1.45625	0.15607
C	0.8452	-2.5322	0.03042
C	-0.51883	-1.89803	-0.22201
O	-1.46472	-2.80871	-0.43309
O	-0.70728	-0.69103	-0.22333
H	1.41971	-0.52397	0.11338

O	3.58021	-2.78961	-0.35601
C	0.82547	-3.45158	1.26513
H	0.55838	-2.88582	2.16421
H	0.10487	-4.26208	1.12616
H	1.82232	-3.87808	1.39874
H	1.1023	-3.1445	-0.84377
H	-2.34332	-2.34663	-0.5821
C	-3.98607	-0.42841	-1.04792
N	-3.96772	-1.61452	-0.68814
C	-5.08517	-2.27421	0.01005
C	-4.70066	-2.63287	1.44511
H	-3.79833	-3.2529	1.46081
H	-4.50484	-1.73113	2.0351
H	-5.98034	-1.64014	-0.00324
H	-5.32111	-3.18542	-0.55103
N	-3.9573	0.66911	-1.56426
C	-3.47841	1.9549	-1.06638
H	-2.63814	2.25589	-1.69887
H	-4.27584	2.68698	-1.24286
C	-3.05257	1.95421	0.40388
H	-2.31562	1.15852	0.55695
H	-3.91701	1.71221	1.03727
C	4.03022	-0.45917	-0.05676
C	5.28029	-0.55919	-0.68147
C	3.68116	0.73586	0.58791
C	6.15677	0.52319	-0.6835
H	5.54155	-1.49881	-1.15698
C	4.5625	1.81719	0.59187
H	2.73631	0.81972	1.11789
C	5.79875	1.71529	-0.04864
H	7.12099	0.43764	-1.17744
H	4.28612	2.73632	1.10154
H	6.4836	2.55922	-0.04648
H	-5.51168	-3.19094	1.92616
C	-2.49824	3.31381	0.84928
H	-3.28947	4.06795	0.74529
H	-2.25148	3.26652	1.92989
C	-1.0882	5.18419	0.27583
H	-0.27449	5.51072	-0.38085
H	-1.97801	5.77561	0.03377

H	-0.79603	5.41595	1.31967
C	-0.1564	2.9718	0.28382
H	-0.33376	1.92212	0.03548
H	0.64907	3.33758	-0.36194
H	0.1963	3.02486	1.33424
N	-1.357	3.76945	0.054

Transition state 1 (TS1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.4377	-1.0231	0.4765
N	2.07691	-1.06844	0.40746
C	1.34268	-2.30528	0.63479
C	-0.02609	-2.21719	-0.0577
O	-0.7662	-3.23602	0.00927
O	-0.32898	-1.12656	-0.64628
H	1.56417	-0.37455	-0.12253
O	4.1141	-1.98871	0.83186
C	1.18253	-2.62382	2.12978
H	0.64702	-1.81599	2.64149
H	0.62154	-3.55407	2.25285
H	2.17069	-2.73365	2.58345
H	1.89124	-3.13387	0.16848
H	-2.02082	-2.74394	-0.67655
C	-2.2938	-0.95357	-1.51987
N	-2.76542	-2.08651	-1.12621
C	-4.21201	-2.32016	-0.94814
C	-4.62352	-2.27727	0.5228
H	-4.04885	-3.00156	1.10888
H	-4.45633	-1.2823	0.94891
H	-4.75571	-1.57579	-1.53726
H	-4.42623	-3.30309	-1.38047
N	-2.30087	0.06869	-2.15169
C	-1.71749	1.39165	-2.01396
H	-0.65989	1.29179	-2.28029
H	-2.18724	2.03277	-2.76723
C	-1.85209	1.99724	-0.61232
H	-1.37167	1.31338	0.09511
H	-1.28695	2.93735	-0.59376
C	4.08011	0.28601	0.09676

C	5.4416	0.2632	-0.23216
C	3.39462	1.5087	0.08081
C	6.10098	1.43546	-0.59458
H	5.96097	-0.68863	-0.19182
C	4.05689	2.68425	-0.27448
H	2.35073	1.55484	0.37917
C	5.40938	2.64934	-0.61875
H	7.15573	1.40472	-0.85489
H	3.51894	3.62877	-0.27362
H	5.92412	3.56545	-0.89659
H	-5.68722	-2.52106	0.62158
C	-3.30241	2.29674	-0.21609
H	-3.89703	1.35882	-0.21914
H	-3.74366	2.94345	-0.98569
C	-3.06794	2.15602	2.19919
H	-2.03573	1.80446	2.12026
H	-3.14994	2.73975	3.12182
H	-3.72698	1.26874	2.29696
C	-4.74574	3.56993	1.23197
H	-4.78223	4.14011	2.16632
H	-4.96455	4.25637	0.40686
H	-5.55012	2.80784	1.26733
N	-3.41601	2.99788	1.06106

Activated amino acid – conformation 1 (C1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C							
N	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
O	4	B4	3	A3	2	D2	0
C	5	B5	4	A4	3	D3	0
N	6	B6	5	A5	4	D4	0
C	7	B7	6	A6	5	D5	0
C	8	B8	7	A7	6	D6	0
C	9	B9	8	A8	7	D7	0
N	10	B10	9	A9	8	D8	0
C	11	B11	10	A10	9	D9	0

H 12 B12 11 A11 10 D10 0
H 12 B13 11 A12 10 D11 0
H 12 B14 11 A13 10 D12 0
C 11 B15 10 A14 9 D13 0
H 16 B16 11 A15 10 D14 0
H 16 B17 11 A16 10 D15 0
H 16 B18 11 A17 10 D16 0
H 10 B19 9 A18 8 D17 0
H 10 B20 9 A19 8 D18 0
H 9 B21 8 A20 7 D19 0
H 9 B22 8 A21 7 D20 0
H 8 B23 7 A22 6 D21 0
H 8 B24 7 A23 6 D22 0
N 6 B25 5 A24 4 D23 0
H 26 B26 6 A25 5 D24 0
C 26 B27 6 A26 5 D25 0
H 28 B28 26 A27 6 D26 0
H 28 B29 26 A28 6 D27 0
C 28 B30 26 A29 6 D28 0
H 31 B31 28 A30 26 D29 0
H 31 B32 28 A31 26 D30 0
H 31 B33 28 A32 26 D31 0
O 4 B34 3 A33 2 D32 0
H 2 B35 1 A34 3 D33 0
O 1 B36 2 A35 3 D34 0
C 1 B37 37 A36 2 D35 0
C 38 B38 1 A37 37 D36 0
C 38 B39 1 A38 37 D37 0
C 39 B40 38 A39 1 D38 0
H 39 B41 38 A40 1 D39 0
C 40 B42 38 A41 1 D40 0
H 40 B43 38 A42 1 D41 0
C 43 B44 40 A43 38 D42 0
H 41 B45 39 A44 38 D43 0
H 43 B46 40 A45 38 D44 0
H 45 B47 43 A46 40 D45 0
C 3 B48 2 A47 1 D46 0
H 49 B49 3 A48 2 D47 0
H 49 B50 3 A49 2 D48 0
H 49 B51 3 A50 2 D49 0

H	3	B52	2	A51	1	D50	0

Variables:

B1	1.34416
B2	1.44983
B3	1.5055
B4	1.36168
B5	1.4055
B6	1.2493
B7	1.45601
B8	1.52808
B9	1.52819
B10	1.45958
B11	1.45484
B12	1.08218
B13	1.09379
B14	1.0821
B15	1.45552
B16	1.09396
B17	1.07948
B18	1.08204
B19	1.08501
B20	1.09679
B21	1.08275
B22	1.08268
B23	1.08593
B24	1.08628
B25	1.36091
B26	0.99188
B27	1.45785
B28	1.08348
B29	1.08172
B30	1.52544
B31	1.08308
B32	1.08477
B33	1.08316
B34	1.20582
B35	0.99331
B36	1.22922
B37	1.52
B38	1.39516

B39	1.39483
B40	1.39471
B41	1.09966
B42	1.39514
B43	1.0996
B44	1.39483
B45	1.09968
B46	1.09976
B47	1.09968
B48	1.54
B49	1.07
B50	1.07
B51	1.07
B52	1.07
A1	122.0968
A2	107.08537
A3	111.6537
A4	123.30182
A5	117.51614
A6	128.1747
A7	108.80449
A8	111.89498
A9	113.30634
A10	113.74745
A11	109.62514
A12	113.0679
A13	109.86639
A14	115.27395
A15	112.68364
A16	110.68868
A17	109.34908
A18	108.61681
A19	109.81924
A20	107.91934
A21	109.17287
A22	109.58914
A23	112.08591
A24	107.94364
A25	115.18133
A26	126.75817

A27	110.96404
A28	109.06578
A29	109.84607
A30	110.34895
A31	111.01995
A32	110.87935
A33	125.21785
A34	118.65395
A35	124.22241
A36	124.71291
A37	119.99722
A38	120.00432
A39	120.00863
A40	119.98077
A41	120.00002
A42	120.008
A43	120.0047
A44	120.01279
A45	119.98395
A46	120.02486
A47	108.62389
A48	109.4712
A49	109.4712
A50	109.47123
A51	112.15936
D1	153.31462
D2	-158.32945
D3	-153.7833
D4	49.92681
D5	-173.50503
D6	149.08332
D7	-178.79007
D8	-171.84204
D9	161.45764
D10	-172.30607
D11	67.09486
D12	-53.87692
D13	-65.46322
D14	-64.2869
D15	57.11733

D16	175.4841
D17	-52.94552
D18	63.25704
D19	-55.91637
D20	60.26433
D21	-91.37891
D22	27.79737
D23	-132.76587
D24	10.77511
D25	-161.44214
D26	-86.18831
D27	32.27061
D28	152.4083
D29	179.32866
D30	60.03984
D31	-60.60292
D32	19.0521
D33	177.19768
D34	0.64693
D35	179.86379
D36	0.08503
D37	-179.92024
D38	-179.97293
D39	-0.05203
D40	-179.97984
D41	-0.00555
D42	-0.03761
D43	179.96185
D44	179.97501
D45	-179.95633
D46	36.63931
D47	52.94095
D48	172.94096
D49	-67.05904
D50	-82.54427

Activated amino acid – conformation 2 (C2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	4.76716	0.49878	0.79983
N	3.51865	-0.07166	0.80918
C	2.78673	-0.6675	-0.29188
C	1.29826	-0.41303	-0.06516
O	0.61195	-0.53932	-1.22403
C	-0.80634	-0.55108	-1.11536
N	-1.33913	-1.69816	-1.03215
C	-2.79059	-1.80398	-1.04515
C	-3.37752	-2.0111	0.36331
C	-3.06878	-0.89481	1.36732
N	-3.47054	0.45798	0.93679
C	-2.95334	1.45339	1.87879
H	-3.21318	2.46019	1.53326
H	-1.86327	1.3723	1.93431
H	-3.36244	1.32591	2.89784
C	-4.9192	0.59487	0.79025
H	-5.29197	-0.08929	0.02361
H	-5.46129	0.389	1.73209
H	-5.15883	1.61589	0.47539
H	-3.54129	-1.14445	2.33683
H	-1.98713	-0.8666	1.53619
H	-4.46011	-2.16755	0.26912
H	-2.96722	-2.93847	0.78167
H	-3.27334	-0.93949	-1.52742
H	-3.04807	-2.68586	-1.64539
N	-1.36873	0.69239	-1.19015
H	-2.24837	0.76021	-0.66134
C	-0.60291	1.93152	-1.31167
H	-0.08724	2.17722	-0.37073
H	0.16719	1.78876	-2.07531
C	-1.52181	3.08284	-1.71565
H	-0.94772	4.01043	-1.81224
H	-2.30191	3.25131	-0.96369
H	-2.01119	2.87388	-2.67252
O	0.80065	-0.17568	1.01273
H	3.034	-0.03542	1.69946
O	5.25215	0.96948	1.8197
C	3.01299	-2.19029	-0.42676
H	4.07286	-2.39353	-0.60707
H	2.71869	-2.69786	0.49738

H	2.42554	-2.59794	-1.25479
H	3.06819	-0.18148	-1.23068
C	5.5104	0.53147	-0.54856
C	6.39937	-0.49157	-0.87961
C	5.29366	1.58262	-1.43925
C	7.072	-0.46283	-2.1012
H	6.56977	-1.32045	-0.17742
C	5.96695	1.61166	-2.66115
H	4.59251	2.3887	-1.17865
C	6.85605	0.58907	-2.99185
H	7.77281	-1.26898	-2.3622
H	5.79595	2.44058	-3.36325
H	7.38684	0.61168	-3.95478

Activated amino acid – conformation 3 (C3)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.67972	1.64331	0.04197
C	2.84208	0.22747	-1.52517
H	2.58137	-0.3301	-2.46531
O	2.65521	1.69014	0.83405
N	1.59719	0.90797	-1.15534
C	3.26471	-0.91001	-0.533
O	4.40752	-1.06237	-0.16454
C	4.01049	1.15653	-1.86669
H	3.69848	1.85462	-2.6608
H	4.30559	1.72364	-0.9667
H	4.88763	0.5775	-2.21033
C	0.42623	2.42347	0.37628
C	0.26813	2.80374	1.71342
C	-0.53523	2.78835	-0.5667
C	-0.84996	3.53291	2.10554
H	1.03897	2.52459	2.41837
C	-1.65512	3.52654	-0.18373
H	-0.37887	2.5157	-1.61184
C	-1.8115	3.8932	1.15413
H	-0.97425	3.82942	3.14336
H	-2.38208	3.8313	-0.92444
H	-2.68351	4.47313	1.45472

O	2.34804	-1.46624	0.18384
H	0.88399	0.14879	-1.18687
C	1.0679	-1.78061	-0.20632
N	0.39613	-1.06182	-1.03717
N	0.65823	-2.90109	0.41651
H	-0.34248	-3.06764	0.38752
C	-0.94767	-1.45787	-1.47443
H	-1.09432	-0.99979	-2.46325
H	-0.99556	-2.5481	-1.6382
C	-2.06932	-0.99029	-0.52493
H	-1.94944	0.08957	-0.37584
C	1.41017	-3.65249	1.44237
H	1.05957	-4.67949	1.38455
H	2.46031	-3.63931	1.15654
C	1.22542	-3.08531	2.85101
H	1.78012	-3.69797	3.5693
H	1.61386	-2.05947	2.91587
H	0.17407	-3.07966	3.15147
C	-3.46135	-1.32194	-1.06541
H	-3.61121	-0.81108	-2.04541
H	-3.51585	-2.40139	-1.269
H	-1.95467	-1.46094	0.46525
N	-4.53109	-1.00819	-0.12647
C	-5.78318	-1.64402	-0.50154
H	-6.54812	-1.4415	0.26301
H	-6.18746	-1.29047	-1.4751
H	-5.64743	-2.73084	-0.56081
C	-4.72254	0.43135	0.05468
H	-5.03346	0.94244	-0.88172
H	-5.50883	0.60544	0.80472
H	-3.80949	0.90511	0.41241

Transition state 2 (TS2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.65966	1.60392	0.07567
C	3.07492	0.55186	-1.36257
H	2.99789	-0.12361	-2.21204
O	2.41916	1.30647	1.00429

N	1.82789	1.21641	-1.17428
C	3.47836	-0.37005	-0.22111
O	4.38564	-0.72466	0.35474
C	4.26018	1.5009	-1.58741
H	4.02368	2.12076	-2.44273
H	4.40014	2.13584	-0.72319
H	5.18189	0.9635	-1.78541
C	0.4156	2.3962	0.37346
C	0.05087	2.60529	1.69765
C	-0.37656	2.92366	-0.64161
C	-1.09654	3.31834	2.00548
H	0.67684	2.20614	2.4724
C	-1.52124	3.64056	-0.33472
H	-0.08127	2.77456	-1.66247
C	-1.88453	3.83648	0.98971
H	-1.37203	3.47403	3.03363
H	-2.12456	4.05216	-1.12482
H	-2.77222	4.39617	1.22776
O	2.23955	-1.56967	0.01957
H	0.70186	-0.241	-1.32731
C	1.0734	-1.89736	-0.32328
N	0.33271	-1.17052	-1.14353
N	0.61194	-3.06103	0.15278
H	-0.34863	-3.2731	0.01851
C	-1.03064	-1.45151	-1.55951
H	-1.17633	-0.91534	-2.48878
H	-1.12733	-2.50503	-1.80225
C	-2.08505	-1.01499	-0.539
H	-1.91212	0.02847	-0.30616
C	1.34988	-3.88129	1.10909
H	0.97428	-4.89159	1.00049
H	2.38766	-3.88496	0.81536
C	1.20217	-3.40502	2.54943
H	1.7487	-4.06412	3.21662
H	1.59654	-2.40276	2.66261
H	0.16053	-3.4043	2.856
C	-3.50236	-1.23571	-1.06686
H	-3.67261	-0.59577	-1.94027
H	-3.58536	-2.261	-1.41683
H	-1.97099	-1.56748	0.38925

N	-4.5233	-1.04111	-0.05509
C	-5.80061	-1.5729	-0.481
H	-6.5225	-1.474	0.32117
H	-6.20393	-1.06543	-1.36259
H	-5.70477	-2.62745	-0.71366
C	-4.65132	0.33911	0.37018
H	-4.94164	1.00635	-0.4471
H	-5.40701	0.40677	1.14383
H	-3.72337	0.70379	0.78838

Molecular complex 2 (MC2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.67972	1.50331	-0.13803
C	2.94208	0.44747	-1.60517
H	2.78137	-0.4301	-2.28531
O	2.51521	0.99014	0.75405
N	1.73719	1.22797	-1.43534
C	3.44471	-0.13001	-0.253
O	4.44752	-0.58237	0.15546
C	4.11049	1.31653	-2.12669
H	3.79848	1.77462	-3.0808
H	4.32559	2.12364	-1.4067
H	5.00763	0.7175	-2.29033
C	0.54623	2.36347	0.33628
C	0.38813	2.68374	1.69342
C	-0.41523	2.82835	-0.5867
C	-0.70996	3.43291	2.12554
H	1.13897	2.32459	2.39837
C	-1.51512	3.56654	-0.14373
H	-0.27887	2.5957	-1.63184
C	-1.6715	3.8732	1.21413
H	-0.81425	3.66942	3.18336
H	-2.26208	3.9113	-0.86444
H	-2.52351	4.45312	1.55472
O	2.16804	-1.44624	0.26384
H	0.52399	-0.45121	-1.34687
C	1.0479	-1.86061	-0.10632
N	0.27613	-1.26182	-1.05717

N	0.57823	-3.02109	0.43651
H	-0.40248	-3.22764	0.34752
C	-1.06767	-1.61787	-1.47443
H	-1.19432	-1.21979	-2.48325
H	-1.13556	-2.7081	-1.5582
C	-2.14932	-1.05029	-0.54493
H	-1.98944	0.02957	-0.45584
C	1.33017	-3.71249	1.48237
H	0.97957	-4.75949	1.48455
H	2.38031	-3.71931	1.17654
C	1.18542	-3.08531	2.87101
H	1.76012	-3.65797	3.6093
H	1.55386	-2.05947	2.85587
H	0.13407	-3.07966	3.19147
C	-3.56135	-1.36194	-1.06541
H	-3.71121	-0.87108	-2.04541
H	-3.63585	-2.44139	-1.249
H	-2.05467	-1.46094	0.46525
N	-4.61109	-1.00819	-0.10647
C	-5.88318	-1.62402	-0.48154
H	-6.62812	-1.4015	0.28301
H	-6.26746	-1.27047	-1.4551
H	-5.76743	-2.71084	-0.54081
C	-4.76254	0.43135	0.05468
H	-5.05346	0.94244	-0.88172
H	-5.52883	0.62544	0.80472
H	-3.82949	0.88511	0.41241

Azlactone

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.00774	-0.17968	1.10242
C	-2.32423	-0.11946	1.1013
H	-2.93759	0.12361	2.00441
O	-0.4188	-1.56036	1.10242
N	-1.07122	0.65259	1.10212
C	-1.85076	-1.58487	1.10241
O	-2.60185	-2.59454	1.10319
C	-3.16638	0.21409	-0.14414

H	-4.13705	-0.22541	-0.04651
H	-3.26311	1.2758	-0.2354
H	-2.6841	-0.17635	-1.01584
C	1.48977	0.23889	1.10282
C	2.48943	-0.73432	1.10309
C	1.83271	1.5909	1.1028
C	3.83172	-0.35551	1.10402
H	2.21873	-1.80014	1.10388
C	3.17536	1.96999	1.10274
H	1.04495	2.35807	1.10241
C	4.17484	0.99707	1.10348
H	4.61972	-1.12255	1.10486
H	3.44546	3.03607	1.10231
H	5.23325	1.29551	1.10416

EDC urea

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.85699	1.87359	-0.07493
N	2.33985	0.69579	-0.76928
C	3.63811	0.0989	-0.496
C	3.50873	-1.42982	-0.53216
C	4.84096	-2.12562	-0.23717
N	4.81093	-3.57174	-0.45901
C	6.15387	-4.13383	-0.4358
H	6.10951	-5.20346	-0.66921
H	6.66234	-4.02113	0.54365
H	6.7741	-3.64625	-1.19614
C	3.94371	-4.27021	0.48096
H	4.25979	-4.14736	1.53726
H	2.91411	-3.91399	0.39086
H	3.94705	-5.34112	0.25059
H	5.60673	-1.71413	-0.90891
H	5.17004	-1.88169	0.79626
H	2.73948	-1.71886	0.19273
H	3.14884	-1.73764	-1.52035
H	4.36005	0.41335	-1.26471
H	4.04937	0.40779	0.47789
N	2.48077	2.8484	0.79864

H	1.83616	3.52196	1.18946
C	3.8736	3.29197	0.69912
H	4.46844	2.87815	1.52391
H	4.29336	2.90159	-0.23175
C	3.96452	4.81805	0.70986
H	5.01121	5.137	0.66628
H	3.53173	5.23332	1.62858
H	3.43569	5.25094	-0.14607
O	0.65615	2.20281	-0.25702
H	1.75634	0.27646	-1.46475

R = Me

N-Protected alanine

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-4.7399	-1.9254	-0.22034
N	-3.70175	-1.23954	0.34107
C	-3.22965	0.01385	-0.21984
C	-1.8001	0.2197	0.26356
O	-1.26672	1.34018	-0.29952
O	-1.23646	-0.48306	1.06764
H	-3.09736	-1.67261	1.02792
O	-5.39361	-1.47516	-1.15597
C	-4.13575	1.20422	0.15085
H	-4.17121	1.3399	1.23731
H	-3.77338	2.12517	-0.31449
H	-5.14378	0.99456	-0.21326
H	-3.20926	-0.07026	-1.31382
C	-5.03811	-3.28368	0.39702
H	-6.08638	-3.30678	0.70955
H	-4.90945	-4.05479	-0.36931
H	-4.40385	-3.52575	1.25533
H	-0.32163	1.48585	-0.21485

Molecular complex 1 (MC1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C

N 1 B1

C 2 B2 1 A1

C 3 B3 2 A2 1 D1 0

O 4 B4 3 A3 2 D2 0

O 4 B5 3 A4 2 D3 0

H 2 B6 1 A5 3 D4 0

O 1 B7 2 A6 3 D5 0

C 3 B8 2 A7 1 D6 0

H 9 B9 3 A8 2 D7 0

H 9 B10 3 A9 2 D8 0

H 9 B11 3 A10 2 D9 0

H 3 B12 2 A11 1 D10 0

C 1 B13 8 A12 2 D11 0

H 14 B14 1 A13 8 D12 0

H 14 B15 1 A14 8 D13 0

H 14 B16 1 A15 8 D14 0

H 5 B17 4 A16 3 D15 0

C 6 B18 4 A17 3 D16 0

N 19 B19 6 A18 4 D17 0

C 20 B20 19 A19 6 D18 0

C 21 B21 20 A20 19 D19 0

C 22 B22 21 A21 20 D20 0

N 23 B23 22 A22 21 D21 0

C 24 B24 23 A23 22 D22 0

H 25 B25 24 A24 23 D23 0

H 25 B26 24 A25 23 D24 0

H 25 B27 24 A26 23 D25 0

C 24 B28 23 A27 22 D26 0

H 29 B29 24 A28 23 D27 0

H 29 B30 24 A29 23 D28 0

H 29 B31 24 A30 23 D29 0

H 23 B32 22 A31 21 D30 0

H 23 B33 22 A32 21 D31 0

H 22 B34 21 A33 20 D32 0

H 22 B35 21 A34 20 D33 0

H 21 B36 20 A35 19 D34 0

H 21 B37 20 A36 19 D35 0

N 19 B38 6 A37 4 D36 0

C	39	B39	19	A38	6	D37	0
H	40	B40	39	A39	19	D38	0
H	40	B41	39	A40	19	D39	0
C	40	B42	39	A41	19	D40	0
H	43	B43	40	A42	39	D41	0
H	43	B44	40	A43	39	D42	0
H	43	B45	40	A44	39	D43	0

Variables:

B1	1.36212
B2	1.45293
B3	1.52513
B4	1.32785
B5	1.22312
B6	1.0125
B7	1.22653
B8	1.53957
B9	1.0954
B10	1.09378
B11	1.09261
B12	1.09768
B13	1.52378
B14	1.09437
B15	1.09461
B16	1.09452
B17	1.00537
B18	2.81952
B19	1.24375
B20	1.47212
B21	1.53216
B22	1.53317
B23	1.46155
B24	1.45751
B25	1.09543
B26	1.10848
B27	1.09545
B28	1.4578
B29	1.10876
B30	1.09369
B31	1.09514
B32	1.09782

B33	1.11064
B34	1.0964
B35	1.09668
B36	1.09811
B37	1.09597
B38	1.21018
B39	1.45727
B40	1.09583
B41	1.09535
B42	1.5276
B43	1.09324
B44	1.09594
B45	1.09603
A1	122.98221
A2	106.08222
A3	114.25918
A4	121.95763
A5	120.51582
A6	122.82674
A7	112.91251
A8	110.66083
A9	110.51788
A10	108.59874
A11	109.2364
A12	122.29085
A13	109.01396
A14	108.73056
A15	113.67445
A16	106.90875
A17	113.88843
A18	90.7124
A19	121.86034
A20	112.05349
A21	111.11193
A22	113.47711
A23	111.21513
A24	109.54534
A25	113.42621
A26	109.82288
A27	112.62357

A28	112.98637
A29	110.57074
A30	109.42436
A31	108.17611
A32	109.76653
A33	108.72975
A34	109.63889
A35	110.44421
A36	107.01706
A37	89.72976
A38	132.92037
A39	106.18867
A40	106.89498
A41	115.43351
A42	110.36594
A43	111.14195
A44	109.81529
D1	-155.92186
D2	175.76961
D3	-5.08313
D4	-162.43832
D5	-8.27679
D6	81.47477
D7	59.51088
D8	-179.68892
D9	-59.92135
D10	-39.00132
D11	179.6357
D12	-57.71545
D13	58.96025
D14	-179.44006
D15	177.37375
D16	-176.06574
D17	5.36228
D18	152.08794
D19	-99.2683
D20	-179.93802
D21	-172.44496
D22	163.36641
D23	-176.55795

D24	62.93433
D25	-58.06929
D26	-71.65447
D27	-61.79728
D28	59.46658
D29	177.84861
D30	-53.6847
D31	61.87337
D32	-56.94877
D33	59.76389
D34	23.80055
D35	140.12589
D36	-166.06475
D37	-55.05172
D38	103.23126
D39	-142.93097
D40	-19.12658
D41	61.25233
D42	-59.7078
D43	-179.14169

Transition state 1 (TS1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C							
N	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
O	4	B4	3	A3	2	D2	0
O	4	B5	3	A4	2	D3	0
H	2	B6	1	A5	3	D4	0
O	1	B7	2	A6	3	D5	0
C	3	B8	2	A7	1	D6	0
H	9	B9	3	A8	2	D7	0
H	9	B10	3	A9	2	D8	0
H	9	B11	3	A10	2	D9	0
H	3	B12	2	A11	1	D10	0
C	1	B13	8	A12	2	D11	0
H	14	B14	1	A13	8	D12	0

H	14	B15	1	A14	8	D13	0
H	14	B16	1	A15	8	D14	0
H	5	B17	4	A16	3	D15	0
C	6	B18	4	A17	3	D16	0
N	19	B19	6	A18	4	D17	0
C	20	B20	19	A19	6	D18	0
C	21	B21	20	A20	19	D19	0
C	22	B22	21	A21	20	D20	0
N	23	B23	22	A22	21	D21	0
C	24	B24	23	A23	22	D22	0
H	25	B25	24	A24	23	D23	0
H	25	B26	24	A25	23	D24	0
H	25	B27	24	A26	23	D25	0
C	24	B28	23	A27	22	D26	0
H	29	B29	24	A28	23	D27	0
H	29	B30	24	A29	23	D28	0
H	29	B31	24	A30	23	D29	0
H	23	B32	22	A31	21	D30	0
H	23	B33	22	A32	21	D31	0
H	22	B34	21	A33	20	D32	0
H	22	B35	21	A34	20	D33	0
H	21	B36	20	A35	19	D34	0
H	21	B37	20	A36	19	D35	0
N	19	B38	6	A37	4	D36	0
C	39	B39	19	A38	6	D37	0
H	40	B40	39	A39	19	D38	0
H	40	B41	39	A40	19	D39	0
C	40	B42	39	A41	19	D40	0
H	43	B43	40	A42	39	D41	0
H	43	B44	40	A43	39	D42	0
H	43	B45	40	A44	39	D43	0

Variables:

B1	1.34496
B2	1.44829
B3	1.52828
B4	1.22558
B5	1.26318
B6	0.9934
B7	1.20417
B8	1.53206

B9	1.08636
B10	1.08276
B11	1.08206
B12	1.08206
B13	1.51597
B14	1.08243
B15	1.08439
B16	1.08375
B17	1.71876
B18	2.03615
B19	1.29311
B20	1.46515
B21	1.52706
B22	1.5289
B23	1.4505
B24	1.44811
B25	1.08362
B26	1.09412
B27	1.0839
B28	1.44895
B29	1.09425
B30	1.08182
B31	1.08339
B32	1.08585
B33	1.09605
B34	1.08414
B35	1.08575
B36	1.08268
B37	1.0821
B38	1.16669
B39	1.44595
B40	1.08118
B41	1.08051
B42	1.5227
B43	1.08278
B44	1.0842
B45	1.08503
A1	122.93568
A2	109.97074
A3	117.26699

A4	117.57915
A5	120.55271
A6	123.25254
A7	112.29078
A8	110.50604
A9	110.14065
A10	109.56728
A11	108.95621
A12	120.94913
A13	108.67454
A14	108.57524
A15	113.47706
A16	99.22019
A17	124.39231
A18	99.06467
A19	120.91605
A20	112.77254
A21	111.34875
A22	113.16257
A23	111.50411
A24	109.64714
A25	113.0667
A26	109.97623
A27	113.27697
A28	112.75374
A29	110.83381
A30	109.38023
A31	108.32723
A32	109.63982
A33	108.32359
A34	109.78473
A35	108.35249
A36	105.93699
A37	107.11965
A38	142.88253
A39	106.80644
A40	107.37976
A41	111.96666
A42	110.38268
A43	110.95103

A44	109.55828
D1	-158.38136
D2	169.39178
D3	-11.90021
D4	-170.00644
D5	-4.35981
D6	79.01221
D7	60.52833
D8	-179.21615
D9	-59.1704
D10	-41.27028
D11	-179.4734
D12	-48.84101
D13	68.02031
D14	-170.70886
D15	177.23694
D16	-176.93086
D17	2.0158
D18	158.25553
D19	-84.03538
D20	-176.65237
D21	-170.61181
D22	164.95467
D23	-176.06363
D24	63.36937
D25	-57.62562
D26	-68.94831
D27	-60.893
D28	60.58911
D29	178.83816
D30	-51.71916
D31	64.11963
D32	-54.04036
D33	62.82853
D34	39.47267
D35	154.45079
D36	-176.22665
D37	-21.78455
D38	60.91274
D39	176.87809

D40	-60.88483
D41	61.10387
D42	-59.75003
D43	-179.22194

Activated amino acid – conformation 1 (C1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.87599	0.53419	-0.6211
N	-2.70334	0.74478	0.0514
C	-1.72773	1.7001	-0.44533
C	-0.37203	1.2985	0.12098
O	0.59907	2.14272	-0.32459
C	1.95302	1.77152	-0.11928
N	2.37288	0.7474	-0.72303
C	3.67114	0.15052	-0.44975
C	3.54175	-1.37821	-0.48591
C	4.87399	-2.07401	-0.19092
N	4.84396	-3.52013	-0.41276
C	6.1869	-4.08222	-0.38954
H	6.14253	-5.15185	-0.62296
H	6.69536	-3.96952	0.5899
H	6.80713	-3.59463	-1.14988
C	3.97674	-4.2186	0.52722
H	4.29281	-4.09574	1.58351
H	2.94714	-3.86237	0.43711
H	3.98008	-5.28951	0.29685
H	5.63975	-1.66252	-0.86266
H	5.20306	-1.83008	0.84251
H	2.77251	-1.66725	0.23898
H	3.18187	-1.68603	-1.47409
H	4.39308	0.46496	-1.21846
H	4.08239	0.4594	0.52414
N	2.54378	2.69473	0.70805
H	1.89916	3.36828	1.09886
C	3.93661	3.13829	0.60852
H	4.53144	2.72447	1.43331
H	4.35637	2.74791	-0.32235
C	4.02753	4.66437	0.61926

H	5.07422	4.98332	0.57568
H	3.59473	5.07964	1.53798
H	3.49869	5.09726	-0.23667
O	-0.19018	0.38354	0.88833
H	-2.33423	0.0383	0.67607
O	-4.19229	1.21151	-1.59854
C	-2.09834	3.15216	-0.09008
H	-2.14786	3.28449	0.99611
H	-1.36546	3.84979	-0.50457
H	-3.07897	3.37125	-0.51791
H	-1.67043	1.62211	-1.53931
C	-4.781	-0.59086	-0.08554
H	-5.76328	-0.48443	-0.49627
H	-4.37646	-1.53979	-0.36974
H	-4.83207	-0.53004	0.98151

Activated amino acid – conformation 2 (C2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.26608	0.78241	1.00293
N	-2.57423	1.94997	0.76481
C	-1.63539	2.14365	-0.32334
C	-0.32552	1.38387	-0.08311
O	0.37642	1.28553	-1.24363
C	1.70047	0.79255	-1.13088
N	2.60909	1.67036	-1.0157
C	4.00102	1.24618	-1.01579
C	4.60192	1.20721	0.40158
C	3.88835	0.2722	1.38421
N	3.77849	-1.13088	0.94228
C	2.90228	-1.87089	1.85333
H	2.78464	-2.90107	1.49875
H	1.91773	-1.39364	1.88004
H	3.29761	-1.90858	2.88521
C	5.07871	-1.7899	0.83057
H	5.70044	-1.2848	0.08677
H	5.62955	-1.80568	1.78979
H	4.93614	-2.82507	0.50288
H	4.39863	0.32575	2.36534

H	2.86736	0.63877	1.53259
H	5.66811	0.95755	0.32188
H	4.55276	2.21566	0.83078
H	4.14778	0.2732	-1.51064
H	4.56838	1.98477	-1.59661
N	1.78856	-0.56921	-1.23492
H	2.57084	-0.9564	-0.69158
C	0.63191	-1.44758	-1.39326
H	0.03629	-1.49755	-0.46856
H	-0.01596	-1.02998	-2.16948
C	1.08584	-2.84919	-1.79675
H	0.2197	-3.50774	-1.92326
H	1.73217	-3.29397	-1.03061
H	1.64388	-2.82239	-2.73839
O	0.04983	0.96041	0.98485
H	-2.38091	2.45087	1.62295
O	-3.84297	0.55675	2.05153
C	-1.33685	3.64038	-0.5092
H	-2.26413	4.17778	-0.72745
H	-0.89344	4.06423	0.39956
H	-0.63135	3.78843	-1.3303
H	-2.08365	1.74997	-1.2378
C	-3.23508	-0.12901	-0.23802
H	-3.12314	0.46983	-1.11766
H	-2.41152	-0.80783	-0.16149
H	-4.14902	-0.68228	-0.29712

Activated amino acid – conformation 3 (C3)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.0853	-1.79202	1.07708
C	-2.76383	-0.91067	-1.07947
H	-2.3002	-0.79224	-2.07289
O	-3.07372	-1.29833	1.60586
N	-1.72359	-1.62033	-0.30347
C	-2.92375	0.53826	-0.56105
O	-4.04572	1.02729	-0.38475
C	-4.08071	-1.67016	-1.26864
H	-3.87654	-2.63092	-1.76124

H	-4.56978	-1.85387	-0.31559
H	-4.76084	-1.09285	-1.90565
O	-1.94178	1.11884	-0.03294
H	-1.14055	-1.41135	-0.41378
C	-0.596	0.95774	-0.42365
N	-0.11061	-0.17472	-0.72212
N	0.00679	2.18589	-0.36026
H	1.01508	2.13979	-0.37548
C	1.25375	-0.20516	-1.26322
H	1.33105	-1.10556	-1.87662
H	1.43817	0.65353	-1.93467
C	2.38126	-0.25968	-0.19924
H	2.13861	-1.08106	0.49639
C	-0.5733	3.45176	0.09835
H	-0.03719	4.25128	-0.43874
H	-1.61141	3.48265	-0.22667
C	-0.4788	3.66278	1.60546
H	-0.89844	4.63526	1.8798
H	-1.0344	2.88877	2.14269
H	0.56876	3.63703	1.94915
C	3.7728	-0.46798	-0.82032
H	3.81812	-1.46847	-1.29974
H	3.9171	0.26603	-1.61482
H	2.40458	0.65296	0.40142
N	4.87825	-0.27307	0.13804
C	6.15853	-0.19893	-0.54701
H	6.95317	0.01738	0.18581
H	6.44338	-1.13403	-1.07392
H	6.1475	0.61379	-1.28162
C	4.9097	-1.29213	1.18206
H	5.05169	-2.31692	0.78477
H	5.72999	-1.0815	1.86598
H	3.97885	-1.28543	1.75587
C	-1.13858	-2.68033	1.8731
H	-0.75529	-2.10688	2.72976
H	-1.73978	-3.51423	2.28222
H	-0.30238	-3.09086	1.28625

Transition state 2 (TS2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.67972	1.57331	-0.04803
C	2.89208	0.33747	-1.56517
H	2.68137	-0.3801	-2.37531
O	2.58521	1.34014	0.79405
N	1.66719	1.06797	-1.29534
C	3.35471	-0.52001	-0.393
O	4.42752	-0.82237	-0.00454
C	4.06049	1.23653	-1.99669
H	3.74848	1.81462	-2.8708
H	4.31559	1.92364	-1.1867
H	4.94763	0.6475	-2.25033
O	2.25804	-1.45624	0.22384
H	0.70399	-0.15121	-1.26687
C	1.0579	-1.82061	-0.15632
N	0.33613	-1.16182	-1.04717
N	0.61823	-2.96109	0.42651
H	-0.37248	-3.14764	0.36752
C	-1.00767	-1.53787	-1.47443
H	-1.14432	-1.10979	-2.47325
H	-1.06556	-2.6281	-1.5982
C	-2.10932	-1.02029	-0.53493
H	-1.96944	0.05957	-0.41584
C	1.37017	-3.68249	1.46237
H	1.01957	-4.71949	1.43455
H	2.42031	-3.67931	1.16654
C	1.20542	-3.08531	2.86101
H	1.77012	-3.67797	3.5893
H	1.58386	-2.05947	2.88587
H	0.15407	-3.07966	3.17147
C	-3.51135	-1.34194	-1.06541
H	-3.66121	-0.84108	-2.04541
H	-3.57585	-2.42139	-1.259
H	-2.00467	-1.46094	0.46525
N	-4.57109	-1.00819	-0.11647
C	-5.83318	-1.63402	-0.49154
H	-6.58812	-1.4215	0.27301
H	-6.22746	-1.28047	-1.4651
H	-5.70743	-2.72084	-0.55081
C	-4.74254	0.43135	0.05468

H	-5.04346	0.94244	-0.88172
H	-5.51883	0.61544	0.80472
H	-3.81949	0.89511	0.41241
C	0.45727	2.41338	0.36609
H	-0.33536	1.76297	0.67204
H	0.72491	3.05616	1.17856
H	0.13289	3.00469	-0.46459

Molecular complex 2 (MC2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.1653	-1.79202	0.91708
C	-2.86383	-1.13067	-1.03947
H	-2.4002	-0.71224	-1.97289
O	-2.95372	-0.83833	1.40586
N	-1.98359	-2.04033	-0.34347
C	-3.30375	0.07826	-0.20105
O	-4.12572	0.92729	-0.26475
C	-4.20071	-1.81016	-1.40864
H	-3.97654	-2.71092	-1.98124
H	-4.70978	-2.09387	-0.47559
H	-4.86084	-1.15285	-1.98565
O	-1.74178	1.11884	0.10706
H	-0.14056	-0.59135	-0.75378
C	-0.596	1.13774	-0.32365
N	0.06939	0.02528	-0.80212
N	0.10679	2.28589	-0.38026
H	1.11508	2.25979	-0.45548
C	1.41375	-0.12516	-1.32322
H	1.39105	-1.02556	-1.95662
H	1.61817	0.71353	-1.99467
C	2.46126	-0.25968	-0.21924
H	2.17861	-1.08106	0.43639
C	-0.5133	3.53176	0.09835
H	0.00281	4.35128	-0.39874
H	-1.55141	3.52265	-0.24667
C	-0.4588	3.68278	1.62546
H	-0.91844	4.63526	1.9198
H	-1.0144	2.86877	2.10269

H	0.56876	3.67703	1.98915
C	3.8528	-0.46798	-0.82032
H	3.89812	-1.46847	-1.29974
H	3.9971	0.26603	-1.63482
H	2.48458	0.65296	0.40142
N	4.91825	-0.27307	0.13804
C	6.21853	-0.19893	-0.52701
H	6.99317	0.01738	0.20581
H	6.48338	-1.13403	-1.05392
H	6.2075	0.61379	-1.26162
C	4.9297	-1.29213	1.18206
H	5.07169	-2.31692	0.78477
H	5.74999	-1.0815	1.88598
H	3.99885	-1.26543	1.75587
C	-1.37858	-2.64033	1.9131
H	-0.85529	-1.98688	2.62976
H	-2.03978	-3.29423	2.50222
H	-0.66238	-3.27086	1.36625

Azlactone

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.34009	0.10574	-0.15607
C	2.44815	0.69418	-0.35712
H	2.87452	0.88615	-1.3518
O	1.0101	-1.11163	-0.04274
N	1.05965	1.14677	-0.33228
C	2.3659	-0.81867	-0.15406
O	3.21891	-1.6559	-0.08004
C	3.32458	1.37716	0.69957
H	4.33773	0.96562	0.66435
H	3.36485	2.45286	0.50872
H	2.91561	1.21883	1.70236
C	-1.19505	0.04146	-0.05217
H	-1.57877	-0.59008	-0.82601
H	-1.47163	-0.35558	0.90217
H	-1.60138	1.02536	-0.16049

R = OtBu

N-Protected alanine

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.8577	0.10707	0.1916
N	2.66689	0.44101	-0.385
C	1.79611	1.42759	0.22534
C	0.38117	1.15222	-0.2695
O	-0.49607	2.02832	0.29857
O	0.08409	0.30861	-1.07956
H	2.24708	-0.18992	-1.05614
O	4.34645	0.70308	1.14114
C	2.24064	2.87084	-0.07876
H	2.22607	3.0596	-1.15763
H	1.5882	3.5914	0.42204
H	3.2614	3.00097	0.28785
H	1.79621	1.29337	1.31518
O	4.39424	-0.95337	-0.46034
C	5.69916	-1.50391	-0.0664
C	5.63377	-2.03741	1.36901
H	6.568	-2.55618	1.6125
H	5.48547	-1.22495	2.08188
H	4.81083	-2.75351	1.47065
C	6.79227	-0.44419	-0.2421
H	7.77431	-0.8926	-0.05317
H	6.7862	-0.05848	-1.26764
H	6.64515	0.38649	0.44978
C	5.88911	-2.6505	-1.06322
H	6.84284	-3.15617	-0.87872
H	5.08263	-3.38471	-0.9665
H	5.8894	-2.27322	-2.09107
H	-1.43516	1.84936	0.21093

Molecular complex 1 (MC1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C

N	1	B1						
C	2	B2	1	A1				
C	3	B3	2	A2	1	D1	0	
O	4	B4	3	A3	2	D2	0	
O	4	B5	3	A4	2	D3	0	
H	2	B6	1	A5	3	D4	0	
O	1	B7	2	A6	3	D5	0	
C	3	B8	2	A7	1	D6	0	
H	9	B9	3	A8	2	D7	0	
H	9	B10	3	A9	2	D8	0	
H	9	B11	3	A10	2	D9	0	
H	3	B12	2	A11	1	D10	0	
H	5	B13	4	A12	3	D11	0	
C	6	B14	4	A13	3	D12	0	
N	15	B15	6	A14	4	D13	0	
C	16	B16	15	A15	6	D14	0	
C	17	B17	16	A16	15	D15	0	
C	18	B18	17	A17	16	D16	0	
N	19	B19	18	A18	17	D17	0	
C	20	B20	19	A19	18	D18	0	
H	21	B21	20	A20	19	D19	0	
H	21	B22	20	A21	19	D20	0	
H	21	B23	20	A22	19	D21	0	
C	20	B24	19	A23	18	D22	0	
H	25	B25	20	A24	19	D23	0	
H	25	B26	20	A25	19	D24	0	
H	25	B27	20	A26	19	D25	0	
H	19	B28	18	A27	17	D26	0	
H	19	B29	18	A28	17	D27	0	
H	18	B30	17	A29	16	D28	0	
H	18	B31	17	A30	16	D29	0	
H	17	B32	16	A31	15	D30	0	
H	17	B33	16	A32	15	D31	0	
N	15	B34	6	A33	4	D32	0	
C	35	B35	15	A34	6	D33	0	
H	36	B36	35	A35	15	D34	0	
H	36	B37	35	A36	15	D35	0	
C	36	B38	35	A37	15	D36	0	
H	39	B39	36	A38	35	D37	0	

H	39	B40	36	A39	35	D38	0
H	39	B41	36	A40	35	D39	0
O	1	B42	8	A41	2	D40	0
C	43	B43	1	A42	8	D41	0
C	44	B44	43	A43	1	D42	0
H	45	B45	44	A44	43	D43	0
H	45	B46	44	A45	43	D44	0
H	45	B47	44	A46	43	D45	0
C	44	B48	43	A47	1	D46	0
H	49	B49	44	A48	43	D47	0
H	49	B50	44	A49	43	D48	0
H	49	B51	44	A50	43	D49	0
C	44	B52	43	A51	1	D50	0
H	53	B53	44	A52	43	D51	0
H	53	B54	44	A53	43	D52	0
H	53	B55	44	A54	43	D53	0

Variables:

B1	1.35828
B2	1.45078
B3	1.52635
B4	1.33057
B5	1.22038
B6	1.01249
B7	1.22085
B8	1.53996
B9	1.09536
B10	1.0934
B11	1.09272
B12	1.09759
B13	1.00401
B14	3.39533
B15	1.23975
B16	1.47214
B17	1.53264
B18	1.53341
B19	1.46169
B20	1.45744
B21	1.09538
B22	1.10846
B23	1.09554

B24	1.45812
B25	1.10875
B26	1.09349
B27	1.09506
B28	1.09808
B29	1.11086
B30	1.096
B31	1.09658
B32	1.0977
B33	1.0965
B34	1.21316
B35	1.4611
B36	1.09603
B37	1.09606
B38	1.52671
B39	1.09409
B40	1.09632
B41	1.09571
B42	1.36341
B43	1.44193
B44	1.54
B45	1.07
B46	1.07
B47	1.07
B48	1.54
B49	1.07
B50	1.07
B51	1.07
B52	1.54
B53	1.07
B54	1.07
B55	1.07
A1	121.37307
A2	107.5141
A3	111.95379
A4	123.38891
A5	120.00759
A6	125.37474
A7	112.58819
A8	110.58092

A9	110.4674
A10	108.71202
A11	109.36182
A12	109.31192
A13	102.87208
A14	80.68973
A15	123.77842
A16	111.11246
A17	111.582
A18	113.36946
A19	111.1212
A20	109.54757
A21	113.38838
A22	109.83837
A23	112.84074
A24	113.04904
A25	110.65007
A26	109.29445
A27	108.58213
A28	109.4659
A29	108.24177
A30	109.70532
A31	110.79107
A32	107.00893
A33	98.93946
A34	130.70297
A35	106.4064
A36	106.83457
A37	114.9183
A38	110.4212
A39	110.97822
A40	109.9616
A41	124.39814
A42	114.81563
A43	109.41453
A44	109.4712
A45	109.4712
A46	109.47123
A47	108.6058
A48	109.4712

A49	109.4712
A50	109.47123
A51	108.54687
A52	109.4712
A53	109.4712
A54	109.47123
D1	-157.77456
D2	175.07233
D3	-5.3503
D4	-164.07578
D5	-7.05464
D6	79.13511
D7	60.52678
D8	-178.62021
D9	-58.91073
D10	-41.05371
D11	178.87204
D12	177.10538
D13	19.13203
D14	144.65727
D15	-109.775
D16	-174.0326
D17	-170.95156
D18	166.98044
D19	-176.13449
D20	63.33524
D21	-57.63248
D22	-68.00132
D23	-60.7623
D24	60.64077
D25	178.95262
D26	-52.07232
D27	63.62143
D28	-51.50497
D29	65.01921
D30	13.53987
D31	130.27484
D32	-152.11652
D33	-55.54958
D34	119.09556

D35	-127.4871
D36	-3.57428
D37	58.97967
D38	-61.72869
D39	178.88643
D40	179.18859
D41	-0.36432
D42	-65.61568
D43	-50.19788
D44	69.80213
D45	-170.19788
D46	172.77456
D47	179.73601
D48	-60.26398
D49	59.73602
D50	51.08047
D51	-91.47132
D52	28.52869
D53	148.52869

Transition state 1 (TS1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C							
N	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
O	4	B4	3	A3	2	D2	0
O	4	B5	3	A4	2	D3	0
H	2	B6	1	A5	3	D4	0
O	1	B7	2	A6	3	D5	0
C	3	B8	2	A7	1	D6	0
H	9	B9	3	A8	2	D7	0
H	9	B10	3	A9	2	D8	0
H	9	B11	3	A10	2	D9	0
H	3	B12	2	A11	1	D10	0
H	5	B13	4	A12	3	D11	0
C	6	B14	4	A13	3	D12	0
N	15	B15	6	A14	4	D13	0

C 16 B16 15 A15 6 D14 0
C 17 B17 16 A16 15 D15 0
C 18 B18 17 A17 16 D16 0
N 19 B19 18 A18 17 D17 0
C 20 B20 19 A19 18 D18 0
H 21 B21 20 A20 19 D19 0
H 21 B22 20 A21 19 D20 0
H 21 B23 20 A22 19 D21 0
C 20 B24 19 A23 18 D22 0
H 25 B25 20 A24 19 D23 0
H 25 B26 20 A25 19 D24 0
H 25 B27 20 A26 19 D25 0
H 19 B28 18 A27 17 D26 0
H 19 B29 18 A28 17 D27 0
H 18 B30 17 A29 16 D28 0
H 18 B31 17 A30 16 D29 0
H 17 B32 16 A31 15 D30 0
H 17 B33 16 A32 15 D31 0
N 15 B34 6 A33 4 D32 0
C 35 B35 15 A34 6 D33 0
H 36 B36 35 A35 15 D34 0
H 36 B37 35 A36 15 D35 0
C 36 B38 35 A37 15 D36 0
H 39 B39 36 A38 35 D37 0
H 39 B40 36 A39 35 D38 0
H 39 B41 36 A40 35 D39 0
O 1 B42 8 A41 2 D40 0
C 43 B43 1 A42 8 D41 0
C 44 B44 43 A43 1 D42 0
H 45 B45 44 A44 43 D43 0
H 45 B46 44 A45 43 D44 0
H 45 B47 44 A46 43 D45 0
C 44 B48 43 A47 1 D46 0
H 49 B49 44 A48 43 D47 0
H 49 B50 44 A49 43 D48 0
H 49 B51 44 A50 43 D49 0
C 44 B52 43 A51 1 D50 0
H 53 B53 44 A52 43 D51 0
H 53 B54 44 A53 43 D52 0
H 53 B55 44 A54 43 D53 0

Variables:

B1	1.35475
B2	1.45468
B3	1.53804
B4	1.26161
B5	1.27384
B6	1.01207
B7	1.22087
B8	1.53685
B9	1.09597
B10	1.09325
B11	1.09304
B12	1.09762
B13	1.51476
B14	2.16268
B15	1.28905
B16	1.47527
B17	1.53228
B18	1.53395
B19	1.46105
B20	1.45781
B21	1.09524
B22	1.10821
B23	1.09557
B24	1.45882
B25	1.10842
B26	1.09347
B27	1.0949
B28	1.09824
B29	1.1108
B30	1.0958
B31	1.09672
B32	1.09481
B33	1.09539
B34	1.20105
B35	1.45254
B36	1.09546
B37	1.0941
B38	1.52787
B39	1.0936

B40	1.09529
B41	1.09537
B42	1.37045
B43	1.43841
B44	1.54
B45	1.07
B46	1.07
B47	1.07
B48	1.54
B49	1.07
B50	1.07
B51	1.07
B52	1.54
B53	1.07
B54	1.07
B55	1.07
A1	122.1626
A2	108.96271
A3	116.7732
A4	117.94682
A5	119.67781
A6	125.88088
A7	112.53724
A8	110.54439
A9	109.82499
A10	109.36855
A11	109.30101
A12	101.3546
A13	118.12724
A14	97.86496
A15	121.93207
A16	112.19147
A17	111.51403
A18	113.21045
A19	111.09673
A20	109.50523
A21	113.3648
A22	109.85706
A23	112.85264
A24	113.0241

A25	110.6822
A26	109.24252
A27	108.63075
A28	109.42177
A29	108.31391
A30	109.73265
A31	108.49173
A32	106.37415
A33	106.39529
A34	136.03313
A35	106.47854
A36	107.15484
A37	113.49517
A38	110.05662
A39	111.08613
A40	109.73034
A41	124.20526
A42	115.31951
A43	108.55121
A44	109.4712
A45	109.4712
A46	109.47123
A47	109.05867
A48	109.4712
A49	109.4712
A50	109.47123
A51	109.23595
A52	109.4712
A53	109.4712
A54	109.47123
D1	-159.13439
D2	176.4347
D3	-4.16133
D4	-162.14858
D5	-8.5191
D6	77.65982
D7	59.57676
D8	179.80136
D9	-60.13845
D10	-42.51015

D11	175.41531
D12	-175.17125
D13	3.00836
D14	151.38364
D15	-93.98584
D16	-174.23893
D17	-170.98445
D18	167.00871
D19	-176.17557
D20	63.31567
D21	-57.6837
D22	-67.96646
D23	-60.6441
D24	60.81319
D25	179.09196
D26	-52.12223
D27	63.60402
D28	-51.75488
D29	64.89156
D30	29.45492
D31	144.82654
D32	-172.6498
D33	-37.07455
D34	79.97326
D35	-165.32818
D36	-42.02123
D37	61.03493
D38	-59.83815
D39	-179.3894
D40	179.28883
D41	-2.21608
D42	36.93162
D43	-78.48055
D44	41.51946
D45	161.51945
D46	158.95448
D47	56.4771
D48	176.47712
D49	-63.52289
D50	-79.75865

D51	-158.74312
D52	-38.7431
D53	81.25689

Activated amino acid – conformation 1 (C1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.87599	0.53419	-0.6211
N	-2.70334	0.74478	0.0514
C	-1.72773	1.7001	-0.44533
C	-0.37203	1.2985	0.12098
O	0.59907	2.14272	-0.32459
C	1.95302	1.77152	-0.11928
N	2.37288	0.7474	-0.72303
C	3.67114	0.15052	-0.44975
C	3.54175	-1.37821	-0.48591
C	4.87399	-2.07401	-0.19092
N	4.84396	-3.52013	-0.41276
C	6.1869	-4.08222	-0.38954
H	6.14253	-5.15185	-0.62296
H	6.69536	-3.96952	0.5899
H	6.80713	-3.59463	-1.14988
C	3.97674	-4.2186	0.52722
H	4.29281	-4.09574	1.58351
H	2.94714	-3.86237	0.43711
H	3.98008	-5.28951	0.29685
H	5.63975	-1.66252	-0.86266
H	5.20306	-1.83008	0.84251
H	2.77251	-1.66725	0.23898
H	3.18187	-1.68603	-1.47409
H	4.39308	0.46496	-1.21846
H	4.08239	0.4594	0.52414
N	2.54378	2.69473	0.70805
H	1.89916	3.36828	1.09886
C	3.93661	3.13829	0.60852
H	4.53144	2.72447	1.43331
H	4.35637	2.74791	-0.32235
C	4.02753	4.66437	0.61926
H	5.07422	4.98332	0.57568

H	3.59473	5.07964	1.53798
H	3.49869	5.09726	-0.23667
O	-0.19018	0.38354	0.88833
H	-2.33423	0.0383	0.67607
O	-4.19229	1.21151	-1.59854
C	-2.09834	3.15216	-0.09008
H	-2.14786	3.28449	0.99611
H	-1.36546	3.84979	-0.50457
H	-3.07897	3.37125	-0.51791
H	-1.67043	1.62211	-1.53931
O	-4.71636	-0.5105	-0.12379
C	-6.06474	-0.27672	-0.53865
C	-6.1619	-0.41368	-2.06947
H	-7.04435	-0.96307	-2.32312
H	-6.20783	0.55926	-2.51241
H	-5.30101	-0.93238	-2.43651
C	-6.49108	1.14329	-0.12223
H	-7.54028	1.15359	0.08746
H	-5.94956	1.43602	0.75297
H	-6.27962	1.82688	-0.91777
C	-6.99335	-1.30802	0.12896
H	-8.00031	-1.14208	-0.1926
H	-6.68828	-2.29523	-0.14897
H	-6.93667	-1.20329	1.19231

Activated amino acid – conformation 2 (C2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.26608	0.78241	-1.00293
N	2.57423	1.94997	-0.76481
C	1.63539	2.14365	0.32334
C	0.32552	1.38387	0.08311
O	-0.37642	1.28553	1.24363
C	-1.70047	0.79255	1.13088
N	-2.60909	1.67036	1.0157
C	-4.00102	1.24618	1.01579
C	-4.60192	1.20721	-0.40158
C	-3.88835	0.2722	-1.38421
N	-3.77849	-1.13088	-0.94228

C	-2.90228	-1.87089	-1.85333
H	-2.78464	-2.90107	-1.49875
H	-1.91773	-1.39364	-1.88004
H	-3.29761	-1.90858	-2.88521
C	-5.07871	-1.7899	-0.83057
H	-5.70044	-1.2848	-0.08677
H	-5.62955	-1.80568	-1.78979
H	-4.93614	-2.82507	-0.50288
H	-4.39863	0.32575	-2.36534
H	-2.86736	0.63877	-1.53259
H	-5.66811	0.95755	-0.32188
H	-4.55276	2.21566	-0.83078
H	-4.14778	0.2732	1.51064
H	-4.56838	1.98477	1.59661
N	-1.78856	-0.56921	1.23492
H	-2.57084	-0.9564	0.69158
C	-0.63191	-1.44758	1.39326
H	-0.03629	-1.49755	0.46856
H	0.01596	-1.02998	2.16948
C	-1.08584	-2.84919	1.79675
H	-0.2197	-3.50774	1.92326
H	-1.73217	-3.29397	1.03061
H	-1.64388	-2.82239	2.73839
O	-0.04983	0.96041	-0.98485
H	2.38091	2.45087	-1.62295
O	3.84297	0.55675	-2.05153
C	1.33685	3.64038	0.5092
H	2.26413	4.17778	0.72745
H	0.89344	4.06423	-0.39956
H	0.63135	3.78843	1.3303
H	2.08365	1.74997	1.2378
O	3.2388	-0.01956	0.089
C	3.99559	-1.28289	0.11484
C	3.7047	-1.8159	1.5201
H	4.05347	-1.11115	2.28205
H	2.62992	-1.97188	1.66068
H	4.2156	-2.7723	1.67332
C	5.49228	-1.00381	-0.05844
H	5.7035	-0.60293	-1.05066
H	5.83578	-0.28683	0.69551

H	6.05642	-1.93382	0.07525
C	3.45409	-2.2385	-0.95357
H	3.94056	-3.21546	-0.8534
H	2.37505	-2.38015	-0.82539
H	3.64115	-1.85115	-1.95597

Activated amino acid – conformation 3 (C3)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.99833	1.05676	-0.46539
C	2.39985	-0.84769	-1.7859
H	1.84271	-1.44605	-2.57141
O	2.90621	0.80108	0.30979
N	1.53504	0.31093	-1.54521
C	2.43763	-1.87107	-0.56162
O	3.54634	-2.27241	-0.15122
C	3.77915	-0.52738	-2.36996
H	3.63692	0.0355	-3.30747
H	4.364	0.08966	-1.66465
H	4.3571	-1.43821	-2.58528
O	1.55309	-1.91536	0.22579
H	0.51118	-0.21171	-1.37807
C	0.19635	-1.85052	-0.08453
N	-0.30329	-1.05875	-0.97395
N	-0.5164	-2.69569	0.69209
H	-1.50634	-2.52717	0.68392
C	-1.71422	-1.10244	-1.35352
H	-1.7503	-0.73083	-2.38053
H	-2.07416	-2.14356	-1.38834
C	-2.6437	-0.23895	-0.47282
H	-2.19364	0.7649	-0.41224
C	-0.01911	-3.53443	1.80386
H	-0.67648	-4.4133	1.83397
H	0.9835	-3.88167	1.53284
C	-0.01002	-2.79905	3.14684
H	0.34486	-3.47066	3.92935
H	0.65923	-1.93894	3.10381
H	-1.01011	-2.45177	3.41374
C	-4.07959	-0.17166	-1.01662

H	-4.06866	0.31399	-2.01524
H	-4.43514	-1.19589	-1.18263
H	-2.68286	-0.62423	0.56238
N	-5.01828	0.47066	-0.09573
C	-6.40138	0.24007	-0.51124
H	-7.07538	0.68193	0.24047
H	-6.64519	0.68142	-1.48793
H	-6.59801	-0.8348	-0.55966
C	-4.75937	1.90636	0.05964
H	-4.85856	2.45956	-0.89061
H	-5.48101	2.32282	0.77424
H	-3.7637	2.07796	0.45739
O	1.21608	2.18467	-0.32989
C	1.42402	2.98119	0.88202
C	0.43131	4.13738	0.68594
H	0.46908	4.82667	1.53695
H	0.67612	4.6935	-0.22202
H	-0.59108	3.75894	0.57873
C	2.85049	3.53153	0.97336
H	3.56845	2.72309	1.12138
H	3.11039	4.05361	0.04726
H	2.91902	4.24581	1.79729
C	1.05082	2.16791	2.13243
H	0.02699	1.77961	2.02659
H	1.73788	1.33361	2.26028
H	1.0766	2.80427	3.02441

Transition state 2 (TS2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.98624	1.14413	-0.3778
C	2.77166	-0.58835	-1.63163
H	2.393	-1.3226	-2.3396
O	2.81328	0.908	0.4957
N	1.80809	0.44223	-1.4858
C	2.99367	-1.42852	-0.37429
O	3.76211	-1.94875	0.26338
C	4.1651	-0.13607	-2.09211
H	4.03591	0.3859	-3.0317

H	4.60041	0.54032	-1.37074
H	4.83713	-0.97465	-2.24667
O	1.40855	-2.07257	0.14385
H	0.3069	-0.50994	-1.35514
C	0.18884	-2.0837	-0.168
N	-0.32747	-1.25852	-1.06149
N	-0.58301	-3.00388	0.4306
H	-1.56708	-2.93084	0.32075
C	-1.71835	-1.17178	-1.46384
H	-1.71821	-0.72633	-2.4507
H	-2.13064	-2.16913	-1.58256
C	-2.57536	-0.32704	-0.5175
H	-2.08793	0.63383	-0.40013
C	-0.09316	-3.90533	1.46736
H	-0.74484	-4.77086	1.45724
H	0.89335	-4.23641	1.18351
C	-0.06626	-3.27207	2.85369
H	0.28065	-3.9936	3.58679
H	0.60301	-2.4207	2.87099
H	-1.05635	-2.93996	3.15122
C	-4.00117	-0.16653	-1.04484
H	-3.98549	0.42468	-1.96737
H	-4.38162	-1.14767	-1.31517
H	-2.61835	-0.78249	0.468
N	-4.91507	0.39336	-0.06692
C	-6.29307	0.24857	-0.48695
H	-6.95239	0.61069	0.29317
H	-6.52148	0.79842	-1.40487
H	-6.52097	-0.7978	-0.65557
C	-4.61694	1.77043	0.27186
H	-4.67203	2.44034	-0.59146
H	-5.32505	2.11933	1.014
H	-3.62809	1.85429	0.70235
O	1.10321	2.14544	-0.2689
C	1.09988	3.06806	0.82675
C	-0.03595	4.02296	0.46193
H	-0.15015	4.78984	1.22121
H	0.16494	4.50382	-0.48869
H	-0.9732	3.48349	0.37516
C	2.41953	3.8369	0.90186

H	3.23658	3.18851	1.1795
H	2.64177	4.28699	-0.06065
H	2.33905	4.63347	1.63583
C	0.78261	2.35558	2.14212
H	-0.13683	1.78529	2.04427
H	1.57893	1.68435	2.42552
H	0.64062	3.08667	2.93272

Molecular complex 2 (MC2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.97833	0.95676	-0.60539
C	2.57985	-0.70769	-1.8859
H	2.04271	-1.60605	-2.29141
O	2.76621	0.34108	0.26979
N	1.75504	0.45093	-1.78521
C	3.15763	-1.07107	-0.46162
O	3.82634	-1.93241	-0.01122
C	3.87915	-0.42738	-2.68996
H	3.59692	-0.06451	-3.68747
H	4.464	0.34966	-2.18465
H	4.4771	-1.33821	-2.78528
O	1.23309	-1.81536	0.42579
H	0.03118	-0.55171	-1.31807
C	0.07635	-1.93052	0.09547
N	-0.48329	-1.21875	-0.93395
N	-0.7364	-2.83569	0.73209
H	-1.74634	-2.72717	0.68392
C	-1.87422	-1.18244	-1.35352
H	-1.8903	-0.85083	-2.40053
H	-2.27416	-2.20356	-1.34834
C	-2.7237	-0.23895	-0.49282
H	-2.25364	0.7449	-0.49224
C	-0.17911	-3.59443	1.84386
H	-0.81648	-4.4733	1.99397
H	0.8035	-3.94167	1.53284
C	-0.05002	-2.79905	3.14684
H	0.36486	-3.43066	3.94935
H	0.61923	-1.93894	3.00381
H	-1.03011	-2.43177	3.49374

C	-4.15959	-0.17166	-1.01662
H	-4.16866	0.31399	-2.01524
H	-4.53514	-1.19589	-1.16263
H	-2.74286	-0.58423	0.54238
N	-5.07828	0.49066	-0.09573
C	-6.46138	0.28007	-0.49124
H	-7.13538	0.72193	0.24047
H	-6.70519	0.72142	-1.48793
H	-6.67801	-0.7948	-0.53966
C	-4.79937	1.90636	0.05964
H	-4.87856	2.47956	-0.89061
H	-5.50101	2.34282	0.77424
H	-3.7837	2.05796	0.45739
O	1.33608	2.10467	-0.30989
C	1.48402	2.90119	0.90202
C	0.51131	4.05738	0.66594
H	0.52908	4.74667	1.51695
H	0.77612	4.6135	-0.24202
H	-0.51108	3.67894	0.55873
C	2.93049	3.41153	0.99336
H	3.62845	2.58309	1.12138
H	3.19039	3.97361	0.08726
H	3.03902	4.08581	1.85729
C	1.07082	2.08791	2.13243
H	0.04699	1.71961	2.02659
H	1.73788	1.23361	2.28028
H	1.1166	2.72427	3.02441

Azlactone

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	0.34009	0.10574	-0.15607
C	2.44815	0.69418	-0.35712
H	2.87452	0.88615	-1.3518
O	1.0101	-1.11163	-0.04274
N	1.05965	1.14677	-0.33228
C	2.3659	-0.81867	-0.15406
O	3.21891	-1.6559	-0.08004
C	3.32458	1.37716	0.69957

H	4.33773	0.96562	0.66435
H	3.36485	2.45286	0.50872
H	2.91561	1.21883	1.70236
O	-1.0854	0.04605	-0.05959
C	-1.66801	0.66748	-1.2082
C	-1.42584	2.18712	-1.14795
H	-0.59794	2.44154	-1.77625
H	-2.3012	2.70146	-1.48573
H	-1.21011	2.47423	-0.14002
C	-1.02306	0.09507	-2.48412
H	-0.79633	-0.94003	-2.33563
H	-1.70287	0.19724	-3.30407
H	-0.12185	0.63031	-2.69918
C	-3.18256	0.38947	-1.22947
H	-3.62761	0.7698	-0.33382
H	-3.62166	0.87089	-2.07819
H	-3.35072	-0.66543	-1.29118

R = OBn

N-Protected alanine

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.93204	-0.17722	-0.74911
N	-1.83063	0.19451	-0.04344
C	-0.95754	1.24961	-0.52351
C	0.41311	1.0223	0.10286
O	1.29791	1.95854	-0.34271
O	0.66922	0.16107	0.90841
H	-1.45087	-0.43648	0.65158
O	-3.36522	0.4149	-1.72722
C	-1.50811	2.65415	-0.213
H	-1.61237	2.79761	0.8678
H	-0.84793	3.4265	-0.61717
H	-2.49252	2.75	-0.67692
H	-0.84041	1.16064	-1.61148
O	-3.47929	-1.29582	-0.20403

C	-4.68907	-1.78728	-0.83555
C	-5.93505	-1.23647	-0.18505
C	-6.58736	-1.95897	0.82111
C	-6.45313	0.00705	-0.57411
C	-7.73672	-1.45348	1.4302
H	-6.19308	-2.92563	1.12736
C	-7.60106	0.51412	0.03459
H	-5.94313	0.57278	-1.34827
C	-8.24556	-0.21461	1.0371
H	-8.23471	-2.02658	2.20794
H	-7.99588	1.47789	-0.27649
H	-9.14211	0.18034	1.50795
H	-4.64961	-1.53583	-1.8972
H	-4.63359	-2.87162	-0.71369
H	2.23215	1.80753	-0.18155

Molecular complex 1 (MC1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C								
N	1	B1						
C	2	B2	1	A1				
C	3	B3	2	A2	1	D1	0	
O	4	B4	3	A3	2	D2	0	
O	4	B5	3	A4	2	D3	0	
H	2	B6	1	A5	3	D4	0	
O	1	B7	2	A6	3	D5	0	
C	3	B8	2	A7	1	D6	0	
H	9	B9	3	A8	2	D7	0	
H	9	B10	3	A9	2	D8	0	
H	9	B11	3	A10	2	D9	0	
H	3	B12	2	A11	1	D10	0	
H	5	B13	4	A12	3	D11	0	
C	6	B14	4	A13	3	D12	0	
N	15	B15	6	A14	4	D13	0	
C	16	B16	15	A15	6	D14	0	
C	17	B17	16	A16	15	D15	0	
C	18	B18	17	A17	16	D16	0	
N	19	B19	18	A18	17	D17	0	

C	20	B20	19	A19	18	D18	0
H	21	B21	20	A20	19	D19	0
H	21	B22	20	A21	19	D20	0
H	21	B23	20	A22	19	D21	0
C	20	B24	19	A23	18	D22	0
H	25	B25	20	A24	19	D23	0
H	25	B26	20	A25	19	D24	0
H	25	B27	20	A26	19	D25	0
H	19	B28	18	A27	17	D26	0
H	19	B29	18	A28	17	D27	0
H	18	B30	17	A29	16	D28	0
H	18	B31	17	A30	16	D29	0
H	17	B32	16	A31	15	D30	0
H	17	B33	16	A32	15	D31	0
N	15	B34	6	A33	4	D32	0
C	35	B35	15	A34	6	D33	0
H	36	B36	35	A35	15	D34	0
H	36	B37	35	A36	15	D35	0
C	36	B38	35	A37	15	D36	0
H	39	B39	36	A38	35	D37	0
H	39	B40	36	A39	35	D38	0
H	39	B41	36	A40	35	D39	0
O	1	B42	8	A41	2	D40	0
C	43	B43	1	A42	8	D41	0
H	44	B44	43	A43	1	D42	0
H	44	B45	43	A44	1	D43	0
C	44	B46	43	A45	1	D44	0
C	47	B47	44	A46	43	D45	0
C	47	B48	44	A47	43	D46	0
C	48	B49	47	A48	44	D47	0
H	48	B50	47	A49	44	D48	0
C	49	B51	47	A50	44	D49	0
H	49	B52	47	A51	44	D50	0
C	52	B53	49	A52	47	D51	0
H	50	B54	48	A53	47	D52	0
H	52	B55	49	A54	47	D53	0
H	54	B56	52	A55	49	D54	0

Variables:

B1	1.36322
B2	1.45189

B3	1.52499
B4	1.33041
B5	1.22144
B6	1.01231
B7	1.22745
B8	1.54077
B9	1.0955
B10	1.09359
B11	1.0923
B12	1.09705
B13	1.00354
B14	3.38635
B15	1.23953
B16	1.4723
B17	1.53249
B18	1.53345
B19	1.46182
B20	1.45756
B21	1.0954
B22	1.10847
B23	1.09554
B24	1.45836
B25	1.10866
B26	1.09346
B27	1.09503
B28	1.09806
B29	1.11083
B30	1.09596
B31	1.09658
B32	1.09772
B33	1.09657
B34	1.21329
B35	1.46078
B36	1.09598
B37	1.09616
B38	1.5268
B39	1.0942
B40	1.0963
B41	1.09578
B42	1.43

B43	1.43239
B44	1.0953
B45	1.0981
B46	1.51062
B47	1.40096
B48	1.40035
B49	1.3954
B50	1.08519
B51	1.39591
B52	1.08814
B53	1.39596
B54	1.08711
B55	1.087
B56	1.08688
A1	121.92725
A2	107.67964
A3	112.15383
A4	123.35368
A5	121.51042
A6	122.49415
A7	112.61741
A8	110.63129
A9	110.45369
A10	108.56941
A11	108.908
A12	109.23887
A13	103.31244
A14	81.18961
A15	123.79597
A16	111.07749
A17	111.61664
A18	113.31987
A19	111.11245
A20	109.55559
A21	113.37908
A22	109.84504
A23	112.7835
A24	112.99935
A25	110.65029
A26	109.30068

A27	108.57228
A28	109.51062
A29	108.26174
A30	109.72609
A31	110.81388
A32	107.03854
A33	98.25231
A34	130.67332
A35	106.41223
A36	106.85909
A37	114.94158
A38	110.41681
A39	110.98078
A40	109.9599
A41	122.00248
A42	109.47122
A43	110.20679
A44	109.08369
A45	108.72472
A46	121.33576
A47	119.74232
A48	120.41668
A49	119.12891
A50	120.73493
A51	119.53991
A52	120.04393
A53	119.6455
A54	119.77717
A55	120.20238
D1	-158.97349
D2	172.97265
D3	-7.72288
D4	-167.85532
D5	-4.83962
D6	78.00051
D7	60.33394
D8	-178.86804
D9	-59.1879
D10	-41.80424
D11	178.31364

D12	178.81445
D13	15.90508
D14	146.43146
D15	-111.57018
D16	-174.15897
D17	-171.77387
D18	166.55486
D19	-176.24966
D20	63.23109
D21	-57.73572
D22	-68.54237
D23	-60.86963
D24	60.52448
D25	178.86662
D26	-52.88282
D27	62.84147
D28	-51.62487
D29	64.89615
D30	11.76012
D31	128.50792
D32	-155.43718
D33	-56.92286
D34	120.44168
D35	-126.13671
D36	-2.2334
D37	59.16871
D38	-61.5098
D39	179.117
D40	179.51144
D41	-21.82004
D42	-57.99491
D43	58.80031
D44	180.0000
D45	-32.39786
D46	149.79886
D47	-177.82462
D48	2.92273
D49	177.42448
D50	-2.59226
D51	0.51161

D52	-179.78707
D53	-179.9662
D54	179.7386

Transition state 1 (TS1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C								
N	1	B1						
C	2	B2	1	A1				
C	3	B3	2	A2	1	D1	0	
O	4	B4	3	A3	2	D2	0	
O	4	B5	3	A4	2	D3	0	
H	2	B6	1	A5	3	D4	0	
O	1	B7	2	A6	3	D5	0	
C	3	B8	2	A7	1	D6	0	
H	9	B9	3	A8	2	D7	0	
H	9	B10	3	A9	2	D8	0	
H	9	B11	3	A10	2	D9	0	
H	3	B12	2	A11	1	D10	0	
H	5	B13	4	A12	3	D11	0	
C	6	B14	4	A13	3	D12	0	
N	15	B15	6	A14	4	D13	0	
C	16	B16	15	A15	6	D14	0	
C	17	B17	16	A16	15	D15	0	
C	18	B18	17	A17	16	D16	0	
N	19	B19	18	A18	17	D17	0	
C	20	B20	19	A19	18	D18	0	
H	21	B21	20	A20	19	D19	0	
H	21	B22	20	A21	19	D20	0	
H	21	B23	20	A22	19	D21	0	
C	20	B24	19	A23	18	D22	0	
H	25	B25	20	A24	19	D23	0	
H	25	B26	20	A25	19	D24	0	
H	25	B27	20	A26	19	D25	0	
H	19	B28	18	A27	17	D26	0	
H	19	B29	18	A28	17	D27	0	
H	18	B30	17	A29	16	D28	0	
H	18	B31	17	A30	16	D29	0	

H	17	B32	16	A31	15	D30	0
H	17	B33	16	A32	15	D31	0
N	15	B34	6	A33	4	D32	0
C	35	B35	15	A34	6	D33	0
H	36	B36	35	A35	15	D34	0
H	36	B37	35	A36	15	D35	0
C	36	B38	35	A37	15	D36	0
H	39	B39	36	A38	35	D37	0
H	39	B40	36	A39	35	D38	0
H	39	B41	36	A40	35	D39	0
O	1	B42	8	A41	2	D40	0
C	43	B43	1	A42	8	D41	0
H	44	B44	43	A43	1	D42	0
H	44	B45	43	A44	1	D43	0
C	44	B46	43	A45	1	D44	0
C	47	B47	44	A46	43	D45	0
C	47	B48	44	A47	43	D46	0
C	48	B49	47	A48	44	D47	0
H	48	B50	47	A49	44	D48	0
C	49	B51	47	A50	44	D49	0
H	49	B52	47	A51	44	D50	0
C	52	B53	49	A52	47	D51	0
H	50	B54	48	A53	47	D52	0
H	52	B55	49	A54	47	D53	0
H	54	B56	52	A55	49	D54	0

Variables:

B1	1.36095
B2	1.45504
B3	1.53585
B4	1.26171
B5	1.27545
B6	1.01178
B7	1.22813
B8	1.53831
B9	1.09619
B10	1.09348
B11	1.0927
B12	1.0968
B13	1.50585
B14	2.15871

B15	1.2884
B16	1.4752
B17	1.5322
B18	1.53393
B19	1.46116
B20	1.45798
B21	1.09528
B22	1.10827
B23	1.09552
B24	1.45873
B25	1.10839
B26	1.09343
B27	1.0949
B28	1.09811
B29	1.1107
B30	1.09598
B31	1.0966
B32	1.09483
B33	1.09552
B34	1.20219
B35	1.45194
B36	1.09567
B37	1.0942
B38	1.5281
B39	1.09356
B40	1.09527
B41	1.09551
B42	1.43
B43	1.43239
B44	1.0953
B45	1.0981
B46	1.51062
B47	1.40096
B48	1.40035
B49	1.3954
B50	1.08519
B51	1.39591
B52	1.08814
B53	1.39596
B54	1.08711

B55	1.087
B56	1.08688
A1	122.46094
A2	109.40089
A3	116.85755
A4	118.01434
A5	121.32827
A6	122.90194
A7	112.54299
A8	110.62115
A9	109.85315
A10	109.17862
A11	108.72594
A12	101.61056
A13	118.03389
A14	97.9658
A15	121.96422
A16	112.0261
A17	111.56522
A18	113.11982
A19	111.19153
A20	109.50818
A21	113.39689
A22	109.84899
A23	112.7681
A24	112.98831
A25	110.68909
A26	109.28918
A27	108.55021
A28	109.54976
A29	108.32789
A30	109.72634
A31	108.48284
A32	106.51742
A33	106.6934
A34	135.74354
A35	106.53011
A36	107.16867
A37	113.53578
A38	110.01014

A39	111.0516
A40	109.81012
A41	121.63182
A42	109.47122
A43	110.20679
A44	109.08369
A45	108.72472
A46	121.33576
A47	119.74232
A48	120.41668
A49	119.12891
A50	120.73493
A51	119.53991
A52	120.04393
A53	119.6455
A54	119.77717
A55	120.20238
D1	-158.84974
D2	173.54639
D3	-7.40907
D4	-166.16617
D5	-5.6696
D6	77.84086
D7	59.88416
D8	-179.87697
D9	-59.89598
D10	-41.7648
D11	175.41309
D12	-175.19195
D13	3.27598
D14	151.67904
D15	-96.92991
D16	-174.95741
D17	-172.61549
D18	165.45124
D19	-176.39564
D20	63.09987
D21	-57.91905
D22	-69.55462
D23	-61.26298

D24	60.17073
D25	178.46313
D26	-53.75263
D27	61.98184
D28	-52.35961
D29	64.18136
D30	26.43648
D31	141.89073
D32	-172.51955
D33	-37.4132
D34	81.43732
D35	-163.94144
D36	-40.65044
D37	60.76633
D38	-59.97857
D39	-179.5019
D40	179.44013
D41	-22.69689
D42	-57.99491
D43	58.80031
D44	180.
D45	-32.39786
D46	149.79886
D47	-177.82462
D48	2.92273
D49	177.42448
D50	-2.59226
D51	0.51161
D52	-179.78707
D53	-179.9662
D54	179.7386

Activated amino acid – conformation 1 (C1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1			
C	3.8577	0.10707	0.1916
N	2.66689	0.44101	-0.385
C	1.79611	1.42759	0.22534
C	0.38117	1.15222	-0.2695

O	-0.49607	2.02832	0.29857
C	-1.88277	1.76406	0.16915
N	-2.33326	0.72621	0.72609
C	-3.68527	0.23944	0.4992
C	-3.66023	-1.29241	0.41076
C	-5.05302	-1.87803	0.16004
N	-5.10331	-3.33688	0.26366
C	-6.47863	-3.81385	0.29901
H	-6.48838	-4.89967	0.44584
H	-7.04645	-3.59226	-0.6278
H	-7.01034	-3.35333	1.13912
C	-4.35438	-4.00448	-0.79334
H	-4.73778	-3.7744	-1.80863
H	-3.29978	-3.71908	-0.75605
H	-4.41146	-5.08887	-0.64915
H	-5.74204	-1.47857	0.91671
H	-5.43512	-1.52916	-0.82384
H	-2.96187	-1.57055	-0.38653
H	-3.25772	-1.70018	1.34491
H	-4.33323	0.53806	1.33711
H	-4.13455	0.65107	-0.41842
N	-2.465	2.78422	-0.54317
H	-1.80258	3.43784	-0.93832
C	-3.80335	3.32264	-0.28636
H	-4.49302	3.03683	-1.09136
H	-4.1807	2.87744	0.63789
C	-3.76679	4.84516	-0.15117
H	-4.77668	5.2373	0.00921
H	-3.37247	5.31369	-1.06154
H	-3.13941	5.15142	0.69283
O	0.08409	0.30861	-1.07956
H	2.24708	-0.18992	-1.05614
O	4.34645	0.70308	1.14114
C	2.24064	2.87084	-0.07876
H	2.22607	3.0596	-1.15763
H	1.5882	3.5914	0.42204
H	3.2614	3.00097	0.28785
H	1.79621	1.29337	1.31518
O	4.39424	-0.95337	-0.46034
C	5.69916	-1.50391	-0.0664

C	6.79757	-0.43905	-0.24295
C	6.54442	0.70536	-0.99972
C	8.04546	-0.61859	0.35378
C	7.53921	1.66964	-1.16024
H	5.56075	0.84625	-1.47068
C	9.04034	0.34636	0.19413
H	8.24509	-1.52042	0.95042
C	8.78748	1.4903	-0.56284
H	7.33996	2.57141	-1.75724
H	10.02402	0.20472	0.66508
H	9.57167	2.25076	-0.68949
H	5.65351	-1.87634	0.93565
H	5.8319	-2.30517	-0.763

Activated amino acid – conformation 2 (C2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.26608	0.78241	1.00293
N	-2.57423	1.94997	0.76481
C	-1.63539	2.14365	-0.32334
C	-0.32552	1.38387	-0.08311
O	0.37642	1.28553	-1.24363
C	1.70047	0.79255	-1.13088
N	2.60909	1.67036	-1.0157
C	4.00102	1.24618	-1.01579
C	4.60192	1.20721	0.40158
C	3.88835	0.2722	1.38421
N	3.77849	-1.13088	0.94228
C	2.90228	-1.87089	1.85333
H	2.78464	-2.90107	1.49875
H	1.91773	-1.39364	1.88004
H	3.29761	-1.90858	2.88521
C	5.07871	-1.7899	0.83057
H	5.70044	-1.2848	0.08677
H	5.62955	-1.80568	1.78979
H	4.93614	-2.82507	0.50288
H	4.39863	0.32575	2.36534
H	2.86736	0.63877	1.53259

H	5.66811	0.95755	0.32188
H	4.55276	2.21566	0.83078
H	4.14778	0.2732	-1.51064
H	4.56838	1.98477	-1.59661
N	1.78856	-0.56921	-1.23492
H	2.57084	-0.9564	-0.69158
C	0.63191	-1.44758	-1.39326
H	0.03629	-1.49755	-0.46856
H	-0.01596	-1.02998	-2.16948
C	1.08584	-2.84919	-1.79675
H	0.2197	-3.50774	-1.92326
H	1.73217	-3.29397	-1.03061
H	1.64388	-2.82239	-2.73839
O	0.04983	0.96041	0.98485
H	-2.38091	2.45087	1.62295
O	-3.84297	0.55675	2.05153
C	-1.33685	3.64038	-0.5092
H	-2.26413	4.17778	-0.72745
H	-0.89344	4.06423	0.39956
H	-0.63135	3.78843	-1.3303
H	-2.08365	1.74997	-1.2378
O	-3.2388	-0.01956	-0.089
C	-3.99559	-1.28289	-0.11484
H	-3.61746	-1.95019	0.63123
H	-3.79227	-1.65544	-1.09707
C	-5.49978	-1.00241	0.05931
C	-6.20466	-0.33324	-0.94161
C	-6.1576	-1.41868	1.21655
C	-7.56728	-0.07987	-0.78469
H	-5.68594	-0.00553	-1.85412
C	-7.52069	-1.16476	1.37379
H	-5.60221	-1.94668	2.00525
C	-8.22524	-0.49533	0.37328
H	-8.12295	0.44768	-1.57339
H	-8.03913	-1.49302	2.28635
H	-9.29952	-0.29506	0.49692

Activated amino acid – conformation 3 (C3)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.29508	-1.79397	-0.31387
C	-3.24728	-1.14982	-1.43784
H	-3.50942	-0.47683	-2.32096
O	-1.85291	-2.17207	0.71225
N	-1.78809	-1.2182	-1.4579
C	-3.86489	-0.35206	-0.20285
O	-4.75407	-0.87726	0.46609
C	-3.93972	-2.50342	-1.68685
H	-3.56984	-2.90632	-2.64329
H	-3.68987	-3.20866	-0.86793
H	-5.03062	-2.40002	-1.72614
O	-3.23384	0.5308	0.36994
H	-1.46897	0.03197	-1.44626
C	-2.26051	1.3775	-0.09813
N	-1.49158	1.15546	-1.10844
N	-2.23281	2.50684	0.6441
H	-1.42053	3.08581	0.47678
C	-0.42945	2.08427	-1.53612
H	-0.24135	1.84394	-2.58173
H	-0.79487	3.12333	-1.50563
C	0.87543	1.91503	-0.72322
H	1.13091	0.85529	-0.71932
C	-2.9787	2.78901	1.87956
H	-3.05059	3.88479	1.94291
H	-3.9883	2.3958	1.76245
C	-2.30734	2.20895	3.13246
H	-2.89554	2.47188	4.02318
H	-2.25524	1.12275	3.07028
H	-1.30126	2.61316	3.26395
C	2.03275	2.76257	-1.29024
H	2.27963	2.40478	-2.30978
H	1.68282	3.80134	-1.41534
H	0.72269	2.20946	0.3289
N	3.20011	2.79708	-0.41206
C	4.14409	3.83799	-0.82439
H	4.97565	3.87921	-0.11257
H	4.56956	3.66696	-1.83353
H	3.64071	4.80657	-0.83646
C	3.87252	1.50898	-0.31753

H	4.26252	1.14739	-1.29337
H	4.7222	1.58694	0.36851
H	3.20463	0.74152	0.08311
O	0.09819	-1.85872	-0.38716
C	0.65296	-2.30976	0.84547
H	0.31803	-1.6785	1.67593
H	0.27234	-3.31397	1.07049
C	2.14748	-2.30559	0.72997
C	2.7699	-2.58833	-0.49051
C	2.93535	-2.04958	1.86196
C	4.16177	-2.62335	-0.57323
H	2.15557	-2.77536	-1.3653
C	4.32768	-2.08327	1.77222
H	2.45315	-1.81384	2.80354
C	4.94061	-2.37417	0.55222
H	4.64164	-2.84843	-1.52736
H	4.93198	-1.88248	2.65316
H	6.03456	-2.40469	0.47846

Transition state 2 (TS2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.2417	-2.00411	-0.24189
C	-3.17771	-1.54497	-1.35098
H	-3.54091	-0.85145	-2.10577
O	-1.84445	-2.37391	0.75592
N	-1.75989	-1.52129	-1.35636
C	-3.81301	-0.99756	-0.07197
O	-4.63534	-1.13791	0.68292
C	-3.82207	-2.91823	-1.59002
H	-3.45098	-3.2825	-2.53953
H	-3.53665	-3.61103	-0.8115
H	-4.90503	-2.85912	-1.63678
O	-3.1888	0.66098	0.18971
H	-1.38953	0.23803	-1.38558
C	-2.318	1.49201	-0.18058
N	-1.42327	1.22241	-1.11505
N	-2.35347	2.70353	0.39365
H	-1.60192	3.32754	0.21649

C	-0.33545	2.07888	-1.55162
H	-0.06605	1.73808	-2.5433
H	-0.69323	3.09707	-1.67053
C	0.88943	2.02251	-0.63486
H	1.1707	0.98246	-0.5195
C	-3.27339	3.05283	1.47012
H	-3.38713	4.1299	1.44141
H	-4.23407	2.61741	1.24425
C	-2.79184	2.60258	2.84455
H	-3.49953	2.91174	3.60746
H	-2.70058	1.52398	2.88242
H	-1.82713	3.03988	3.08331
C	2.04533	2.85234	-1.19361
H	2.40366	2.39937	-2.12504
H	1.66825	3.83719	-1.45627
H	0.64086	2.3961	0.35468
N	3.12415	3.04452	-0.24333
C	4.04054	4.07353	-0.68622
H	4.79443	4.24245	0.07385
H	4.55314	3.81902	-1.619
H	3.50752	5.00543	-0.83862
C	3.83235	1.81881	0.073
H	4.30329	1.36471	-0.80325
H	4.60773	2.03071	0.79967
H	3.16731	1.08852	0.51169
O	0.10337	-1.9977	-0.25881
C	0.75969	-2.48261	0.88804
H	0.44399	-1.92791	1.76118
H	0.48617	-3.51834	1.05094
C	2.25225	-2.35451	0.68841
C	2.82916	-2.44523	-0.57339
C	3.07995	-2.18698	1.7917
C	4.20441	-2.37136	-0.72308
H	2.19839	-2.56636	-1.43351
C	4.45631	-2.11793	1.64354
H	2.64799	-2.10898	2.77503
C	5.02357	-2.20912	0.38342
H	4.63689	-2.44273	-1.70563
H	5.0813	-1.98866	2.5095
H	6.09113	-2.15365	0.26435

Molecular complex 2 (MC2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.37508	-1.73397	-0.45387
C	-3.26728	-1.40982	-1.49784
H	-3.72942	-0.49683	-1.96096
O	-2.15291	-1.77207	0.61225
N	-1.84809	-1.4582	-1.6379
C	-3.64489	-1.39206	0.03715
O	-4.63407	-1.31726	0.68609
C	-3.95972	-2.70342	-1.98685
H	-3.68984	-2.86632	-3.04329
H	-3.60987	-3.56867	-1.40793
H	-5.05062	-2.62002	-1.90614
O	-3.05383	0.7708	0.38994
H	-1.48897	0.53197	-1.48626
C	-2.24051	1.5975	0.02187
N	-1.47158	1.41546	-1.10844
N	-2.11281	2.78684	0.6841
H	-1.32053	3.38581	0.51678
C	-0.34945	2.22426	-1.53612
H	-0.18135	2.00394	-2.60173
H	-0.63487	3.28333	-1.50563
C	0.93543	1.97503	-0.74322
H	1.15091	0.89529	-0.77932
C	-2.8787	2.96901	1.91956
H	-2.95059	4.04479	2.10291
H	-3.8883	2.5958	1.72245
C	-2.28734	2.24895	3.13246
H	-2.89554	2.43188	4.02318
H	-2.25524	1.16275	2.95028
H	-1.26126	2.59316	3.34395
C	2.09275	2.80257	-1.29024
H	2.35963	2.44478	-2.30978
H	1.76282	3.84134	-1.39534
H	0.78269	2.22946	0.3089
N	3.26011	2.81708	-0.41206
C	4.20409	3.83799	-0.82439

H	5.03565	3.87921	-0.11257
H	4.62956	3.66696	-1.83353
H	3.72071	4.82657	-0.81646
C	3.91252	1.50898	-0.31753
H	4.28252	1.14739	-1.29337
H	4.7622	1.58694	0.36851
H	3.22463	0.76152	0.08311
O	-0.04181	-1.89872	-0.34716
C	0.55296	-2.28976	0.90547
H	0.23803	-1.5985	1.69593
H	0.19234	-3.29397	1.17049
C	2.06748	-2.28559	0.74997
C	2.6899	-2.58833	-0.47051
C	2.87535	-2.02958	1.86196
C	4.08177	-2.62335	-0.57323
H	2.07557	-2.77536	-1.3453
C	4.26768	-2.08327	1.77222
H	2.41315	-1.79384	2.82354
C	4.88061	-2.37417	0.55222
H	4.54164	-2.84843	-1.52736
H	4.87198	-1.88248	2.65316
H	5.95456	-2.40469	0.47846

Azlactone

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.15856	-0.35202	0.03217
C	-2.02649	0.69581	0.47136
H	-2.35866	0.8341	1.51001
O	-1.1004	-1.34323	-0.19199
N	-0.56886	0.79957	0.40026
C	-2.33348	-0.74741	0.06473
O	-3.37104	-1.33236	-0.05083
C	-2.75143	1.71001	-0.42015
H	-3.83317	1.55643	-0.36016
H	-2.51398	2.72616	-0.09332
H	-2.43832	1.60103	-1.46348
O	1.05414	-0.81282	-0.19113
C	2.25885	0.03932	-0.02672

C	3.39384	-0.93503	-0.39282
C	3.09561	-2.24931	-0.75367
C	4.71996	-0.50362	-0.36379
C	4.12338	-3.1321	-1.08473
H	2.05008	-2.58933	-0.77571
C	5.74809	-1.38628	-0.69588
H	4.95518	0.53225	-0.07958
C	5.45004	-2.70039	-1.05619
H	3.88843	-4.16822	-1.36856
H	6.79355	-1.04574	-0.6733
H	6.26022	-3.3966	-1.31732
H	2.21524	0.85884	-0.71329
H	2.33656	0.35973	0.99122

R = OFm

N-Protected alanine

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.40741	-1.22421	-1.01957
N	0.23806	-1.28565	-0.32646
C	-0.89523	-2.03228	-0.84105
C	-2.14306	-1.47783	-0.16374
O	-3.25444	-2.11507	-0.62602
O	-2.14192	-0.62441	0.68993
H	0.04483	-0.59953	0.3926
O	1.66913	-1.87224	-2.01913
C	-0.74642	-3.54954	-0.6216
H	-0.67379	-3.7794	0.44687
H	-1.59752	-4.08683	-1.0487
H	0.16872	-3.88228	-1.11656
H	-0.99757	-1.85069	-1.91932
O	2.26005	-0.34137	-0.42903
C	3.55273	-0.23018	-1.05429
H	4.03862	-1.21009	-1.07342
C	4.37279	0.78266	-0.24972
H	3.77438	1.70253	-0.17371
C	4.78923	0.3027	1.13392

C	5.71446	1.07102	-0.90859
C	6.1951	0.30935	1.24882
C	3.99814	-0.10181	2.20437
C	6.76847	0.78361	-0.01755
C	5.98179	1.54799	-2.18707
C	6.81228	-0.08982	2.43586
H	2.91641	-0.11081	2.11764
C	4.61945	-0.50333	3.39272
C	8.0953	0.97486	-0.40763
H	5.17439	1.77707	-2.87863
C	7.31286	1.73696	-2.57733
H	7.89529	-0.08444	2.53003
C	6.01367	-0.49675	3.5066
H	4.01183	-0.82196	4.23557
H	8.91319	0.75759	0.2746
C	8.35891	1.45177	-1.69367
H	7.53434	2.10942	-3.57377
H	6.47984	-0.80963	4.43725
H	9.38729	1.60436	-2.01044
H	3.42105	0.10346	-2.08833
H	-4.11115	-1.73736	-0.41394

Molecular complex 1 (MC1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C								
N	1	B1						
C	2	B2	1	A1				
C	3	B3	2	A2	1	D1	0	
O	4	B4	3	A3	2	D2	0	
O	4	B5	3	A4	2	D3	0	
H	2	B6	1	A5	3	D4	0	
O	1	B7	2	A6	3	D5	0	
C	3	B8	2	A7	1	D6	0	
H	9	B9	3	A8	2	D7	0	
H	9	B10	3	A9	2	D8	0	
H	9	B11	3	A10	2	D9	0	
H	3	B12	2	A11	1	D10	0	
H	5	B13	4	A12	3	D11	0	

C	6	B14	4	A13	3	D12	0	
N	15	B15	6	A14	4	D13	0	
C	16	B16	15	A15	6	D14	0	
C	17	B17	16	A16	15	D15	0	
C	18	B18	17	A17	16	D16	0	
N	19	B19	18	A18	17	D17	0	
C	20	B20	19	A19	18	D18	0	
H	21	B21	20	A20	19	D19	0	
H	21	B22	20	A21	19	D20	0	
H	21	B23	20	A22	19	D21	0	
C	20	B24	19	A23	18	D22	0	
H	25	B25	20	A24	19	D23	0	
H	25	B26	20	A25	19	D24	0	
H	25	B27	20	A26	19	D25	0	
H	19	B28	18	A27	17	D26	0	
H	19	B29	18	A28	17	D27	0	
H	18	B30	17	A29	16	D28	0	
H	18	B31	17	A30	16	D29	0	
H	17	B32	16	A31	15	D30	0	
H	17	B33	16	A32	15	D31	0	
N	15	B34	6	A33	4	D32	0	
C	35	B35	15	A34	6	D33	0	
H	36	B36	35	A35	15	D34	0	
H	36	B37	35	A36	15	D35	0	
C	36	B38	35	A37	15	D36	0	
H	39	B39	36	A38	35	D37	0	
H	39	B40	36	A39	35	D38	0	
H	39	B41	36	A40	35	D39	0	
O	1	B42	8	A41	2	D40	0	
C	43	B43	1	A42	8	D41	0	
H	44	B44	43	A43	1	D42	0	
H	44	B45	43	A44	1	D43	0	
C	44	B46	43	A45	1	D44	0	
H	47	B47	44	A46	43	D45	0	
C	47	B48	44	A47	43	D46	0	
C	47	B49	44	A48	43	D47	0	
C	49	B50	47	A49	44	D48	0	
C	49	B51	47	A50	44	D49	0	
C	50	B52	47	A51	44	D50	0	
C	8	B53	1	A52	2	D51	0	

C	51	B54	49	A53	47	D52	0
H	52	B55	49	A54	47	D53	0
C	52	B56	49	A55	47	D54	0
C	53	B57	50	A56	47	D55	0
H	54	B58	8	A57	1	D56	0
C	54	B59	8	A58	1	D57	0
H	55	B60	51	A59	49	D58	0
C	55	B61	51	A60	49	D59	0
H	57	B62	52	A61	49	D60	0
H	58	B63	53	A62	50	D61	0
C	58	B64	53	A63	50	D62	0
H	60	B65	54	A64	8	D63	0
H	62	B66	55	A65	51	D64	0
H	65	B67	58	A66	53	D65	0

Variables:

B1	1.36322
B2	1.45189
B3	1.52499
B4	1.33041
B5	1.22144
B6	1.01231
B7	1.22745
B8	1.54077
B9	1.0955
B10	1.09359
B11	1.0923
B12	1.09705
B13	1.00354
B14	3.38635
B15	1.23953
B16	1.4723
B17	1.53249
B18	1.53345
B19	1.46182
B20	1.45756
B21	1.0954
B22	1.10847
B23	1.09554
B24	1.45836
B25	1.10866

B26	1.09346
B27	1.09503
B28	1.09806
B29	1.11083
B30	1.09596
B31	1.09658
B32	1.09772
B33	1.09657
B34	1.21329
B35	1.46078
B36	1.09598
B37	1.09616
B38	1.5268
B39	1.0942
B40	1.0963
B41	1.09578
B42	1.43
B43	1.41016
B44	1.08207
B45	1.08111
B46	1.52661
B47	1.08805
B48	1.51953
B49	1.52056
B50	1.39495
B51	1.38138
B52	1.39513
B53	5.22809
B54	1.38487
B55	1.07619
B56	1.38929
B57	1.38529
B58	1.07359
B59	1.38898
B60	1.07565
B61	1.38693
B62	1.07549
B63	1.0758
B64	1.38601
B65	1.07567

B66	1.0756
B67	1.07573
A1	121.92725
A2	107.67964
A3	112.15383
A4	123.35368
A5	121.51042
A6	122.49415
A7	112.61741
A8	110.63129
A9	110.45369
A10	108.56941
A11	108.908
A12	109.23887
A13	103.31244
A14	81.18961
A15	123.79597
A16	111.07749
A17	111.61664
A18	113.31987
A19	111.11245
A20	109.55559
A21	113.37908
A22	109.84504
A23	112.7835
A24	112.99935
A25	110.65029
A26	109.30068
A27	108.57228
A28	109.51062
A29	108.26174
A30	109.72609
A31	110.81388
A32	107.03854
A33	98.25231
A34	130.67332
A35	106.41223
A36	106.85909
A37	114.94158
A38	110.41681

A39	110.98078
A40	109.9599
A41	122.00248
A42	109.47122
A43	109.73718
A44	110.40145
A45	107.15623
A46	107.65698
A47	112.71266
A48	114.46382
A49	110.61721
A50	129.0682
A51	110.4967
A52	37.09456
A53	120.62402
A54	120.96905
A55	119.12772
A56	120.80549
A57	58.43286
A58	147.33823
A59	120.96458
A60	118.87922
A61	119.77257
A62	121.01216
A63	118.74198
A64	119.59271
A65	119.73345
A66	119.7538
D1	-158.97349
D2	172.97265
D3	-7.72288
D4	-167.85532
D5	-4.83962
D6	78.00051
D7	60.33394
D8	-178.86804
D9	-59.1879
D10	-41.80424
D11	178.31364
D12	178.81445

D13	15.90508
D14	146.43146
D15	-111.57018
D16	-174.15897
D17	-171.77387
D18	166.55486
D19	-176.24966
D20	63.23109
D21	-57.73572
D22	-68.54237
D23	-60.86963
D24	60.52448
D25	178.86662
D26	-52.88282
D27	62.84147
D28	-51.62487
D29	64.89615
D30	11.76012
D31	128.50792
D32	-155.43718
D33	-56.92286
D34	120.44168
D35	-126.13671
D36	-2.2334
D37	59.16871
D38	-61.5098
D39	179.117
D40	179.51144
D41	19.2728
D42	-59.74989
D43	59.09813
D44	180.
D45	53.63732
D46	175.28285
D47	-68.93836
D48	123.34266
D49	-57.10133
D50	-122.22789
D51	148.64021
D52	179.69955

D53	0.24467
D54	-179.71391
D55	-179.65707
D56	4.41988
D57	-94.12701
D58	-179.98963
D59	0.06041
D60	-179.87084
D61	179.99756
D62	-0.05356
D63	78.80949
D64	179.8965
D65	-179.9407

Transition state 1 (TS1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C								
N	1	B1						
C	2	B2	1	A1				
C	3	B3	2	A2	1	D1	0	
O	4	B4	3	A3	2	D2	0	
O	4	B5	3	A4	2	D3	0	
H	2	B6	1	A5	3	D4	0	
O	1	B7	2	A6	3	D5	0	
C	3	B8	2	A7	1	D6	0	
H	9	B9	3	A8	2	D7	0	
H	9	B10	3	A9	2	D8	0	
H	9	B11	3	A10	2	D9	0	
H	3	B12	2	A11	1	D10	0	
H	5	B13	4	A12	3	D11	0	
C	6	B14	4	A13	3	D12	0	
N	15	B15	6	A14	4	D13	0	
C	16	B16	15	A15	6	D14	0	
C	17	B17	16	A16	15	D15	0	
C	18	B18	17	A17	16	D16	0	
N	19	B19	18	A18	17	D17	0	
C	20	B20	19	A19	18	D18	0	
H	21	B21	20	A20	19	D19	0	

H 21 B22 20 A21 19 D20 0
H 21 B23 20 A22 19 D21 0
C 20 B24 19 A23 18 D22 0
H 25 B25 20 A24 19 D23 0
H 25 B26 20 A25 19 D24 0
H 25 B27 20 A26 19 D25 0
H 19 B28 18 A27 17 D26 0
H 19 B29 18 A28 17 D27 0
H 18 B30 17 A29 16 D28 0
H 18 B31 17 A30 16 D29 0
H 17 B32 16 A31 15 D30 0
H 17 B33 16 A32 15 D31 0
N 15 B34 6 A33 4 D32 0
C 35 B35 15 A34 6 D33 0
H 36 B36 35 A35 15 D34 0
H 36 B37 35 A36 15 D35 0
C 36 B38 35 A37 15 D36 0
H 39 B39 36 A38 35 D37 0
H 39 B40 36 A39 35 D38 0
H 39 B41 36 A40 35 D39 0
O 1 B42 8 A41 2 D40 0
C 43 B43 1 A42 8 D41 0
H 44 B44 43 A43 1 D42 0
H 44 B45 43 A44 1 D43 0
C 44 B46 43 A45 1 D44 0
H 47 B47 44 A46 43 D45 0
C 47 B48 44 A47 43 D46 0
C 47 B49 44 A48 43 D47 0
C 49 B50 47 A49 44 D48 0
C 49 B51 47 A50 44 D49 0
C 50 B52 47 A51 44 D50 0
C 8 B53 1 A52 2 D51 0
C 51 B54 49 A53 47 D52 0
H 52 B55 49 A54 47 D53 0
C 52 B56 49 A55 47 D54 0
C 53 B57 50 A56 47 D55 0
H 54 B58 8 A57 1 D56 0
C 54 B59 8 A58 1 D57 0
H 55 B60 51 A59 49 D58 0
C 55 B61 51 A60 49 D59 0

H	57	B62	52	A61	49	D60	0
H	58	B63	53	A62	50	D61	0
C	58	B64	53	A63	50	D62	0
H	60	B65	54	A64	8	D63	0
H	62	B66	55	A65	51	D64	0
H	65	B67	58	A66	53	D65	0

Variables:

B1	1.36095
B2	1.45504
B3	1.53585
B4	1.26171
B5	1.27545
B6	1.01178
B7	1.22813
B8	1.53831
B9	1.09619
B10	1.09348
B11	1.0927
B12	1.0968
B13	1.50585
B14	2.15871
B15	1.2884
B16	1.4752
B17	1.5322
B18	1.53393
B19	1.46116
B20	1.45798
B21	1.09528
B22	1.10827
B23	1.09552
B24	1.45873
B25	1.10839
B26	1.09343
B27	1.0949
B28	1.09811
B29	1.1107
B30	1.09598
B31	1.0966
B32	1.09483
B33	1.09552

B34	1.20219
B35	1.45194
B36	1.09567
B37	1.0942
B38	1.5281
B39	1.09356
B40	1.09527
B41	1.09551
B42	1.43
B43	1.41016
B44	1.08207
B45	1.08111
B46	1.52661
B47	1.08805
B48	1.51953
B49	1.52056
B50	1.39495
B51	1.38138
B52	1.39513
B53	5.22743
B54	1.38487
B55	1.07619
B56	1.38929
B57	1.38529
B58	1.07359
B59	1.38898
B60	1.07565
B61	1.38693
B62	1.07549
B63	1.0758
B64	1.38601
B65	1.07567
B66	1.0756
B67	1.07573
A1	122.46094
A2	109.40089
A3	116.85755
A4	118.01434
A5	121.32827
A6	122.90194

A7	112.54299
A8	110.62115
A9	109.85315
A10	109.17862
A11	108.72594
A12	101.61056
A13	118.03389
A14	97.9658
A15	121.96422
A16	112.0261
A17	111.56522
A18	113.11982
A19	111.19153
A20	109.50818
A21	113.39689
A22	109.84899
A23	112.7681
A24	112.98831
A25	110.68909
A26	109.28918
A27	108.55021
A28	109.54976
A29	108.32789
A30	109.72634
A31	108.48284
A32	106.51742
A33	106.6934
A34	135.74354
A35	106.53011
A36	107.16867
A37	113.53578
A38	110.01014
A39	111.0516
A40	109.81012
A41	121.63182
A42	109.47122
A43	109.73718
A44	110.40145
A45	107.15623
A46	107.65698

A47	112.71266
A48	114.46382
A49	110.61721
A50	129.0682
A51	110.4967
A52	37.16525
A53	120.62402
A54	120.96905
A55	119.12772
A56	120.80549
A57	58.4438
A58	147.46693
A59	120.96458
A60	118.87922
A61	119.77257
A62	121.01216
A63	118.74198
A64	119.59271
A65	119.73345
A66	119.7538
D1	-158.84974
D2	173.54639
D3	-7.40907
D4	-166.16617
D5	-5.6696
D6	77.84086
D7	59.88416
D8	-179.87697
D9	-59.89598
D10	-41.7648
D11	175.41309
D12	-175.19195
D13	3.27598
D14	151.67904
D15	-96.92991
D16	-174.95741
D17	-172.61549
D18	165.45124
D19	-176.39564
D20	63.09987

D21	-57.91905
D22	-69.55462
D23	-61.26298
D24	60.17073
D25	178.46313
D26	-53.75263
D27	61.98184
D28	-52.35961
D29	64.18136
D30	26.43648
D31	141.89073
D32	-172.51955
D33	-37.4132
D34	81.43732
D35	-163.94144
D36	-40.65044
D37	60.76633
D38	-59.97857
D39	-179.5019
D40	179.44013
D41	19.77142
D42	-59.74989
D43	59.09813
D44	180.0000
D45	53.63732
D46	175.28285
D47	-68.93836
D48	123.34266
D49	-57.10133
D50	-122.22789
D51	148.96601
D52	179.69955
D53	0.24467
D54	-179.71391
D55	-179.65707
D56	5.08661
D57	-93.42683
D58	-179.98963
D59	0.06041
D60	-179.87084

D61	179.99756
D62	-0.05356
D63	78.86586
D64	179.8965
D65	-179.9407

Activated amino acid – conformation 1 (C1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.93204	-0.17722	-0.74911
N	-1.83063	0.19451	-0.04344
C	-0.95754	1.24961	-0.52351
C	0.41311	1.0223	0.10286
O	1.29791	1.95854	-0.34271
C	2.67839	1.73539	-0.10457
N	3.21128	0.7427	-0.67067
C	4.55619	0.28526	-0.35709
C	4.57649	-1.24911	-0.35187
C	5.96455	-1.80654	-0.02258
N	6.07055	-3.2561	-0.19184
C	7.45959	-3.69031	-0.14443
H	7.51574	-4.76702	-0.33982
H	7.94965	-3.49713	0.83182
H	8.037	-3.17456	-0.91979
C	5.26568	-3.99787	0.77026
H	5.55763	-3.80306	1.82261
H	4.20732	-3.74745	0.65977
H	5.37515	-5.07162	0.58336
H	6.69561	-1.34957	-0.70346
H	6.25916	-1.4968	1.00365
H	3.828	-1.59145	0.37157
H	4.26168	-1.61628	-1.33523
H	5.25971	0.64931	-1.1211
H	4.91478	0.65848	0.61524
N	3.15745	2.73719	0.70275
H	2.44039	3.34801	1.06983
C	4.49737	3.32145	0.6054
H	5.11766	3.00376	1.45375
H	4.97126	2.94227	-0.3037
C	4.42759	4.84792	0.55753

H	5.43559	5.27415	0.51823
H	3.93533	5.24881	1.45235
H	3.87321	5.19047	-0.32282
O	0.66922	0.16107	0.90841
H	-1.45087	-0.43648	0.65158
O	-3.36522	0.4149	-1.72722
C	-1.50811	2.65415	-0.213
H	-1.61237	2.79761	0.8678
H	-0.84793	3.4265	-0.61717
H	-2.49252	2.75	-0.67692
H	-0.84041	1.16064	-1.61148
O	-3.47929	-1.29582	-0.20403
C	-4.67198	-1.78034	-0.82663
H	-5.43598	-1.03505	-0.75079
C	-5.15595	-3.06846	-0.15133
H	-4.39858	-3.84161	-0.35091
C	-5.35896	-2.90137	1.34701
C	-6.5261	-3.54465	-0.6121
C	-6.67985	-3.24423	1.70281
C	-4.45402	-2.48522	2.3173
C	-7.40269	-3.64458	0.48844
C	-6.96425	-3.86152	-1.89439
C	-7.09453	-3.17163	3.03406
H	-3.43325	-2.22061	2.05108
C	-4.87218	-2.41008	3.65129
C	-8.72115	-4.06807	0.30965
H	-6.29309	-3.76918	-2.74217
C	-8.2875	-4.28315	-2.06996
H	-8.11074	-3.4359	3.3157
C	-6.18192	-2.75116	4.0043
H	-4.17389	-2.08462	4.41775
H	-9.40087	-4.14771	1.15447
C	-9.15647	-4.38697	-0.9782
H	-8.64393	-4.53074	-3.06646
H	-6.49264	-2.68867	5.04399
H	-10.18039	-4.71717	-1.13371
H	-4.47429	-1.97763	-1.85953

Activated amino acid – conformation 2 (C2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.26608	0.78241	1.00293
N	-2.57423	1.94997	0.76481
C	-1.63539	2.14365	-0.32334
C	-0.32552	1.38387	-0.08311
O	0.37642	1.28553	-1.24363
C	1.70047	0.79255	-1.13088
N	2.60909	1.67036	-1.0157
C	4.00102	1.24618	-1.01579
C	4.60192	1.20721	0.40158
C	3.88835	0.2722	1.38421
N	3.77849	-1.13088	0.94228
C	2.90228	-1.87089	1.85333
H	2.78464	-2.90107	1.49875
H	1.91773	-1.39364	1.88004
H	3.29761	-1.90858	2.88521
C	5.07871	-1.7899	0.83057
H	5.70044	-1.2848	0.08677
H	5.62955	-1.80568	1.78979
H	4.93614	-2.82507	0.50288
H	4.39863	0.32575	2.36534
H	2.86736	0.63877	1.53259
H	5.66811	0.95755	0.32188
H	4.55276	2.21566	0.83078
H	4.14778	0.2732	-1.51064
H	4.56838	1.98477	-1.59661
N	1.78856	-0.56921	-1.23492
H	2.57084	-0.9564	-0.69158
C	0.63191	-1.44758	-1.39326
H	0.03629	-1.49755	-0.46856
H	-0.01596	-1.02998	-2.16948
C	1.08584	-2.84919	-1.79675
H	0.2197	-3.50774	-1.92326
H	1.73217	-3.29397	-1.03061
H	1.64388	-2.82239	-2.73839
O	0.04983	0.96041	0.98485
H	-2.38091	2.45087	1.62295
O	-3.84297	0.55675	2.05153
C	-1.33685	3.64038	-0.5092

H	-2.26413	4.17778	-0.72745
H	-0.89344	4.06423	0.39956
H	-0.63135	3.78843	-1.3303
H	-2.08365	1.74997	-1.2378
O	-3.2388	-0.01956	-0.089
C	-3.97355	-1.2461	-0.11409
C	-5.41967	-1.02008	-0.56501
H	-3.49806	-1.92518	-0.79059
H	-5.95245	-1.97542	-0.44873
C	-6.14835	0.08989	0.18014
C	-5.49102	-0.54077	-2.0081
C	-6.57676	1.08377	-0.72451
C	-6.41653	0.2137	1.53958
C	-6.1677	0.69389	-2.08025
C	-5.00043	-1.14472	-3.16051
C	-7.27419	2.20456	-0.26984
H	-6.08541	-0.54795	2.23814
C	-7.11428	1.33927	1.99307
C	-6.35448	1.32626	-3.31087
H	-4.48195	-2.09953	-3.11413
C	-5.18657	-0.5081	-4.39332
H	-7.60829	2.97218	-0.96335
C	-7.53907	2.3249	1.09588
H	-7.32909	1.44721	3.05294
H	-6.87716	2.27722	-3.37468
C	-5.85773	0.71696	-4.46535
H	-4.80792	-0.97035	-5.30086
H	-8.08158	3.19155	1.46457
H	-5.99552	1.19887	-5.42969
H	-3.97551	-1.67307	0.86703

Activated amino acid – conformation 3 (C3)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.15445	-1.85976	-0.49691
C	-1.98346	-2.99363	-1.43398
H	-2.8416	-2.75316	-2.14547
O	0.04511	-2.68809	0.38741
N	-1.14236	-1.78638	-1.45766

C	-2.74719	-3.20971	-0.03916
O	-2.68937	-4.32138	0.50471
C	-1.30661	-4.26346	-1.96546
H	-0.96121	-4.06261	-2.99217
H	-0.44268	-4.5231	-1.33076
H	-2.00489	-5.11181	-1.97593
O	-2.96374	-2.28264	0.67724
H	-2.00329	-0.91581	-1.24451
C	-3.42267	-1.04051	0.27904
N	-2.98178	-0.40651	-0.75378
N	-4.34512	-0.5663	1.12798
H	-4.54248	0.42019	1.01672
C	-3.57175	0.85198	-1.23519
H	-3.36006	0.87565	-2.3134
H	-4.66403	0.81056	-1.126
C	-3.00048	2.11659	-0.57863
H	-1.91133	2.06827	-0.64469
C	-4.83114	-1.17655	2.38222
H	-5.87806	-0.8678	2.49293
H	-4.81802	-2.2556	2.25077
C	-3.99965	-0.76366	3.59882
H	-4.41181	-1.22361	4.50675
H	-2.9543	-1.10739	3.48469
H	-3.99424	0.31925	3.73979
C	-3.54447	3.40312	-1.23007
H	-3.20283	3.4414	-2.27874
H	-4.64182	3.34553	-1.25284
H	-3.24018	2.156	0.497
N	-3.19197	4.62041	-0.49084
C	-3.96226	5.76215	-0.96168
H	-3.71896	6.63668	-0.34889
H	-3.74808	6.03059	-2.0196
H	-5.02548	5.56584	-0.86147
C	-1.75992	4.90799	-0.53014
H	-1.37797	5.08014	-1.55763
H	-1.56029	5.80927	0.05516
H	-1.18511	4.09513	-0.08333
O	0.68081	-0.76139	-0.59793
C	1.63139	-0.73631	0.47309
H	1.10835	-0.62487	1.43158

H	2.17826	-1.68653	0.52039
C	2.57978	0.42582	0.22567
H	1.9562	1.32273	0.07349
C	3.54808	0.64416	1.36597
C	3.50995	0.22497	-0.96376
C	4.87467	0.5909	0.89932
C	4.85453	0.32651	-0.54521
C	5.88226	0.1827	-1.4698
H	6.92039	0.26624	-1.16056
C	3.18753	-0.04593	-2.28454
H	2.15316	-0.15461	-2.59433
C	5.56469	-0.07713	-2.80448
H	6.3615	-0.19495	-3.53599
C	4.23074	-0.20207	-3.20799
H	4.00121	-0.41914	-4.25001
C	5.94603	0.7791	1.77245
H	6.97108	0.73867	1.42165
C	3.29094	0.873	2.71147
H	2.27067	0.9094	3.08642
C	4.36636	1.05857	3.59626
H	4.16725	1.23442	4.65016
C	5.68201	1.01674	3.12332
H	6.5072	1.16093	3.82375

Transition state 2 (TS2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.56792	-2.0346	-0.25196
C	-2.38941	-3.01269	-1.20897
H	-3.20134	-2.74859	-1.88276
O	-0.65621	-2.74001	0.74211
N	-1.38761	-2.0113	-1.28922
C	-3.09827	-3.09028	0.14385
O	-3.51436	-3.77893	0.93033
C	-1.92868	-4.44232	-1.52881
H	-1.50366	-4.42427	-2.52428
H	-1.17054	-4.76139	-0.82827
H	-2.75168	-5.15007	-1.51218
O	-3.76659	-1.46961	0.50959

H	-2.37724	-0.52081	-1.2407
C	-3.83344	-0.29127	0.07163
N	-3.10674	0.13351	-0.94736
N	-4.70955	0.53051	0.66855
H	-4.67557	1.4962	0.4405
C	-3.07556	1.47678	-1.4947
H	-2.72642	1.37741	-2.51477
H	-4.08444	1.8726	-1.55872
C	-2.15462	2.42642	-0.72423
H	-1.18156	1.9547	-0.65019
C	-5.50363	0.14607	1.83025
H	-6.37965	0.78355	1.82993
H	-5.83874	-0.86887	1.6853
C	-4.7475	0.27655	3.14734
H	-5.3931	0.00457	3.97652
H	-3.88523	-0.37877	3.15858
H	-4.40949	1.29635	3.30478
C	-2.05984	3.79204	-1.40456
H	-1.56552	3.68321	-2.37647
H	-3.06655	4.14543	-1.60976
H	-2.51546	2.56783	0.29074
N	-1.41054	4.79705	-0.58422
C	-1.61551	6.12794	-1.1166
H	-1.17969	6.85985	-0.44678
H	-1.16952	6.26727	-2.10586
H	-2.67651	6.33719	-1.19273
C	-0.00135	4.53556	-0.36816
H	0.57203	4.50863	-1.2994
H	0.41606	5.312	0.26158
H	0.14008	3.59282	0.14324
O	0.41027	-1.11818	-0.35014
C	1.36945	-1.0837	0.68298
H	0.88747	-0.84216	1.62119
H	1.84225	-2.04996	0.79067
C	2.39338	-0.01414	0.3113
H	1.85072	0.90838	0.1155
C	3.42944	0.20978	1.40006
C	3.26651	-0.36619	-0.88276
C	4.71731	0.01842	0.89941
C	4.61514	-0.33936	-0.5266

C	5.60071	-0.62149	-1.45831
H	6.64163	-0.60172	-1.18731
C	2.8921	-0.67797	-2.17699
H	1.85493	-0.7127	-2.45205
C	5.22263	-0.9331	-2.75483
H	5.97448	-1.15583	-3.49125
C	3.88097	-0.96196	-3.11014
H	3.60353	-1.20932	-4.11955
C	5.82313	0.17682	1.7179
H	6.81864	0.03079	1.33757
C	3.24066	0.56276	2.72217
H	2.25203	0.71672	3.1185
C	4.34896	0.72002	3.545
H	4.21387	0.99263	4.57656
C	5.62904	0.52803	3.04551
H	6.47812	0.65303	3.69387

Molecular complex 2 (MC2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.25445	-1.89976	-0.61691
C	-1.80346	-3.11363	-1.53398
H	-2.8816	-2.93316	-1.78547
O	-0.45489	-2.70809	0.40741
N	-0.98236	-1.96638	-1.69766
C	-1.72719	-3.60971	-0.03916
O	-2.24937	-4.46138	0.60471
C	-1.24661	-4.34346	-2.30546
H	-1.16121	-4.08261	-3.37217
H	-0.24268	-4.6031	-1.93076
H	-1.90489	-5.21181	-2.19593
O	-2.94374	-1.92264	0.85724
H	-2.40329	-0.61581	-1.16451
C	-3.50267	-0.92051	0.45904
N	-3.16178	-0.28651	-0.71378
N	-4.56512	-0.3863	1.16798
H	-4.82248	0.58019	1.03672
C	-3.69175	0.95198	-1.23519
H	-3.52006	0.95565	-2.3134

H	-4.78403	0.97056	-1.106
C	-3.04048	2.19659	-0.59863
H	-1.95133	2.10827	-0.72469
C	-4.93114	-1.03655	2.42222
H	-5.95806	-0.7278	2.65293
H	-4.93802	-2.1156	2.23077
C	-3.99965	-0.72366	3.59882
H	-4.35181	-1.22361	4.50675
H	-2.9943	-1.06739	3.38469
H	-3.97424	0.35925	3.79979
C	-3.56447	3.48312	-1.23007
H	-3.24283	3.5414	-2.29874
H	-4.66182	3.44553	-1.25284
H	-3.24018	2.216	0.477
N	-3.19197	4.68041	-0.49084
C	-3.94226	5.84215	-0.96168
H	-3.69896	6.71668	-0.34889
H	-3.74808	6.09058	-2.0196
H	-5.02548	5.64584	-0.86147
C	-1.75992	4.94799	-0.53014
H	-1.37797	5.10014	-1.55763
H	-1.54029	5.84927	0.05516
H	-1.20511	4.11513	-0.08333
O	0.68081	-0.92139	-0.55793
C	1.61139	-0.85631	0.53309
H	1.06835	-0.70487	1.47158
H	2.17826	-1.78653	0.60039
C	2.53978	0.34582	0.24567
H	1.8962	1.22273	0.09349
C	3.52808	0.60416	1.38597
C	3.46995	0.16497	-0.94376
C	4.85467	0.5709	0.89932
C	4.81453	0.30651	-0.54521
C	5.86226	0.1827	-1.4698
H	6.90038	0.28624	-1.16056
C	3.16753	-0.08593	-2.28454
H	2.13316	-0.19461	-2.59433
C	5.54469	-0.07713	-2.80448
H	6.3415	-0.17495	-3.53599
C	4.21074	-0.20207	-3.20799

H	3.98121	-0.39914	-4.25001
C	5.92603	0.7791	1.77245
H	6.95108	0.75867	1.40165
C	3.27094	0.853	2.73147
H	2.25067	0.8894	3.10642
C	4.34636	1.05857	3.59626
H	4.16725	1.25442	4.65016
C	5.66201	1.01674	3.12332
H	6.4872	1.18093	3.80375

Azlactone

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.32798	0.166	-0.07203
C	-3.3611	-0.41455	-0.60096
H	-3.78638	-0.1374	-1.57576
O	-2.06304	1.12847	0.58679
N	-1.93843	-0.72376	-0.75187
C	-3.39734	0.82404	0.30029
O	-4.31069	1.46251	0.73358
C	-4.17517	-1.57369	-0.01553
H	-5.21916	-1.27228	0.11316
H	-4.12952	-2.43368	-0.68924
H	-3.77385	-1.87567	0.95716
O	-0.03073	0.32437	0.11552
C	0.79471	-0.63761	-0.5464
H	0.93974	-1.47937	0.09804
C	2.15831	-0.03459	-0.90209
H	1.97848	0.74881	-1.65385
C	2.87266	0.54784	0.30813
C	3.17456	-1.03992	-1.42451
C	4.14318	-0.04552	0.45848
C	2.44077	1.52245	1.20096
C	4.33079	-1.02852	-0.61668
C	3.08684	-1.8947	-2.51918
C	4.98361	0.33972	1.50477
H	1.46301	1.98583	1.0908
C	3.28341	1.90553	2.25132
C	5.40698	-1.86993	-0.90564

H	2.19035	-1.91338	-3.13046
C	4.16673	-2.73864	-2.80406
H	5.96487	-0.11229	1.62577
C	4.54393	1.31781	2.39979
H	2.9556	2.66512	2.95599
H	6.30094	-1.86471	-0.28685
C	5.31595	-2.72476	-2.00597
H	4.1104	-3.41364	-3.6541
H	5.18789	1.6254	3.21961
H	6.14504	-3.38653	-2.24324
H	0.30839	-0.9607	-1.44306

R = OPh

N-Protected alanine

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	3.39631	-0.56703	-0.13513
N	2.1701	-0.78949	0.40441
C	1.22625	-1.69089	-0.23174
C	-0.1627	-1.30802	0.26724
O	-1.10771	-2.09573	-0.3156
O	-0.38605	-0.45521	1.0916
H	1.79688	-0.13946	1.08553
O	3.87369	-1.16771	-1.07795
C	1.5516	-3.17088	0.04269
H	1.51773	-3.38086	1.11711
H	0.84304	-3.82352	-0.47435
H	2.55882	-3.37885	-0.32554
H	1.24155	-1.53138	-1.31797
O	4.0129	0.44138	0.56984
C	5.30334	0.85039	0.24225
C	5.52714	2.22627	0.27108
C	6.3432	-0.04432	-0.01348
C	6.81132	2.71753	0.03758
H	4.69491	2.89136	0.47921
C	7.62131	0.46273	-0.25274

H	6.15214	-1.1092	-0.03983
C	7.86225	1.83774	-0.22785
H	6.98692	3.78957	0.0616
H	8.43454	-0.2283	-0.45776
H	8.86192	2.22042	-0.41324
H	-2.02762	-1.836	-0.22668

Molecular complex 1 (MC1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C							
N	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
O	4	B4	3	A3	2	D2	0
O	4	B5	3	A4	2	D3	0
H	2	B6	1	A5	3	D4	0
O	1	B7	2	A6	3	D5	0
C	3	B8	2	A7	1	D6	0
H	9	B9	3	A8	2	D7	0
H	9	B10	3	A9	2	D8	0
H	9	B11	3	A10	2	D9	0
H	3	B12	2	A11	1	D10	0
H	5	B13	4	A12	3	D11	0
C	6	B14	4	A13	3	D12	0
N	15	B15	6	A14	4	D13	0
C	16	B16	15	A15	6	D14	0
C	17	B17	16	A16	15	D15	0
C	18	B18	17	A17	16	D16	0
N	19	B19	18	A18	17	D17	0
C	20	B20	19	A19	18	D18	0
H	21	B21	20	A20	19	D19	0
H	21	B22	20	A21	19	D20	0
H	21	B23	20	A22	19	D21	0
C	20	B24	19	A23	18	D22	0
H	25	B25	20	A24	19	D23	0
H	25	B26	20	A25	19	D24	0
H	25	B27	20	A26	19	D25	0

H	19	B28	18	A27	17	D26	0
H	19	B29	18	A28	17	D27	0
H	18	B30	17	A29	16	D28	0
H	18	B31	17	A30	16	D29	0
H	17	B32	16	A31	15	D30	0
H	17	B33	16	A32	15	D31	0
N	15	B34	6	A33	4	D32	0
C	35	B35	15	A34	6	D33	0
H	36	B36	35	A35	15	D34	0
H	36	B37	35	A36	15	D35	0
C	36	B38	35	A37	15	D36	0
H	39	B39	36	A38	35	D37	0
H	39	B40	36	A39	35	D38	0
H	39	B41	36	A40	35	D39	0
O	1	B42	8	A41	2	D40	0
C	43	B43	1	A42	8	D41	0
C	44	B44	43	A43	1	D42	0
C	44	B45	43	A44	1	D43	0
C	45	B46	44	A45	43	D44	0
H	45	B47	44	A46	43	D45	0
C	46	B48	44	A47	43	D46	0
H	46	B49	44	A48	43	D47	0
C	49	B50	46	A49	44	D48	0
H	47	B51	45	A50	44	D49	0
H	49	B52	46	A51	44	D50	0
H	51	B53	49	A52	46	D51	0

Variables:

B1	1.35828
B2	1.45078
B3	1.52635
B4	1.33057
B5	1.22038
B6	1.01249
B7	1.22085
B8	1.53996
B9	1.09536
B10	1.0934
B11	1.09272
B12	1.09759
B13	1.00401

B14	3.39533
B15	1.23975
B16	1.47214
B17	1.53264
B18	1.53341
B19	1.46169
B20	1.45744
B21	1.09538
B22	1.10846
B23	1.09554
B24	1.45812
B25	1.10875
B26	1.09349
B27	1.09506
B28	1.09808
B29	1.11086
B30	1.096
B31	1.09658
B32	1.0977
B33	1.0965
B34	1.21316
B35	1.4611
B36	1.09603
B37	1.09606
B38	1.52671
B39	1.09409
B40	1.09632
B41	1.09571
B42	1.36341
B43	1.43
B44	1.39516
B45	1.39471
B46	1.39483
B47	1.09961
B48	1.39543
B49	1.09968
B50	1.39483
B51	1.0996
B52	1.09968
B53	1.09976

A1	121.37307
A2	107.5141
A3	111.95379
A4	123.38891
A5	120.00759
A6	125.37474
A7	112.58819
A8	110.58092
A9	110.4674
A10	108.71202
A11	109.36182
A12	109.31192
A13	102.87208
A14	80.68973
A15	123.77842
A16	111.11246
A17	111.582
A18	113.36946
A19	111.1212
A20	109.54757
A21	113.38838
A22	109.83837
A23	112.84074
A24	113.04904
A25	110.65007
A26	109.29445
A27	108.58213
A28	109.4659
A29	108.24177
A30	109.70532
A31	110.79107
A32	107.00893
A33	98.93946
A34	130.70297
A35	106.4064
A36	106.83457
A37	114.9183
A38	110.4212
A39	110.97822
A40	109.9616

A41	124.39814
A42	114.81563
A43	119.98077
A44	120.01055
A45	119.99846
A46	119.99722
A47	119.99416
A48	120.01279
A49	119.99399
A50	120.008
A51	119.98114
A52	120.01134
D1	-157.77456
D2	175.07233
D3	-5.3503
D4	-164.07578
D5	-7.05464
D6	79.13511
D7	60.52678
D8	-178.62021
D9	-58.91073
D10	-41.05371
D11	178.87204
D12	177.10538
D13	19.13203
D14	144.65727
D15	-109.775
D16	-174.0326
D17	-170.95156
D18	166.98044
D19	-176.13449
D20	63.33524
D21	-57.63248
D22	-68.00132
D23	-60.7623
D24	60.64077
D25	178.95262
D26	-52.07232
D27	63.62143
D28	-51.50497

D29	65.01921
D30	13.53987
D31	130.27484
D32	-152.11652
D33	-55.54958
D34	119.09556
D35	-127.4871
D36	-3.57428
D37	58.97967
D38	-61.72869
D39	178.88643
D40	179.18859
D41	-0.36432
D42	89.30246
D43	-90.77665
D44	179.95325
D45	-0.05203
D46	-179.97772
D47	0.04098
D48	0.03411
D49	179.98918
D50	-179.99644
D51	-179.99951

Transition state 1 (TS1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C							
N	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
O	4	B4	3	A3	2	D2	0
O	4	B5	3	A4	2	D3	0
H	2	B6	1	A5	3	D4	0
O	1	B7	2	A6	3	D5	0
C	3	B8	2	A7	1	D6	0
H	9	B9	3	A8	2	D7	0
H	9	B10	3	A9	2	D8	0
H	9	B11	3	A10	2	D9	0

H 3 B12 2 A11 1 D10 0
H 5 B13 4 A12 3 D11 0
C 6 B14 4 A13 3 D12 0
N 15 B15 6 A14 4 D13 0
C 16 B16 15 A15 6 D14 0
C 17 B17 16 A16 15 D15 0
C 18 B18 17 A17 16 D16 0
N 19 B19 18 A18 17 D17 0
C 20 B20 19 A19 18 D18 0
H 21 B21 20 A20 19 D19 0
H 21 B22 20 A21 19 D20 0
H 21 B23 20 A22 19 D21 0
C 20 B24 19 A23 18 D22 0
H 25 B25 20 A24 19 D23 0
H 25 B26 20 A25 19 D24 0
H 25 B27 20 A26 19 D25 0
H 19 B28 18 A27 17 D26 0
H 19 B29 18 A28 17 D27 0
H 18 B30 17 A29 16 D28 0
H 18 B31 17 A30 16 D29 0
H 17 B32 16 A31 15 D30 0
H 17 B33 16 A32 15 D31 0
N 15 B34 6 A33 4 D32 0
C 35 B35 15 A34 6 D33 0
H 36 B36 35 A35 15 D34 0
H 36 B37 35 A36 15 D35 0
C 36 B38 35 A37 15 D36 0
H 39 B39 36 A38 35 D37 0
H 39 B40 36 A39 35 D38 0
H 39 B41 36 A40 35 D39 0
O 1 B42 8 A41 2 D40 0
C 43 B43 1 A42 8 D41 0
C 44 B44 43 A43 1 D42 0
C 44 B45 43 A44 1 D43 0
C 45 B46 44 A45 43 D44 0
H 45 B47 44 A46 43 D45 0
C 46 B48 44 A47 43 D46 0
H 46 B49 44 A48 43 D47 0
C 49 B50 46 A49 44 D48 0
H 47 B51 45 A50 44 D49 0

H	49	B52	46	A51	44	D50	0
H	51	B53	49	A52	46	D51	0

Variables:

B1	1.35475
B2	1.45468
B3	1.53804
B4	1.26161
B5	1.27384
B6	1.01207
B7	1.22087
B8	1.53685
B9	1.09597
B10	1.09325
B11	1.09304
B12	1.09762
B13	1.51476
B14	2.16268
B15	1.28905
B16	1.47527
B17	1.53228
B18	1.53395
B19	1.46105
B20	1.45781
B21	1.09524
B22	1.10821
B23	1.09557
B24	1.45882
B25	1.10842
B26	1.09347
B27	1.0949
B28	1.09824
B29	1.1108
B30	1.0958
B31	1.09672
B32	1.09481
B33	1.09539
B34	1.20105
B35	1.45254
B36	1.09546
B37	1.0941

B38	1.52787
B39	1.0936
B40	1.09529
B41	1.09537
B42	1.37045
B43	1.43
B44	1.39516
B45	1.39471
B46	1.39483
B47	1.09961
B48	1.39543
B49	1.09968
B50	1.39483
B51	1.0996
B52	1.09968
B53	1.09976
A1	122.1626
A2	108.96271
A3	116.7732
A4	117.94682
A5	119.67781
A6	125.88088
A7	112.53724
A8	110.54439
A9	109.82499
A10	109.36855
A11	109.30101
A12	101.3546
A13	118.12724
A14	97.86496
A15	121.93207
A16	112.19147
A17	111.51403
A18	113.21045
A19	111.09673
A20	109.50523
A21	113.3648
A22	109.85706
A23	112.85264
A24	113.0241

A25	110.6822
A26	109.24252
A27	108.63075
A28	109.42177
A29	108.31391
A30	109.73265
A31	108.49173
A32	106.37415
A33	106.39529
A34	136.03313
A35	106.47854
A36	107.15484
A37	113.49517
A38	110.05662
A39	111.08613
A40	109.73034
A41	124.20526
A42	115.31951
A43	119.98077
A44	120.01055
A45	119.99846
A46	119.99722
A47	119.99416
A48	120.01279
A49	119.99399
A50	120.008
A51	119.98114
A52	120.01134
D1	-159.13439
D2	176.4347
D3	-4.16133
D4	-162.14858
D5	-8.5191
D6	77.65982
D7	59.57676
D8	179.80136
D9	-60.13845
D10	-42.51015
D11	175.41531
D12	-175.17125

D13	3.00836
D14	151.38364
D15	-93.98584
D16	-174.23893
D17	-170.98445
D18	167.00871
D19	-176.17557
D20	63.31567
D21	-57.6837
D22	-67.96646
D23	-60.6441
D24	60.81319
D25	179.09196
D26	-52.12223
D27	63.60402
D28	-51.75488
D29	64.89156
D30	29.45492
D31	144.82654
D32	-172.6498
D33	-37.07455
D34	79.97326
D35	-165.32818
D36	-42.02123
D37	61.03493
D38	-59.83815
D39	-179.3894
D40	179.28883
D41	-2.21608
D42	89.55078
D43	-90.52832
D44	179.95325
D45	-0.05203
D46	-179.97772
D47	0.04098
D48	0.03411
D49	179.98918
D50	-179.99644
D51	-179.99951

Activated amino acid – conformation 1 (C1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.93204	-0.17722	-0.74911
N	-1.83063	0.19451	-0.04344
C	-0.95754	1.24961	-0.52351
C	0.41311	1.0223	0.10286
O	1.29791	1.95854	-0.34271
C	2.67839	1.73539	-0.10457
N	3.21128	0.7427	-0.67067
C	4.55619	0.28526	-0.35709
C	4.57649	-1.24911	-0.35187
C	5.96455	-1.80654	-0.02258
N	6.07055	-3.2561	-0.19184
C	7.45959	-3.69031	-0.14443
H	7.51574	-4.76702	-0.33982
H	7.94965	-3.49713	0.83182
H	8.037	-3.17456	-0.91979
C	5.26568	-3.99787	0.77026
H	5.55763	-3.80306	1.82261
H	4.20732	-3.74745	0.65977
H	5.37515	-5.07162	0.58336
H	6.69561	-1.34957	-0.70346
H	6.25916	-1.4968	1.00365
H	3.828	-1.59145	0.37157
H	4.26168	-1.61628	-1.33523
H	5.25971	0.64931	-1.1211
H	4.91478	0.65848	0.61524
N	3.15745	2.73719	0.70275
H	2.44039	3.34801	1.06983
C	4.49737	3.32145	0.6054
H	5.11766	3.00376	1.45375
H	4.97126	2.94227	-0.3037
C	4.42759	4.84792	0.55753
H	5.43559	5.27415	0.51823
H	3.93533	5.24881	1.45235
H	3.87321	5.19047	-0.32282
O	0.66922	0.16107	0.90841
H	-1.45087	-0.43648	0.65158
O	-3.36522	0.4149	-1.72722

C	-1.50811	2.65415	-0.213
H	-1.61237	2.79761	0.8678
H	-0.84793	3.4265	-0.61717
H	-2.49252	2.75	-0.67692
H	-0.84041	1.16064	-1.61148
O	-3.47929	-1.29582	-0.20403
C	-4.67198	-1.78034	-0.82663
C	-4.58851	-2.70332	-1.86951
C	-5.91839	-1.33162	-0.39035
C	-5.75167	-3.17691	-2.47641
H	-3.60575	-3.0573	-2.21303
C	-7.08204	-1.80501	-0.99783
H	-5.98428	-0.60459	0.43208
C	-6.9985	-2.7274	-2.04078
H	-5.68606	-3.90422	-3.29851
H	-8.06467	-1.45102	-0.65371
H	-7.91541	-3.10067	-2.51976

Activated amino acid – conformation 2 (C2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-3.26608	0.78241	1.00293
N	-2.57423	1.94997	0.76481
C	-1.63539	2.14365	-0.32334
C	-0.32552	1.38387	-0.08311
O	0.37642	1.28553	-1.24363
C	1.70047	0.79255	-1.13088
N	2.60909	1.67036	-1.0157
C	4.00102	1.24618	-1.01579
C	4.60192	1.20721	0.40158
C	3.88835	0.2722	1.38421
N	3.77849	-1.13088	0.94228
C	2.90228	-1.87089	1.85333
H	2.78464	-2.90107	1.49875
H	1.91773	-1.39364	1.88004
H	3.29761	-1.90858	2.88521
C	5.07871	-1.7899	0.83057
H	5.70044	-1.2848	0.08677
H	5.62955	-1.80568	1.78979

H	4.93614	-2.82507	0.50288
H	4.39863	0.32575	2.36534
H	2.86736	0.63877	1.53259
H	5.66811	0.95755	0.32188
H	4.55276	2.21566	0.83078
H	4.14778	0.2732	-1.51064
H	4.56838	1.98477	-1.59661
N	1.78856	-0.56921	-1.23492
H	2.57084	-0.9564	-0.69158
C	0.63191	-1.44758	-1.39326
H	0.03629	-1.49755	-0.46856
H	-0.01596	-1.02998	-2.16948
C	1.08584	-2.84919	-1.79675
H	0.2197	-3.50774	-1.92326
H	1.73217	-3.29397	-1.03061
H	1.64388	-2.82239	-2.73839
O	0.04983	0.96041	0.98485
H	-2.38091	2.45087	1.62295
O	-3.84297	0.55675	2.05153
C	-1.33685	3.64038	-0.5092
H	-2.26413	4.17778	-0.72745
H	-0.89344	4.06423	0.39956
H	-0.63135	3.78843	-1.3303
H	-2.08365	1.74997	-1.2378
O	-3.2388	-0.01956	-0.089
C	-3.97355	-1.2461	-0.11409
C	-3.85917	-2.14908	0.94327
C	-4.80557	-1.53888	-1.19449
C	-4.57643	-3.34512	0.91964
H	-3.20348	-1.91786	1.79519
C	-5.52276	-2.73566	-1.2184
H	-4.89626	-0.82691	-2.02766
C	-5.40798	-3.63859	-0.16148
H	-4.48626	-4.057	1.75284
H	-6.17866	-2.96631	-2.07039
H	-5.97308	-4.58188	-0.18004

Activated amino acid – conformation 3 (C3)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.10915	-1.87644	-0.70704
C	-2.95437	-0.58736	-1.7041
H	-2.99658	0.39184	-2.19081
O	-1.80946	-2.77273	-0.26658
N	-1.53653	-0.84073	-1.48935
C	-3.75313	-0.41082	-0.40556
O	-4.89112	-0.75887	-0.26259
C	-3.61476	-1.63841	-2.60259
H	-3.07778	-1.68391	-3.55474
H	-3.58495	-2.6208	-2.12744
H	-4.65763	-1.37357	-2.79087
O	-3.11238	0.14573	0.70121
H	-0.94048	-0.02356	-1.50937
C	-2.24649	1.21358	0.69076
N	-1.98693	1.86326	-0.38068
N	-1.81814	1.4553	1.96844
H	-1.02744	2.07624	2.04794
C	-1.15778	3.05881	-0.29564
H	-1.43912	3.7094	-1.13297
H	-1.36485	3.63925	0.62076
C	0.3508	2.76226	-0.38767
H	0.52618	2.16593	-1.29121
C	-2.14029	0.64061	3.14277
H	-1.9621	1.27608	4.01736
H	-3.2091	0.41822	3.11711
C	-1.33183	-0.65598	3.25311
H	-1.58696	-1.17988	4.18183
H	-1.55361	-1.32371	2.41506
H	-0.2549	-0.44973	3.26486
C	1.19112	4.04441	-0.41364
H	0.97992	4.60396	-1.34958
H	0.8676	4.69287	0.41184
H	0.67783	2.14663	0.46109
N	2.6233	3.80828	-0.23642
C	3.33625	5.05781	-0.00515
H	4.39273	4.84657	0.19317
H	3.28495	5.75974	-0.86169
H	2.92111	5.56524	0.87272
C	3.21745	3.07253	-1.34626

H	3.12062	3.59922	-2.31732
H	4.28393	2.92013	-1.14977
H	2.75619	2.08613	-1.4449
O	0.2318	-1.77211	-0.4953
C	0.80977	-2.83105	0.27249
C	0.69583	-4.15124	-0.16407
C	1.4886	-2.54403	1.45657
C	1.26028	-5.18432	0.58405
H	0.16098	-4.37727	-1.09787
C	2.05286	-3.57759	2.20529
H	1.57898	-1.50341	1.80041
C	1.9385	-4.89749	1.76902
H	1.17043	-6.22491	0.24021
H	2.58799	-3.35105	3.13889
H	2.38309	-5.71227	2.35888

Transition state 2 (TS2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.40695	1.49296	-0.67529
C	3.18041	0.32236	-1.4941
H	3.36464	-0.54696	-2.12039
O	2.00444	1.80666	0.33833
N	1.82738	0.71862	-1.65533
C	3.52488	-0.20034	-0.09924
O	4.2933	-0.19285	0.72268
C	4.22839	1.39735	-1.81615
H	4.05419	1.71588	-2.83597
H	4.11476	2.24685	-1.15803
H	5.24163	1.01625	-1.73645
O	2.42574	-1.55733	0.27134
H	0.92171	-0.84114	-1.49587
C	1.34204	-2.1134	-0.05062
N	0.61807	-1.72445	-1.08602
N	0.95841	-3.16343	0.68814
H	0.05948	-3.55072	0.52274
C	-0.69425	-2.219	-1.46424
H	-0.81906	-1.96509	-2.50909

H	-0.70968	-3.30348	-1.41439
C	-1.82887	-1.60404	-0.64102
H	-1.72216	-0.5271	-0.68662
C	1.67761	-3.61741	1.8734
H	1.43	-4.66423	2.00165
H	2.73492	-3.55509	1.66901
C	1.3277	-2.82759	3.12924
H	1.86818	-3.22536	3.98243
H	1.59783	-1.78517	3.0124
H	0.26547	-2.8878	3.34555
C	-3.20135	-2.04452	-1.14837
H	-3.36495	-1.6437	-2.15516
H	-3.20555	-3.12705	-1.24373
H	-1.73755	-1.88855	0.40353
N	-4.28168	-1.68742	-0.24858
C	-5.5097	-2.3677	-0.60153
H	-6.27728	-2.13714	0.12792
H	-5.88716	-2.08637	-1.58931
H	-5.35495	-3.44084	-0.5934
C	-4.49128	-0.25605	-0.14493
H	-4.75256	0.20251	-1.10325
H	-5.29832	-0.06204	0.55149
H	-3.60824	0.23826	0.23619
O	0.12221	1.88929	-0.88075
C	-0.52268	2.70019	0.01328
C	-1.0883	3.85951	-0.48495
C	-0.70107	2.34501	1.34092
C	-1.83632	4.67435	0.35009
H	-0.93894	4.10731	-1.51957
C	-1.44667	3.1674	2.1677
H	-0.243	1.453	1.7203
C	-2.01824	4.33279	1.67923
H	-2.27421	5.57549	-0.04119
H	-1.5793	2.89581	3.20001
H	-2.59616	4.96589	2.32839

Molecular complex 2 (MC2)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.9972	-2.20188	-0.34462
C	-3.12176	-1.93786	-0.80825
H	-3.63525	-1.09499	-0.32041
O	-1.57603	-3.15124	0.46906
N	-1.74987	-1.51141	-1.10546
C	-2.96427	-3.06443	0.20473
O	-3.74739	-3.79604	0.73029
C	-3.90911	-2.37234	-2.04767
H	-4.01773	-1.52268	-2.72693
H	-3.39495	-3.17973	-2.57952
H	-4.90374	-2.72074	-1.75368
O	-3.5359	1.0632	0.30534
H	-1.6786	0.49712	-1.17612
C	-2.67768	1.86279	-0.08925
N	-1.71613	1.50126	-0.99683
N	-2.68219	3.18617	0.31929
H	-1.81533	3.70022	0.24734
C	-0.62073	2.31209	-1.49671
H	-0.34522	1.91211	-2.48018
H	-0.98076	3.33329	-1.67907
C	0.624	2.33024	-0.5894
H	0.92046	1.29125	-0.40283
C	-3.58952	3.60792	1.3819
H	-3.73416	4.69028	1.28216
H	-4.54915	3.12478	1.18711
C	-3.1053	3.25698	2.79211
H	-3.82151	3.60716	3.54521
H	-3.00232	2.1724	2.89245
H	-2.13518	3.72174	3.00839
C	1.77157	3.13107	-1.21453
H	2.10734	2.62843	-2.14664
H	1.38646	4.11428	-1.51811
H	0.37656	2.76934	0.38616
N	2.88848	3.37247	-0.30115
C	3.80555	4.36463	-0.84636
H	4.59566	4.57504	-0.11707
H	4.29094	4.04287	-1.78983
H	3.26865	5.29907	-1.04395
C	3.60283	2.15125	0.05107
H	4.05449	1.64356	-0.82492

H	4.4083	2.39315	0.75307
H	2.93526	1.44013	0.54426
O	0.3194	-2.06673	-0.26096
C	1.04639	-2.95684	0.58998
C	1.5293	-4.16467	0.08559
C	1.27407	-2.6169	1.92333
C	2.2393	-5.03271	0.91501
H	1.35007	-4.43229	-0.96579
C	1.98394	-3.48553	2.75327
H	0.89402	-1.6646	2.32081
C	2.46628	-4.69327	2.24905
H	2.61982	-5.9848	0.51768
H	2.16328	-3.21731	3.80455
H	3.02577	-5.37807	2.90289

Azlactone

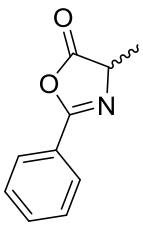
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.32808	0.16462	-0.07016
C	-3.36137	-0.41834	-0.59579
H	-3.78817	-0.14267	-1.57034
O	-2.06315	1.12717	0.58855
N	-1.93862	-0.72644	-0.74821
C	-3.39755	0.82123	0.30413
O	-4.3109	1.45937	0.73789
C	-4.17363	-1.57755	-0.008
H	-5.21773	-1.27694	0.12171
H	-4.12809	-2.43826	-0.6808
H	-3.77077	-1.87808	0.96451
O	-0.03073	0.32437	0.11552
C	0.79471	-0.63761	-0.5464
C	1.20118	-0.41922	-1.86305
C	1.1947	-1.79304	0.12457
C	2.00713	-1.35683	-2.50872
H	0.88609	0.49201	-2.39173
C	2.00057	-2.73131	-0.52152
H	0.87488	-1.96494	1.16258
C	2.40652	-2.51314	-1.83801
H	2.32744	-1.18496	-3.5465

H	2.31578	-3.64228	0.0077
H	3.04163	-3.25243	-2.34749

NMR and IR data for 2-phenyl azlactone



4-methyl-2-phenyloxazol-5(4H)-one

4-Methyl-2-phenyloxazol-5(4*H*)-one

The product was obtained after liquid-liquid extraction in dichloromethane/water as a white solid (191 mg; 87%); mp 36.1-36.4 °C; IR (KBr) ν / cm^{-1} 3064, 2982, 2936, 2901, 1810, 1654, 1495, 1450, 1322, 1253, 1106; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (d, 2H, *J* 7.5 Hz), 7.60-7.46 (m, 3H), 4.45 (q, 1H, *J* 7.5 Hz), 1.58 (d, 3H, *J* 7.8 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 179.1, 161.7, 133.0, 129.0, 128.0, 126.0, 61.1, 17.0.

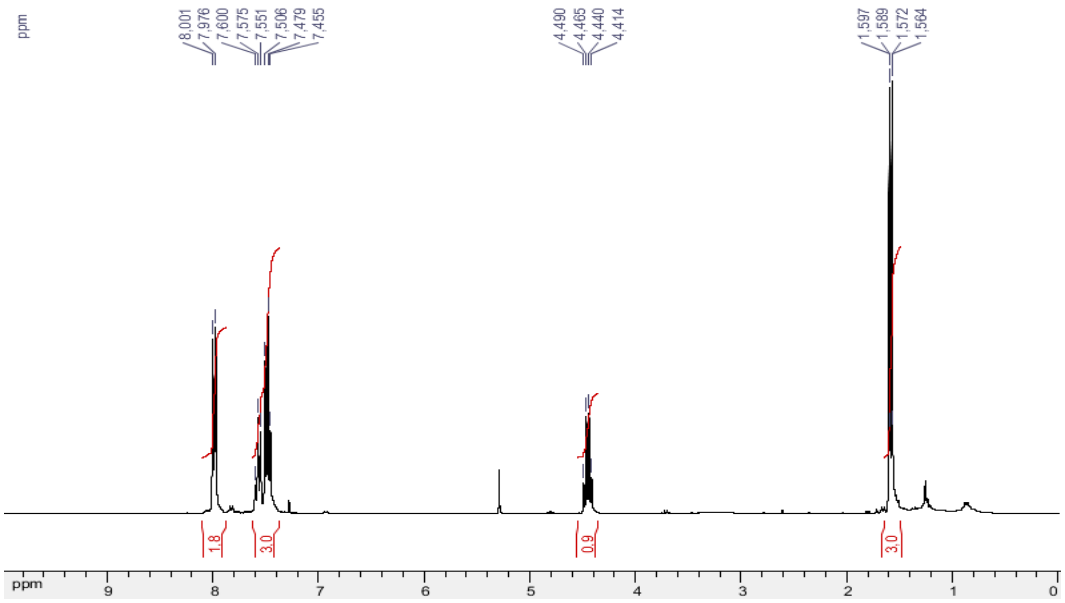


Figure S8. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum for 4-methyl-2-phenyloxazol-5(4*H*)-one.

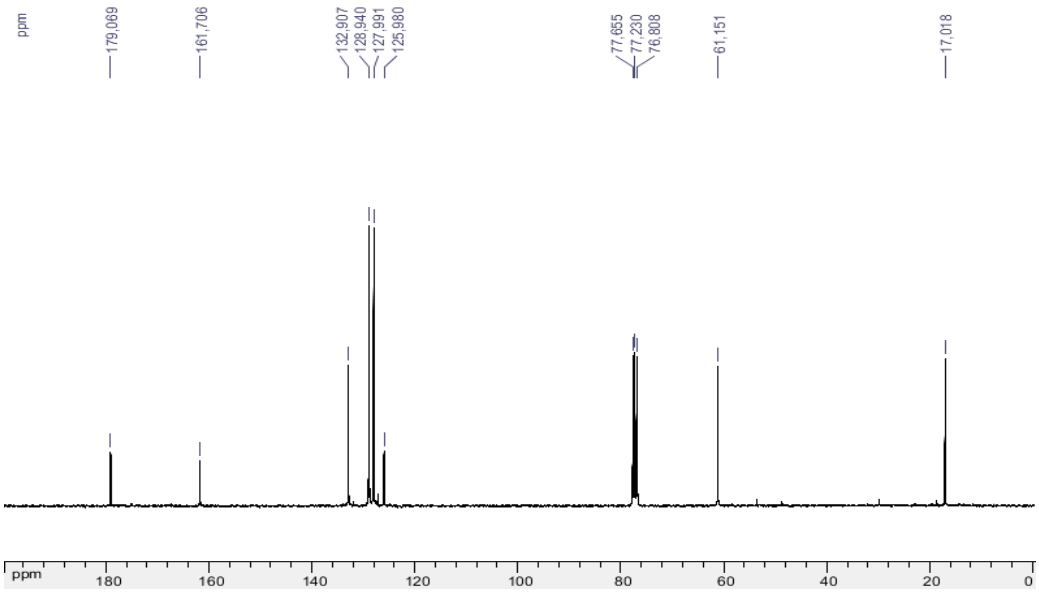


Figure S9. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum for 4-methyl-2-phenyloxazol-5(4*H*)-one.

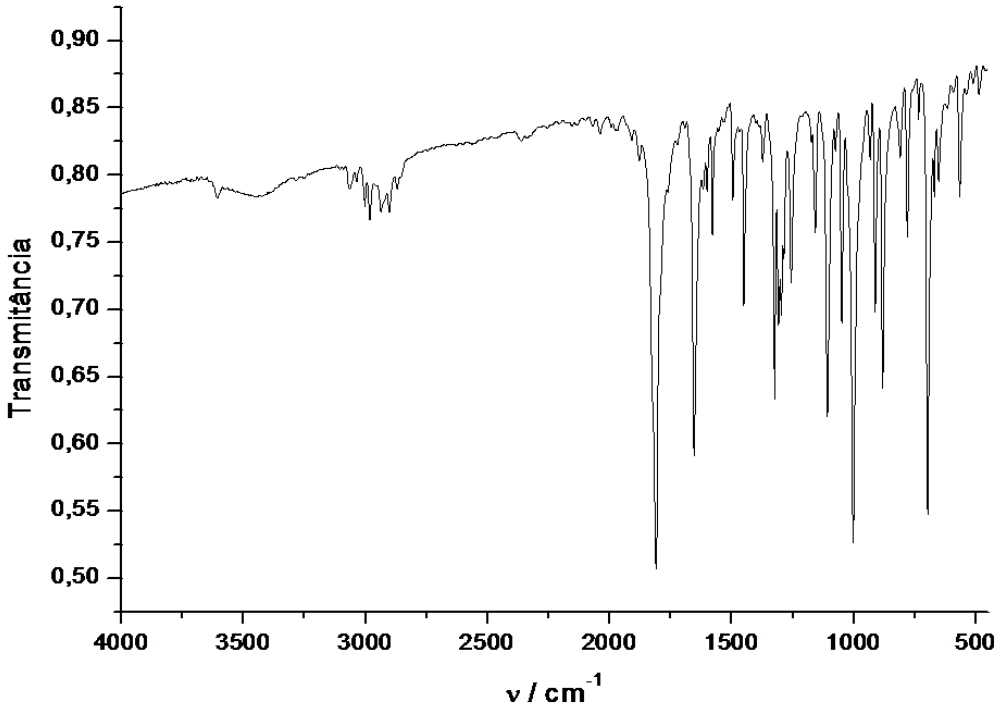


Figure S10. IR (KBr) spectrum for 4-methyl-2-phenyloxazol-5(4*H*)-one.