Supporting Information

Table S1 The relative energy of all the conformers.

Conformers	Relative energy / $kJmol^{-1}$
I	0
II	1.654048
III	1.89034
IV	1.94285
V	1.995359
VI	2.021614
VII	2.494199
VIII	2.520454
IX	2.546708
X	2.572963
XI	2.809256
XII	2.83551
XIII	3.150567
XIV	3.308095
XV	3.413114
XVI	3.596897
XVII	3.83319
XVIII	4.725851
XIX	6.72121
XX	11.47332
XXI	15.67407
XXII	20.55745
XXIII	23.8918
XXIV	25.75589
XXV	33.68481
XXVI	41.56123

Table S2 Bond length, bond angle, and dihedral angle of conformers V and I.

Parameters											
Bond length / Å	V	I		V	I		V	I		V	I
R(1,7)	1.464	1.464	A(28,27,31)	112.347	112.431	D(7,1,15,89)	21.25	21.16	D(44,43,89,90)	-156.91	-157.10
R(1,8)	1.460	1.460	A(29,27,31)	109.508	109.525	D(7,1,15,92)	-138.22	-139.64	D(45,43,89,15)	127.73	128.30
R(1,15)	1.712	1.711	A(11,30,12)	110.893	110.557	D(8,1,15,89)	152.08	151.94	D(45,43,89,90)	-39.14	-39.27
R(1,78)	1.796	1.796	A(11,30,31)	103.934	103.911	D(8,1,15,92)	-7.40	-8.86	D(43,45,47,30)	-37.49	-36.67
R(2,9)	1.463	1.462	A(11,30,47)	116.785	116.272	D(78,1,15,89)	-93.46	-93.54	D(43,45,47,48)	-154.99	-154.14
R(2,10)	1.470	1.471	A(12,30,31)	102.290	102.688	D(78,1,15,92)	107.06	105.66	D(43,45,47,49)	83.98	85.13
R(2,12)	1.683	1.692	A(12,30,47)	115.533	115.864	D(7,1,78,79)	17.34	16.93	D(46,45,47,30)	77.89	78.85
R(2,32)	1.802	1.799	A(31,30,47)	105.393	105.685	D(7,1,78,87)	-167.68	-167.88	D(46,45,47,48)	-39.61	-38.62
R(3,20)	1.447	1.445	A(27,31,30)	102.935	103.020	D(8,1,78,79)	-113.85	-114.18	D(46,45,47,49)	-160.64	-159.35
R(3,23)	1.357	1.358	A(27,31,43)	115.253	115.218	D(8,1,78,87)	61.14	61.01	D(55,45,47,30)	-165.92	-165.00
R(4,23)	1.221	1.223	A(27,31,68)	111.118	111.008	D(15,1,78,79)	132.26	131.90	D(55,45,47,48)	76.58	77.54
R(5,107)	1.362	1.362	A(30,31,43)	105.948	105.891	D(15,1,78,87)	-52.76	-52.91	D(55,45,47,49)	-44.45	-43.19
R(5,108)	1.442	1.441	A(30,31,68)	103.131	102.916	D(9,2,12,30)	23.13	30.35	D(43,45,55,52)	-63.37	-63.65
R(6,107)	1.225	1.225	A(43,31,68)	116.535	116.819	D(9,2,12,69)	-156.84	-148.08	D(43,45,55,56)	177.48	177.19
R(11,23)	1.367	1.361	A(2,32,33)	122.212	120.709	D(10,2,12,30)	152.52	159.19	D(43,45,55,60)	58.75	58.49
R(11,24)	1.470	1.470	A(2,32,41)	116.391	117.604	D(10,2,12,69)	-27.45	-19.24	D(46,45,55,52)	174.92	174.70
R(11,30)	1.464	1.465	A(33,32,41)	121.332	121.570	D(32,2,12,30)	-93.77	-86.96	D(46,45,55,56)	55.77	55.54
R(12,30)	1.516	1.514	A(32,33,34)	120.753	120.903	D(32,2,12,69)	86.26	94.61	D(46,45,55,60)	-62.95	-63.15
R(12,69)	1.435	1.435	A(32,33,35)	118.992	118.909	D(9,2,32,33)	-136.54	-165.11	D(47,45,55,52)	58.24	58.08
R(13,14)	1.013	1.014	A(34,33,35)	120.250	120.184	D(9,2,32,41)	46.38	18.77	D(47,45,55,56)	-60.91	-61.08
R(13,104)	1.454	1.453	A(33,35,36)	119.439	119.581	D(10,2,32,33)	94.89	65.78	D(47,45,55,60)	-179.63	-179.77
R(13,107)	1.361	1.360	A(33,35,37)	120.300	120.201	D(10,2,32,41)	-82.20	-110.33	D(30,47,49,50)	-50.37	-52.73
R(15,89)	1.449	1.449	A(36,35,37)	120.261	120.218	D(12,2,32,33)	-18.39	-46.99	D(30,47,49,51)	133.41	132.20
R(15,92)	1.418	1.418	A(35,37,38)	119.931	119.878	D(12,2,32,41)	164.52	136.90	D(45,47,49,50)	-166.83	-169.38
R(16,17)	1.093	1.094	A(35,37,39)	120.106	120.138	D(23,3,20,16)	83.50	-179.61	D(45,47,49,51)	16.95	15.55
R(16,18)	1.095	1.094	A(38,37,39)	119.962	119.984	D(23,3,20,21)	-39.49	58.94	D(48,47,49,50)	70.83	68.26
R(16,19)	1.094	1.094	A(37,39,40)	120.211	120.195	D(23,3,20,22)	-156.05	-58.09	D(48,47,49,51)	-105.39	-106.80
R(16,20)	1.520	1.517	A(37,39,41)	120.197	120.243	D(20,3,23,4)	-0.28	0.31	D(47,49,51,52)	-2.39	-2.10
R(20,21)	1.092	1.094	A(40,39,41)	119.592	119.561	D(20,3,23,11)	-179.82	179.94	D(47,49,51,64)	177.80	177.48
R(20,22)	1.092	1.094	A(32,41,39)	119.073	118.937	D(108,5,107,6)	0.70	1.16	D(50,49,51,52)	-178.57	-177.08
R(24,25)	1.097	1.097	A(32,41,42)	120.130	119.680	D(108,5,107,13)	-178.17	-177.73	D(50,49,51,64)	1.63	2.50
R(24,26)	1.092	1.092	A(39,41,42)	120.795	121.373	D(107,5,108,109)	-38.48	-38.06	D(49,51,52,53)	-107.82	-107.03
R(24,27)	1.527	1.529	A(31,43,44)	105.304	105.345	D(107,5,108,110)	-155.19	-154.83	D(49,51,52,54)	138.41	139.11
R(27,28)	1.088	1.088	A(31,43,45)	105.247	105.316	D(107,5,108,111)	84.38	84.75	D(49,51,52,55)	16.14	17.07
R(27,29)	1.094	1.093	A(31,43,89)	118.146	117.926	D(24,11,23,3)	172.66	-8.43	D(64,51,52,53)	71.99	73.37

R(27,31)	1.549	1.548	A(44,43,45)	107.097	107.065	D(24,11,23,4)	-6.88	171.20	D(64,51,52,54)	-41.77	-40.50
R(30,31)	1.579	1.574	A(44,43,89)	106.731	106.814	D(30,11,23,3)	-1.14	177.21	D(64,51,52,55)	-164.04	-162.53
R(30,47)	1.552	1.552	A(45,43,89)	113.567	113.634	D(30,11,23,4)	179.32	-3.17	D(49,51,64,65)	2.97	3.00
R(31,43)	1.592	1.591	A(43,45,46)	108.466	108.546	D(23,11,24,25)	86.17	86.13	D(49,51,64,66)	-118.05	-117.97
R(31,68)	1.512	1.511	A(43,45,47)	105.271	105.445	D(23,11,24,26)	-32.61	-33.39	D(49,51,64,67)	123.91	123.94
R(32,33)	1.394	1.396	A(43,45,55)	117.457	117.231	D(23,11,24,27)	-153.79	-154.02	D(52,51,64,65)	-176.84	-177.40
R(32,41)	1.398	1.394	A(46,45,47)	107.256	107.182	D(30,11,24,25)	-99.19	-99.09	D(52,51,64,66)	62.14	61.63
R(33,34)	1.083	1.084	A(46,45,55)	106.448	106.425	D(30,11,24,26)	142.02	141.39	D(52,51,64,67)	-55.91	-56.45
R(33,35)	1.396	1.394	A(47,45,55)	111.537	111.613	D(30,11,24,27)	20.85	20.76	D(51,52,55,45)	-43.18	-44.17
R(35,36)	1.085	1.086	A(30,47,45)	103.956	103.849	D(23,11,30,12)	-75.94	-74.58	D(51,52,55,56)	75.51	74.51
R(35,37)	1.396	1.397	A(30,47,48)	109.501	109.475	D(23,11,30,31)	174.82	175.87	D(51,52,55,60)	-167.07	-167.97
R(37,38)	1.086	1.086	A(30,47,49)	112.398	112.596	D(23,11,30,47)	59.25	60.23	D(53,52,55,45)	79.92	79.21
R(37,39)	1.397	1.396	A(45,47,48)	110.720	110.827	D(24,11,30,12)	109.93	110.44	D(53,52,55,56)	-161.38	-162.11
R(39,40)	1.086	1.086	A(45,47,49)	111.779	112.072	D(24,11,30,31)	0.70	0.90	D(53,52,55,60)	-43.96	-44.59
R(39,41)	1.394	1.394	A(48,47,49)	108.446	108.004	D(24,11,30,47)	-114.87	-114.75	D(54,52,55,45)	-165.63	-166.37
R(41,42)	1.085	1.083	A(47,49,50)	116.883	116.599	D(2,12,30,11)	94.10	95.71	D(54,52,55,56)	-46.93	-47.69
R(43,44)	1.091	1.091	A(47,49,51)	124.693	124.752	D(2,12,30,31)	-155.60	-153.95	D(54,52,55,60)	70.49	69.83
R(43,45)	1.577	1.578	A(50,49,51)	118.320	118.472	D(2,12,30,47)	-41.70	-39.30	D(45,55,56,57)	66.33	66.15
R(43,89)	1.522	1.522	A(49,51,52)	122.050	121.976	D(69,12,30,11)	-85.92	-85.69	D(45,55,56,58)	-54.64	-54.72
R(45,46)	1.090	1.089	A(49,51,64)	121.865	121.898	D(69,12,30,31)	24.38	24.65	D(45,55,56,59)	-173.91	-174.00
R(45,47)	1.547	1.548	A(52,51,64)	116.085	116.125	D(69,12,30,47)	138.28	139.31	D(52,55,56,57)	-53.39	-53.57
R(45,55)	1.558	1.557	A(51,52,53)	108.869	109.160	D(2,12,69,68)	162.05	160.68	D(52,55,56,58)	-174.36	-174.44
R(47,48)	1.090	1.090	A(51,52,54)	109.255	109.189	D(2,12,69,70)	-20.31	-21.37	D(52,55,56,59)	66.37	66.29
R(47,49)	1.513	1.512	A(51,52,55)	114.206	114.016	D(30,12,69,68)	-17.93	-18.04	D(60,55,56,57)	-171.95	-172.24
R(49,50)	1.086	1.086	A(53,52,54)	104.674	104.656	D(30,12,69,70)	159.71	159.91	D(60,55,56,58)	67.08	66.89
R(49,51)	1.340	1.340	A(53,52,55)	110.463	110.497	D(14,13,104,101)	-70.84	-71.48	D(60,55,56,59)	-52.19	-52.39
R(51,52)	1.511	1.511	A(54,52,55)	108.936	108.898	D(14,13,104,105)	167.11	166.49	D(45,55,60,61)	178.01	177.47
R(51,64)	1.507	1.507	A(45,55,52)	109.989	109.988	D(14,13,104,106)	50.68	50.11	D(45,55,60,62)	58.86	58.25
R(52,53)	1.100	1.100	A(45,55,56)	108.343	108.315	D(107,13,104,101)	83.39	84.96	D(45,55,60,63)	-62.33	-62.89
R(52,54)	1.100	1.100	A(45,55,60)	112.377	112.281	D(107,13,104,105)	-38.66	-37.08	D(52,55,60,61)	-59.52	-60.09
R(52,55)	1.545	1.545	A(52,55,56)	109.079	109.105	D(107,13,104,106)	-155.08	-153.46	D(52,55,60,62)	-178.67	-179.31
R(55,56)	1.547	1.547	A(52,55,60)	109.390	109.456	D(14,13,107,5)	-16.64	-15.39	D(52,55,60,63)	60.13	59.55
R(55,60)	1.539	1.539	A(56,55,60)	107.579	107.617	D(14,13,107,6)	164.50	165.74	D(56,55,60,61)	58.84	58.36
R(56,57)	1.093	1.093	A(55,56,57)	112.141	112.202	D(104,13,107,5)	-170.99	-171.87	D(56,55,60,62)	-60.31	-60.86
R(56,58)	1.095	1.095	A(55,56,58)	111.142	111.079	D(104,13,107,6)	10.15	9.26	D(56,55,60,63)	178.49	178.00
R(56,59)	1.096	1.096	A(55,56,59)	110.028	110.045	D(1,15,89,43)	30.26	28.63	D(31,68,69,12)	2.92	2.98
R(60,61)	1.097	1.096	A(57,56,58)	107.975	107.900	D(1,15,89,90)	-160.09	-161.18	D(31,68,69,70)	-174.95	-175.20
R(60,62)	1.095	1.095	A(57,56,59)	107.630	107.665	D(92,15,89,43)	-167.99	-168.46	D(76,68,69,12)	179.58	179.49
R(60,63)	1.092	1.092	A(58,56,59)	107.756	107.781	D(92,15,89,90)	1.66	1.73	D(76,68,69,70)	1.71	1.32
R(64,65)	1.094	1.094	A(55,60,61)	109.780	109.830	D(1,15,92,91)	162.24	163.31	D(31,68,76,74)	175.24	175.20
R(64,66)	1.098	1.098	A(55,60,62)	111.415	111.402	D(1,15,92,93)	-21.09	-19.92	D(31,68,76,77)	-4.51	-4.60

R(64,67)	1.098	1.098	A(55,60,63)	112.448	112.395	D(89,15,92,91)	-0.34	-0.45	D(69,68,76,74)	-0.74	-0.64
R(68,69)	1.398	1.399	A(61,60,62)	107.644	107.683	D(89,15,92,93)	176.33	176.33	D(69,68,76,77)	179.50	179.57
R(68,76)	1.391	1.391	A(61,60,63)	107.525	107.511	D(17,16,20,3)	-65.05	-60.12	D(12,69,70,71)	2.67	3.56
R(69,70)	1.396	1.397	A(62,60,63)	107.834	107.827	D(17,16,20,21)	56.49	59.29	D(12,69,70,72)	-178.81	-178.76
R(70,71)	1.082	1.081	A(51,64,65)	111.968	111.944	D(17,16,20,22)	179.10	-179.80	D(68,69,70,71)	-179.93	-178.69
R(70,72)	1.399	1.399	A(51,64,66)	111.064	111.071	D(18,16,20,3)	175.66	-179.87	D(68,69,70,72)	-1.41	-1.01
R(72,73)	1.086	1.086	A(51,64,67)	110.952	111.011	D(18,16,20,21)	-62.79	-60.45	D(69,70,72,73)	-179.65	-179.61
R(72,74)	1.396	1.395	A(65,64,66)	108.154	108.123	D(18,16,20,22)	59.82	60.46	D(69,70,72,74)	0.20	0.06
R(74,75)	1.085	1.085	A(65,64,67)	108.147	108.133	D(19,16,20,3)	56.12	60.42	D(71,70,72,73)	-1.12	-1.90
R(74,76)	1.398	1.398	A(66,64,67)	106.331	106.332	D(19,16,20,21)	177.66	179.83	D(71,70,72,74)	178.74	177.77
R(76,77)	1.085	1.086	A(31,68,69)	110.733	110.796	D(19,16,20,22)	-59.72	-59.26	D(70,72,74,75)	-179.69	-179.63
R(78,79)	1.395	1.395	A(31,68,76)	128.835	128.519	D(11,24,27,28)	-156.02	-156.07	D(70,72,74,76)	0.73	0.60
R(78,87)	1.398	1.397	A(69,68,76)	120.332	120.576	D(11,24,27,29)	83.38	83.32	D(73,72,74,75)	0.16	0.04
R(79,80)	1.084	1.084	A(12,69,68)	109.391	109.294	D(11,24,27,31)	-33.83	-33.86	D(73,72,74,76)	-179.42	-179.73
R(79,81)	1.396	1.396	A(12,69,70)	129.499	130.062	D(25,24,27,28)	-36.83	-36.96	D(72,74,76,68)	-0.45	-0.31
R(81,82)	1.086	1.086	A(68,69,70)	121.069	120.613	D(25,24,27,29)	-157.43	-157.58	D(72,74,76,77)	179.30	179.48
R(81,83)	1.396	1.395	A(69,70,71)	121.639	121.605	D(25,24,27,31)	85.37	85.24	D(75,74,76,68)	179.96	179.92
R(83,84)	1.086	1.086	A(69,70,72)	118.044	118.267	D(26,24,27,28)	85.59	85.27	D(75,74,76,77)	-0.28	-0.29
R(83,85)	1.398	1.398	A(71,70,72)	120.301	120.088	D(26,24,27,29)	-35.01	-35.34	D(1,78,79,80)	-4.52	-4.33
R(85,86)	1.085	1.085	A(70,72,73)	118.794	118.698	D(26,24,27,31)	-152.21	-152.52	D(1,78,79,81)	175.54	175.75
R(85,87)	1.393	1.393	A(70,72,74)	121.311	121.408	D(24,27,31,30)	34.37	34.65	D(87,78,79,80)	-179.41	-179.42
R(87,88)	1.085	1.085	A(73,72,74)	119.895	119.893	D(24,27,31,43)	149.20	149.45	D(87,78,79,81)	0.65	0.66
R(89,90)	1.374	1.374	A(72,74,75)	120.115	120.198	D(24,27,31,68)	-75.42	-74.90	D(1,78,87,85)	-175.79	-175.99
R(90,91)	1.448	1.447	A(72,74,76)	119.937	119.766	D(28,27,31,30)	156.86	157.03	D(1,78,87,88)	4.66	4.50
R(90,101)	1.504	1.504	A(75,74,76)	119.947	120.036	D(28,27,31,43)	-88.31	-88.16	D(79,78,87,85)	-0.97	-0.96
R(91,92)	1.408	1.408	A(68,76,74)	119.287	119.358	D(28,27,31,68)	47.06	47.48	D(79,78,87,88)	179.48	179.53
R(91,99)	1.406	1.406	A(68,76,77)	119.887	119.846	D(29,27,31,30)	-82.95	-82.62	D(78,79,81,82)	-179.84	-179.94
R(92,93)	1.400	1.400	A(74,76,77)	120.825	120.795	D(29,27,31,43)	31.89	32.19	D(78,79,81,83)	-0.06	-0.08
R(93,94)	1.081	1.081	A(1,78,79)	118.344	118.356	D(29,27,31,68)	167.26	167.84	D(80,79,81,82)	0.23	0.14
R(93,95)	1.393	1.393	A(1,78,87)	119.790	119.797	D(11,30,31,27)	-21.63	-21.92	D(80,79,81,83)	-179.99	-180.00
R(95,96)	1.086	1.086	A(79,78,87)	121.670	121.666	D(11,30,31,43)	-143.02	-143.29	D(79,81,83,84)	179.91	179.88
R(95,97)	1.404	1.404	A(78,79,80)	119.763	119.742	D(11,30,31,68)	94.04	93.58	D(79,81,83,85)	-0.20	-0.18
R(97,98)	1.086	1.086	A(78,79,81)	118.853	118.859	D(12,30,31,27)	-137.11	-137.17	D(82,81,83,84)	-0.31	-0.26
R(97,99)	1.389	1.389	A(80,79,81)	121.384	121.400	D(12,30,31,43)	101.50	101.46	D(82,81,83,85)	179.58	179.69
R(99,100)	1.086	1.086	A(79,81,82)	119.627	119.639	D(12,30,31,68)	-21.44	-21.67	D(81,83,85,86)	-179.97	179.99
R(101,102)	1.098	1.098	A(79,81,83)	120.137	120.137	D(47,30,31,27)	101.73	100.98	D(81,83,85,87)	-0.13	-0.14
R(101,103)	1.088	1.088	A(82,81,83)	120.236	120.224	D(47,30,31,43)	-19.66	-20.39	D(84,83,85,86)	-0.08	-0.06
R(101,104)	1.547	1.547	A(81,83,84)	119.891	119.899	D(47,30,31,68)	-142.60	-143.52	D(84,83,85,87)	179.76	179.81
R(104,105)	1.090	1.090	A(81,83,85)	120.310	120.302	D(11,30,47,45)	150.10	150.00	D(83,85,87,78)	0.70	0.69
R(104,106)	1.091	1.091	A(84,83,85)	119.798	119.800	D(11,30,47,48)	-91.55	-91.61	D(83,85,87,88)	-179.75	-179.80
R(108,109)	1.093	1.093	A(83,85,86)	120.177	120.177	D(11,30,47,49)	29.04	28.54	D(86,85,87,78)	-179.46	-179.44

R(108,110)	1.093	1.093	A(83,85,87)	120.202	120.212	D(12,30,47,45)	-76.75	-77.59	D(86,85,87,88)	0.09	0.07
R(108,111)	1.521	1.521	A(86,85,87)	119.621	119.611	D(12,30,47,48)	41.59	40.81	D(15,89,90,91)	-2.27	-2.29
R(111,112)	1.093	1.093	A(78,87,85)	118.823	118.819	D(12,30,47,49)	162.19	160.96	D(15,89,90,101)	179.55	179.44
R(111,113)	1.096	1.096	A(78,87,88)	120.564	120.561	D(31,30,47,45)	35.35	35.34	D(43,89,90,91)	165.91	166.55
R(111,114)	1.094	1.094	A(85,87,88)	120.612	120.618	D(31,30,47,48)	153.69	153.74	D(43,89,90,101)	-12.27	-11.73
Bond Angle / ◦			A(15,89,43)	120.624	120.821	D(31,30,47,49)	-85.71	-86.11	D(89,90,91,92)	2.12	2.07
A(7,1,8)	120.074	120.015	A(15,89,90)	107.375	107.327	D(27,31,43,44)	-3.27	-2.21	D(89,90,91,99)	-174.35	-174.52
A(7,1,15)	108.163	108.220	A(43,89,90)	130.978	130.937	D(27,31,43,45)	-116.25	-115.20	D(101,90,91,92)	-179.49	-179.45
A(7,1,78)	107.872	107.826	A(89,90,91)	108.479	108.510	D(27,31,43,89)	115.74	116.80	D(101,90,91,99)	4.04	3.96
A(8,1,15)	107.215	107.205	A(89,90,101)	130.826	130.785	D(30,31,43,44)	109.82	110.93	D(89,90,101,102)	122.29	122.26
A(8,1,78)	108.005	108.049	A(91,90,101)	120.670	120.683	D(30,31,43,45)	-3.16	-2.06	D(89,90,101,103)	3.70	3.84
A(15,1,78)	104.452	104.480	A(90,91,92)	108.579	108.589	D(30,31,43,89)	-131.17	-130.06	D(89,90,101,104)	-118.01	-118.00
A(9,2,10)	118.770	119.029	A(90,91,99)	131.423	131.379	D(68,31,43,44)	-136.17	-135.22	D(91,90,101,102)	-55.70	-55.83
A(9,2,12)	109.704	109.245	A(92,91,99)	119.909	119.949	D(68,31,43,45)	110.84	111.79	D(91,90,101,103)	-174.29	-174.26
A(9,2,32)	107.796	107.969	A(15,92,91)	106.601	106.574	D(68,31,43,89)	-17.17	-16.21	D(91,90,101,104)	64.00	63.91
A(10,2,12)	106.006	105.171	A(15,92,93)	131.716	131.793	D(27,31,68,69)	121.93	121.95	D(90,91,92,15)	-1.04	-0.94
A(10,2,32)	106.643	106.794	A(91,92,93)	121.602	121.557	D(27,31,68,76)	-54.36	-54.22	D(90,91,92,93)	-178.12	-178.12
A(12,2,32)	107.399	108.205	A(92,93,94)	121.843	121.840	D(30,31,68,69)	12.27	12.34	D(99,91,92,15)	175.91	176.10
A(20,3,23)	116.110	114.985	A(92,93,95)	117.480	117.490	D(30,31,68,76)	-164.02	-163.83	D(99,91,92,93)	-1.17	-1.08
A(107,5,108)	115.812	115.767	A(94,93,95)	120.668	120.661	D(43,31,68,69)	-103.32	-103.18	D(90,91,99,97)	177.03	177.08
A(23,11,24)	119.353	124.931	A(93,95,96)	118.747	118.737	D(43,31,68,76)	80.39	80.66	D(90,91,99,100)	-2.17	-2.21
A(23,11,30)	127.245	121.631	A(93,95,97)	121.632	121.648	D(2,32,33,34)	3.82	4.70	D(92,91,99,97)	0.89	0.82
A(24,11,30)	113.149	113.228	A(96,95,97)	119.621	119.615	D(2,32,33,35)	-177.01	-176.10	D(92,91,99,100)	-178.31	-178.47
A(2,12,30)	129.934	129.233	A(95,97,98)	119.671	119.671	D(41,32,33,34)	-179.24	-179.35	D(15,92,93,94)	5.40	5.27
A(2,12,69)	121.558	122.506	A(95,97,99)	120.658	120.641	D(41,32,33,35)	-0.06	-0.14	D(15,92,93,95)	-175.67	-175.83
A(30,12,69)	108.508	108.246	A(98,97,99)	119.672	119.689	D(2,32,41,39)	176.90	175.80	D(91,92,93,94)	-178.35	-178.35
A(14,13,104)	117.843	118.037	A(91,99,97)	118.710	118.708	D(2,32,41,42)	-3.72	-5.37	D(91,92,93,95)	0.58	0.55
A(14,13,107)	117.373	117.859	A(91,99,100)	120.727	120.740	D(33,32,41,39)	-0.22	-0.28	D(92,93,95,96)	179.98	-179.99
A(104,13,107)	119.738	119.883	A(97,99,100)	120.558	120.548	D(33,32,41,42)	179.16	178.55	D(92,93,95,97)	0.26	0.22
A(1,15,89)	126.126	126.431	A(90,101,102)	108.998	109.020	D(32,33,35,36)	-179.29	-179.73	D(94,93,95,96)	-1.07	-1.08
A(1,15,92)	122.312	122.312	A(90,101,103)	112.469	112.288	D(32,33,35,37)	0.32	0.50	D(94,93,95,97)	179.20	179.14
A(89,15,92)	108.916	108.949	A(90,101,104)	113.313	113.382	D(34,33,35,36)	-0.11	-0.52	D(93,95,97,98)	179.33	179.41
A(17,16,18)	108.236	108.344	A(102,101,103)	107.087	107.026	D(34,33,35,37)	179.50	179.70	D(93,95,97,99)	-0.51	-0.47
A(17,16,19)	109.163	108.316	A(102,101,104)	107.539	107.528	D(33,35,37,38)	179.95	179.59	D(96,95,97,98)	-0.39	-0.37
A(17,16,20)	110.486	110.983	A(103,101,104)	107.142	107.304	D(33,35,37,39)	-0.31	-0.42	D(96,95,97,99)	179.76	179.75
A(18,16,19)	108.245	108.293	A(13,104,101)	111.852	111.893	D(36,35,37,38)	-0.43	-0.19	D(95,97,99,91)	-0.07	-0.06
A(18,16,20)	109.756	109.781	A(13,104,105)	107.459	107.428	D(36,35,37,39)	179.31	179.80	D(95,97,99,100)	179.13	179.23
A(19,16,20)	110.886	111.038	A(13,104,106)	108.642	108.677	D(35,37,39,40)	-179.72	-179.56	D(98,97,99,91)	-179.92	-179.95
A(3,20,16)	111.559	107.317	A(101,104,105)	110.989	110.969	D(35,37,39,41)	0.02	-0.01	D(98,97,99,100)	-0.71	-0.65
A(3,20,21)	108.701	108.836	A(101,104,106)	109.928	109.940	D(38,37,39,40)	0.02	0.43	D(90,101,104,13)	-172.23	-172.50
A(3,20,22)	103.969	109.074	A(105,104,106)	107.839	107.800	D(38,37,39,41)	179.76	179.98	D(90,101,104,105)	-52.22	-52.52

A(16,20,21)	111.214	112.044	A(5,107,6)	124.142	124.117	D(37,39,41,32)	0.24	0.35	D(90,101,104,106)	67.00	66.64
A(16,20,22)	111.633	111.990	A(5,107,13)	110.402	110.438	D(37,39,41,42)	-179.14	-178.46	D(102,101,104,13)	-51.70	-51.91
A(21,20,22)	109.489	107.517	A(6,107,13)	125.445	125.435	D(40,39,41,32)	179.98	179.91	D(102,101,104,105)	68.31	68.07
A(3,23,4)	124.634	123.970	A(5,108,109)	109.061	109.058	D(40,39,41,42)	0.60	1.10	D(102,101,104,106)	-172.48	-172.77
A(3,23,11)	111.227	111.473	A(5,108,110)	104.399	104.448	D(31,43,45,46)	-89.58	-90.74	D(103,101,104,13)	63.13	62.93
A(4,23,11)	124.138	124.556	A(5,108,111)	111.614	111.531	D(31,43,45,47)	24.96	23.84	D(103,101,104,105)	-176.86	-177.09
A(11,24,25)	110.853	110.927	A(109,108,110)	109.289	109.313	D(31,43,45,55)	149.76	148.72	D(103,101,104,106)	-57.64	-57.93
A(11,24,26)	109.553	110.139	A(109,108,111)	110.883	110.890	D(44,43,45,46)	158.70	157.47	D(5,108,111,112)	-64.85	-64.68
A(11,24,27)	102.982	102.764	A(110,108,111)	111.375	111.382	D(44,43,45,47)	-86.76	-87.95	D(5,108,111,113)	175.70	175.86
A(25,24,26)	107.749	108.011	A(108,111,112)	110.249	110.250	D(44,43,45,55)	38.04	36.94	D(5,108,111,114)	55.89	56.03
A(25,24,27)	112.082	111.993	A(108,111,113)	110.019	110.055	D(89,43,45,46)	41.13	39.79	D(109,108,111,112)	56.96	57.08
A(26,24,27)	113.588	112.977	A(108,111,114)	110.851	110.846	D(89,43,45,47)	155.68	154.37	D(109,108,111,113)	-62.49	-62.39
A(24,27,28)	112.790	112.698	A(112,111,113)	108.363	108.349	D(89,43,45,55)	-79.53	-80.75	D(109,108,111,114)	177.70	177.78
A(24,27,29)	109.666	109.641	A(112,111,114)	108.962	108.937	D(31,43,89,15)	-108.30	-107.76	D(110,108,111,112)	178.90	179.06
A(24,27,31)	104.314	104.255	A(113,111,114)	108.335	108.340	D(31,43,89,90)	84.83	84.67	D(110,108,111,113)	59.44	59.59
A(28,27,29)	108.152	108.224	**Dihedral Angle** / °			D(44,43,89,15)	9.96	10.47	D(110,108,111,114)	-60.36	-60.24

Table S3 Second order perturbation theory analysis of Fock matrix in NBO Basis of Conformer I.

Donor NBO (i)	ED(i)/e	Acceptor NBO (j)	ED(j)/e	E(2)[a] / kJmol^{-1}	E(j)-E(i)[b]	F(i,j)[c]
π(C32 - C41)	1.67073	π *(C33 - C35)	0.31452	89.418	0.29	0.070
π(C32 - C41)	1.67073	π *(C37 - C39)	0.31867	73.500	0.29	0.064
π(C33 - C35)	1.66161	π *(C37 - C39)	0.31867	85.596	0.28	0.068
π(C33 - C35)	1.66161	π *(C32 - C41)	0.36802	79.422	0.28	0.065
π(C37 - C39)	1.65143	π *(C32 - C41)	0.36802	97.146	0.27	0.071
π(C37 - C39)	1.65143	π *(C33 - C35)	0.31452	82.740	0.28	0.067
σ(C49 - H50)	1.97701	σ*(C51 - C52)	0.02573	26.670	0.94	0.069
π(C68 - C76)	1.67209	π *(C69 - C70)	0.38726	93.576	0.27	0.071
π(C68 - C76)	1.67209	π *(C72 - C74)	0.33923	79.338	0.28	0.065
σ(C69 - C70)	1.97507	σ*(C68 - C69)	0.02940	21.840	1.28	0.073
π(C69 - C70)	1.66291	π *(C72 - C74)	0.33923	87.360	0.29	0.070
π(C69 - C70)	1.66291	π *(C68 - C76)	0.34352	79.338	0.30	0.067
σ(C70 - C72)	1.97482	σ*(N12 - C69)	0.03438	28.098	1.07	0.076
π(C72 - C74)	1.67327	π *(C68 - C76)	0.34352	86.814	0.29	0.069
π (C72 - C74)	1.67327	π *(C69 - C70)	0.38726	78.246	0.27	0.065
π(C78 - C79)	1.69133	π *(C85 - C87)	0.29750	84.462	0.30	0.069
π(C78 - C79)	1.69133	π *(C81 - C83)	0.31009	69.804	0.30	0.063
π(C81 - C83)	1.64831	π *(C78 - C79)	0.38246	99.414	0.27	0.071
π(C81 - C83)	1.64831	π *(C85 - C87)	0.29750	79.590	0.28	0.066
π(C85 - C87)	1.65106	π *(C81 - C83)	0.31009	86.814	0.28	0.069
π(C85 - C87)	1.65106	π *(C78 - C79)	0.38246	81.732	0.27	0.065
π(C89 - C90)	1.85484	π *(C91 - C92)	0.46143	62.202	0.30	0.064
σ(C90 - C91)	1.96345	σ*(C43 - C89)	0.02429	25.410	1.05	0.071
π (C91 - C92)	1.61385	π *(C93 - C95)	0.32966	79.002	0.28	0.066
π(C91 - C92)	1.61385	π *(C97 - C99)	0.30119	76.314	0.29	0.066
π(C91 - C92)	1.61385	π *(C89 - C90)	0.24494	71.526	0.29	0.065
σ(C93 - C95)	1.97508	σ*(N15 - C92)	0.03246	29.568	1.08	0.078
π(C93 - C95)	1.70815	π *(C91 - C92)	0.46143	82.236	0.28	0.069
π(C93 - C95)	1.70815	π *(C97 - C99)	0.30119	75.726	0.29	0.065
π(C97 - C99)	1.70292	π *(C93 - C95)	0.32966	86.016	0.28	0.068

π(C97 - C99)	1.70292	π *(C91 - C92)	0.46143	78.918	0.27	0.067
LP(1) O 3	1.96103	σ*(O4 - C23)	0.03189	34.818	1.14	0.087
LP(2) O 3	1.82444	π *(O4 - C23)	0.36695	177.912	0.34	0.112
LP(2) O 4	1.83514	σ*(O3 - C23)	0.10151	136.752	0.61	0.128
LP(2) O 4	1.83514	σ*(N11 - C23)	0.07461	94.836	0.73	0.117
LP(1) O 5	1.96185	σ*(O6 - C107)	0.11417	30.534	1.01	0.078
LP(2) O 5	1.82733	π *(O6 - C107)	0.29753	102.144	0.46	0.097
LP(2) O 5	1.82733	σ*(C108 - C111)	0.01527	24.906	0.70	0.060
LP(2) O 6	1.83602	σ*(O5 - C107)	0.10342	135.492	0.61	0.127
LP(2) O 6	1.83602	σ*(N13 - C107)	0.06867	90.720	0.73	0.115
LP(2) O 7	1.81575	σ*(S1 - C78)	0.20147	76.440	0.45	0.081
LP(2) O 7	1.81575	σ*(S1 - N15)	0.28093	31.080	0.41	0.050
LP(2) O 7	1.81575	σ*(S1 - O8)	0.14801	21.756	0.58	0.049
LP(3) O 7	1.78519	σ*(S1 - N15)	0.28093	83.328	0.40	0.081
LP(3) O 7	1.78519	σ*(S1 - O8)	0.14801	68.166	0.58	0.088
LP(2) O 8	1.80487	σ*(S1 - C78)	0.20147	78.456	0.45	0.082
LP(2) O 8	1.80487	σ*(S1 - N15)	0.28093	34.104	0.40	0.052
LP(2) O 8	1.80487	σ*(S1 - O7)	0.15443	22.176	0.57	0.049
LP(3) O 8	1.77011	σ*(S1 - N15)	0.28093	84.798	0.40	0.081
LP(3) O 8	1.77011	σ*(S1 - O7)	0.15443	72.828	0.56	0.090
LP(2) O 9	1.81463	σ*(S2 - C32)	0.20272	79.170	0.45	0.083
LP(2) O 9	1.81463	σ*(S2 - N12)	0.26558	31.038	0.42	0.051
LP(2) O 9	1.81463	σ*(S2 - O10)	0.15948	25.074	0.56	0.052
LP(3) O 9	1.77373	σ*(S2 - N12)	0.26558	84.630	0.41	0.082
LP(3) O 9	1.77373	σ*(S2 - O10)	0.15948	71.568	0.56	0.089
LP(2) O10	1.82180	σ*(S2 - C32)	0.20272	72.324	0.45	0.079
LP(2) O10	1.82180	σ*(S2 - N12)	0.26558	33.810	0.42	0.053
LP(3) O10	1.78640	σ*(S 2 - O9)	0.14640	72.114	0.57	0.090
LP(3) O10	1.78640	σ*(S2 - N12)	0.26558	71.988	0.42	0.077
LP(1) N11	1.70408	π *(O4 - C23)	0.36695	268.548	0.27	0.119
LP(1) N11	1.70408	σ*(N12 - C30)	0.06714	45.444	0.52	0.071
LP(1) N11	1.70408	σ*(C24 - H25)	0.02230	24.654	0.70	0.062

LP(1) N11	1.70408	σ*(C30 - C47)	0.04151	24.276	0.61	0.057
LP(1) N12	1.79121	π *(C69 - C70)	0.38726	109.662	0.30	0.083
LP(1) N12	1.79121	σ*(N 11 - C30)	0.05333	38.934	0.62	0.070
LP(1) N12	1.79121	σ*(S2 - C32)	0.20272	36.918	0.43	0.055
LP(1) N13	1.73099	π *(O6 - C107)	0.29753	125.538	0.40	0.098
LP(1) N13	1.73099	π *(C101 - C104)	0.03022	33.768	0.62	0.067
LP(1) N13	1.73099	σ*(O6 - C107)	0.11417	33.180	0.70	0.069
LP(1) N15	1.70626	π *(C91 - C92)	0.46143	98.112	0.33	0.082
LP(1) N15	1.70626	π *(C89 - C90)	0.24494	85.932	0.34	0.075
LP(1) N15	1.70626	σ*(S1 - C78)	0.20147	26.964	0.43	0.048
σ*(O6 - C107)	0.11417	σ*(N13 - C107)	0.06867	44.814	0.03	0.056
σ*(S2 - N12)	0.26558	σ*(N12 - C30)	0.06714	25.872	0.15	0.067
σ*(S2 - N12)	0.26558	σ*(S2 - C 32)	0.20272	22.932	0.03	0.024
π *(C69 - C70)	0.38726	π *(C68 - C76)	0.34352	908.460	0.01	0.082
π *(C78 - C79)	0.38246	π *(C81 - C83)	0.31009	793.506	0.02	0.083
π *(C78 - C79)	0.38246	π *(C85 - C87)	0.29750	668.178	0.02	0.078
π *(C91 - C92)	0.46143	π *(C97 - C99)	0.30119	994.896	0.01	0.081
π *(C91 - C92)	0.46143	π *(C89 - C90)	0.24494	662.550	0.01	0.064
π *(O6 - C107)	0.29753	σ*(O6 - C107)	0.11417	217.014	0.30	0.247

[a]E(2) means energy of hyper conjugative interaction (stabilization energy).

[b]Energy difference between donor (i) and acceptor (j) NBO orbitals.

[c]F(i,j) is the Fock matrix element between i and j NBO orbitals.

Table S4 Second order perturbation theory analysis of Fock matrix in NBO Basis of Conformer V.

Donor NBO (i)	ED(i)/e	Acceptor NBO (j)	ED(j)/e	E(2)[a]/kJmol^{-1}	E(j)-E(i)[b]	F(i,j)[c]
π (C32 - C33)	1.68591	π *(C35 - C37)	0.31418	73.290	0.30	0.064
π (C32 - C33)	1.68591	π *(C39 - C41)	0.3081	83.958	0.30	0.069
π (C35 - C37)	1.64763	π *(C32 - C33)	0.38206	96.684	0.27	0.071
π (C35 - C37)	1.64763	π *(C39 - C41)	0.3081	82.236	0.28	0.067
π (C39 - C41)	1.65403	π *(C32 - C33)	0.38206	82.656	0.27	0.066
π (C39 - C41)	1.65403	π *(C35 - C37)	0.31418	85.428	0.28	0.068
σ (C49 - H50)	1.97714	σ*(C51 - C52)	0.0257	26.628	0.94	0.069
π (C68 - C76)	1.66972	π *(C69 - C70)	0.38688	94.374	0.27	0.071
π (C68 - C76)	1.66972	π *(C72 - C74)	0.33859	80.094	0.28	0.066
σ (C69 - C70)	1.97498	σ*(C68 - C69)	0.02977	22.386	1.28	0.074
π (C69 - C70)	1.66532	π *(C68 - C76)	0.34253	79.800	0.30	0.067
π (C69 - C70)	1.66532	π *(C72 - C74)	0.33859	86.184	0.29	0.069
σ (C70 - C72)	1.9748	σ*(N12 - C69)	0.03477	28.308	1.07	0.076
π (C72 - C74)	1.67247	π *(C68 - C76)	0.34253	86.478	0.29	0.069
π (C72 - C74)	1.67247	π *(C69 - C70)	0.38688	78.834	0.27	0.065
π (C78 - C79)	1.69122	π *(C81 - C83)	0.31003	69.804	0.30	0.063
π (C78 - C79)	1.69122	π *(C85 - C87)	0.29771	84.588	0.30	0.069
π (C81 - C83)	1.64819	π *(C78 - C79)	0.38204	99.498	0.27	0.071
π (C81 - C83)	1.64819	π *(C85 - C87)	0.29771	79.632	0.28	0.066
π (C85 - C87)	1.65141	π *(C78 - C79)	0.38204	81.648	0.27	0.065
π (C85 - C87)	1.65141	π *(C81 - C83)	0.31003	86.772	0.28	0.069
π (C89 - C90)	1.85516	π *(C91 - C92)	0.46146	61.908	0.30	0.064
σ (C90 - C91)	1.96344	σ*(C43 - C89)	0.02439	25.452	1.05	0.071
π (C91 - C92)	1.61423	π *(C89 - C90)	0.24513	71.652	0.29	0.065
π (C91 - C92)	1.61423	π *(C93 - C95)	0.32883	78.834	0.28	0.066
π (C91 - C92)	1.61423	π *(C97 - C99)	0.3011	76.272	0.29	0.066
σ (C93 - C95)	1.97509	σ*(N15 - C92)	0.03242	29.526	1.08	0.078
π (C93 - C95)	1.70732	π *(C91 - C92)	0.46146	82.572	0.28	0.069
π (C93 - C95)	1.70732	π *(C97 - C99)	0.3011	75.894	0.29	0.065

π (C97 - C99)	1.70288	π *(C91 - C92)	0.46146	78.918	0.27	0.067
π (C97 - C99)	1.70288	π *(C93 - C95)	0.32883	85.932	0.28	0.068
LP (1) O3	1.95746	σ*(O4 - C23)	0.02001	36.498	1.16	0.090
LP (2) O3	1.82347	π *(O4 - C23)	0.36913	187.866	0.33	0.113
LP (2) O3	1.82347	σ*(C16 - C20)	0.01399	23.058	0.71	0.058
LP (2) O4	1.83222	σ*(O3 - C23)	0.10552	136.122	0.61	0.128
LP (2) O4	1.83222	σ*(N11 - C23)	0.07821	99.288	0.72	0.119
LP (1) O5	1.96182	σ*(O6 - C107)	0.11312	30.702	1.01	0.078
LP (2) O5	1.82694	π *(O6 - C107)	0.29671	103.278	0.46	0.098
LP (2) O5	1.82694	σ*(C108 - C111)	0.01525	24.864	0.70	0.060
LP (2) O6	1.83615	σ*(O5 - C107)	0.10339	135.618	0.61	0.127
LP (2) O6	1.83615	σ*(N13 - C107)	0.0688	90.930	0.73	0.115
LP (2) O7	1.81541	σ*(S1 - O8)	0.14793	21.756	0.58	0.049
LP (2) O7	1.81541	σ*(S1 - N15)	0.28203	31.290	0.41	0.050
LP (2) O7	1.81541	σ*(S1 - C78)	0.20131	76.566	0.45	0.081
LP (3) O7	1.7848	σ*(S1 - O8)	0.14793	68.292	0.58	0.088
LP (3) O7	1.7848	σ*(S1 - N15)	0.28203	83.412	0.40	0.081
LP (2) O8	1.80462	σ*(S1 - O7)	0.15472	22.680	0.57	0.050
LP (2) O8	1.80462	σ*(S1 - N15)	0.28203	33.600	0.40	0.052
LP (2) O8	1.80462	σ*(S1 - C78)	0.20131	78.540	0.45	0.082
LP (3) O8	1.77001	σ*(S1 - O7)	0.15472	72.324	0.57	0.090
LP (3) O8	1.77001	σ*(S1 - N15)	0.28203	85.554	0.40	0.081
LP (2) O9	1.81238	σ*(S2 - O10)	0.1629	29.400	0.56	0.056
LP (2) O9	1.81238	σ*(S2 - N12)	0.25922	23.982	0.43	0.045
LP (2) O9	1.81238	σ*(S2 - C32)	0.20742	80.304	0.45	0.083
LP (3) O9	1.77585	σ*(S2 - O10)	0.1629	66.906	0.56	0.086
LP (3) O9	1.77585	σ*(S2 - N12)	0.25922	90.888	0.42	0.086
LP (2) O10	1.81866	σ*(S2 - N12)	0.25922	34.902	0.43	0.054
LP (2) O10	1.81866	σ*(S2 - C32)	0.20742	73.416	0.45	0.079
LP (3) O10	1.78446	σ*(S2 - O9)	0.14727	73.290	0.57	0.091
LP (3) O10	1.78446	σ*(S2 - N12)	0.25922	72.324	0.43	0.077
LP (1) N11	1.70805	π *(O4 - C23)	0.36913	285.852	0.26	0.120

LP (1) N11	1.70805	σ*(N12 - C30)	0.06947	47.502	0.52	0.072
LP (1) N11	1.70805	σ*(C24 - H25)	0.02185	24.402	0.71	0.061
LP (1) N11	1.70805	σ*(C30 - C47)	0.04158	24.570	0.61	0.057
LP (1) N12	1.79392	σ*(S2 - C32)	0.20742	39.228	0.43	0.057
LP (1) N12	1.79392	σ*(N11 - C30)	0.05578	38.514	0.62	0.070
LP (1) N12	1.79392	π *(C69 - C70)	0.38688	107.562	0.31	0.083
LP (1) N13	1.73374	σ*(O6 - C107)	0.11312	33.432	0.71	0.070
LP (1) N13	1.73374	π *(O6 - C107)	0.29671	122.682	0.40	0.097
LP (1) N13	1.73374	σ*(C101 - C104)	0.03008	33.642	0.62	0.067
LP (1) N15	1.70767	σ*(S1 - C78)	0.20131	26.460	0.43	0.048
LP (1) N15	1.70767	π *(C89 - C90)	0.24513	84.840	0.34	0.075
LP (1) N15	1.70767	π *(C91 - C92)	0.46146	97.146	0.33	0.082
σ*(S2 - N12)	0.25922	σ*(S2 - C32)	0.20742	27.384	0.02	0.021
σ*(S2 - N12)	0.25922	σ*(N12 - C30)	0.06947	28.224	0.14	0.067
σ*(O6 - C107)	0.11312	σ*(N13 - C107)	0.0688	49.728	0.03	0.056
π *(O6 - C107)	0.29671	σ*(O6 - C107)	0.11312	213.276	0.31	0.246
π * (C32 - C33)	0.38206	π *(C35 - C37)	0.31418	902.034	0.01	0.083
π * (C32 - C33)	0.38206	π *(C39 - C41)	0.3081	901.992	0.01	0.079
π * (C69 - C70)	0.38688	π *(C68 - C76)	0.34253	858.102	0.02	0.082
π * (C78 - C79)	0.38204	π *(C81 - C83)	0.31003	796.026	0.02	0.083
π * (C78 - C79)	0.38204	π *(C85 - C87)	0.29771	678.006	0.02	0.078
π * (C91 - C92)	0.46146	π *(C89 - C90)	0.24513	688.968	0.01	0.064
π * (C91 - C92)	0.46146	π *(C97 - C99)	0.3011	982.758	0.01	0.081

[a]E(2) means energy of hyper conjugative interaction (stabilization energy).

[b]Energy difference between donor (i) and acceptor (j) NBO orbitals.

[c]F(i,j) is the Fock matrix element between i and j NBO orbitals.