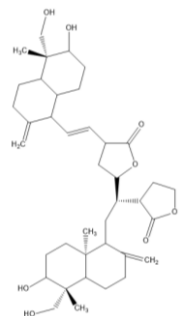
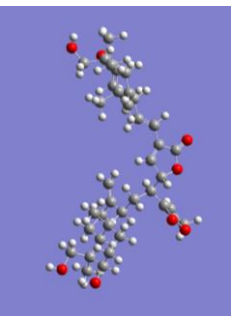
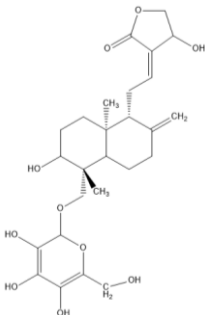
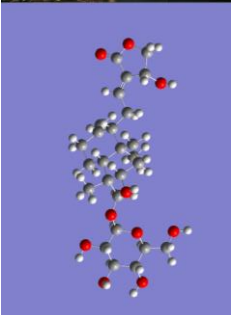
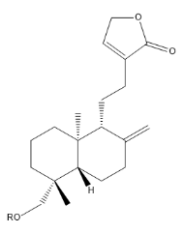
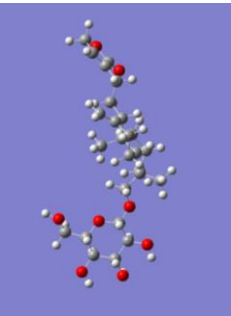
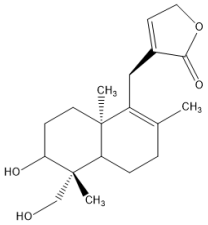
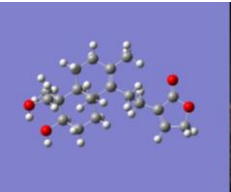
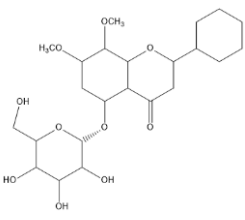
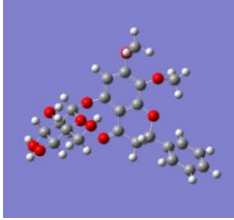
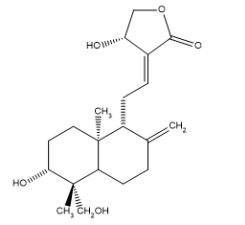
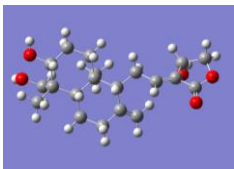
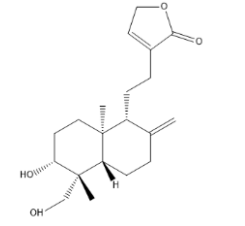
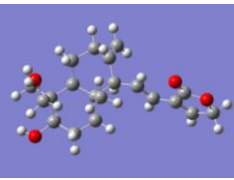
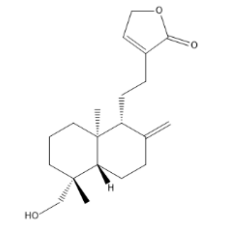
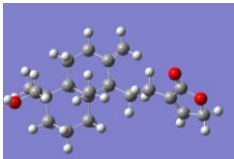
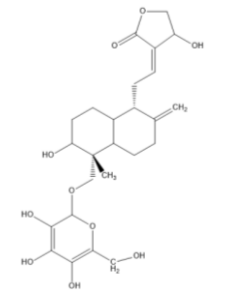
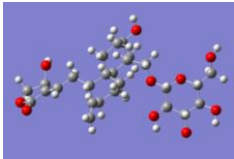
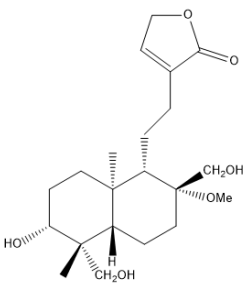
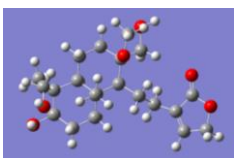


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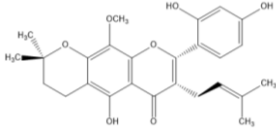
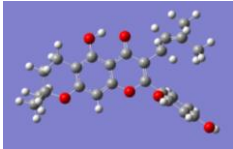
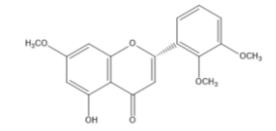
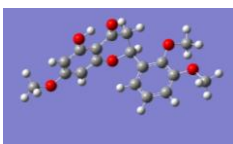
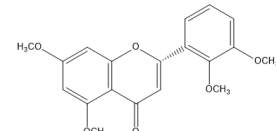
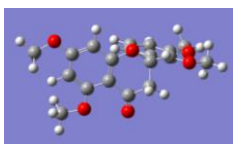
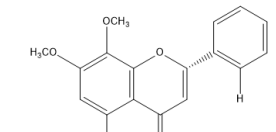
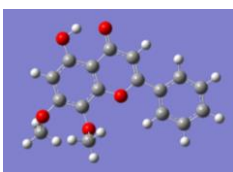
Lampiran 1 Senyawa Uji

Terpen dari *andrographis paniculata*

Senyawa	Struktur 2D	Struktur 3D	Referensi
L1			(Okhwarobo dkk., 2014)
L3			(Okhwarobo dkk., 2014)
L4			(Koteswara dkk., 2004)
L5			(Okhwarobo dkk., 2014)

L6			(Okhwarobo dkk., 2014)
L7			(Reddy dkk., 2003)
L8			(Koteswara dkk., 2004)
L9			(Aromdee, 2012)
L10			(Koteswara dkk., 2004)
L11			(Okhwarobo dkk., 2014)

Flavonoid dari andrographis paniculata

Senyawa	Struktur 2D	Struktur 3D	Referensi
L2	 2-(2,3-dimethoxyphenyl)-5-hydroxy-7-methoxy-4H-chromen-4-one		(Kishore dkk., 2003)
L12	 2-(2,3-dimethoxyphenyl)-5-hydroxy-7-methoxy-4H-chromen-4-one		(Koteswara dkk., 2004)
L13	 2-(2,3-dimethoxyphenyl)-5,7-dimethoxy-4H-chromen-4-one		(Koteswara dkk., 2004)
L14	 5-hydroxy-7,8-dimethoxy-2-phenyl-4H-chromen-4-one		(Koteswara dkk., 2004)

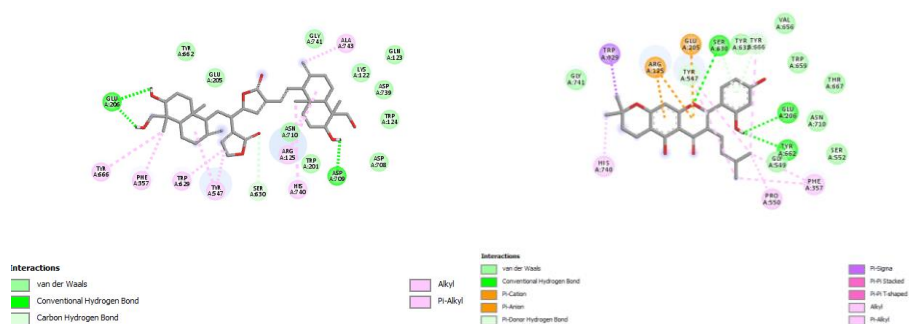
Lampiran 2 Penambatan Ulang Ligan Alami

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	88	-6,72	0	1,76	RANKING
1	2	31	-6,58	0,61	1,59	RANKING
1	3	72	-6,57	0,59	1,6	RANKING
1	4	81	-6,57	0,44	1,65	RANKING
1	5	3	-6,54	0,49	1,66	RANKING
1	6	22	-6,52	0,54	1,64	RANKING
1	7	57	-6,5	1,03	1,75	RANKING
1	8	23	-6,47	1,05	1,76	RANKING
1	9	36	-6,46	1,07	1,74	RANKING
1	10	87	-6,46	1,09	1,73	RANKING
1	11	29	-6,45	1,35	1,93	RANKING
1	12	74	-6,45	1,07	1,72	RANKING
1	13	58	-6,44	1,07	1,73	RANKING
1	14	91	-6,44	1,09	1,74	RANKING
1	15	41	-6,41	1,13	1,7	RANKING
1	16	92	-6,39	1,14	1,69	RANKING
1	17	7	-6,39	1,07	1,71	RANKING
1	18	40	-6,38	1,16	1,68	RANKING
1	19	52	-6,37	0,9	1,62	RANKING
1	20	27	-6,36	0,54	1,62	RANKING
1	21	25	-6,3	0,86	1,54	RANKING
1	22	12	-6,17	1,08	1,5	RANKING
1	23	98	-6,1	1,76	1,9	RANKING
1	24	53	-6,09	1,71	1,97	RANKING
1	25	28	-6,09	1,7	1,91	RANKING
1	26	43	-6,04	0,34	1,71	RANKING
1	27	60	-6,03	1,6	1,94	RANKING
1	28	96	-6,02	1,15	1,88	RANKING
1	29	49	-5,98	1,74	1,88	RANKING
1	30	55	-5,93	1,44	1,62	RANKING
1	31	65	-5,91	1,7	2	RANKING

1	32	2	-5,86	1,48	1,52	RANKING
2	1	17	-6,62	0	3,93	RANKING
2	2	24	-6,59	0,19	3,91	RANKING
2	3	11	-6,58	0,09	3,94	RANKING
2	4	82	-6,58	0,14	3,87	RANKING
2	5	5	-6,57	0,41	3,8	RANKING
2	6	47	-6,52	0,19	4,01	RANKING
2	7	10	-6,45	0,3	4,04	RANKING
2	8	14	-6,31	1,67	3,8	RANKING
2	9	69	-6,31	1,68	3,8	RANKING
2	10	8	-6,31	1,66	4,47	RANKING
2	11	76	-6,29	1,66	3,81	RANKING
2	12	59	-6,29	1,65	3,77	RANKING
2	13	21	-6,29	1,66	3,78	RANKING
2	14	48	-6,28	1,66	3,72	RANKING
2	15	94	-6,28	1,42	3,58	RANKING
2	16	100	-6,28	1,67	3,76	RANKING
2	17	80	-6,28	1,67	3,72	RANKING
2	18	99	-6,28	1,65	3,83	RANKING
2	19	62	-6,27	1,69	3,76	RANKING
2	20	33	-6,27	1,67	3,79	RANKING
2	21	64	-6,26	1,68	3,77	RANKING
2	22	95	-6,26	1,67	3,71	RANKING
2	23	45	-6,25	1,68	3,72	RANKING
2	24	73	-6,25	1,67	4,41	RANKING
2	25	15	-6,25	1,67	3,77	RANKING
2	26	86	-6,25	1,66	3,74	RANKING
2	27	90	-6,25	1,66	3,72	RANKING
2	28	9	-6,25	1,63	3,69	RANKING
2	29	56	-6,25	1,69	3,72	RANKING
2	30	1	-6,25	1,7	3,76	RANKING
2	31	6	-6,24	1,7	4,25	RANKING
2	32	85	-6,24	1,7	3,7	RANKING
2	33	44	-6,22	1,44	3,65	RANKING

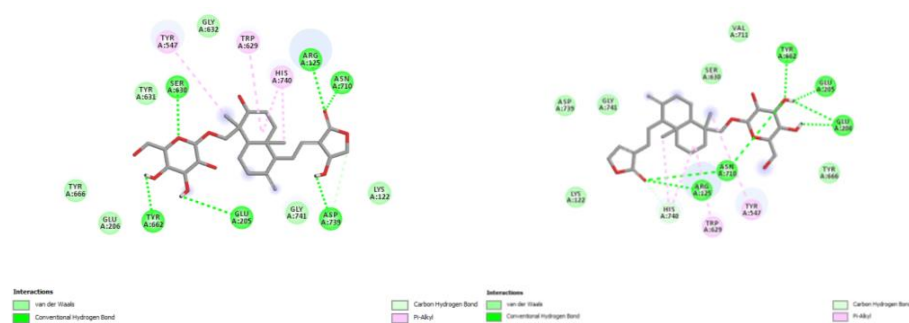
2	34	19	-6,22	1,69	4,24	RANKING
2	35	66	-6,21	1,7	4,23	RANKING
2	36	42	-6,21	1,7	4,23	RANKING
2	37	50	-6,2	1,7	4,14	RANKING
2	38	70	-6,2	1,69	4,17	RANKING
2	39	84	-6,2	1,7	4,16	RANKING
2	40	54	-6,2	1,71	4,15	RANKING
2	41	51	-6,2	1,71	4,16	RANKING
2	42	4	-6,19	1,72	4,3	RANKING
2	43	68	-6,19	1,72	4,17	RANKING
2	44	34	-6,18	1,74	4,18	RANKING
2	45	26	-6,18	1,7	4,24	RANKING
2	46	13	-6,18	1,69	4,29	RANKING
2	47	78	-6,18	1,33	3,83	RANKING
2	48	89	-6,17	1,38	3,83	RANKING
2	49	75	-6,17	1,75	4,24	RANKING
2	50	46	-6,16	1,37	4	RANKING
2	51	37	-6,15	1,75	4,26	RANKING
2	52	77	-6,14	1,63	4,32	RANKING
2	53	71	-6,13	1,42	3,74	RANKING
2	54	38	-6,05	1,77	4,39	RANKING
2	55	39	-6	1,3	3,65	RANKING
2	56	83	-5,99	1,75	4,41	RANKING
2	57	16	-5,97	1,75	4,37	RANKING
2	58	61	-5,93	1,74	4,45	RANKING
2	59	97	-5,8	1,95	4,28	RANKING
3	1	30	-6,53	0	3,81	RANKING
3	2	20	-5,91	1,46	3,91	RANKING
4	1	63	-6,19	0	2,56	RANKING
4	2	18	-6,15	0,19	2,55	RANKING
4	3	32	-6,06	0,27	2,49	RANKING
4	4	93	-5,5	1,86	2,1	RANKING
4	5	35	-5,48	1,9	2,17	RANKING
5	1	67	-6,13	0	4,5	RANKING

Lampiran 3 Interaksi Senyawa Uji – Target Uji



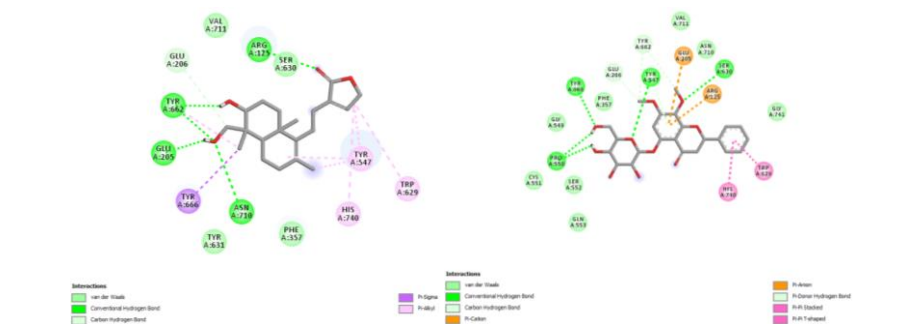
L1

L2



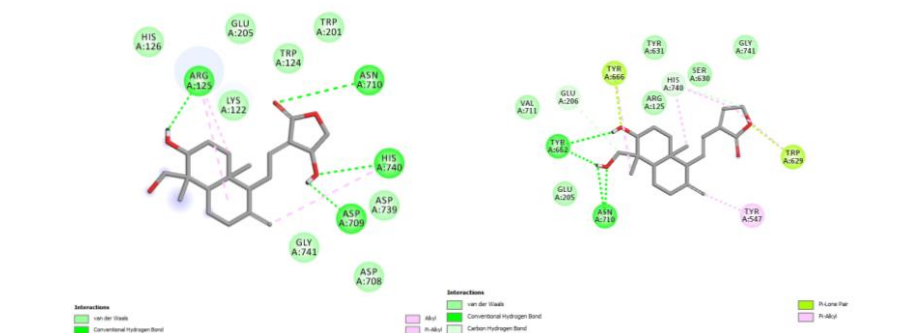
L3

L4



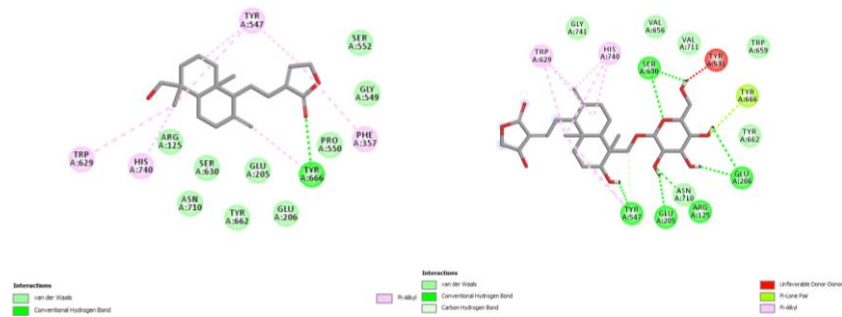
L5

L6



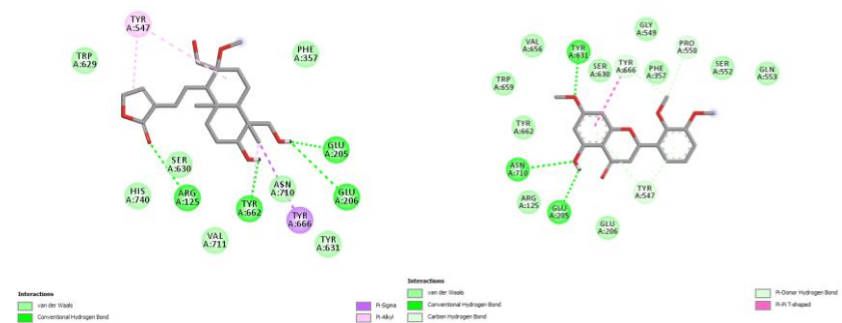
L7

L8



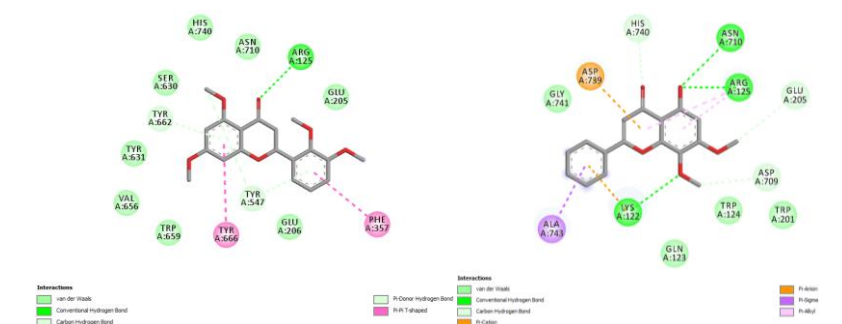
L9

L10



L11

L12



L13

L14

Lampiran 4 Tabel Interaksi Reseptor-Ligan

Senyawa	#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
LF7	GLU_168@OE2	LF7_729@H27	LF7_729@N2	3856	0,08	2,82	158,26
	GLU_167@OE2	LF7_729@H16	LF7_729@N12	2279	0,05	2,87	158,04
	LF7_729@O20	TYR_509@HH	TYR_509@OH	1884	0,04	2,71	163,35
	LF7_729@O20	SER_592@HG	SER_592@OG	1108	0,02	2,72	163,14
	LF7_729@N2	TYR_624@HH	TYR_624@OH	432	0,01	2,79	163,77
	GLY_703@O	LF7_729@H27	LF7_729@N2	302	0,01	2,85	156,68
	LF7_729@N15	SER_592@HG	SER_592@OG	136	0,00	2,92	158,95
	TYR_509@OH	LF7_729@H16	LF7_729@N12	123	0,00	2,93	160,00
	LF7_729@N15	TYR_624@HH	TYR_624@OH	45	0,00	2,92	143,93
	LF7_729@O20	TYR_624@HH	TYR_624@OH	34	0,00	2,84	144,71
	ASN_672@OD1	LF7_729@H16	LF7_729@N12	33	0,00	2,89	156,84
	SER_171@OG	LF7_729@H13	LF7_729@O4	27	0,00	2,83	160,07
	GLU_167@O	LF7_729@H13	LF7_729@O4	27	0,00	2,84	166,69
	LF7_729@O4	TYR_509@HH	TYR_509@OH	22	0,00	2,85	158,23
	LF7_729@N2	TYR_509@HH	TYR_509@OH	19	0,00	2,84	157,30
	LF7_729@N2	TYR_628@HH	TYR_628@OH	18	0,00	2,87	163,38
	GLY_703@O	LF7_729@H13	LF7_729@O4	14	0,00	2,84	155,50
	GLU_167@OE1	LF7_729@H13	LF7_729@O4	7	0,00	2,78	163,93
	TYR_509@OH	LF7_729@H13	LF7_729@O4	7	0,00	2,86	152,31
	HID_702@O	LF7_729@H13	LF7_729@O4	5	0,00	2,82	154,60
	HID_702@NE2	LF7_729@H16	LF7_729@N12	5	0,00	2,91	167,25
	TRP_591@O	LF7_729@H13	LF7_729@O4	5	0,00	2,93	146,77
	GLU_167@O	LF7_729@H27	LF7_729@N2	4	0,00	2,85	164,77
	TYR_509@OH	LF7_729@H27	LF7_729@N2	4	0,00	2,90	154,09
	HID_702@NE2	LF7_729@H13	LF7_729@O4	3	0,00	2,87	157,56
	LF7_729@O4	ARG_87@HH22	ARG_87@NH2	2	-	2,88	147,69
	HID_702@O	LF7_729@H27	LF7_729@N2	2	-	2,93	166,37
	PRO_512@O	LF7_729@H27	LF7_729@N2	2	-	2,93	157,35
	HID_702@NE2	LF7_729@H27	LF7_729@N2	1	-	2,90	143,99
	LF7_729@N2	SER_514@HG	SER_514@OG	1	-	2,91	138,88
	LF7_729@N12	ARG_87@HH21	ARG_87@NH2	1	-	2,92	138,33
	LF7_729@O4	HIE_88@HE2	HIE_88@NE2	1	-	2,93	173,06
	TRP_591@NE1	LF7_729@H27	LF7_729@N2	1	-	2,98	161,79
	TYR_624@OH	LF7_729@H27	LF7_729@N2	1	-	2,99	138,95

Senyawa	#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
L1	ASP_671@OD1	RES_729@H101	RES_729@O4	12786	0,26	2,65	165,05
	RES_729@O3	GLN_515@H	GLN_515@N	4309	0,09	2,90	154,01
	RES_729@O2	ASN_672@HD22	ASN_672@ND2	3132	0,06	2,88	160,06
	RES_729@O8	ARG_87@HH12	ARG_87@NH1	2550	0,05	2,85	152,79
	ASP_671@OD2	RES_729@H101	RES_729@O4	2130	0,04	2,67	164,63
	GLU_167@OE2	RES_729@H95	RES_729@O2	1501	0,03	2,75	162,70
	ASP_671@OD2	RES_729@H95	RES_729@O2	870	0,02	2,73	157,86
	GLN_515@O	RES_729@H96	RES_729@O3	749	0,02	2,75	155,73
	RES_729@O3	LYS_516@HZ2	LYS_516@NZ	687	0,01	2,87	152,83
	RES_729@O3	LYS_516@HZ3	LYS_516@NZ	635	0,01	2,86	152,93
	RES_729@O3	LYS_516@HZ1	LYS_516@NZ	571	0,01	2,86	151,97
	GLN_85@O	RES_729@H95	RES_729@O2	492	0,01	2,76	160,75
	RES_729@O6	ARG_87@HH12	ARG_87@NH1	475	0,01	2,89	148,62
	ASP_671@OD1	RES_729@H95	RES_729@O2	445	0,01	2,76	157,85
	RES_729@O7	ARG_87@HH11	ARG_87@NH1	399	0,01	2,85	146,63
	RES_729@O8	ARG_87@HH11	ARG_87@NH1	381	0,01	2,86	153,63
	RES_729@O2	TRP_163@HE1	TRP_163@NE1	380	0,01	2,90	155,44
	RES_729@O6	ARG_87@HH22	ARG_87@NH2	241	0,00	2,90	149,76
	RES_729@O7	LYS_84@HZ1	LYS_84@NZ	234	0,00	2,85	152,44
	RES_729@O2	ASN_672@HD21	ASN_672@ND2	195	0,00	2,88	150,40
	SER_514@OG	RES_729@H96	RES_729@O3	191	0,00	2,85	153,50
	RES_729@O7	LYS_84@HZ2	LYS_84@NZ	189	0,00	2,83	150,18
	RES_729@O7	LYS_84@HZ3	LYS_84@NZ	183	0,00	2,83	149,28
	ALA_705@O	RES_729@H95	RES_729@O2	176	0,00	2,79	156,14
	GLU_167@OE1	RES_729@H95	RES_729@O2	164	0,00	2,78	158,44
	ASP_701@OD2	RES_729@H101	RES_729@O4	126	0,00	2,72	162,30
	RES_729@O8	ARG_87@HH22	ARG_87@NH2	123	0,00	2,87	150,66
	TRP_86@O	RES_729@H95	RES_729@O2	120	0,00	2,76	160,48
	RES_729@O4	LYS_84@HZ2	LYS_84@NZ	105	0,00	2,86	153,93
	RES_729@O1	LYS_516@HZ2	LYS_516@NZ	79	0,00	2,88	157,23
	RES_729@O4	LYS_84@HZ3	LYS_84@NZ	71	0,00	2,86	154,22
	TYR_509@OH	RES_729@H96	RES_729@O3	59	0,00	2,83	154,22
	RES_729@O4	LYS_84@HZ1	LYS_84@NZ	58	0,00	2,86	154,95
	RES_729@O7	ARG_87@HH12	ARG_87@NH1	55	0,00	2,86	149,89
	GLN_515@O	RES_729@H90	RES_729@O1	50	0,00	2,79	149,32
	ASP_671@O	RES_729@H101	RES_729@O4	44	0,00	2,72	159,11
	RES_729@O3	SER_514@HG	SER_514@OG	43	0,00	2,83	151,47
	RES_729@O4	TRP_163@HE1	TRP_163@NE1	37	0,00	2,91	147,18
	RES_729@O3	TYR_509@HH	TYR_509@OH	35	0,00	2,80	151,19
	RES_729@O1	LYS_516@HZ1	LYS_516@NZ	29	0,00	2,88	154,48

RES_729@O2	LYS_84@HZ1	LYS_84@NZ	27	0,00	2,87	154,84
RES_729@O2	LYS_84@HZ2	LYS_84@NZ	18	0,00	2,93	153,17
RES_729@O1	LYS_516@HZ3	LYS_516@NZ	15	0,00	2,90	147,64
RES_729@O7	ARG_87@HH22	ARG_87@NH2	12	0,00	2,84	151,67
RES_729@O6	ASN_672@HD21	ASN_672@ND2	12	0,00	2,91	144,92
ASP_701@OD1	RES_729@H101	RES_729@O4	11	0,00	2,80	159,19
RES_729@O2	LYS_84@HZ3	LYS_84@NZ	10	0,00	2,90	155,12
CYS_513@O	RES_729@H96	RES_729@O3	9	0,00	2,88	147,14
RES_729@O6	ARG_87@HH11	ARG_87@NH1	7	0,00	2,91	140,84
RES_729@O4	ASP_671@H	ASP_671@N	7	0,00	2,95	148,21
RES_729@O4	ASN_672@HD21	ASN_672@ND2	5	0,00	2,90	160,46
ASN_672@OD1	RES_729@H95	RES_729@O2	4	0,00	2,82	156,31
GLN_85@O	RES_729@H101	RES_729@O4	3	0,00	2,80	146,45
ASN_672@ND2	RES_729@H101	RES_729@O4	2	-	2,78	151,40
TYR_509@OH	RES_729@H90	RES_729@O1	2	-	2,80	149,81
ASN_672@OD1	RES_729@H101	RES_729@O4	2	-	2,84	144,96
RES_729@O1	TYR_509@HH	TYR_509@OH	2	-	2,90	150,89
LYS_84@O	RES_729@H95	RES_729@O2	1	-	2,77	164,70
RES_729@O1	GLN_515@HE21	GLN_515@NE2	1	-	2,87	149,63
SER_706@OG	RES_729@H95	RES_729@O2	1	-	2,96	158,83

Senyawa	#Acceptor	DonorH	Donor	Frames	Frac	AvgDist	AvgAng
L3	ASP_625@OD1	RES_729@H74	RES_729@O7	22592	0,45	2,75	159,10
	ASP_625@OD1	RES_729@H73	RES_729@O6	20261	0,41	2,79	160,41
	ASP_625@OD2	RES_729@H74	RES_729@O7	19134	0,38	2,76	159,29
	ASP_625@OD2	RES_729@H73	RES_729@O6	18716	0,37	2,78	160,44
	ASN_672@OD1	RES_729@H58	RES_729@O1	8090	0,16	2,84	150,36
	TYR_624@OH	RES_729@H76	RES_729@O10	4869	0,10	2,88	150,66
	ASP_671@OD2	RES_729@H75	RES_729@O8	1332	0,03	2,72	162,22
	GLU_168@OE2	RES_729@H73	RES_729@O6	803	0,02	2,74	158,50
	GLU_168@OE2	RES_729@H74	RES_729@O7	695	0,01	2,75	160,49
	TYR_624@OH	RES_729@H74	RES_729@O7	389	0,01	2,88	151,16
	RES_729@O7	TYR_624@HH	TYR_624@OH	237	0,00	2,90	155,51
	HIE_88@ND1	RES_729@H75	RES_729@O8	180	0,00	2,86	147,01
	RES_729@O3	ASN_672@HD21	ASN_672@ND2	124	0,00	2,95	147,87
	SER_592@OG	RES_729@H76	RES_729@O10	113	0,00	2,92	152,46
	TYR_509@OH	RES_729@H58	RES_729@O1	108	0,00	2,85	146,12
	ARG_87@O	RES_729@H75	RES_729@O8	96	0,00	2,83	145,77
	ASN_672@OD1	RES_729@H76	RES_729@O10	87	0,00	2,84	153,16

ASP_701@OD1	RES_729@H75	RES_729@O8	80	0,00	2,72	159,48
ASP_701@OD2	RES_729@H75	RES_729@O8	69	0,00	2,72	158,95
GLY_703@O	RES_729@H75	RES_729@O8	57	0,00	2,82	148,03
RES_729@O10	TYR_624@HH	TYR_624@OH	41	0,00	2,88	148,53
RES_729@O1	SER_592@HG	SER_592@OG	32	0,00	2,88	150,89
RES_729@O10	SER_592@HG	SER_592@OG	20	0,00	2,90	145,54
RES_729@O9	ARG_87@HH22	ARG_87@NH2	17	0,00	2,89	149,32
RES_729@O9	ASN_672@HD22	ASN_672@ND2	17	0,00	2,93	152,03
RES_729@O5	LYS_84@HZ1	LYS_84@NZ	15	0,00	2,93	142,84
RES_729@O7	ASN_672@HD21	ASN_672@ND2	9	0,00	2,97	145,68
HID_702@NE2	RES_729@H58	RES_729@O1	8	0,00	2,91	159,98
TYR_628@OH	RES_729@H76	RES_729@O10	8	0,00	2,93	154,82
RES_729@O10	ASN_672@HD21	ASN_672@ND2	7	0,00	2,91	155,55
RES_729@O9	ARG_87@HH12	ARG_87@NH1	7	0,00	2,94	156,78
RES_729@O5	LYS_84@HZ3	LYS_84@NZ	7	0,00	2,94	146,27
GLU_167@OE2	RES_729@H70	RES_729@O4	5	0,00	2,82	141,98
GLU_168@OE2	RES_729@H70	RES_729@O4	4	0,00	2,91	148,48
RES_729@O5	LYS_84@HZ2	LYS_84@NZ	4	0,00	2,92	138,48
ARG_87@NH1	RES_729@H58	RES_729@O1	4	0,00	2,95	166,83
RES_729@O4	ASN_672@HD21	ASN_672@ND2	4	0,00	2,97	150,21
TRP_86@O	RES_729@H75	RES_729@O8	2	-	2,73	161,45
HID_702@NE2	RES_729@H76	RES_729@O10	2	-	2,84	169,06
RES_729@O6	ASN_672@HD21	ASN_672@ND2	2	-	2,88	143,38
GLU_167@OE1	RES_729@H70	RES_729@O4	2	-	2,88	151,01
RES_729@O9	ASN_672@HD21	ASN_672@ND2	2	-	2,90	146,98
RES_729@O8	ARG_87@HH12	ARG_87@NH1	2	-	2,97	156,89
RES_729@O8	GLY_703@H	GLY_703@N	1	-	2,79	139,00
GLU_168@OE1	RES_729@H70	RES_729@O4	1	-	2,81	135,37
ASP_671@OD1	RES_729@H75	RES_729@O8	1	-	2,82	135,14
ASP_671@O	RES_729@H75	RES_729@O8	1	-	2,83	155,81
RES_729@O10	TYR_628@HH	TYR_628@OH	1	-	2,86	156,70
RES_729@O1	ARG_87@HE	ARG_87@NE	1	-	2,90	145,60
TYR_509@OH	RES_729@H76	RES_729@O10	1	-	2,96	145,38
RES_729@O6	ASN_672@HD22	ASN_672@ND2	1	-	2,97	141,33
RES_729@O9	LYS_84@HZ3	LYS_84@NZ	1	-	2,97	146,93
RES_729@O2	ARG_87@HE	ARG_87@NE	1	-	2,99	136,24
RES_729@O8	ARG_87@HH22	ARG_87@NH2	1	-	2,99	137,45
RES_729@O9	LYS_84@HZ1	LYS_84@NZ	1	-	2,99	146,33
RES_729@O1	TYR_509@HH	TYR_509@OH	1	-	2,99	149,83

