Benchmarking Computational Methods and Influence of Guest Conformation on Chirogenesis in Zinc Porphyrin Complexes

Irina Osadchuk, Victor Borovkov, Riina Aav, and Eric Clot

Supporting Information

Contents

Table S1. Electronic energy (a.u.), ZPE correction (a.u.), relative energy (kcal mol^{-1}) and Boltzman distribution (298 K) of the various conformers optimized for the six systems host+guest considered at the BP86/def2-SV(P)//BP86/def2-TZVP and COSMO solvent (chloroform) model.

Host	Guest	conf.	E_{el}	ZPE	ΔE	Boltz. Pop. (%)
Host A	L-Ala-OMe	a	-4363.6638	0.873747	0.00	100
		b	-4362.84559	0.87383	5.36	0
	L-Leu-OMe	a	-4481.52056	0.956945	0.00	72
		b	-4481.51816	0.956866	0.51	28
		c	-4481.50887	0.956767	5.84	0
		d	-4481.5049	0.956619	6.44	0
	S-Leucinol	a	-4368.22467	0.946776	0.00	99
		b	-4368.22738	0.947345	3.06	1
		c	-4368.22205	0.946809	5.48	0
		d	-4368.22089	0.946601	6.24	0
	L-Phe-OMe	a	-4594.57577	0.953991	0.00	81
		b	-4594.57526	0.954369	1.03	12
		c	-4594.56866	0.953376	1.74	3
		d	-4594.56934	0.953567	1.81	3
Host B	L-Phe-OMe	a	-4672.19889	1.007658	0.00	89
		b	-4672.19725	1.008383	1.48	6
		c	-4672.19614	1.008485	2.23	2
		d	-4672.19615	1.008301	2.12	2
		e	-4672.19551	1.00831	2.52	1
		f	-4672.19263	1.008351	4.35	0
		g	-4672.19314	1.008488	4.11	0
		h	-4672.19327	1.00821	3.86	0
Host C	L-Phe-OMe	a	-3675.32607	0.69513	0.00	93
		b	-3675.31984	0.694803	1.77	4
		c	-3675.31884	0.69485	1.80	3

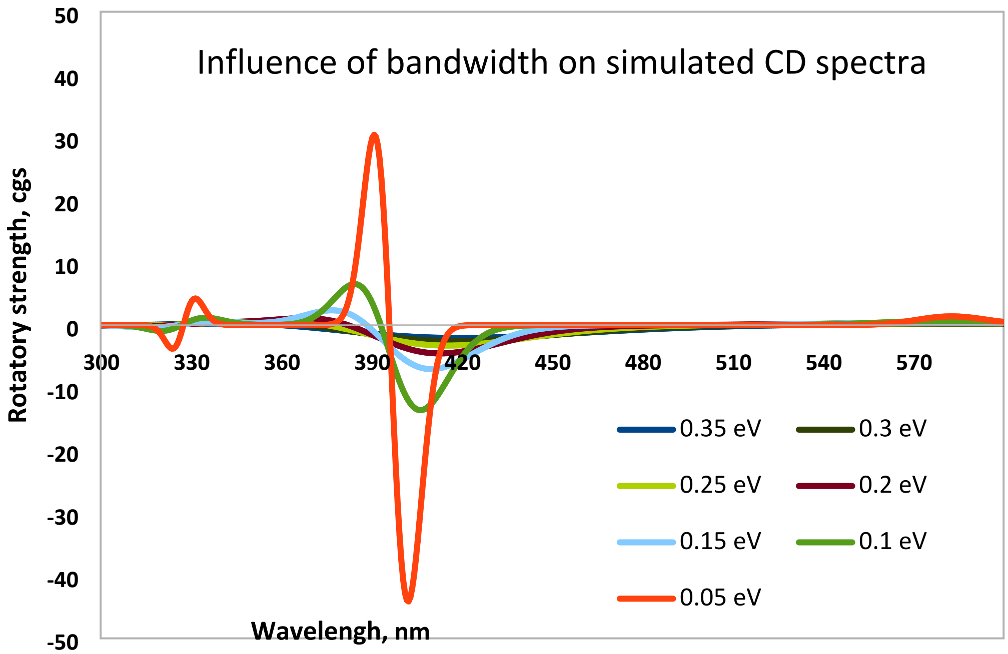
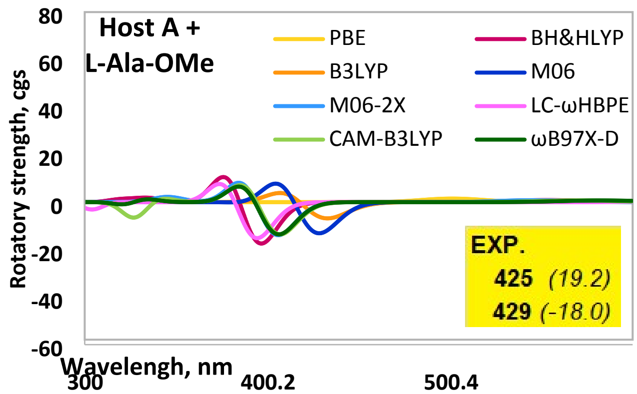
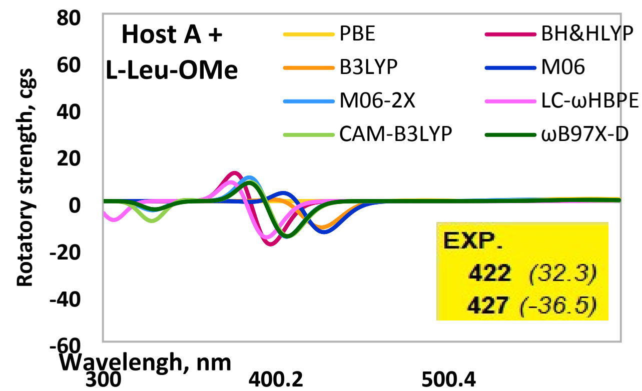


Figure S1. Influence of the bandwidth on simulated CD spectra A/L-Ala-OMe as an illustrative example.

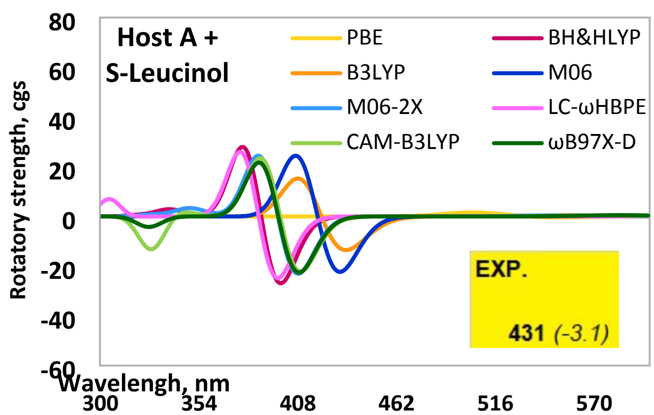
a)

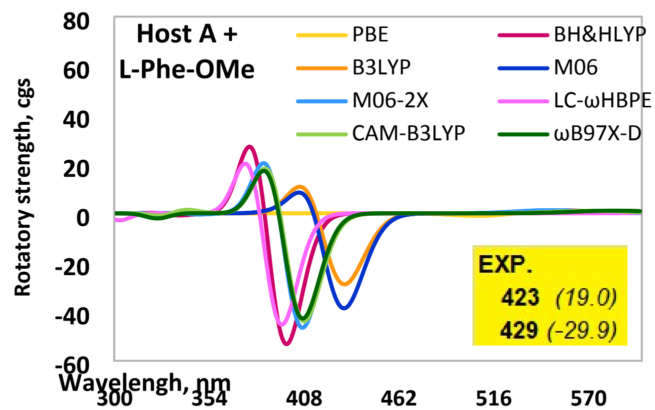
b)





c)



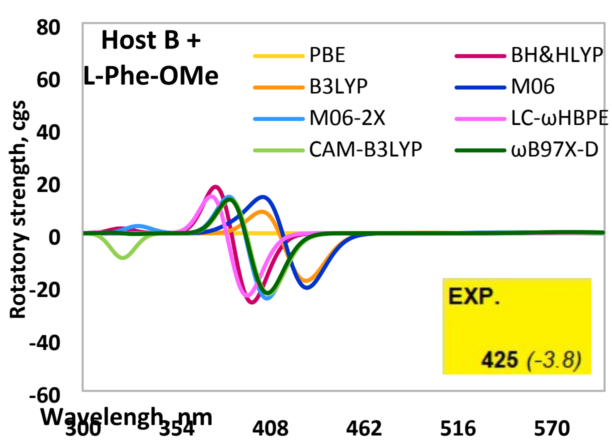


d)

e)

f)

Figure S2. Simulated CD spectra calculated using different functionals, SMD solvent model and cc-pVDZ basis set a) A/L-Ala-OMe, b) A/L-Leu-OME, c) A/S-Leucinol, d) A/L-Phe-OMe e) B/L-Phe-OMe, f) C/L-Phe-OMe



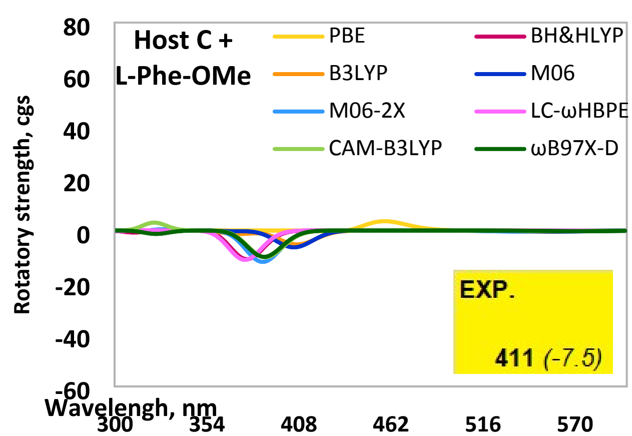


Table S2. Transition energies (nm) , oscillator strengths and rotational strengths (cgs) calculated using different functionals, SMD solvent model and cc-pVDZ basis set

	Host A/L-Ala-OMe					Host A/L-Leu-OMe			
Functional	**Excit. en.**	**osc. str.**	Rv	Rl	**Functional**	**Excit. en.**	**osc. str.**	Rv	Rl
PBE	587	0.00	1	1	**PBE**	587	0.00	1	0
EXP.	585	0.00	0	1	**EXP.**	585	0.00	2	2
425 *(19.2)*	**538**	**0.01**	**-1**	**-2**	**422** *(32.3)*	**546**	**0.00**	**-2**	-2
429 *(-18.0)*	**537**	**0.00**	**1**	**2**	**427** *(-36.5)*	**543**	**0.00**	**3**	4
	505	0.00	1	1		508	0.00	-2	-2
	499	0.00	2	2		500	0.00	2	3
BH&HLYP	553	0.02	1	1	**BH&HLYP**	554	0.02	0	0
	552	0.02	1	1		552	0.02	1	1
	390	**2.04**	**-69**	**-72**		**390**	**1.99**	**-73**	-75
	384	**1.19**	**60**	**62**		**384**	**1.17**	**64**	66
	335	0.00	2	3		337	0.00	0	0
	320	0.00	1	1		321	0.01	0	1
B3LYP	554	0.00	1	1	**B3LYP**	554	0.00	1	1
	553	0.00	0	0		553	0.00	0	0
	429	**0.03**	**-12**	**-12**		**433**	**0.00**	**5**	5
	423	**0.98**	**-4**	**-4**		**426**	**0.61**	**-26**	-27
	416	0.58	-22	-23		418	0.93	-8	-8
	415	0.84	33	35		415	0.81	14	13
CAM-B3LYP	569	0.01	1	1	**CAM-B3LYP**	569	0.01	1	1
	568	0.01	0	1		567	0.01	0	0
	400	**1.89**	**-59**	**-61**		**400**	**1.84**	**-64**	-65
	395	**1.11**	**50**	**52**		**395**	**1.09**	**54**	56
	338	0.00	4	5		340	0.00	2	3
	328	0.00	-10	-12		329	0.01	-12	-13
M06	569	0.01	1	1	**M06**	569	0.01	1	1
	568	0.01	0	0		568	0.00	0	0
	421	**1.69**	**-53**	**-53**		**421**	**1.63**	**-50**	-51
	414	**0.96**	**35**	**35**		**414**	**0.93**	**47**	47
	410	0.02	11	12		414	0.01	-7	-7
	398	0.02	-2	-2		401	0.05	-4	-4
M06-2X	546	0.01	1	1	**M06-2X**	546	0.01	1	1
	544	0.01	0	0		544	0.01	0	0
	398	**1.93**	**-66**	**-66**		**399**	**1.88**	**-72**	-71
	394	**1.13**	**58**	**58**		**394**	**1.11**	**65**	64
	345	0.00	3	3		347	0.00	0	1
	329	0.00	0	0		329	0.00	-5	-3
wB97-XD	583	0.01	1	1	**wB97-XD**	583	0.01	1	1
	581	0.01	0	0		581	0.00	0	0
	399	**1.90**	**-60**	**-61**		**400**	**1.85**	**-65**	-66
	394	**1.11**	**50**	**51**		**394**	**1.09**	**54**	56
	329	0.00	6	7		330	0.00	-4	-2

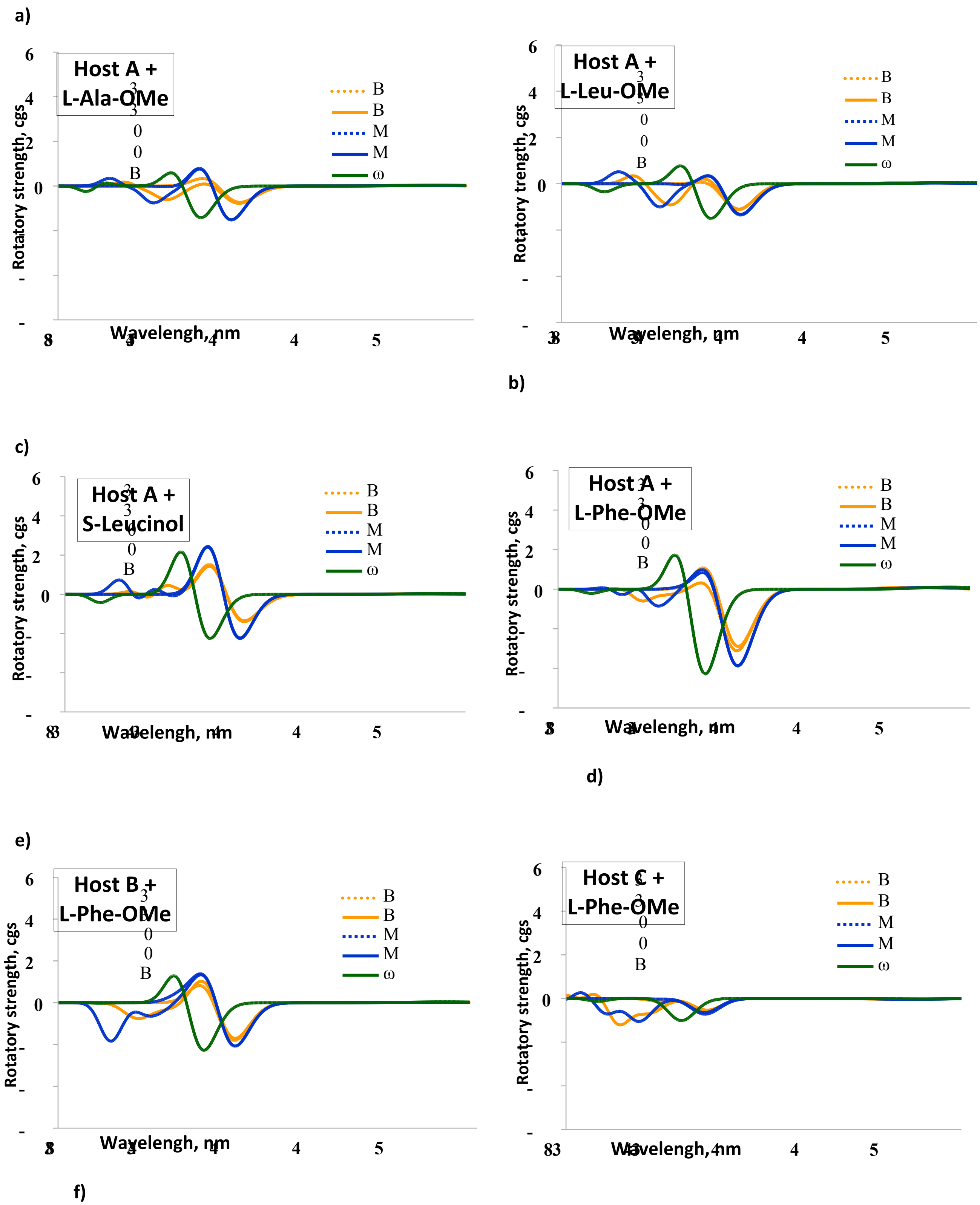
	326	0.01	-5	-5		327	0.01	0	0
LC-wHPBE	643	0.02	1	1	**LC-wHPBE**	643	0.02	1	1
	640	0.01	1	1		640	0.01	1	1
	388	**1.99**	**-65**	**-66**		**388**	**1.94**	**-64**	-65
	383	**1.18**	**54**	**56**		**383**	**1.16**	**54**	56
	307	0.00	4	4		308	0.00	-1	-1
	305	0.01	-8	-7		306	0.01	-8	-8

	Host A/S-leucinol					Host A/L-Phe-OMe			
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
PBE	589	0.00	0	0	**PBE**	591	0.00	1	1
EXP.	586	0.00	0	0	**EXP.**	587	0.00	1	1
	548	**0.00**	**1**	**1**	**423** *(19.0)*	**541**	**0.00**	**-1**	**-1**
431 *(-3.1)*	**545**	**0.00**	**-2**	**-2**	**429** *(-29.9)*	**540**	**0.01**	**3**	**4**
	509	0.00	2	2		513	0.01	2	2
	501	0.00	2	2		512	0.02	-4	-5
BH&HLYP	554	0.02	1	1	**BH&HLYP**	555	0.02	4	4
	553	0.02	0	0		553	0.02	-2	-2
	391	**2.00**	**-127**	**-131**		**392**	**2.01**	**-207**	**-211**
	385	**1.17**	**127**	**131**		**386**	**1.16**	**170**	**176**
	338	0.00	4	4		335	0.00	-1	-1
	321	0.00	1	2		327	0.00	1	1
B3LYP	555	0.00	0	0	**B3LYP**	556	0.00	2	2
	553	0.00	0	0		554	0.00	0	0
	435	**0.03**	**-14**	**-15**		**432**	**0.30**	**-4**	**-4**
	426	**0.35**	**0**	**1**		**425**	**0.65**	**-70**	**-72**
	420	1.15	-83	-86		421	0.62	-12	-12
	416	0.81	96	101		416	0.47	59	61
CAM-B3LYP	570	0.01	1	1	**CAM-B3LYP**	570	0.01	3	3
	568	0.01	0	0		568	0.01	-1	-1
	401	**1.84**	**-120**	**-125**		**401**	**1.87**	**-187**	**-190**
	395	**1.09**	**120**	**125**		**396**	**1.08**	**151**	**156**
	341	0.00	4	4		338	0.00	3	3
	328	0.02	-18	-16		329	0.00	-2	-2
M06	569	0.01	1	1	**M06**	570	0.01	3	3
	568	0.00	0	0		569	0.00	-1	-1
	422	**1.56**	**-108**	**-109**		**424**	**1.55**	**-142**	**-143**
	416	**0.52**	**13**	**13**		**417**	**0.90**	**121**	**122**
	414	0.50	98	100		411	0.10	-27	-27
	403	0.03	-3	-3		399	0.03	4	4
M06-2X	547	0.01	1	1	**M06-2X**	548	0.01	4	4
	545	0.01	0	0		545	0.01	-1	-1
	399	**1.88**	**-131**	**-130**		**400**	**1.90**	**-207**	**-203**
	394	**1.11**	**131**	**131**		**395**	**1.10**	**170**	**169**

	349	0.00	5	4		346	0.00	-1	-1
	329	0.00	1	1		336	0.00	0	1
wB97-XD	584	0.01	1	1	**wB97-XD**	584	0.01	3	3
	582	0.00	0	0		582	0.00	0	0
	400	**1.85**	**-122**	**-126**		**400**	**1.88**	**-187**	**-191**
	395	**1.09**	**119**	**123**		**396**	**1.09**	**152**	**156**
	330	0.01	4	3		329	0.00	2	4
	328	0.03	-9	-10		326	0.00	-4	-4
LC-wHPBE	645	0.01	1	1	**LC-wHPBE**	644	0.02	3	3
	642	0.01	0	0		640	0.01	-1	-1
	389	**1.95**	**-133**	**-137**		**389**	**1.96**	**-197**	**-200**
	384	**1.16**	**132**	**137**		**384**	**1.16**	**163**	**168**
	309	0.01	-10	-10		305	0.00	6	6
	307	0.01	17	18		304	0.00	-9	-7

	Host B/L-Phe-OMe					**Host C/L-Phe-OMe**			
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
PBE	588	0.00	0	0	**PBE**	578	0.00	0	0
EXP.	583	0.00	1	0	**EXP.**	577	0.00	0	0
	524	**0.00**	**0**	**0**		**498**	**0.00**	**-2**	**-2**
425 *(-3.8)*	**515**	**0.01**	**-1**	**-1**	**411** *(-7.5)*	**497**	**0.00**	**2**	**3**
	510	0.00	1	1		451	0.35	23	24
	506	0.00	1	1		448	0.41	-18	-18
BH&HLYP	551	0.02	2	2	**BH&HLYP**	549	0.04	1	1
	551	0.01	-2	-2		548	0.04	-2	-2
	391	**2.04**	**-95**	**-97**		**380**	**1.24**	**21**	**23**
	384	**1.16**	**82**	**86**		**379**	**1.26**	**-37**	**-38**
	321	0.00	3	3		315	0.01	0	1
	320	0.00	-1	-1		312	0.00	-1	-2
B3LYP	554	0.00	0	0	**B3LYP**	548	0.01	0	0
	551	0.00	0	0		547	0.01	-1	-1
	422	**1.48**	**-71**	**-72**		**411**	**0.91**	**21**	**23**
	417	**0.65**	**46**	**48**		**410**	**0.95**	**-29**	**-30**
	407	0.05	7	7		374	0.00	1	1
	407	0.03	4	5		373	0.00	-3	-3
CAM-B3LYP	567	0.01	1	1	**CAM-B3LYP**	564	0.02	1	1
	566	0.00	-1	-1		562	0.03	-2	-1
	400	**1.89**	**-88**	**-90**		**391**	**1.15**	**19**	**21**
	394	**1.08**	**74**	**77**		**389**	**1.17**	**-34**	**-35**
	326	0.00	4	4		325	0.00	-2	-2
	324	0.01	-16	-16		324	0.00	5	5
M06	570	0.00	1	1	**M06**	562	0.02	1	1
	568	0.00	-1	-1		561	0.02	-2	-2
	424	**1.70**	**-79**	**-80**		**409**	**0.99**	**24**	**26**

	417	**0.92**	**56**	**55**		**408**	**1.03**	**-34**	**-33**
	397	0.02	9	9		363	0.01	-2	-2
	394	0.04	-5	-5		362	0.01	2	1
M06-2X	545	0.01	1	1	**M06-2X**	540	0.03	1	1
	543	0.00	-1	-1		539	0.03	-2	-2
	399	**1.92**	**-99**	**-96**		**389**	**1.18**	**21**	**23**
	393	**1.10**	**83**	**83**		**388**	**1.21**	**-39**	**-38**
	332	0.00	4	3		324	0.01	2	1
	330	0.00	0	0		321	0.00	-1	-1
wB97-XD	581	0.01	1	1	**wB97-XD**	576	0.02	1	1
	579	0.00	0	0		575	0.02	-1	-1
	399	**1.90**	**-88**	**-90**		**390**	**1.16**	**19**	**21**
	393	**1.09**	**74**	**77**		**389**	**1.18**	**-34**	**-35**
	323	0.00	-3	-4		325	0.00	0	0
	322	0.00	3	3		324	0.00	-2	-2
LC-wHPBE	640	0.01	2	2	**LC-wHPBE**	636	0.03	1	**1**
	637	0.01	-1	-1		634	0.03	-2	**-2**
	388	**1.99**	**-91**	**-93**		**379**	**1.23**	**17**	**19**
	382	**1.15**	**77**	**80**		**377**	**1.26**	**-33**	**-34**
	304	0.00	2	2		307	0.00	3	2
	301	0.00	-1	-2		306	0.00	-3	-3



a)
Host A +
L-Ala-OMe
b)
Host A +
L-Leu-OMe
c)
Host A +
S-Leucinol
d)
Host A +
L-Phe-OMe
e)
Host B +
L-Phe-OMe
f)
Host C +
L-Phe-OMe
Rotatory strength, cgs
Wavelengh, nm
B
B
M
M
ω

Figure S3. Simulated CD spectra calculated using 20 and 6 excited states and B3LYP and M06 functionals, SMD solvent model and cc-pVDZ basis set of **a)** Host A/L-Ala-OMe, **b)** Host A/L -Leu-OME, **c)** Host A/S-Leucinol, **d)** Host A/L-Phe-OMe **e)** Host B/L-Phe-OMe, **f)** Host C/L-Phe-OMe

Table S3. Transition energies (nm), oscillator strengths and rotational strengths (cgs) calculated for first 20 excited states using B3LYP and M06 functionals, SMD solvent model and cc-pVDZ basis set

	Host A/L-Ala-OMe					Host A/L-Leu-OMe			
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
B3LYP	554	0.00	1	1		554	0.00	1	1
	553	0.00	0	0		553	0.00	0	0
	429	0.03	-12	-12		433	0.00	5	5
	423	0.98	-5	-5		426	0.61	-26	-27
	416	0.58	-22	-24		418	0.93	-8	-8
	415	0.84	33	35		415	0.81	14	13
	403	0.01	-3	-3		403	0.00	1	1
	395	0.01	-1	-1		397	0.02	2	2
	393	0.00	2	2		393	0.00	0	0
	392	0.01	-1	-1		392	0.01	1	2
	378	0.01	-11	-12		379	0.01	-10	-12
	376	0.04	-12	-13		376	0.05	-14	-15
	374	0.02	5	7		375	0.01	4	6
	373	0.01	9	9		373	0.01	8	8
	371	0.02	7	7		370	0.01	1	2
	368	0.00	0	1		367	0.00	-2	-3
	366	0.06	-2	-4		364	0.06	-2	-4
	363	0.06	-5	-4		364	0.06	-1	1
	360	0.01	-4	-4		360	0.03	-5	-5
	355	0.01	8	8		355	0.01	10	10
M06	569	0.01	1	1		569	0.01	1	1
	568	0.01	0	1		568	0.00	0	0
	421	1.69	-53	-54		421	1.63	-51	-52
	414	0.96	35	35		414	0.93	47	48
	410	0.02	11	12		414	0.01	-7	-7
	398	0.02	-2	-2		401	0.05	-4	-4
	387	0.00	-1	-1		387	0.00	1	1
	377	0.00	-1	-1		378	0.00	0	1
	376	0.00	2	2		375	0.00	1	1
	373	0.00	0	0		374	0.00	1	1
	367	0.03	-23	-24		368	0.03	-22	-23
	366	0.02	-4	-4		366	0.02	-1	-1
	364	0.07	2	4		364	0.06	-5	-2
	362	0.07	19	19		362	0.06	15	16
	355	0.05	-1	-1		354	0.08	-3	-3
	354	0.03	0	-2		353	0.03	3	0
	352	0.06	-15	-13		352	0.04	-6	-2
	350	0.03	11	10		349	0.01	4	4
	345	0.01	-3	-3		346	0.02	-3	-3
	341	0.02	9	8		341	0.03	8	8

	Host A/S-Leucinol					Host A/L-Phe-OMe			
Functional	Excit. en.	osc. str.	Rv	Rl	Functional	Excit. en.	osc. str.	Rv	Rl
B3LYP	555	0.00	0	0	**B3LYP**	556	0.00	2	2
	553	0.00	0	0		554	0.00	0	0
	435	0.03	-14	-15		432	0.30	-4	-5
	426	0.35	0	0		425	0.65	-70	-72
	420	1.15	-84	-87		421	0.62	-13	-13
	416	0.81	97	102		416	0.47	60	61
	403	0.01	-2	-2		411	0.31	-11	-11
	398	0.02	1	1		403	0.05	-4	-4
	394	0.00	2	2		389	0.01	3	3
	391	0.01	-2	-2		384	0.01	0	1
	380	0.03	-16	-17		377	0.02	-18	-19
	377	0.04	19	20		376	0.02	5	4
	375	0.00	6	8		374	0.03	3	5
	374	0.00	1	0		373	0.00	5	6
	370	0.01	2	2		371	0.03	6	6
	365	0.06	-12	-12		368	0.00	-2	-4
	364	0.03	11	11		366	0.05	-1	-1
	364	0.04	-14	-14		364	0.04	0	2
	360	0.01	2	2		361	0.03	-16	-16
	355	0.01	4	5		356	0.01	7	8
M06	569	0.01	1	1		570	0.01	3	3
	568	0.00	0	0		569	0.00	-1	-1
	422	1.56	-108	-109		424	1.55	-142	-143
	416	0.52	13	13		417	0.90	122	123
	414	0.50	98	100		411	0.10	-27	-26
	403	0.03	-2	-3		399	0.03	4	5
	387	0.00	-1	-1		396	0.06	3	4
	376	0.00	2	2		384	0.01	-3	-4
	376	0.00	-1	-1		371	0.00	-1	-1
	375	0.00	0	0		368	0.01	-11	-6
	369	0.07	-29	-30		367	0.02	-14	-19
	367	0.03	28	29		366	0.01	2	3
	365	0.00	0	-1		363	0.08	2	5
	364	0.05	14	15		361	0.08	16	16
	355	0.15	-36	-37		355	0.03	8	8
	353	0.05	17	18		354	0.01	3	1
	350	0.01	0	1		352	0.06	-19	-17
	348	0.01	1	1		350	0.01	7	7
	346	0.01	3	3		346	0.02	-10	-10
	341	0.03	8	8		342	0.02	7	7

	Host B/L-Phe-OMe				Host C/L-Phe-OMe				
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
B3LYP	554	0.00	0	0	**B3LYP**	548	0.01	0	0
	551	0.00	0	0		547	0.01	-1	-1
	422	1.48	-71	-70		411	0.91	21	23
	417	0.65	46	48		410	0.96	-29	-30
	407	0.05	7	7		374	0.00	1	1
	407	0.03	4	5		373	0.00	-3	-3
	404	0.00	2	2		372	0.01	1	1
	401	0.09	14	15		367	0.00	-1	-1
	400	0.08	-7	-9		363	0.06	-7	-7
	399	0.04	-6	-7		362	0.09	-1	-2
	398	0.01	2	2		357	0.01	2	2
	393	0.06	-4	-5		351	0.01	-5	-5
	372	0.04	-14	-15		342	0.41	12	12
	372	0.00	2	2		340	0.36	-26	-26
	370	0.03	14	15		320	0.00	5	6
	367	0.03	-2	-1		317	0.00	-1	-1
	364	0.08	-6	-6		315	0.01	-1	-2
	361	0.04	-4	-3		314	0.00	0	0
	357	0.00	-1	-1		301	0.01	2	2
	351	0.01	-4	-4		298	0.00	0	0
M06	567	0.00	1	0		562	0.02	1	1
	566	0.00	0	0		561	0.02	-2	-2
	422	1.72	-79	-78		409	0.99	23	25
	414	0.92	66	67		408	1.03	-34	-34
	391	0.01	5	5		363	0.01	-2	-2
	388	0.00	1	1		362	0.01	2	1
	384	0.01	0	0		360	0.03	-5	-5
	383	0.01	0	0		358	0.00	1	2
	383	0.01	-4	-5		354	0.14	-10	-10
	380	0.00	-1	-1		353	0.11	-3	-3
	379	0.02	2	2		343	0.01	3	3
	378	0.01	-2	-2		337	0.02	-7	-7
	363	0.00	10	10		333	0.28	10	10
	362	0.05	-32	-32		331	0.24	-15	-14
	360	0.08	12	13		312	0.00	2	3
	356	0.09	5	5		308	0.00	2	2
	353	0.07	1	2		301	0.00	-2	-2
	349	0.04	-6	-6		298	0.00	-1	-1
	342	0.00	1	1		292	0.01	2	2
	338	0.01	-23	-23		286	0.00	1	1

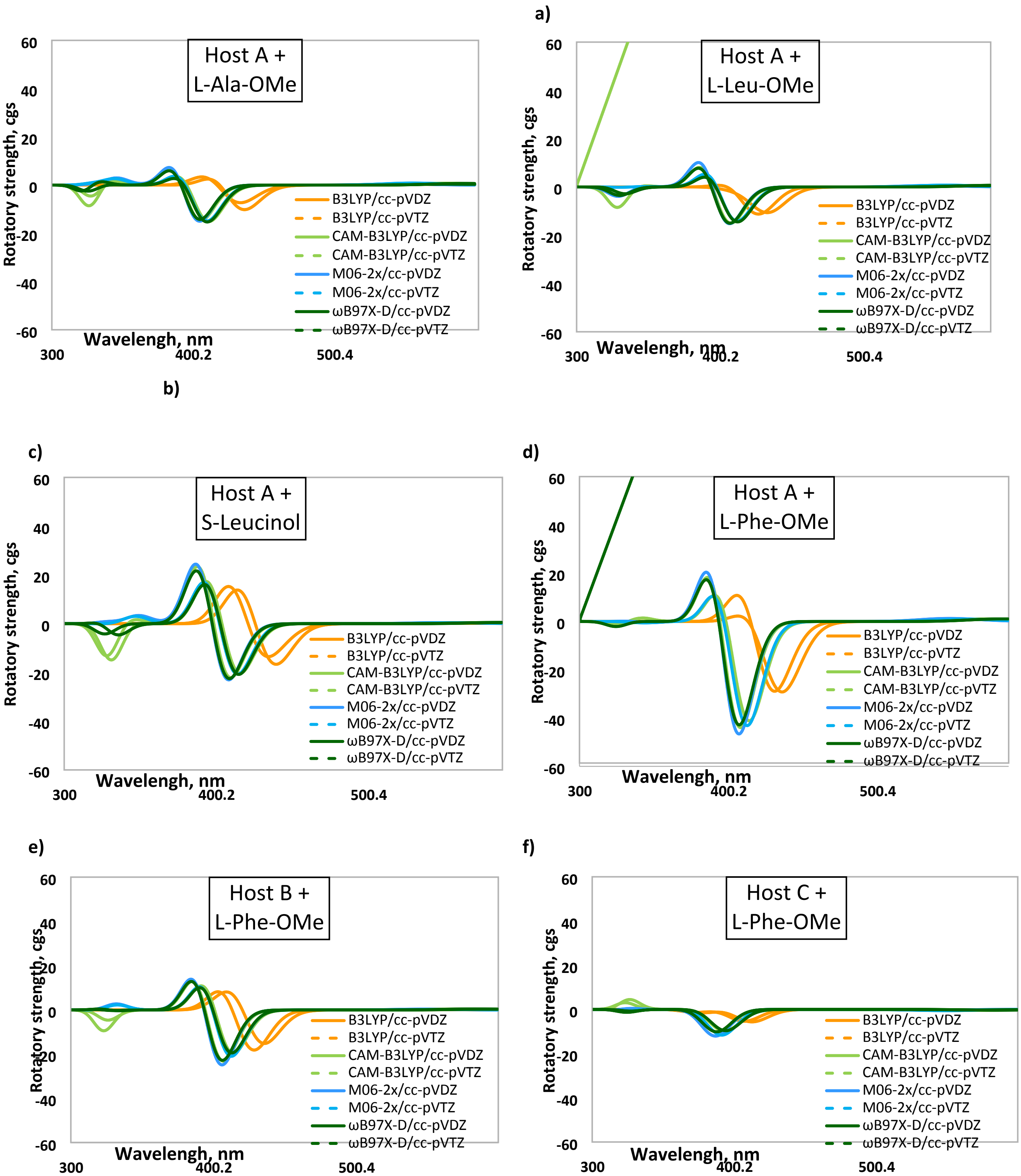


Figure S4. Simulated CD spectra calculated using cc-pVDZ and cc-pVTZ basis sets with B3LYP, CAM-B3LYP, M06-2X and ωB97X-D functionals and SMD solvent model of a) A/L-Ala-OMe, b) A/L-Leu-OME, c) A/S-Leucinol, d) A/L--Phe-OMe e) B/L-Phe-OMe, f) C/L-Phe-OMe

Table S4. Transition energies (nm), oscillator strengths and rotational strengths (cgs) calculated for the various complexes and the various functionals with cc-pVDZ and cc-pVTZ basis sets.

	Host A/L-Ala-OMe					**Host A/L-Leu-OMe**			
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
B3LYP					**B3LYP**				
/cc-pVDZ	554	0.00	1	1	**/cc-pVDZ**	554	0.00	1	1
	553	0.00	0	0		553	0.00	0	1
	429	**0.03**	**-12**	**-12**		**433**	**0.00**	**5**	**5**
	423	**0.98**	**-4**	**-4**		**426**	**0.61**	**-26**	**-22**
	416	0.58	-22	-23		418	0.93	-8	-16
	415	0.84	33	35		415	0.81	14	17
/cc-pVTZ	594	0.01	2	2	**/cc-pVTZ**	562	0.00	1	1
	592	0.01	1	1		560	0.00	0	0
	405	**1.88**	**-66**	**-66**		**431**	0.06	18	**14**
	401	**1.09**	**50**	**50**		**429**	1.08	-61	**-53**
	332	0.00	2	1		423	0.81	68	70
	329	0.00	5	5		420	0.41	-43	-50
CAM-B3LYP					**CAM-B3LYP**				
/cc-pVDZ	569	0.01	1	1	**/cc-pVDZ**	569	0.01	1	1
	568	0.01	0	1		567	0.01	0	0
	400	**1.89**	**-59**	**-61**		**400**	**1.84**	**-64**	**-65**
	395	**1.11**	**50**	**52**		**395**	**1.09**	**54**	**56**
	338	0.00	4	5		340	0.00	2	3
	328	0.00	-10	-12		329	0.01	-12	-13
/cc-pVTZ	580	0.01	1	1	**/cc-pVTZ**	569	0.01	1	1
	578	0.01	1	1		567	0.01	0	0
	406	**1.88**	**-67**	**-68**		**400**	**1.84**	**-64**	**-65**
	402	**1.09**	**52**	**52**		**395**	**1.09**	**54**	**56**
	338	0.00	4	5		340	0.00	2	3
	331	0.00	-11	-11		329	0.01	-12	-13
M06-2X					**M06-2X**				
/cc-pVDZ	546	0.01	1	1	**/cc-pVDZ**	546	0.01	1	1
	544	0.01	0	0		544	0.01	0	0
	398	**1.93**	**-66**	**-66**		**399**	**1.88**	**-72**	**-70**
	394	**1.13**	**58**	**58**		**394**	**1.11**	**65**	**64**
	345	0.00	3	3		347	0.00	0	1
	329	0.00	0	0		329	0.00	-5	-1
/cc-pVTZ	557	0.01	2	2	**/cc-pVTZ**	557	0.01	1	2
	555	0.01	1	1		555	0.01	0	0
	404	**1.92**	**-75**	**-72**		**405**	**1.87**	**-76**	**-72**
	400	**1.11**	**60**	**58**		**401**	**1.09**	**63**	**61**
	344	0.00	2	2		346	0.00	0	0
	330	0.01	0	1		331	0.01	0	-2

wB97-XD					wB97-XD				
/cc-pVDZ	583	0.01	1	1	/cc-pVDZ	583	0.01	1	1
	581	0.01	0	0		581	0.00	0	0
	399	**1.90**	**-60**	**-61**		**400**	**1.85**	**-65**	**-65**
	394	**1.11**	**50**	**51**		**394**	**1.09**	**54**	**56**
	329	0.00	6	7		330	0.00	-4	-1
	326	0.01	-5	-5		327	0.01	0	1
/cc-pVTZ	594	0.01	2	2	/cc-pVTZ	594	0.01	1	1
	592	0.01	1	1		592	0.01	0	0
	405	**1.88**	**-66**	**-66**		**406**	1.83	-67	**-66**
	401	**1.09**	**50**	**50**		**401**	1.07	52	**52**
	332	0.00	2	1		332	0.00	-6	-6
	329	0.00	5	5		330	0.00	2	0

	Host A/S-Leucinol					Host A/L-Phe-OMe			
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
B3LYP					B3LYP				
/cc-pVDZ	555	0.00	0	0	/cc-pVDZ	556	0.00	2	2
	553	0.00	0	0		554	0.00	0	0
	435	**0.03**	**-14**	**-15**		**432**	**0.30**	**-4**	**-4**
	426	**0.35**	**0**	**1**		**425**	**0.65**	**-70**	**-72**
	420	1.15	-83	-86		421	0.62	-12	-12
	416	0.81	96	101		416	0.47	59	61
/cc-pVTZ	563	0.00	0	0	/cc-pVTZ	564	0.00	2	2
	560	0.00	0	0		561	0.00	0	0
	432	**0.31**	**-58**	**-58**		**434**	**0.90**	**-61**	**-61**
	428	**0.89**	**-7**	**-7**		**428**	**0.42**	**-1**	**-1**
	424	0.74	25	25		425	0.70	10	9
	421	0.38	34	34		419	0.22	10	10
CAM-B3LYP					CAM-B3LYP				
/cc-pVDZ	570	0.01	1	1	/cc-pVDZ	570	0.01	3	3
	568	0.01	0	0		568	0.01	-1	-1
	401	**1.84**	**-120**	**-125**		**401**	**1.87**	**-187**	**-190**
	395	**1.09**	**120**	**125**		**396**	**1.08**	**151**	**156**
	341	0.00	4	4		338	0.00	3	3
	328	0.02	-18	-16		329	0.00	-2	-2
/cc-pVTZ	580	0.01	1	1	/cc-pVTZ	581	0.01	3	3
	578	0.01	0	0		579	0.01	-1	-1
	407	**1.83**	**-137**	**-138**		**407**	**1.85**	**-195**	**-195**
	402	**1.07**	**132**	**133**		**403**	**1.06**	**153**	**153**
	340	0.00	4	4		338	0.00	3	3
	331	0.04	-21	-21		331	0.01	-3	-3
M06-2X					M06-2X				

/cc-pVDZ	547	0.01	1	1	/cc-pVDZ	548	0.01	4	4
	545	0.01	0	0		545	0.01	-1	-1
	399	**1.88**	**-131**	**-130**		**400**	**1.90**	**-207**	**-203**
	394	**1.11**	**131**	**131**		**395**	**1.10**	**170**	**169**
	349	0.00	5	4		346	0.00	-1	-1
	329	0.00	1	1		336	0.00	0	1
/cc-pVTZ	558	0.01	1	1	/cc-pVTZ	558	0.01	4	4
	556	0.01	0	0		556	0.01	-2	-2
	405	**1.87**	**-152**	**-147**		**406**	**1.89**	**-216**	**-208**
	401	**1.09**	**146**	**141**		**402**	**1.09**	**171**	**164**
	347	0.00	4	4		345	0.00	-1	-1
	330	0.01	0	1		336	0.00	0	0
wB97-XD					wB97-XD				
/cc-pVDZ	584	0.01	1	1	/cc-pVDZ	584	0.01	3	3
	582	0.00	0	0		582	0.00	0	0
	400	**1.85**	**-122**	**-126**		**400**	**1.88**	**-187**	**-191**
	395	**1.09**	**119**	**123**		**396**	**1.09**	**152**	**156**
	330	0.01	4	3		329	0.00	2	4
	328	0.03	-9	-10		326	0.00	-4	-4
/cc-pVTZ	595	0.01	1	1	/cc-pVTZ	595	0.01	3	3
	593	0.01	0	0		593	0.01	-1	-1
	406	**1.83**	**-139**	**-140**		**407**	**1.85**	**-195**	**-195**
	402	**1.07**	**132**	**132**		**403**	**1.07**	**152**	**152**
	333	0.02	-13	-13		330	0.00	0	0
	330	0.00	8	7		329	0.00	-3	-3

	Host B/L-Phe-OMe				Host C/L-Phe-OMe				
Functional	Excit. en.	osc. str.	Rv	Rl	Functional	Excit. en.	osc. str.	Rv	Rl
B3LYP					B3LYP				
/cc-pVDZ	554	0.00	0	0	/cc-pVDZ	548	0.01	0	0
	551	0.00	0	0		547	0.01	-1	-1
	422	**1.48**	**-71**	**-72**		**411**	**0.91**	**21**	**23**
	417	**0.65**	**46**	**48**		**410**	**0.95**	**-29**	**-30**
	407	0.05	7	7		374	0.00	1	1
	407	0.03	4	5		373	0.00	-3	-3
/cc-pVTZ	561	0.00	0	0	/cc-pVTZ	554	0.01	0	0
	558	0.00	0	0		553	0.01	-1	-1
	428	**1.48**	**-76**	**-77**		**416**	**0.90**	**19**	**20**
	424	**0.70**	**58**	**59**		**415**	**0.95**	**-28**	**-28**
	411	0.05	4	4		380	0.00	4	4
	407	0.00	4	4		379	0.00	-7	-7
CAM-B3LYP					CAM-B3LYP				
/cc-pVDZ	567	0.01	1	1	/cc-pVDZ	564	0.02	1	1
	566	0.00	-1	-1		562	0.03	-2	-1

	400	**1.89**	**-88**	**-90**		**391**	**1.15**	**19**	**21**
	394	**1.08**	**74**	**77**		**389**	**1.17**	**-34**	**-35**
	326	0.00	4	4		325	0.00	-2	-2
	324	0.01	-16	-16		324	0.00	5	5
/cc-pVTZ	578	0.01	2	2	**/cc-pVTZ**	573	0.03	1	1
	576	0.01	-1	-1		572	0.03	-2	-2
	406	**1.87**	**-97**	**-98**		**395**	**1.14**	**21**	**21**
	401	**1.07**	**85**	**85**		**394**	**1.16**	**-36**	**-35**
	328	0.00	2	2		328	0.00	-9	-9
	326	0.01	-8	-8		327	0.01	14	14
M06-2X					**M06-2X**				
/cc-pVDZ	545	0.01	1	1	**/cc-pVDZ**	540	0.03	1	1
	543	0.00	-1	-1		539	0.03	-2	-2
	399	**1.92**	**-99**	**-96**		**389**	**1.18**	**21**	**23**
	393	**1.10**	**83**	**83**		**388**	**1.21**	**-39**	**-38**
	332	0.00	4	3		324	0.01	2	1
	330	0.00	0	0		321	0.00	-1	-1
/cc-pVTZ	556	0.01	2	2	**/cc-pVTZ**	550	0.03	1	1
	554	0.01	-1	-1		550	0.03	-2	-2
	405	**1.91**	**-111**	**-107**		**393**	**1.17**	**25**	**24**
	401	**1.09**	**96**	**93**		**392**	**1.20**	**-43**	**-41**
	332	0.00	3	3		326	0.01	0	0
	330	0.00	0	-1		324	0.00	-1	-1
wB97-XD					**wB97-XD**				
/cc-pVDZ	581	0.01	1	1	**/cc-pVDZ**	576	0.02	1	1
	579	0.00	0	0		575	0.02	-1	-1
	399	**1.90**	**-88**	**-90**		**390**	**1.16**	**19**	**21**
	393	**1.09**	**74**	**77**		**389**	**1.18**	**-34**	**-35**
	323	0.00	-3	-4		325	0.00	0	0
	322	0.00	3	3		324	0.00	-2	-2
/cc-pVTZ	592	0.01	0	0	**/cc-pVTZ**	588	0.02	1	1
	590	0.00	0	0		586	0.02	-1	-1
	405	**1.88**	**2**	**2**		**396**	1.16	20	20
	401	**1.07**	**1**	**1**		**395**	1.18	-35	-34
	327	0.01	0	0		330	0.00	2	1
	325	0.00	0	0		329	0.00	-2	-2

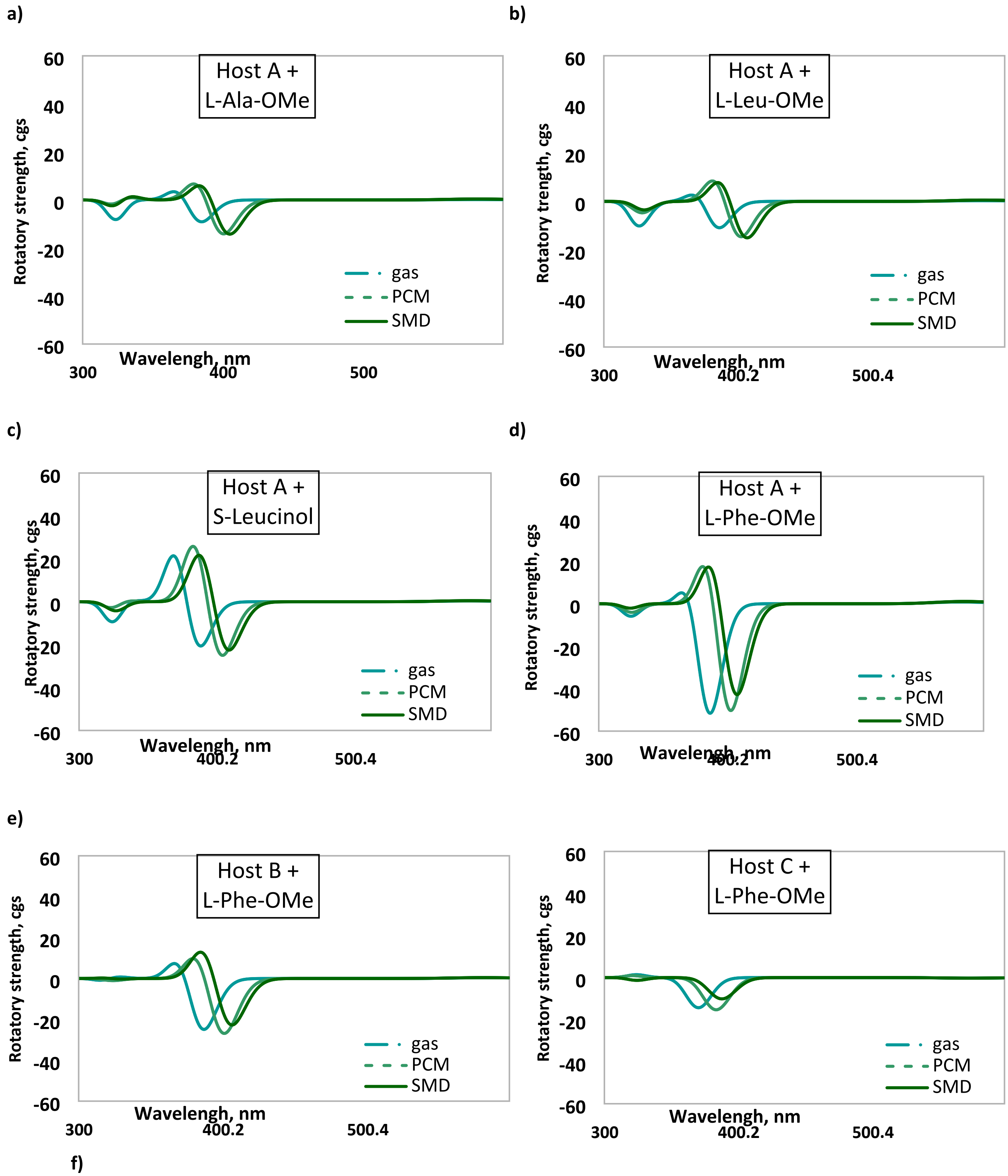


Figure S5. Simulated CD spectra calculated in gas phase and using PCM and SMD solvent models, ωB97X-D functional and cc-pVDZ basis set of a) A/L-Ala-OMe, b) A/L-Leu-OME, c) A/S-Leucinol, d) A/L--Phe-OMe e) B/L-Phe-OMe, f) C/L-Phe-OMe.

Table S5. Transition energies (nm), oscillator strengths and rotational strengths (cgs) calculated in gas phase and using PCM and SMD solvent models, ωB97X-D functional and cc-pVDZ basis set.

Host A/L-Ala-OMe					Host A/L-Leu-OMe				
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
wB97-XD/cc-pVDZ					**wB97-XD/cc-pVDZ**				
gas	581	0.01	1	1	**gas**	582	0.01	0	0
	579	0.01	0	0		579	0.01	0	1
	380	**1.47**	**-34**	**-35**		**381**	**1.41**	**-31**	**-32**
	375	**0.76**	**28**	**29**		**376**	**0.74**	**20**	**21**
	329	0.01	1	3		330	0.01	-2	0
	325	0.02	-13	-13		325	0.01	-11	-12
PCM	582	0.01	1	1	**PCM**	582	0.01	1	1
	580	0.01	0	1		579	0.01	0	0
	395	**1.87**	**-56**	**-58**		**395**	**1.82**	**-56**	**-57**
	389	**1.06**	**47**	**49**		**389**	**1.05**	**47**	**49**
	328	0.00	3	5		329	0.00	-4	-2
	325	0.01	-6	-6		326	0.01	-2	-2
SMD	583	0.01	1	1	**SMD**	583	0.01	1	1
	581	0.01	0	0		581	0.00	0	0
	399	1.90	-60	-61		**400**	**1.85**	**-65**	**-66**
	394	1.11	50	51		**394**	**1.09**	**54**	**56**
	329	0.00	6	7		330	0.00	-4	-2
	326	0.01	-5	-5		327	0.01	0	0

Host A/S-Leucinol					Host A/L-Phe-OMe				
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
wB97-XD/cc-pVDZ					**wB97-XD/cc-pVDZ**				
gas	581	0.00	1	1	**gas**	582	0.00	0	0
	579	0.01	0	0		580	0.01	2	2
	381	**1.43**	**-91**	**-95**		**382**	**1.42**	**-147**	**-149**
	375	**0.75**	**91**	**94**		**378**	**0.74**	**85**	**88**
	332	0.01	4	4		329	0.02	1	3
	325	0.01	-14	-14		325	0.02	-9	-9
PCM	582	0.01	1	1	**PCM**	583	0.01	2	2
	580	0.01	0	0		580	0.01	0	0
	396	**1.82**	**-119**	**-124**		**396**	**1.84**	**-187**	**-190**
	390	**1.05**	**119**	**123**		**391**	**1.04**	**142**	**146**
	329	0.01	5	4		328	0.01	0	2
	326	0.03	-8	-8		325	0.01	-5	-5
SMD	584	0.01	1	1	**SMD**	584	0.01	3	3
	582	0.00	0	0		582	0.00	0	0
	400	**1.85**	**-122**	**-126**		**400**	**1.88**	**-187**	**-191**

395	**1.09**	**119**	**123**		**396**	**1.09**	**152**	**156**
330	0.01	4	3		329	0.00	2	4
328	0.03	-9	-10		326	0.00	-4	-4

	Host B/L-Phe-OMe					**Host C/L-Phe-OMe**			
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
wB97-XD/cc-pVDZ					**wB97-XD/cc-pVDZ**				
gas	580	0.00	1	1	**gas**	576	0.02	0	0
	578	0.00	0	0		574	0.01	-1	-1
	382	**1.47**	**-76**	**-77**		**372**	**0.80**	**20**	**22**
	376	**0.73**	**53**	**55**		**371**	**0.81**	**-41**	**-42**
	322	0.01	8	7		323	0.00	3	2
	320	0.01	-8	-8		322	0.00	-1	-1
PCM	579	0.01	1	1	**PCM**	575	0.02	1	1
	578	0.00	0	0		573	0.02	-1	-1
	395	**1.88**	**-86**	**-87**		**385**	**1.11**	**19**	**21**
	389	**1.04**	**62**	**64**		**384**	**1.13**	**-42**	**-43**
	323	0.00	-2	-3		324	0.00	-2	-2
	321	0.01	1	1		322	0.00	3	3
SMD	581	0.01	1	1	**SMD**	576	0.02	1	1
	579	0.00	0	0		575	0.02	-1	-1
	399	**1.90**	**-88**	**-90**		**390**	**1.16**	**19**	**21**
	393	**1.09**	**74**	**77**		**389**	**1.18**	**-34**	**-35**
	323	0.00	-3	-4		325	0.00	0	0
	322	0.00	3	3		324	0.00	-2	-2

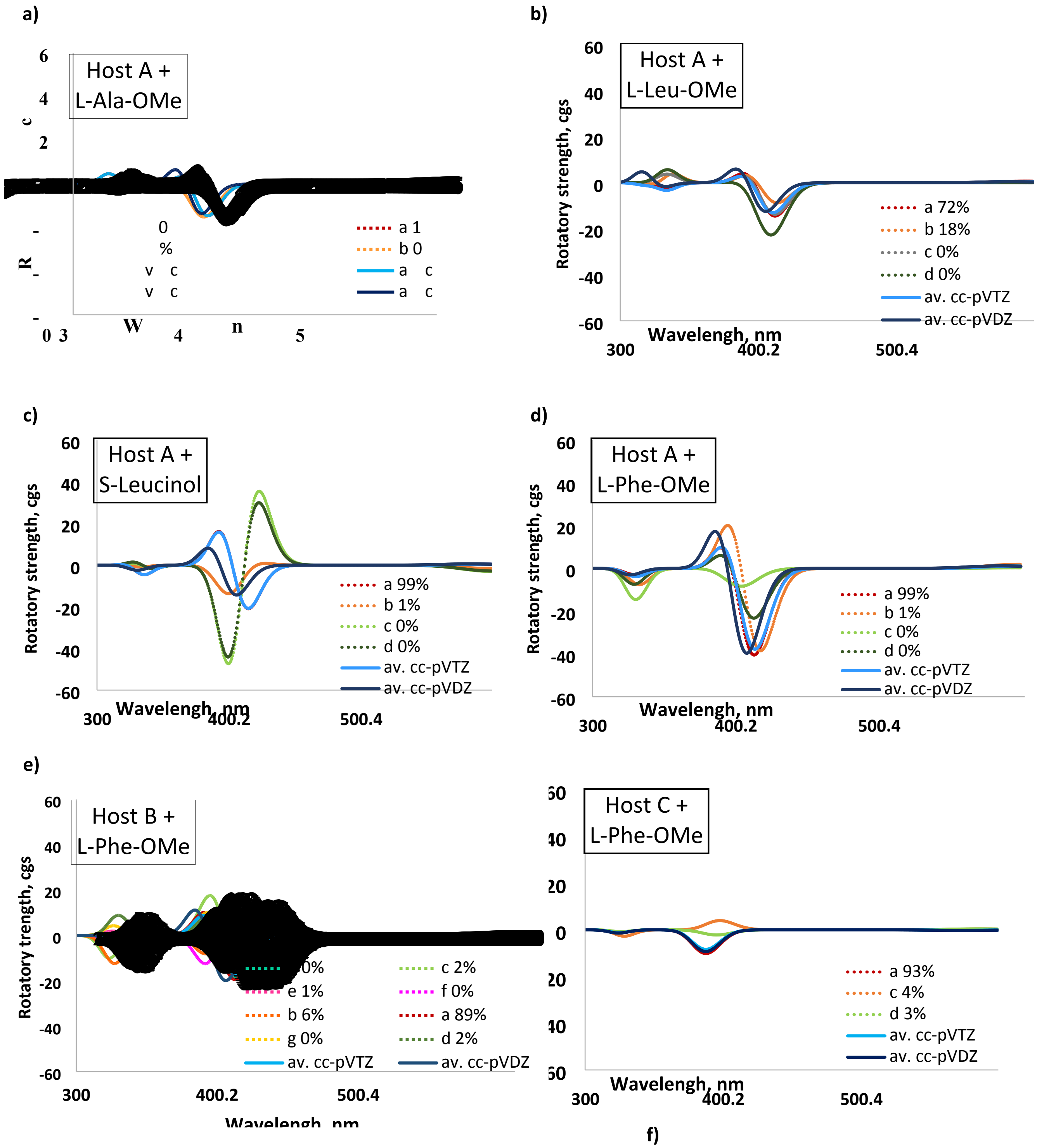


Figure S6. Simulated CD spectra of complexes with varying conformations of guests (**a-g**) and average CD spectra calculated using the cc-pVDZ and cc-pVTZ basis sets, ωB97X-D functional and SMD solvent model of **a)** A/L-Ala-OMe, **b)** A/L-Leu-OME, **c)** A/S-Leucinol, **d)** A/L-Phe-OMe **e)** B/L-Phe-OMe, **f)** C/L-Phe-OMe. Simulated spectra of the lowest-energy conformers (red dots) are not clearly seen because they coincide with the average CD spectra calculated using the cc-pVTZ basis set.

Table S6. Transition energies (nm), oscillator strengths and rotational strengths (cgs) calculated for complexes with varying conformations of guests calculated using the cc-pVDZ and cc-pVTZ basis sets, ωB97X-D functional and SMD solvent model

Host A/L-Ala-OMe

	Excit. en.	osc. str.	Rv	Rl
conf. a				
/cc-pVTZ	593	0.01	1	1
	591	0.01	0	0
	404	**1.91**	**-65**	**-65**
	400	**1.10**	**47**	**47**
	331	0.00	3	3
	328	0.01	-6	-6
/cc-pVDZ	581	0.01	1	1
	579	0.00	0	0
	398	**1.93**	**-58**	**-60**
	393	**1.12**	**47**	**49**
	329	0.01	8	9
	325	0.01	-9	-9
conf. b				
/cc-pVTZ	594	0.01	-1	-1
	592	0.01	0	0
	404	**1.88**	**-37**	**-37**
	401	**1.11**	**13**	**14**
	333	0.00	8	8
	330	0.00	-5	-5
/cc-pVDZ	582	0.01	0	0
	580	0.01	0	0
	398	**1.90**	**-41**	**-43**
	394	**1.13**	**14**	**15**
	332	0.00	5	5
	327	0.00	-6	-6

Host A/L-Leu-OMe

Functional	Excit. en.	osc. str.	Rv	Rl
conf. a				
/cc-pVTZ	594	0.01	1	1
	592	0.01	0	0
	406	**1.83**	**-67**	**-67**
	401	**1.07**	**52**	**52**
	332	0.00	-6	-6
	330	0.00	2	2
/cc-pVDZ	583	0.01	1	1
	581	0.00	0	0
	400	**1.85**	**-65**	**-66**
	394	**1.09**	**54**	**56**
	330	0.00	-4	-2
	327	0.01	0	0
conf. b				
/cc-pVTZ	595	0.01	2	2
	594	0.01	0	0
	407	**1.82**	**-35**	**-35**
	402	**1.06**	**27**	**28**
	334	0.01	17	16
	332	0.03	-13	-13
/cc-pVDZ	584	0.01	1	1
	582	0.01	0	0
	401	**1.84**	**-32**	**-32**
	395	**1.08**	**22**	**24**
	332	0.03	29	28
	328	0.03	-9	-9
conf. c				
/cc-pVTZ	595	0.01	0	0
	593	0.01	0	1
	406	**1.80**	**-65**	**-65**
	402	**1.08**	**49**	**50**
	334	0.00	4	3
	332	0.00	1	1
/cc-pVDZ	584	0.01	0	0
	582	0.01	0	0
	400	**1.82**	**-67**	**-70**
	395	**1.10**	**50**	**52**
	334	0.00	3	3
	329	0.00	-6	-6
conf. d				
/cc-pVTZ	596	0.01	-1	-1

	595	0.01	1	1
	406	**1.80**	**-65**	**-65**
	403	**1.08**	**31**	**31**
	335	0.00	6	5
	332	0.00	2	2
/cc-pVDZ	585	0.01	-1	-1
	583	0.01	1	1
	400	**1.82**	**-65**	**-67**
	396	**1.10**	**28**	**30**
	333	0.00	7	7
	329	0.00	-6	-7

Host A/S-Leucinol					Host A/L-Phe-OMe				
Functional	**Excit. en.**	**osc. str.**	**Rv**	**Rl**	**Functional**	**Excit. en.**	**osc. str.**	**Rv**	**Rl**
conf. a					**conf. a**				
/cc-pVTZ	595	0.01	1	1	**/cc-pVTZ**	584	0.01	3	3
	593	0.01	0	0		582	0.00	0	0
	406	**1.83**	**-139**	**-140**		**400**	**1.88**	**-187**	**-191**
	402	**1.07**	**132**	**132**		**396**	**1.09**	**152**	**156**
	333	0.02	-13	-13		329	0.00	2	4
	330	0.00	8	7		326	0.00	-4	-4
/cc-pVDZ	584	0.01	1	1	**/cc-pVDZ**	584	0.01	3	3
	582	0.00	0	0		582	0.00	0	0
	400	**1.85**	**-122**	**-126**		**400**	**1.88**	**-187**	**-191**
	395	**1.09**	**119**	**123**		**396**	**1.09**	**152**	**156**
	330	0.01	4	3		329	0.00	2	4
	328	0.03	-9	-10		326	0.00	-4	-4
conf. b					**conf. b**				
/cc-pVTZ	585	0.01	-4	-4	**/cc-pVTZ**	600	0.01	5	5
	584	0.01	0	0		595	0.00	0	0
	403	**1.86**	**27**	**27**		**410**	**1.82**	**-202**	**-202**
	396	**1.07**	**-51**	**-52**		**405**	**1.03**	**175**	**176**
	329	0.02	-12	-10		333	0.03	-9	-9
	327	0.01	-10	-10		331	0.00	-1	-1
/cc-pVDZ	585	0.01	-4	-4	**/cc-pVDZ**	588	0.01	5	5
	584	0.01	0	0		584	0.00	1	1
	403	**1.86**	**27**	**27**		**404**	**1.85**	**-186**	**-189**
	396	**1.07**	**-51**	**-52**		**398**	**1.04**	**169**	**175**
	329	0.02	-12	-10		**331**	0.02	-13	-11
	327	0.01	-10	-10		328	0.01	-2	-2
conf. c									
/cc-pVTZ	602	0.01	-5	-4		595	0.01	1	1
	599	0.00	-3	-3		592	0.01	0	0
	413	**1.81**	**232**	**232**		**406**	**1.82**	**-7**	**-7**
	407	**1.02**	**-245**	**-245**		**402**	**1.05**	**-7**	**-6**

	336	0.00	-8	-8		333	0.01	-4	-5
	334	0.04	7	7		329	0.03	-15	-15
/cc-pVDZ	591	0.01	-5	-5		583	0.01	0	0
	589	0.00	-3	-3		581	0.01	-1	-1
	407	**1.83**	**223**	**226**		**400**	**1.84**	**-1**	**-2**
	401	**1.03**	**-247**	**-253**		**395**	**1.07**	**-10**	**-9**
	333	0.00	-13	-13		330	0.01	0	1
	331	0.04	6	4		327	0.02	-6	-6
conf. d									
/cc-pVTZ	602	0.01	-4	-4		594	0.01	3	3
	598	0.00	-2	-2		593	0.01	0	0
	412	**1.83**	**215**	**216**		**407**	**1.82**	**-94**	**-93**
	407	**1.04**	**-232**	**-232**		**402**	**1.10**	**69**	**69**
	336	0.00	-9	-9		332	0.00	3	3
	333	0.04	9	9		330	0.02	-13	-12
/cc-pVDZ	591	0.01	-5	-5		583	0.01	3	3
	588	0.00	-2	-3		582	0.00	0	0
	406	**1.86**	**209**	**212**		**401**	**1.84**	**-91**	**-93**
	400	**1.04**	**-235**	**-241**		**395**	**1.11**	**76**	**78**
	333	0.00	-15	-15		330	0.01	11	12
	331	0.04	8	7		327	0.02	-15	-15

Host B/L-Phe-OMe					Host C/L-Phe-OMe				
Functional	Excit. en.	osc. str.	Rv	Rl	Functional	Excit. en.	osc. str.	Rv	Rl
conf. a					conf. a				
/cc-pVTZ	592	0.01	2	2	/cc-pVTZ	576	0	1	1
	590	0.00	-1	-1		575	0	-1	-1
	405	**1.88**	**-95**	**-96**		**390**	**1**	**19**	**21**
	401	**1.07**	**82**	**82**		**389**	**1**	**-34**	**-35**
	327	0.01	-4	-4		325	0	0	0
	325	0.00	4	3		324	0	-2	-2
/cc-pVDZ	**581**	0.01	1	1	/cc-pVDZ	576	**0**	1	1
	579	0.00	0	0		575	0	-1	-1
	399	**1.90**	**-88**	**-90**		**390**	**1**	**19**	**21**
	393	**1.09**	**74**	**77**		**389**	**1**	**-34**	**-35**
	323	0.00	-3	-4		325	0	0	0
	322	0.00	3	3		324	0	-2	-2
conf. b					conf. b				
	594	0.01	-1	-1	/cc-pVTZ	587	0.02	1	1
	592	0.00	1	1		586	0.02	-1	-1
	406	**1.92**	**84**	**84**		**395**	**1.22**	**62**	**62**
	402	**1.09**	**-75**	**-75**		**395**	**1.21**	**-56**	**-56**
	329	0.01	-6	-6		329	0.00	5	5
	326	0.00	-10	-10		329	0.00	-9	-9
	582	0.01	-1	-1	/cc-pVDZ	575	0.02	1	1

	581	0.00	0	0	574	0.02	-1	-1
	400	**1.94**	**70**	**73**	**389**	**1.22**	**59**	**61**
	395	**1.11**	**-67**	**-70**	**388**	**1.21**	**-52**	**-53**
	325	0.01	-13	-15	325	**0.00**	4	4
	323	0.00	-5	-5	324	0.00	-8	-8
conf. c								
/cc-pVTZ	596	0.01	2	2	587	0.02	0	0
	593	0.00	0	0	586	0.02	1	1
	408	**1.94**	**-128**	**-128**	**395**	**1.19**	**-5**	**-5**
	404	**1.04**	**127**	**127**	**394**	**1.18**	**2**	**2**
	329	0.02	8	9	329	0.00	4	4
	325	0.00	-19	-19	328	0.00	-5	-5
/cc-pVDZ	583	0.01	3	3	575	0.02	0	0
	582	0.00	0	0	574	0.02	1	1
	401	**1.84**	**-93**	**-91**	**389**	**1.19**	**-7**	**-5**
	395	**1.11**	**78**	**76**	**388**	**1.18**	**4**	**4**
	330	0.01	12	11	325	0.00	4	4
	327	0.02	-15	-15	324	0.00	-5	-5
conf. d								
/cc-pVTZ	594	0.01	0	0				
	591	0.00	0	0				
	406	**1.88**	**-44**	**-44**				
	402	**1.04**	**49**	**49**				
	329	0.01	13	14				
	327	0.01	-2	-2				
/cc-pVDZ	582	0.01	0	0				
	580	0.00	0	-1				
	400	**1.90**	**-48**	**-49**				
	395	**1.06**	**52**	**54**				
	326	0.01	15	17				
	324	0.00	-3	-4				
conf. e								
/cc-pVTZ	592	0.01	1	1				
	590	0.01	0	0				
	404	**1.92**	**-47**	**-47**				
	400	**1.12**	**41**	**40**				
	327	0.00	1	1				
	326	0.00	2	1				
/cc-pVDZ	581	0.01	0	0				
	579	0.00	0	0				
	398	**1.95**	**-50**	**-51**				
	393	**1.14**	**48**	**48**				
	324	0.00	2	1				
	322	0.00	1	1				
conf. f								
/cc-pVTZ	592	0.01	-1	-1				

	590	0.01	1	1
	404	**1.91**	**94**	**94**
	400	**1.07**	**-94**	**-94**
	328	0.00	-8	-8
	325	0.00	1	1
/cc-pVDZ	581	0.01	-1	-1
	579	0.00	0	0
	398	**1.94**	**92**	**93**
	393	**1.09**	**-94**	**-96**
	324	0.00	-11	-10
	322	0.00	3	3
conf. g				
/cc-pVTZ	596	0.01	1	1
	593	0.01	0	0
	407	**1.79**	**-103**	**-103**
	403	**1.08**	**96**	**96**
	332	0.01	-5	-5
	329	0.01	10	10
/cc-pVDZ	585	0.01	1	1
	582	0.00	0	0
	401	**1.83**	**-110**	**-110**
	396	**1.09**	**109**	**110**
	328	0.02	-7	-7
	326	0.01	5	6
conf. h				
/cc-pVTZ	595	0.01	1	1
	592	0.01	-1	-1
	406	**1.93**	**-97**	**-97**
	403	**1.07**	**77**	**77**
	327	0.00	1	1
	326	0.00	-6	-7
/cc-pVDZ	588	0.01	5	5
	584	0.00	1	1
	404	**1.85**	**-186**	**-189**
	398	**1.04**	**169**	**175**
	331	0.02	-13	-11
	328	0.01	-2	-2

Table S7. Orbitals participation in transitions calculated using the cc-pVDZ and cc-pVTZ basis sets, ωB97X-D functional and SMD solvent model

Host A/L-Ala-OMe

Conformer a
(ωB97-XD/cc-pVTZ)
Excited State 1:
228 -> 230 -0.24926
228 -> 231 0.40608
229 -> 230 0.44807
229 -> 231 0.27171
Excited State 2:
228 -> 230 -0.40780
228 -> 231 -0.24589
229 -> 230 -0.27441
229 -> 231 0.44629
Excited State 3:
228 -> 230 0.29245
228 -> 231 0.41684
229 -> 230 -0.38388
229 -> 231 0.27113
Excited State 4:
228 -> 230 0.41660
228 -> 231 -0.29442
229 -> 230 0.27264
229 -> 231 0.38996
Excited State 5:
220 -> 230 0.36386
223 -> 230 -0.31776
224 -> 230 0.33334
224 -> 231 0.13877
225 -> 231 0.12040
225 -> 234 -0.11020
227 -> 230 0.16787
227 -> 231 0.17306
Excited State 6:
220 -> 230 -0.27615
221 -> 231 -0.12645
222 -> 234 -0.11720
223 -> 231 0.34615
224 -> 230 -0.17331
224 -> 231 0.28809
225 -> 231 0.25960
225 -> 234 -0.10245
227 -> 231 0.19627

Conformer a
(ωB97-XD/cc-pVDZ)
Excited State 1:
228 -> 230 0.12335
228 -> 231 -0.46168
229 -> 230 0.50523
229 -> 231 0.13111
Excited State 2:
228 -> 230 0.46747
228 -> 231 0.12183
229 -> 230 -0.13268
229 -> 231 0.49946
Excited State 3:
222 -> 230 0.10403
228 -> 230 0.48928
228 -> 231 -0.10347
229 -> 231 -0.46869
Excited State 4:
222 -> 231 0.11775
228 -> 230 0.10333
228 -> 231 0.49788
229 -> 230 0.46564
Excited State 5:
220 -> 230 0.18504
221 -> 230 -0.10820
223 -> 230 -0.11755
223 -> 231 -0.29009
224 -> 230 -0.31281
225 -> 230 0.11246
225 -> 234 -0.11817
227 -> 230 0.41312
227 -> 234 -0.12990
Excited State 6:
220 -> 230 -0.22001
220 -> 231 -0.18304
221 -> 231 0.10845
222 -> 234 -0.14194
223 -> 230 0.34880
223 -> 231 -0.13270
224 -> 231 0.34617
225 -> 230 0.19342
225 -> 231 -0.14853
227 -> 230 0.12113

Conformer b
(ωB97-XD/cc-pVTZ)
Excited State 1:
228 -> 230 -0.44379
228 -> 231 -0.18650
229 -> 230 -0.20929
229 -> 231 0.47549
Excited State 2:
228 -> 230 -0.19069
228 -> 231 0.43106
229 -> 230 0.48676
229 -> 231 0.20553
Excited State 3:
228 -> 231 0.51027
229 -> 230 -0.46167
Excited State 4:
221 -> 230 0.10327
228 -> 230 0.50271
229 -> 231 0.47811
Excited State 5:
220 -> 230 -0.21546
220 -> 231 0.17893
222 -> 231 -0.10776
223 -> 230 -0.24764
224 -> 230 0.15775
224 -> 231 -0.23277
225 -> 231 0.12463
227 -> 231 0.43703
227 -> 234 -0.13706
Excited State 6:
220 -> 230 0.50404
224 -> 230 -0.23396
227 -> 231 0.35465
227 -> 234 -0.11126

Conformer b
(ωB97-XD/cc-pVDZ)
Excited State 1:
228 -> 230 -0.47175
228 -> 231 -0.10707
229 -> 230 -0.11731
229 -> 231 0.50303
Excited State 2:
228 -> 230 -0.10841
228 -> 231 0.46447
229 -> 230 0.50947
229 -> 231 0.11619
Excited State 3:
221 -> 231 0.10243
228 -> 230 0.16026
228 -> 231 0.47923
229 -> 230 -0.44757
229 -> 231 0.15204
Excited State 4:
221 -> 230 0.11040
228 -> 230 0.47676
228 -> 231 -0.16511
229 -> 230 0.15090
229 -> 231 0.45754
Excited State 5:
220 -> 231 0.12610
223 -> 230 0.14590
224 -> 231 -0.14379
227 -> 230 0.10929
227 -> 231 0.58995
227 -> 234 -0.19079
Excited State 6:
220 -> 230 0.39012
220 -> 231 -0.11305
222 -> 231 0.12394
223 -> 230 -0.26245
224 -> 230 -0.20088
224 -> 231 0.30119
225 -> 230 -0.11281
227 -> 231 0.21054

Host A/L-Leu-OMe

Conformer a
(ωB97-XD/cc-pVTZ)
Excited State 1:
240 -> 242 -0.36851
240 -> 243 0.30437
241 -> 242 0.33882
241 -> 243 0.39797
Excited State 2:
240 -> 242 0.31011
240 -> 243 0.36071
241 -> 242 0.40466
241 -> 243 -0.33344
Excited State 3:
234 -> 243 0.10161
240 -> 242 0.21422
240 -> 243 0.46310
241 -> 242 -0.42366
241 -> 243 0.19976
Excited State 4:
234 -> 242 0.11271
240 -> 242 0.45845
240 -> 243 -0.21802
241 -> 242 0.19726
241 -> 243 0.43521
Excited State 5:
232 -> 242 0.42416
235 -> 242 0.24347
236 -> 242 0.34415
236 -> 243 0.18386
237 -> 242 -0.14205
239 -> 243 0.16176
Excited State 6:
232 -> 242 0.29390
232 -> 243 -0.27932
233 -> 243 0.10203
235 -> 242 -0.17085
235 -> 243 0.18953
236 -> 242 0.13880
236 -> 243 -0.28809
239 -> 243 -0.29295

Conformer a
(ωB97-XD/cc-pVDZ) 4
Excited State 1:

240 -> 242 -0.10435
240 -> 243 0.46721
241 -> 242 0.50910
241 -> 243 0.11163
Excited State 2:
240 -> 242 -0.47230
240 -> 243 -0.10180
241 -> 242 -0.11370
241 -> 243 0.50406
Excited State 3:
240 -> 242 0.43471
240 -> 243 0.24965
241 -> 242 -0.23600
241 -> 243 0.41448
Excited State 4:
234 -> 243 0.10302
240 -> 242 -0.24831
240 -> 243 0.44094
241 -> 242 -0.41271
241 -> 243 -0.24133
Excited State 5:
232 -> 242 0.23434
233 -> 242 -0.10236
235 -> 242 0.20534
235 -> 243 -0.19297
236 -> 242 0.33207
237 -> 243 0.11432
237 -> 246 -0.10991
239 -> 242 0.35582
239 -> 243 0.21438
239 -> 246 -0.13188
Excited State 6:
232 -> 242 0.29543
232 -> 243 -0.27821
235 -> 242 0.15680
235 -> 243 0.16465
236 -> 242 0.24484
236 -> 243 -0.25871
237 -> 242 -0.17580
239 -> 242 -0.19612
239 -> 243 -0.18475

Conformer b
(ωB97-XD/cc-pVTZ)
Excited State 1:
233 -> 235 -0.10978
233 -> 236 0.45856
234 -> 235 0.51465
234 -> 236 0.11965
Excited State 2:
233 -> 235 -0.46384
233 -> 236 -0.10534
234 -> 235 -0.12328
234 -> 236 0.50965
Excited State 3:
233 -> 235 0.40840
233 -> 236 0.30490
234 -> 235 -0.27834
234 -> 236 0.37585
Excited State 4:
233 -> 235 -0.30315
233 -> 236 0.41270
234 -> 235 -0.37440
234 -> 236 -0.28648
Excited State 5:
225 -> 236 0.29326
228 -> 236 0.25799
229 -> 236 0.42597
230 -> 236 0.28435
230 -> 239 -0.13268
232 -> 236 0.13006
Excited State 6:
225 -> 235 0.46641
225 -> 236 -0.22013
226 -> 235 0.10974
226 -> 236 -0.10157
229 -> 235 0.23427
230 -> 235 -0.12659
230 -> 236 0.30160

Conformer b
(ωB97-XD/cc-pVDZ)
Excited State 1:
233 -> 235 0.12884
233 -> 236 0.45490
234 -> 235 0.50808
234 -> 236 -0.13780
Excited State 2:
233 -> 235 -0.46487
233 -> 236 0.12814
234 -> 235 0.13878
234 -> 236 0.49860
Excited State 3:
227 -> 235 0.10900
233 -> 235 0.49135
234 -> 236 0.46815
Excited State 4:
227 -> 236 0.11642
233 -> 236 0.50262
234 -> 235 -0.46122
Excited State 5:
225 -> 236 0.13535
228 -> 236 0.26303
229 -> 235 0.22345
229 -> 236 0.30941
230 -> 235 0.22412
230 -> 236 0.34099
230 -> 239 -0.15815
232 -> 235 0.14274
232 -> 236 0.10647
Excited State 6:
225 -> 235 0.30685
225 -> 236 -0.44970
227 -> 235 -0.10099
229 -> 235 0.18335
229 -> 236 -0.22756
230 -> 236 0.22910

Conformer c
(ωB97-XD/cc-pVTZ)
Excited State 1:
240 -> 242 -0.43232
240 -> 243 0.21438
241 -> 242 0.24275
241 -> 243 0.45805
Excited State 2:
240 -> 242 0.22243
240 -> 243 0.41602
241 -> 242 0.47262
241 -> 243 -0.23541
Excited State 3:
240 -> 243 0.51502
241 -> 242 -0.46276
Excited State 4:
233 -> 242 0.10086
240 -> 242 0.50251
241 -> 243 0.48407
Excited State 5:
232 -> 242 0.32988
232 -> 243 0.16801
235 -> 242 -0.18209
236 -> 242 0.24574
236 -> 243 0.22401
237 -> 242 -0.10300
239 -> 243 0.37147
239 -> 247 -0.11053
Excited State 6:
232 -> 242 0.44941
232 -> 243 -0.12571
235 -> 242 0.11112
235 -> 243 -0.10919
236 -> 242 0.23729
239 -> 243 -0.37477
239 -> 247 0.11076

Conformer c
(ωB97-XD/cc-pVDZ)
Excited State 1:
240 -> 242 0.44641
240 -> 243 0.18963
241 -> 242 -0.20905
241 -> 243 0.47102
Excited State 2:
240 -> 242 0.19433
240 -> 243 -0.43563
241 -> 242 0.48074
241 -> 243 0.20473
Excited State 3:
233 -> 243 0.10342
240 -> 243 0.50708
241 -> 242 0.47003
Excited State 4:
233 -> 242 0.11382
240 -> 242 0.50015
241 -> 243 -0.48488
Excited State 5:
232 -> 243 0.12184
235 -> 242 0.14135
236 -> 243 -0.13489
239 -> 243 0.60158
239 -> 246 -0.19331
Excited State 6:
232 -> 242 0.48637
235 -> 243 0.11996
236 -> 242 -0.35400
236 -> 243 0.19774
239 -> 243 0.15142

Conformer d
(ωB97-XD/cc-pVTZ)
Excited State 1:
240 -> 242 -0.44550
240 -> 243 0.18362
241 -> 242 0.20851
241 -> 243 0.47534
Excited State 2:
240 -> 242 0.18946
240 -> 243 0.42978
241 -> 242 0.48939
241 -> 243 -0.20332
Excited State 3:
240 -> 243 0.50665
241 -> 242 -0.45439
Excited State 4:
240 -> 242 0.49572
241 -> 243 0.47379
Excited State 5:
232 -> 242 0.38605
232 -> 243 0.17270
235 -> 242 0.21680
236 -> 242 0.26208
236 -> 243 0.24766
237 -> 242 -0.11511
239 -> 243 0.26268
Excited State 6:
232 -> 242 -0.41303
232 -> 243 0.23700
236 -> 242 -0.14142
236 -> 243 0.11263
239 -> 243 0.43020
239 -> 247 0.12144

Conformer d
(ωB97-XD/cc-pVTZ)
Excited State 1:
240 -> 242 -0.46724
240 -> 243 -0.12745
241 -> 242 -0.14144
241 -> 243 0.49622
Excited State 2:
240 -> 242 -0.13010
240 -> 243 0.45679
241 -> 242 0.50566
241 -> 243 0.13915
Excited State 3:
233 -> 243 -0.10183
240 -> 242 0.14971
240 -> 243 0.48478
241 -> 242 -0.44849
241 -> 243 0.14153
Excited State 4:
233 -> 242 -0.11060
240 -> 242 0.47898
240 -> 243 -0.15518
241 -> 242 0.13945
241 -> 243 0.46168
Excited State 5:
232 -> 243 0.15803
235 -> 242 -0.14803
236 -> 243 0.17943
239 -> 243 0.57215
239 -> 246 -0.18261
Excited State 6:
232 -> 242 0.47107
235 -> 242 0.16213
236 -> 242 0.27524
236 -> 243 -0.22342
239 -> 243 0.23366

Host A/s-leucinol

Conformer a
(ωB97-XD/cc-pVTZ)
Excited State 1:
233 -> 235 -0.42998
233 -> 236 0.22181
234 -> 235 0.24377
234 -> 236 0.45631
Excited State 2:
233 -> 235 0.22540
233 -> 236 0.42104
234 -> 235 0.46416
234 -> 236 -0.24039
Excited State 3:
227 -> 236 0.11326
233 -> 236 0.50638
234 -> 235 -0.46934
Excited State 4:
227 -> 235 0.12553
233 -> 235 0.50064
234 -> 236 0.48129
Excited State 5:
225 -> 235 0.53382
226 -> 235 0.11034
227 -> 236 0.10552
228 -> 235 0.11039
229 -> 235 0.18544
229 -> 236 0.10839
230 -> 235 -0.30949
Excited State 6:
225 -> 235 -0.16578
225 -> 236 0.39104
228 -> 235 0.24251
229 -> 236 0.29848
232 -> 236 0.33876
232 -> 239 -0.10777

Conformer a
(ωB97-XD/cc-pVDZ)
Excited State 1:
233 -> 235 0.32806
233 -> 236 -0.35826
234 -> 235 0.37905
234 -> 236 0.34824
Excited State 2:
233 -> 235 0.35680
233 -> 236 0.32734
234 -> 235 -0.34880
234 -> 236 0.38002
Excited State 3:
227 -> 235 0.11483
233 -> 235 0.49554
234 -> 236 -0.47661
Excited State 4:
227 -> 236 0.12484
233 -> 236 0.49747
234 -> 235 0.47978
Excited State 5:
225 -> 235 0.11468
225 -> 236 0.13222
228 -> 236 0.24092
229 -> 235 0.21286
230 -> 235 0.11076
232 -> 235 0.50783
232 -> 236 0.13088
232 -> 239 -0.16559
Excited State 6:
225 -> 236 0.51648
226 -> 236 0.11305
229 -> 236 0.20876
230 -> 236 -0.29983
232 -> 235 -0.16948

Conformer b
(ωB97-XD/cc-pVTZ)
Excited State 1:
233 -> 235 -0.24769
233 -> 236 0.41520
234 -> 235 0.44893
234 -> 236 0.25354
Excited State 2:
233 -> 235 -0.42280
233 -> 236 -0.24266
234 -> 235 -0.25875
234 -> 236 0.44167
Excited State 3:
227 -> 235 0.11428
233 -> 235 0.49217
234 -> 236 0.48449
Excited State 4:
227 -> 236 0.12706
233 -> 236 0.50210
234 -> 235 -0.47737
Excited State 5:
224 -> 236 0.21186
227 -> 236 0.11152
228 -> 235 -0.15292
228 -> 236 -0.33002
229 -> 235 0.35347
229 -> 236 -0.15881
230 -> 236 0.19865
230 -> 239 -0.13836
231 -> 235 0.21928
Excited State 6:
224 -> 235 0.36937
224 -> 236 0.19333
225 -> 235 0.13596
225 -> 236 0.10840
228 -> 235 -0.18487
229 -> 235 -0.20804
229 -> 236 0.14638
230 -> 235 0.28075
230 -> 236 0.23662

Conformer b
(ωB97-XD/cc-pVDZ)
Excited State 1:
233 -> 235 -0.24769
233 -> 236 0.41520
234 -> 235 0.44893
234 -> 236 0.25354
Excited State 2:
233 -> 235 -0.42280
233 -> 236 -0.24266
234 -> 235 -0.25875
234 -> 236 0.44167
Excited State 3:
227 -> 235 0.11428
233 -> 235 0.49217
234 -> 236 0.48449
Excited State 4:
227 -> 236 0.12706
233 -> 236 0.50210
234 -> 235 -0.47737
Excited State 5:
224 -> 236 0.21186
227 -> 236 0.11152
228 -> 235 -0.15292
228 -> 236 -0.33002
229 -> 235 0.35347
229 -> 236 -0.15881
230 -> 236 0.19865
230 -> 239 -0.13836
231 -> 235 0.21928
Excited State 6:
224 -> 235 0.36937
224 -> 236 0.19333
225 -> 235 0.13596
225 -> 236 0.10840
228 -> 235 -0.18487
229 -> 235 -0.20804
229 -> 236 0.14638
230 -> 235 0.28075
230 -> 236 0.23662

Conformer c
(ωB97-XD/cc-pVTZ)
Excited State 1:

233 -> 235 -0.11631
233 -> 236 0.45902
234 -> 235 0.51034
234 -> 236 0.12061
Excited State 2:
233 -> 235 -0.47936
233 -> 236 -0.11383
234 -> 235 -0.12314
234 -> 236 0.49107
Excited State 3:
227 -> 235 0.10232
233 -> 235 0.41203
233 -> 236 -0.27806
234 -> 235 0.25185
234 -> 236 0.40966
Excited State 4:
227 -> 236 0.10651
233 -> 235 0.26796
233 -> 236 0.42716
234 -> 235 -0.39619
234 -> 236 0.26634
Excited State 5:
224 -> 235 -0.26458
224 -> 236 -0.11560
226 -> 235 -0.17490
228 -> 235 0.32394
228 -> 236 0.12315
229 -> 235 0.26631
230 -> 235 0.26658
230 -> 236 0.20337
231 -> 235 -0.14352
Excited State 6:
224 -> 235 -0.12622
226 -> 235 -0.12308
226 -> 236 0.11079
228 -> 236 -0.22247
229 -> 236 0.37118
230 -> 235 0.25578
230 -> 236 -0.35841
230 -> 239 0.11919

Conformer c
(ωB97-XD/cc-pVDZ)
Excited State 1:
233 -> 235 -0.22831
233 -> 236 0.42133
234 -> 235 0.46516
234 -> 236 0.22898
Excited State 2:
233 -> 235 0.44433
233 -> 236 0.21816
234 -> 235 0.23885
234 -> 236 -0.44297
Excited State 3:
227 -> 235 0.10531
233 -> 235 0.41361
233 -> 236 -0.26286
234 -> 235 0.23934
234 -> 236 0.42416
Excited State 4:
227 -> 236 0.11259
233 -> 235 0.25155
233 -> 236 0.43356
234 -> 235 -0.40598
234 -> 236 0.25466
Excited State 5:
224 -> 235 -0.24375
224 -> 236 -0.12547
228 -> 235 0.33377
228 -> 236 0.17409
229 -> 235 0.31089
230 -> 235 0.18269
230 -> 236 0.24075
230 -> 239 -0.12040
231 -> 235 -0.17687
Excited State 6:
224 -> 235 -0.17505
228 -> 235 0.10505
228 -> 236 -0.19562
229 -> 236 0.37466
230 -> 235 0.32408
230 -> 236 -0.30315
230 -> 239 0.11364

Conformer d
(ωB97-XD/cc-pVTZ)
Excited State 1:
233 -> 235 -0.10659
233 -> 236 0.45678
234 -> 235 0.51673
234 -> 236 0.11019
Excited State 2:
233 -> 235 -0.48238
233 -> 236 -0.10363
234 -> 235 -0.11314
234 -> 236 0.49261

Excited State 3:
227 -> 235 0.10141
233 -> 235 0.40040
233 -> 236 -0.29787
234 -> 235 0.26519
234 -> 236 0.39913
Excited State 4:
227 -> 236 0.10422
233 -> 235 0.28433
233 -> 236 0.41882
234 -> 235 -0.38200
234 -> 236 0.28369
Excited State 5:
224 -> 235 -0.24643
225 -> 235 -0.11557
226 -> 235 -0.19267
228 -> 235 0.34100
228 -> 236 0.10174
229 -> 235 0.26739
230 -> 235 0.26366
230 -> 236 0.18040
231 -> 235 -0.14697
Excited State 6:
225 -> 235 0.11121
225 -> 236 -0.13795
228 -> 236 0.19680
229 -> 236 -0.36033
230 -> 235 -0.24669
230 -> 236 0.39560
230 -> 239 -0.12496

Conformer d
(ωB97-XD/cc-pVDZ)
Excited State 1:
233 -> 235 -0.20560
233 -> 236 0.42809
234 -> 235 0.48016
234 -> 236 0.20570
Excited State 2:
233 -> 235 0.45575
233 -> 236 0.19486
234 -> 235 0.21602
234 -> 236 -0.45362
Excited State 3:
227 -> 235 0.10379
233 -> 235 0.39835
233 -> 236 -0.28966
234 -> 235 0.26001
234 -> 236 0.40924
Excited State 4:
227 -> 236 0.10974
233 -> 235 0.27486
233 -> 236 0.42088
234 -> 235 -0.38825
234 -> 236 0.27922
Excited State 5:
224 -> 235 -0.24893
224 -> 236 -0.10231
228 -> 235 0.35602
228 -> 236 0.15177
229 -> 235 0.30626
230 -> 235 0.18040
230 -> 236 0.22731
230 -> 239 -0.12039
231 -> 235 -0.18172
Excited State 6:
224 -> 235 -0.17472
228 -> 236 -0.16982
229 -> 236 0.36319
230 -> 235 0.31850
230 -> 236 -0.34226
230 -> 239 0.11529

Host A/L-Phe-OMe

Conformer a
(ωB97-XD/cc-pVTZ)
Excited State 1:
248 -> 250 0.14257
248 -> 251 -0.45730
249 -> 250 0.49707
249 -> 251 0.15389
Excited State 2:
248 -> 250 0.45927
248 -> 251 0.14304
249 -> 250 -0.15345
249 -> 251 0.49486
Excited State 3:
242 -> 250 0.10558
248 -> 250 0.49639
249 -> 251 -0.47130
Excited State 4:
242 -> 251 0.11793
248 -> 251 0.50142
249 -> 250 0.47259
Excited State 5:
239 -> 250 -0.15456
241 -> 250 -0.12469
243 -> 251 -0.32703
244 -> 250 0.32479
245 -> 250 0.13031
245 -> 254 -0.13398
247 -> 250 0.40505
247 -> 254 -0.12591
Excited State 6:
239 -> 251 -0.31028
241 -> 251 -0.11426
242 -> 254 -0.14345
243 -> 250 -0.33857
244 -> 250 0.12084
244 -> 251 0.39776
245 -> 250 -0.16878

Conformer a
(ωB97-XD/cc-pVDZ)
Excited State 1:
248 -> 250 0.14257
248 -> 251 -0.45730
249 -> 250 0.49707
249 -> 251 0.15389
Excited State 2:
248 -> 250 0.45927
248 -> 251 0.14304
249 -> 250 -0.15345
249 -> 251 0.49486
Excited State 3:
242 -> 250 0.10558
248 -> 250 0.49639
249 -> 251 -0.47130
Excited State 4:
242 -> 251 0.11793
248 -> 251 0.50142
249 -> 250 0.47259
Excited State 5:
239 -> 250 -0.15456
241 -> 250 -0.12469
243 -> 251 -0.32703
244 -> 250 0.32479
245 -> 250 0.13031
245 -> 254 -0.13398
247 -> 250 0.40505
247 -> 254 -0.12591
Excited State 6:
239 -> 251 -0.31028
241 -> 251 -0.11426
242 -> 254 -0.14345
243 -> 250 -0.33857
244 -> 250 0.12084
244 -> 251 0.39776
245 -> 250 -0.16878

Conformer b
(ωB97-XD/cc-pVTZ)
Excited State 1:
248 -> 250 -0.18017
248 -> 251 -0.43176
249 -> 250 0.49478
249 -> 251 -0.19139
Excited State 2:
248 -> 250 0.44918
248 -> 251 -0.16948
249 -> 250 0.20075
249 -> 251 0.47850
Excited State 3:
248 -> 250 0.45258
248 -> 251 -0.22389
249 -> 250 -0.20137
249 -> 251 -0.42831
Excited State 4:
248 -> 250 0.21693
248 -> 251 0.46828
249 -> 250 0.41432
249 -> 251 -0.21573
Excited State 5:
240 -> 251 -0.21549
243 -> 250 -0.11791
243 -> 251 -0.13682
244 -> 251 0.48053
245 -> 251 0.25754
245 -> 254 0.12674
247 -> 250 0.14342
247 -> 251 -0.17473
Excited State 6:
240 -> 250 -0.46432
240 -> 251 -0.13407
243 -> 250 0.36818
244 -> 250 0.14047
245 -> 250 0.21294
245 -> 251 0.10539
247 -> 250 -0.11513

Conformer b
(ωB97-XD/cc-pVDZ)
Excited State 1:
248 -> 251 -0.45823
249 -> 250 0.51931
249 -> 251 -0.10138
Excited State 2:
248 -> 250 0.47849
249 -> 250 0.10836
249 -> 251 0.50018
Excited State 3:
248 -> 250 0.47684
248 -> 251 -0.14088
249 -> 250 -0.13076
249 -> 251 -0.46192
Excited State 4:
248 -> 250 0.13557
248 -> 251 0.49606
249 -> 250 0.44574
249 -> 251 -0.14244
Excited State 5:
240 -> 251 -0.13123
243 -> 250 -0.16312
243 -> 251 -0.15845
244 -> 250 -0.18298
244 -> 251 0.39929
245 -> 251 0.24159
245 -> 254 -0.14091
247 -> 250 0.25540
247 -> 251 -0.17324
Excited State 6:
240 -> 250 -0.27463
240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297
245 -> 251 0.21252
247 -> 250 -0.15451

Conformer c
(ωB97-XD/cc-pVTZ)
Excited State 1:
248 -> 250 -0.38391
248 -> 251 0.28586
249 -> 250 0.31556
249 -> 251 0.41576
Excited State 2:
248 -> 250 0.28814
248 -> 251 0.37782
249 -> 250 0.42091
249 -> 251 -0.31344

Excited State 3:
242 -> 251 0.10696
248 -> 251 0.50751
249 -> 250 -0.46636
Excited State 4:
242 -> 250 0.11744
248 -> 250 0.50511
249 -> 251 0.47542
Excited State 5:
240 -> 250 0.39270
240 -> 251 0.11988
243 -> 250 0.27554
244 -> 250 0.30506
244 -> 251 0.23877
245 -> 250 -0.15573
247 -> 251 0.16427
Excited State 6:
240 -> 250 0.10723
240 -> 251 -0.38768
243 -> 251 -0.28099
244 -> 250 -0.14003
245 -> 250 -0.20249
245 -> 251 0.33346

Conformer c
(ωB97-XD/cc-pVDZ)
Excited State 1:
248 -> 250 0.17764
248 -> 251 -0.44644
249 -> 250 0.48357
249 -> 251 0.18981
Excited State 2:
248 -> 250 0.44814
248 -> 251 0.17622
249 -> 250 -0.19126
249 -> 251 0.48160
Excited State 3:
242 -> 250 0.10470
248 -> 250 0.48900
248 -> 251 -0.10909
249 -> 250 -0.10344
249 -> 251 -0.46617
Excited State 4:
242 -> 251 0.11834
248 -> 250 0.11021
248 -> 251 0.49409
249 -> 250 0.46654
249 -> 251 -0.10381
Excited State 5:
240 -> 250 0.20090
240 -> 251 0.15393
241 -> 250 -0.10045
243 -> 250 0.10885
243 -> 251 0.28156
244 -> 250 0.33061
244 -> 251 0.11380
245 -> 251 -0.12306
245 -> 254 -0.10401
247 -> 250 0.37106
247 -> 254 -0.10867
Excited State 6:
240 -> 250 0.20492
240 -> 251 0.21274
242 -> 254 0.11288
243 -> 250 0.28399
243 -> 251 -0.12322
244 -> 250 0.11627
244 -> 251 0.31342
245 -> 250 -0.23657
245 -> 251 0.11842
247 -> 250 -0.24511

Conformer d
(ωB97-XD/cc-pVTZ)
Excited State 1:
248 -> 250 -0.42760
248 -> 251 -0.21360
249 -> 250 -0.23838
249 -> 251 0.46476
Excited State 2:
248 -> 250 -0.21464
248 -> 251 0.42158
249 -> 250 0.47006
249 -> 251 0.23710
Excited State 3:
248 -> 250 -0.30852
248 -> 251 0.40645
249 -> 250 -0.37004
249 -> 251 -0.28836
Excited State 4:
248 -> 250 0.40312
248 -> 251 0.31330
249 -> 250 -0.28823
249 -> 251 0.37796
Excited State 5:
240 -> 250 0.15799
240 -> 251 0.34425
243 -> 250 -0.17700
243 -> 251 -0.30946
244 -> 251 0.33560
245 -> 250 -0.15337
247 -> 251 0.16746
Excited State 6:
240 -> 250 0.45783
240 -> 251 -0.15903
242 -> 250 0.11577
243 -> 250 -0.22689
243 -> 251 0.15608
244 -> 251 -0.13621
245 -> 250 -0.30990

Conformer d
(ωB97-XD/cc-pVDZ)
Excited State 1:
248 -> 250 0.23624
248 -> 251 -0.41616
249 -> 250 0.45819
249 -> 251 0.24816
Excited State 2:
248 -> 250 0.42240
248 -> 251 0.23009
249 -> 250 -0.25395
249 -> 251 0.45204
Excited State 3:
242 -> 250 0.10154
248 -> 250 0.48105
248 -> 251 0.13984
249 -> 250 0.12673
249 -> 251 -0.46120
Excited State 4:
242 -> 251 0.11377
248 -> 250 -0.13533
248 -> 251 0.49093
249 -> 250 0.45650
249 -> 251 0.13200
Excited State 5:
240 -> 250 -0.11982
240 -> 251 -0.19485
243 -> 251 0.35377
244 -> 250 -0.28202
244 -> 251 -0.17029
245 -> 250 -0.12901
245 -> 254 0.10812
247 -> 250 -0.33410
247 -> 251 -0.10941
Excited State 6:
239 -> 250 0.10957
240 -> 250 -0.22297
240 -> 251 -0.12097
242 -> 254 -0.12163
243 -> 250 0.39924
244 -> 250 0.10982
244 -> 251 -0.29051
245 -> 250 0.26476
245 -> 251 -0.10267

Host B/L-Phe-OMe

Conformer a
(ωB97-XD/cc-pVTZ)
Excited State 1:
256 -> 258 -0.45072
256 -> 259 -0.19007
257 -> 258 -0.20882
257 -> 259 0.46704
Excited State 2:
256 -> 258 -0.19586
256 -> 259 0.43664
257 -> 258 0.47989
257 -> 259 0.20335
Excited State 3:
250 -> 259 0.10135
256 -> 259 0.50774
257 -> 258 -0.47107
Excited State 4:
250 -> 258 0.11366
256 -> 258 0.49832
257 -> 259 0.49017
Excited State 5:
249 -> 258 0.56418
251 -> 258 0.23048
251 -> 259 -0.14106
252 -> 258 -0.14546
252 -> 259 0.11480
253 -> 258 0.20620
Excited State 6:
249 -> 258 -0.14834
249 -> 259 -0.13622
251 -> 258 0.33782
252 -> 258 0.23947
252 -> 259 0.44125
253 -> 263 0.13519
255 -> 259 -0.10826

Conformer a
(ωB97-XD/cc-pVDZ)
Excited State 1:
256 -> 258 0.42022
256 -> 259 -0.25074
257 -> 258 0.26630
257 -> 259 0.43576
Excited State 2:
256 -> 258 -0.25382
256 -> 259 -0.41484
257 -> 258 0.44055
257 -> 259 -0.26330
Excited State 3:
250 -> 259 0.10237
256 -> 259 0.49662
257 -> 258 0.47799
Excited State 4:
250 -> 258 0.11647
256 -> 258 0.49544
257 -> 259 -0.48805
Excited State 5:
249 -> 258 0.21622
251 -> 258 0.42561
252 -> 259 -0.42497
253 -> 258 -0.10606
253 -> 262 -0.13635
255 -> 259 0.10621
Excited State 6:
249 -> 258 0.42012
251 -> 259 0.28647
252 -> 258 -0.34969
252 -> 259 0.21711
253 -> 258 -0.13298

Conformer b
(ωB97-XD/cc-pVTZ)

Excited State 1:
256 -> 258 -0.48390
257 -> 259 0.50135
Excited State 2:
256 -> 259 0.46913
257 -> 258 0.51492
Excited State 3:
256 -> 258 0.14290
256 -> 259 0.48643
257 -> 258 -0.45190
257 -> 259 0.13616
Excited State 4:
250 -> 258 -0.11226
256 -> 258 0.47713
256 -> 259 -0.14517
257 -> 258 0.13576
257 -> 259 0.47015
Excited State 5:
248 -> 258 0.41890
249 -> 258 -0.29003
251 -> 258 -0.28157
252 -> 259 0.20000
253 -> 258 0.25407
Excited State 6:
248 -> 258 -0.11828
248 -> 259 0.25883
249 -> 259 -0.19122
250 -> 262 0.11708
251 -> 258 -0.19046
251 -> 259 -0.30905
252 -> 258 0.35544
252 -> 259 0.10938
253 -> 259 0.11793
254 -> 259 -0.12775
255 -> 259 0.12460

Conformer b
(ωB97-XD/cc-pVDZ)
Excited State 1:
256 -> 258 -0.44484
256 -> 259 0.20638
257 -> 258 0.21603
257 -> 259 0.46113
Excited State 2:
256 -> 258 0.20631
256 -> 259 0.43938
257 -> 258 0.46603
257 -> 259 -0.21619
Excited State 3:
256 -> 258 0.24774
256 -> 259 0.43196
257 -> 258 -0.41713
257 -> 259 0.23892
Excited State 4:
250 -> 258 0.10771
256 -> 258 0.43060
256 -> 259 -0.24963
257 -> 258 0.24098
257 -> 259 0.42565
Excited State 5:
248 -> 258 -0.27434
248 -> 259 0.11840
251 -> 258 0.38458
251 -> 259 -0.13496
252 -> 258 -0.15603
252 -> 259 -0.32396
253 -> 258 -0.13342
253 -> 262 -0.14445
254 -> 259 0.12766
Excited State 6:
248 -> 258 -0.16230
248 -> 259 0.29082
250 -> 262 -0.13809
251 -> 258 -0.17025
251 -> 259 -0.33197
252 -> 258 0.37110
253 -> 259 0.10402
254 -> 258 -0.10239
255 -> 259 0.10335

Conformer c
(ωB97-XD/cc-pVTZ)
Excited State 1:
256 -> 258 -0.43173
256 -> 259 0.21963
257 -> 258 0.24630
257 -> 259 0.45202
Excited State 2:
256 -> 258 0.22934
256 -> 259 0.41968
257 -> 258 0.46302
257 -> 259 -0.23694
Excited State 3:
256 -> 259 0.50081
257 -> 258 -0.46144
Excited State 4:
250 -> 258 0.10853
256 -> 258 0.49272
257 -> 259 0.48062
Excited State 5:
249 -> 258 0.18377
249 -> 259 -0.15583
251 -> 258 0.19689
251 -> 259 -0.14438
252 -> 258 -0.24466
252 -> 259 0.38794
253 -> 258 -0.15501
253 -> 259 0.22587
253 -> 263 -0.11441
255 -> 259 0.16972
Excited State 6:
249 -> 258 -0.15032
250 -> 263 0.10363
251 -> 258 0.46712
251 -> 259 0.30257
252 -> 258 0.21340
252 -> 259 0.13454
254 -> 259 0.14846

Conformer c
(ωB97-XD/cc-pVDZ)
Excited State 1:
240 -> 250 -0.27463
240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297
245 -> 251 0.21252
247 -> 250 -0.15451
Excited State 2:
240 -> 250 -0.27463
240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297
245 -> 251 0.21252
247 -> 250 -0.15451
Excited State 3:
240 -> 250 -0.27463
240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297
245 -> 251 0.21252
247 -> 250 -0.15451
Excited State 4:
240 -> 250 -0.27463
240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297
245 -> 251 0.21252
247 -> 250 -0.15451
Excited State 5:
240 -> 250 -0.27463
240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297
245 -> 251 0.21252
247 -> 250 -0.15451
Excited State 6:
240 -> 250 -0.27463
240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297
245 -> 251 0.21252
247 -> 250 -0.15451

Conformer d
(ωB97-XD/cc-pVTZ)
Excited State 1:
256 -> 258 -0.47591
256 -> 259 -0.11748
257 -> 258 -0.12568
257 -> 259 0.49487
Excited State 2:
256 -> 258 -0.11771
256 -> 259 0.46167
257 -> 258 0.50789
257 -> 259 0.12549
Excited State 3:
256 -> 259 0.50642
257 -> 258 -0.47038
Excited State 4:
250 -> 258 0.11141
256 -> 258 0.49826
257 -> 259 0.48773
Excited State 5:
248 -> 258 0.22520
249 -> 258 0.36961
249 -> 259 -0.13642
251 -> 258 -0.26828
251 -> 259 0.20883
252 -> 258 -0.21219
252 -> 259 0.19469
253 -> 258 0.19322
Excited State 6:
248 -> 258 0.18558
248 -> 259 0.17488
249 -> 258 0.28200
249 -> 259 0.31597
250 -> 259 0.10222
251 -> 258 0.19414
252 -> 259 -0.26400
253 -> 258 0.16686
253 -> 259 0.18489
255 -> 259 0.16254

Conformer d
(ωB97-XD/cc-pVDZ)
Excited State 1:
256 -> 258 -0.48282
257 -> 259 0.50064
Excited State 2:
256 -> 259 0.47542
257 -> 258 0.50739
Excited State 3:
250 -> 259 0.10048
256 -> 258 0.11837
256 -> 259 0.48424
257 -> 258 -0.46523
257 -> 259 0.11711
Excited State 4:
250 -> 258 0.11364
256 -> 258 0.48270
256 -> 259 -0.12402
257 -> 258 0.11377
257 -> 259 0.47495
Excited State 5:
248 -> 258 -0.22123
248 -> 259 0.16538
249 -> 258 0.15866
249 -> 259 -0.15662
251 -> 258 0.30966
251 -> 259 -0.27047
252 -> 258 0.12830
252 -> 259 -0.30239
253 -> 258 0.13150
253 -> 259 -0.10505
255 -> 259 0.12650
Excited State 6:
248 -> 258 -0.22783
249 -> 258 0.20380
251 -> 258 -0.24984
251 -> 259 -0.18173
252 -> 258 0.39368
252 -> 259 0.28206
253 -> 258 0.10541

Conformer e
(ωB97-XD/cc-pVTZ)
Excited State 1:
256 -> 258 -0.47417
256 -> 259 -0.12741
257 -> 258 -0.14303
257 -> 259 0.48977
Excited State 2:
256 -> 258 -0.13266
256 -> 259 0.45513
257 -> 258 0.50708
257 -> 259 0.13810

Excited State 3:
250 -> 259 -0.10168
256 -> 259 0.51083
257 -> 258 -0.46735
Excited State 4:
250 -> 258 -0.11284
256 -> 258 0.49786
257 -> 259 0.49087
Excited State 5:
249 -> 258 0.59118
251 -> 258 0.11396
252 -> 258 0.18380
252 -> 259 0.11271
253 -> 258 -0.21028
Excited State 6:
249 -> 258 -0.16426
249 -> 259 0.17193
251 -> 258 0.41185
252 -> 259 0.39549
253 -> 259 0.10101
253 -> 262 0.12612
255 -> 259 0.19539

Conformer e
(ωB97-XD/cc-pVDZ)
Excited State 1:
256 -> 258 0.45657
256 -> 259 -0.17902
257 -> 258 0.19381
257 -> 259 0.47178
Excited State 2:
256 -> 258 -0.18277
256 -> 259 -0.44635
257 -> 258 0.48102
257 -> 259 -0.19017
Excited State 3:
250 -> 259 0.10304
256 -> 259 0.50110
257 -> 258 0.47500
Excited State 4:
250 -> 258 0.11535
256 -> 258 0.49607
257 -> 259 -0.48965
Excited State 5:
248 -> 259 -0.12536
251 -> 258 0.41529
252 -> 259 -0.40820
253 -> 259 -0.13063
253 -> 262 0.16550
255 -> 259 -0.21461
Excited State 6:
248 -> 258 0.53108
251 -> 258 -0.10814
251 -> 259 -0.19184
252 -> 258 0.31469
253 -> 258 -0.12333

Conformer f
(ωB97-XD/cc-pVTZ)
Excited State 1:
256 -> 258 -0.49009
257 -> 259 0.50395
Excited State 2:
256 -> 259 0.46980
257 -> 258 0.52253
Excited State 3:
250 -> 259 0.10174
256 -> 259 0.50084
257 -> 258 -0.45970
Excited State 4:
250 -> 258 0.11469
256 -> 258 0.48756
257 -> 259 0.48314
Excited State 5:
249 -> 258 0.52351
251 -> 258 -0.23691
252 -> 258 0.18977
252 -> 259 -0.19009
253 -> 258 -0.18689
Excited State 6:
249 -> 258 0.26777
249 -> 259 0.15257
251 -> 258 0.34660
251 -> 259 0.12044
252 -> 258 0.21628
252 -> 259 0.34746
253 -> 259 0.11313
253 -> 263 -0.13398
255 -> 259 0.17454

Conformer f
(ωB97-XD/cc-pVDZ)
Excited State 1:
256 -> 258 -0.49200
257 -> 259 0.50631
Excited State 2:
256 -> 259 0.48041
257 -> 258 0.51694
Excited State 3:
250 -> 259 0.10332
256 -> 258 0.10806
256 -> 259 0.48912
257 -> 258 -0.46530
257 -> 259 0.10630
Excited State 4:
250 -> 258 0.11733
256 -> 258 0.48368
256 -> 259 -0.11121
257 -> 258 0.10340
257 -> 259 0.48012
Excited State 5:
248 -> 258 -0.27243
248 -> 259 0.11473
251 -> 258 0.38748
252 -> 259 0.36242
253 -> 258 0.13426
253 -> 259 0.10938
253 -> 262 0.14876
255 -> 259 0.17488
Excited State 6:
248 -> 258 0.36016
250 -> 262 -0.12765
251 -> 258 0.17114
251 -> 259 0.28993
252 -> 258 0.38763
252 -> 259 0.13452
253 -> 259 0.10919
255 -> 259 0.10131

Conformer g
(ωB97-XD/cc-pVTZ)
Excited State 1:
256 -> 258 -0.44800
256 -> 259 -0.19914
257 -> 258 -0.21923
257 -> 259 0.46134
Excited State 2:
256 -> 258 -0.20415
256 -> 259 0.43022
257 -> 258 0.47747
257 -> 259 0.21455
Excited State 3:
256 -> 258 0.17148
256 -> 259 0.47717
257 -> 258 -0.44090
257 -> 259 0.16788
Excited State 4:
250 -> 258 0.11068
256 -> 258 0.46699
256 -> 259 -0.18019
257 -> 258 0.15971
257 -> 259 0.46069
Excited State 5:
248 -> 258 0.45030
249 -> 258 -0.23623
251 -> 258 -0.11055
251 -> 259 0.13108
252 -> 258 0.13746
253 -> 258 -0.38233
Excited State 6:
248 -> 259 0.30390
249 -> 259 -0.18653
251 -> 258 0.32901
251 -> 259 -0.10055
252 -> 259 0.30440
253 -> 258 -0.10418
253 -> 259 -0.29374
253 -> 262 0.13676

Conformer g
(ωB97-XD/cc-pVDZ)
Excited State 1:
256 -> 258 -0.44984
256 -> 259 -0.19822
257 -> 258 -0.21292
257 -> 259 0.46203
Excited State 2:
256 -> 258 -0.20083
256 -> 259 0.43814
257 -> 258 0.47265
257 -> 259 0.21048
Excited State 3:
256 -> 258 0.19931
256 -> 259 0.45836
257 -> 258 -0.43702
257 -> 259 0.19461
Excited State 4:
250 -> 258 0.11308
256 -> 258 0.45383
256 -> 259 -0.20688
257 -> 258 0.18899
257 -> 259 0.45040
Excited State 5:
248 -> 258 0.44099
249 -> 258 -0.14287
251 -> 259 0.17297
252 -> 258 0.18380
253 -> 258 -0.40396
Excited State 6:
248 -> 259 0.22776
249 -> 259 -0.10787
251 -> 258 0.38989
251 -> 259 -0.10024
252 -> 259 0.36126
253 -> 259 -0.23490
253 -> 262 -0.16190
254 -> 259 -0.11834

Conformer h
(ωB97-XD/cc-pVTZ)
Excited State 1:
256 -> 258 -0.48408
257 -> 259 0.49909
Excited State 2:
256 -> 259 0.46295
257 -> 258 0.51844
Excited State 3:
256 -> 259 0.50521
257 -> 258 -0.45988
Excited State 4:
250 -> 258 -0.11210
256 -> 258 0.49011
257 -> 259 0.48456
Excited State 5:
248 -> 258 0.48475
249 -> 258 -0.10415
251 -> 258 -0.23504
251 -> 259 0.19312
252 -> 258 0.29939
255 -> 258 0.10295
255 -> 259 -0.10018
Excited State 6:
248 -> 258 0.21918
248 -> 259 0.21088
251 -> 258 0.36046
252 -> 259 0.40355
253 -> 258 0.13613
253 -> 262 0.15023
255 -> 259 0.14459

Conformer h
(ωB97-XD/cc-pVDZ)
Excited State 1:
248 -> 251 -0.45823
249 -> 250 0.51931
249 -> 251 -0.10138
Excited State 2:
248 -> 250 0.47849
249 -> 250 0.10836
249 -> 251 0.50018
Excited State 3:
248 -> 250 0.47684
248 -> 251 -0.14088
249 -> 250 -0.13076
249 -> 251 -0.46192
Excited State 4:
248 -> 250 0.13557
248 -> 251 0.49606
249 -> 250 0.44574
249 -> 251 -0.14244
Excited State 5:
240 -> 251 -0.13123
243 -> 250 -0.16312
243 -> 251 -0.15845

244 -> 250 -0.18298
244 -> 251 0.39929
245 -> 251 0.24159
245 -> 254 -0.14091

247 -> 250 0.25540
247 -> 251 -0.17324
Excited State 6:
240 -> 250 -0.27463

240 -> 251 -0.17965
242 -> 254 -0.11761
243 -> 250 0.44315
244 -> 251 0.23297

245 -> 251 0.21252
247 -> 250 -0.15451

Host C/L-Phe-OMe

Conformer a
(ωB97-XD/cc-pVTZ)
Excited State 1:
174 -> 176 -0.28334
174 -> 177 0.36082
175 -> 176 0.42767
175 -> 177 0.32991
Excited State 2:
174 -> 176 -0.36336
174 -> 177 -0.27998
175 -> 176 -0.33269
175 -> 177 0.42541
Excited State 3:
170 -> 176 0.11950
174 -> 176 0.51230
174 -> 177 -0.10764
175 -> 177 0.44756
Excited State 4:
170 -> 177 0.11483
174 -> 176 0.10947
174 -> 177 0.51539
175 -> 176 -0.44332
Excited State 5:
169 -> 176 0.63771
171 -> 176 -0.19190
172 -> 176 0.12007
173 -> 176 -0.12141
Excited State 6:
169 -> 177 0.65294
171 -> 177 -0.10450
172 -> 177 0.13792
173 -> 177 -0.13267

Conformer a
(ωB97-XD/cc-pVDZ) 4
Excited State 1:
174 ->176 -0.31484
174 ->177 0.34140
175 ->176 0.39581
175 ->177 0.35912
Excited State 2:
174 ->176 -0.31484
174 ->177 0.34140
175 ->176 0.39581
175 ->177 0.35912
Excited State 3:
174 ->176 -0.31484
174 ->177 0.34140
175 ->176 0.39581
175 ->177 0.35912
Excited State 4:
174 ->176 -0.31484
174 ->177 0.34140
175 ->176 0.39581
175 ->177 0.35912
Excited State 5:
174 ->176 -0.31484
174 ->177 0.34140
175 ->176 0.39581
175 ->177 0.35912
Excited State 6:
169 ->176 -0.11571
169 ->177 0.63792
171 ->177 -0.11678
172 ->177 0.16688
173 ->177 -0.10606

Conformer b
(ωB97-XD/cc-pVTZ)
Excited State 1:
174 -> 177 -0.45612
175 -> 176 0.54178
Excited State 2:
174 -> 176 0.45962
175 -> 177 0.53873
Excited State 3:
170 -> 177 0.11522
174 -> 176 -0.19965
174 -> 177 0.48786
175 -> 176 0.41940
175 -> 177 0.17353
Excited State 4:
170 -> 176 0.11159
174 -> 176 0.48514
174 -> 177 0.20071
175 -> 176 0.17141
175 -> 177 -0.42255
Excited State 5:
169 -> 176 0.63907
170 -> 176 0.13378
172 -> 176 0.11330
173 -> 176 -0.17795
Excited State 6:
169 -> 177 0.63245
172 -> 177 0.21372
173 -> 177 -0.16010

Conformer b
(ωB97-XD/cc-pVDZ)
Excited State 1:
174 ->177 0.46098
175 ->176 0.53703
Excited State 2:
174 ->176 -0.46547
175 ->177 0.53303
Excited State 3:
170 ->177 0.11711
174 ->176 0.19381
174 ->177 0.48391
175 ->176 -0.42533
175 ->177 0.17289
Excited State 4:
170 ->176 0.11589
174 ->176 0.48039
174 ->177 -0.19520
175 ->176 0.17040
175 ->177 0.42940
Excited State 5:
169 ->176 0.64252
170 ->176 0.12449
172 ->176 0.11368
173 ->176 0.17142
Excited State 6:
169 ->177 0.61080
172 ->177 0.28438
173 ->177 0.13041

Conformer c
(ωB97-XD/cc-pVTZ)
Excited State 1:
174 -> 176 0.30240
174 -> 177 -0.34609
175 -> 176 0.40735
175 -> 177 0.35376
Excited State 2:
174 -> 176 0.34715
174 -> 177 0.30054
175 -> 176 -0.35524
175 -> 177 0.40637
Excited State 3:
170 -> 176 0.10067
174 -> 176 0.43002
174 -> 177 -0.29969
175 -> 176 -0.25955
175 -> 177 -0.37560
Excited State 4:
170 -> 177 0.10319
174 -> 176 0.30012
174 -> 177 0.43160
175 -> 176 0.37361
175 -> 177 -0.26059
Excited State 5:
169 -> 176 0.61534
169 -> 177 0.15003
172 -> 176 -0.20573
172 -> 177 -0.11819
173 -> 176 0.14237
Excited State 6:
169 -> 176 -0.17384
169 -> 177 0.63347
172 -> 177 -0.11441
173 -> 177 0.16475

Conformer c
(ωB97-XD/cc-pVDZ)
Excited State 1:
174 ->176 0.38759
174 ->177 -0.25761
175 ->176 0.29660
175 ->177 0.44363
Excited State 2:
174 ->176 -0.25843
174 ->177 -0.38530
175 ->176 0.44554
175 ->177 -0.29586
Excited State 3:
170 ->176 0.11736
174 ->176 0.48531
174 ->177 -0.17998
175 ->176 -0.15959
175 ->177 -0.43424
Excited State 4:
170 ->177 0.12084
174 ->176 0.18073
174 ->177 0.48736
175 ->176 0.43195
175 ->177 -0.16031
Excited State 5:
169 ->176 0.53300
169 ->177 0.27616
172 ->176 -0.21496
172 ->177 -0.21959
173 ->176 0.13595
Excited State 6:
169 ->176 -0.33131
169 ->177 0.56256
172 ->177 -0.13524
173 ->176 -0.10366
173 ->177 0.14660

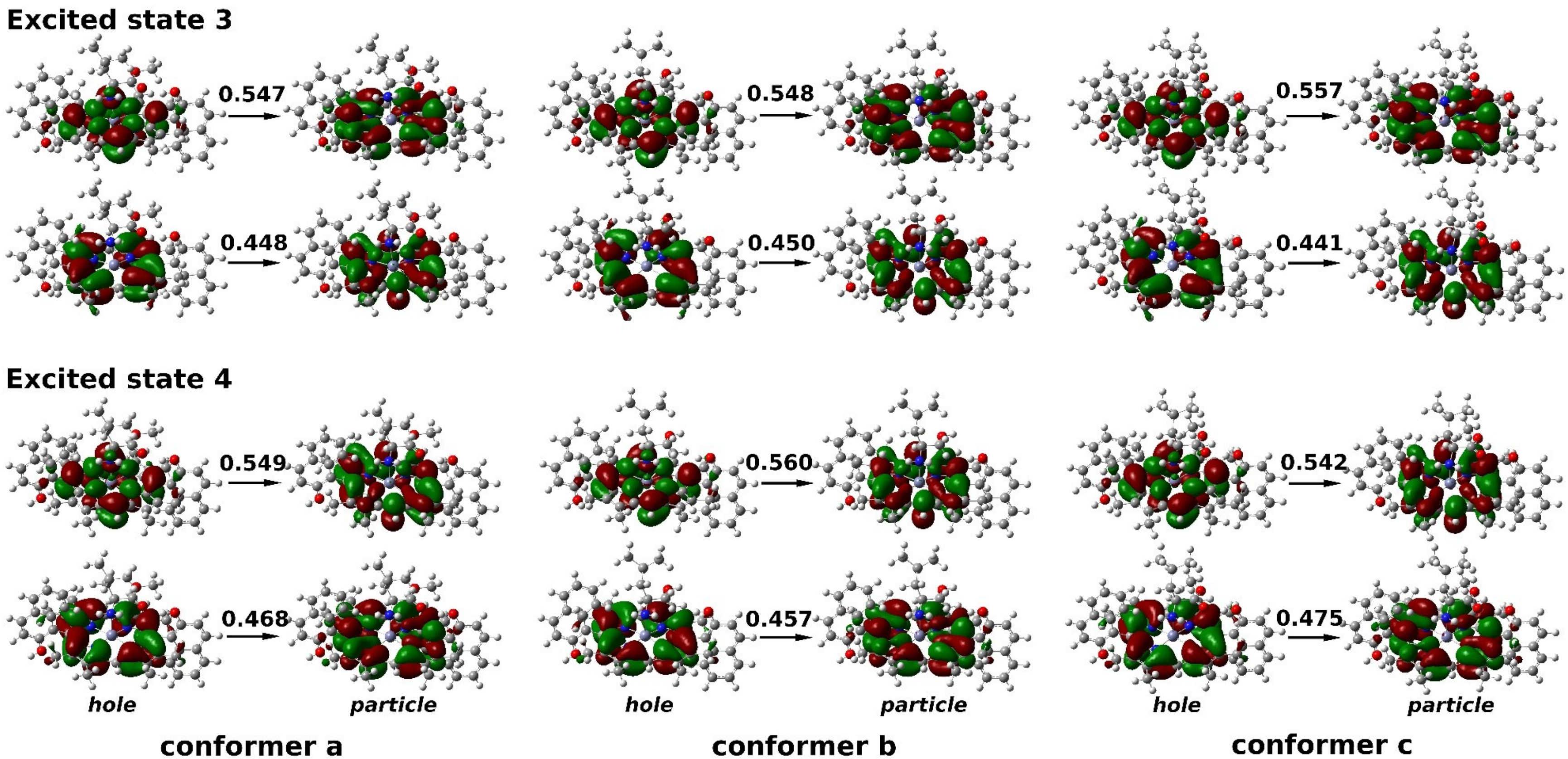


Figure S7. NTO analysis for several conformers of complex A/S-Leucinol calculated using ωB97X-D/cc-pVTZ and SMD solvent model

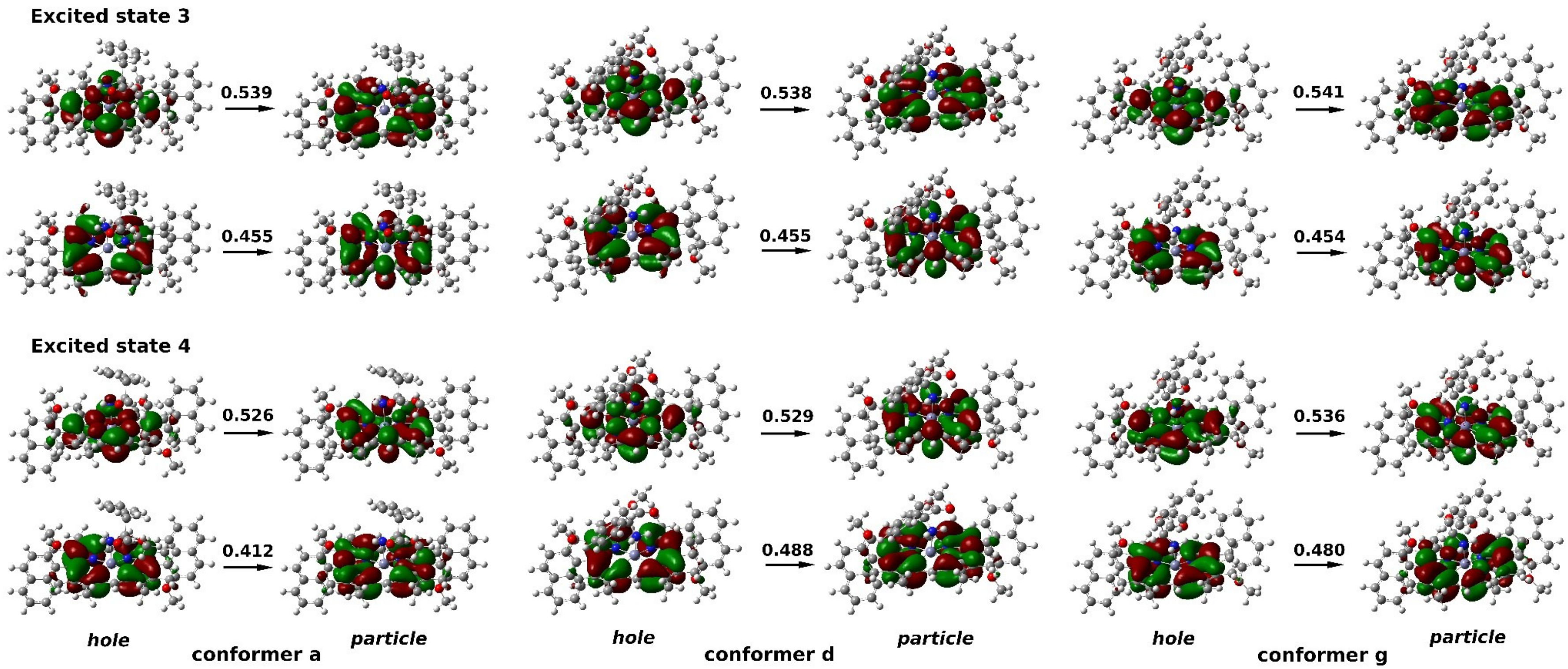


Figure S8. NTO analysis for several conformers of complex B/L-Phe-OMe calculated using ωB97X-D/cc-pVTZ and SMD solvent mode

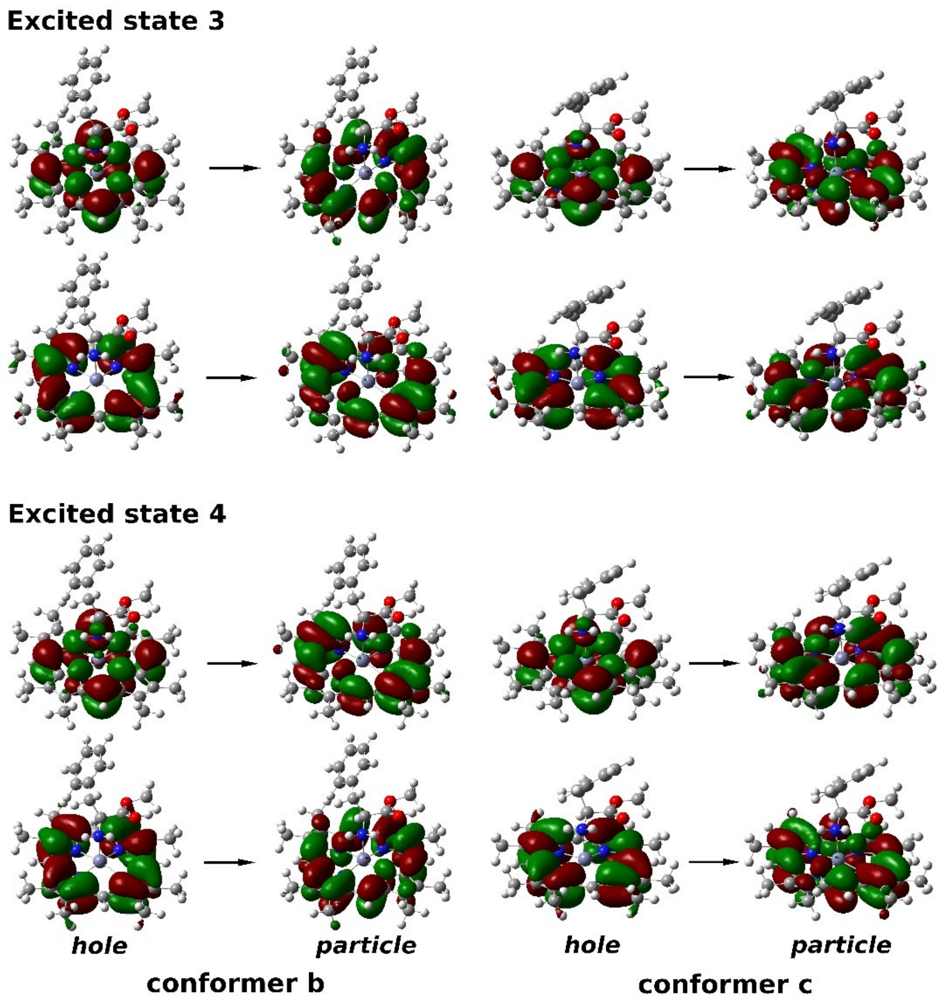


Figure S9. NTO analysis for several conformers of complex C/ʟ-Phe-OMe calculated using ωB97X-D/cc-pVTZ and SMD solvent model