Electronic Supplementary Material (ESI) for RSC Advances.

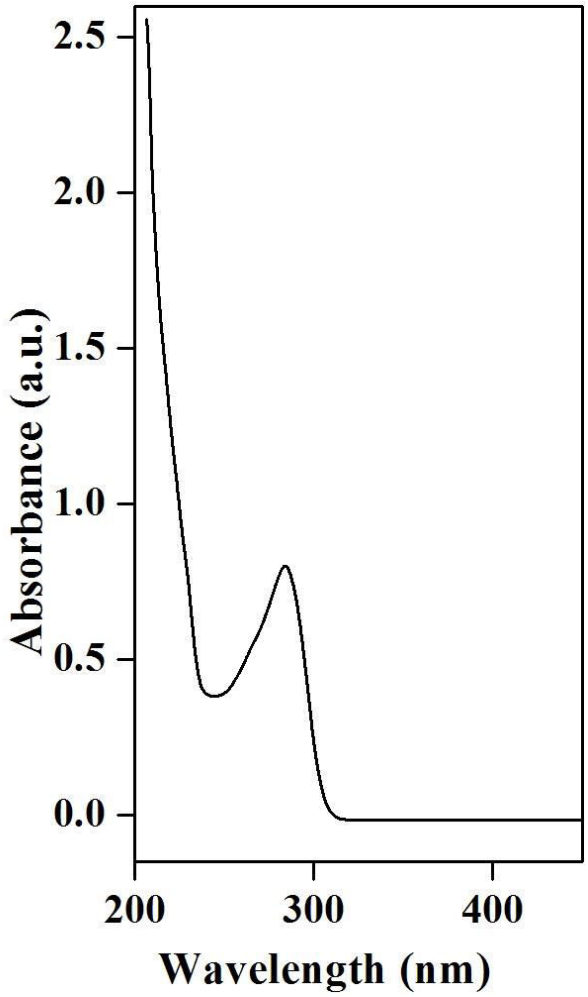


Fig. S1: UV–vis transmission spectrum of LSP in Ethanol solution

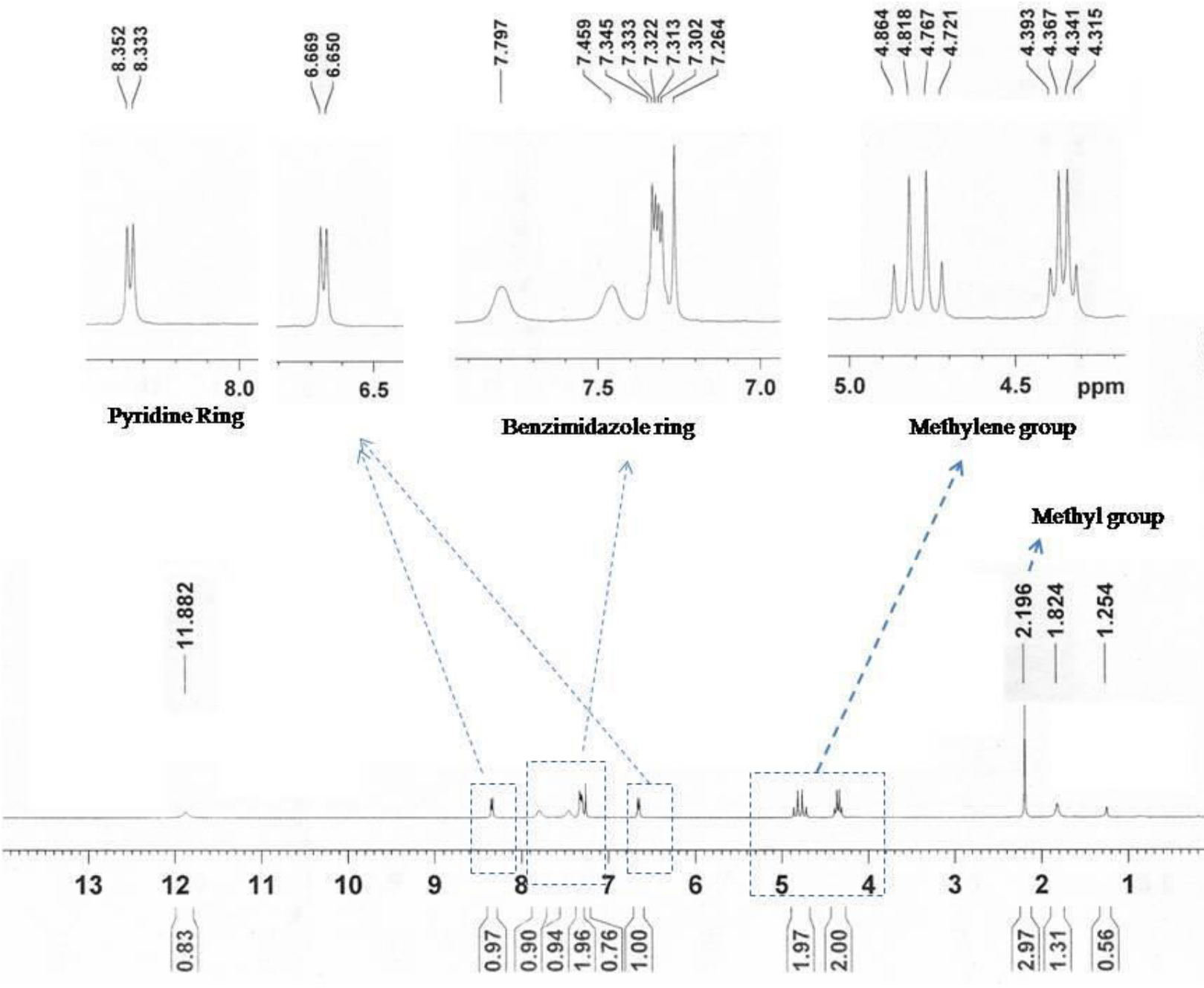


Fig. S2: ^{1}H NMR spectrum of LSP

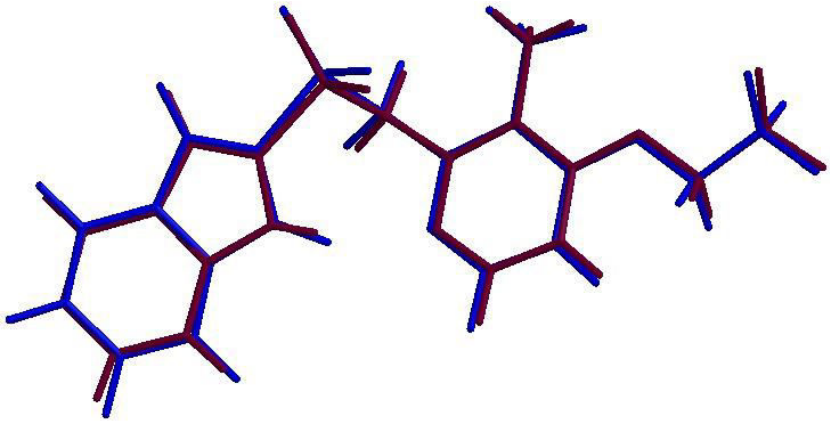


Fig. S3: Comparison of the experimental (in red) and the optimized (in blue) structure of LSP (hydrogen atoms are not shown)

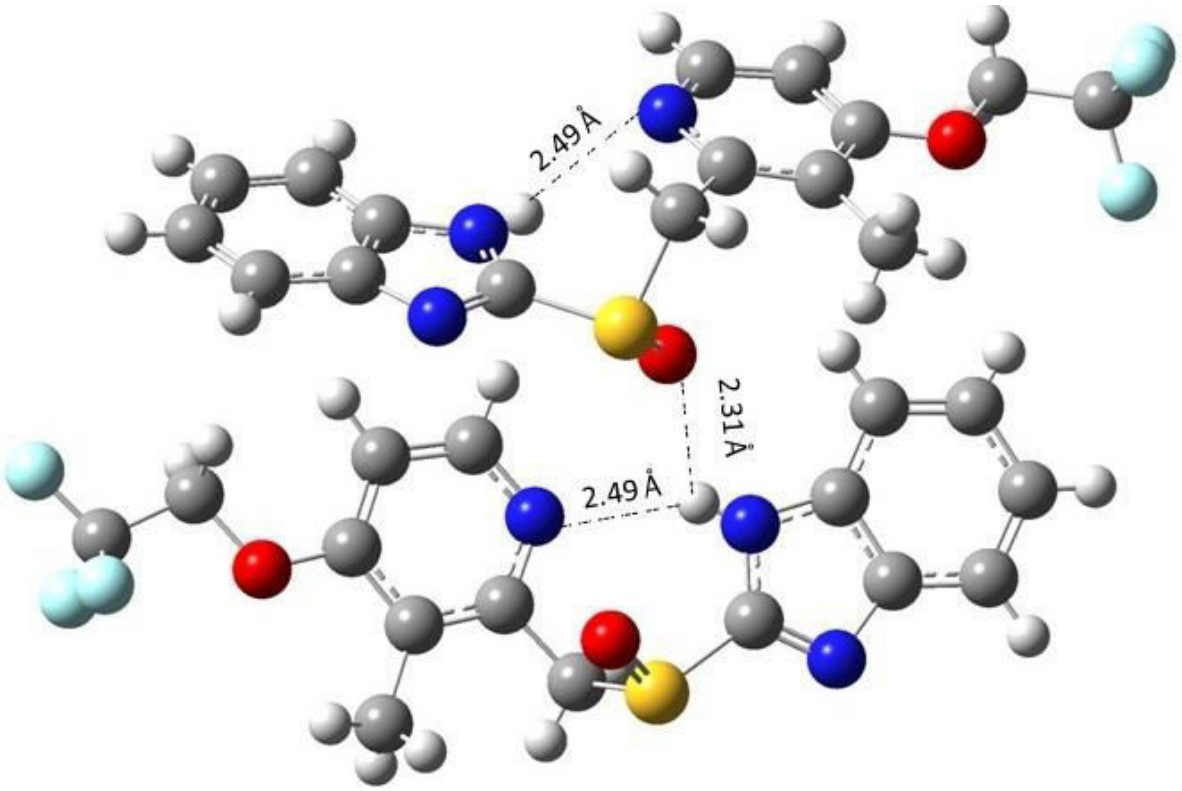
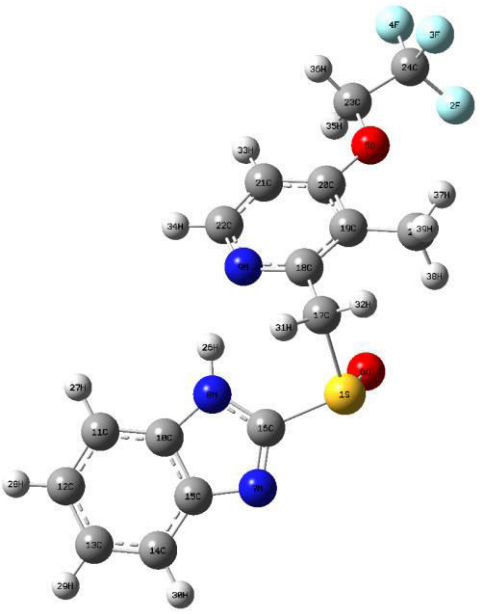
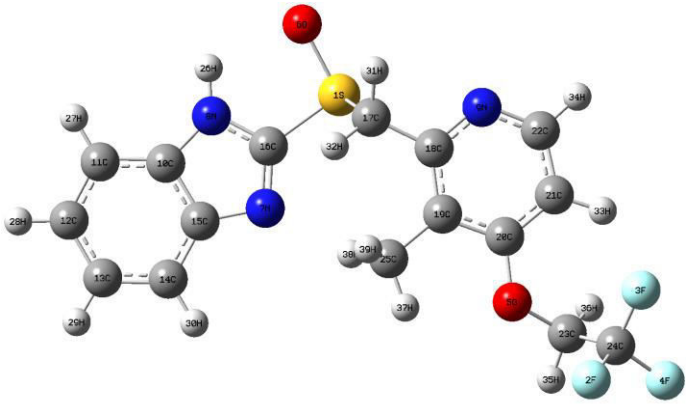


Fig. S4: Dimer structure of LSP exhibiting intra and intermolecular interactions.

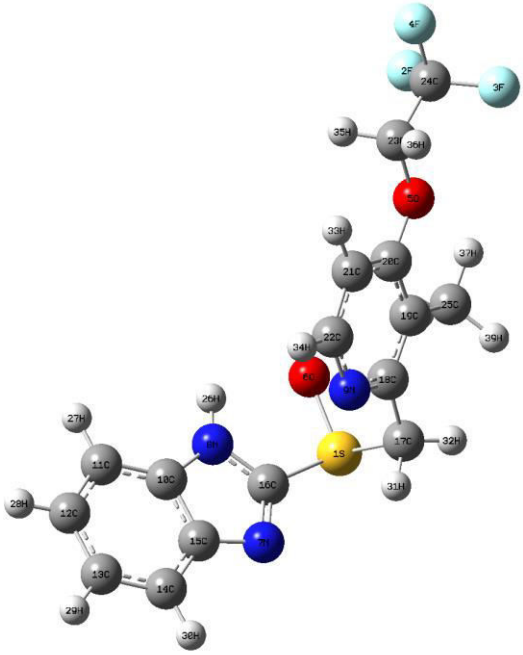
Conformer 1
D1= -146.67729°, D2= -88.98879°
D3= -88.51928°, D4= -179.39567°,
Energy= -1630.10021899 a.u.



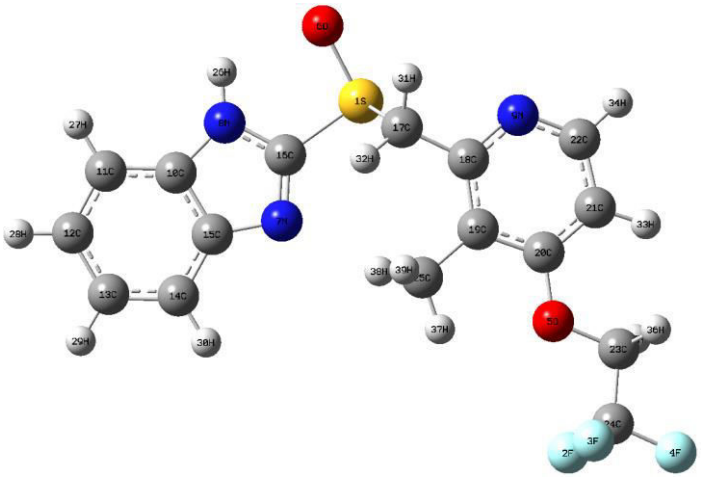
Conformer 2
D1= -64.23331°, D2= 116.83465°
D3= -103.44262°, D4= 98.48725°,
Energy= -1630.09952096 a.u.



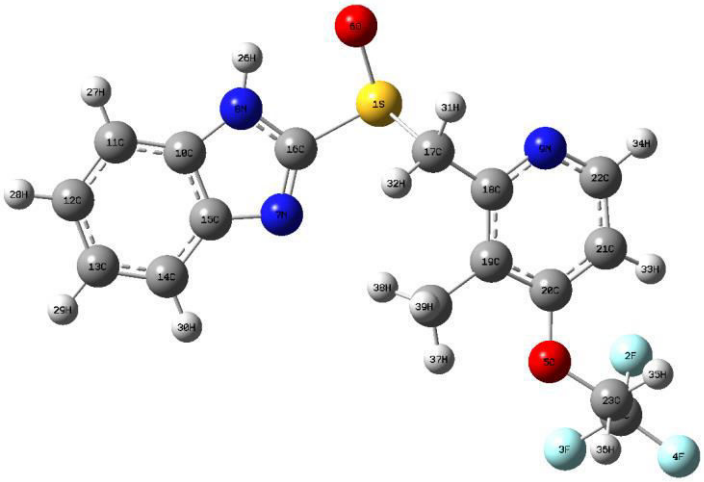
Conformer 3
D1= -69.10399°, D2= -76.57527°
D3= -82.92743° D4= 178.15086°,
Energy= -1630.10121361 a.u.



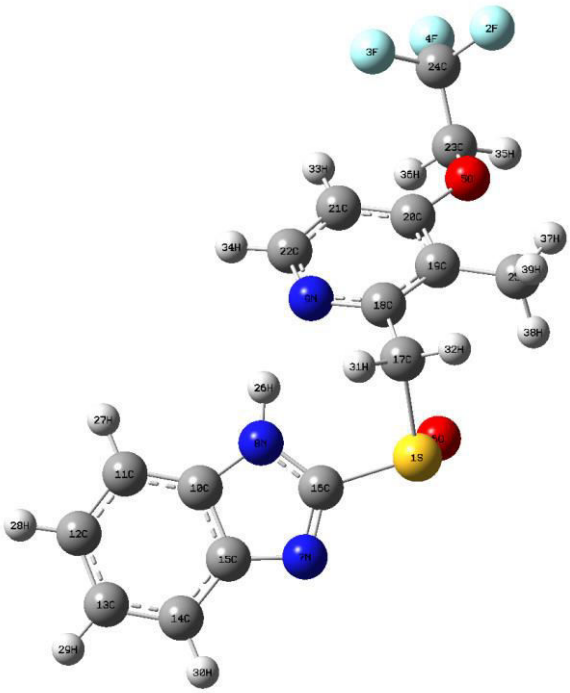
Conformer 4
D1= -63.80397°, D2= 117.59324°
D3= -103.42753°, D4= 179.65972°,
Energy= -1630.09916402 a.u.



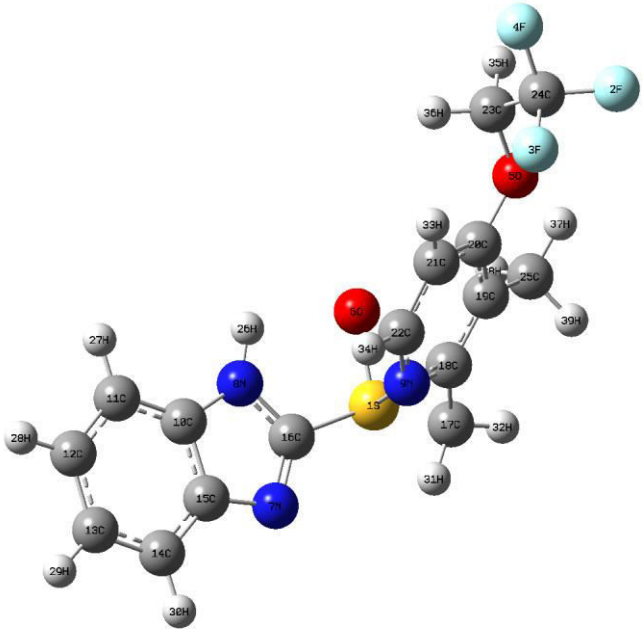
Conformer 5
D1= -63.52218°, D2= 118.31458°
D3= -102.95647°, D4= -96.81477°,
Energy= -1630.09920707a.u.



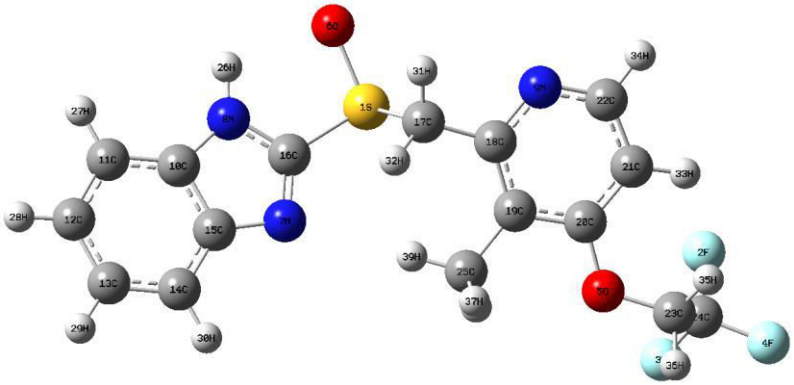
Conformer 6
D1= -146.60983°, D2= -89.17417°
D3= -88.51772°, D4= 99.01331°,
Energy= -1630.10140877 a.u.



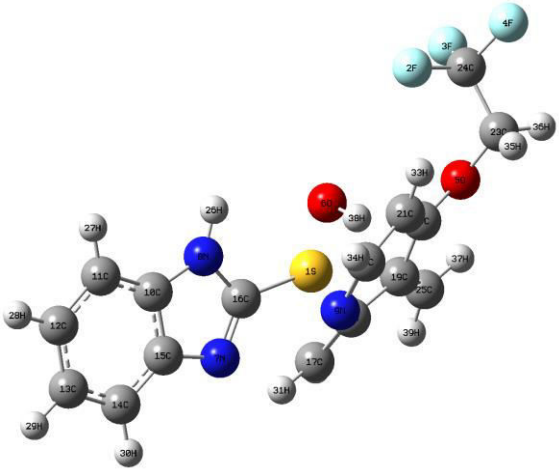
Conformer 7
D1= -69.30829°, D2= -76.32036°
D3= -83.04116°, D4= 99.94559°,
Energy= -1630.10180096 a.u.



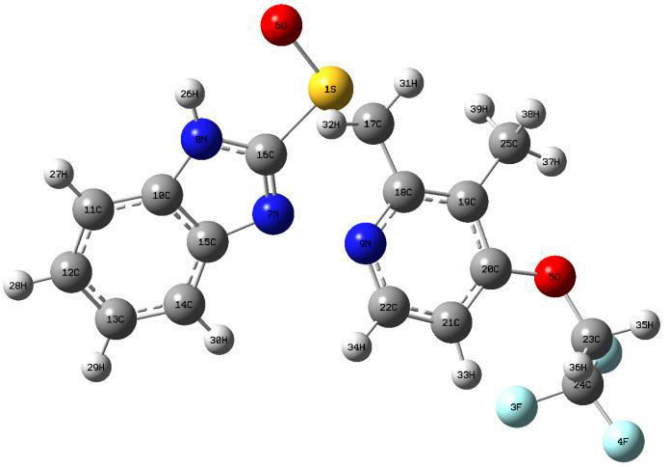
Conformer 8
D1= -60.99464°, D2= 135.08909°
D3= -86.30392°, D4= -94.99218°,
Energy= -1630.09907528 a.u.



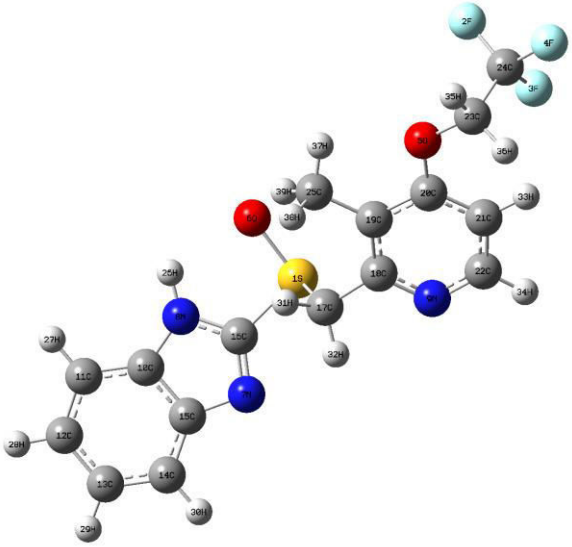
Conformer 9
D1= -84.47611°, D2= -130.29230°
D3= -27.27487°, D4= -94.47761°
Energy= -1630.08687659 a.u.



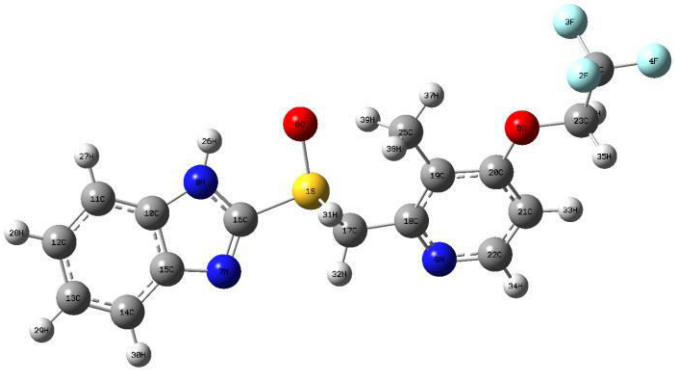
Conformer 10
D1= -82.66247°, D2= 61.00618°
D3= 79.43098°, D4= 96.32184°
Energy= -1630.09707468 a.u.



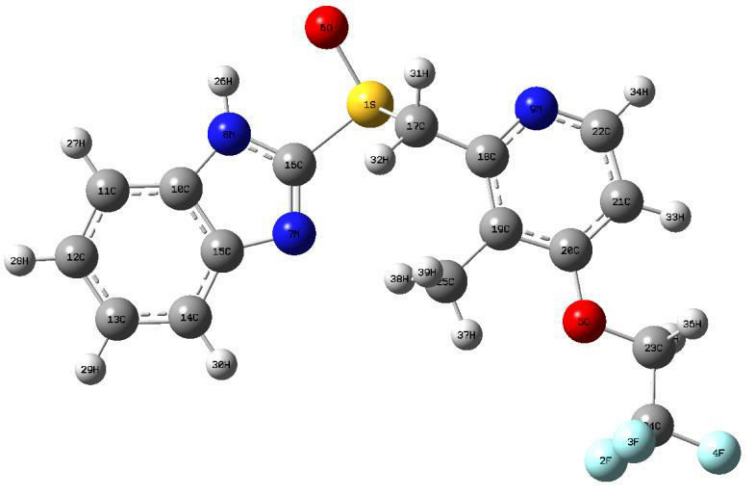
Conformer 11
D1= -65.61287°, D2= 173.55014°
D3= 88.70853°, D4= 96.07098°
Energy= -1630.10167194 a.u.



Conformer 12
D1= -66.03562°, D2= 174.01252°
D3= 89.40534°, D4= 179.55037°
Energy= -1630.10162461 a.u.



Conformer 13
D1= -63.81090°, D2= 117.57720°
D3= -103.43550°, D4= 179.62235°,
Energy= -1630.09916404 a.u.



Conformer 14
D1= -71.67822°, D2= -86.09530°
D3= 90.36915°, D4= 90.78730°
Energy= -1630.09670008 a.u.

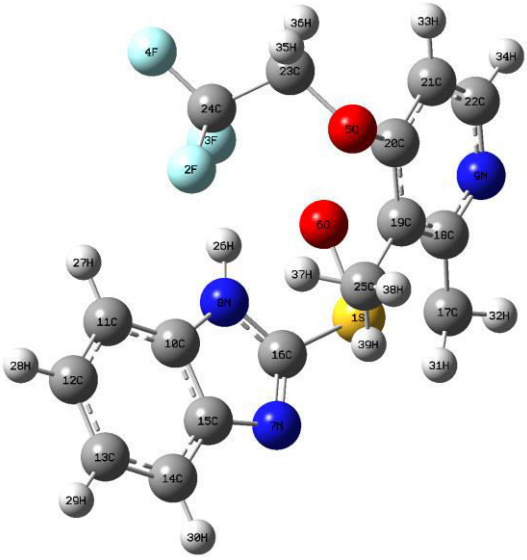


Fig. S5: Various possible conformers of LSP based on potential energy scan results

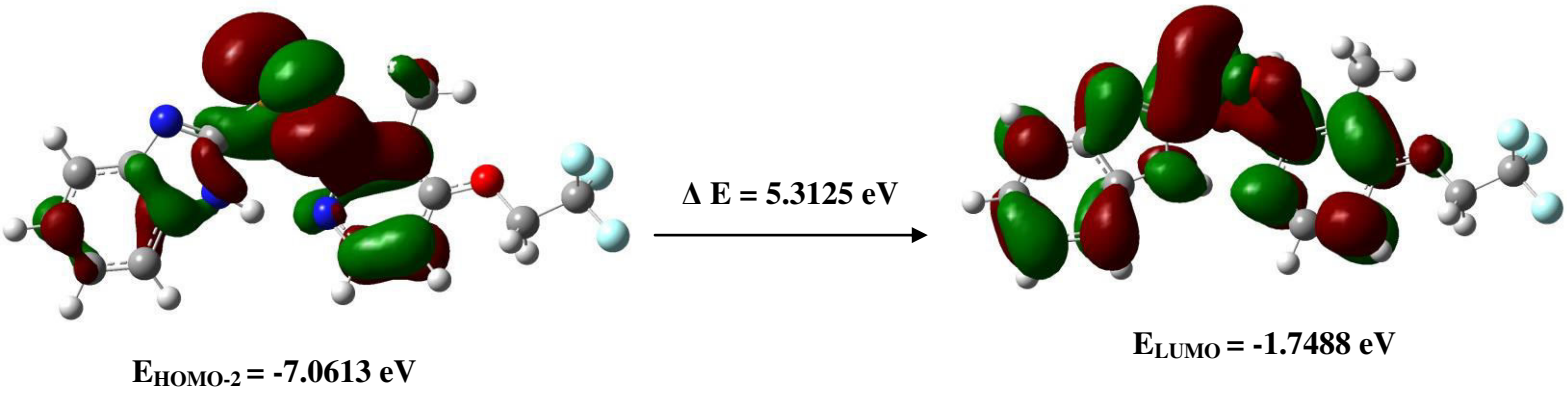


Fig. S6: The atomic orbital composition of the molecular orbitals and the electronic transitions for LSP

Table 1: Optimized geometrical parameters of LSP by DFT with B3LYP/6-311++G(d,p) method in comparison with XRD data.*

Geometrical parameters	Optimized Values	XRD Values	Geometrical Parameters	Optimized Values	XRD Values	Geometrical Parameters	Optimized Values	XRD Values
Bond Length(Å)			**Bond Angles(◦)**			**Dihedral Angles(◦)**		
H27-C11	1.085	0.958	C10-C11-C12	116.756	116.138	C10-C11-C12-C13	0.056	0.219
H28-C12	1.084	0.875	C10-N8-C16	106.017	105.703	C11-C12-C13-C14	0.131	-0.155
H29-C13	1.084	0.990	C10-C15-N7	110.030	110.157	C12-C13-C14-C15	-0.129	-0.791
H30-C14	1.083	0.988	C10-C15-C14	120.142	120.148	C12-C13-C14-H30	179.983	-179.981
C10-C11	1.397	1.399	C10-C11-H27	121.899	119.053	C13-C14-C15-C10	-0.053	1.668
C11-C12	1.388	1.375	C10-N8-H26	129.9079	140.806	C13-C14-C15-N7	179.548	-178.302
C12-C13	1.411	1.393	C11-C12-C13	121.727	122.103	C14-C15-C10-N8	179.939	179.775
C13-C14	1.387	1.368	C11-C12-H28	119.192	121.305	C15-C10-C11-C12	-0.242	0.694
C14-C15	1.400	1.399	C11-C10-C15	122.120	122.3318	C15-C10-C11-H27	179.858	177.743
C10-C15	1.417	1.388	C11-C10-N8	132.736	131.919	C15-N7-C16-N8	-0.182	-0.298
N8-H26	1.027	0.794	C12-C13-C14	121.405	121.516	C15-N7-C16-S1	-176.962	-177.801
N8-C10	1.379	1.370	C12-C13-H29	118.978	119.460	N7-C16-N8-C10	0.354	0.155
N8-C16	1.371	1.345	C13-C14-C15	117.847	117.740	N7-C16-N8-H26	175.589	175.214
N7-C16	1.308	1.304	C13-C14-H30	121.819	119.640	C16-N8-C10-C11	179.290	-178.291
N7-C15	1.385	1.391	C14-C15-N7	129.825	129.694	C16-S1-C17-C18	-90.247	-95.965
C16-S1	1.815	1.787	C14-C13-H29	119.616	118.970	N8-C10-C11-C12	-179.838	178.822
S1-O6	1.513	1.492	C15-N7-C16	104.393	103.055	N8-C10-C11-H27	0.262	-4.127
S1-C17	1.907	1.844	N7-C16-N8	114.415	115.354	C10-C15-N7-C16	-0.059	0.328
C17-H31	1.088	0.955	C16-N8-H26	123.868	113.191	N8-C16-S1-C17	41.584	70.407
C17-H32	1.087	0.932	C16-S1-O6	109.428	107.118	N8-C16-S1-O6	-68.439	-40.521
C17-C18	1.499	1.494	C16-S1-C17	97.536	99.125	S1-C17-C18-C19	-92.058	-93.495
C18-C19	1.401	1.393	S1-C16-N8	125.652	124.475	S1-C17-C18-N9	86.808	85.476
C19-C20	1.407	1.395	S1-C17-C18	112.255	110.760	O6-S1-C17-C18	22.533	15.153
C20-C21	1.394	1.378	S1-C17-H31	106.957	108.675	C17-C18-C19-C20	-179.123	-178.053
C21-C22	1.389	1.385	C17-S1-O6	106.052	106.880	C17-C18-N9-C22	179.478	179.341
C22-N9	1.329	1.325	C17-C18-N9	115.633	114.275	C18-C19-C20-C21	-0.835	-2.446
N9-C18	1.348	1.343	C18-C19-C20	116.574	116.089	C18-C19-C20-O5	179.239	177.213
C22-H34	1.086	0.980	C18-N9-C22	118.389	117.054	C18-N9-C22-C21	-0.044	-0.343
C21-H33	1.081	1.001	C18-C19-C25	122.516	123.314	C18-C19-C25-H39	-61.194	-68.720
C19-C25	1.508	1.503	C18-C17-H31	111.777	109.719	C19-C20-C21-C22	-0.701	0.662

C25-H37	1.087	0.938	C19-C18-N9	123.421	124.379	C19-C20-C21-H33	-179.732	-175.883
C25-H38	1.093	0.925	C19-C25-H37	111.017	113.055	C19-C20-O5-C23	178.154	-175.457
C25-H39	1.094	0.939	C19-C20-O5	116.266	115.380	C20-C21-C22-N9	1.208	0.838
C20-O5	1.363	1.369	C20-C19-C25	120.899	120.590	C20-C21-C22-H34	-178.716	-177.848
O5-C23	1.411	1.410	C20-O5-C23	119.041	117.289	C20-O5-C23-C24	179.617	173.476
C23-H35	1.095	0.976	C20-C21-H33	122.535	122.489	C20-O5-C23-H36	61.505	55.009
C23-H36	1.095	0.872	C21-C22-N9	123.453	124.068	C20-O5-C23-H35	-62.023	-67.102
C23-C24	1.520	1.480	C21-C20-O5	123.474	123.931	C22-N9-C18-C19	-1.685	-1.723
C24-F2	1.343	1.325	O5-C23-H35	111.766	111.901	N9-C18-C19-C25	-176.773	-177.699
C24-F3	1.345	1.317	O5-C23-C24	107.451	106.915	O5-C23-C24-F3	-61.205	-64.116
C24-F4	1.352	1.326	C23-C24-F2	112.327	113.373	O5-C23-C24-F4	179.743	177.719

* K. Vyas, A. Sivalakshmidevi and G. O. Reddy, Cryst. Struct. Commun., 2000, C56, e572-e573

Table S2: Observed and Calculated Normal frequencies of LSP with their Potential Energy Distribution

DFT		**Obs**		
Unscaled	**Scaled**	**Raman**	**IR**	**Assignment (%PED)**
3303	3154		3224	ν(N8H26)(99)
3212	3072	3071		ν(C21H33)(97)
3197	3058		3068	ν(C14H30)(68)+ν(C13H29)(22)+ν(C12H28)(7)
3189	3051			ν(C11H27)(45)+ν(C12H28)(34)+ν(C14H30)(18)
3179	3041			ν(C13H29)(44)+ν(C11H27)(37)+ν(C14H30)(12)+ν(C12H28)(7)
3167	3031			ν(C12H28)(51)+ν(C13H29)(30)+ν(C11H27)(14)
3159	3024			ν(C22H34)(70)+ν(C17H32)(16)+ν(C17H31)(12)
3158	3023			ν(C17H32)(40)+ν(C17H31)(31)+ν(C22H34)(27)
3150	3016	2986	2986	ν(C25H37)(89)+ν(C25H38)(7)
3098	2969	2969		ν(C17H31)(56)+ν(C17H32)(42)
3089	2961		2955	ν(C25H38)(65)+ν(C25H39)(32)
3085	2957	2932	2932	ν(C23H35)(52)+ν(C23H36)(47)
3033	2909			ν(C25H39)(62)+ν(C25H38)(24)+ν(C25H37)(7)
3032	2909			ν(C23H36)(49)+ν(C23H35)(44)+ν(C25H39)(5)
1656	1626			ν(C10C11)(21)+ν(C13C14)(13)+ν(C14C15)(13)+ν(C11C12)(8)+ν(N8C10)(7)+δ_{asym}(ring1)(6)+δin(C14H30)(5)+ δin(C11H27)(5)+δ'(ring3)(5)
1622	1593	1584	1580	ν(N9C22)(19)+ν(C19C20)(18)+ν(C21C22)(12)+δin(C22H34)(10)+ν(C18C19)(6)+ δ'_{asym}(ring2)(5)
1616	1588			ν(C12C13)(15)+ν(C10C15)(15)+ν(C14C15)(13)+ν(C11C12)(8)+δin(C12H28)(7)+ν(C10C11)(7)
1611	1583			ν(C20C21)(26)+ν(C18C19)(13)+ν(C21C22)(12)+ν(N9C18)(11)+δin(C21H33)(9)+δ_{asym}(ring2)(6)+ δ'_{asym}(ring2)(5)
1536	1511			δ_{in}(N8H26)(27)+δ_{in}(C13H29)(17)+ν(C11C12)(11)+ν(C13C14)(9)+ν(C14C15)(6)
1511	1487	1495		$\delta'_{asym}(C25H_3)$(33)+δ_{in}(C22H34)(13)+δ_{in}(C21H33)(8)+$S(C23H_2)$(7)+ν(C19C20)(7)+ν(N9C22)(5)
1505	1482		1475	$\delta'_{asym}(C25H_3)$(17)+ν(N7C16)(15)+$S(C23H_2)$(9)+ $\delta_{asym}(C25H_3)$(9)+(C10C11)(8)+ν(C13C14)(6)+δ_{in}(C12H28)(5)
1504	1480			$\delta'_{asym}(C25H_3)$(14)+ν(N7C16)(14)+$S(C23H_2)$(13)+ $\delta_{asym}(C25H_3)$(12)+ ν(C10C11)(7)+ν(C13C14)(5)

1498	1474			S($C23H_2$)(45)+ δ_{asym}($C25H_3$)(41)
1487	1464	1468		S($C23H_2$)(24)+ δ_{asym}($C25H_3$)(15)+ δ'_{asym}($C25H_3$)(9)+δ_{in}(C21H33)(9)+ S($C17H_2$)(7)+ν(C19C20)(6)
1476	1453		1456	S($C17H_2$)(61)+ν(C17C18)(8)+ν(C18C19)(7)
1461	1439	1436		ν(N7C16)(38)+ν(N8C16)(16)+δ_{in}(C12H28)(9)+δ_{in}(N8H26)(9)+δ_{in}(C11H27)(5)
1449	1427			δ_{in}(N8H26)(17)+δ_{in}(C14H30)(13)+ν(C11C12)(7)+ν(C10C15)(7)+ν(C14C15)(5)+δ_{in}(C13H29)(5)+δ_{in}(C22H34)(5)
1440	1419			ω($C23H_2$)(58)+ν(C23C24)(15)
1438	1417			ν(C18C19)(14)+S($C17H_2$)(13)+δ_{in}(C22H34)(12)+δ_{in}(N8H26)(6)+ω($C23H_2$)(6) +δ'_{asym}($C25H_3$)(6)+ν(N9C18)(5)
1411	1391	1402	1402	δ_{sym} ($C25H_3$)(85)+ν(C19C25)(7)
1383	1364	1362		ν(C12C13)(17)+ν(C14C15)(13)+ν(C10C15)(10)+ν(C13C14)(10)+ν(C10C11)(8)+ν(N 8C16)(7)+δ_{in}(C12H28)(7)+ν(C11C12)(7)+δ_{in}(C13H29)(6)+δ'(ring3)(5)
1329	1312	1308	1310	ν(O5C20)(22)+ν(N9C22)(18)+ν(C20C21)(12)+δ_{tri}(ring2)(9)+ν(C18C19)(5)+ ν(N9C18)(5)+δ_{in}(C21H33)(5)
1319	1302		1300	δ_{in}(C11H27)(21)+ν(N8C10)(13)+ν(C11C12)(11)+δ_{in}(C13H29)(10)+ δ_{in}(C12H28)(7)+ δ_{tri}(ring1)(7)+δ_{in}(C14H30)(6)
1307	1290			(N9C22)(19)+ν(C21C22)(12)+ν(C19C20)(11)+δ_{in}(C22H34)(9)+ν(O5C20)(8)+ν_{asym}(F 2C24)(5)+t($C23H_2$)(5)
1306	1289		1283	t($C23H_2$)(60)+ν_{asym}(F3C24)(13)+ν(F2C24)(9)
1290	1274	1272		ν(N7C15)(21)+ν(N8C10)(15)+ν(C10C15)(14)+ν(C13C14)(11)+ δ_{in}(C14H30)(10)+δ_{in}(C13H29)(6)+ δ(ring3)(6)+ν(C11C12)(6)
1284	1268		1265	ν(N9C18)(24)+δ_{in}(C22H34)(17)+ν_{asym}(C17C18)(10)+t($C17H_2$)(9)+ν(C19C20)(7)+ν(C20C21)(7)
1265	1250		1252	ν(C23C24)(18)+ δ_{sym}($C24F_3$)(18)+ω($C23H_2$)(14)+ν_{asym}(F3C24)(10) +ν_{asym}(F2C24)(10)+ν(O5C20)(9)
1252	1238			ω($C17H_2$)(29)+ν(N7C15)(18)+ν(C10C11)(6)+ δ_{tri}(ring1)(5)+δin(C14H30)(5)
1245	1231	1229		ω($C17H_2$)(40)+ν(N7C15)(13)+ δ_{tri}(ring1)(7)
1211	1197	1196	1198	ν(C19C25)(28)+ δ_{tri}(ring2)(18)+δin(C21H33)(18)+ν(C20C21)(11)
1203	1190			ν(N8C16)(37)+δ_{in}(N8H26)(11)+ν(N8C10)(10)+ν(S1C16)(7)+δ_{in}(C12H28)(6)+δ_{tri} (ring1)(5)

1176	1164	1162	1163	t($C17H_2$)(30)+ω($C17H_2$)(10)+ν(O5C23)(8)+δ_{in}(C21H33)(7)+ δ_{tri}(ring2)(6)+ρ($C25H_3$)(6)
1171	1159			ρ($C23H_2$)(27)+ν(F2C24)(21)+ν_{asym}(F3C24)(20)+t($C23H_2$)(14)+ δ'_{asym}($C24F_3$)(7)+ρ($C24F_3$)(7)
1168	1156			δ_{in}(C12H28)(25)+δ_{in}(C13H29)(18)+δ_{in}(C11H27)(13)+ν(C12C13)(10)+δ_{in}(C14H30)(9)+ν(N8C10)(5)+ν(N7C15)(5)
1148	1137	1142		ν(F4C24)(55)+ δ_{asym}($C24F_3$)(12)+ν_{asym}(F3C24)(7)+ρ'($C24F_3$)(6) +ν_{asym}(F2C24)(6)+S(C23C24O5)(6)
1135	1124			δ_{in}(C13H29)(16)+δ_{in}(C14H30)(15)+ν(C13C14)(14)+ν(C11C12)(13)+ δ_{tri} (ring1)(12)+δ_{in}(C11H27)(9)+δ_{in}(C12H28)(8)
1132	1121	1115	1117	ν(O5C23)(35)+ν(C21C22)(9)+δ_{in}(C21H33)(9)+ν(C17C18)(7)+δ_{in}(O5C20)(6)+t(C17 H_2)(5)
1098	1088	1086	1088	t($C17H_2$)(37)+ν(N9C18)(13)+ν(C21C22)(11)+ν(N9C22)(6)+δ_{in}(C21H33)(6)+ δ_{tri} (ring2)(5)+δ_{in}(C17C18)(5)
1058	1049			ρ($C25H_3$)(38)+ν(O5C23)(27)+ν_{asym}(C17C18)(6)+ν(O5C20)(5)
1055	1046		1038	ρ'($C25H_3$)(73)+ω(C19C25)(9)+ δ_{asym}($C25H_3$)(6)+ δ_{puck}(ring2)(5)
1031	1022	1046		ν(S1O6)(88)
1026	1018	1008	1003	ν(C12C13)(40)+ν(C13C14)(12)+δ_{in}(C14H30)(12)+ν(C11C12)(12)+δ_{in}(C11H27)(11)
981	974		970	ρ($C23H_2$)(44)+ν_{asym}(F2C24)(20)+ν(F3C24)(20)+t($C23H_2$)(5)
976	969	965		ω(C13H29)(38)+ω(C12H28)(25)+ω(C14H30)(19)+ δ_{puck}(ring1)(10)+ω(C11H27)(5)
970	963			δ(ring3)(40)+δ'(ring3)(19)+ν(C10C15)(11)+ν(S1C16)(8)+ν(N8C16)(7)
962	955			ω(C22H34)(69)+ω(C21H33)(16)+ δ_{puck} (ring2)(6)
944	938			ω(C12H28)(31)+ω(C14H30)(30)+ω(C11H27)(25)+τ'_{asym}(ring1)(7)+ω(C13H29)(5)
933	927	923	922	ρ($C25H_3$)(21)+ν(C17C18)(11)+ν(O5C20)(10)+ν(C19C20)(7)+ρ($C17H_2$)(7)+ν(C18C1 9)(7)+ν(O5C23)(5)+ν(C20C21)(5)
907	901	897		δ_{tri}(ring1)(56)+ν(N7C15)(8)+δ'(ring3)(8)+ν(N8C10)(6)+δ_{asym}(ring1)(6)
881	876	880		ρ($C17H_2$)(67)+τ(S1C17)(6)
858	853	859	858	ν(C23C24)(19)+ν(F3C24)(17)+ν(F2C24)(16)+S(C23C24O5)(8)+δ(C20O5C23)(7)+δ_{t} $_{ri}$(ring2)(5)+ν(C17C18)(5)
855	850			ω(C11H27)(34)+ω(C14H30)(24)+ω(C13H29)(15)+ δ_{puck}(ring1)(10)+τ_{asym}(ring1)(5)
850	846	842	841	δ_{tri}(ring2)(26)+δ'_{asym}(ring2)(16)+ν(C19C25)(12)+δ_{asym}(ring2)(7)

821	817		814	ω(C21H33)(52)+ δ_{puck}(ring2)(17)+ω(O5C20)(13)+ω(C22H34)(6)
814	811			ν(C10C15)(19)+ν(C14C15)(16)+ν(C10C11)(16)+δ'_{asym}(ring1)(10)+ ν(N8C10)(8)+ν(N7C15)(6)+ν(S1C16)(5)
810	807	803	800	ω(N8H26)(65)+ δ_{puck}(ring2)(8)
784	781			δ_{puck}(ring2)(37)+ω(C17C18)(20)+ω(C22H34)(8)+ω(C19C25)(6)+S(C17C18S1)(6)
772	769	774	768	δ_{puck}(ring1)(46)+τ(ring3)(28)+ω(C12H28)(10)+ω(N8H26)(5)
752	749		748	ω(C13H29)(27)+ω(C11H27)(18)+ω(C12H28)(16)+ω(C14H30)(11)+ δ_{puck}(ring1)(10)+τ'(ring3)(7)
742	739	739		δ_{puck}(ring2)(17)+ν(C19C25)(9)+δ(C20O5C23)(6)+ν_{asym}(C17C18)(6)+ν(C18C19)(6)+ ν(C20C21)(5)+ν(F4C24)(5)+ω(O5C20)(5)+δ_{sym}($C24F_3$)(5)
682	681	676	677	ω(O5C20)(23)+S(C17C18S1)(8)+δ_{puck}(ring2)(8)+τ'(ring3)(8)+ω(C17C18)(6)+ω(S1O 6)(6)+τ_{asym}(ring2)(6)
676	674			τ'(ring3)(33)+ω(N8H26)(15)+ω(S1C16)(14)+τ(ring3)(13)
649	648	658	658	δ_{sym}($C24F_3$)(26)+ω(O5C20)(9)+ν(S1C17)(8)+ω(C17C18)(6)+ν(F4C24)(6)+δ_{asym} (ring2)(5)+S(C23C24O5)(5)+ν(C19C25)(5)
630	629		636	δ'(ring3)(31)+δ_{asym}(ring1)(22)+δ(ring3)(13)+δ'_{asym}(ring1)(12)+ν(C14C15)(8)+ν(C10 C11)(8)
598	597	608	615	δ'_{asym}(ring1)(19)+ν(S1C17)(17)+ δ'_{asym}(ring2)(12)+ δ_{asym} (ring1)(7)+ δ_{asym} (ring2)(7)+ν(S1C16)(6)
589	589	589		δ'_{asym}(ring1)(20)+ δ_{asym}(ring1)(12)+ δ'_{asym} (ring2)(10)+ν(S1C17)(8)+ω(S1O6)(8)+ δ_{asym}(ring2)(6)+ν(S1C16)(5)
583	583			δ_{puck}(ring1)(30)+τ_{asym}(ring1)(21)+τ'(ring3)(13)+τ(ring3)(6)+τ'_{asym}(ring1)(6)+ω(C13H 29)(5)
576	575		577	δ_{asym} ($C24F_3$)(19)+δ_{in}(O5C20)(13)+ δ_{asym}(ring2)(10)+ δsym($C24F_3$)(9)+ δ(C20O5C23)(8)+ρ'($C24F_3$)(6)
563	562	566	565	τ_{asym}(ring2)(21)+ω(O5C20)(15)+ν(S1C17)(15)+ δ_{puck}(ring2)(10)+ τ'_{asym} (ring2)(7)+ω(C19C25)(6)+S(C17C18S1)(5)
533	533	529	528	δ'_{asym}($C24F_3$)(30)+ δ_{asym}(ring2)(15)+ δ_{asym}($C24F_3$)(8)
532	532			δ'_{asym}($C24F_3$)(40)+ δ_{asym}(ring2)(11)+ δ_{asym}($C24F_3$)(6)
511	512	512	513	δ_{in}(C17C18)(12)+ δ_{asym}($C24F_3$)(11)+δ_{in}(C19C25)(11)+δ_{in}(O5C20)(10)+ τ(S1C17)(8)+ δ'_{asym}(ring2)(8)+ρ($C17H_2$)(7)

505	505			δ_{in}(S1C16)(17)+ω(S1O6)(14)+ δ_{asym}(ring1)(9)+ δ_{asym}(C24F_3)(9)+ δ'_{asym}(ring1)(8
488	488	494	492	τ'_{asym}(ring2)(29)+ν(S1C17)(18)+ω(C19C25)(15)+ω(C17C18)(8)+ δ'_{asym}(ring2)(5)
444	444	448	447	τ'_{asym}(ring1)(28)+τ(C10C15)(25)+τ_{asym}(ring1)(15)+δ(C16S1C17)(5)+ω(S1O6)(5)
413	414			ω(S1O6)(29)+ τ'_{asym}(ring1)(16)+ν(S1C16)(9)+δ_{asym}(ring1)(9)
408	409	408	415	δ_{in}(C19C25)(16)+ δ_{asym}(C24F_3)(15)+ρ'(C24F_3)(14)+δ_{in}(C17C18)(7)+ τ(S1C17)(5)+δ(C20O5C23)(5)+ρ(C24F_3)(5)
382	383	394	403	ρ(S1O6)(17)+τ(S1C17)(9)+ω(S1O6)(7)+ω(C19C25)(6)+δ_{in}(C17C18)(5)+ δ_{in}(C19C25)(5)+ τ'_{asym}(ring2)(5)
371	372			δ(C16S1C17)(30)+τ(S1C17)(25)+δ_{in}(C17C18)(9)+τ(C17C18)(6)+δ_{in}(C19C25)(5)+ τ'_{asym}(ring1)(5)
364	365			ρ(C24F_3)(50)+ρ'(C24F_3)(18)+δ'_{asym}(C24F_3)(16)+ρ(C23H_2)(6)
331	332			ν(S1C16)(17)+δ_{in}(C17C18)(15)+τ'_{asym}(ring1)(11)+τ(C10C15)(8)+δ_{in}(C19C25)(8)+δ(C16S1C17)(6)+ω(S1C16)(6)+τ(S1C17)(5)+ ω(S1O6)(5)
294	295			ω(C19C25)(29)+ω(O5C20)(13)+ω(C17C18)(10)+ω(C21H33)(6)+ω(S1O6)(6)+ τ(O5C20)(6)+τ'_{asym}(ring2)(5)
266	267	271		δ_{in}(C19C25)(17)+ρ'(C24F_3)(16)+δ_{in}(O5C20)(8)+ν(O5C23)(7)+ δ_{asym}(C24F_3)(5)+ ρ(C24F_3)(5)
258	259	250		τ_{asym}(ring1)(35)+τ(C10C15)(16)+ω(N8H26)(14)+τ'(ring3)(10)+τ(ring3)(6)+τ(S1C16)(6)+ τ'_{asym}(ring1)(6)+δ_{puck}(ring1)(5
238	239			τ_{asym}(ring2)(27)+ω(S1O6)(10)+ τ'_{asym}(ring2)(9)+δ(C16S1C17)(5)
213	214	215		ρ(S1O6)(33)+τ(C10C15)(11)+ν(S1C16)(9)+ τ_{asym}(ring2)(7)+ω(S1C16)(6)
205	206			S(C23C24O5)(16)+δ(C20O5C23)(11)+τ(S1C17)(11)+ρ'(C24F_3)(9)+δ_{in}(O5C20)(8)+ν(C23C24)(6)+τ(C10C15)(5)
180	181	184		δ(C16S1C17)(39)+ω(S1O6)(14)+δ_{in}(S1C16)(12)+τ(C10C15)(9)
153	154			τ(O5C20)(30)+τ(C23C24)(26)+ τ'_{asym}(ring2)(10)+ τ_{asym}(ring2)(5)+τ(O5C23)(5
130	131			τ(S1C17)(26)+δ_{in}(S1C16)(21)+δ(C16S1C17)(9)
117	118			τ(S1C17)(19)+S(C17C18S1)(16)+ω(S1O6)(9)+τ(C23C24)(9)+ τ'_{asym} (ring2)(6)+δ_{in}(S1C16)(5)+ τ_{asym}(ring2)(5
113	113			τ(C19C25)(76)
87	87			S(C23C24O5)(15)+ω(S1C16)(12)+δ(C20O5C23)(9)+δ_{in}(S1C16)(9)+ω(S1O6)(8)+ τ(C17C18)(6)+τ(C10C15)(6)+τ(S1C17)(5)

67	67			τ(S1C17)(24)+τ(S1C16)(16)+S(C17C18S1)(10)+ω(S1C16)(7)+δ(C16S1C17)(5)+ω(S1O6)(5)
64	65			ω(N8H26)(24)+τ(S1C16)(13)+τ(C19C25)(8)+ω(S1C16)(7)+δ(C16S1C17)(6)+τ(O5C23)(6)+asymτ'(ring2)(5
54	54			τ(S1C16)(30)+ω(N8H26)(24)+τ(C17C18)(16)+τ(O5C23)(8)
44	44			τ(S1C16)(32)+ω(N8H26)(24)+τ(O5C23)(10)+τ(O5C20)(7)+τ(C17C18)(6)+S(C17C18S1)(5)
38	38			τ(C23C24)(23)+τ(S1C16)(20)+τ(O5C20)(19)+ω(N8H26)(11)+τ(O5C23)(6)+τ(S1C17)(5
27	27			τ(S1C17)(37)+τ(S1C16)(19)+τ(O5C23)(14)+τ(O5C20)(10)+S(C17C18S1)(6)
14	15			τ(S1C16)(30)+τ(S1C17)(29)+τ(C17C18)(13)+τ(O5C20)(6)+τ(O5C23)(5)+δ(C16S1C17)(5)

Note: All wavenumbers are in cm^{-1}. Vibrations with PED contribution ≥ 5 are included. Types of vibration: ν_{sym}, ν_{asym} symmetric and asymmetric stretching; δ, deformation; δ_{sym}, δ_{asym}, δ'_{asym}, symmetric, asymmetric and asymmetric' deformation; δ_{in}, δ_{oop} in plane and out of plane bending; ω wagging; δ_{sciss}, scissoring; ρ, ρ' rocking and rocking'; τ, torsion; τ_{asym} , τ'_{asym} asymmetric and asymmetric' torsion; δ_{tri}, trigonal deformation; and δ_{puck}, Puckring.

Table S3: Calculated absorption wavelength, energy and oscillator strength of electronic transition in LSP in gas phase and solvent

	Excitation Transition		λ (nm)		E(ev)	Oscillator strength (f)	Transition type/ assignments
			Exp[a]	Cal			
Gas Phase	93→96	H-2→L	-	286.79	4.3232	0.0373	π→π*
Ethanol	93→96	H-2→L	284	287.10	4.3185	0.0794	π→π*

Table S4: Comparison between calculated and experimental ^{1}H NMR chemical shifts (ppm) for LSP

Atom no.	Chemical Shifts (ppm)		Atom no.	Chemical Shifts (ppm)	
	Cal	Exp		Cal	Exp
H(26)	13.281	11.882	H(33)	6.464	6.659
H(27)	7.595	7.264-7.797	H(34)	8.68	8.343
H(28)	7.453		H(35)	4.111	4.315-4.393
H(29)	7.372		H(36)	4.117	
H(30)	7.960		H(37)	3.051	2.196
H(31)	4.278	4.721-4.864	H(38)	2.372	
H(32)	4.543		H(39)	1.849	