Stark spectroscopy of Lumichrome - a possible candidate for stand-off detection of bacterial quorum sensing.

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Supporting Information

Table S1. Molecular geometry of Lumichrome optimized in the gas phase at the B3LYP/6-311+G(2d,p) level of theory using Gaussian16. A frequency calculation was conducted to verify that the optimized geometry is a minimum on the nuclear geometry potential energy surface. Coordinates are in angstroms.

Atom	X	Y	Z
C	3.908134	2.988834	0.000000
C	2.547934	2.345093	0.000000
C	1.366475	3.162481	0.000000
C	0.133851	2.560858	0.000000
C	0.000000	1.152087	0.000000
C	1.175041	0.340892	0.000000
C	2.435675	0.974576	0.000000
H	3.317287	0.344753	0.000000
N	1.088214	-1.011596	0.000000
C	-0.120409	-1.520622	0.000000
N	-0.245437	-2.897479	0.000000
C	-1.440517	-3.585008	0.000000
N	-2.567694	-2.770965	0.000000
C	-2.636550	-1.376029	0.000000
C	-1.299000	-0.716646	0.000000
N	-1.228572	0.592992	0.000000
O	-3.699264	-0.802759	0.000000
H	-3.451816	-3.263606	0.000000
O	-1.508489	-4.794555	0.000000
H	0.597983	-3.454754	0.000000
H	-0.777180	3.147367	0.000000
C	1.481644	4.664027	0.000000
H	2.024281	5.025421	0.878275
H	0.496142	5.129128	0.000000
H	2.024281	5.025421	-0.878275
H	4.047148	3.626584	-0.877668
H	4.697515	2.237690	0.000000
H	4.047148	3.626584	0.877668

Table S2. Molecular geometry of Lumiflavin optimized in the gas phase at the B3LYP/6-311+G(2d,p) level of theory using Gaussian16. A frequency calculation was conducted to verify that the optimized geometry is a minimum on the nuclear geometry potential energy surface. Coordinates are in angstroms.

Atom	X	Y	Z
C	-0.039452	0.000000	0.004482
C	2.070364	-0.000148	-1.916940
C	4.650650	-0.000178	-1.143382
C	5.320818	-0.000083	1.627970
H	4.543741	1.663658	2.592499
H	4.543930	-1.663882	2.592558
H	7.368622	0.000034	1.910397
C	6.577083	-0.000304	-2.941022
C	6.033327	-0.000413	-5.541686
C	3.466394	-0.000379	-6.322184
C	1.539611	-0.000249	-4.480369
H	-0.395867	-0.000231	-5.164934
N	2.798667	-0.000458	-8.820730
C	4.583776	-0.000594	-10.506800
C	7.287552	-0.000652	-9.925361
N	7.902593	-0.000533	-7.382632
C	10.577272	-0.000528	-6.639793
H	10.993135	-1.690684	-5.523249
H	10.993152	1.689686	-5.523345
H	11.708303	-0.000589	-8.355484
N	9.106723	-0.000722	-11.599637
C	8.523321	-0.000693	-14.143567
N	5.938596	-0.000584	-14.833383
C	3.864879	-0.000914	-13.248821
O	1.696205	-0.000364	-14.027161
H	5.583823	-0.000450	-16.719859
O	10.117677	-0.000711	-15.810672
H	8.520417	-0.000321	-2.294477
H	0.045121	1.666263	1.237181
H	-1.884347	-0.000144	-0.927904
H	0.045206	-1.665991	1.237539

Table S3. First 10 excited states of gas phase Lumichrome calculated at the B3LYP/6-311+G(2d,p) level of theory using Gaussian16.

Excited State	Wavelength (nm)	Oscillator Strength
1	367.00	0.0649
2	362.79	0.0011
3	321.84	0.2235
4	311.12	0.0001
5	258.57	0.0290
6	254.38	0.0000
7	250.81	0.0000
8	248.89	0.2674
9	243.26	0.0000
10	240.99	0.2555

Table S4. First 10 excited states of gas phase Lumiflavin calculated at the B3LYP/6-311+G(2d,p) level of theory using Gaussian16.

Excited State	Wavelength (nm)	Oscillator Strength
1	412.92	0.1993
2	391.09	0.0003
3	373.81	0.0003
4	325.27	0.1464
5	315.72	0.0000
6	306.18	0.0110
7	268.28	0.0002
8	264.81	0.0936
9	256.45	0.5767
10	249.32	0.0329

Table S5. Transition dipole moments ($\vec{m}$) and difference permanent dipole moments ($\Delta\vec{\mu}$) of the two lowest experimentally-measurable electronic transitions of gas phase Lumichrome and Lumiflavin calculated at the B3LYP/6-311+G(2d,p) level of theory using Gaussian16. Vector components are given in the above standard orientation. The finite field method was used to compute the difference permanent dipole moments. Coordinates are in units of Debye.

Compound	Transition	Vector	X	Y	Z
Lumichrome	S_{10}	$\vec{m}$	-0.83	0.29	0.00
		$\Delta\vec{\mu}$	-1.43	1.22	0.00
	S_{30}	$\vec{m}$	-1.44	-0.53	0.00
		$\Delta\vec{\mu}$	-5.36	-0.26	0.00
Lumiflavin	S_{10}	$\vec{m}$	-1.58	-0.47	0.00
		$\Delta\vec{\mu}$	-1.17	1.33	0.00
	S_{40}	$\vec{m}$	-1.25	0.10	0.00
		$\Delta\vec{\mu}$	-4.15	1.22	0.00

Figure S1. Standard Orientations of Lumichrome and Lumiflavin

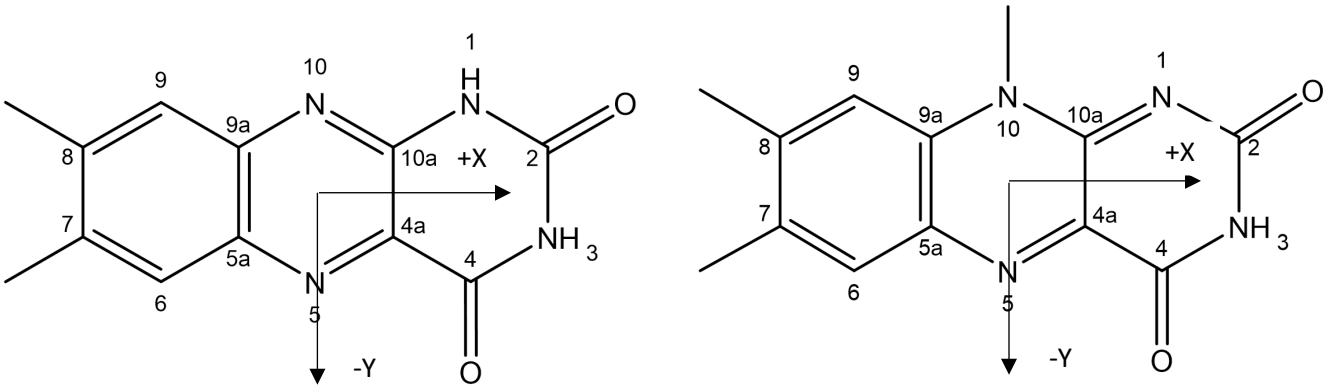

Figure S2. Possible orientations of the experimentally measured difference permanent dipole moments of the lumichrome S_{10} (red) and S_{30} (blue) transitions, relative to the theoretically determined transition dipole moments. In these figures, the solid lines represent the difference permanent dipole moment possibilities and the dotted line represent the transition dipole moment possibilities.