

Supporting Information

Atomistic modeling of metal-ligand chirality transfer and chiroptical properties of lead and tin hybrid perovskites

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1. Additional simulation details

1.1 Details on the density of states calculations

The densities of states (DOSs) were calculated under periodic boundary conditions including SOC effects and in the cluster models, both including and not accounting for SOC effects. The comparison of the DOSs calculated with periodic conditions and the DOSs calculated for the molecular clusters of lead- and tin- based perovskites are reported in Figures S1 a) and b), respectively.

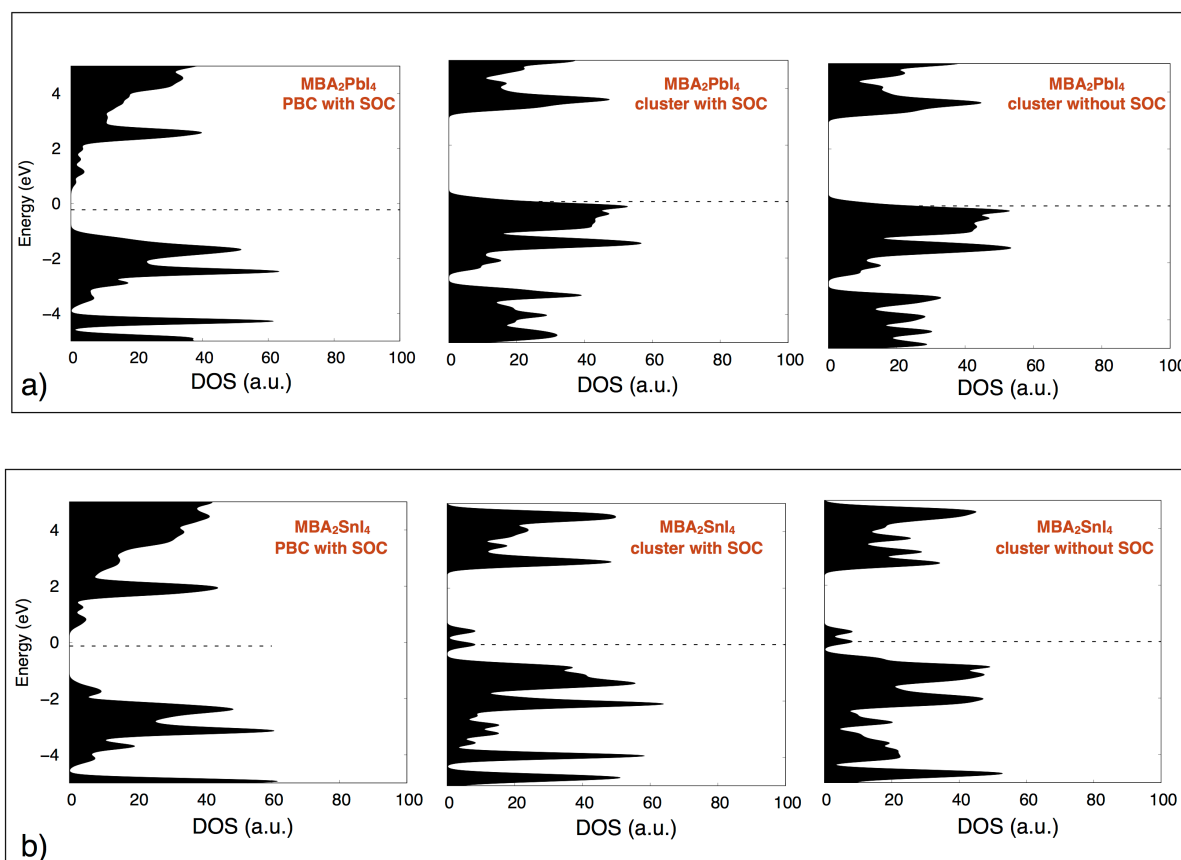


Figure S1. Comparisons between DOSs calculated in periodic conditions accounting SOC effects and DOSs computed for the investigated molecular clusters both including SOC and also not accounting for SOC effects for a) lead- and b) tin- based perovskites.

A convergence test on the vacuum dimension were performed. The DOSs calculated for the molecular clusters of lead- and tin- based perovskites by considering the vacuum values of 12 Å, 14 Å and 16 Å are reported in Figures S2 a) and b), respectively.

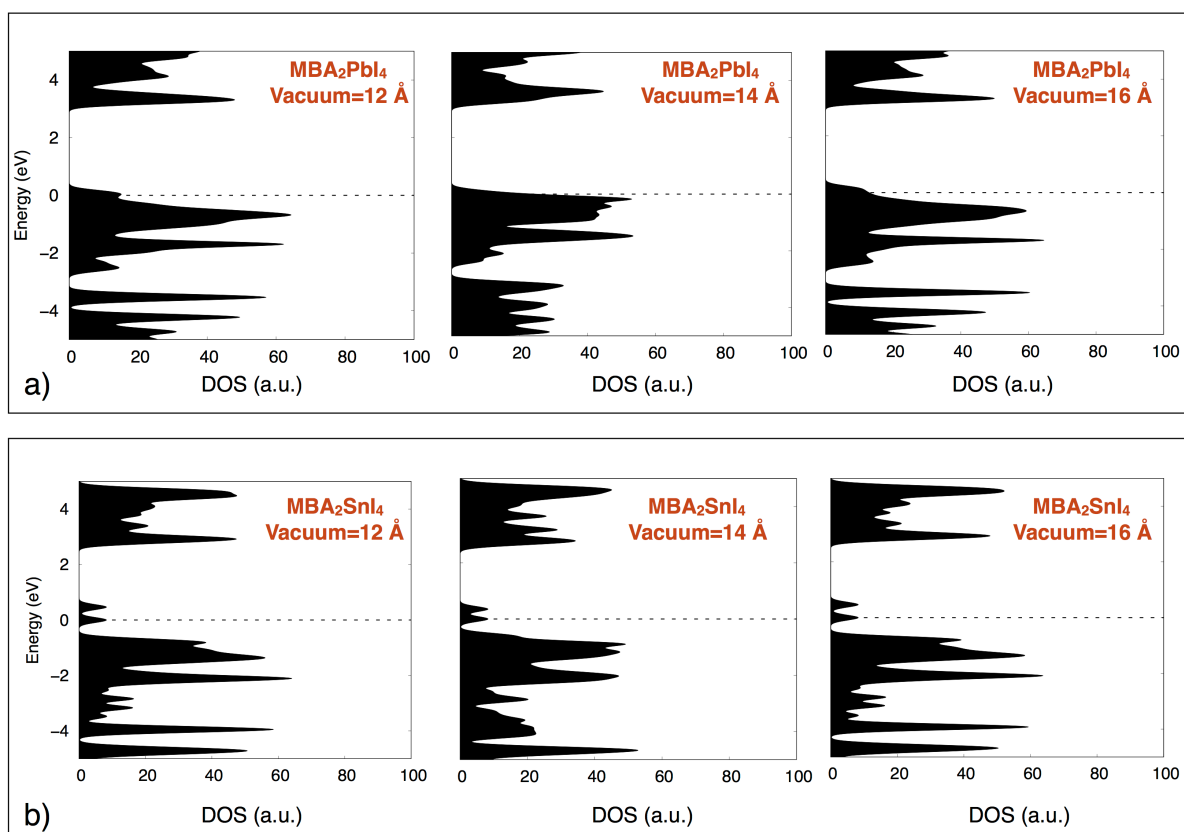


Figure S2. DOSs calculated varying the vacuum values from 12 Å, 14 Å and 16 Å for the molecular clusters of a) lead- and b) tin- based perovskites.

1.2 Energy and temperature evolution plots of the ab-initio trajectories

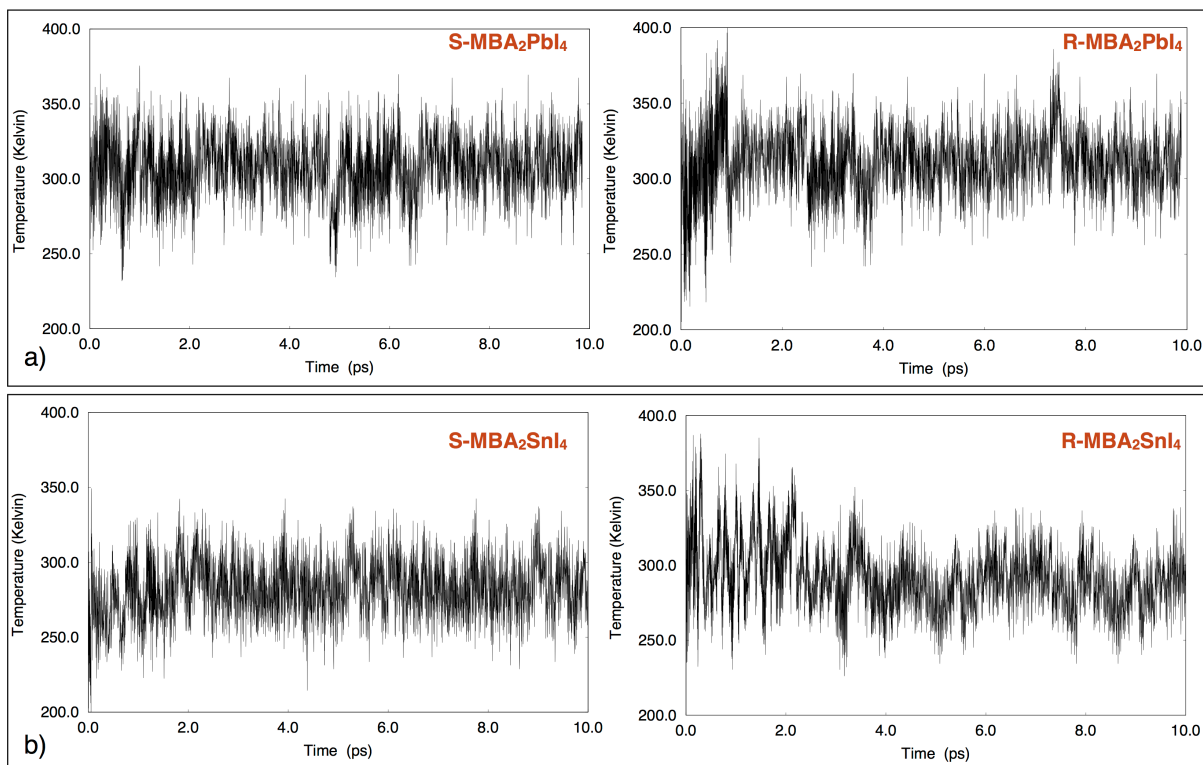


Figure S3. Temperature evolution plots of ab-initio molecular dynamic trajectories computed for a) S- and R- lead-based perovskite models and b) S- and R- tin-based perovskite models.

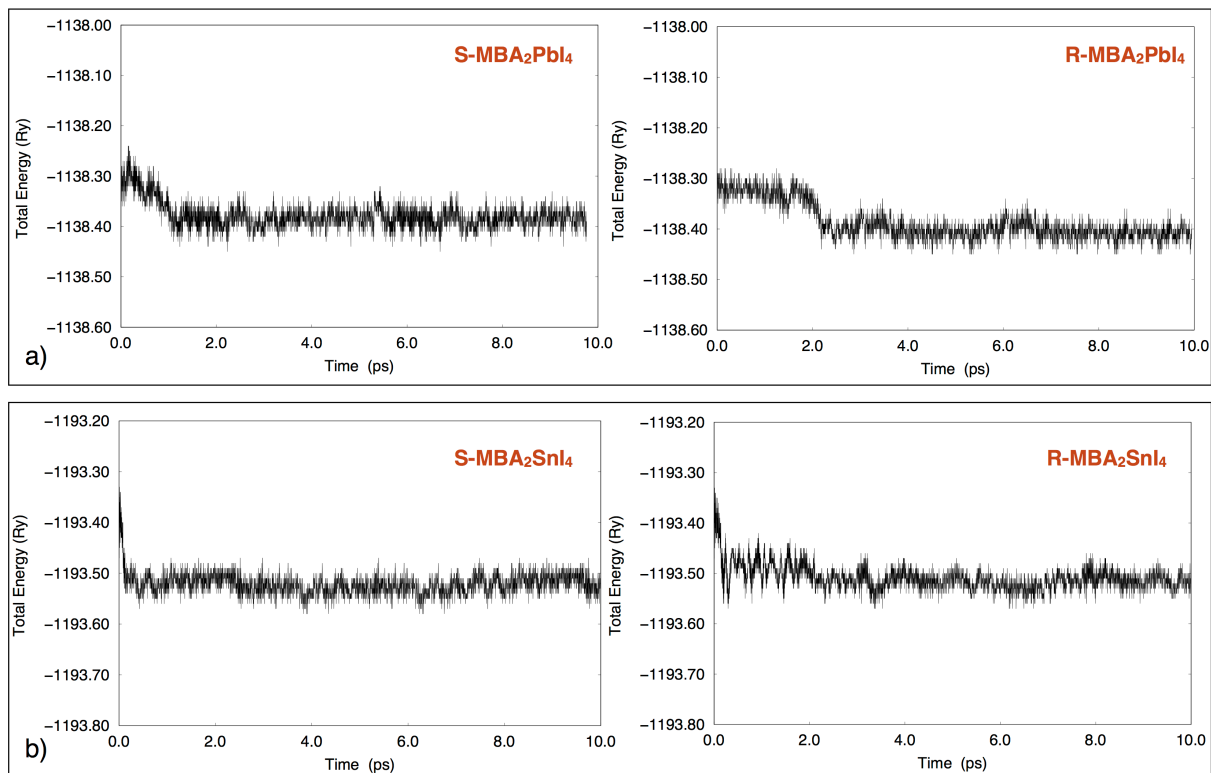


Figure S4. Energy evolution plots of ab-initio molecular dynamic trajectories computed for a) S- and R- lead-based perovskite models and b) S- and R- tin-based perovskite models.

2. Benchmark of the exchange-density functionals

Table S1. Vertical excitation energies (VEE) computed with the benchmarked exchange density functionals compared with the experimental band positions.

S- and R-(MBA ⁺) ₂ PbI ₄ [Experimental band position: 510-550 nm] ¹		S- and R-(MBA ⁺) ₂ SnI ₄ [Experimental band position: 350-600 nm] ²
XC functionals	VEE /nm	VEE /nm
HSE06	417-586	296-1053
HSE06-SOC	416-585	297-1049
LC- ω HPBE	206-267	173-312
ω B97xD	239-297	201-354
cam-B3LYP	263-309	216-416
MN15	309-367	245-505
B97D3	612-966	377-1511

3. Simulations of the ECD spectra

The calculations of the ECD spectra were performed at the HSE06/ LANL2DZ³ level of theory within Gaussian v. 16⁴ by considering the first 100 electronic states for the lead-based coordinates and the first 200 electronic states for the tin-based ones, to compute the vertical excitation energies and the rotatory strengths from the ground to the excited states. Rotatory strengths are reported in the usual c.g.s. units of 10⁻⁴⁰ esu.cm.erg/Gauss.

The electric transition dipole moment μ^{0n} associated with an electronic transition 0 $\rightarrow$ n is given in the dipole-length form⁵ by:

$$\mu_l^{0n} = - \int d^3r \rho^{0n}(\mathbf{r}) \mathbf{r} \quad 1)$$

and in the velocity length formalism⁴ by:

$$\mu_v^{0n} = \frac{1}{i\omega^{0n}} \int d^3r \mathbf{j}^{0n}(\mathbf{r}) \quad 2)$$

The magnetic transition dipole moments m^{0n} are calculated from

$$\mathbf{m}^{0n} = \frac{1}{2c} \int d^3r \mathbf{r} \times \mathbf{j}^{0n}(\mathbf{r}) \quad 3)$$

where $\rho^{0n}(\mathbf{r})$ and $\mathbf{j}^{0n}(\mathbf{r})$ are the changes in charge and current density associated with the nth excitation from the ground state and ω^{0n} are the excitation energies for the specific transition.^{5,6}

The rotatory strengths R^{0n} and the oscillator strengths f^{0n} are related to the transition dipole moment⁵ by equations:^{5,6}

$$R^{0n} = \text{Im}(\mu^{0n} \cdot \mathbf{m}^{0n*}) \quad 4)$$

$$f^{0n} = \frac{2}{3} \omega^{0n} |\mu^{0n}|^2 \quad 5)$$

The spectra here shown are in the dipole-length formalism, however no important differences are observed with the dipole-velocity framework. Moreover, dipole-length formalism is generally observed with superior robustness in comparison to dipole-velocity values.⁷ The ECD spectrum was simulated by assuming gaussian bands with 900 cm⁻¹ full width at half-height for all transition centered in each excitation wavelength. A factor of 2.278 was applied during the conversion of rotatory strength and $\Delta\epsilon$ values.⁸ The calculations of electronic UV spectra were done in the same way, assuming the factor 2.8710⁴ accounting for the conversion between oscillator strengths and the molar extinction coefficients.⁹

3.1 ECD spectra calculated with spin-orbit coupling

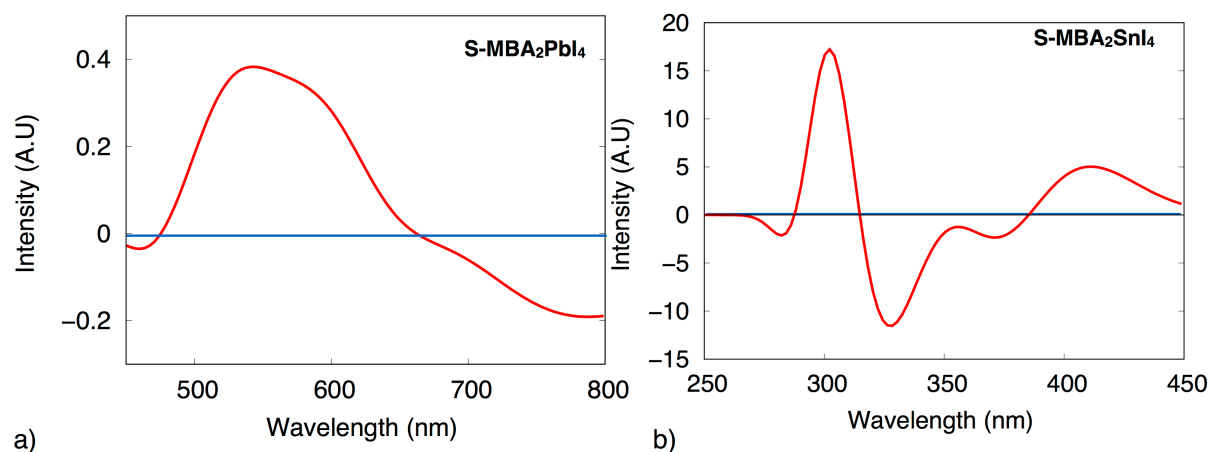


Figure S5. ECD spectra computed by including SOC effects for a) S-enantiomer of lead-based perovskite cluster coordinates and b) S- enantiomer of tin-based perovskite cluster coordinates. All the coordinates include 2 octahedra and four chiral MBA⁺ ligand.

3.2 Values of the calculated rotational strengths

Table S2. Calculated rotational strengths and wavelengths for S-MBA₂PbI₄.

S-MBA₂PbI₄	
R strengths	Wavelength / nm
0.0745	404.0790
0.2667	404.3028
0.1795	406.7405
-0.0254	409.1538
-0.4885	410.1272
0.1391	410.4934
0.1536	412.0469
-0.0961	413.0341
0.1581	413.6397
-0.2718	415.1060
0.2188	419.1147
0.1382	421.5200
0.0098	422.1508
0.3418	423.4469
-0.4999	423.6637
-0.0079	425.7709
0.0374	425.8732
-0.0724	428.9046
-0.1328	430.3321
0.2504	431.5440
0.1201	433.1554
-0.4329	435.3277
-0.2649	436.2917
0.0977	437.5683
-0.2095	441.6945
-0.1904	442.7186
-0.6065	444.9563
-0.0667	445.9314
0.0984	446.0596
-0.4851	447.8945
-0.2387	448.8663
0.0493	452.4000
-0.0723	452.5320
-0.0417	454.2377
2.4280	457.5025
-1.1606	458.1949
-0.0906	459.0422
0.0205	460.7632
0.1549	462.9457
0.0171	465.5851
-0.0320	465.9872
0.0837	469.3704
0.0206	469.6723
0.0221	472.4432
-0.0110	473.5607
1.6326	474.0852
0.1157	480.8065
0.2722	482.1137
-0.1417	485.7171

-0.0655	486.1546
-0.1535	487.8169
1.0910	489.4133
-0.1338	489.9736
0.0728	491.0396
-0.0113	495.5881
0.4280	496.0635
-0.8541	496.5993
-0.2387	499.0752
0.2134	499.8792
-0.0150	500.6453
-0.0170	501.8193
0.1171	509.2308
0.0889	509.8792
0.0340	510.8866
-0.0260	513.3375
0.1188	517.5541
0.3116	519.4819
-0.1351	526.4665
0.2844	529.7017
-0.0087	529.8148
0.2285	530.5621
-0.0449	533.3434
-0.1085	540.7083
2.0E-4	541.0383
0.0244	547.6022
0.0546	551.9120
0.0266	554.1789
0.1358	556.0907
-0.2002	559.8025
0.0075	564.4098
0.2681	565.1036
0.4733	577.0572
-0.2915	577.1108
0.1044	584.8332
0.0853	586.6298
0.4229	594.7247
-0.1263	595.6094
-0.0854	600.7696
-0.0998	610.3107
0.1486	620.4389
0.0137	652.5682
0.0598	724.5637
0.0207	864.1997
0.1399	868.6144
-0.1287	913.3554
0.1252	936.1566
-0.1403	961.8365
-0.4075	1020.0937
0.1167	1136.9882
0.0910	406.5540
-0.1275	406.8205
-1.2437	406.9272
0.1966	413.8190
0.0488	414.3716

-0.0256	415.7456
-0.0418	416.0243
-0.0324	416.1219
-0.0388	416.2754
-0.0641	417.0867
-0.0669	419.7809
-3.0E-4	421.0196
0.1397	421.4341
-1.7525	422.4094
0.0094	423.1438
-0.2222	424.9255
0.2761	425.5228
0.0299	426.6930
-0.6480	427.8992
0.1759	429.7808
0.0426	430.4664
-0.3713	432.1149
-0.0042	437.0752
0.0331	437.3833
0.1342	438.4183
-0.0686	454.9536
-0.0037	456.5265
-0.1107	456.7617
-0.1028	456.8626
-0.2659	462.9630
0.0257	462.9975
0.1056	465.4978
0.0097	466.6529
0.0403	467.0919
-0.1232	467.2326
-0.0416	467.9195
-0.0117	469.0334
0.0615	471.7250
0.0022	473.7776
-0.3754	473.8500
0.1397	475.3744
-0.1255	476.2499
0.1602	477.6978
5.3342	480.9742
-0.1557	487.4337
0.1741	488.4503
-0.0709	490.7290
0.1267	494.4037
-0.0299	499.0150
0.0334	503.0395
0.1365	504.4706
-0.0146	504.5116
-0.0609	509.1472
-0.3262	512.6802
0.2033	517.4462
-0.0904	518.4837
0.0057	519.2211
0.0252	520.1785
0.0993	523.8005
-0.2680	523.8889

0.2165	526.1987
-0.1051	531.2661
-0.0032	533.2288
0.0748	536.9193
0.0072	537.9898
-0.0173	540.3788
0.0629	545.6524
-0.0334	547.6022
0.3275	555.2946
-0.0033	557.9906
-0.2309	559.4997
-0.0982	560.3332
-0.1409	564.9235
-0.2257	575.6922
0.2080	576.8963
0.1441	580.1589
0.1035	582.9928
-0.0516	583.7331
-0.2889	589.6114
0.1862	594.1838
-0.0114	595.5237
-0.0844	606.5530
0.1568	612.6302
0.1217	614.7237
0.0292	624.9056
-0.3065	645.4423
-0.0913	647.9693
0.2741	657.6856
-0.2948	671.0910
-0.2502	695.1445
0.3944	699.0201
-1.0452	701.5883
-0.1236	796.2856
-0.0718	806.4778
-0.0095	815.2174
-0.2972	857.2169
3.0E-4	958.8644
0.0440	1007.5899
0.1975	1017.5014
-0.3444	1024.4718
0.1703	401.5041
-0.2754	402.2197
-0.4150	403.1341
-0.0031	404.0264
-0.3734	407.6890
-0.4910	408.1046
-0.0887	410.4798
-0.6323	411.1869
-0.0120	412.9791
-0.0270	416.0103
0.0039	416.4430
0.1407	416.6667
0.0735	417.7605
0.7799	420.8768
-0.1253	423.2159

-0.3027	423.8373
-1.5998	425.4353
0.1694	426.7810
0.0266	427.3394
-0.4432	427.4571
0.2994	427.6633
-0.1501	428.7565
0.0524	429.5726
0.0023	432.9136
0.0459	433.5487
3.3366	438.0006
-0.6399	440.7222
-0.0220	442.5291
-0.0337	446.0596
-0.0774	446.4125
-0.0490	446.5249
0.0175	447.0395
0.3270	448.8501
-0.0858	450.9701
0.0334	451.6921
-0.1272	453.8391
-0.7203	455.0537
-0.0165	459.9437
0.0110	460.5068
-0.0189	460.5410
0.1028	462.2733
0.2333	464.2443
0.0131	466.2322
-0.2265	467.3029
0.0485	469.4059
0.0337	470.6161
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0.0234	475.9394
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0.2046	497.0567
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-0.0921	575.1054
-0.0162	578.0515
0.6561	578.4556
0.0652	581.7632
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0.2114	599.2903
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0.0263	407.3545
0.1784	412.5673
-0.5843	413.1578
-0.0410	413.2679
-0.2487	413.6259
-1.3506	414.0536
0.0991	415.5229
-0.2434	415.8988
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0.0129	419.9513
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0.0460	465.8123
-0.4575	467.8137
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0.1001	475.7205
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0.6221	478.3053
0.0124	478.7296
5.1867	479.2101
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0.0980	490.7678
-0.0971	493.9709
0.1527	497.6945
0.0059	499.2760
0.1332	501.5759
-0.0035	504.6552
0.0775	506.4259
8.0E-4	509.0011
-0.0169	509.6071
-0.0366	513.3799
0.0474	518.4837
-0.0159	519.8300
-0.0925	523.8668
0.0106	524.8858
0.0407	531.1524
-0.3223	532.8854
-0.1164	535.8762
0.0184	537.8033
0.1392	540.8497
0.1421	546.3970
0.9327	546.6617
-0.1043	546.8784
0.1295	548.6673
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0.1870	562.0840
-0.0181	564.2302
0.0171	565.1036

-0.1221	567.7660
0.0529	569.9559
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0.2702	575.9059
0.1266	581.1640
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0.4838	597.4729
0.0681	598.2216
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0.0129	420.6344
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-0.0505	480.2670
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-0.0388	490.2058
0.0173	495.3903
0.1902	495.9247
0.0901	496.2023
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0.0983	502.6321
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-0.0041	514.8279
0.0674	519.5906
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-0.3950	521.1614
0.1354	523.6016
-0.1151	525.1523
0.0037	525.2412
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0.1000	535.7143
0.0291	537.4540
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0.0450	546.7098
0.0040	547.3125
0.9470	552.3540
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0.0689	564.8207
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-0.3096	584.2001
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0.3936	589.0798
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0.0156	598.3081

0.9854	599.0878
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0.1174	628.0994
0.0363	628.1947
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-0.2032	682.6056
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-0.0867	785.6510
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-0.0025	820.6069
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0.0954	981.7686
-0.1037	1025.6569
-0.1046	1046.3205
-0.2599	402.9378
-0.1584	405.2267
-0.6226	407.6087
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0.1328	419.0864
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-0.1944	420.5631
-0.0012	420.7057
-2.0259	422.5244
0.0057	423.3892
-0.0799	423.9966
0.2254	424.0400
0.0223	424.2284
-0.5137	424.4606
-0.2762	426.4292
0.0902	429.8255
-0.3058	430.3918
-0.5965	431.7091
0.1343	433.0043
0.5303	433.3822
0.2193	434.7636
-0.5730	436.0925
0.0012	436.4605
0.3485	446.2520
-0.3551	449.3538
-0.0191	455.6718
-0.2014	457.3002
-0.1382	462.5489
0.3179	463.4124
0.1017	464.1575
0.0498	466.6704
-0.0765	469.5657
1.7630	469.7968

-2.3156	469.9746
-0.0088	470.9375
0.0848	471.6175
-0.4996	475.0832
5.8762	476.3961
0.0496	476.7437
-0.0312	477.8265
0.0512	478.1579
-0.0187	481.8143
-0.2586	485.1665
0.0284	488.1622
0.0611	491.0979
-0.0103	495.5485
0.1341	495.9247
0.0668	497.4551
0.0064	498.7744
0.1990	502.3880
0.2220	504.2247
0.0601	504.3886
-0.1031	509.5234
-0.1219	511.0548
-0.0079	511.6869
0.0373	520.5494
-0.0760	521.4679
-0.0134	523.1823
0.0473	526.1987
-0.0126	526.6452
-0.0053	527.5405
-0.0560	533.0685
0.0182	545.5804
0.0375	547.1677
-0.2475	550.1019
-0.0919	557.2641
-0.4125	564.2302
-0.0205	568.2078
-0.0220	569.7728
0.8015	570.1392
0.0607	582.7738
0.1538	586.3527
-0.2684	590.8463
-0.2284	595.1239
-0.0599	595.2666
0.1881	598.6544
-0.0102	601.0605
0.0217	605.7242
-0.2062	622.2116
-0.0155	641.5392
-0.4384	647.6312
-0.0958	656.0171
-0.0049	675.9885
-0.0446	681.3691
-0.0842	687.3304
-0.0305	719.1483
0.0572	724.2677
-0.6737	765.6366

-0.2644	809.2118
-0.1413	817.4723
-0.0259	832.0485
-0.2365	994.7508
0.1864	998.7528
-0.1022	1035.9289
0.0156	1069.2135
-0.0039	1163.7446
-0.1855	403.3831
-0.3444	405.0416
0.2404	405.1341
0.1261	408.6689
-0.2506	411.0644
-0.4978	412.1563
-0.0110	413.1441
0.2940	417.2129
0.4529	419.4546
-0.2680	419.6957
-0.7099	421.4914
-0.6577	422.4525
0.0048	424.0400
0.2558	424.4896
-0.0311	425.0856
0.1192	425.5520
-0.1284	426.6197
0.1573	432.5214
-0.2904	432.9589
-0.7462	433.9883
0.3766	434.2464
0.0519	435.6333
0.0221	437.7535
-0.0930	437.7998
-0.0617	440.6596
0.0279	440.9101
-0.2519	441.6631
-0.6970	442.2296
-0.0026	442.4818
0.1160	443.8901
-0.0759	445.1158
-1.2899	452.8787
-0.6553	454.6204
0.7397	454.8203
-0.0045	456.3755
1.0150	456.9803
0.0502	457.4350
-0.2890	459.6201
0.0367	460.0630
-0.1725	460.4214
0.0162	461.7574
0.0676	462.0840
0.0094	467.4437
0.0066	469.3349
-0.1685	473.0193
0.4301	475.1742
-0.0303	475.5201

1.2618	477.8081
1.9335	478.3237
0.0649	479.0621
-0.8056	480.4157
-0.0351	485.4321
0.0212	485.5841
0.0010	486.5930
0.0880	487.5103
0.2529	488.3543
-0.1512	490.0509
0.1320	494.6402
0.0105	496.5596
-0.0625	498.4539
-0.0238	498.8947
-0.0294	499.6578
0.8529	507.1502
0.0134	510.0049
-0.7897	510.3195
0.0436	510.9707
0.1285	513.3799
0.1199	514.2946
0.5220	515.9192
-0.0944	517.0367
0.4030	519.1994
-0.0929	520.7896
-0.1241	524.5974
-0.0268	527.6526
0.0862	531.3798
0.0655	535.2523
-0.9611	536.6871
0.0015	536.8032
0.6770	537.6635
0.0868	544.6468
-0.1197	547.6747
-0.0334	547.8681
-0.1759	550.9076
0.0387	559.4997
-0.0175	560.5356
-0.0324	569.5898
-0.0920	572.7436
-0.0465	583.1024
-0.0033	584.1726
-0.0797	592.7934
-0.0893	624.2456
-0.1642	628.7675
-0.0280	635.2354
-0.2058	658.5579
-0.0124	668.8851
-0.5945	671.5631
0.0478	702.7800
0.0567	812.1238
-0.3978	864.7415
-0.1594	882.2589
-0.2528	900.3046
0.0637	956.0579

-0.1870	959.3832
0.2414	972.6902
0.0980	1050.6602

Table S3. Calculated rotational strengths and wavelengths for R-MBA₂PbI₄

R-MBA ₂ PbI ₄	
R strenghts	Wavelength/nm
-0.0431	401.6990
-0.1511	402.6372
-0.5150	404.6982
-0.0111	406.2214
0.0018	407.9168
0.2398	414.8979
0.1831	417.2830
-0.0444	417.6480
0.0064	419.2279
0.0072	421.4771
0.8668	422.3806
-0.1594	425.2750
-9.0E-4	425.7417
-0.0141	425.8586
-1.8661	426.8985
-0.1552	427.4424
1.1300	432.8985
-0.0388	433.7457
1.3842	435.2209
0.1522	438.3254
-0.0427	439.1940
-0.0157	440.1128
0.1784	441.1765
0.0442	441.4275
0.7557	442.1036
-0.0822	443.0188
-0.2776	444.4783
0.0070	444.5419
-0.2323	447.1040
0.6711	449.7120
-0.1361	450.1523
0.0268	451.8895
-0.2869	452.7301
0.2721	454.6370
0.5328	456.2580
-1.1940	457.9244
0.8616	458.2287
-0.0744	461.0370
-0.0153	463.0666
0.0816	465.0967
0.0090	467.0216
-0.3090	467.5670
-0.0200	469.0157
0.0141	471.5816
0.0442	471.9043
0.0620	474.5202

0.0719	476.5973
-0.0308	481.1793
0.1517	482.6949
-0.0224	482.7700
0.0832	483.5034
0.0996	492.5986
0.0785	493.1466
-0.1702	494.3643
0.1448	496.2221
-2.1930	498.0939
0.9610	498.2739
0.1909	501.0900
-0.0457	501.4746
-0.5322	501.6773
0.1734	511.6447
-0.0783	511.8346
0.2522	511.8768
0.0234	515.0629
0.0349	516.4344
0.2437	517.4894
-0.1305	518.2239
0.0611	529.2726
-0.4361	529.3403
0.3237	532.6339
-0.5198	533.0227
0.0168	534.0318
-0.8192	536.8961
0.6092	539.6270
0.0145	546.9748
0.1555	549.7365
-0.4757	552.3540
0.3596	555.3443
-0.0406	563.3084
-0.0683	566.1345
-0.0559	566.9879
-0.0053	572.2419
0.4137	592.9066
0.1661	596.7835
0.4657	599.6956
-0.0232	606.3159
0.0684	608.9932
-0.0265	623.9632
0.3026	625.3149
-0.2883	639.3911
0.1029	641.8046
-0.1284	645.9125
0.3405	653.1520
-0.0663	671.5267
0.1090	672.2177
-0.0575	691.5427
-0.0096	718.7735
0.1273	803.3981
-0.0846	886.7972
0.7704	894.7236
0.0435	907.9438

-0.0266	942.7693
0.1432	951.3681
-0.1137	999.6376
-0.0074	400.4161
0.3694	402.8594
-0.0272	403.4224
-0.1846	405.3458
1.4448	406.8872
-0.0253	407.2877
-0.1388	407.7694
0.1698	409.1404
1.4970	412.1426
0.0501	413.0203
-0.3814	413.1303
0.0214	413.6948
-0.3009	413.8052
-1.1233	414.9256
-0.1127	415.7874
0.7689	417.6059
0.3768	417.7746
-0.1419	418.1123
-0.1038	422.9708
-0.1434	426.6050
-0.0198	430.4664
-0.0046	431.2591
-0.0940	436.8445
-0.0425	440.0971
0.2449	441.8990
0.0352	443.6363
-0.0505	445.0360
0.3199	445.3873
0.2358	446.4286
0.0183	448.0238
-0.0835	449.2237
-0.0930	450.2993
0.0138	451.0356
-0.1827	451.4293
-0.0876	451.6757
0.0107	452.8622
0.5904	454.4706
-0.0219	456.3922
-0.3288	456.6441
0.7990	457.7218
-0.0548	458.2287
-0.2654	463.1530
0.1879	472.1916
0.0454	473.2177
-0.0145	473.5427
0.1801	481.8891
0.0518	483.2399
-0.1191	485.0717
-0.0683	487.6252
0.6625	488.3735
0.0226	488.5272
-0.3885	488.5849

-0.1229	489.7802
0.0758	491.0396
0.0152	491.3312
-0.0113	492.0128
-0.1730	503.6723
-8.0E-4	505.3332
0.6142	506.5500
-6.0011	507.0673
2.3966	507.2123
0.4705	508.1259
-0.2518	521.7967
0.3345	522.5656
0.0041	522.7416
-0.0014	523.2926
-0.1073	524.8636
-0.1050	528.5514
0.3109	531.7440
0.0483	534.4456
-0.6548	542.5281
-0.2623	545.1970
0.5807	546.3248
0.0363	550.2239
-0.3163	554.2284
0.1932	555.8168
0.0074	558.4676
-0.5482	570.4798
-0.1061	572.0573
0.2835	575.8525
0.0072	578.9142
-0.1404	583.4587
0.2483	584.6679
-0.1188	591.0714
0.0413	594.2123
-0.0731	596.5254
0.2175	600.5080
0.1570	603.0462
-0.1001	616.9235
0.0099	639.5229
0.0134	642.3692
-0.4175	650.6867
-0.1780	652.4310
-0.0087	672.3634
0.0789	681.1073
-0.0663	732.2577
-0.0283	737.5223
0.1116	743.6643
0.1952	776.0238
-0.0406	879.5083
-0.1416	923.4804
0.0366	931.5896
0.0069	1084.4400
0.1542	1099.1322
0.1524	401.6600
0.1718	402.3240
-0.3916	402.7809

0.0143	404.3950
0.0191	405.7035
0.9456	406.3144
-0.1113	407.8096
-0.0457	408.2119
0.3379	408.4268
0.8838	408.6823
-0.2402	409.2483
0.0172	409.6670
-0.0787	413.0066
0.0706	413.2816
-0.0178	416.3033
0.0102	416.4151
0.0237	421.3769
-0.1975	421.5200
0.6571	431.6941
0.4730	431.8443
-0.0256	432.5516
-0.7389	432.6722
-0.0013	433.7608
-0.0176	435.3125
0.0615	436.1844
0.1086	436.6601
-0.0658	437.2138
-0.2807	440.3938
0.3691	440.7848
0.5178	441.6945
0.7905	443.1769
-0.0056	447.1201
-0.3798	448.7203
-0.0235	450.9537
-0.2310	454.4206
-0.0386	462.3766
0.1799	465.7074
-0.0287	467.6550
0.1528	468.0783
0.0158	469.0334
0.0309	470.8125
0.0835	472.1197
-0.0075	473.8138
-0.1037	475.7388
-0.0167	476.1768
0.2185	477.3855
-0.0632	479.8585
0.0012	481.3472
-3.5889	485.7741
-0.0939	486.2880
0.5984	492.3446
-0.7209	492.6768
0.0049	493.6565
-0.1041	494.3643
-0.1034	495.5881
0.0611	501.0900
0.1953	507.5027
0.2465	509.4189

-0.1015	511.0548
-0.1593	513.2101
0.1952	518.2239
0.0567	521.7090
0.0307	522.9398
-0.1010	529.1597
0.1256	531.0388
-0.1715	531.1978
0.3022	533.0685
-0.0886	540.0026
-0.0297	541.5103
-0.0213	542.5281
0.0184	542.8840
0.0913	554.8974
-0.0145	557.0890
-0.0362	559.3988
0.0553	560.7128
0.1535	578.3478
-0.0603	581.4634
0.1028	583.0750
0.0127	584.7506
0.2520	585.8822
-0.0653	590.3967
-0.0345	597.9046
-0.3959	599.3771
0.0182	617.5373
-0.1563	627.1156
0.0787	631.5830
-0.4080	639.1607
0.5893	643.0681
0.0091	646.6191
0.1051	655.0823
-0.0657	706.8622
0.1074	718.0251
0.2398	760.0576
-0.0318	777.9693
-0.0198	796.7456
0.6348	869.2836
-0.0042	873.1359
0.0240	873.6275
0.0796	1019.1723
0.1546	1033.6859
0.0408	403.5404
-0.1169	404.5136
-0.0154	404.5532
-0.0109	405.9557
-0.2227	406.7405
-0.1500	408.2656
-0.0156	409.4238
0.4445	409.7752
0.5514	409.7887
0.0161	411.2959
0.4983	411.3505
-0.1844	415.5646
-0.5064	417.7746

-0.0399	419.1430
0.0223	421.9499
-0.0116	425.4790
0.0607	429.1567
-0.1288	437.1830
-0.4014	437.2446
-0.0230	438.0470
-0.0126	439.2561
-0.0047	439.9100
0.0055	441.0041
0.0866	441.3804
0.0095	441.4746
0.0989	444.4942
-0.3673	453.1763
-0.2839	453.9387
-0.0459	455.7387
0.0012	459.5180
0.1693	468.0077
-0.0910	469.0866
0.1864	472.6411
-0.0449	475.6476
0.2787	476.4144
0.0548	476.6156
-0.2067	476.6705
0.0241	478.2316
0.1785	481.8704
-0.0107	481.9265
-0.0410	485.2424
-0.0017	485.3372
-0.1357	486.4023
0.0172	491.4285
-1.6376	493.0682
-1.3791	493.3426
-0.0142	495.1137
-0.2678	496.9970
-0.2419	500.4031
0.0480	511.0548
0.0177	511.4339
-0.1550	514.1242
0.3083	514.7211
0.0061	515.8334
-0.0574	515.8763
0.2376	524.7305
0.0395	527.6750
0.1213	532.3826
6.0E-4	534.4456
-0.0772	535.8993
-0.3148	536.3856
-0.0131	542.9790
0.1952	546.5413
-0.1375	546.9266
0.0333	548.8371
-0.0410	564.3071
-0.0517	566.6514
0.0721	567.5583

0.0136	573.9088
0.2790	578.4825
-0.0711	588.8841
0.0885	590.8182
0.2648	592.7367
-0.0719	596.0670
-0.5114	607.4138
-0.0563	613.1446
0.0191	628.1630
-0.1547	637.4865
0.1428	639.0290
-0.3156	644.2363
0.3548	651.2329
-0.0023	658.1040
0.0967	666.0853
-0.0643	718.5239
0.1126	729.1605
0.0345	760.4767
0.1681	763.1417
-0.0272	826.6733
0.1270	883.9553
0.6864	888.7019
-0.1449	891.7666
0.0684	1048.0875
0.1495	1061.4418
0.1456	401.1927
-0.1590	401.3483
0.1115	404.3028
-0.0000	405.8097
-0.1217	406.4475
0.0678	406.6606
-0.0211	409.3292
-0.0722	409.9511
-0.0092	411.5278
0.2769	411.5550
0.0105	417.6762
0.7978	417.9152
-0.0347	422.3375
0.3251	423.6493
0.1083	423.9676
0.2929	426.3706
-0.0131	428.4161
0.0440	431.4990
0.4869	433.2763
-1.0E-4	433.3217
-0.0375	433.5184
-0.0694	436.5833
0.0015	436.7062
0.8492	436.9522
-0.1104	439.7853
-0.0394	440.8005
-0.2879	441.2078
-0.0728	441.7731
0.0351	447.7652
-0.0134	449.3701

0.0969	449.5817
0.5916	451.4950
-0.0451	454.8369
0.0514	457.4688
-0.0167	459.5690
-0.0165	460.9685
0.0437	467.6727
-0.2880	468.3962
-2.9039	469.2639
-1.6186	469.3704
0.0350	470.7589
-0.0297	473.0914
0.1301	480.3599
-0.9838	485.9833
1.4568	486.4404
-0.0039	487.7402
0.0536	488.5080
-0.5123	493.9316
0.1394	495.8059
0.1117	499.0351
0.0330	500.3426
-0.0505	502.3880
-0.1059	506.4259
0.2862	509.5025
0.2107	509.5443
0.5318	510.8445
-0.0087	515.7048
-0.3932	519.5689
-0.2855	520.7459
-0.0198	521.2051
0.1187	523.8447
0.1232	527.4732
-0.0071	530.0410
-0.0224	534.3766
9.0E-4	545.8923
0.4996	546.3008
0.0056	550.0288
0.3639	558.3168
0.0880	568.5722
0.0341	571.0310
0.1142	571.6621
-0.1600	582.0360
0.0042	593.4168
-0.0502	597.0993
0.0916	615.1502
-0.1922	620.6250
-0.0479	630.9409
0.0831	634.9754
0.4241	646.7539
0.3548	666.6219
-0.0989	676.5411
0.0681	700.9148
-0.0157	742.8631
0.0939	759.1743
0.6741	840.2153

-0.0025	852.1557
0.0366	873.3816
-0.0035	913.5571
0.0811	945.8584
0.1372	985.9015
-0.3879	401.8161
0.7525	404.7642
-0.1226	405.6903
-0.3297	406.1150
0.9296	408.5747
-0.1269	408.6554
0.1221	409.0864
-0.7582	409.8970
-0.0050	410.9691
0.5836	414.6484
0.6663	415.1754
-0.3970	416.5967
-0.0632	416.6946
0.0267	419.4404
-0.0703	421.1339
-0.1054	421.3197
0.0914	424.6639
-0.0385	427.5307
0.0815	429.6916
-0.8264	430.4664
0.3406	432.3708
-0.1985	432.6571
-2.4580	435.7098
0.1130	438.2635
-0.0399	438.7593
0.0363	440.8474
-0.0091	442.2296
-0.0783	442.8291
0.0014	447.6683
0.9063	448.5905
-0.0059	450.0054
-0.1717	450.7735
0.0761	455.3876
-0.0172	457.1318
0.1895	459.3989
-0.0561	459.7052
-0.0012	466.2497
-0.0526	468.6084
0.1770	474.0309
-0.1000	475.4290
-0.0214	476.2864
0.1622	477.2203
0.0136	477.3855
-0.4128	480.3041
-1.8400	484.2391
0.1016	487.3955
0.2499	487.6635
-0.0379	489.0469
0.0074	492.2079
0.3361	493.9119

0.5119	496.4206
0.0954	500.5646
-0.0948	503.8154
0.0630	506.0956
1.1806	507.8764
-1.5673	508.2091
0.1580	509.4816
0.0758	511.2232
0.2572	520.4839
-0.3897	524.3758
0.1466	526.7346
-0.3968	527.9893
-0.5317	528.9117
0.1099	531.9263
0.0347	535.1138
-0.1350	544.0261
0.5119	546.8784
0.1604	550.1019
-0.1247	552.4524
0.0019	559.7520
0.0522	563.3084
-0.1883	568.1038
0.1210	569.6682
0.2979	570.2439
0.0346	571.0047
-0.3635	574.8657
0.0485	576.4408
0.1036	582.5277
-0.0272	582.6644
-0.2184	593.1900
0.1712	600.1596
0.0754	603.4860
0.0080	605.5469
0.0232	622.1493
-0.3944	624.5283
-0.2309	638.9304
-0.1883	648.7482
0.0045	650.6526
-0.1751	654.1502
0.0247	657.7901
-0.1181	664.0186
-0.6147	683.9974
0.0279	686.7220
0.3406	715.6654
-0.0502	730.9210
0.3614	759.4995
-0.0053	764.6461
-0.0064	824.8056
0.5099	866.1898
0.1765	880.0695
0.0813	912.9523
0.1366	996.6677
-0.0349	1084.8191
0.0147	1102.7452
0.0071	406.6606

0.2633	406.8472
1.0163	407.3946
-0.2002	413.7224
-0.0478	414.3854
0.0439	415.6064
0.0239	415.8431
0.0149	416.1219
0.0629	416.1637
0.0578	417.1428
0.0672	419.6957
2.0E-4	421.0482
-0.2439	421.4914
1.8503	422.9419
0.0035	423.2015
0.4444	425.2750
-0.5446	425.6979
-0.0301	426.6490
0.6864	427.3688
-0.1746	429.8404
-0.0233	430.3321
0.3564	432.0848
0.0166	436.5680
-0.0405	437.2754
-0.1343	438.1398
0.0638	454.6870
0.0062	456.3755
0.1470	456.7449
0.0688	456.8290
0.2820	462.7041
-0.0442	462.8594
-0.1210	465.9872
0.0298	466.7055
0.1301	467.3557
0.0183	467.5317
-0.0486	467.8666
0.0193	468.4316
-0.0622	471.8864
4.0E-4	473.8138
0.3894	474.3751
-0.1508	475.3198
0.1274	476.0307
-0.1605	476.9636
-5.3533	480.3041
0.1478	487.3955
-0.1705	488.4503
0.0706	490.7096
-0.1274	494.2856
0.0305	498.8345
-0.0357	503.0803
-0.0059	504.0814
-0.1127	504.6347
0.0624	509.0637
0.3244	512.4474
-0.4933	517.8564
0.3756	518.4187

-0.0076	519.0040
-0.0251	520.2439
0.1524	522.8297
0.0232	523.9995
-0.2147	526.0203
0.1071	531.2206
-0.0020	534.0318
-0.0500	536.3161
-0.0347	537.7567
0.0181	539.9556
-0.0632	545.5085
0.0335	547.7472
-0.3831	555.9661
0.0017	558.0407
0.2805	559.3232
0.1151	559.9792
0.2230	563.7945
0.2284	575.6388
-0.1993	577.7286
-0.1482	580.1047
-0.0307	582.6097
-0.0302	583.0750
0.2895	589.2755
-0.1980	594.4115
0.0098	595.4951
0.0527	606.5530
-0.1699	611.4532
-0.1201	614.5715
-0.0300	624.6540
-0.1347	646.6191
0.5356	646.7876
-0.2874	657.8250
0.2942	670.6559
0.2708	696.4316
-0.2307	697.5666
0.8662	701.4693
0.1244	795.9792
0.0748	806.2683
0.0099	814.5754
0.2965	856.3298
-3.0E-4	957.2376
-0.0221	1009.4746
-0.2236	1015.9191
0.3454	1021.0167

Table S4. Calculated rotational strengths and wavelengths for S-MBA₂SnI₄

S-MBA ₂ SnI ₄	
R strenghts	Wavelength/nm
-0.2751	260.5315
5.9480	262.7818
-0.1076	263.1439
-0.2540	265.5307
40.1898	267.6838

-1.4407	268.0075
2.1695	268.0886
-45.4223	268.7503
-0.0842	269.4094
0.3605	270.3954
1.4319	270.9975
-4.1735	271.4598
-0.0602	272.4370
0.4567	273.0242
0.4479	273.0482
-0.5242	273.9461
-5.2428	275.1241
0.6953	275.2767
-2.4927	275.3499
12.0187	276.0603
0.1702	277.1575
0.6271	277.8524
-1.0494	278.3571
1.1584	279.9391
-0.5372	280.0086
0.8289	281.5137
-0.6744	283.3193
-1.3132	284.2405
-0.7892	284.6904
9.6078	285.4301
-5.2187	287.1469
4.6087	287.2267
-0.1874	287.5594
-0.1461	289.5516
-0.3306	289.8221
-0.1039	290.1337
0.0164	291.5717
0.5288	291.6197
-0.4578	292.4304
0.1338	293.6827
0.3577	295.1071
1.4039	296.7936
-1.4221	297.6333
-0.3696	298.3917
-16.2883	299.9058
-88.6784	300.4211
-29.1316	301.8677
7.4190	302.0000
0.4737	302.4562
-0.9233	302.4783
0.0742	303.1136
1.7408	305.5911
-36.6656	306.0809
-6.6331	306.7238
-1.8623	308.5154
-1.4467	308.7072
0.3645	310.4289
0.7481	310.9344
0.4875	311.4024
1.0575	311.8484

0.1606	312.5551
3.4919	312.8781
137.9083	314.0338
25.3930	314.6946
0.2723	315.1261
-0.8473	315.8558
7.4691	316.0327
0.3735	316.9365
0.2208	318.5715
-0.6543	318.7187
1.1516	319.6379
0.1582	319.6791
1.4523	319.9263
-0.0605	320.8442
-2.4711	322.7295
31.7126	323.4865
0.2076	326.3613
0.2178	327.6882
0.0348	327.9046
0.0339	328.5729
-1.0389	330.0582
1.5405	330.0933
-0.6940	333.5707
0.0290	333.9207
-0.0986	336.4915
0.1001	338.4643
-0.1923	339.5475
-0.6938	340.0592
-0.8678	340.3856
0.6913	340.6191
-0.7817	341.4154
-0.0410	341.5188
-0.0662	341.6598
2.5769	343.6842
33.4373	344.8108
-18.0219	345.4538
9.9184	345.8388
0.9340	347.1251
2.6410	347.3874
0.1769	347.7670
-0.0220	348.8421
-0.4190	349.0579
-0.0125	350.5168
0.2059	351.0918
-1.1648	351.3800
-0.4905	351.4497
1.4234	353.4210
0.9190	353.8139
0.4719	354.3796
1.2534	355.1096
0.1164	355.1502
0.1585	357.1018
-0.6269	359.2515
-2.1351	359.4908
-1.1993	360.4199

-0.3541	361.6380
-0.3799	361.9016
2.5509	362.5252
-1.3430	363.5658
1.0688	363.7789
-0.2189	365.8483
-61.6986	366.6588
1.8228	367.1251
-0.3972	367.5273
1.2241	368.4437
-0.1010	368.9255
-0.1511	369.2658
-0.2636	369.5296
-0.7145	370.3676
0.1349	372.9830
-0.1059	373.2073
-0.0242	373.3756
-0.0839	374.2876
0.5643	374.9320
-4.5516	375.3515
0.1035	376.0110
-0.9091	377.7274
-0.0250	378.1993
-0.0024	378.3030
0.0743	379.8195
0.0984	381.3481
0.1615	381.9583
-0.0651	382.9482
-0.1179	383.3977
0.1011	384.5498
-0.6967	386.5498
0.1634	387.6483
0.1071	388.1211
0.6700	392.1305
-0.2964	392.7633
-0.2394	393.6602
-1.3968	394.5737
-0.0371	395.4537
-0.0892	396.1478
0.8885	396.3376
-0.1049	398.8849
-0.1110	401.2445
0.5360	402.0894
0.2209	404.1975
-0.9138	404.3686
0.0092	405.7831
0.0874	407.7962
0.2458	408.2791
-0.2085	409.0864
-0.3882	409.4643
0.4137	411.2006
-0.1935	411.2823
-0.3019	412.0606
-0.0227	413.6535
0.0268	414.1227

-0.1344	415.2588
0.4509	415.5646
0.0873	417.0026
0.1575	417.3111
-0.2415	420.1361
0.0114	420.7770
0.1731	421.1482
-0.4690	421.7062
0.0550	422.0503
0.2170	424.5041
0.9416	426.2242
0.0270	426.4878
0.2366	426.6490
0.1520	429.1271
0.5176	430.7353
-0.1216	431.5290
-0.0351	431.8443
-0.3419	436.9675
-0.1907	437.0445
0.5462	437.8770
-0.2588	438.4803
0.2323	438.7593
-0.6225	438.9299
0.6119	442.0878
0.6194	443.7790
-0.0721	444.7012
-1.2086	449.1099
-0.7260	449.7609
0.1846	449.8260
0.2941	451.2488
-0.1070	451.4950
0.4646	455.5380
-0.0288	457.6543
0.3903	458.3810
0.1793	459.3649
-0.0817	459.5350
-0.0174	461.9292
0.2630	462.7213
-0.2201	465.8997
0.0958	466.1097
0.2296	467.7784
-0.0850	472.5871
0.0068	474.1758
0.0089	474.3933
-0.3742	476.2133
0.2522	477.2937
-0.8615	477.8081
1.5192	486.5548
0.0114	486.6884
0.3218	487.3189
-0.0715	489.3554
-0.8279	500.3830
-0.1116	500.5444
-0.2883	502.1847
0.3624	509.0011

-0.2372	510.9497
0.1069	516.8214
-0.0500	518.5054
-0.1708	522.1040
0.4315	527.4284
0.0073	532.6110
-0.0460	542.1016
-0.3804	562.4660
-0.1454	600.3628
4.5961	625.4094
-0.5329	760.1041
-8.8103	843.8137
-1.0004	871.9092
4.9840	896.2741
-0.3335	916.6605
-0.8438	957.0162
-1.2428	1009.8853
0.7783	1108.0611
-0.0222	1234.7061
6.7436	1371.0925
-5.7702	1416.7903
0.2335	1517.4205
0.7640	1598.3132
0.1291	1754.1690
-0.6401	2567.2182
-0.6516	258.6099
0.2494	258.6854
-0.4762	261.0575
-0.4065	261.4920
-0.1700	262.4041
-0.2411	264.0508
32.4121	264.5404
-3.8218	265.8720
0.8908	265.8948
-0.0711	266.3741
-38.4954	266.5571
-0.2346	267.2056
-0.3744	267.9902
-0.3754	268.8085
0.2895	271.8284
0.9378	272.6763
1.5972	272.8262
-4.8800	273.1023
-0.3954	273.8917
-2.7416	273.9945
-5.0216	274.0974
-0.9263	274.5582
1.4279	275.5945
-0.0221	275.7966
-28.7821	277.0029
32.6121	277.8959
5.9778	278.5820
2.0296	279.2903
-0.3626	280.8766
0.4304	281.4562

-0.0587	281.8077
0.2634	282.7642
1.2603	282.8995
-0.2361	284.8668
0.0158	286.1342
0.2046	287.1801
-7.4808	288.0666
2.8684	288.4884
-2.7090	289.2817
-1.0791	289.4639
1.1181	292.7960
1.1720	293.0656
-0.3631	293.5577
1.2421	294.7427
1.0978	295.7188
0.1062	296.2481
-0.0721	296.3754
-9.1532	297.8190
1.8820	297.9334
-61.6955	298.1767
-25.4998	299.4644
-7.8447	299.5873
2.2920	301.3620
0.7721	301.9559
-0.0870	302.6996
2.5889	303.2913
-2.1880	304.3398
0.3096	304.9530
-0.4404	306.6859
-2.2867	309.1609
-4.7750	309.5387
9.3981	309.8168
2.7729	309.8864
103.1457	312.2563
5.4673	312.9807
4.1415	313.1544
0.4789	313.5895
3.2877	314.9901
0.9121	315.1821
-0.2860	315.9603
3.5166	316.1212
-0.8455	316.2098
-12.3149	318.3100
-1.0779	319.0628
1.7536	319.6956
-0.8929	322.3524
22.2005	322.4277
0.6051	323.1917
-0.1997	325.0707
0.0119	325.4031
-0.0159	325.9243
0.0383	326.1384
0.0249	326.7651
-0.0265	327.4461
-0.2089	327.8699

-0.9382	328.7557
1.4397	330.0144
9.4476	331.5304
6.3344	332.4985
-1.7014	333.1320
2.8805	333.8040
-0.2232	334.0555
0.4754	335.5092
-2.7928	335.7906
-0.3069	336.2545
0.3565	338.2429
-0.3078	338.8338
2.3654	339.2413
-0.2712	339.6219
-1.2957	340.0592
0.6118	341.3122
-3.5137	341.7915
3.5537	342.4988
-2.6179	344.9258
-4.9736	345.2040
8.2904	346.3599
-2.0145	346.9602
0.3789	347.1640
-1.7338	347.6696
-0.3984	348.0791
0.1533	348.7245
-0.4043	350.4079
-0.1424	350.4574
-0.0500	350.8338
-0.7558	351.1911
-1.1301	352.6579
-1.3586	355.4757
0.2129	356.0263
-0.9416	356.3943
0.8762	358.3803
-0.0187	358.7635
1.5195	359.5637
-0.7124	360.3989
0.0095	360.8914
-0.1435	361.0909
-0.3329	362.0810
0.7130	364.3876
-0.0819	364.5589
0.2442	364.7946
-0.1601	365.4820
0.5125	367.2446
-7.4942	368.6078
-1.9214	369.5186
-26.9594	369.6727
1.8210	370.7770
0.2482	371.4204
0.3438	372.9830
-0.0849	373.7354
-0.1444	374.5700
-0.0323	375.0113

0.4068	375.4083
-0.7717	375.8858
0.3171	376.6500
0.1081	377.2338
-0.3291	377.9114
-0.9745	379.1697
-0.2731	380.9619
-0.0146	381.1139
-0.0723	381.1139
-2.3484	381.7586
-0.1682	381.9231
0.0445	383.2793
-0.0605	383.7414
-0.0292	384.0620
0.3217	384.4784
0.1586	385.5293
1.4036	386.8389
0.9128	387.1888
-0.6274	387.2492
0.0074	389.0212
-1.0275	389.2408
-0.0557	391.6604
-0.0853	394.5236
0.5236	394.5737
-0.6947	394.9504
-0.0137	396.4768
0.1221	398.2194
1.3897	400.8817
0.4458	402.1285
-0.9932	403.8424
0.3633	404.8963
-0.2335	405.7964
-0.2938	406.0486
-0.1688	406.1416
0.0773	406.2214
-0.4835	409.9647
-0.0357	410.9827
0.1953	412.5947
-0.1224	412.7868
-0.2274	413.1166
0.1239	416.1917
-0.5027	417.0447
1.1640	417.5497
-0.4511	418.4365
0.0948	419.1996
-0.1813	419.6957
0.5498	419.7383
0.1523	420.1503
0.0874	421.6059
-0.3069	425.2021
-0.0886	425.8148
-0.2847	425.8586
-0.5582	426.0340
-0.9628	428.2979
0.2433	428.5049

0.6998	433.3671
0.0230	434.1401
0.1320	435.3277
1.0811	436.0925
0.1664	436.4145
-0.9826	438.1552
1.9586	438.8834
-0.0647	442.9872
-0.0483	444.7012
-0.1693	446.0115
-0.6621	447.1201
-0.0325	451.3144
-0.1181	451.4786
0.1998	452.9779
0.5725	454.4373
-0.3557	456.8290
-0.3586	461.7574
-0.0362	462.3594
-1.3360	462.5144
0.1900	462.9630
0.0184	465.5328
-0.0715	466.1272
0.0013	472.6411
0.0976	474.1577
-0.1443	474.8106
0.0879	476.7071
-0.4333	481.5900
-0.1828	482.2448
-0.2594	482.4510
-0.2253	492.9703
0.3058	495.2520
-0.0025	498.9549
-0.1046	506.9430
-0.3959	509.4398
0.6101	509.5653
-0.0696	529.1372
-0.2678	530.0863
0.5343	543.3831
0.0249	571.7675
-1.3415	650.1414
5.4613	740.2493
-1.7308	749.4566
4.5987	795.1634
-1.3298	867.8249
3.5480	933.7621
0.6114	938.0668
-0.8705	979.9084
-1.4144	1078.9725
-9.8427	1104.2167
2.8333	1142.7454
-2.1957	1251.2601
1.4316	1461.8420
-0.4186	1655.4415
0.9656	1800.4787
-0.6191	2150.0953

2.3501	260.2310
0.1856	260.5096
-0.2923	261.3268
10.0943	262.8931
0.4906	263.2835
-0.0154	263.3338
9.4390	263.9497
29.0418	264.1969
-70.9575	266.4827
-0.1691	266.6430
0.0065	267.0274
-7.5600	267.3034
-0.7442	267.5684
-0.4719	270.6135
0.8171	271.3886
-3.3776	272.4549
0.8658	272.6284
14.1466	272.7183
0.0127	273.0603
-0.0105	273.9885
1.1847	274.9961
1.8464	275.5333
0.3608	276.0726
3.7902	277.3061
27.1568	277.4797
0.5419	278.3134
-0.8110	279.3280
-0.4677	279.7183
-1.7585	281.0483
0.4891	281.7757
2.7936	283.2546
-3.8618	283.8246
-0.1249	285.1613
1.1688	286.3718
-0.1378	286.4643
-7.1271	288.2873
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6.7436	1371.0925
-5.7702	1416.7903
0.2335	1517.4205
0.7640	1598.3132
0.1291	1754.1690
-0.6401	2567.2182
-0.4616	267.2343
-16.5077	268.2566
0.3770	268.5119
-19.5999	270.9029
-120.8619	271.0686
-0.3319	271.9594
-1.3938	272.0488
-0.1239	272.7782
-1.0064	274.0127
-0.9890	274.6311
3.3016	275.8885
99.0529	276.1586
-0.1619	277.1761
43.7239	277.5790
6.2187	277.7653
-0.2876	277.9084
0.3273	281.1056
-0.5785	281.5328
-2.5700	283.3581
-1.2614	283.6624

0.1200	283.8440
-3.9684	285.5023
-0.5261	285.7390
-1.2603	286.4313
-0.3391	286.8682
1.0161	287.1137
-0.6256	289.0527
-4.2864	289.3289
-0.2743	289.8830
-0.0722	291.3732
1.6826	292.2238
-13.4040	292.9342
-2.0378	295.5568
-0.0167	296.4533
-0.5937	297.6833
-5.1487	297.8118
0.0228	298.0407
0.4622	300.5011
74.6543	301.9706
4.4295	302.8769
-0.5096	303.4989
-104.613	304.7134
-8.9498	304.9455
-24.2288	305.2529
-20.6466	305.5610
2.2531	306.2244
-68.3881	308.0713
-40.9239	309.2379
-57.3207	309.3150
-1.7292	312.1071
0.1348	313.8750
84.2861	314.5192
4.0313	314.7186
1.4842	314.8383
-1.4043	315.2541
6.0439	315.3102
4.4853	315.9522
168.8343	316.3791
5.8910	317.5608
0.7038	321.0351
-0.3346	321.8842
-0.2314	322.1683
1.2729	322.7211
-0.4611	323.3601
1.6221	323.9339
0.0735	324.3996
0.8266	324.6881
-1.6884	325.6506
-0.7583	327.1786
1.0268	328.9212
-0.7201	331.2915
0.5108	331.9560
-12.1894	332.3115
2.1401	332.6945
7.8259	332.7391

0.6914	333.1589
-0.9015	334.1634
12.5568	334.2714
0.3342	335.8360
0.6221	336.1362
-0.0324	337.5071
-6.7431	338.8616
0.0213	339.3526
0.6645	342.5177
0.2930	342.9531
1.1226	344.5141
0.2042	346.0895
189.0895	347.6988
4.2148	349.8450
1.1767	350.5366
6.5485	353.3908
-4.9055	354.4909
-0.3373	354.9674
-0.8434	355.5164
5.1616	355.8732
-65.2944	357.6162
-96.2727	357.7089
-45.4968	358.3906
-4.1244	358.6806
-0.3274	359.2100
0.7887	360.3571
0.3733	360.9649
-1.5098	362.0916
-0.0117	362.2395
0.3238	364.0136
0.0324	364.2914
-1.0391	366.3774
0.6484	366.7671
-2.2448	367.4838
0.4508	369.8159
-0.1529	369.9151
1.1681	370.5334
-0.0325	370.6441
0.1642	372.2447
-0.1670	373.0502
0.1551	373.3644
0.6741	374.0282
0.0657	375.8630
0.1305	376.7414
-0.0292	378.0265
0.1595	379.0771
0.0828	379.5059
0.1910	380.2849
-0.6648	380.5064
0.8786	381.7821
-0.3950	383.3740
0.4611	383.7651
-0.3551	384.3712
0.4509	384.8360
-0.1657	385.5772

0.2787	386.7184
1.4294	386.8148
-1.0497	386.9233
0.5517	388.8506
0.0950	389.0090
-0.0919	389.1188
-0.1853	389.8398
-0.2591	390.7972
0.6135	391.0804
-0.0306	391.8087
0.0724	392.8752
0.5029	393.8351
-0.0704	396.5782
-0.2233	397.2254
0.9197	397.4289
-0.1124	399.4754
0.0600	399.8872
-0.9035	400.8299
0.1920	401.7770
-0.2135	403.7899
-0.4725	403.8424
-1.0091	406.3144
0.0192	406.7538
0.0666	407.9436
0.0529	408.3731
-5.3764	411.0372
0.4404	412.2385
0.4061	412.6770
0.0312	412.6908
0.0861	413.7086
0.1145	414.5792
0.2404	415.8849
-1.1365	419.1571
0.2396	419.5396
-0.0387	419.6531
-0.0829	421.8638
-0.0776	422.3806
0.9981	422.7115
-0.0251	423.6204
0.1005	424.5331
0.0166	425.9609
0.3369	426.7810
-0.0550	426.8398
-0.1431	427.7517
-0.1328	429.2903
0.7851	431.0794
-0.1752	431.7992
-0.0720	433.2007
-0.0364	436.4451
0.6088	436.5065
-0.1995	437.0906
-0.0757	439.4428
-0.1259	442.6870
0.3804	443.9695
-0.0595	444.8925

-2.5841	445.9634
1.3762	446.5410
0.1467	446.8786
0.1812	449.0774
0.3914	450.2176
-0.5293	451.0848
0.2428	451.3636
0.1696	453.4247
-0.6519	455.2039
0.0542	456.1742
-1.2866	456.9635
0.3003	457.0981
0.2418	459.1610
-0.2969	460.6435
0.3468	461.1569
-0.1542	462.1012
-0.0764	464.8354
0.3323	465.0270
0.6106	466.3023
0.3255	467.4965
-0.0786	468.0783
-0.0163	471.4025
-0.0598	472.8391
0.4152	473.1996
-0.3094	476.1950
0.2400	477.1102
-0.3372	478.8404
-0.3480	481.9827
-0.2835	482.0763
0.1013	483.6541
-0.1770	485.6791
0.0115	487.8552
-0.4920	488.1814
-0.1021	490.7678
-0.1129	496.6589
0.1328	500.4637
0.1730	503.8768
-0.0411	506.8188
0.3318	506.9430
-0.0288	510.3404
-0.0355	511.1811
0.1792	511.3707
-0.0436	517.4894
-0.5965	533.1143
0.0376	535.7837
-0.0511	543.5021
-0.1023	545.6524
-0.0265	566.8844
0.4340	576.1465
-1.0034	697.5666
4.5256	800.3417
3.3824	937.0046
0.9722	942.6977
0.5708	970.7124
-0.3982	1033.3417

-0.9437	1066.6409
-5.1186	1091.6887
-0.5946	1164.8367
0.0930	1198.8121
1.2005	1411.7948
-2.7539	1475.9215
2.4402	1659.2033
-1.5609	1711.3608
-0.3762	2013.0555
0.0246	2129.0738

Table S5. Calculated rotational strengths and wavelengths for R-MBA₂SnI₄

R-MBA ₂ SnI ₄	
R strenghts	Wavelength/nm
0.0016	260.5643
-2.7169	264.0227
-3.4532	264.7209
-0.1258	265.5421
-53.5092	265.9062
4.5312	266.3284
41.9798	266.8150
0.4331	266.9757
-0.2622	267.9844
0.0844	268.7095
0.5524	269.4270
1.6871	269.4621
-1.1313	269.8194
18.1059	270.4189
-0.8169	272.2637
-0.6241	272.8442
0.8318	273.1384
0.7428	273.8736
-5.7902	274.4064
-10.9152	274.4186
3.3287	275.2400
-0.8749	275.4783
-23.6835	276.5092
-0.6011	277.2132
0.4048	277.9582
2.6539	278.2011
-0.8960	279.7561
2.3245	282.2177
0.4077	284.0909
-0.0095	284.7361
0.6522	286.0287
0.0858	286.5371
-0.5499	286.8881
0.7139	286.9279
4.2286	289.3289
-0.0743	289.3829
0.1859	289.4706
-1.0881	290.3237
2.9113	291.0931

-1.1133	291.1819
-0.9212	291.2433
9.3374	291.4280
1.6435	293.3565
-0.2002	295.2194
-0.1820	296.8361
0.7113	298.8372
23.0513	299.4500
-4.5716	299.9203
98.6615	300.2177
-0.6727	300.9821
-0.2950	302.3973
-1.0373	303.2839
-1.1090	305.3806
16.3658	305.9602
-6.1549	306.1338
20.8088	307.0501
0.6022	307.3238
-0.5676	308.5844
0.2454	308.6381
-0.6953	309.4075
-15.0996	310.3280
-11.4595	310.3901
-2.7989	311.0045
-0.2106	311.3399
0.2016	312.3349
-0.9577	312.6259
-8.2862	312.9886
-125.3331	313.6291
-4.6303	316.0166
1.3554	316.5081
-10.0678	317.7885
-4.4076	318.5796
0.0554	319.8933
0.0296	320.3639
0.0631	320.7779
0.6303	321.3259
0.4388	323.2169
0.3230	324.7900
0.2108	327.1441
0.3603	327.4548
-0.825	327.7834
0.3829	328.7296
-1.1178	329.4538
-1.3940	331.0000
9.5721	332.6499
-1.0251	333.0516
-29.7271	333.1857
1.8588	333.6604
-1.2371	334.7041
0.1375	336.6010
-0.9617	336.7472
0.5448	339.4547
1.1298	340.1244
-0.4391	340.4789

0.1325	341.8291
0.0152	342.6879
2.0551	343.4180
0.4023	344.1607
5.7025	345.3865
-14.8436	345.5981
-1.4320	346.9020
-2.6043	347.0766
2.6764	347.9522
-0.5871	348.2353
0.4988	348.3526
-1.3822	350.9429
-0.6982	351.3005
-0.1240	351.7584
-1.8581	352.1476
0.4533	352.5677
0.8305	353.5418
-1.2693	355.6183
2.6257	355.7916
-0.2863	356.1182
-0.7638	358.0908
-1.2638	359.7826
1.4853	359.8974
0.8529	361.3537
2.3457	362.2395
-0.0014	364.0029
-2.3482	364.7195
2.5726	365.6220
1.0093	365.8375
0.2161	366.1180
0.3462	366.6696
40.7838	367.8650
4.4021	368.2688
-1.0980	368.4656
-0.8645	369.4526
0.2439	369.8930
1.9588	370.0805
6.0E-4	370.5998
0.1041	370.6662
0.0150	371.5094
0.5777	373.1960
-0.0305	374.0507
-0.1748	374.1861
0.2497	375.7834
0.0367	376.6843
3.6933	377.0046
-0.8012	377.4402
0.0045	378.5684
0.5566	379.0655
-0.2442	379.7033
0.0715	381.7469
0.4740	383.0191
0.3615	383.5635
-0.0419	385.9728
0.0137	386.9474

-0.1720	386.9595
-0.1846	390.0358
-0.1451	390.0971
0.1534	392.0191
-0.2329	394.8624
1.1643	395.3403
0.2649	395.5167
0.1417	395.6554
-0.7445	399.0901
0.5491	400.3257
0.1582	400.3516
-0.0703	400.5324
0.2963	404.6059
0.2912	405.5975
0.1610	405.7964
-0.1102	405.8229
-0.1341	405.9955
-0.1689	406.2613
0.0426	406.5806
-0.1914	407.8230
-0.0569	410.8875
-0.0213	410.9691
0.0628	411.8418
-0.2734	412.0606
-0.5289	412.9791
0.0128	415.7317
0.2761	417.9574
0.1564	418.4929
0.0477	418.9873
-0.0871	419.8092
-1.0536	423.5481
0.4339	424.8092
-0.1657	424.9110
0.2935	426.2974
-0.1937	427.2511
-0.9735	428.9639
-0.1346	429.1864
-0.1268	431.3940
0.1323	431.5290
-0.0756	432.2503
0.6085	435.1751
0.1590	437.5837
-0.1859	438.8989
-0.5771	440.0191
-0.0390	442.6238
-0.8307	442.8449
0.1121	443.8901
0.9234	446.0115
-0.4806	447.5715
-0.1644	448.0562
0.3008	448.7527
0.0285	451.8401
1.0464	451.9553
-0.7585	453.8059
-0.0243	454.6204

-0.2342	454.8536
-0.3267	455.5715
0.2680	457.0981
0.0864	461.2769
-0.0800	462.3077
0.3659	463.5335
0.4141	463.7933
-0.1208	468.3432
-0.1809	472.0659
1.2861	472.4432
0.0484	476.5790
0.1156	476.9636
0.0908	478.5081
-0.2054	479.7472
-1.8517	480.0441
-0.1676	483.3152
0.1360	487.0512
0.0335	488.6042
0.8612	496.6589
-0.1831	504.3886
0.3790	505.4979
0.0049	506.0130
0.1042	509.7327
0.2153	510.2146
-0.1687	514.9347
-0.0105	517.2953
-0.5103	533.9169
0.0340	543.8116
0.3554	544.1215
0.1026	582.4184
-4.6673	627.2107
0.4693	727.2381
6.8652	849.1244
3.2815	863.4182
-5.1346	873.9966
0.4177	901.5471
0.9484	968.6671
1.1940	1005.1421
-0.9511	1060.2631
-0.0393	1147.3932
-5.6020	1346.6963
5.6521	1395.7607
-0.5526	1515.5678
-1.1950	1679.1802
0.1678	1794.2324
0.5052	2308.8728
0.2662	265.4967
1.1306	265.9176
0.6846	266.1799
-1.4138	268.3146
-63.7848	268.4364
0.8146	268.5351
-0.3229	268.7386
-6.6676	268.9716
-0.2239	269.3042

0.0432	269.4445
-1.2274	270.4484
47.7129	272.2039
176.2872	272.3831
-0.0631	275.2950
-20.3441	276.0235
-96.6489	276.7127
-3.2133	277.4611
-2.8996	279.3909
-11.2783	279.5860
-0.0229	280.2362
0.6472	280.6861
2.0777	281.5839
-0.4054	281.6989
-0.7672	282.3204
-2.1784	283.2740
-1.4307	283.7208
0.1470	284.0844
9.5993	286.6628
1.5497	288.5755
3.8966	289.0258
-0.0610	289.3357
12.0032	290.7998
3.4165	291.3185
-0.2028	292.6993
0.8801	293.1486
1.2794	293.1833
-0.4122	293.2318
-0.7272	294.0584
23.6374	295.0159
-0.4289	297.1204
0.5537	297.4194
-0.2975	298.9883
-0.8510	299.6813
-6.9627	300.6686
7.5067	300.9529
3.0093	301.1427
1.2907	301.5671
2.1934	301.9118
198.0840	302.5963
-3.0830	303.0839
1.9527	305.1554
-90.5787	306.8603
0.6488	307.1413
-1.8069	307.2021
6.9336	308.8916
-79.7904	310.1419
-1.0744	311.3009
14.5727	311.5587
-75.5000	312.1228
-71.3398	312.3899
-7.3196	313.6767
1.3507	313.8115
1.5557	314.2246
-2.0760	314.7585

-0.9163	315.1901
30.8026	315.6229
2.2334	315.6871
0.4523	316.7262
-0.6559	318.7760
0.3890	320.7199
-0.8841	321.4341
0.2132	321.6757
0.5591	322.0095
0.4442	322.6289
0.8056	325.3093
0.6654	325.7447
-1.5493	327.0406
7.5570	328.2341
-17.5625	328.4251
0.2001	332.4628
-0.0529	333.0159
-1.3654	334.4245
-0.5640	336.4824
0.8245	336.8842
1.4907	339.2506
-0.0310	339.4733
0.0726	339.5754
0.2757	341.6222
-0.0927	343.5891
-0.0502	344.0272
-37.6855	345.1368
-9.2965	345.9448
-14.1785	346.1185
0.0853	347.1931
0.0636	347.5917
-0.1344	347.8060
1.5892	348.2940
1.8669	348.9402
-0.5808	349.1856
-0.1370	350.4079
0.9252	351.1713
-1.1536	351.6887
0.4328	352.3276
-3.0671	353.4311
0.6805	354.2987
-1.3656	354.4707
-0.5900	356.0773
0.1199	356.4352
-0.8797	356.5786
0.0630	356.9580
-2.5118	357.8946
-2.3020	358.8672
88.1588	359.9182
0.3565	362.3876
3.5572	363.0341
-0.6598	363.4061
-0.3963	365.2132
-0.3642	365.3422
-0.1537	365.6004

0.2746	366.3341
0.8967	369.6066
1.3456	370.8213
-0.0124	371.5427
0.2444	372.3899
0.0381	372.5576
-0.2049	374.1184
-0.0189	374.4909
0.7029	374.5813
-0.4947	375.3402
0.2480	375.4764
0.5813	375.8630
0.2119	377.6125
-0.4033	378.3491
-0.7162	379.1697
1.0676	379.8660
-1.3980	380.5531
0.5690	380.8450
0.2800	381.0204
-0.3668	382.0054
0.3523	384.1571
-0.3262	384.5618
-0.7012	384.6333
0.2097	385.1943
-0.0322	385.2660
0.2352	385.6131
-0.3055	388.4733
0.3003	389.5951
0.2376	389.6930
1.2035	390.2443
-0.6745	390.7603
0.1066	392.7136
0.1818	395.1012
3.2999	396.4515
-1.8173	400.6100
0.2276	400.7393
-0.0148	401.5171
0.0216	406.0752
-0.5901	406.3277
-0.0062	406.7805
0.1736	407.2476
1.0799	409.0190
0.1697	411.2687
0.0540	411.4323
-0.0756	411.5960
0.0258	412.1837
0.2009	412.2932
0.1199	413.4330
0.2587	416.1219
-0.0313	417.1428
0.6384	417.1848
-0.1843	417.3953
0.7143	417.9434
0.0182	418.5211
0.2191	421.1482

0.2715	423.0717
0.0178	423.5192
-0.0105	423.6637
0.1288	424.2574
-0.9673	424.7511
0.8993	425.3041
-0.6188	426.6930
-0.0340	428.8009
0.1239	429.1716
0.1276	431.8743
0.1110	436.5219
-1.4342	437.0445
-0.2632	438.0315
-0.2501	438.4493
0.5450	442.1036
-0.0141	442.4660
-0.2099	443.6680
0.7063	444.1602
-0.4301	444.4464
-0.5948	445.6112
0.1836	448.1047
-0.2827	449.1912
-0.3725	450.7244
-0.2882	452.1034
-0.0546	453.9221
0.9122	455.9061
0.0188	456.3251
0.2079	456.3587
-0.3295	456.9635
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0.1315	466.1797
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2.9247	291.8116
1.0302	291.9901
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-1.2486	308.1631
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-0.1010	406.6872
1.7423	406.8472
0.5145	407.5819
-0.8197	408.4672
-0.0698	409.2618
0.0156	411.6779
0.1791	412.2111
-0.1705	412.4439
0.1415	412.7868
-0.9007	413.9432
0.5268	415.1893
-1.0978	415.3005
-0.1133	415.7874
-1.1353	417.1708
-0.5460	418.5211
0.9367	418.5494
-0.1323	419.5822
-0.1268	420.7912
0.4845	421.0053
-0.6107	422.0216
0.1608	425.0128
0.5397	425.5082
0.0895	425.5374
0.0901	427.8992
0.3223	430.0787
0.1686	430.1830
0.1195	433.4427
0.2180	436.6908
0.1562	437.5529
0.8658	437.8307
0.0228	438.4958

-0.2096	439.6140
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-0.2222	443.9060
-0.2392	444.3192
-0.1370	445.2276
-0.1728	446.7338
0.7246	446.9752
-0.1292	450.3973
-0.4708	453.3253
0.0244	454.8203
0.0252	455.8726
-0.0545	455.9899
0.0546	458.2626
0.0952	459.5010
-0.1268	459.7903
0.2238	461.8777
-0.0835	463.1876
0.0365	463.8280
0.0217	464.7310
-0.0460	466.6178
-0.2391	466.8811
-0.1557	472.1197
0.8350	476.0672
-0.1654	476.3412
-0.0271	476.9086
-0.0853	480.3227
0.1057	484.8822
0.5701	490.0703
-0.1788	491.4090
0.0945	495.5288
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-0.1189	500.5444
-0.0446	506.6533
0.1368	508.5214
0.0389	511.0128
0.0142	517.5325
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-0.0261	527.1596
-0.4355	560.3079
0.0592	572.3211
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0.5948	830.9902
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0.2551	1126.2590
7.4014	1134.1831
1.1468	1180.0076
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1.9935	1347.8662
1.5357	1493.3229
0.0764	1586.2620
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-0.2830	418.6199
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-0.2913	507.7726
-0.2543	512.5108
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0.0573	527.1148
0.0449	533.8480
0.6076	540.2612
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-0.1830	593.1616
0.8711	706.7012
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7.0914	1093.6123
1.0438	1189.1646
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-1.9002	1396.5459
1.7240	1425.5771
-1.3736	1741.1278
0.7688	2463.7753
0.5135	2595.1286

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