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Supporting Information

Discovery of an Allosteric Ligand Binding Site in SMYD3 Lysine Methyltransferase

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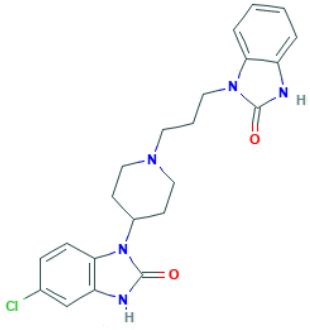
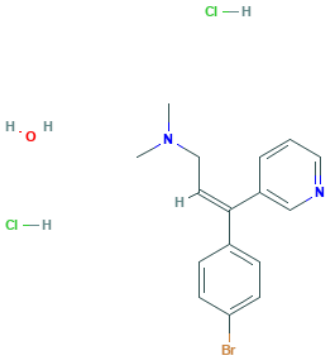
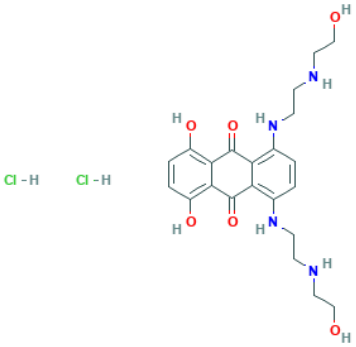
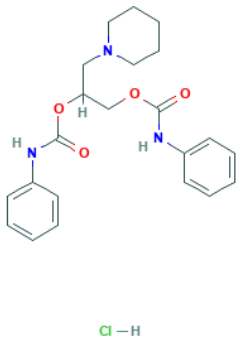
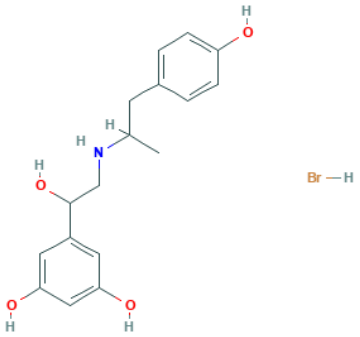
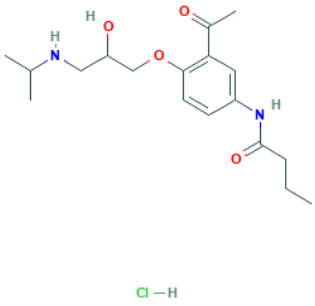
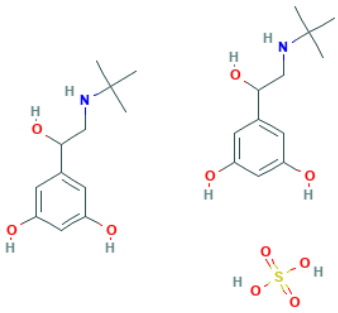
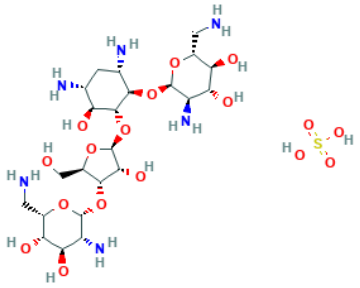
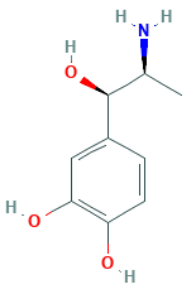
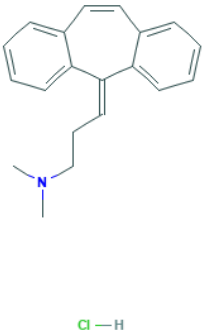
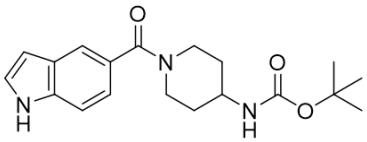
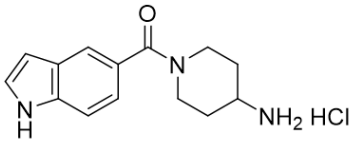
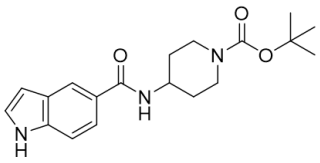
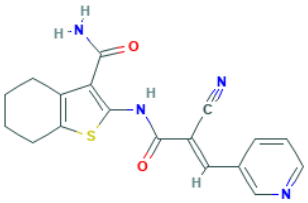
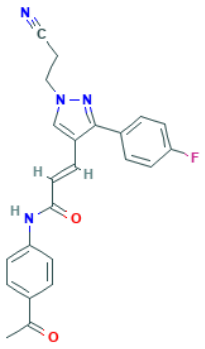
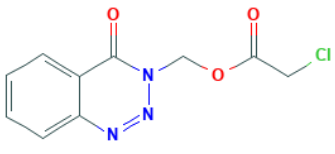
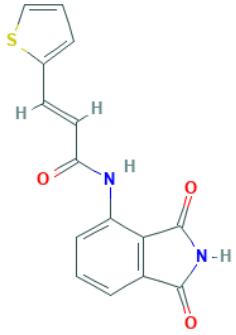
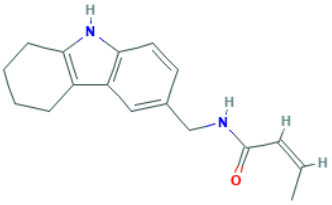
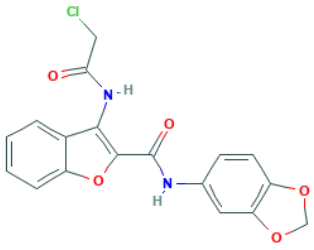
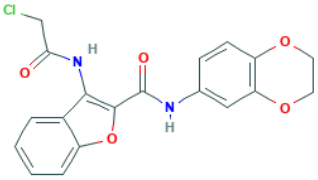
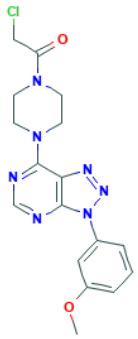
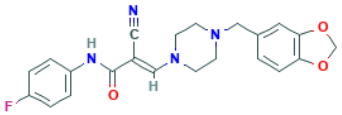
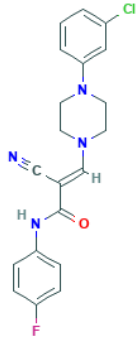
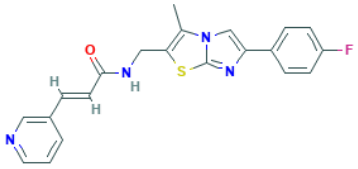
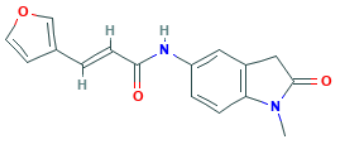
Identities of the compounds screened with the developed SPR biosensor-based assay.

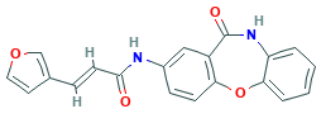
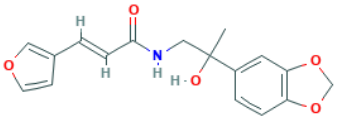
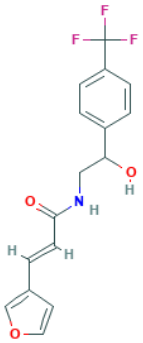
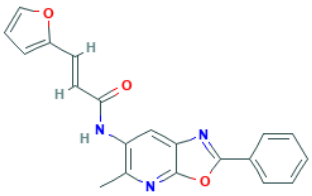
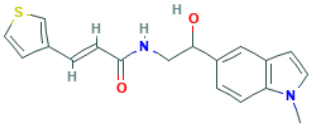
Compound number	Compound name or compound commercial ID or compound internal ID	MW	Structure
1	Domperidone	425.92	
2	Zimelidine dihydrochloride monohydrate	408.17	
3	Mitoxantrone dihydrochloride	517.41	
4	Diperodon hydrochloride	433.94	

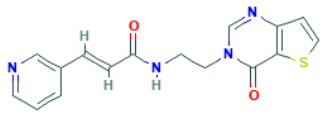
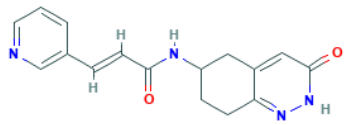
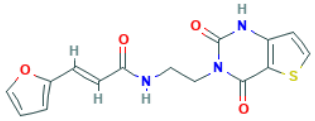
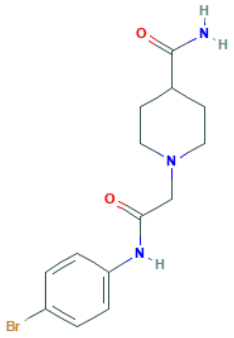
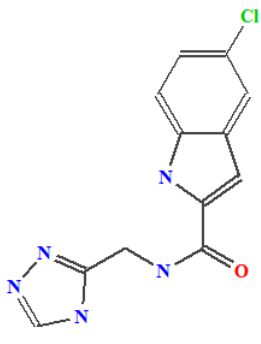
5	Fenoterol hydrobromide	384.27	
6	Acebutolol hydrochloride	327.90	
7	Terbutaline hemisulfate	548.66	
8	Neomycin sulfate	712.73	
9	Levonordefrin	183.21	

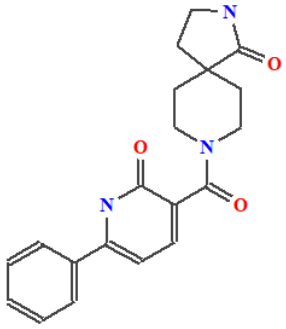
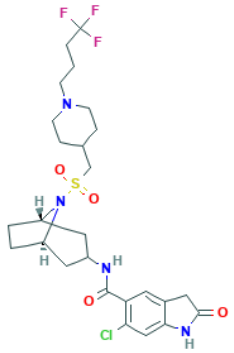
10	Cyclobenzaprine hydrochloride	311.86	
11	EM74	343.43	
12	EM77	279.77	
13	EM80	343.43	
14	F1736-2038	352.41	
15	F1683-0387	402.43	

16	F1045-0033	253.64	
17	F0440-0176	298.32	
18	F0651-0368	268.36	
19	F1883-1392	372.76	
20	F1883-1544	386.79	

21	F2865-0951	387.83	
22	F3225-7671	408.43	
23	F3225-7672	384.84	
24	F6262-6388	392.45	
25	F6436-1245	282.30	

26	F6436-1315	346.34	
27	F6436-2198	315.33	
28	F6436-3052	325.29	
29	F6442-4214	345.36	
30	F6521-7418	326.41	

31	F6523-3565	326.37	
32	F6523-4183	296.33	
33	F6524-3792	331.35	
34	BCI-121	340.22	
35	BB0304929	275.70	

36	BB0304996	351.41	
37	EPZ031686	591.09	
38	NP-6	647.69	Peptide NAFEAP
39	SV-6	708.73	Peptide SNNFEV
40	NK-6	797.87	Peptide NFFDQK

Tables

Figures

Table S1. Results of the conformational search on the low-energy conformers of (*R*)-diperodon in conjugate acid form: relative MM energies (ΔE_{MM}, MMFF94s), absolute and relative DFT electronic energies (E and ΔE, B97D/def2-TZVP/IEFPCM[H_2O], Boltzmann populations at equilibrium based on DFT electronic energies (χ_E), and DFT free energies (G, B97D/def2-TZVP/IEFPCM[H_2O]).

Conf.	ΔE_{MM}, kcal mol^{-1}	E, E_h (ΔE, kcal mol^{-1})	χ_E, %	G, E_h	Notes
c002	1.268	−1319.8695264 (0.866)	2.79	−1319.459604	
c003	1.283	−1319.8690060 (1.192)	1.61	−1319.458514	
c004	1.954	—	—	—	clustered (**c002**, RMSD = 0.000 33 Å)
c005	2.074	−1319.8674716 (2.155)	0.32	−1319.456486	
c006	2.340	−1319.8684047 (1.570)	0.85	−1319.457351	
c007	2.391	—	—	—	clustered (**c002**, RMSD = 0.000 27 Å)
c008	2.496	−1319.8697703 (0.713)	3.61	−1319.458383	
c009	2.694	−1319.8675451 (2.109)	0.34	−1319.456338	
c010	2.725	−1319.8682160 (1.688)	0.70	−1319.456049	
c011	3.268	−1319.8674729 (2.154)	0.32	−1319.456877	
c012	3.507	−1319.8653931 (3.459)	0.04	−1319.453317	
c013	4.168	−1319.8676041 (2.072)	0.36	−1319.454716	
c014	4.184	−1319.8629220 (5.010)	0.00	−1319.452554	
c015	4.296	−1319.8709060 (0.000)	12.03	−1319.457503	
c016	4.300	−1319.8700556 (0.534)	4.89	−1319.458327	
c017	4.394	−1319.8684440 (1.545)	0.89	−1319.459551	
c018	4.443	−1319.8685366 (1.487)	0.98	−1319.454913	
c019	5.056	−1319.8656911 (3.272)	0.05	−1319.453266	
c020	5.146	−1319.8701049 (0.503)	5.15	−1319.455084	
c021	5.262	−1319.8688457 (1.293)	1.36	−1319.457893	
c022	5.413	−1319.8683196 (1.623)	0.78	−1319.456529	
c023	5.730	−1319.8682274 (1.681)	0.71	−1319.459619	
c024	5.751	−1319.8678406 (1.924)	0.47	−1319.456768	
c025	5.790	−1319.8631467 (4.869)	0.00	−1319.450516	
c026	5.798	−1319.8694420 (0.919)	2.55	−1319.455205	
c027	5.934	−1319.8637083 (4.517)	0.01	−1319.454523	
c028	5.943	−1319.8678374 (1.926)	0.47	−1319.458310	
c029	5.973	−1319.8650627 (3.667)	0.02	−1319.453160	
c030	6.176	−1319.8668309 (2.557)	0.16	−1319.457610	
c031	6.179	−1319.8672179 (2.314)	0.24	−1319.456196	
c032	6.201	−1319.8687732 (1.338)	1.26	−1319.454877	
c033	6.220	—	—	—	clustered (**c030**, RMSD = 0.004 15 Å)
c034	6.225	−1319.8692663 (1.029)	2.12	−1319.454340	
c035	6.245	−1319.8677130 (2.004)	0.41	−1319.457628	
c036	6.270	−1319.8693763 (0.960)	2.38	−1319.458977	
c037	6.275	−1319.8666268 (2.685)	0.13	−1319.455643	
c038	6.377	—	—	—	clustered (**c045**, RMSD = 0.000 78 Å)
c039	6.492	−1319.8564210 (9.089)	0.00	−1319.445844	
c040	6.605	—	—	—	discarded (imaginary frequency)
c041	6.852	−1319.8657252 (3.251)	0.05	−1319.455794	
c042	7.179	−1319.8669852 (2.460)	0.19	−1319.454533	
c043	7.202	−1319.8649106 (3.762)	0.02	−1319.453210	
c044	7.213	−1319.8598861 (6.915)	0.00	−1319.449137	
c045	7.276	−1319.8673750 (2.216)	0.29	−1319.456160	
c046	7.296	−1319.8608397 (6.317)	0.00	−1319.451472	
c047	7.297	−1319.8622176 (5.452)	0.00	−1319.454033	
c048	7.323	−1319.8624830 (5.286)	0.00	−1319.453618	
c049	7.327	—	—	—	discarded (imaginary frequency)
c050	7.376	−1319.8615641 (5.862)	0.00	−1319.451188	
c051	7.534	−1319.8660844 (3.026)	0.07	−1319.454398	
c052	7.670	—	—	—	clustered (**c034**, RMSD = 0.000 43 Å)
c053	7.705	−1319.8675127 (2.129)	0.33	−1319.453255	
c054	7.720	−1319.8682880 (1.643)	0.75	−1319.454355	
c055	7.727	−1319.8669795 (2.464)	0.19	−1319.456214	
c056	7.790	−1319.8660706 (3.034)	0.07	−1319.454376	
c057	7.832	−1319.8658051 (3.201)	0.05	−1319.454016	

Table S1. (*Continued*)

Conf.	ΔE_{MM}, kcal mol^{-1}	E, E_h (ΔE, kcal mol^{-1})	χ_E, %	G, E_h	Notes
c058	7.882	−1319.8591729 (7.363)	0.00	−1319.448316	
c059	7.893	−1319.8632453 (4.807)	0.00	−1319.450879	
c060	7.939	−1319.8668650 (2.536)	0.17	−1319.454806	
c061	7.947	−1319.8620434 (5.561)	0.00	−1319.450489	
c062	7.963	−1319.8608719 (6.296)	0.00	−1319.450945	
c063	8.003	−1319.8629887 (4.968)	0.00	−1319.450293	
c064	8.095	−1319.8658471 (3.175)	0.06	−1319.453765	
c065	8.096	−1319.8663687 (2.847)	0.10	−1319.455591	
c066	8.167	−1319.8654229 (3.441)	0.04	−1319.453361	
c067	8.217	−1319.8663302 (2.871)	0.09	−1319.453179	
c068	8.310	−1319.8671323 (2.368)	0.22	−1319.458063	
c069	8.327	—	—	—	clustered (**c074**, RMSD = 0.000 66 Å)
c070	8.327	—	—	—	clustered (**c074**, RMSD = 0.000 72 Å)
c071	8.351	−1319.8700254 (0.553)	4.74	−1319.454541	
c072	8.398	−1319.8680357 (1.801)	0.58	−1319.456248	
c073	8.414	−1319.8590182 (7.460)	0.00	−1319.447012	
c074	8.423	−1319.8672536 (2.292)	0.25	−1319.456102	
c075	8.473	−1319.8670840 (2.398)	0.21	−1319.454919	
c076	8.489	−1319.8593942 (7.224)	0.00	−1319.448903	
c077	8.562	−1319.8600411 (6.818)	0.00	−1319.449496	
c078	8.639	−1319.8673315 (2.243)	0.27	−1319.453213	
c079	8.640	—	—	—	clustered (**c078**, RMSD = 0.000 82 Å)
c080	8.950	−1319.8585472 (7.755)	0.00	−1319.447192	
c081	8.950	−1319.8615106 (5.896)	0.00	−1319.451227	
c082	9.049	−1319.8647461 (3.865)	0.02	−1319.452645	
c083	9.101	−1319.8684360 (1.550)	0.88	−1319.454185	
c084	9.114	−1319.8589894 (7.478)	0.00	−1319.448519	
c085	9.153	−1319.8591140 (7.400)	0.00	−1319.448909	
c086	9.165	−1319.8630730 (4.915)	0.00	−1319.452966	
c087	9.166	−1319.8617350 (5.755)	0.00	−1319.449401	
c088	9.208	—	—	—	clustered (**c053**, RMSD = 0.000 48 Å)
c089	9.300	−1319.8650024 (3.705)	0.02	−1319.453980	
c090	9.310	−1319.8584467 (7.818)	0.00	−1319.446486	
c091	9.334	−1319.8606955 (6.407)	0.00	−1319.448114	
c092	9.344	−1319.8632868 (4.781)	0.00	−1319.452452	
c093	9.450	−1319.8591194 (7.396)	0.00	−1319.447762	
c094	9.502	−1319.8600951 (6.784)	0.00	−1319.448573	
c095	9.532	−1319.8676082 (2.069)	0.37	−1319.455350	
c096	9.542	−1319.8674433 (2.173)	0.31	−1319.457879	
c097	9.562	−1319.8660410 (3.053)	0.07	−1319.453498	
c098	9.570	−1319.8577996 (8.224)	0.00	−1319.446779	
c099	9.658	−1319.8595498 (7.126)	0.00	−1319.449649	
c100	9.717	−1319.8569040 (8.786)	0.00	−1319.444068	
c101	9.718	−1319.8602128 (6.710)	0.00	−1319.449842	
c102	9.789	−1319.8608533 (6.308)	0.00	−1319.449713	
c103	9.845	−1319.8565824 (8.988)	0.00	−1319.446059	
c104	9.869	−1319.8537864 (10.743)	0.00	−1319.442011	
c105	9.961	−1319.8586321 (7.702)	0.00	−1319.447537	
c106	9.976	—	—	—	discarded (imaginary frequency)
c107	10.011	−1319.8700331 (0.548)	4.77	−1319.454205	
c108	10.033	−1319.8672694 (2.282)	0.26	−1319.456664	
c109	10.186	−1319.8642409 (4.182)	0.01	−1319.454025	
c110	10.202	−1319.8652644 (3.540)	0.03	−1319.455521	
c111	10.253	−1319.8677304 (1.993)	0.42	−1319.457106	
c112	10.286	−1319.8605442 (6.502)	0.00	−1319.448637	
c113	10.289	−1319.8621018 (5.525)	0.00	−1319.450305	
c114	10.313	−1319.8662496 (2.922)	0.09	−1319.452053	
c115	10.319	−1319.8655166 (3.382)	0.04	−1319.452587	
c116	10.353	−1319.8648457 (3.803)	0.02	−1319.454267	

Table S1. (*Continued*)

Conf.	ΔE_{MM}, kcal mol^{-1}	E, E_h (ΔE, kcal mol^{-1})	χ_E, %	G, E_h	Notes
c117	10.390	−1319.8704828 (0.266)	7.69	−1319.457231	
c118	10.460	−1319.8665369 (2.742)	0.12	−1319.454774	
c119	10.501	—	—	—	clustered (**c185**, RMSD = 0.000 27 Å)
c120	10.551	−1319.8609791 (6.229)	0.00	−1319.448870	
c121	10.597	−1319.8564880 (9.047)	0.00	−1319.445753	
c122	10.607	−1319.8696335 (0.799)	3.13	−1319.458032	
c123	10.638	−1319.8629667 (4.982)	0.00	−1319.450517	
c124	10.694	−1319.8579142 (8.152)	0.00	−1319.447232	
c125	10.707	−1319.8580819 (8.047)	0.00	−1319.448331	
c126	10.714	−1319.8647567 (3.859)	0.02	−1319.448945	
c127	10.720	−1319.8695246 (0.867)	2.79	−1319.456125	
c128	10.747	−1319.8669692 (2.470)	0.19	−1319.452501	
c129	10.761	—	—	—	clustered (**c026**, RMSD = 0.000 76 Å)
c130	10.795	−1319.8609832 (6.227)	0.00	−1319.448132	
c131	10.818	−1319.8594919 (7.162)	0.00	−1319.448332	
c132	10.844	−1319.8676802 (2.024)	0.40	−1319.454470	
c133	10.861	−1319.8555780 (9.618)	0.00	−1319.444381	
c134	10.865	—	—	—	clustered (**c185**, RMSD = 0.001 06 Å)
c135	10.873	−1319.8586867 (7.668)	0.00	−1319.449848	
c136	10.910	—	—	—	clustered (**c185**, RMSD = 0.000 95 Å)
c137	10.954	−1319.8693354 (0.986)	2.28	−1319.457749	
c138	10.966	−1319.8630814 (4.910)	0.00	−1319.453233	
c139	11.004	−1319.8663244 (2.875)	0.09	−1319.453089	
c140	11.060	−1319.8633123 (4.765)	0.00	−1319.450109	
c141	11.120	−1319.8610957 (6.156)	0.00	−1319.449170	
c142	11.122	−1319.8606647 (6.427)	0.00	−1319.448830	
c143	11.125	−1319.8625030 (5.273)	0.00	−1319.450726	
c144	11.148	−1319.8688959 (1.261)	1.43	−1319.455340	
c145	11.149	−1319.8655512 (3.360)	0.04	−1319.451631	
c146	11.165	−1319.8590451 (7.443)	0.00	−1319.447680	
c147	11.168	−1319.8600550 (6.809)	0.00	−1319.449479	
c148	11.335	−1319.8585912 (7.728)	0.00	−1319.445555	
c149	11.377	−1319.8655778 (3.343)	0.04	−1319.452847	
c150	11.384	—	—	—	clustered (**c217**, RMSD = 0.000 30 Å)
c151	11.408	−1319.8610373 (6.193)	0.00	−1319.449455	
c152	11.466	−1319.8652215 (3.567)	0.03	−1319.454487	
c153	11.467	−1319.8656304 (3.310)	0.05	−1319.455135	
c154	11.499	—	—	—	clustered (**c122**, RMSD = 0.001 41 Å)
c155	11.602	−1319.8647062 (3.890)	0.02	−1319.455694	
c156	11.608	−1319.8582780 (7.924)	0.00	−1319.444654	
c157	11.664	−1319.8642910 (4.151)	0.01	−1319.452966	
c158	11.670	—	—	—	clustered (**c169**, RMSD = 0.000 80 Å)
c159	11.678	−1319.8589823 (7.482)	0.00	−1319.448061	
c160	11.680	−1319.8589776 (7.485)	0.00	−1319.446829	
c161	11.774	−1319.8625375 (5.251)	0.00	−1319.452248	
c162	11.789	−1319.8605051 (6.527)	0.00	−1319.450194	
c163	11.883	−1319.8596589 (7.058)	0.00	−1319.447785	
c164	11.902	−1319.8570223 (8.712)	0.00	−1319.446068	
c165	11.963	−1319.8605624 (6.491)	0.00	−1319.448348	
c166	11.968	−1319.8634067 (4.706)	0.00	−1319.451493	
c167	11.972	−1319.8601014 (6.780)	0.00	−1319.449570	
c168	11.984	−1319.8602152 (6.709)	0.00	−1319.448726	
c169	12.013	−1319.8597708 (6.987)	0.00	−1319.449443	
c170	12.043	−1319.8543669 (10.378)	0.00	−1319.443880	
c171	12.057	−1319.8653847 (3.465)	0.03	−1319.452584	
c172	12.107	−1319.8584162 (7.837)	0.00	−1319.447353	
c173	12.112	−1319.8621370 (5.503)	0.00	−1319.451515	
c174	12.165	−1319.8617947 (5.717)	0.00	−1319.448997	
c175	12.226	−1319.8584371 (7.824)	0.00	−1319.447072	

Table S1. (*Continued*)

Conf.	ΔE_{MM}, kcal mol^{-1}	E, E_h (ΔE, kcal mol^{-1})	χ_E, %	G, E_h	Notes
c176	12.240	−1319.8661554 (2.981)	0.08	−1319.453571	
c177	12.244	−1319.8688248 (1.306)	1.33	−1319.455031	
c178	12.309	−1319.8635968 (4.587)	0.01	−1319.449947	
c179	12.311	−1319.8631807 (4.848)	0.00	−1319.448883	
c180	12.312	−1319.8667830 (2.587)	0.15	−1319.454565	
c181	12.343	−1319.8561221 (9.277)	0.00	−1319.445759	
c182	12.351	—	—	—	clustered (**c261**, RMSD = 0.001 39 Å)
c183	12.363	−1319.8613089 (6.022)	0.00	−1319.448912	
c184	12.366	−1319.8681867 (1.706)	0.68	−1319.456148	
c185	12.372	−1319.8684621 (1.534)	0.90	−1319.454878	
c186	12.399	−1319.8651406 (3.618)	0.03	−1319.451520	
c187	12.399	—	—	—	clustered (**c053**, RMSD = 0.000 64 Å)
c188	12.417	—	—	—	clustered (**c261**, RMSD = 0.001 25 Å)
c189	12.420	−1319.8580849 (8.045)	0.00	−1319.447990	
c190	12.454	−1319.8650097 (3.700)	0.02	−1319.455682	
c191	12.474	−1319.8557274 (9.525)	0.00	−1319.444283	
c192	12.476	−1319.8582448 (7.945)	0.00	−1319.447385	
c193	12.492	−1319.8624195 (5.325)	0.00	−1319.450500	
c194	12.528	−1319.8582953 (7.913)	0.00	−1319.445955	
c195	12.553	−1319.8674226 (2.186)	0.30	−1319.456558	
c196	12.571	−1319.8590395 (7.446)	0.00	−1319.446776	
c197	12.681	−1319.8640136 (4.325)	0.01	−1319.451326	
c198	12.709	−1319.8578536 (8.191)	0.00	−1319.448555	
c199	12.741	−1319.8663365 (2.867)	0.10	−1319.451812	
c200	12.784	−1319.8674610 (2.162)	0.31	−1319.454681	
c201	12.787	−1319.8574689 (8.432)	0.00	−1319.445933	
c202	12.839	−1319.8662595 (2.916)	0.09	−1319.451634	
c203	12.859	−1319.8581935 (7.977)	0.00	−1319.448236	
c204	12.877	−1319.8639076 (4.392)	0.01	−1319.451710	
c205	12.908	−1319.8672380 (2.302)	0.25	−1319.452764	
c206	12.912	−1319.8594856 (7.166)	0.00	−1319.446752	
c207	12.935	−1319.8671693 (2.345)	0.23	−1319.451666	
c208	13.004	−1319.8580848 (8.045)	0.00	−1319.446305	
c209	13.063	−1319.8581443 (8.008)	0.00	−1319.449132	
c210	13.065	−1319.8635650 (4.607)	0.01	−1319.450725	
c211	13.072	−1319.8575252 (8.397)	0.00	−1319.446068	
c212	13.189	−1319.8652355 (3.558)	0.03	−1319.451897	
c213	13.194	−1319.8656933 (3.271)	0.05	−1319.451584	
c214	13.210	−1319.8604875 (6.538)	0.00	−1319.449938	
c215	13.234	−1319.8639820 (4.345)	0.01	−1319.448675	
c216	13.257	−1319.8640352 (4.311)	0.01	−1319.452871	
c217	13.314	−1319.8669905 (2.457)	0.19	−1319.453004	
c218	13.352	−1319.8616272 (5.823)	0.00	−1319.449622	
c219	13.475	−1319.8510990 (12.429)	0.00	−1319.442746	
c220	13.477	−1319.8568340 (8.830)	0.00	−1319.446257	
c221	13.537	−1319.8652590 (3.544)	0.03	−1319.453066	
c222	13.542	−1319.8650983 (3.644)	0.03	−1319.453369	
c223	13.550	—	—	—	clustered (**c074**, RMSD = 0.000 86 Å)
c224	13.554	−1319.8590075 (7.466)	0.00	−1319.444077	
c225	13.559	−1319.8620549 (5.554)	0.00	−1319.451716	
c226	13.598	−1319.8564140 (9.094)	0.00	−1319.443954	
c227	13.635	−1319.8567126 (8.906)	0.00	−1319.447865	
c228	13.678	−1319.8620605 (5.551)	0.00	−1319.450485	
c229	13.703	−1319.8513742 (12.256)	0.00	−1319.441156	
c230	13.709	−1319.8641816 (4.220)	0.01	−1319.450048	
c231	13.715	−1319.8683214 (1.622)	0.78	−1319.454169	
c232	13.718	−1319.8582351 (7.951)	0.00	−1319.448424	
c233	13.737	−1319.8578942 (8.165)	0.00	−1319.446778	
c234	13.787	−1319.8648352 (3.809)	0.02	−1319.453726	

Table S1. (*Continued*)

Conf.	ΔE_{MM}, kcal mol^{-1}	E, E_h (ΔE, kcal mol^{-1})	χ_E, %	G, E_h	Notes
c235	13.792	—	—	—	clustered (**c240**, RMSD = 0.001 05 Å)
c236	13.810	—	—	—	clustered (**c240**, RMSD = 0.000 69 Å)
c237	13.823	−1319.8592526 (7.313)	0.00	−1319.445299	
c238	13.841	−1319.8632962 (4.775)	0.00	−1319.448387	
c239	13.866	−1319.8524923 (11.555)	0.00	−1319.441682	
c240	13.881	−1319.8607141 (6.395)	0.00	−1319.446889	
c241	13.883	—	—	—	clustered (**c225**, RMSD = 0.000 31 Å)
c242	13.884	−1319.8689825 (1.207)	1.57	−1319.454777	
c243	13.905	−1319.8617108 (5.770)	0.00	−1319.449827	
c244	13.905	—	—	—	discarded (imaginary frequency)
c245	13.959	−1319.8626553 (5.177)	0.00	−1319.450522	
c246	13.963	−1319.8650831 (3.654)	0.03	−1319.450399	
c247	13.966	−1319.8686896 (1.391)	1.15	−1319.455140	
c248	13.980	−1319.8677599 (1.974)	0.43	−1319.454536	
c249	14.010	−1319.8656311 (3.310)	0.05	−1319.452136	
c250	14.021	−1319.8603998 (6.593)	0.00	−1319.449784	
c251	14.033	−1319.8589534 (7.500)	0.00	−1319.448665	
c252	14.047	−1319.8613044 (6.025)	0.00	−1319.451089	
c253	14.050	—	—	—	clustered (**c271**, RMSD = 0.000 21 Å)
c254	14.091	−1319.8609480 (6.249)	0.00	−1319.447479	
c255	14.097	−1319.8627614 (5.111)	0.00	−1319.453503	
c256	14.141	−1319.8517716 (12.007)	0.00	−1319.441342	
c257	14.147	−1319.8537728 (10.751)	0.00	−1319.441793	
c258	14.150	−1319.8676994 (2.012)	0.40	−1319.454283	
c259	14.159	−1319.8596518 (7.062)	0.00	−1319.443760	
c260	14.163	−1319.8606344 (6.445)	0.00	−1319.448760	
c261	14.182	−1319.8666639 (2.662)	0.13	−1319.452512	
c262	14.186	−1319.8583337 (7.889)	0.00	−1319.445820	
c263	14.311	−1319.8669970 (2.453)	0.19	−1319.455111	
c264	14.352	−1319.8567527 (8.881)	0.00	−1319.445032	
c265	14.355	−1319.8642580 (4.172)	0.01	−1319.451902	
c266	14.360	−1319.8595055 (7.154)	0.00	−1319.445491	
c267	14.370	−1319.8629609 (4.986)	0.00	−1319.451755	
c268	14.377	−1319.8581518 (8.003)	0.00	−1319.444820	
c269	14.405	—	—	—	discarded (imaginary frequency)
c270	14.421	—	—	—	discarded (imaginary frequency)
c271	14.440	−1319.8567337 (8.893)	0.00	−1319.446537	
c272	14.486	−1319.8613667 (5.986)	0.00	−1319.448933	
c273	14.499	−1319.8586650 (7.681)	0.00	−1319.448023	
c274	14.500	—	—	—	clustered (**c273**, RMSD = 0.000 53 Å)
c275	14.542	−1319.8646063 (3.953)	0.02	−1319.453248	
c276	14.542	−1319.8604673 (6.550)	0.00	−1319.449334	
c277	14.585	−1319.8570739 (8.680)	0.00	−1319.444144	
c278	14.679	−1319.8600121 (6.836)	0.00	−1319.449301	
c279	14.680	−1319.8654580 (3.419)	0.04	−1319.449731	
c280	14.691	−1319.8644153 (4.073)	0.01	−1319.452152	
c281	14.726	−1319.8598409 (6.943)	0.00	−1319.448587	
c282	14.737	−1319.8611860 (6.099)	0.00	−1319.445546	
c283	14.750	−1319.8580983 (8.037)	0.00	−1319.448189	
c284	14.803	−1319.8701662 (0.464)	5.50	−1319.455179	
c285	14.832	—	—	—	clustered (**c222**, RMSD = 0.000 71 Å)
c286	14.854	−1319.8594435 (7.193)	0.00	−1319.447266	
c287	14.861	−1319.8582337 (7.952)	0.00	−1319.444248	
c288	14.924	—	—	—	discarded (imaginary frequency)
c289	14.935	—	—	—	discarded (imaginary frequency)
c290	14.950	−1319.8607980 (6.343)	0.00	−1319.449140	
c291	14.952	−1319.8590032 (7.469)	0.00	−1319.448659	
c292	14.954	−1319.8598171 (6.958)	0.00	−1319.443600	
c293	14.972	−1319.8567109 (8.908)	0.00	−1319.446058	

Table S2. Oscillator strengths (f_j), rotational strengths in dipole length form (R_j), and excitation wavelengths (λ_j) for the first 50 excited states of the conformers of (*R*)-diperodon, as calculated by TD-DFT calculations at the PBE0/def2-TZVP/IEFPCM[H_2O] level after DFT optimization at the B97D/def2-TZVP/IEFPCM[H_2O] level.

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c001	**c002**	**c003**	**c005**	**c006**
1	0.0179; −8.3627 (246.39)	0.0164; 6.2154 (246.18)	0.0202; 7.7549 (246.21)	0.0184; −8.4074 (246.50)	0.0193; −6.9010 (246.00)
2	0.0188; 11.0196 (244.46)	0.0193; 5.4865 (244.31)	0.0218; −10.5837 (244.50)	0.0204; 11.3659 (244.43)	0.0201; −2.9549 (244.22)
3	0.5325; −220.2807 (233.74)	0.9421; −118.5613 (233.70)	0.8728; 149.0347 (233.72)	0.5120; −213.4147 (233.86)	1.1007; −46.3212 (233.26)
4	0.5263; 159.3615 (230.55)	0.1689; 95.4984 (230.67)	0.2517; −128.7751 (230.72)	0.5596; 154.1575 (230.59)	0.0495; 20.9642 (230.41)
5	0.0068; 1.4259 (226.83)	0.0015; −0.7594 (222.99)	0.0019; 0.8404 (223.18)	0.0104; 2.0775 (227.62)	0.0021; 0.0604 (221.63)
6	0.0000; −0.0010 (216.00)	0.0000; 0.0176 (212.25)	0.0000; −0.0034 (212.83)	0.0000; −0.0023 (216.47)	0.0000; 0.0023 (211.34)
7	0.0001; 0.1378 (213.11)	0.0000; 0.0289 (210.94)	0.0000; 0.0557 (210.97)	0.0001; 0.1210 (213.08)	0.0000; −0.0738 (209.66)
8	0.0000; 0.0000 (208.44)	0.0001; 0.0066 (205.79)	0.0000; 0.0069 (206.04)	0.0000; −0.0029 (208.48)	0.0001; 0.0047 (204.85)
9	0.2024; −33.9448 (196.75)	0.2528; 59.2399 (197.02)	0.2398; 62.0668 (196.90)	0.2019; −19.8079 (196.89)	0.2498; 21.2133 (196.67)
10	0.0935; 21.4739 (195.47)	0.2359; −43.0985 (195.28)	0.2674; −0.5588 (195.14)	0.0264; 4.5850 (195.81)	0.2515; −77.6714 (195.15)
11	0.1849; 45.5025 (194.96)	0.0027; −0.2517 (192.99)	0.0172; 6.2716 (192.86)	0.2537; 46.6443 (195.00)	1.0511; −45.3543 (192.28)
12	0.5455; −256.2324 (192.40)	0.9181; −209.0616 (192.42)	0.8324; 141.2125 (192.35)	0.5231; −204.8485 (192.44)	0.0036; −1.7917 (192.04)
13	0.0184; 53.2617 (192.20)	0.0525; 79.2908 (192.19)	0.1626; 0.2452 (191.11)	0.0107; 26.5872 (192.15)	0.1646; −6.2953 (190.86)
14	0.7253; 135.6322 (190.76)	0.2816; 157.7922 (190.96)	0.2454; −178.8436 (190.87)	0.7587; 122.4090 (190.75)	0.0679; 63.8924 (190.32)
15	0.0009; 4.9653 (188.07)	0.0035; −12.8702 (187.15)	0.0020; −11.7512 (187.57)	0.0010; 2.7501 (188.52)	0.0020; 12.9434 (187.47)
16	0.0000; −0.0092 (187.80)	0.0095; −13.3841 (186.45)	0.0007; −0.3766 (186.03)	0.0000; −0.0160 (188.03)	0.0003; −0.0033 (185.39)
17	0.0006; 0.0158 (187.58)	0.0001; 0.2326 (186.32)	0.0000; −0.0026 (185.54)	0.0005; −0.0033 (187.65)	0.0015; 4.1030 (184.90)
18	0.0000; −0.0026 (184.44)	0.0000; 0.0022 (185.32)	0.0196; −7.5063 (182.90)	0.0000; −0.0037 (184.55)	0.0000; 0.0148 (184.67)
19	0.0121; 9.9026 (183.60)	0.0000; −0.0111 (182.66)	0.0001; −0.0262 (182.55)	0.0143; 11.2492 (184.10)	0.0050; 4.7666 (181.93)
20	0.0053; 6.2964 (182.42)	0.0147; 9.9247 (182.21)	0.0112; 4.7009 (182.52)	0.0098; 7.6652 (181.83)	0.0000; 0.0129 (181.92)
21	0.1284; −0.0490 (176.58)	0.1224; −2.6155 (176.33)	0.0449; −6.4464 (177.49)	0.0053; −2.4682 (177.45)	0.1306; −0.5468 (176.38)
22	0.0230; −8.8019 (176.22)	0.0320; −15.7618 (175.91)	0.1227; 2.0297 (176.21)	0.1339; −2.4460 (176.71)	0.0029; −1.4658 (175.00)
23	0.0273; 10.5777 (175.77)	0.0502; 4.1061 (174.32)	0.0112; −3.2786 (173.60)	0.0441; 5.4890 (175.84)	0.0460; 10.6489 (174.30)
24	0.0010; −0.2272 (174.15)	0.0004; 1.3381 (173.55)	0.0006; −0.0337 (173.09)	0.0008; −0.3277 (174.07)	0.0136; 1.6469 (172.81)
25	0.0305; 7.7666 (172.35)	0.0013; 1.0383 (173.51)	0.0270; −1.6330 (172.52)	0.0023; −4.0960 (172.04)	0.0066; 1.8964 (172.50)
26	0.0008; −0.4651 (171.69)	0.0015; −2.7845 (172.03)	0.0005; −0.3172 (171.67)	0.0250; 11.8937 (171.80)	0.0028; −1.5777 (171.58)
27	0.0002; −1.2818 (170.16)	0.0026; 2.2367 (171.26)	0.0008; −0.2070 (169.84)	0.0026; −1.6671 (170.78)	0.0017; −0.4111 (171.20)
28	0.0003; 0.2009 (169.49)	0.0011; −1.8910 (169.62)	0.0003; −1.8313 (169.61)	0.0003; −1.4967 (170.55)	0.0007; −1.0693 (168.93)
29	0.0014; −2.9736 (169.15)	0.0006; −0.1420 (169.19)	0.0011; −1.3705 (168.18)	0.0005; 0.0938 (169.30)	0.0007; 2.5041 (168.48)
30	0.0012; 0.1128 (168.33)	0.0001; 0.7057 (168.75)	0.0011; −0.9674 (168.05)	0.0006; −0.9078 (168.67)	0.0014; 0.5583 (168.02)
31	0.0001; 0.4891 (168.26)	0.0015; −1.4159 (167.82)	0.0003; 1.4756 (166.79)	0.0011; −0.0736 (168.43)	0.0001; −0.0656 (166.54)
32	0.0005; 0.5941 (167.25)	0.0026; 3.9368 (167.09)	0.0000; 0.1031 (166.61)	0.0137; −2.8808 (165.95)	0.0004; 0.3659 (165.84)
33	0.0002; 0.2099 (166.11)	0.0026; −0.6276 (166.05)	0.0419; 1.3215 (165.66)	0.0312; 1.1283 (165.78)	0.0462; 4.3087 (165.67)
34	0.0421; −1.3665 (165.65)	0.0424; −1.0474 (165.82)	0.0002; 1.0121 (164.60)	0.0001; 0.9190 (165.58)	0.0006; −0.7311 (165.48)
35	0.0006; −0.0941 (164.68)	0.0006; −3.0380 (165.02)	0.0008; −0.3571 (163.84)	0.0010; −0.1631 (163.80)	0.0007; −1.3865 (164.73)
36	0.0008; 0.0229 (163.20)	0.0004; −1.7066 (164.18)	0.0010; −0.3945 (163.18)	0.0007; 0.7192 (163.46)	0.0006; −2.3848 (163.15)
37	0.0002; −0.7898 (162.80)	0.0005; 1.2231 (163.20)	0.0163; −3.9434 (162.16)	0.0003; −1.3515 (162.81)	0.0009; 0.5976 (162.56)
38	0.0017; −0.1072 (162.48)	0.0004; −0.1036 (162.85)	0.0071; 5.0549 (162.09)	0.0017; −0.0990 (162.64)	0.0008; 0.8734 (162.22)
39	0.0020; 2.3152 (161.80)	0.0192; 6.5530 (162.17)	0.0003; 0.0088 (162.03)	0.0006; 3.3433 (162.16)	0.0034; −0.4586 (161.86)
40	0.0007; −1.1655 (161.59)	0.0008; −1.9604 (162.03)	0.0013; −1.6959 (161.56)	0.0044; 0.8641 (161.99)	0.0010; −6.0434 (161.62)
41	0.0044; 6.9917 (160.87)	0.0010; 0.1119 (161.53)	0.0161; 7.5032 (160.83)	0.0013; −0.5607 (161.42)	0.0003; −1.5129 (161.40)
42	0.0062; −4.8677 (160.82)	0.0015; −0.9229 (161.16)	0.0124; 2.5340 (160.53)	0.0013; −0.7600 (160.99)	0.0086; 0.8175 (160.67)
43	0.0029; 2.0310 (160.51)	0.0055; 0.3121 (160.89)	0.0054; 6.6125 (159.95)	0.0076; −0.9816 (160.78)	0.0248; −2.4949 (160.60)
44	0.0053; −3.2231 (159.94)	0.0005; −1.1367 (160.67)	0.0002; −0.0604 (159.85)	0.0031; 7.0664 (160.28)	0.0003; 0.1125 (160.22)
45	0.0120; 3.4304 (159.92)	0.0011; 2.4771 (160.54)	0.0018; −6.4790 (159.65)	0.0066; −11.2115 (160.23)	0.0070; 2.8612 (159.96)
46	0.0058; −9.3199 (159.70)	0.0126; −0.7399 (160.06)	0.0057; 8.0630 (159.62)	0.0064; 1.1115 (160.12)	0.0004; −1.6486 (159.81)
47	0.0014; 1.6706 (159.56)	0.0072; 1.2153 (159.44)	0.0074; 3.2286 (158.73)	0.0063; −5.1264 (159.62)	0.0008; 0.1675 (159.17)
48	0.0105; 10.5140 (158.58)	0.0081; −5.6468 (158.41)	0.0039; −2.0304 (158.20)	0.0085; 10.3955 (158.60)	0.0095; −5.9036 (158.18)
49	0.0009; −1.6238 (158.23)	0.0113; 17.8137 (158.10)	0.0150; 24.9758 (157.68)	0.0057; −0.1383 (158.51)	0.0034; 8.5213 (157.86)
50	0.0046; 5.4539 (157.68)	0.0050; 7.9117 (157.67)	0.0202; −9.9410 (157.56)	0.0161; 5.9300 (158.10)	0.0647; −2.3305 (157.26)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c008	**c009**	**c010**	**c011**	**c013**
1	0.0194; −6.7187 (245.72)	0.0169; 0.7217 (245.83)	0.0153; 9.2280 (245.98)	0.0201; 8.3827 (246.30)	0.0181; −6.7285 (246.02)
2	0.0202; −4.9228 (244.38)	0.0198; −9.1524 (244.76)	0.0196; −1.2225 (244.46)	0.0227; −13.1127 (244.49)	0.0188; 3.0300 (244.16)
3	1.0972; −54.2085 (233.34)	0.8690; −196.6172 (233.40)	1.0185; −95.7638 (233.62)	0.8628; 190.6939 (233.65)	1.0760; −118.1373 (233.57)
4	0.0578; 16.9210 (230.55)	0.2558; 165.6116 (230.53)	0.0997; 97.2719 (230.88)	0.2616; −164.0617 (230.79)	0.0466; 48.8127 (230.83)
5	0.0002; −0.0908 (221.02)	0.0005; 0.1360 (221.45)	0.0009; −0.5394 (220.51)	0.0017; 0.8668 (223.07)	0.0015; 0.0295 (220.87)
6	0.0000; −0.0076 (210.96)	0.0000; 0.0602 (212.76)	0.0002; 0.1227 (213.43)	0.0000; −0.0062 (212.87)	0.0000; −0.0623 (210.90)
7	0.0000; 0.0728 (210.59)	0.0000; 0.0144 (212.12)	0.0000; 0.0115 (210.50)	0.0000; 0.0601 (211.58)	0.0000; 0.0088 (210.56)
8	0.0000; −0.0095 (205.00)	0.0001; −0.0150 (206.97)	0.0001; 0.0180 (207.26)	0.0000; 0.0073 (206.52)	0.0000; 0.0246 (205.54)
9	0.2594; 29.3519 (196.79)	0.2599; −39.9998 (196.51)	0.2284; 331.4878 (196.54)	0.2318; 51.7055 (196.69)	0.2458; 29.7811 (197.12)
10	0.2534; −31.4531 (195.30)	0.2489; 60.0700 (195.19)	0.2322; −312.8116 (196.25)	0.2688; −10.8426 (195.28)	0.2410; 15.5766 (195.60)
11	1.0707; −15.1580 (192.40)	0.9145; −237.6691 (192.29)	0.0315; −42.2983 (193.37)	0.0228; 11.4183 (192.78)	1.1344; −120.0610 (192.51)
12	0.0003; 0.0960 (191.88)	0.0006; −0.1120 (192.00)	0.9901; −55.6717 (192.75)	0.8256; 182.5207 (192.40)	0.0011; 1.6472 (191.82)
13	0.0531; 2.6727 (191.03)	0.0520; 22.7720 (191.00)	0.0443; 3.8373 (191.80)	0.2989; −85.7588 (191.28)	0.0809; 49.8330 (191.36)
14	0.1493; −32.3925 (190.93)	0.3520; 165.9617 (190.82)	0.1043; 116.1482 (191.59)	0.0819; −112.3491 (191.08)	0.0044; −22.4226 (191.18)
15	0.0161; 12.6693 (187.12)	0.0000; 0.0006 (187.14)	0.0672; −19.9685 (188.44)	0.0007; −0.4346 (187.62)	0.0307; 21.2518 (188.82)
16	0.0023; −3.5860 (186.57)	0.0000; −0.0038 (185.38)	0.0004; 0.2604 (187.83)	0.0007; −0.0196 (186.44)	0.0068; −22.3367 (187.01)
17	0.0000; −0.0164 (186.06)	0.0001; 1.9466 (185.28)	0.0011; 6.2234 (187.42)	0.0438; −28.6391 (186.09)	0.0006; −0.3703 (186.48)
18	0.0006; 9.4514 (185.66)	0.0000; −0.0005 (183.01)	0.0000; 0.0081 (184.59)	0.0000; −0.0069 (185.58)	0.0000; 0.0013 (184.37)
19	0.0000; 0.0103 (184.65)	0.0005; −0.3624 (181.86)	0.0000; 0.0001 (183.43)	0.0000; −0.0130 (182.88)	0.0000; 0.0060 (182.59)
20	0.0000; −0.0006 (182.01)	0.0019; 2.9239 (180.96)	0.0131; 8.9949 (181.33)	0.0127; 8.3631 (182.12)	0.0389; 14.8326 (181.58)
21	0.0074; 0.9677 (177.30)	0.0097; −5.7601 (176.30)	0.1181; −6.7707 (177.87)	0.0590; −3.9774 (177.03)	0.1072; −16.7865 (176.24)
22	0.1274; 8.3565 (176.28)	0.1194; 12.6114 (176.19)	0.1116; −8.1734 (176.37)	0.1214; 0.1558 (176.36)	0.0097; 8.6516 (175.36)
23	0.0717; 9.1343 (173.94)	0.0629; −2.5242 (174.78)	0.0071; 4.5954 (175.74)	0.0192; −6.2086 (174.27)	0.0668; 14.1495 (174.78)
24	0.0002; −0.0996 (172.49)	0.0003; −0.5282 (172.94)	0.0029; −2.2296 (173.80)	0.0006; −0.1333 (172.98)	0.0026; −4.4983 (172.76)
25	0.0008; −0.7073 (172.25)	0.0006; 0.2750 (172.33)	0.0005; −0.0379 (173.17)	0.0158; −0.1123 (172.43)	0.0007; −0.4567 (172.50)
26	0.0013; −0.7503 (172.17)	0.0003; −1.2994 (171.92)	0.0071; 1.4159 (172.39)	0.0015; −0.2122 (172.13)	0.0029; −1.0835 (172.45)
27	0.0005; −0.7629 (171.42)	0.0094; 4.0746 (171.69)	0.0036; 0.8613 (171.97)	0.0021; −0.0286 (170.15)	0.0050; 2.9687 (170.97)
28	0.0002; 1.0541 (170.93)	0.0005; 1.1632 (170.17)	0.0003; −0.2263 (170.82)	0.0003; 0.0595 (169.07)	0.0021; −0.5676 (169.40)
29	0.0011; −0.7492 (167.55)	0.0004; −0.2831 (168.08)	0.0010; −0.6510 (168.59)	0.0008; 2.3773 (168.81)	0.0003; −0.1632 (169.19)
30	0.0016; 0.8174 (167.40)	0.0013; −0.0408 (167.83)	0.0014; −0.0849 (168.23)	0.0011; −0.3571 (168.22)	0.0013; 0.8731 (168.05)
31	0.0073; −0.0580 (166.23)	0.0015; −0.2805 (167.54)	0.0002; 1.1381 (167.47)	0.0008; −0.3284 (166.58)	0.0038; −0.0385 (167.84)
32	0.0011; −0.3012 (165.87)	0.0005; −0.4370 (166.55)	0.0045; 0.6276 (167.28)	0.0001; 0.3450 (166.35)	0.0003; −1.0399 (166.44)
33	0.0404; −2.8568 (165.48)	0.0013; −2.3575 (166.31)	0.0067; 9.4240 (166.61)	0.0041; −5.3846 (165.68)	0.0419; −1.7204 (166.09)
34	0.0006; 2.7972 (164.80)	0.0315; 10.9447 (165.23)	0.0009; 1.4603 (165.75)	0.0361; 6.7197 (165.54)	0.0022; −1.9322 (165.48)
35	0.0019; 0.0313 (164.07)	0.0058; −8.8288 (164.96)	0.0147; 24.4790 (165.42)	0.0019; 1.4888 (165.00)	0.0012; 0.4425 (165.20)
36	0.0002; 0.0776 (163.56)	0.0002; 0.2226 (164.81)	0.0300; −33.2920 (165.40)	0.0039; 0.5925 (164.36)	0.0022; −0.2731 (163.69)
37	0.0003; −0.1777 (163.34)	0.0008; −1.5498 (163.64)	0.0007; −1.5416 (164.38)	0.0024; 0.6710 (163.88)	0.0041; 0.6392 (163.13)
38	0.0014; −0.5202 (163.06)	0.0006; 0.4604 (162.65)	0.0008; −1.6707 (163.41)	0.0005; 0.5451 (162.65)	0.0009; 2.2891 (162.86)
39	0.0006; 0.9944 (162.26)	0.0005; 1.2853 (162.15)	0.0011; −1.0153 (161.62)	0.0105; −0.3915 (161.83)	0.0005; 0.7653 (162.73)
40	0.0002; 0.4598 (162.01)	0.0003; 0.1388 (161.85)	0.0021; 3.4691 (161.51)	0.0004; −0.9177 (161.63)	0.0276; −0.6468 (162.27)
41	0.0003; 0.1562 (161.34)	0.0005; 0.5881 (161.09)	0.0008; −1.6122 (161.27)	0.0033; 6.0072 (161.14)	0.0139; 3.9019 (161.00)
42	0.0085; −1.2798 (160.83)	0.0002; −0.1014 (161.03)	0.0054; 0.5514 (160.92)	0.0004; −2.2436 (161.05)	0.0008; 0.5164 (160.89)
43	0.0150; −0.8213 (160.46)	0.0003; 0.0510 (160.68)	0.0002; −0.5678 (160.57)	0.0123; 3.8017 (160.87)	0.0124; −0.0339 (160.47)
44	0.0154; 6.5381 (159.93)	0.0059; −2.6846 (160.09)	0.0027; 1.8983 (160.39)	0.0235; 2.8460 (160.42)	0.0004; 3.0141 (160.30)
45	0.0050; −1.0205 (159.45)	0.0053; 4.1125 (159.90)	0.0009; −3.1371 (160.37)	0.0010; 1.4388 (160.18)	0.0082; 2.5848 (160.14)
46	0.0022; −0.3266 (159.17)	0.0269; 10.6528 (159.01)	0.0046; 0.4581 (160.17)	0.0001; 0.0926 (159.68)	0.0022; 1.4413 (159.44)
47	0.0008; 0.0510 (159.03)	0.0010; −2.2663 (158.90)	0.0004; −0.4976 (158.63)	0.0036; −5.0587 (159.42)	0.0043; 4.8502 (158.71)
48	0.0070; 4.4129 (158.21)	0.0036; 0.9433 (158.00)	0.0040; −1.7832 (158.48)	0.0147; −15.4591 (158.34)	0.0107; 8.0836 (158.29)
49	0.0037; 9.5229 (157.81)	0.0024; 4.0574 (157.63)	0.0310; −19.1087 (158.34)	0.0006; 1.7707 (158.29)	0.0110; 18.3779 (158.08)
50	0.0638; −1.9408 (157.31)	0.0304; −26.6348 (157.04)	0.0231; −4.3723 (158.12)	0.0195; 9.2181 (158.24)	0.0043; 3.6925 (157.71)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c015	**c016**	**c017**	**c018**	**c020**
1	0.0157; 16.9946 (247.47)	0.0206; −7.9260 (245.87)	0.0174; −11.5370 (246.75)	0.0190; −9.9121 (245.60)	0.0153; −5.6494 (247.36)
2	0.0242; −2.1943 (244.70)	0.0220; 14.6297 (244.65)	0.0220; −9.5637 (244.46)	0.0202; −4.2079 (244.43)	0.0059; 6.1839 (244.80)
3	0.0591; −11.3255 (236.15)	0.7886; 196.0143 (233.61)	0.5045; 102.3680 (233.90)	1.1313; −51.7539 (233.41)	0.0091; 14.7539 (241.93)
4	0.0015; 3.1673 (234.08)	0.3211; −155.6097 (230.39)	0.5429; −105.3433 (230.41)	0.0276; 12.8126 (230.75)	0.0686; −79.4529 (236.85)
5	0.7004; −51.9813 (230.34)	0.0018; 0.3853 (222.67)	0.0008; −0.2333 (227.95)	0.0001; −0.0359 (219.93)	0.1130; −417.7516 (233.83)
6	0.0092; 2.4527 (227.48)	0.0000; 0.0097 (212.67)	0.0000; −0.0010 (216.91)	0.0000; 0.0529 (211.93)	0.6456; 523.3167 (230.27)
7	0.0570; −12.3425 (224.93)	0.0000; 0.0457 (211.54)	0.0000; 0.0027 (212.76)	0.0000; −0.0060 (210.12)	0.0052; 3.0251 (217.23)
8	0.0069; 0.7378 (222.72)	0.0000; 0.0047 (206.41)	0.0000; −0.0009 (208.62)	0.0000; 0.0032 (205.69)	0.0040; −3.7640 (212.25)
9	0.0690; −64.2282 (204.41)	0.2384; −2.0843 (196.96)	0.2241; −47.4280 (197.04)	0.2526; 51.3945 (196.65)	0.0266; −9.5598 (208.34)
10	0.0238; −20.6406 (202.15)	0.2808; −44.0589 (195.04)	0.0001; 0.1632 (195.86)	0.2481; −74.2146 (195.72)	0.0289; 0.2110 (203.50)
11	0.0335; 80.1551 (201.74)	0.0207; −13.3952 (192.77)	0.2627; −69.8137 (194.79)	1.1799; −4.1088 (192.42)	0.1415; 129.1586 (198.81)
12	0.1486; 59.7817 (198.42)	0.7328; 228.8078 (192.57)	0.5620; 269.7194 (192.47)	0.0004; −3.6259 (191.69)	0.1513; −196.0630 (196.98)
13	0.0296; 112.6334 (195.91)	0.3676; −180.1192 (190.81)	0.0722; 39.0820 (191.37)	0.0024; −0.9294 (191.45)	0.1505; −82.9333 (194.62)
14	0.0406; −12.8379 (195.76)	0.1713; 29.1134 (190.64)	0.6479; −231.4680 (190.63)	0.0607; −20.7422 (191.29)	0.2074; −145.2862 (193.11)
15	0.1707; −210.1137 (194.28)	0.0006; 0.1792 (186.55)	0.0001; −0.0389 (188.28)	0.0235; 12.4742 (187.74)	0.3500; 174.4118 (192.58)
16	0.7006; 46.7071 (191.36)	0.0022; −2.2108 (186.21)	0.0018; −12.3761 (187.91)	0.0000; 0.0089 (186.98)	0.2339; 119.2010 (190.91)
17	0.3021; 96.2399 (190.33)	0.0001; −1.4917 (186.07)	0.0000; −0.0147 (187.36)	0.0003; 4.2141 (185.76)	0.0088; −13.1835 (190.62)
18	0.0280; −42.2341 (189.00)	0.0000; 0.0001 (185.70)	0.0297; 13.3398 (186.25)	0.0041; 8.5315 (185.57)	0.1959; 29.6984 (188.59)
19	0.0333; −17.9255 (184.62)	0.0000; −0.0008 (182.90)	0.0000; −0.0097 (184.65)	0.0000; 0.0083 (184.35)	0.0803; −44.4813 (186.42)
20	0.0405; 27.2373 (182.30)	0.0049; 5.8516 (182.42)	0.0150; 10.2916 (183.69)	0.0000; −0.0055 (182.44)	0.0982; 43.6603 (184.17)
21	0.0166; −10.9241 (181.48)	0.0001; −0.0895 (179.55)	0.0028; −0.7628 (176.64)	0.0338; 4.8146 (176.73)	0.0236; 35.8005 (182.39)
22	0.1299; 42.4329 (178.30)	0.1387; −12.4824 (176.86)	0.1328; 7.8910 (176.43)	0.1273; 1.4423 (176.09)	0.0363; 19.2307 (178.63)
23	0.0057; −1.3026 (177.11)	0.0258; 1.5003 (174.42)	0.0010; −0.0106 (175.20)	0.0645; 7.8357 (174.43)	0.1000; −32.7320 (177.84)
24	0.0965; −50.5745 (176.40)	0.0425; 3.2792 (173.18)	0.0021; −0.0354 (174.18)	0.0007; 0.6475 (172.87)	0.0124; 9.0128 (177.09)
25	0.0019; −2.3551 (173.66)	0.0000; −0.0998 (172.99)	0.0453; 5.9326 (173.44)	0.0004; −0.1485 (172.32)	0.0025; 1.3863 (173.26)
26	0.0001; −0.1818 (173.34)	0.0006; 0.0520 (172.43)	0.0013; −2.0167 (172.15)	0.0006; −0.1450 (172.07)	0.0063; −1.1226 (172.20)
27	0.0046; 0.3765 (171.74)	0.0010; 1.5268 (171.32)	0.0001; −0.0984 (171.01)	0.0012; 2.3862 (170.73)	0.0033; −4.7080 (171.42)
28	0.0022; 3.5980 (170.32)	0.0013; 0.0000 (169.55)	0.0077; 2.8497 (170.46)	0.0004; 0.9741 (169.82)	0.0039; −0.1376 (171.11)
29	0.0566; 13.2788 (169.41)	0.0004; −0.2235 (168.61)	0.0006; −2.3178 (170.33)	0.0008; −0.5047 (168.49)	0.0250; −1.6672 (170.82)
30	0.0022; 6.0893 (168.60)	0.0013; 0.1776 (167.59)	0.0003; −0.4420 (169.56)	0.0013; 0.1545 (167.49)	0.0030; −4.0087 (169.72)
31	0.0237; −14.2409 (168.32)	0.0106; −5.8467 (166.65)	0.0011; −0.9478 (168.16)	0.0012; −0.9237 (167.36)	0.0027; 1.6242 (168.76)
32	0.0146; −2.9406 (167.88)	0.0008; 0.3020 (166.01)	0.0001; 0.9255 (166.72)	0.0362; −1.6389 (165.49)	0.0002; −0.2989 (167.75)
33	0.0362; −5.6644 (167.25)	0.0285; 5.1279 (165.88)	0.0455; −4.1941 (165.98)	0.0010; −1.0134 (165.21)	0.0007; 0.0663 (167.23)
34	0.0086; −6.6135 (166.68)	0.0009; 2.3096 (165.41)	0.0011; 2.4021 (165.95)	0.0019; 0.5139 (165.13)	0.0143; 0.5751 (166.50)
35	0.0196; 0.5666 (166.15)	0.0089; −5.1420 (164.81)	0.0003; 0.5727 (164.82)	0.0063; −1.2913 (164.89)	0.0011; −0.4309 (165.89)
36	0.0074; 0.4769 (165.33)	0.0010; 0.6217 (164.06)	0.0136; −7.4550 (163.55)	0.0011; 0.1498 (164.79)	0.0015; 2.6679 (165.41)
37	0.0032; −1.1972 (164.60)	0.0004; 0.5454 (163.72)	0.0004; 0.1101 (163.44)	0.0036; 4.0195 (163.71)	0.0014; −0.2464 (165.03)
38	0.0033; 1.8153 (164.34)	0.0002; 0.8060 (162.66)	0.0047; −3.6219 (163.30)	0.0018; −2.7487 (163.10)	0.0075; −13.1022 (164.56)
39	0.0070; 2.1063 (163.86)	0.0001; 0.4656 (162.23)	0.0017; −3.4321 (162.65)	0.0004; 2.1454 (162.72)	0.0110; 31.4662 (163.92)
40	0.0030; −2.5324 (163.58)	0.0042; −1.0286 (161.41)	0.0019; 0.6713 (162.44)	0.0003; 0.7315 (161.84)	0.0057; −1.3869 (163.54)
41	0.0048; 0.8946 (163.17)	0.0018; 0.4397 (160.92)	0.0383; 13.1535 (162.13)	0.0008; 1.6027 (161.30)	0.0363; −26.0986 (163.39)
42	0.0114; −4.0690 (162.95)	0.0003; 0.2725 (160.56)	0.0007; −4.4306 (161.94)	0.0004; −1.4908 (161.01)	0.0258; 4.4997 (163.22)
43	0.0026; −5.8629 (162.34)	0.0010; −1.7636 (160.44)	0.0038; 3.1932 (161.29)	0.0008; 0.6432 (160.96)	0.0136; −4.0319 (162.94)
44	0.0011; −0.2889 (161.64)	0.0164; 0.8160 (159.99)	0.0178; −4.7208 (161.00)	0.0282; 5.4727 (159.59)	0.0536; 37.7889 (162.65)
45	0.0041; 2.2291 (161.42)	0.0013; 0.1702 (159.43)	0.0024; −4.0222 (160.81)	0.0025; 2.8353 (158.89)	0.0019; −1.0141 (161.99)
46	0.0115; 5.1053 (160.87)	0.0000; −0.0241 (159.07)	0.0011; 2.1277 (160.40)	0.0031; −0.5631 (158.62)	0.0034; −4.4361 (161.58)
47	0.0297; −6.3385 (160.24)	0.0400; 1.8540 (158.24)	0.0048; 3.2683 (158.76)	0.0054; 1.3974 (158.07)	0.0129; 0.3239 (160.80)
48	0.0301; −1.4815 (160.14)	0.0055; −6.6616 (158.13)	0.0006; −0.7684 (158.29)	0.0028; 1.8482 (158.00)	0.0124; 28.4434 (160.31)
49	0.0294; −11.7192 (159.74)	0.0001; −0.4197 (157.62)	0.0086; −11.7621 (157.97)	0.0362; 21.1529 (157.25)	0.0599; −36.6142 (160.26)
50	0.0017; −4.3663 (159.48)	0.0481; −41.0587 (157.34)	0.0153; 25.2191 (157.95)	0.0678; 13.0780 (157.17)	0.0010; 3.9020 (160.04)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c021	**c022**	**c023**	**c024**	**c026**
1	0.0174; −5.5212 (246.29)	0.0178; −0.1058 (244.44)	0.0217; −4.2564 (246.82)	0.0154; −7.8307 (245.50)	0.0286; 6.0104 (249.48)
2	0.0110; 8.2566 (243.20)	0.0116; −3.3649 (242.64)	0.0228; −7.1039 (244.42)	0.0176; 6.5870 (244.42)	0.0187; 6.0696 (244.45)
3	0.3426; −662.7031 (232.98)	0.6294; 33.7415 (232.87)	0.7778; 41.7299 (233.56)	0.1799; 343.8345 (233.92)	0.0523; 261.3872 (236.68)
4	0.2520; 217.8791 (232.38)	0.2664; −89.4919 (227.65)	0.3343; −38.5211 (230.58)	0.6362; −251.7578 (231.61)	0.1523; −33.6544 (234.86)
5	0.3599; 326.9878 (229.97)	0.0000; 0.0223 (216.70)	0.0019; 0.0655 (224.94)	0.0607; −24.2117 (228.42)	0.4307; −188.3857 (231.84)
6	0.0022; 1.3444 (221.20)	0.0001; 0.0936 (212.73)	0.0000; −0.0019 (214.41)	0.0043; −1.0000 (218.99)	0.1741; −74.5758 (230.02)
7	0.0017; 0.0836 (214.06)	0.0001; 0.0155 (209.03)	0.0000; 0.0059 (209.10)	0.0028; −0.6446 (217.57)	0.0010; 2.7229 (226.05)
8	0.0004; 0.1009 (208.98)	0.0001; −0.0637 (206.47)	0.0000; 0.0079 (205.43)	0.0009; 0.6594 (214.71)	0.0076; 5.1461 (222.18)
9	0.0560; −23.5988 (198.56)	0.2667; 49.5948 (196.98)	0.2571; 33.5675 (196.93)	0.0223; 12.2132 (200.34)	0.0512; −14.1535 (203.21)
10	0.2873; 50.6335 (197.82)	0.2546; −21.1455 (195.65)	0.2635; −91.2437 (194.82)	0.2699; 124.0221 (197.69)	0.0469; −52.7362 (201.51)
11	0.1333; 55.1054 (195.09)	0.0002; 0.1263 (192.95)	0.0072; −4.7489 (193.42)	0.2059; −317.2571 (196.73)	0.0270; −34.6166 (200.14)
12	0.4244; −435.7930 (193.38)	0.8239; 103.7515 (192.61)	0.7170; 129.2399 (192.34)	0.1430; 272.5791 (193.26)	0.0965; 92.9995 (198.66)
13	0.0261; 12.1090 (192.24)	0.2567; −185.1299 (191.65)	0.0209; 70.0941 (192.07)	0.2441; −35.2608 (192.38)	0.2356; 52.3844 (195.68)
14	0.0304; −54.9450 (191.45)	0.0001; −0.0472 (187.69)	0.5451; −136.6548 (190.64)	0.0467; 120.3107 (192.06)	0.1061; 189.9109 (193.91)
15	0.1004; 34.7870 (191.11)	0.0509; 69.4524 (186.56)	0.0016; −9.2600 (187.57)	0.5561; −283.2886 (191.44)	0.3704; −249.8142 (193.77)
16	0.6589; 371.0754 (190.90)	0.0069; 14.2460 (186.49)	0.0000; −0.0012 (186.03)	0.1434; 119.2461 (190.15)	0.0527; 170.6421 (192.11)
17	0.0192; 14.1303 (188.33)	0.0014; −13.9357 (185.43)	0.0010; 1.3153 (185.10)	0.0746; −7.6937 (189.21)	0.4673; −17.9469 (189.99)
18	0.0003; 0.7192 (187.81)	0.0000; −0.0085 (184.95)	0.0002; −0.0456 (184.80)	0.0038; −14.1960 (187.81)	0.1095; −119.8845 (189.31)
19	0.0098; 22.7733 (185.59)	0.0000; 0.0018 (184.93)	0.0123; 8.3110 (182.94)	0.0010; −0.9023 (186.14)	0.0095; 4.4048 (184.30)
20	0.0078; −9.0992 (181.63)	0.0006; 1.8214 (184.77)	0.0000; −0.0034 (182.24)	0.0005; −1.5802 (184.06)	0.0035; −2.2818 (182.37)
21	0.0380; −4.9165 (181.22)	0.0204; −17.0288 (180.28)	0.0120; −3.7022 (177.38)	0.0263; −30.5522 (178.75)	0.0876; 27.0050 (181.24)
22	0.0777; −7.5245 (179.67)	0.1277; 3.6719 (176.35)	0.1243; 5.1928 (176.31)	0.0376; 19.9104 (178.20)	0.0658; 31.9253 (178.94)
23	0.0543; 5.5887 (176.90)	0.0025; −2.5129 (174.23)	0.0193; −0.7150 (174.61)	0.1461; 47.1439 (177.81)	0.1391; −54.1538 (178.54)
24	0.0006; −1.7276 (174.96)	0.0004; 0.7493 (172.65)	0.0086; 0.4454 (174.46)	0.0139; 1.1131 (176.68)	0.0031; 0.2480 (175.14)
25	0.0008; 1.5093 (173.73)	0.0037; 1.6213 (172.10)	0.0237; 3.2428 (173.34)	0.0109; −6.3136 (174.67)	0.0089; −9.2080 (171.92)
26	0.0435; −0.2759 (172.88)	0.0003; 0.9429 (171.39)	0.0010; 0.4391 (171.50)	0.0016; −1.2856 (171.15)	0.0050; 3.4413 (170.28)
27	0.0073; 2.2530 (172.02)	0.0008; −1.8089 (171.06)	0.0078; −6.6975 (171.31)	0.0391; −2.3801 (170.68)	0.0040; −2.4572 (169.98)
28	0.0061; −4.7347 (170.28)	0.0305; 9.4993 (169.46)	0.0002; 0.1777 (170.65)	0.0068; −1.4459 (169.87)	0.0038; 3.7106 (169.87)
29	0.0173; −4.7895 (169.62)	0.0042; −3.1508 (169.04)	0.0014; 2.8998 (168.87)	0.0015; 1.4549 (169.44)	0.0463; −4.2226 (169.26)
30	0.0008; 1.2187 (169.41)	0.0018; −0.4662 (167.20)	0.0004; 0.0884 (168.45)	0.0004; −1.9850 (168.84)	0.0017; 5.3720 (168.72)
31	0.0003; 1.6673 (168.95)	0.0327; −10.2522 (167.08)	0.0012; −0.7658 (167.93)	0.0008; −0.5113 (168.01)	0.0085; −39.4858 (167.37)
32	0.0516; −8.4306 (166.54)	0.0054; 3.4782 (166.63)	0.0002; 0.8294 (167.05)	0.0009; 1.5951 (167.84)	0.0028; −6.1730 (167.35)
33	0.0144; −0.8448 (165.33)	0.0171; 15.1119 (166.45)	0.0009; −1.2305 (166.28)	0.0161; 12.8378 (166.55)	0.0352; 27.2237 (166.77)
34	0.0129; −2.8574 (165.23)	0.0145; 25.7509 (166.05)	0.0447; 0.1376 (165.80)	0.0465; −13.6600 (166.36)	0.0020; −4.0582 (166.26)
35	0.0023; −2.4599 (164.84)	0.0305; −6.4433 (165.61)	0.0008; 1.1940 (162.90)	0.0746; −16.3697 (165.85)	0.0112; −9.5570 (165.38)
36	0.0003; 0.9813 (164.54)	0.0253; 2.4077 (165.14)	0.0006; 3.6747 (162.58)	0.0045; 1.3102 (165.66)	0.0038; −3.0850 (165.18)
37	0.0013; 1.7580 (164.25)	0.0117; 9.3910 (164.67)	0.0034; −4.9865 (162.46)	0.0053; 2.2901 (165.30)	0.0283; 1.5569 (165.05)
38	0.0014; −2.2175 (164.07)	0.0026; −3.2669 (164.20)	0.0056; 6.0540 (161.91)	0.0018; 3.9523 (164.90)	0.0160; 1.1471 (164.98)
39	0.1128; 5.4080 (162.89)	0.0003; −0.3561 (164.04)	0.0067; −0.4606 (161.88)	0.0072; 1.3373 (164.86)	0.0008; 4.0012 (164.32)
40	0.0003; −1.3186 (162.52)	0.0712; 48.8470 (163.47)	0.0068; −2.3127 (161.81)	0.0039; 0.1350 (162.44)	0.0012; 0.6610 (163.79)
41	0.0006; 1.9644 (162.44)	0.0451; −29.6525 (162.61)	0.0002; 0.0662 (161.66)	0.0123; −12.1185 (162.29)	0.0077; 7.1462 (162.75)
42	0.0086; 4.0336 (161.54)	0.0408; −28.2519 (162.45)	0.0014; −3.1866 (160.64)	0.0110; 10.8937 (162.13)	0.0057; −4.5899 (162.13)
43	0.0087; −2.6949 (161.38)	0.0134; 5.3207 (161.58)	0.0006; 0.1968 (160.54)	0.0339; −6.5732 (161.72)	0.0056; −2.5884 (161.86)
44	0.0007; 1.5633 (160.85)	0.0034; 0.4515 (161.06)	0.0027; 1.1512 (160.47)	0.0017; 0.5375 (161.21)	0.0073; −1.7200 (161.73)
45	0.0007; 0.4155 (160.72)	0.0079; 1.3435 (160.76)	0.0402; −2.2551 (159.04)	0.0030; −0.9770 (160.97)	0.0048; 3.6145 (161.55)
46	0.0003; 0.1935 (160.41)	0.0034; −1.8884 (159.47)	0.0087; −3.9482 (158.42)	0.0006; −1.2957 (160.76)	0.0078; 0.2899 (161.47)
47	0.0002; 0.1866 (160.31)	0.0109; 2.8779 (159.38)	0.0094; 6.7443 (158.26)	0.0007; −0.4659 (160.50)	0.0019; −1.9869 (160.98)
48	0.0255; 9.6723 (159.54)	0.0038; −2.7581 (158.63)	0.0102; −2.1945 (157.76)	0.0041; −0.2081 (159.97)	0.0124; −12.3929 (160.94)
49	0.0006; −2.5434 (159.33)	0.0023; 8.7921 (158.41)	0.0204; 15.2257 (157.73)	0.0053; 0.3679 (159.89)	0.0016; −0.5470 (160.58)
50	0.0136; 5.4344 (158.68)	0.0009; 3.3194 (158.23)	0.0047; 15.3601 (157.41)	0.0022; 3.9685 (159.53)	0.0027; −6.6076 (160.34)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c028	**c031**	**c032**	**c034**	**c035**
1	0.0215; 2.6760 (246.90)	0.0191; 4.0032 (246.28)	0.0156; 19.0996 (247.56)	0.0178; −1.3135 (244.46)	0.0207; 3.0865 (246.68)
2	0.0185; 4.6136 (244.11)	0.0088; −3.0799 (242.37)	0.0258; −3.5076 (244.65)	0.0109; 2.4540 (242.58)	0.0216; 0.5535 (244.30)
3	0.5709; 19.0233 (233.37)	0.4894; 475.4519 (232.14)	0.0574; −12.1670 (236.32)	0.6300; −86.9151 (232.80)	1.0277; −24.4642 (233.25)
4	0.4978; −22.3281 (230.52)	0.5149; −308.0613 (229.61)	0.0018; 3.5287 (234.06)	0.2407; 85.2932 (227.11)	0.1175; 2.9947 (230.49)
5	0.0178; −1.0612 (226.65)	0.0026; −0.1257 (225.47)	0.7123; −51.5841 (230.50)	0.0003; 0.0041 (216.65)	0.0024; −0.0323 (223.28)
6	0.0000; 0.0026 (216.24)	0.0003; −0.3540 (217.55)	0.0115; 1.6606 (227.82)	0.0002; −0.0160 (213.98)	0.0000; −0.0006 (212.87)
7	0.0001; −0.0374 (209.71)	0.0002; 0.0871 (210.90)	0.0597; −12.9476 (225.15)	0.0000; 0.0375 (213.78)	0.0000; 0.0489 (207.90)
8	0.0000; 0.0034 (206.27)	0.0000; 0.0000 (205.64)	0.0088; 0.6458 (222.46)	0.0001; 0.0764 (203.56)	0.0000; 0.0020 (204.16)
9	0.2500; −30.0606 (196.80)	0.3440; −19.0819 (196.36)	0.0676; −71.4614 (204.56)	0.2327; 35.2949 (196.80)	0.2414; 2.1899 (196.79)
10	0.1487; −4.2813 (195.21)	0.1698; −27.6647 (195.35)	0.0229; −13.2999 (202.60)	0.2066; −48.9604 (195.51)	0.2703; 30.7954 (194.76)
11	0.1201; 2.9068 (194.15)	0.0133; −0.3325 (194.19)	0.0365; 75.9740 (202.07)	0.4851; −12.6113 (192.99)	0.0517; 16.2133 (192.44)
12	0.4893; 72.1231 (192.35)	0.5416; 586.0368 (192.57)	0.1500; 62.5141 (198.47)	0.4765; 69.1118 (192.01)	0.9008; −128.8089 (192.24)
13	0.1021; −218.1569 (192.13)	0.6382; −525.7577 (191.11)	0.0099; 62.5877 (196.01)	0.0001; −0.0284 (190.39)	0.0002; 0.9809 (191.84)
14	0.7098; 146.2394 (190.54)	0.0424; 40.3248 (190.96)	0.0568; 30.4992 (195.84)	0.0004; −0.3696 (189.75)	0.3478; 59.4751 (190.60)
15	0.0037; 16.1345 (187.99)	0.0082; 3.9795 (189.19)	0.1734; −183.6744 (194.43)	0.0001; −0.0955 (188.45)	0.0009; 2.7532 (187.29)
16	0.0000; 0.0218 (187.28)	0.0008; 0.1294 (188.51)	0.7448; 35.2199 (191.38)	0.1319; −95.4568 (187.78)	0.0004; 0.0745 (186.31)
17	0.0017; 0.4100 (185.50)	0.0358; −22.3697 (188.46)	0.2400; 91.9089 (190.27)	0.0103; −1.6740 (187.66)	0.0000; 0.0012 (185.05)
18	0.0012; −0.1282 (183.60)	0.0000; 0.0161 (185.22)	0.0539; −48.1431 (189.52)	0.0072; −9.0871 (183.30)	0.0006; 0.0729 (184.05)
19	0.0000; 0.0217 (183.17)	0.0331; −51.4203 (183.79)	0.0280; −18.6574 (184.39)	0.0149; 11.5133 (182.22)	0.0073; 6.4204 (182.05)
20	0.0022; 3.4462 (182.04)	0.0112; 12.4256 (182.34)	0.0106; 8.8942 (181.60)	0.0000; −0.0296 (181.84)	0.0000; 0.0029 (181.38)
21	0.1482; 19.9402 (176.87)	0.0396; −5.8580 (178.59)	0.0729; 13.4436 (181.38)	0.0035; 13.7752 (178.39)	0.1289; 1.9649 (176.32)
22	0.0040; −14.6917 (176.52)	0.0496; 26.7929 (177.75)	0.1100; 39.9649 (178.09)	0.0585; 2.6940 (177.00)	0.0003; 0.1565 (175.26)
23	0.0026; 1.4416 (176.06)	0.0251; −8.2377 (177.09)	0.0039; −0.4554 (177.11)	0.0627; −8.7099 (175.74)	0.0062; 0.9869 (174.34)
24	0.0008; 0.2392 (174.78)	0.0056; 1.6961 (173.52)	0.0999; −51.5148 (176.37)	0.0124; 8.2981 (174.89)	0.0005; −0.2414 (174.14)
25	0.0452; −5.4059 (172.55)	0.0046; 0.4901 (172.94)	0.0028; −3.2407 (173.83)	0.0008; −0.3322 (171.96)	0.0554; −1.2837 (173.05)
26	0.0019; −1.5531 (171.35)	0.0317; −0.3541 (172.44)	0.0001; −0.1043 (173.39)	0.0008; −0.0083 (170.98)	0.0016; −1.2586 (171.65)
27	0.0003; 0.2938 (169.51)	0.0009; −0.8658 (170.52)	0.0017; 0.1006 (172.02)	0.0383; −4.3176 (170.23)	0.0007; 1.2866 (170.64)
28	0.0012; 2.2772 (169.09)	0.0025; −1.6165 (170.37)	0.0002; 0.1987 (170.25)	0.0027; −1.6866 (169.25)	0.0008; 0.3562 (169.89)
29	0.0009; −1.0715 (168.88)	0.0060; 1.9628 (168.91)	0.0599; 19.1295 (169.56)	0.0129; 5.1177 (169.18)	0.0005; −0.5789 (168.65)
30	0.0014; 1.1326 (168.25)	0.0011; 0.4972 (168.00)	0.0002; 1.7722 (168.96)	0.0012; −0.8277 (168.08)	0.0016; −0.1082 (167.79)
31	0.0003; 0.1334 (167.62)	0.0007; −0.4955 (167.65)	0.0276; −4.8679 (168.77)	0.0724; −29.8985 (167.59)	0.0006; 0.3183 (167.65)
32	0.0001; −0.3144 (166.22)	0.0163; 0.4777 (166.04)	0.0213; −18.0777 (167.99)	0.0005; 3.0449 (166.84)	0.0015; 1.1039 (167.45)
33	0.0464; −0.6300 (165.93)	0.0001; −1.6150 (165.28)	0.0142; −5.2604 (167.72)	0.0042; −8.2568 (166.51)	0.0003; 0.3709 (166.28)
34	0.0006; −0.9208 (165.77)	0.0353; −20.7702 (164.79)	0.0263; 1.7581 (167.39)	0.0368; −0.4074 (165.73)	0.0007; −2.5016 (166.12)
35	0.0002; 0.5713 (163.51)	0.0074; −0.7412 (164.57)	0.0130; −9.6690 (166.59)	0.0356; 33.0864 (165.33)	0.0463; 2.0519 (165.68)
36	0.0003; −0.1129 (162.60)	0.0219; 8.8055 (164.30)	0.0026; 0.9909 (165.32)	0.0601; −62.7323 (165.28)	0.0000; −0.0458 (164.71)
37	0.0004; 0.3491 (162.10)	0.0084; −0.7006 (164.27)	0.0062; −1.7387 (164.65)	0.0154; 11.2895 (164.78)	0.0025; 0.0638 (161.70)
38	0.0017; 0.7830 (161.91)	0.0515; 0.0815 (163.04)	0.0002; 1.2084 (164.28)	0.0027; 1.3973 (164.32)	0.0019; 1.7649 (161.68)
39	0.0099; 0.1905 (161.72)	0.0006; −1.5400 (162.30)	0.0082; 1.4832 (163.97)	0.0040; −1.5569 (164.10)	0.0010; −4.5284 (161.48)
40	0.0001; −0.1441 (161.56)	0.0583; −1.9651 (162.19)	0.0071; 5.6442 (163.63)	0.0134; 1.1595 (163.40)	0.0061; 4.6711 (161.47)
41	0.0029; −2.4438 (161.52)	0.0016; 2.4532 (162.12)	0.0018; −3.2980 (163.23)	0.0112; −18.8180 (163.00)	0.0008; 1.0339 (161.02)
42	0.0005; −1.8489 (160.77)	0.0321; −10.1735 (161.23)	0.0139; −12.0373 (162.81)	0.0065; −11.3516 (162.06)	0.0010; −0.1211 (160.96)
43	0.0032; −0.3756 (160.46)	0.0069; −3.0202 (160.86)	0.0091; 10.4478 (162.25)	0.0036; 10.5470 (162.00)	0.0001; −0.0808 (160.79)
44	0.0015; −0.9823 (160.04)	0.0001; 0.4611 (160.52)	0.0008; −1.9413 (161.71)	0.0055; −0.1640 (161.77)	0.0004; 0.0753 (160.35)
45	0.0380; 2.0198 (159.65)	0.0014; 0.1951 (160.49)	0.0111; 3.6798 (160.80)	0.0009; 0.8073 (161.18)	0.0003; 0.3349 (159.85)
46	0.0023; −0.3385 (159.47)	0.0153; 3.0611 (160.04)	0.0113; −9.4322 (160.72)	0.0084; 9.4364 (160.25)	0.0419; −0.7810 (158.63)
47	0.0014; 2.4209 (159.27)	0.0182; 4.0575 (159.76)	0.0439; −12.2646 (160.41)	0.0040; −2.1893 (160.00)	0.0041; −0.1053 (158.30)
48	0.0096; −15.7664 (158.54)	0.0155; −4.1569 (158.58)	0.0456; 1.1777 (159.80)	0.0020; −5.2513 (159.34)	0.0040; 7.2892 (158.29)
49	0.0038; −1.4557 (158.44)	0.0027; −1.9857 (158.44)	0.0226; −40.1029 (159.57)	0.0008; 1.0422 (159.11)	0.0088; 3.0964 (158.11)
50	0.0067; −0.4721 (158.22)	0.0034; 0.1602 (158.33)	0.0028; −0.0535 (159.51)	0.0218; −9.7771 (158.93)	0.0496; 1.3829 (157.31)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c036	**c042**	**c045**	**c053**	**c054**
1	0.0200; 1.0360 (245.78)	0.0175; −4.7066 (246.29)	0.0174; 0.1860 (246.11)	0.0258; 4.8419 (249.20)	0.0119; 3.0691 (244.67)
2	0.0223; −2.1731 (244.55)	0.0090; 8.3328 (242.72)	0.0071; 4.5444 (241.88)	0.0170; 5.6243 (244.25)	0.0162; −10.0750 (243.86)
3	1.0669; −51.7448 (233.68)	0.3379; −729.2010 (232.54)	0.8123; −459.3612 (231.85)	0.0698; 298.4370 (236.17)	0.7377; −78.4429 (232.29)
4	0.1011; 22.0618 (230.28)	0.2870; 295.0841 (231.99)	0.2095; 383.8614 (229.84)	0.0407; −11.8536 (234.93)	0.2056; 97.2578 (228.76)
5	0.0042; −0.3152 (221.54)	0.3223; 317.0704 (229.66)	0.0062; −2.6130 (224.10)	0.6440; −308.2329 (232.09)	0.0002; 0.1348 (218.67)
6	0.0001; −0.0095 (211.36)	0.0024; 1.5325 (221.11)	0.0000; −0.0238 (214.73)	0.0640; −18.0874 (228.92)	0.0002; 0.1465 (211.91)
7	0.0001; 0.0990 (210.51)	0.0017; −0.0878 (213.47)	0.0000; −0.0440 (207.94)	0.0063; −5.3251 (224.93)	0.0000; −0.0074 (209.19)
8	0.0001; −0.0404 (205.30)	0.0003; 0.1164 (208.37)	0.0002; 0.1400 (202.64)	0.0043; 2.5295 (222.38)	0.0000; 0.0057 (208.24)
9	0.2465; 2.3138 (196.89)	0.0664; −27.7530 (198.21)	0.2873; 41.3785 (196.74)	0.0688; −16.7456 (202.39)	0.2226; 19.1186 (196.70)
10	0.2693; 3.0168 (195.02)	0.2807; 55.5213 (197.55)	0.2405; 28.8172 (195.17)	0.0273; 8.7285 (201.39)	0.2324; −85.8818 (195.67)
11	1.0377; −55.1288 (192.44)	0.1350; 69.4818 (195.04)	0.0014; −1.4414 (193.72)	0.0587; −45.2434 (199.76)	0.7958; 6.5049 (192.81)
12	0.0104; 0.0589 (192.12)	0.4185; −453.9741 (193.30)	0.8536; −245.1513 (192.70)	0.0818; −13.7192 (198.91)	0.0189; 0.3798 (191.98)
13	0.2145; 46.9335 (190.78)	0.0245; 13.9881 (192.29)	0.0075; 1.9650 (192.04)	0.2327; 97.0879 (195.95)	0.2421; 53.1835 (191.88)
14	0.0381; −10.9682 (190.45)	0.0432; −65.3701 (191.38)	0.3499; 241.4189 (190.94)	0.3030; −127.1270 (193.99)	0.0710; −90.8175 (187.49)
15	0.0022; 2.6031 (186.38)	0.2385; 120.0884 (191.03)	0.0001; −0.1865 (187.13)	0.1933; 121.4836 (193.64)	0.0002; 1.1521 (187.33)
16	0.0107; −6.9724 (185.91)	0.5144; 295.6824 (190.85)	0.0000; −0.0313 (186.87)	0.0246; 101.4053 (192.11)	0.0131; 59.2855 (187.28)
17	0.0009; 0.3717 (185.74)	0.0237; 16.9612 (188.48)	0.0127; −18.1532 (186.70)	0.5141; −21.8935 (189.76)	0.0144; −31.0275 (185.88)
18	0.0002; −3.8907 (185.58)	0.0003; 0.6381 (187.73)	0.0235; 43.5297 (184.40)	0.0732; −92.2258 (188.87)	0.0000; 0.0060 (185.38)
19	0.0000; 0.0059 (184.84)	0.0128; 27.6845 (185.64)	0.0000; 0.0045 (182.98)	0.0137; 2.2962 (184.32)	0.0000; 0.0000 (184.15)
20	0.0000; 0.0023 (182.01)	0.0025; −5.7332 (182.39)	0.0664; −43.5931 (180.17)	0.0053; −0.3359 (182.84)	0.0042; 4.7767 (180.59)
21	0.0001; 0.4566 (177.66)	0.0807; −17.3372 (180.61)	0.0097; −3.2884 (178.81)	0.1468; 33.4229 (180.62)	0.0151; 20.9166 (179.18)
22	0.1266; 7.4363 (176.26)	0.0292; −2.5595 (179.70)	0.0016; 2.5359 (178.14)	0.0844; −26.7762 (179.23)	0.1326; 9.6612 (177.44)
23	0.0579; −4.0535 (173.92)	0.0550; 5.1507 (176.99)	0.0323; −1.3295 (175.51)	0.0525; −5.6422 (177.55)	0.0097; −1.8006 (175.19)
24	0.0016; 2.8340 (173.16)	0.0004; −0.8603 (174.47)	0.0427; −1.8048 (174.02)	0.0032; 0.2308 (175.00)	0.0006; 0.2651 (173.83)
25	0.0008; −0.1197 (172.34)	0.0004; 1.1388 (173.77)	0.0009; −0.5593 (173.43)	0.0109; −9.0212 (173.27)	0.0074; −1.1661 (172.67)
26	0.0063; −1.8531 (172.03)	0.0433; −1.9506 (172.65)	0.0043; 0.4346 (171.69)	0.0049; 0.7695 (170.92)	0.0005; −1.3330 (170.13)
27	0.0006; 3.2509 (171.12)	0.0071; 2.7715 (171.85)	0.0016; −1.0963 (170.65)	0.0062; 2.1352 (169.84)	0.0014; 0.7620 (168.80)
28	0.0030; −3.9851 (170.93)	0.0052; −10.2901 (170.98)	0.0012; −0.1989 (170.24)	0.0282; 9.2763 (169.54)	0.0016; −0.7470 (168.76)
29	0.0006; 0.1557 (167.93)	0.0013; 6.1120 (170.66)	0.0038; −0.9333 (169.99)	0.0102; −11.2150 (169.45)	0.0115; −10.5761 (168.23)
30	0.0013; −0.5905 (167.30)	0.0136; −3.7859 (170.00)	0.0048; −3.3605 (169.71)	0.0056; 1.0922 (168.99)	0.0019; 1.8470 (168.15)
31	0.0019; 0.2295 (166.91)	0.0005; 1.7820 (168.25)	0.0015; −3.7182 (168.74)	0.0011; 3.7023 (168.36)	0.0016; −0.2411 (167.76)
32	0.0013; −0.4982 (166.72)	0.0004; 0.8711 (166.62)	0.0844; 16.8937 (166.17)	0.0028; −1.0188 (167.42)	0.0086; 5.3191 (166.81)
33	0.0357; −2.2846 (165.56)	0.0590; −3.6468 (166.53)	0.0010; −1.6142 (165.63)	0.0136; −35.8286 (167.18)	0.0478; 0.6228 (166.20)
34	0.0008; 1.8218 (164.67)	0.0110; 2.6041 (165.41)	0.1079; −5.9537 (163.70)	0.0353; 24.1870 (166.54)	0.0017; −0.2344 (166.09)
35	0.0054; 7.7794 (164.45)	0.0206; −5.7954 (165.32)	0.0182; 4.6178 (163.46)	0.0043; −1.9509 (165.86)	0.0067; −8.1691 (165.75)
36	0.0002; −0.2084 (163.69)	0.0036; −1.3088 (164.78)	0.0377; −9.4953 (163.39)	0.0186; −12.9067 (165.42)	0.0001; 0.1058 (165.25)
37	0.0150; −4.8471 (163.17)	0.0004; 2.0308 (164.26)	0.0015; 0.9135 (163.20)	0.0036; 3.5402 (165.11)	0.0220; 22.6532 (164.84)
38	0.0006; 1.3409 (162.87)	0.0015; −3.4631 (164.21)	0.0011; −4.0673 (163.05)	0.0374; −0.0900 (164.99)	0.0440; −21.7916 (164.56)
39	0.0002; 0.1433 (162.43)	0.1162; −10.5180 (163.24)	0.0006; −0.6937 (162.13)	0.0001; 0.0003 (164.37)	0.0004; 1.2826 (163.69)
40	0.0005; −1.1053 (162.12)	0.0023; 5.2927 (162.89)	0.0010; 1.4582 (162.04)	0.0024; 2.0065 (163.60)	0.0720; −24.8857 (163.06)
41	0.0007; −0.5896 (161.65)	0.0007; 2.2319 (162.53)	0.0001; 0.0118 (161.18)	0.0029; −0.8892 (162.88)	0.0212; 3.8320 (162.23)
42	0.0021; 6.0240 (161.29)	0.0001; 0.0491 (162.47)	0.0015; 5.7767 (160.97)	0.0045; 1.9383 (162.48)	0.0046; 3.3230 (161.89)
43	0.0102; 0.6536 (160.77)	0.0044; −0.4088 (161.90)	0.0001; 0.0916 (160.73)	0.0190; 4.8975 (161.72)	0.0003; −0.4878 (161.72)
44	0.0186; 0.5691 (160.26)	0.0113; 10.7542 (161.38)	0.0073; 1.6278 (160.69)	0.0203; 1.0031 (161.63)	0.0017; 1.1191 (161.03)
45	0.0038; −1.0964 (159.74)	0.0020; 0.8727 (161.07)	0.0078; −15.4154 (160.29)	0.0029; −2.3192 (161.52)	0.0090; −3.3732 (160.42)
46	0.0017; −2.1157 (159.68)	0.0002; 0.0373 (160.89)	0.0007; −0.0697 (159.93)	0.0030; −4.7427 (160.99)	0.0001; −0.9401 (160.33)
47	0.0043; 0.4720 (159.61)	0.0001; 0.2393 (160.70)	0.0214; 11.0807 (159.60)	0.0040; 3.2215 (160.71)	0.0161; 9.1488 (160.06)
48	0.0047; −1.7966 (158.13)	0.0165; 3.6300 (159.79)	0.0031; −2.0862 (159.09)	0.0084; −12.1830 (160.61)	0.0252; −6.2429 (159.51)
49	0.0126; 17.4808 (157.70)	0.0027; 2.5238 (159.45)	0.0046; 2.9059 (158.28)	0.0076; 8.7803 (160.56)	0.0109; −12.2931 (158.93)
50	0.0470; 10.3650 (157.31)	0.0108; 4.6830 (158.73)	0.0063; 3.6089 (158.15)	0.0141; −44.3920 (160.08)	0.0213; −8.2448 (158.47)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c055	**c068**	**c071**	**c072**	**c074**
1	0.0174; −8.4065 (244.50)	0.0179; −5.1432 (245.72)	0.0187; 11.8821 (246.29)	0.0159; −4.7794 (244.59)	0.0254; −22.4999 (244.35)
2	0.0066; −0.7560 (238.53)	0.0193; −9.1223 (244.36)	0.0055; 5.7231 (243.77)	0.0146; 4.7177 (244.15)	0.0090; 22.5895 (244.31)
3	0.5308; 58.7206 (232.78)	0.5042; 382.4101 (233.08)	0.1109; −22.8970 (235.73)	0.4291; 347.0174 (233.15)	0.6630; −113.3326 (232.87)
4	0.0044; 8.2514 (223.45)	0.4266; −309.3130 (230.74)	0.0636; −246.2463 (233.69)	0.4930; −182.7646 (229.82)	0.2638; 17.2986 (228.90)
5	0.1800; −93.8057 (222.65)	0.0047; 2.7625 (224.88)	0.3268; 170.0835 (230.73)	0.0019; −0.2128 (223.29)	0.0008; 0.0118 (218.90)
6	0.0018; 1.3692 (219.29)	0.0000; −0.0556 (213.97)	0.1820; −9.6744 (225.73)	0.0000; 0.0221 (214.44)	0.0001; 0.0179 (211.17)
7	0.0031; −1.9475 (215.46)	0.0001; 0.2143 (213.62)	0.0279; −7.0493 (224.49)	0.0000; 0.0131 (212.92)	0.0000; −0.0153 (208.62)
8	0.0002; −0.0105 (204.91)	0.0000; −0.0352 (210.38)	0.0017; 2.9433 (223.44)	0.0002; −0.0620 (210.50)	0.0000; −0.0008 (208.43)
9	0.1814; 26.5677 (197.22)	0.2768; 55.0907 (196.87)	0.0102; 7.0023 (205.63)	0.2261; −92.8013 (197.42)	0.2325; 111.6579 (196.98)
10	0.0414; −78.8459 (197.10)	0.0813; −59.9521 (196.78)	0.0057; 5.3105 (201.23)	0.0445; 0.7776 (196.50)	0.3112; −32.0272 (195.89)
11	0.2012; 25.8979 (195.33)	0.2377; −78.9844 (195.82)	0.0314; 42.0248 (200.25)	0.2934; −22.4741 (195.54)	0.0378; −14.8158 (193.40)
12	0.0220; −7.1526 (194.74)	0.4943; 554.9695 (192.40)	0.0062; 4.8636 (199.09)	0.4207; 407.0296 (192.74)	0.8115; −323.7137 (192.34)
13	0.2690; 269.4237 (193.44)	0.6167; −516.5443 (191.09)	0.0229; −82.5608 (197.52)	0.7691; −281.8967 (191.05)	0.2443; 238.7632 (191.52)
14	0.4042; −282.1713 (192.64)	0.0037; −5.5134 (188.80)	0.3383; 508.9361 (196.17)	0.0024; 0.3945 (189.11)	0.0035; 13.8987 (187.81)
15	0.1591; −35.1275 (191.61)	0.0001; 0.0730 (188.21)	0.1697; −606.8669 (194.54)	0.0000; −0.0361 (188.50)	0.0028; −12.4620 (187.04)
16	0.0674; 24.3684 (189.57)	0.0011; −0.3414 (188.03)	0.5857; 286.1456 (191.31)	0.0192; −19.9531 (188.02)	0.0005; −0.1587 (186.51)
17	0.0035; 6.3600 (188.11)	0.0003; 4.0195 (187.61)	0.1981; −42.8482 (190.36)	0.0043; −18.3478 (187.16)	0.0000; −0.0120 (185.17)
18	0.0240; −4.9464 (188.02)	0.0004; −0.1207 (186.67)	0.0013; 12.7341 (188.07)	0.0007; −0.1890 (186.16)	0.0003; 0.0235 (184.60)
19	0.0032; 19.9651 (187.61)	0.0168; 8.0978 (185.70)	0.0016; −1.9256 (184.80)	0.0063; 28.1189 (184.72)	0.0007; 2.0577 (183.66)
20	0.0084; 7.9830 (181.59)	0.0006; 0.2646 (185.66)	0.0837; 18.6538 (183.82)	0.0036; −2.5190 (184.40)	0.0231; 12.6786 (182.44)
21	0.0082; 1.8357 (180.54)	0.0165; 6.2447 (177.93)	0.0493; −51.7477 (183.79)	0.0103; 8.1600 (180.94)	0.0067; −7.4420 (177.82)
22	0.0098; 5.5154 (180.45)	0.0092; 10.0867 (176.37)	0.1689; −67.7573 (180.38)	0.1260; 5.9565 (177.29)	0.0110; 1.9833 (177.16)
23	0.1620; 36.5675 (176.78)	0.1531; 8.6756 (176.35)	0.0159; −13.6835 (176.38)	0.0265; 9.8904 (176.56)	0.1190; −3.5715 (176.31)
24	0.1039; −5.8305 (174.83)	0.0022; 0.4201 (174.48)	0.0311; 29.8957 (174.63)	0.0069; −2.7485 (175.42)	0.0064; −4.4621 (175.34)
25	0.0017; −4.4464 (174.14)	0.0014; −1.2922 (171.98)	0.0005; −1.7572 (173.77)	0.0023; 0.6027 (173.96)	0.0001; −0.3377 (172.15)
26	0.1628; 44.0865 (173.75)	0.0003; −1.2902 (171.10)	0.0031; −3.2115 (172.55)	0.0062; −0.8210 (173.40)	0.0094; 7.1156 (171.23)
27	0.0305; −26.3920 (170.98)	0.0005; −0.9998 (170.77)	0.0028; −5.6644 (171.71)	0.0002; 0.8962 (170.57)	0.0399; 7.2949 (170.99)
28	0.0059; 10.6780 (170.63)	0.0248; −5.8209 (169.73)	0.0413; −13.8573 (170.59)	0.0099; −2.0875 (168.13)	0.0022; 3.5276 (169.76)
29	0.0003; −1.5907 (170.05)	0.0001; 0.1802 (168.88)	0.0084; 12.9963 (170.40)	0.0297; −5.8418 (167.85)	0.0011; −1.3583 (168.93)
30	0.0011; −0.2180 (169.66)	0.0002; 0.4691 (168.03)	0.0068; −1.1353 (168.68)	0.0045; −0.9159 (167.04)	0.0063; 2.6181 (168.31)
31	0.0049; 9.5455 (169.27)	0.0012; −0.1014 (167.95)	0.0020; 3.1173 (167.92)	0.0029; −0.4965 (166.63)	0.0015; −1.3894 (167.70)
32	0.0126; 18.3984 (168.97)	0.0008; 0.2801 (167.69)	0.0151; 3.5629 (167.63)	0.0014; 3.6572 (166.32)	0.0545; 10.4485 (166.96)
33	0.0018; 1.0155 (168.21)	0.0153; −9.0998 (166.88)	0.0035; 3.9152 (167.24)	0.0038; −4.3130 (165.91)	0.0308; 14.4088 (166.85)
34	0.0427; 12.5562 (167.76)	0.0050; −3.0697 (166.25)	0.0006; −2.2482 (166.30)	0.0006; 1.0218 (165.62)	0.0082; 4.0771 (166.63)
35	0.0345; 13.0234 (167.66)	0.0414; −0.8516 (166.05)	0.0197; 1.9557 (166.18)	0.0091; 1.1028 (165.20)	0.0040; −0.8840 (166.49)
36	0.0158; −3.4255 (166.91)	0.0026; −5.8415 (165.58)	0.0010; 2.1576 (165.66)	0.0129; −0.9723 (165.06)	0.0397; −9.0702 (165.92)
37	0.0290; 20.7840 (166.73)	0.0537; 17.1297 (165.20)	0.0026; −1.7473 (165.44)	0.0168; −1.8104 (164.80)	0.0212; 6.2248 (165.81)
38	0.0059; 6.5510 (165.72)	0.0743; −4.0905 (164.61)	0.0088; 2.3892 (165.01)	0.0189; −4.2785 (164.74)	0.0014; −4.9920 (165.36)
39	0.0032; 1.9357 (165.62)	0.0045; 3.6067 (163.52)	0.0068; 9.1356 (164.12)	0.0148; 8.6151 (164.48)	0.0533; 12.5953 (164.93)
40	0.0133; 3.2109 (165.17)	0.0021; −3.2550 (162.36)	0.0679; 17.3987 (163.84)	0.0527; −12.0106 (163.97)	0.0026; 3.2669 (162.59)
41	0.0222; −23.1651 (164.28)	0.0015; 7.7889 (162.34)	0.0020; −2.7657 (163.26)	0.0004; 2.4173 (163.38)	0.0132; 2.0370 (161.76)
42	0.0062; −1.7530 (164.26)	0.0043; 0.8649 (161.72)	0.0373; 21.1673 (162.92)	0.0477; −11.4478 (162.40)	0.0038; −0.5591 (161.68)
43	0.0051; 4.5691 (163.63)	0.0002; −0.1165 (160.95)	0.0403; −12.6494 (162.45)	0.0457; −8.0797 (160.74)	0.0012; 1.9505 (161.31)
44	0.0006; 0.4904 (162.71)	0.0123; −3.0651 (160.82)	0.0159; −40.6931 (161.65)	0.0131; 5.9322 (160.36)	0.0117; 21.3015 (160.93)
45	0.0057; −5.7102 (162.64)	0.0047; −1.2527 (160.73)	0.0040; 8.7744 (161.41)	0.0023; −0.5773 (160.30)	0.0331; −19.7965 (160.62)
46	0.0023; −5.7239 (162.61)	0.0060; −3.7564 (160.34)	0.0005; −1.6769 (161.01)	0.0021; −4.6098 (160.09)	0.0006; 0.1006 (160.10)
47	0.0011; 3.0134 (162.16)	0.0013; 2.2193 (160.21)	0.0046; 1.7710 (160.79)	0.0028; −1.0951 (159.49)	0.0009; −0.5102 (159.81)
48	0.0028; −0.7578 (161.41)	0.0151; −4.5906 (159.16)	0.0103; 4.3557 (160.56)	0.0018; −2.3821 (158.65)	0.0746; 15.5983 (159.03)
49	0.0001; 0.0079 (161.17)	0.0926; −2.6917 (158.17)	0.0009; −2.5032 (160.32)	0.0271; −40.5822 (158.19)	0.0028; 6.7851 (158.78)
50	0.0000; −0.1881 (160.83)	0.0129; 1.1114 (157.94)	0.0008; −4.0627 (160.12)	0.0813; −4.1490 (157.63)	0.0035; −4.6793 (158.43)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c075	**c078**	**c083**	**c095**	**c096**
1	0.0177; 3.1569 (245.70)	0.0137; −8.0082 (244.51)	0.0046; 29.1834 (247.50)	0.0214; 2.1627 (245.94)	0.0180; 3.1584 (246.19)
2	0.0071; 3.6038 (241.88)	0.0162; 4.6278 (244.38)	0.0022; 9.6689 (247.36)	0.0227; 10.5798 (244.69)	0.0174; 4.1739 (244.49)
3	0.7919; −40.6632 (231.88)	0.6760; −123.3777 (232.44)	0.1878; −0.8123 (241.30)	0.8147; 301.2981 (233.81)	0.1480; −260.4588 (233.74)
4	0.2750; −21.9141 (229.28)	0.2431; 53.5905 (229.90)	0.1341; −63.2676 (232.76)	0.3105; −222.9481 (230.45)	0.0577; −3.7995 (231.80)
5	0.0002; −0.1394 (221.12)	0.0003; −0.0273 (217.49)	0.2019; 88.7162 (230.89)	0.0012; 0.1308 (223.07)	0.6398; 149.5846 (231.25)
6	0.0000; 0.0103 (212.54)	0.0001; 0.0082 (213.34)	0.0117; 3.2216 (226.07)	0.0000; −0.0141 (212.91)	0.0049; −0.3639 (220.58)
7	0.0000; −0.0101 (208.18)	0.0000; −0.0055 (210.01)	0.0518; −15.5929 (224.35)	0.0000; −0.0588 (212.03)	0.0023; 2.2182 (218.56)
8	0.0000; 0.0109 (202.47)	0.0000; −0.0044 (207.62)	0.1515; −18.1848 (218.54)	0.0001; 0.0089 (206.74)	0.0041; −1.4982 (215.89)
9	0.2489; −9.0238 (196.27)	0.2423; 672.2908 (196.56)	0.0286; −60.5594 (209.18)	0.2506; −67.4173 (197.00)	0.0051; −13.1487 (203.11)
10	0.2418; 135.1543 (195.43)	0.2428; −649.5407 (196.45)	0.2158; −205.1395 (203.54)	0.2717; 42.1536 (195.04)	0.3297; 57.1625 (197.92)
11	0.8713; −211.0169 (192.43)	0.4189; −171.6860 (192.48)	0.1057; −72.0102 (200.91)	0.0002; −1.1999 (192.96)	0.2087; −153.8827 (196.76)
12	0.0002; 0.0049 (191.99)	0.3772; −134.8335 (192.15)	0.0224; 10.6794 (198.07)	0.7694; 167.7033 (192.61)	0.0865; 46.7228 (194.42)
13	0.2765; 16.6121 (191.10)	0.3088; 273.9352 (191.62)	0.2425; 443.9959 (195.87)	0.1295; 41.1809 (191.06)	0.2620; −79.8422 (193.34)
14	0.1302; 62.7495 (190.89)	0.0016; −2.7219 (188.25)	0.0825; 261.4369 (194.64)	0.3799; −165.4439 (190.77)	0.0261; −135.8311 (191.89)
15	0.0175; 6.4864 (187.17)	0.0005; 0.1944 (187.92)	0.1166; −206.7613 (193.97)	0.0001; −0.1026 (186.69)	0.5193; 294.4009 (191.38)
16	0.0000; −0.1318 (187.11)	0.0015; 10.2689 (187.19)	0.0551; −234.3197 (190.35)	0.0086; −18.7434 (186.17)	0.0616; 60.7650 (190.06)
17	0.0000; −0.0042 (185.75)	0.0002; 0.0185 (185.43)	0.0243; −14.0617 (188.72)	0.0012; 12.0476 (185.97)	0.2075; −77.0381 (189.70)
18	0.0011; −3.0137 (185.00)	0.0010; −0.0206 (184.83)	0.3547; 80.3001 (188.30)	0.0000; −0.0413 (185.79)	0.0013; 2.6608 (188.41)
19	0.0000; 0.0026 (182.71)	0.0000; −0.0006 (184.60)	0.1839; −65.0628 (187.02)	0.0167; −7.0010 (184.51)	0.0038; −11.5154 (183.93)
20	0.0386; 59.2239 (182.12)	0.0154; 8.9768 (181.37)	0.0225; −0.1534 (184.13)	0.0000; −0.0028 (182.98)	0.0044; 6.8281 (183.60)
21	0.0489; −46.7300 (178.73)	0.0087; −6.9764 (177.63)	0.0327; −24.6580 (182.25)	0.0189; 2.7356 (177.05)	0.0059; −4.0715 (180.31)
22	0.0081; 0.0638 (177.69)	0.0047; −35.6789 (176.34)	0.1201; 74.4838 (182.07)	0.1315; −3.1135 (176.69)	0.1592; 7.9524 (177.69)
23	0.0004; 0.1818 (175.92)	0.1280; 38.3355 (176.21)	0.0046; 6.6573 (178.05)	0.0003; 0.6034 (174.00)	0.0281; −3.9395 (176.46)
24	0.0752; 5.0412 (174.06)	0.0422; 9.4507 (171.76)	0.0648; 1.6465 (176.94)	0.0542; −1.6050 (173.11)	0.0109; −13.5926 (174.84)
25	0.0008; 0.9061 (172.15)	0.0012; 3.5450 (171.54)	0.0325; −11.2374 (175.85)	0.0006; 0.1445 (172.70)	0.0019; −1.5848 (172.31)
26	0.0046; −4.7796 (172.12)	0.0025; 3.9784 (170.95)	0.0023; 1.9775 (174.13)	0.0008; −0.6510 (172.04)	0.0015; −0.4922 (171.73)
27	0.0006; 1.2876 (171.29)	0.0027; −0.7840 (170.73)	0.0126; −17.7138 (171.80)	0.0010; 1.2678 (171.65)	0.0267; −0.6978 (170.89)
28	0.0049; −1.8768 (169.32)	0.0154; 4.8803 (168.78)	0.0030; −8.2616 (171.20)	0.0001; 0.0209 (171.01)	0.0102; 7.9402 (169.64)
29	0.0006; 0.5130 (167.79)	0.0174; −5.6239 (168.57)	0.0034; 0.5721 (170.28)	0.0001; 0.0544 (168.52)	0.0009; −1.4515 (168.49)
30	0.0529; 3.6408 (166.80)	0.0032; 5.9311 (168.54)	0.0015; −1.9770 (169.83)	0.0008; 0.7227 (167.68)	0.0016; −0.7068 (168.21)
31	0.0041; 2.2810 (165.91)	0.0013; 0.1928 (168.12)	0.0009; 3.7235 (169.13)	0.0031; 2.6425 (167.53)	0.0016; 3.2438 (167.34)
32	0.0082; 8.3226 (165.05)	0.0621; 8.5130 (167.38)	0.0040; 2.6066 (168.48)	0.0200; 0.6808 (166.43)	0.0008; −1.9742 (167.23)
33	0.0241; −10.2127 (165.03)	0.0315; 22.2585 (167.05)	0.0491; −3.6832 (168.18)	0.0142; −2.2509 (166.03)	0.0602; 11.3499 (166.74)
34	0.0019; 1.0352 (164.23)	0.0013; 0.7975 (166.32)	0.0099; 19.0717 (167.92)	0.0009; 0.5635 (164.29)	0.0013; 0.5206 (166.04)
35	0.0024; −2.2710 (163.78)	0.0004; 0.9085 (166.19)	0.0045; 6.5823 (167.21)	0.0018; 1.6120 (164.23)	0.0586; −21.5835 (165.30)
36	0.0086; 3.1891 (163.37)	0.0012; 1.1241 (165.50)	0.0075; −2.0656 (166.37)	0.0073; −7.1866 (163.77)	0.0637; 10.1072 (165.03)
37	0.1344; −9.6293 (163.16)	0.0392; −3.7441 (165.37)	0.0183; −3.3141 (165.51)	0.0010; 0.7914 (163.08)	0.0036; −1.6519 (164.35)
38	0.0004; −0.2460 (162.37)	0.0139; 14.4280 (165.25)	0.0191; −30.7926 (165.35)	0.0035; 0.4006 (162.61)	0.0038; 0.4973 (164.26)
39	0.0003; 0.2670 (162.15)	0.0077; −15.3489 (164.16)	0.0078; −12.8841 (164.82)	0.0055; 7.2325 (162.48)	0.0045; −7.5979 (163.18)
40	0.0003; 0.7082 (162.08)	0.0090; −3.3330 (161.99)	0.0354; −26.9388 (164.56)	0.0053; 0.9318 (162.24)	0.0037; 14.7616 (162.95)
41	0.0139; 2.9556 (160.94)	0.0092; −7.5872 (161.45)	0.0222; 3.6943 (164.04)	0.0028; −4.3818 (161.95)	0.0003; 0.6023 (162.83)
42	0.0061; 5.7338 (160.61)	0.0017; 2.0660 (161.43)	0.0212; 6.1796 (163.87)	0.0040; 1.9171 (161.26)	0.0305; 2.0974 (162.38)
43	0.0017; −1.3263 (160.49)	0.0396; 8.5848 (161.17)	0.0078; −4.0420 (163.45)	0.0035; 2.4534 (160.98)	0.0118; 1.8062 (162.07)
44	0.0126; −3.3580 (160.41)	0.0003; −0.3125 (160.55)	0.0299; −6.0522 (163.15)	0.0140; −11.8463 (160.90)	0.0011; 0.7763 (161.79)
45	0.0245; −1.9690 (160.13)	0.0313; 0.0767 (160.03)	0.0120; −9.0530 (162.64)	0.0032; 1.0610 (160.57)	0.0035; 6.2848 (161.23)
46	0.0005; −1.0518 (160.02)	0.0031; −1.2152 (159.92)	0.0121; −6.2909 (162.46)	0.0064; −2.1668 (160.43)	0.0102; −0.3071 (161.00)
47	0.0015; −1.0011 (158.87)	0.0009; −1.2384 (159.15)	0.0056; 2.7439 (162.36)	0.0057; 1.2895 (160.39)	0.0010; 0.2816 (160.54)
48	0.0105; 8.0160 (158.33)	0.0002; −0.1067 (159.01)	0.0045; 1.2212 (161.89)	0.0046; −2.2624 (158.31)	0.0028; −1.7292 (160.23)
49	0.0081; 3.9693 (158.24)	0.0035; −3.8501 (158.87)	0.0043; −6.1985 (161.75)	0.0020; −3.1952 (158.28)	0.0025; −2.3216 (160.02)
50	0.0043; −4.1973 (157.21)	0.0130; −11.2861 (158.60)	0.0106; −6.2266 (161.41)	0.0240; −27.9787 (157.60)	0.0017; 0.1163 (159.83)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c107	**c108**	**c111**	**c117**	**c122**
1	0.0187; −1.4576 (246.82)	0.0194; 6.4195 (246.30)	0.0196; −3.5017 (245.83)	0.0084; −18.5069 (247.92)	0.0159; 8.5855 (247.39)
2	0.0088; 8.1568 (243.90)	0.0091; −3.1705 (242.78)	0.0071; 2.4619 (242.13)	0.0252; 41.1578 (245.01)	0.0046; −0.9762 (241.43)
3	0.0873; 20.3921 (236.32)	0.4601; 589.0322 (232.31)	0.3845; −189.4096 (231.97)	0.0150; 1.5246 (240.29)	0.0408; 61.2627 (235.45)
4	0.0673; −260.7148 (234.36)	0.5481; −433.0479 (230.09)	0.6221; 94.8545 (229.56)	0.1241; −87.2825 (236.26)	0.1057; 155.7423 (230.97)
5	0.3268; 161.1939 (231.21)	0.0046; −0.5150 (226.38)	0.0017; −1.0969 (225.26)	0.0612; −67.9692 (230.56)	0.5935; −131.2379 (228.54)
6	0.2328; −7.9984 (226.40)	0.0004; −0.4328 (218.08)	0.0001; −0.0083 (216.88)	0.4702; 176.0419 (228.79)	0.0044; 11.6027 (227.68)
7	0.0027; −1.0561 (225.48)	0.0002; 0.0859 (211.66)	0.0001; −0.0343 (210.07)	0.0943; 6.7884 (221.68)	0.0037; 16.9822 (216.48)
8	0.0009; −0.3466 (224.04)	0.0000; 0.0062 (206.46)	0.0000; 0.0083 (204.96)	0.0007; −0.4902 (219.56)	0.0281; −4.6398 (213.44)
9	0.0100; −4.9474 (205.98)	0.3602; 10.7705 (196.58)	0.3388; 38.0337 (196.66)	0.0130; 16.2877 (207.93)	0.0854; 14.8892 (203.50)
10	0.0096; −2.9841 (201.78)	0.1273; −2.3644 (195.43)	0.1469; −22.9386 (195.16)	0.1706; −140.9935 (205.55)	0.0263; 8.0660 (199.96)
11	0.0297; 49.9452 (200.13)	0.0505; 10.5323 (194.73)	0.0367; −5.8910 (194.53)	0.0869; 100.3606 (202.43)	0.2253; −98.8671 (199.19)
12	0.0156; 11.6647 (199.53)	0.5046; 616.9993 (192.67)	0.4842; −206.6164 (192.64)	0.1007; 32.5560 (200.54)	0.0444; 41.7621 (197.34)
13	0.0252; −87.8145 (197.83)	0.3197; −164.8586 (191.42)	0.6642; 42.0030 (190.83)	0.0032; −14.2401 (197.16)	0.1230; −154.1532 (195.46)
14	0.3241; 478.1605 (196.08)	0.3072; −375.8316 (191.03)	0.1618; 119.6389 (190.52)	0.2210; 331.2260 (194.44)	0.2351; −100.6974 (194.52)
15	0.1481; −563.0257 (194.54)	0.0988; −73.2687 (189.70)	0.0002; 0.1925 (189.10)	0.0460; −174.4793 (192.25)	0.0690; 415.9844 (192.50)
16	0.3580; 206.3367 (191.54)	0.0069; 7.8180 (189.43)	0.0005; 0.0747 (188.59)	0.3459; −40.5960 (189.74)	0.4388; 12.6150 (189.74)
17	0.4589; 60.6949 (190.84)	0.0012; −0.7828 (188.88)	0.0178; 10.9295 (187.43)	0.1668; −221.0226 (189.26)	0.3455; −153.2258 (188.98)
18	0.0016; −8.1182 (188.49)	0.0000; 0.0761 (185.53)	0.0000; 0.0019 (185.21)	0.2683; 144.4502 (188.93)	0.1005; 31.4206 (186.97)
19	0.0092; −11.7922 (185.21)	0.0284; −49.4299 (184.13)	0.0089; 13.7130 (184.63)	0.0136; −8.7549 (185.18)	0.0166; −28.5700 (184.73)
20	0.1029; 11.4820 (184.18)	0.0097; 11.5031 (183.11)	0.0090; 24.5268 (182.43)	0.2025; −38.9606 (183.62)	0.0009; −4.9371 (182.73)
21	0.0105; −37.1129 (183.95)	0.0504; −8.4221 (179.07)	0.0031; 1.8997 (180.65)	0.0031; 10.7326 (182.94)	0.0183; 5.0629 (181.41)
22	0.1736; −65.6056 (180.58)	0.0597; 25.4119 (178.02)	0.0660; −43.7684 (178.62)	0.0787; 47.9218 (178.55)	0.0434; 34.3327 (178.92)
23	0.0149; −16.9561 (176.27)	0.0193; −6.3109 (177.24)	0.0053; 1.8878 (177.81)	0.0324; −6.2448 (177.48)	0.0254; 3.1087 (176.69)
24	0.0425; 30.7096 (174.66)	0.0104; 2.1209 (175.04)	0.0009; 0.0884 (175.03)	0.0208; −10.2585 (176.23)	0.0011; 3.4394 (175.41)
25	0.0005; −1.8221 (174.34)	0.0100; 0.8329 (173.06)	0.0722; 1.6062 (173.70)	0.0182; 16.6610 (174.30)	0.0119; −1.6082 (174.01)
26	0.0022; −1.9743 (172.89)	0.0275; −0.0130 (172.81)	0.0010; 0.4334 (172.29)	0.0014; −1.9255 (174.12)	0.0017; 1.8866 (172.87)
27	0.0010; −1.5088 (172.33)	0.0021; −0.7919 (170.52)	0.0013; 2.1084 (170.49)	0.0088; −11.3237 (172.85)	0.0052; 0.5676 (171.45)
28	0.0341; −21.3295 (170.62)	0.0011; −1.2624 (170.35)	0.0052; −3.2847 (169.92)	0.0200; −8.6855 (172.71)	0.0011; −0.2542 (170.37)
29	0.0182; 19.6907 (170.37)	0.0096; 1.4225 (168.62)	0.0024; −2.1049 (169.38)	0.0036; −2.5052 (171.91)	0.0005; −0.3642 (169.51)
30	0.0010; −2.4474 (168.24)	0.0011; −0.5106 (168.18)	0.0021; −0.1930 (169.26)	0.0091; −4.0933 (171.61)	0.0036; −0.9667 (168.90)
31	0.0041; 2.0181 (168.04)	0.0014; 0.9114 (168.09)	0.0108; 3.2136 (167.06)	0.0056; −3.5704 (168.53)	0.0031; −4.2392 (168.74)
32	0.0026; 4.9319 (167.46)	0.0095; 0.4888 (166.09)	0.0553; 23.1381 (165.62)	0.0024; −2.5623 (168.27)	0.0334; −11.7282 (168.37)
33	0.0107; 2.6143 (167.32)	0.0010; 1.7942 (165.53)	0.0281; 5.8145 (165.31)	0.0056; −21.3802 (168.05)	0.0030; −5.2459 (167.81)
34	0.0015; 0.4813 (166.89)	0.0018; −1.4136 (165.40)	0.0003; −0.0835 (164.73)	0.0095; 23.0574 (167.57)	0.0778; −65.4255 (166.79)
35	0.0092; −5.6644 (166.31)	0.0077; 5.7862 (165.04)	0.0008; −0.3186 (164.23)	0.0014; 5.0294 (167.25)	0.0527; 9.8838 (166.15)
36	0.0117; 2.6233 (166.22)	0.0020; 3.5339 (164.68)	0.0017; 2.7030 (163.68)	0.0012; −3.8688 (166.30)	0.0019; −5.2226 (165.63)
37	0.0045; 2.0947 (165.45)	0.0381; −19.6284 (164.43)	0.0011; −2.5683 (163.51)	0.0364; −8.9476 (165.72)	0.1253; 24.3220 (165.03)
38	0.0071; 0.6710 (165.12)	0.0358; 1.1979 (163.21)	0.1376; 4.7454 (163.17)	0.0035; −10.9989 (165.03)	0.0095; −2.5397 (164.13)
39	0.0098; 13.4642 (163.84)	0.0010; −1.2786 (163.07)	0.0020; 0.7979 (162.91)	0.0275; −9.9313 (164.89)	0.0033; −6.6161 (163.82)
40	0.0533; 3.1909 (163.63)	0.0003; 0.6492 (162.37)	0.0005; 1.5166 (162.07)	0.0146; −39.4852 (164.32)	0.0125; −5.2409 (163.26)
41	0.0152; 8.9947 (163.58)	0.0799; −0.4492 (162.13)	0.0159; 1.5958 (161.29)	0.0528; −58.1474 (163.96)	0.0483; −18.5397 (162.92)
42	0.0299; 15.2628 (162.59)	0.0252; −17.0129 (161.76)	0.0053; 1.7703 (161.20)	0.0133; −14.6615 (163.71)	0.0105; 9.6602 (162.45)
43	0.0340; −12.2964 (162.33)	0.0055; 3.1084 (161.07)	0.0019; −0.5784 (160.60)	0.0384; 82.9126 (163.45)	0.0095; 21.3476 (161.85)
44	0.0113; −24.4203 (161.89)	0.0002; −0.2694 (160.67)	0.0115; 2.2638 (160.32)	0.0104; 3.3820 (163.21)	0.0214; 5.7070 (161.57)
45	0.0026; −7.4898 (161.19)	0.0016; −0.2191 (160.54)	0.0073; 4.2979 (160.29)	0.0047; −1.1991 (162.62)	0.0058; −2.1574 (161.07)
46	0.0061; −4.9467 (160.85)	0.0091; 1.1165 (160.14)	0.0009; 0.1091 (159.36)	0.0042; −3.1427 (161.89)	0.0306; 2.8722 (160.92)
47	0.0046; −0.9366 (160.75)	0.0295; 10.7061 (160.01)	0.0075; −5.3758 (158.85)	0.0005; −1.0041 (161.71)	0.0126; −4.0552 (160.49)
48	0.0004; −0.4435 (160.63)	0.0047; −3.2629 (158.62)	0.0108; 21.7300 (158.58)	0.0024; −0.0854 (161.46)	0.0014; −1.0605 (160.26)
49	0.0013; 2.2978 (160.53)	0.0013; −7.2000 (158.58)	0.0230; −6.3810 (158.33)	0.0031; −9.1266 (160.96)	0.0033; −8.5855 (159.76)
50	0.0050; 3.6935 (159.92)	0.0009; 3.1095 (158.49)	0.0179; −3.6064 (158.28)	0.0608; 17.5902 (160.75)	0.0042; −0.1581 (159.42)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c127	**c128**	**c132**	**c137**	**c144**
1	0.0154; 1.1441 (247.78)	0.0320; 11.2374 (246.40)	0.0197; 19.6127 (248.12)	0.0120; 5.1649 (246.61)	0.0103; 4.6582 (245.60)
2	0.0063; 3.3170 (241.39)	0.0023; −0.6244 (244.91)	0.0049; −0.6649 (242.39)	0.0088; −7.9837 (242.42)	0.0102; 2.9310 (243.48)
3	0.0169; 4.5492 (234.58)	0.0712; 183.3188 (237.31)	0.0480; 211.9424 (235.15)	0.0441; 22.0896 (235.15)	0.0471; −20.2529 (233.62)
4	0.1983; −220.2606 (231.77)	0.0390; 61.4161 (231.23)	0.0571; 178.4258 (232.03)	0.1308; 70.8633 (233.69)	0.6056; −59.0394 (230.10)
5	0.6071; 125.9492 (229.26)	0.7042; −289.2800 (229.19)	0.5939; −395.7513 (230.34)	0.4940; −95.2692 (228.77)	0.0925; −7.6039 (229.40)
6	0.0033; −4.4291 (227.93)	0.0094; 17.6287 (223.08)	0.0063; −2.8186 (227.01)	0.1079; −8.8922 (226.69)	0.0007; 1.7640 (222.82)
7	0.0069; 7.7512 (215.36)	0.0334; 23.9464 (221.96)	0.0080; 8.8573 (217.04)	0.0061; 7.3749 (219.88)	0.0057; −0.7442 (221.01)
8	0.0194; 6.5047 (211.05)	0.0279; 20.2506 (218.03)	0.0470; −5.7710 (212.28)	0.0006; −0.9555 (216.11)	0.0251; −7.6665 (217.95)
9	0.1086; 1.5103 (201.93)	0.1483; −9.7017 (203.01)	0.0447; −125.0216 (208.37)	0.0133; −6.7852 (203.05)	0.0563; 77.8770 (203.94)
10	0.2387; 55.3511 (198.51)	0.2235; 221.9954 (200.37)	0.0222; 93.0010 (203.15)	0.0370; 27.6391 (200.87)	0.0508; 53.6783 (202.67)
11	0.0648; −43.9251 (197.75)	0.0223; −109.2281 (197.84)	0.1846; −127.2194 (199.89)	0.0429; −15.2076 (199.13)	0.0202; −42.3916 (201.35)
12	0.0613; 15.0736 (196.33)	0.0140; 61.6783 (195.56)	0.0843; 33.6134 (197.66)	0.0890; −75.7996 (197.86)	0.1150; −10.3059 (198.49)
13	0.1480; 543.0479 (195.16)	0.1299; −1.6286 (195.03)	0.1441; 435.2036 (194.57)	0.0499; 75.5154 (196.61)	0.1425; 76.3771 (195.57)
14	0.3087; −331.1330 (193.84)	0.0521; −62.7518 (193.83)	0.1180; −13.9183 (193.65)	0.2544; −389.9577 (195.35)	0.1627; −171.0511 (195.09)
15	0.0509; −344.7369 (191.92)	0.1428; −0.4467 (191.30)	0.8528; −316.4647 (190.88)	0.0447; 295.0773 (192.84)	0.6160; 52.8830 (190.98)
16	0.0309; −76.7650 (190.58)	0.5825; −128.5293 (190.87)	0.0149; 24.5204 (189.92)	0.9296; −83.4756 (190.92)	0.1745; 117.1897 (189.87)
17	0.7299; 233.7090 (189.66)	0.1101; −56.9468 (189.68)	0.0727; −104.0191 (189.32)	0.0724; 91.7474 (189.81)	0.2369; −115.9526 (189.39)
18	0.0256; 39.5530 (184.95)	0.1165; 177.0168 (188.58)	0.0213; −8.4381 (185.35)	0.0343; 16.9001 (185.40)	0.0188; 43.9336 (185.28)
19	0.0018; −0.0215 (183.97)	0.0894; −49.6757 (186.89)	0.0340; 52.1223 (184.07)	0.1193; 52.3252 (183.68)	0.0045; 3.1923 (181.47)
20	0.0088; −3.5800 (182.02)	0.0087; −34.0409 (185.64)	0.0062; 4.8479 (183.02)	0.0160; 24.0445 (182.83)	0.0925; −39.2036 (181.20)
21	0.0809; −49.0299 (180.48)	0.0833; −68.2775 (180.85)	0.0435; −44.3436 (180.64)	0.0066; 4.3460 (182.20)	0.0361; 8.6454 (179.81)
22	0.0048; −3.4872 (178.00)	0.1393; 87.3084 (178.99)	0.0506; 41.3750 (179.87)	0.0709; −47.6010 (179.89)	0.0491; −23.2999 (179.62)
23	0.0198; 6.0043 (175.67)	0.1021; −71.5170 (177.96)	0.0613; −89.9116 (179.64)	0.0403; 4.3785 (177.30)	0.0161; −5.1634 (177.54)
24	0.0015; 0.1027 (175.05)	0.0016; −0.5220 (175.32)	0.0210; −3.1743 (174.26)	0.0083; 2.6518 (174.75)	0.0128; 1.8670 (173.29)
25	0.0008; −0.6633 (172.51)	0.0104; 5.7102 (174.20)	0.0053; −0.2329 (172.28)	0.0025; 2.5388 (173.22)	0.0126; 4.8057 (172.98)
26	0.0215; −6.6107 (172.36)	0.0017; −1.0131 (173.04)	0.0016; 3.6246 (171.19)	0.0004; 0.4660 (172.35)	0.0040; −0.7449 (170.86)
27	0.0047; −2.9837 (171.62)	0.0036; −3.1872 (172.12)	0.0077; −1.0129 (171.00)	0.0001; −2.6584 (171.67)	0.0136; −4.0028 (170.81)
28	0.0038; −3.5756 (168.60)	0.0023; −3.6478 (171.76)	0.0108; 4.5473 (170.40)	0.0018; −3.5635 (171.25)	0.0317; −3.5829 (170.44)
29	0.0009; −2.0817 (168.41)	0.0013; −1.0899 (171.40)	0.0062; 0.1017 (168.10)	0.0056; −4.1125 (170.83)	0.0010; −0.9827 (168.48)
30	0.0009; 1.2015 (168.35)	0.0028; −8.0420 (170.00)	0.0031; 2.9100 (167.83)	0.0129; 2.9542 (170.27)	0.0606; −41.6895 (168.12)
31	0.0874; 26.5563 (167.28)	0.0022; −0.2133 (169.81)	0.0460; −1.4150 (167.54)	0.0033; −0.4063 (169.45)	0.0024; 4.9125 (167.22)
32	0.0305; 16.7338 (165.84)	0.0051; −8.9457 (169.55)	0.0122; −1.9324 (166.95)	0.0030; 2.3095 (168.05)	0.0241; 45.3112 (167.06)
33	0.0545; 11.5961 (165.01)	0.0163; −6.7013 (169.23)	0.0178; −1.8562 (166.17)	0.0135; 4.3941 (167.92)	0.0983; −6.2409 (166.18)
34	0.0796; −20.6670 (164.90)	0.0048; 0.6684 (168.08)	0.0059; 9.1252 (166.10)	0.0506; 14.7461 (165.98)	0.0004; 1.2507 (165.84)
35	0.0591; 6.6754 (164.61)	0.0010; −0.7469 (167.34)	0.0532; 34.8106 (165.92)	0.0010; 0.8421 (165.23)	0.1011; −7.0153 (164.60)
36	0.0056; 2.9893 (164.01)	0.0301; 26.5299 (166.84)	0.0764; 3.7038 (165.50)	0.0092; 10.1431 (164.95)	0.0091; −10.1733 (164.12)
37	0.0077; 4.8954 (163.27)	0.0006; 3.0160 (166.13)	0.0096; 1.6538 (164.87)	0.0074; −2.2988 (164.50)	0.0056; 3.0065 (164.02)
38	0.0008; 3.3163 (162.72)	0.0032; −11.7665 (165.17)	0.0354; −13.9773 (164.17)	0.0095; −13.8427 (164.24)	0.0211; 4.3853 (163.83)
39	0.0008; −0.0449 (162.56)	0.0021; 0.7589 (165.13)	0.0074; 8.0184 (163.89)	0.0794; 65.7719 (164.08)	0.0212; 11.8674 (163.47)
40	0.0023; −2.4648 (162.25)	0.0045; −4.6281 (164.94)	0.0239; −3.1523 (163.60)	0.0134; 14.2737 (163.94)	0.0022; 0.2610 (162.82)
41	0.0003; 0.2318 (161.88)	0.0007; 2.0282 (164.67)	0.0099; −10.2828 (163.32)	0.0742; −55.2663 (163.61)	0.0036; −1.4107 (162.62)
42	0.0178; −15.0186 (161.61)	0.0252; −10.5170 (162.50)	0.0240; 9.4650 (163.27)	0.0217; −16.5240 (163.32)	0.0090; −7.6152 (161.96)
43	0.0108; 13.8954 (161.41)	0.0040; 8.0117 (162.22)	0.0039; −10.2229 (162.85)	0.0027; −2.2526 (162.95)	0.0362; −11.5431 (161.75)
44	0.0018; −1.0350 (161.25)	0.0220; 6.8374 (161.92)	0.0414; −16.2552 (162.75)	0.0202; −1.8405 (162.54)	0.0179; −0.9379 (161.64)
45	0.0341; −11.5121 (160.88)	0.0038; −3.5016 (161.65)	0.0259; −5.6118 (162.47)	0.0196; −16.6128 (162.12)	0.0117; −3.0008 (161.36)
46	0.0247; 1.2556 (160.37)	0.0158; −0.4745 (161.49)	0.0099; −11.2002 (162.27)	0.0078; 0.0705 (161.42)	0.0009; 4.0949 (161.01)
47	0.0025; 1.2217 (159.76)	0.0022; −0.9267 (160.09)	0.0094; 2.6248 (161.40)	0.0097; −1.9540 (161.30)	0.0012; −1.1906 (160.77)
48	0.0130; 15.5780 (159.55)	0.0014; −1.0134 (159.94)	0.0021; −5.7719 (160.98)	0.0056; 20.7178 (160.18)	0.0010; −2.2029 (160.66)
49	0.0001; 0.0554 (159.13)	0.0759; −15.2773 (159.53)	0.0072; −3.9924 (160.70)	0.0062; −10.9056 (159.97)	0.0054; 7.9585 (160.26)
50	0.0046; −1.1348 (158.79)	0.0308; −37.4179 (159.45)	0.0391; 0.8224 (160.50)	0.0438; −10.6804 (159.87)	0.0038; −2.1116 (160.24)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c177	**c184**	**c185**	**c195**	**c200**
1	0.0090; −25.0679 (248.79)	0.0104; 3.7226 (246.21)	0.0150; −15.0801 (247.62)	0.0152; −2.9025 (245.70)	0.0120; 8.1747 (246.78)
2	0.0258; 33.1100 (245.00)	0.0192; −8.0527 (245.75)	0.0104; 2.6055 (244.69)	0.0012; −2.8919 (240.74)	0.0090; −10.1433 (242.33)
3	0.0120; 10.3486 (240.05)	0.6837; 439.2465 (232.14)	0.0079; −79.3220 (237.11)	0.0706; 37.4100 (236.28)	0.0304; 13.7848 (235.29)
4	0.1440; −82.1320 (235.94)	0.1769; −452.6538 (230.40)	0.0272; −269.0740 (233.75)	0.1976; 293.6548 (231.09)	0.1591; 71.9251 (233.93)
5	0.0343; −58.5696 (230.47)	0.0009; 0.7564 (224.12)	0.7000; 374.8839 (231.49)	0.0163; −19.7342 (228.33)	0.4637; −93.3327 (228.65)
6	0.5089; 164.3389 (228.79)	0.0000; 0.0323 (220.42)	0.0631; 32.3777 (228.11)	0.3697; −262.3258 (227.52)	0.1104; −11.3831 (226.76)
7	0.0765; 5.0480 (221.19)	0.0000; −0.0126 (210.65)	0.0091; −0.7602 (220.43)	0.0100; −5.1167 (215.35)	0.0092; 6.7358 (219.54)
8	0.0049; 5.7335 (218.66)	0.0000; 0.0245 (204.89)	0.0347; 1.0995 (216.05)	0.0004; −3.0409 (211.85)	0.0014; −2.0503 (215.68)
9	0.0301; 43.9724 (207.32)	0.1857; 72.7670 (197.75)	0.0251; 86.3334 (209.36)	0.0138; −6.6786 (206.97)	0.0177; −10.4172 (203.18)
10	0.1763; −125.3798 (204.56)	0.2634; −126.3810 (195.45)	0.0194; −73.7010 (204.25)	0.0047; −2.9361 (202.21)	0.0420; 42.6809 (200.92)
11	0.1106; 124.2420 (202.13)	0.0030; −3.6474 (193.97)	0.1993; 65.4914 (199.57)	0.0505; −59.1278 (199.38)	0.0522; −27.4487 (199.13)
12	0.0668; 55.9393 (199.73)	0.5820; 412.4387 (193.52)	0.0946; 115.8274 (197.82)	0.2692; −20.3208 (196.81)	0.0937; −93.9587 (198.06)
13	0.0117; −101.3471 (196.99)	0.2825; −222.8630 (191.64)	0.1540; −346.0475 (195.14)	0.1403; 27.0895 (196.17)	0.0528; 103.9484 (196.45)
14	0.2148; 372.7058 (194.58)	0.0145; −9.5350 (191.49)	0.1238; −28.0272 (193.55)	0.0371; −6.1275 (194.78)	0.2486; −410.7641 (195.23)
15	0.0812; −229.1275 (192.44)	0.0443; −86.0420 (190.99)	0.6952; 60.2600 (190.89)	0.2190; 515.6399 (191.79)	0.0437; 306.4958 (192.74)
16	0.2363; −50.5710 (189.79)	0.2172; −31.2772 (190.12)	0.0499; 52.8659 (190.43)	0.4524; −537.2430 (191.00)	0.8674; −92.9011 (190.89)
17	0.1399; −209.9689 (189.51)	0.0068; −0.2327 (188.59)	0.2804; 165.0480 (189.38)	0.2795; 7.7745 (189.93)	0.0728; 96.0461 (189.87)
18	0.3684; 166.0577 (188.82)	0.0102; −25.9143 (188.21)	0.0051; −20.2723 (184.71)	0.0103; 1.5033 (187.02)	0.0675; 21.8009 (186.32)
19	0.0133; −13.1826 (185.00)	0.0000; −0.1164 (185.95)	0.0162; 21.3850 (183.86)	0.0088; −14.1875 (184.39)	0.0939; 20.3747 (184.15)
20	0.1496; −77.6026 (183.66)	0.0000; −0.0005 (181.74)	0.0076; −8.6345 (182.04)	0.0506; 69.6764 (184.18)	0.0419; 55.0048 (183.19)
21	0.0757; 46.3990 (183.05)	0.0034; −0.1070 (177.68)	0.0106; −4.2404 (181.95)	0.0025; −8.6487 (181.08)	0.0028; 0.2267 (181.91)
22	0.0745; 29.3746 (178.39)	0.0111; −5.7439 (177.32)	0.0791; 8.7897 (178.47)	0.0103; −17.0796 (179.77)	0.0705; −50.3348 (180.15)
23	0.0053; 8.4642 (177.58)	0.0792; 8.4663 (174.40)	0.0845; 43.7928 (177.56)	0.0376; 9.9279 (179.18)	0.0368; 3.7940 (177.32)
24	0.0527; −14.7378 (176.29)	0.0056; 0.1668 (173.71)	0.0061; 2.9570 (173.01)	0.0226; 19.8523 (177.13)	0.0120; 6.8873 (174.14)
25	0.0111; 11.6516 (174.90)	0.0042; 1.0596 (173.39)	0.0017; 0.1660 (172.35)	0.0019; 4.8092 (172.18)	0.0013; 1.1291 (173.40)
26	0.0022; −1.6400 (174.64)	0.0010; −3.8911 (172.23)	0.0118; 0.9714 (172.20)	0.0028; −4.4193 (172.03)	0.0008; −0.4555 (172.43)
27	0.0009; −1.1358 (173.17)	0.0436; 22.0208 (172.11)	0.0026; −0.8421 (170.12)	0.0006; −0.2299 (171.88)	0.0001; −2.8601 (172.18)
28	0.0157; −17.3214 (172.80)	0.0000; 0.1667 (170.63)	0.0012; −1.1239 (169.77)	0.0052; −0.0758 (171.77)	0.0050; −6.8829 (171.33)
29	0.0216; 3.3921 (171.91)	0.0039; 1.5380 (170.06)	0.0193; 14.8803 (169.23)	0.0263; −7.2152 (170.89)	0.0049; −5.1155 (170.92)
30	0.0067; −8.4965 (171.35)	0.0073; 15.5658 (168.70)	0.0097; −7.7205 (168.67)	0.0004; 1.2046 (168.90)	0.0159; 5.5823 (170.72)
31	0.0004; −1.0225 (168.94)	0.0686; −18.0033 (167.41)	0.0103; −12.9438 (168.64)	0.0661; 28.4333 (167.96)	0.0013; 0.7981 (170.04)
32	0.0011; −2.7518 (168.62)	0.0330; 9.9053 (167.05)	0.0093; −3.1892 (167.31)	0.0228; −0.9545 (167.58)	0.0012; 1.5349 (168.14)
33	0.0056; −1.9224 (168.39)	0.0104; −1.2386 (166.88)	0.0119; 4.1592 (166.35)	0.0021; −0.6368 (167.01)	0.0364; 15.6375 (167.27)
34	0.0057; −1.6358 (167.28)	0.0013; −5.4230 (166.77)	0.0553; 3.5496 (166.23)	0.0221; 38.0129 (166.45)	0.0013; −2.3458 (166.46)
35	0.0031; 19.7291 (166.81)	0.0025; 0.5164 (166.42)	0.0021; −2.2433 (165.86)	0.0422; 75.5217 (166.24)	0.0388; 15.0287 (165.70)
36	0.0248; 9.6414 (165.97)	0.0139; −15.2644 (164.84)	0.0073; −2.8260 (165.33)	0.0145; −39.4687 (165.87)	0.0054; 6.9644 (165.25)
37	0.0273; −25.2387 (165.61)	0.0015; 1.5092 (164.35)	0.0095; −1.7710 (164.73)	0.0294; 9.3781 (165.71)	0.0034; 2.7040 (164.72)
38	0.0115; −10.4776 (165.39)	0.0003; −0.0198 (164.20)	0.0179; −9.2372 (164.24)	0.0335; 13.0536 (165.43)	0.0217; −2.4019 (164.53)
39	0.0277; −28.6865 (164.65)	0.0006; 0.0835 (163.85)	0.0088; −11.2370 (164.14)	0.0348; −13.7323 (165.17)	0.0553; 57.9575 (164.24)
40	0.0003; 1.2094 (164.32)	0.0074; −2.2634 (163.77)	0.0109; −4.2568 (163.62)	0.0778; −31.9402 (165.10)	0.0250; −4.4708 (164.10)
41	0.0076; 5.3931 (164.10)	0.0075; 4.2655 (163.54)	0.0265; 2.7049 (163.60)	0.0572; −2.1048 (164.70)	0.0237; −13.1475 (163.99)
42	0.0378; −74.5730 (163.67)	0.0002; 0.7067 (162.39)	0.0346; −37.9483 (163.16)	0.0129; −1.7278 (163.99)	0.0672; −49.0950 (163.68)
43	0.0233; −8.2129 (163.09)	0.0017; −0.2065 (162.09)	0.0076; 3.2906 (162.60)	0.0046; −9.8470 (162.91)	0.0071; 1.0716 (163.00)
44	0.0292; 52.5326 (163.03)	0.0033; −1.1356 (161.79)	0.0305; 32.6862 (162.25)	0.0087; −15.8418 (162.80)	0.0152; 0.0640 (162.92)
45	0.0135; 28.3094 (162.80)	0.0058; 5.7912 (161.00)	0.0123; 2.9855 (162.07)	0.0020; 0.1702 (162.71)	0.0306; −25.0492 (162.59)
46	0.0041; −10.8914 (161.39)	0.0015; −1.4761 (160.74)	0.0064; −7.7931 (161.53)	0.0343; −4.8834 (161.77)	0.0052; −3.0601 (161.76)
47	0.0028; −0.4992 (161.22)	0.0020; −0.8030 (160.49)	0.0058; 2.5330 (161.42)	0.0037; −7.3937 (161.62)	0.0153; 2.4967 (161.38)
48	0.0144; 17.7341 (160.84)	0.0224; 18.8002 (160.30)	0.0030; −0.8196 (161.14)	0.0041; 1.4282 (160.82)	0.0013; 0.5272 (160.78)
49	0.0097; −23.6558 (160.49)	0.0227; −1.8015 (159.81)	0.0048; 8.3858 (161.11)	0.0021; −0.1158 (160.71)	0.0032; 12.1269 (160.58)
50	0.0185; 7.1824 (160.41)	0.0058; −7.6534 (159.77)	0.0079; −4.6581 (160.77)	0.0118; 0.3207 (160.59)	0.0038; −8.5364 (160.31)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c205	**c207**	**c217**	**c231**	**c242**
1	0.0207; 41.6953 (247.37)	0.0105; 11.1202 (245.63)	0.0109; 1.3851 (242.50)	0.0104; −1.2906 (243.58)	0.0091; 2.5450 (243.44)
2	0.0073; −23.4059 (246.17)	0.0117; −0.0212 (243.69)	0.0064; 2.4604 (241.74)	0.0071; −4.1741 (242.85)	0.0063; −4.0538 (241.17)
3	0.0098; −16.8926 (241.74)	0.0750; 18.0652 (234.09)	0.5168; −29.5216 (229.81)	0.1844; −315.5729 (232.67)	0.1495; 123.5800 (232.31)
4	0.0443; 200.1681 (237.84)	0.6310; −95.9636 (230.20)	0.2462; 6.4110 (226.93)	0.1140; 86.8508 (231.04)	0.1874; −132.1859 (228.27)
5	0.2256; −96.5397 (234.09)	0.0443; −5.7879 (229.55)	0.0002; 0.1606 (214.48)	0.2681; 110.0442 (227.79)	0.1102; −24.9382 (225.88)
6	0.5726; −118.0688 (229.55)	0.0003; 1.6626 (223.20)	0.0003; 0.1736 (212.36)	0.0331; −20.3816 (222.11)	0.0264; −37.4282 (225.00)
7	0.0029; 11.8303 (227.71)	0.0005; 0.4708 (221.28)	0.0000; 0.0642 (209.71)	0.0162; 2.0274 (217.56)	0.0986; 53.2091 (219.21)
8	0.0421; 4.6926 (223.67)	0.0320; −11.7165 (218.06)	0.0002; 0.0791 (205.74)	0.0447; 48.6211 (214.52)	0.0056; −22.0054 (216.43)
9	0.0080; −20.5480 (209.09)	0.0768; 50.2790 (204.35)	0.2419; −10.8872 (196.54)	0.0258; 56.7425 (207.73)	0.0096; −23.7109 (206.22)
10	0.0685; 65.7214 (204.23)	0.0344; 28.9641 (202.98)	0.2156; 36.6937 (195.50)	0.0267; 55.3533 (202.34)	0.0028; −36.4399 (203.09)
11	0.0034; 1.9619 (202.71)	0.0386; −0.3220 (201.42)	0.6026; 264.6890 (193.20)	0.1151; 66.2577 (197.97)	0.0251; −24.8180 (199.54)
12	0.0092; −50.0374 (200.24)	0.1152; 4.2313 (198.62)	0.3213; −220.0086 (192.37)	0.1010; −15.3041 (196.75)	0.0758; 37.3120 (197.17)
13	0.0427; 134.0745 (198.87)	0.1143; −7.9778 (195.25)	0.0046; −3.2051 (190.41)	0.2704; −123.6220 (194.52)	0.0883; −49.9719 (195.46)
14	0.2532; −495.7489 (194.75)	0.1824; −72.8410 (194.84)	0.0007; 1.0151 (190.39)	0.0425; −276.3712 (193.33)	0.3909; 177.0091 (193.97)
15	0.1421; 358.4367 (193.40)	0.6550; 25.8549 (191.13)	0.0001; −0.0359 (188.31)	0.2522; −67.6108 (192.25)	0.2108; 117.3334 (193.11)
16	0.0051; 23.9498 (190.99)	0.0534; 92.0267 (189.82)	0.1400; −130.6736 (187.76)	0.4396; 252.8330 (190.44)	0.2960; −270.7441 (192.25)
17	0.9348; −28.6037 (190.58)	0.2955; −87.5092 (189.12)	0.0338; 60.1715 (184.09)	0.0221; 26.7153 (187.70)	0.2150; 19.9615 (188.21)
18	0.0098; 16.0334 (186.98)	0.0113; 30.6603 (186.19)	0.0044; −9.3539 (183.51)	0.0744; 81.3157 (186.01)	0.0384; 65.5327 (184.07)
19	0.0189; −14.1463 (185.87)	0.0161; 11.1460 (181.53)	0.0006; −1.3494 (183.44)	0.0634; −49.1685 (184.91)	0.0187; 8.8829 (183.43)
20	0.0162; 40.0470 (185.31)	0.1504; −59.7109 (180.95)	0.0581; −48.8579 (180.12)	0.0477; 50.4661 (184.32)	0.0129; 14.4548 (182.10)
21	0.0175; 3.4887 (184.30)	0.0105; 0.6367 (180.31)	0.0092; −1.9418 (178.91)	0.0065; −1.1379 (182.16)	0.0013; −0.0988 (181.89)
22	0.2430; −53.9015 (179.63)	0.0300; −9.4539 (179.42)	0.0042; 12.1074 (178.28)	0.0259; −29.5894 (180.97)	0.0054; 4.3661 (180.39)
23	0.0009; −1.9769 (178.05)	0.0164; −1.7359 (177.36)	0.0076; 2.5120 (175.35)	0.0688; 58.3313 (180.48)	0.0054; −15.1761 (179.81)
24	0.0093; −14.0418 (177.59)	0.0039; −8.4323 (173.68)	0.0006; 0.3918 (173.92)	0.0020; −1.0337 (175.43)	0.0147; −19.7016 (179.24)
25	0.0086; −14.1385 (175.92)	0.0216; 15.4823 (173.36)	0.0014; 0.9256 (172.63)	0.0047; 2.5826 (175.03)	0.0023; 0.6252 (174.15)
26	0.0489; 5.2786 (174.90)	0.0011; −2.0265 (171.48)	0.0392; 0.9189 (170.40)	0.0035; −1.1060 (172.88)	0.0138; 8.3225 (172.98)
27	0.0009; −1.7811 (173.38)	0.0277; −2.3946 (171.19)	0.0022; −0.7431 (170.16)	0.0039; −0.9745 (170.84)	0.0100; −18.8418 (172.68)
28	0.0004; 0.7316 (173.22)	0.0333; −9.0806 (170.10)	0.0027; −0.2774 (169.97)	0.0145; 2.2214 (170.75)	0.0378; −6.1355 (172.19)
29	0.0013; 0.7740 (172.72)	0.0021; −0.0608 (169.20)	0.0083; 1.9519 (169.20)	0.0276; 11.1486 (169.62)	0.0133; −3.9132 (170.68)
30	0.0022; −3.3632 (171.78)	0.0566; −32.9450 (168.30)	0.0015; −0.3788 (168.60)	0.0127; −9.0649 (169.11)	0.0087; 15.6029 (170.19)
31	0.0255; −2.6292 (169.32)	0.0037; −0.1035 (167.49)	0.0033; −3.8058 (168.46)	0.0066; 9.9568 (168.41)	0.0405; 31.0541 (169.94)
32	0.0035; 3.1017 (169.14)	0.0233; 43.2133 (166.96)	0.0690; −32.1617 (167.71)	0.0036; 1.2460 (168.15)	0.0041; −2.5943 (169.59)
33	0.0510; 6.7449 (168.53)	0.0017; −1.3380 (166.24)	0.0839; 34.7719 (166.16)	0.0262; −36.6725 (167.40)	0.0421; 5.9919 (168.71)
34	0.0010; −6.4002 (168.12)	0.0727; −1.9106 (165.98)	0.1079; −43.4580 (165.63)	0.0200; 9.0569 (166.87)	0.0020; −4.7910 (168.11)
35	0.0029; 0.1590 (167.33)	0.0042; 2.4673 (165.13)	0.0007; 3.3777 (165.47)	0.0434; 76.8983 (166.48)	0.0086; 9.9813 (167.97)
36	0.0042; 19.7967 (166.95)	0.0185; 9.6064 (164.85)	0.0067; 0.4357 (164.52)	0.0231; 1.5663 (165.58)	0.0098; −13.7305 (167.26)
37	0.0066; 18.2392 (166.70)	0.1020; −38.6431 (164.59)	0.0086; 0.9972 (164.35)	0.0551; 11.0560 (165.17)	0.0348; −1.5337 (166.60)
38	0.0016; 0.8570 (163.94)	0.0147; 7.4016 (163.88)	0.0061; −10.3913 (163.79)	0.0353; −23.0457 (164.71)	0.0275; 39.0951 (166.36)
39	0.0026; 0.7076 (163.85)	0.0202; 15.4392 (163.66)	0.1732; 2.6470 (163.64)	0.0356; −2.0661 (164.39)	0.0173; 24.0310 (165.93)
40	0.0002; 1.5142 (163.41)	0.0115; 5.8317 (163.11)	0.0031; −8.5206 (163.32)	0.0223; 3.3944 (163.42)	0.0014; −3.5993 (165.45)
41	0.0017; −2.7912 (163.28)	0.0004; −2.9994 (162.87)	0.0151; −24.1870 (162.91)	0.0658; −18.9416 (163.26)	0.0449; 53.1346 (165.37)
42	0.0016; −4.2183 (162.20)	0.0068; −4.5242 (162.80)	0.0032; −0.1557 (161.58)	0.0121; 0.6378 (162.93)	0.1113; 9.4752 (164.85)
43	0.0024; −12.4026 (162.00)	0.0028; 0.3513 (162.44)	0.0009; 4.0994 (161.45)	0.0282; 23.5543 (162.83)	0.0409; −5.3761 (164.77)
44	0.0005; −3.3647 (161.78)	0.0099; −6.1130 (161.95)	0.0028; 4.1601 (161.32)	0.0355; −9.0240 (162.79)	0.0074; 3.2824 (164.43)
45	0.0021; −1.3390 (161.60)	0.0352; −8.8863 (161.73)	0.0109; −0.9088 (160.91)	0.0186; 6.0693 (161.74)	0.0825; 18.7146 (163.98)
46	0.0312; −8.8949 (161.43)	0.0221; 3.6668 (161.36)	0.0022; 1.3949 (160.12)	0.0328; −24.7650 (161.53)	0.0232; −31.1909 (163.73)
47	0.0027; 0.4837 (160.71)	0.0029; 5.2191 (160.84)	0.0046; 2.0040 (160.09)	0.0006; −3.4127 (161.22)	0.0487; 15.9391 (163.17)
48	0.0037; −8.1028 (160.56)	0.0008; −1.7298 (160.79)	0.0042; −0.3485 (159.94)	0.0043; −6.3985 (160.51)	0.0034; −6.9706 (162.78)
49	0.0144; 25.2142 (160.28)	0.0020; 1.8374 (160.50)	0.0087; −4.2467 (159.67)	0.0004; −1.0211 (160.48)	0.0025; 2.4279 (162.42)
50	0.0136; 4.1219 (160.12)	0.0047; 2.5975 (160.25)	0.0044; −4.1058 (159.45)	0.0005; 1.4165 (160.06)	0.0100; −9.9264 (162.09)

Table S2. (*Continued*)

j	f_j; R_j, 10^{-40} erg cm^3 (λ_j, nm)				
	c247	**c248**	**c258**	**c263**	**c284**
1	0.0068; 11.6114 (250.17)	0.0158; 6.4668 (244.57)	0.0172; −6.3974 (245.57)	0.0189; −5.2667 (245.34)	0.0145; 5.4107 (247.63)
2	0.0047; −6.8128 (249.07)	0.0041; −0.8056 (243.47)	0.0113; −0.8428 (244.47)	0.0131; −0.7546 (244.01)	0.0113; −5.6907 (242.96)
3	0.1007; −46.0696 (241.09)	0.0291; 178.3205 (233.55)	0.5050; 241.4092 (232.24)	0.4440; 167.0435 (231.95)	0.1820; 268.4576 (233.24)
4	0.0169; −29.5668 (238.38)	0.6290; −214.6973 (230.23)	0.1944; −155.9759 (229.34)	0.3010; −114.5640 (229.09)	0.2387; −94.4743 (230.49)
5	0.1632; −47.9460 (233.77)	0.1085; −15.5304 (225.64)	0.0724; −125.5906 (229.11)	0.0347; 36.4769 (228.84)	0.0373; −30.1173 (222.99)
6	0.3484; 187.3725 (228.26)	0.0191; −3.7611 (220.09)	0.0002; −0.1777 (226.53)	0.0029; −1.9733 (226.44)	0.0023; 1.7635 (222.34)
7	0.0105; −26.7967 (222.86)	0.0059; 3.1499 (218.75)	0.0000; −0.0014 (208.12)	0.0004; −0.2243 (205.93)	0.0639; −37.5537 (219.53)
8	0.0329; 8.9101 (217.65)	0.0081; 2.7164 (216.00)	0.0001; 0.0155 (201.57)	0.0001; 0.1497 (199.58)	0.0275; −7.3890 (217.84)
9	0.0089; 8.5240 (208.76)	0.2088; 7.1478 (203.24)	0.0035; 6.4914 (198.25)	0.0100; −0.0961 (198.38)	0.1122; −122.8316 (204.52)
10	0.0165; 61.4149 (204.02)	0.0006; −17.7430 (200.54)	0.1504; 132.0107 (197.02)	0.2700; −4.8348 (197.47)	0.0088; 25.7610 (202.14)
11	0.0201; 15.7190 (203.70)	0.0651; −6.0875 (199.76)	0.0082; −9.9056 (196.39)	0.0092; 0.4659 (196.47)	0.1381; −40.0276 (200.23)
12	0.0263; −47.3685 (201.78)	0.0531; −8.3410 (196.16)	0.2482; −166.3915 (195.88)	0.2119; 23.8200 (195.56)	0.1174; 3.0659 (198.70)
13	0.0444; 21.3252 (196.85)	0.1165; 181.2642 (195.43)	0.4392; 632.0614 (192.81)	0.2963; 438.2106 (192.92)	0.1838; 143.4599 (194.41)
14	0.1097; 135.7690 (195.58)	0.1892; −98.6077 (194.47)	0.3032; −337.4858 (192.26)	0.1391; −223.8187 (192.33)	0.0907; 22.0928 (193.78)
15	0.0405; −82.3423 (194.36)	0.5759; −98.6031 (190.60)	0.0543; −176.0838 (191.90)	0.0330; −68.0687 (191.46)	0.0832; 394.6248 (192.47)
16	0.2882; −377.1381 (192.60)	0.4845; −8.2240 (189.58)	0.2877; −119.4760 (190.27)	0.5524; −175.3829 (191.11)	0.3280; −405.2140 (190.53)
17	0.4739; 311.1505 (191.89)	0.0065; −11.8211 (187.78)	0.0021; 8.7284 (187.81)	0.0100; 25.9359 (189.22)	0.2544; −95.8496 (189.93)
18	0.2674; −63.7565 (189.82)	0.0058; 7.5853 (185.26)	0.0001; −0.1974 (184.34)	0.0012; 0.5573 (184.34)	0.0231; 6.1507 (188.03)
19	0.0285; −6.8143 (187.44)	0.0082; 25.7111 (182.82)	0.0004; 0.6159 (184.08)	0.0011; −0.9242 (183.57)	0.0118; 31.6903 (187.94)
20	0.1058; −0.1345 (185.37)	0.0245; −13.7221 (181.62)	0.0000; 0.0322 (179.48)	0.0000; −0.0213 (179.36)	0.0105; −11.7572 (186.84)
21	0.0015; 4.1963 (182.27)	0.0117; −3.3344 (179.32)	0.0170; 4.5314 (177.61)	0.0019; −2.6942 (177.60)	0.0127; −10.4311 (179.45)
22	0.0082; −7.0305 (181.02)	0.0889; −38.7026 (178.63)	0.0153; 3.3691 (176.96)	0.0196; −14.2094 (176.58)	0.0100; −1.2064 (177.19)
23	0.0099; 33.0452 (179.38)	0.0240; −3.8343 (177.16)	0.0860; 16.2213 (175.79)	0.0936; 9.7985 (175.55)	0.0039; 7.7787 (174.12)
24	0.1158; −41.7518 (179.26)	0.0042; −1.6674 (176.01)	0.0106; 3.9404 (174.72)	0.0780; −6.1894 (175.12)	0.0499; −17.4094 (173.79)
25	0.0162; −1.1745 (175.54)	0.0031; −3.5176 (173.35)	0.0431; 7.9168 (173.41)	0.0003; 0.1055 (173.82)	0.0065; 0.2777 (172.30)
26	0.0054; −0.6687 (174.19)	0.0470; 6.5657 (170.26)	0.0007; −0.3251 (171.97)	0.0007; −0.4333 (171.59)	0.0471; 17.1051 (172.06)
27	0.0221; −20.1334 (173.49)	0.0011; −1.2352 (169.95)	0.0029; −3.9366 (170.63)	0.0078; −5.6926 (170.84)	0.0047; −3.9579 (171.03)
28	0.0070; −5.5098 (172.21)	0.0110; 1.8495 (169.40)	0.0075; −4.5811 (170.51)	0.0003; 0.9267 (170.20)	0.0152; −2.7543 (169.87)
29	0.0020; 5.6665 (170.85)	0.0019; −1.2317 (169.34)	0.0034; 10.3004 (169.78)	0.1130; −21.2202 (169.91)	0.0191; 17.4567 (169.80)
30	0.0059; 12.0022 (170.47)	0.0362; 14.8011 (168.35)	0.0760; 17.9410 (169.56)	0.0844; −49.2315 (169.58)	0.0061; 22.3427 (169.42)
31	0.0196; −12.9549 (170.30)	0.0083; 2.7452 (167.87)	0.0696; 21.8550 (168.88)	0.0005; −0.6427 (168.73)	0.0663; 16.5317 (168.69)
32	0.0040; −0.6175 (170.12)	0.0084; −2.7226 (167.25)	0.0005; 0.1886 (168.75)	0.0015; 0.0797 (168.62)	0.0194; −49.5434 (168.03)
33	0.0003; 2.6206 (169.22)	0.0842; 4.7018 (166.10)	0.0030; 0.7728 (167.73)	0.0117; −7.4210 (168.06)	0.0104; −14.6432 (167.88)
34	0.0062; −13.8459 (168.61)	0.0177; 14.7758 (166.00)	0.0168; −36.9035 (167.67)	0.0016; −3.0381 (167.50)	0.0382; −55.5874 (167.47)
35	0.0058; 14.7843 (167.60)	0.0312; 0.1159 (165.72)	0.0283; 40.7153 (167.64)	0.0010; −0.4475 (166.86)	0.0485; 11.8895 (167.42)
36	0.0031; −9.3719 (167.28)	0.0048; −3.2273 (165.40)	0.0036; 1.1428 (166.23)	0.0011; 0.7172 (166.01)	0.0170; 7.4816 (166.63)
37	0.0292; −8.6149 (166.58)	0.0093; 10.8056 (164.27)	0.0056; −7.9964 (165.82)	0.0071; 5.5006 (165.35)	0.0011; 2.4814 (165.65)
38	0.0519; −60.0623 (166.03)	0.1290; −20.0242 (163.46)	0.0046; 1.5586 (165.28)	0.0099; 19.5203 (163.89)	0.0022; −11.1012 (165.21)
39	0.0135; −40.8999 (165.77)	0.0091; 19.4347 (163.17)	0.0023; −11.7767 (164.78)	0.0067; 1.4228 (163.39)	0.0005; −0.0644 (164.85)
40	0.0081; 13.6188 (165.52)	0.0044; 1.8938 (162.69)	0.0057; 0.7762 (163.29)	0.0095; −6.5038 (163.20)	0.0035; 10.0634 (164.76)
41	0.0546; 33.9114 (165.06)	0.0011; 1.9464 (162.57)	0.0033; 3.0542 (163.20)	0.0028; −1.3188 (162.11)	0.0922; 22.8822 (163.95)
42	0.0193; 3.6448 (164.92)	0.0116; 15.4935 (162.31)	0.0024; −0.8194 (162.96)	0.0008; 1.7129 (161.95)	0.0164; −7.9617 (163.70)
43	0.0254; 1.9331 (164.05)	0.0205; −13.8923 (162.17)	0.0014; −1.3594 (162.35)	0.0004; −1.4509 (161.91)	0.0348; −11.5368 (163.49)
44	0.0530; 2.5071 (163.70)	0.0318; −16.8302 (161.36)	0.0073; 3.7870 (161.63)	0.0094; 1.2164 (161.83)	0.0052; 3.7840 (163.29)
45	0.0214; −1.4965 (163.56)	0.0005; −0.8851 (161.11)	0.0041; 2.4970 (161.16)	0.0014; 1.4662 (161.00)	0.0072; 10.4075 (162.33)
46	0.0070; −5.7965 (163.18)	0.0157; −12.6384 (160.70)	0.0009; −0.0212 (160.41)	0.0008; −4.4681 (160.46)	0.0260; 28.8343 (161.91)
47	0.0150; 17.1018 (162.94)	0.0062; 8.8510 (160.38)	0.0156; 5.8066 (160.27)	0.0129; −10.0120 (159.79)	0.0177; −13.9870 (161.80)
48	0.0005; −1.7943 (161.75)	0.0008; −3.2938 (160.31)	0.0088; −5.4895 (159.89)	0.0031; −17.8106 (159.62)	0.0065; −13.9344 (161.15)
49	0.0057; −12.1226 (161.70)	0.0027; −2.5105 (159.83)	0.0289; 13.1730 (159.66)	0.0295; 8.2213 (158.91)	0.0022; −0.6190 (160.47)
50	0.0083; 4.9269 (161.21)	0.0067; 2.4735 (159.54)	0.0069; 12.8462 (158.95)	0.0048; 11.1890 (158.55)	0.0116; 0.8256 (160.37)

Figure S1. Preparation of one of the sensing surfaces for the developed assay: blocking of the substrate-binding site of SMYD3 with a tight-binding inhibitor EPZ031686. Injection of 1 µM of EPZ031686 was performed in an interactive run mode, with a standard "Inject" command, the data is unreferenced. Baseline level increment of 58 RU corresponds to saturation of the corresponding binding site. Theoretical increment (R_{max}) for a compound with a similar M_w and SMYD3 immobilization level of approx. 10000 RU is 100 RU, assuming 100% activity of the immobilized protein.

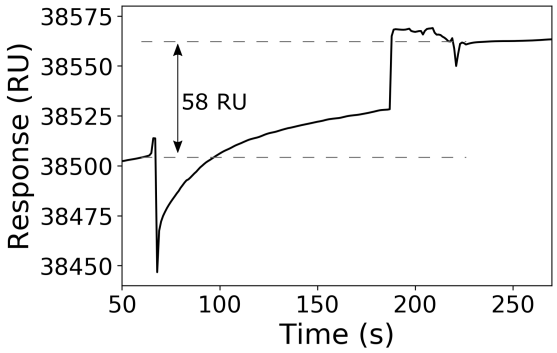


Figure S2. Characterization of the control compound, S-adenosyl-homocysteine (SAH). SAH was injected over SMYD3-functionalized biosensing surface in 2-fold serial dilution series, spanning concentration range 50–0.098 µM. Double-referenced interaction kinetic curves (black) were approximated with a 1:1 kinetic model (red), quantified interaction parameters: association rate constant $k_a = 5.4 \times 10^5\ M^{-1}\ s^{-1}$, dissociation rate constant $k_d = 0.3\ s^{-1}$, dissociation constant $K_D = 560$ nM. The data is referenced against surface with denaturated SMYD3.

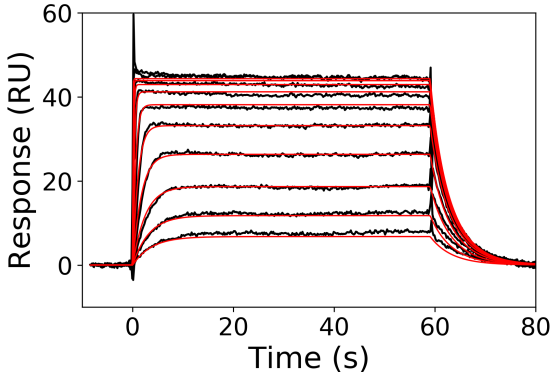


Figure S3. Kinetic curves of a fixed concentration injection of 25 µM SAH in the developed screening setup. (A) Unreferenced data. Responses from two flow cells are shown: reference flow cell containing immobilized SMYD3, denaturated with 6 M guanidine hydrochloride (black), analytical flow cell with SMYD3, immobilized at the same level (red). (B) Referenced sensorgram for the same data.

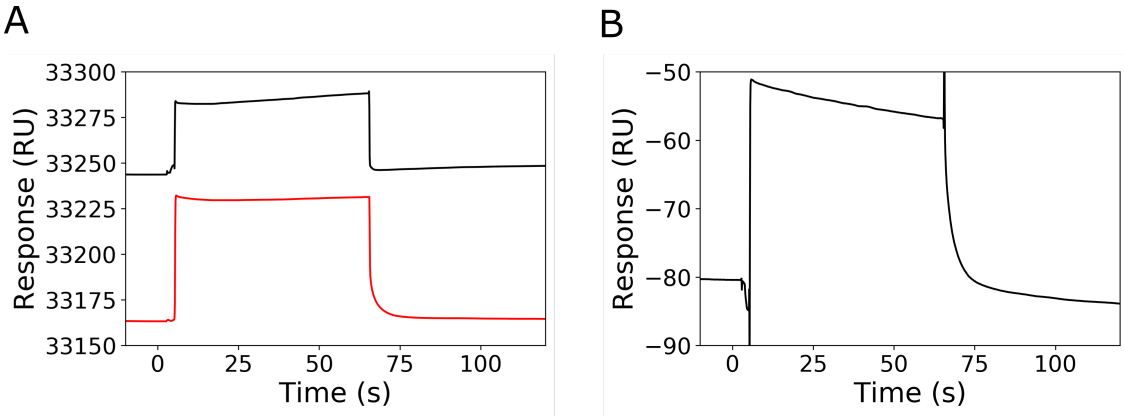


Figure S4. Interaction kinetic analysis of the screening hit, racemic diperodon (*rac*-diperodon) and immobilized SMYD3. The compound was injected in two-fold dilution series, spanning concentration range 100–0.4 µM. The data is referenced against surface with denaturated SMYD3.

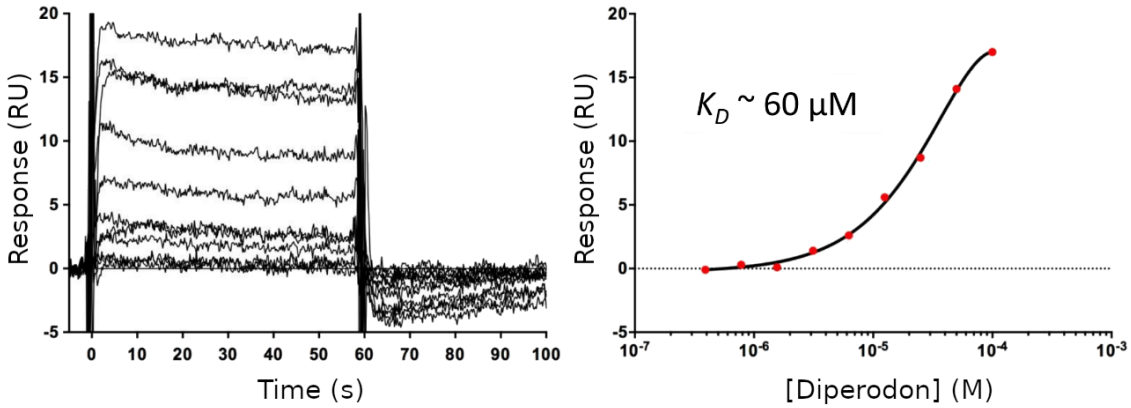


Figure S5. Interaction kinetic analysis of the screening hit, racemic diperodon (*rac*-diperodon) and immobilized SMYD3 with the substrate binding site, blocked with tight-binding SMYD3 inhibitor EPZ031686. The compound was injected in two-fold dilution series, spanning concentration range 100–0.4 µM. The data is referenced against surface with denaturated SMYD3.

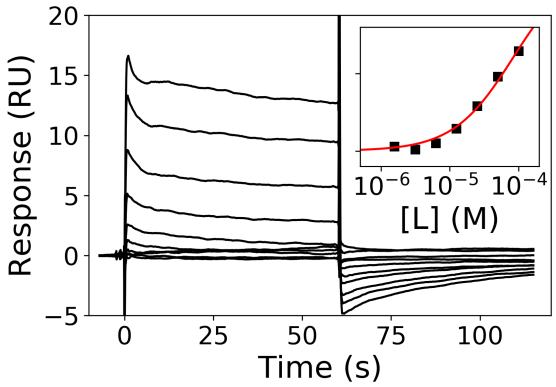


Figure S6. Geometries of the conformers of (*R*)-diperodon (conjugate acid form) having a relative electonic energy below 1 kcal mol^{-1}, as calculated by DFT optimization at the B97D/def2-TZVP/IEFPCM[H_2O] level: **c015** (12.03 %), **c117** (7.69 %), **c284** (5.50 %), **c020** (5.15 %), **c016** (4.89 %), **c107** (4.77 %), **c071** (4.74 %), **c008** (3.61 %), **c122** (3.13 %), **c127** (2.79 %), **c002** (2.79 %), **c026** (2.55 %), **c001** (2.40 %), **c036** (2.38 %), **c137** (2.28 %).

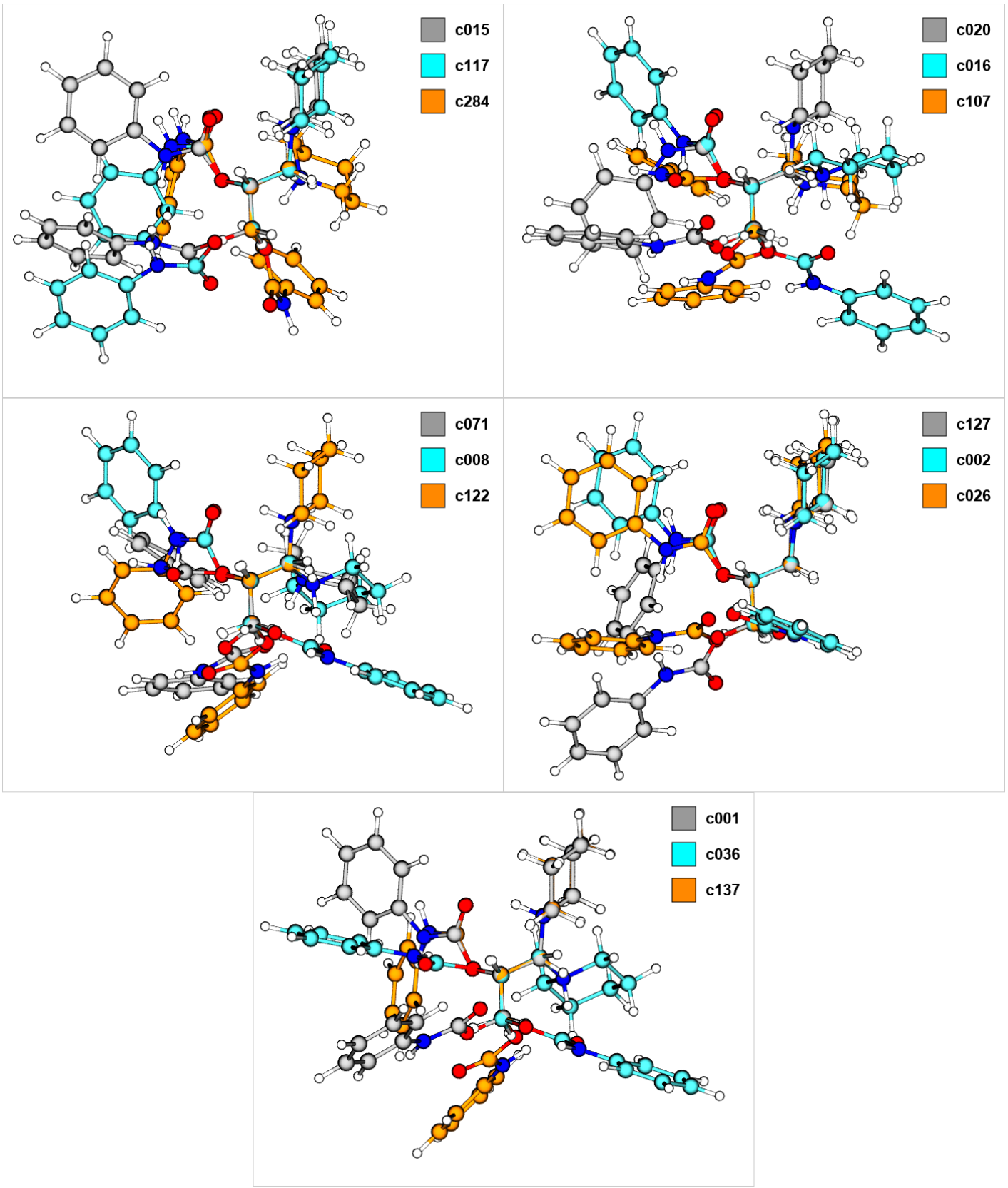


Figure S7. Comparison between the experimental UV spectrum of the first enantiomeric fraction of diperodon on the Lux Cellulose-2 column and the theoretical UV spectrum of (*R*)-diperodon (conjugate acid form), as calculated at the PBE0/def2-TZVP/IEFPCM[H_2O] level of theory after B97D/def2-TZVP/IEFPCM[H_2O] optimization.

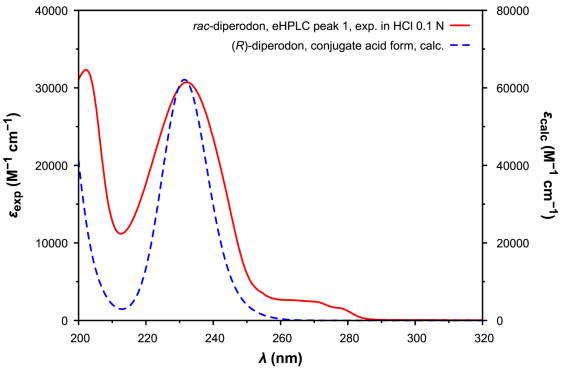


Figure S8. Deconvoluted mass spectra of MAP3K2$_{249-274}$ peptide as substrate for SMYD3 methylation activity in absence (a) and presence (b) of 100 µM of *rac*-diperodon.

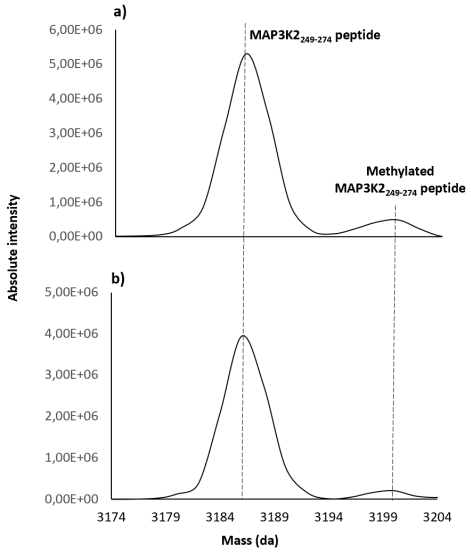


Table S3. Determination of inhibitory potency of diperodon, its individual enantiomers, the reconstituted racemic mixture, and the reference compound EPZ031686. *rac*-Diperodon, (*S*)-diperodon, (*R*)-diperodon and reconstituted *rac*-diperodon were assayed at 100 µM final concentration, while EPZ03168 was assayed at 0.63 µM final concentration, close to its IC_{50}.

	Methylation, %		Inhibition analysis, %	
	Experiment 1	Experiment 2	Inhibition 1	Inhibition 2
Control (2% DMSO)	8.06 ± 0.05	8.06 ± 0.09	-	-
rac-diperodon	4.36 ± 0.08	4.59 ± 0.10	45.9	43.0
(*S*)-diperodon	4.28 ± 0.02	4.45 ± 0.07	46.9	44.8
(*R*)-diperodon	4.74 ± 0.11	4.87 ± 0.01	41.2	39.6
reconstituted *rac*-diperodon	4.95 ± 0.06	4.77 ± 0.07	38.6	40.8
EPZ031686	3.71 ± 0.01	3.90 ± 0.04	54.0	51.6

Figure S9. Interaction of the C-terminal domain of HSP90 with SMYD3 in presence and absence of (*S*)-diperodon. (A) Single-concentration injections of 100 µM of $HSP90_{626-732}$ over surface-immobilized SMYD3 in presence (red) and absence (black) of 100 µM of (*S*)-diperodon. (B) and (C): injection of SMYD3 dilution series over surface-immobilized GST-$HSP90_{626-732}$ in presence (A) and absence (B) of 100 µM of (*S*)-diperodon. For competition experiments, diperodon was added in every analytical injection including blank injections, reference surfaces contained no immobilized protein. No strong evidence of competition between diperodon and C-terminal domain of HSP90 for interaction with SMYD3 was observed.

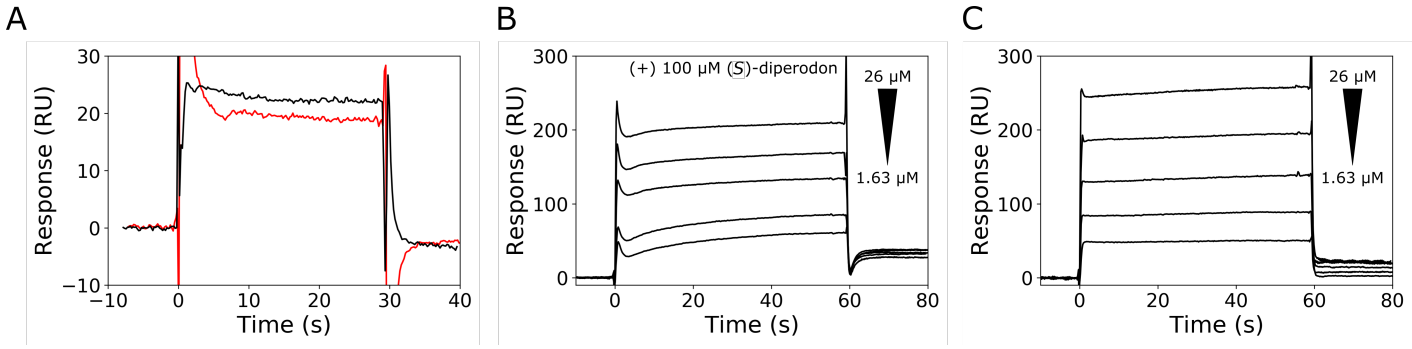


Figure S10. Original uncropped Western Blotting results, providing DMSO controls in the same membranes.

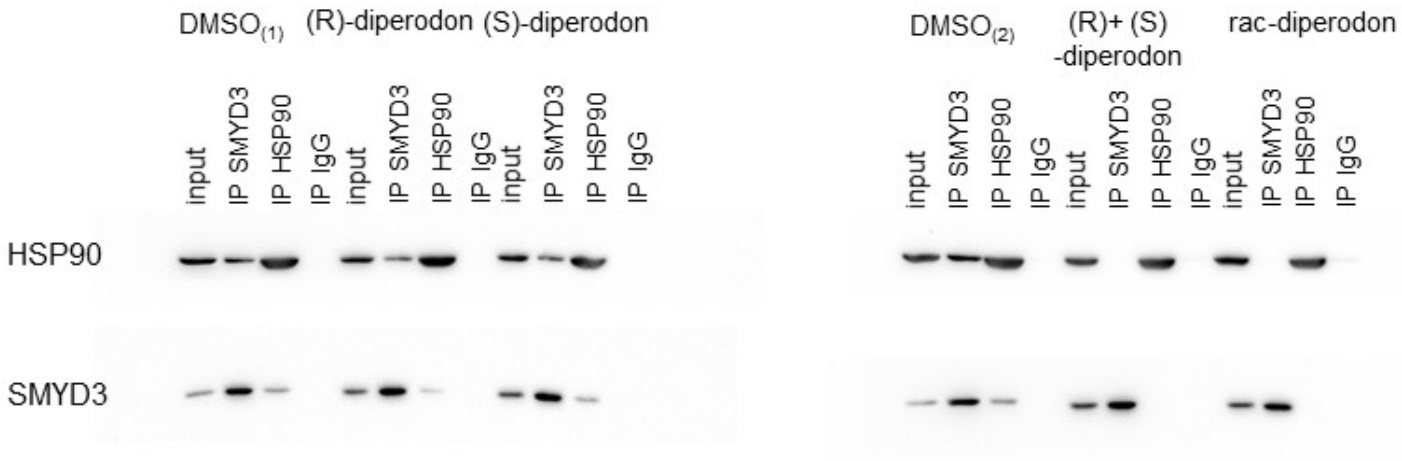


Table S4. Crystallographic data collection and model refinement statistics; values in parenthesis are given for the highest resolution shell.

Data collection		
PDB ID	6Z2R	6YUH
Structure	SMYD3/(*S*)-diperodon	SMYD3/(*R*)-diperodon
Beamline	ESRF ID 29	MAX IV BioMAX
Wavelength, Å	0.976	0.976
Space group	$P2_12_12_1$	$P2_12_12_1$
Unit cell: a, b, c, Å	60.9, 66.05, 102.3	60.14, 66.28, 105.95
Resolution range, Å	44.78-1.61 (1.67-1.61)	105.95-1.93 (1.98-1.93)
Unique reflections	56675 (5553)	32606 (2145)
Multiplicity	5.1 (4.8)	9.3 (7.3)
Completeness, %	99.93 (99.69)	100.0 (100.0)
R_{merge}	0.07 (1.28)	0.192 (1.788)
$CC_{1/2}$	0.99 (0.48)	1 (0.52)
Refinement		
Nr. refl. in test set	2730 (4.8 %)	1621 (5.0 %)
R/R_{free}, %/%	18.4/21.4	18.6/23.0
Nr. non-H atoms/average B-factor, Å^2		
protein	3470/27.1	3458/27.6
H_2O	526/37	256/31.5
ligand	52/44	50/42.3
Ramachandran plot, %		
favoured	98.58	98.58
allowed	1.42	1.42
outliners	0	0
RMS deviations		
bond length, Å	0.01	0.007
bond angles, °	1.41	0.82