Supporting Information

Concentrations and composition profiles of benzotriazole UV stabilizers in municipal sewage sludge in China

Ting Ruan [a], Runzeng Liu [a], Qiang Fu [b], Thanh Wang [a], Yawei Wang [a], Shanjun Song [a], Pu Wang [a], Man Teng [b], Guibin Jiang [a]*

[a] State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China

[b] China National Environmental Monitoring Center, Beijing 100029, China

*Corresponding author

Prof. Guibin Jiang

Research Center for Eco-Environmental Sciences,

Chinese Academy of Sciences

Tel: 8610-6284-9334

Fax: 8610-6284-9179

E-mail: gbjiang@rcees.ac.cn

Table S1: Optimized LC-MS/MS parameters for the benzotriazole compounds.

Analyte	Parent ion (m/z)	Daughter ion (m/z)	Cone voltage (V)	Collision voltage (V)	Retention time (min)	MQL[a] (ng/g)
UV-P	226	107	35	19	6.46	0.47
	226	120	35	21		
UV-PS	268	57	40	22	8.67	0.53
	268	212	40	19		
IS	266	119	35	24	10.79	0.36
	266	238	35	24		
UV-329	324	57	40	28	12.38	0.59
	324	212	40	23		
UV-350	324	212	40	28	14.39	0.69
	324	268	40	21		
UV-320	324	212	40	28	14.89	0.77
	324	268	40	21		
UV-234	448	119	40	40	15.36	0.15
	448	370	40	40		
UV-326	316	57	40	27	15.77	0.63
	316	260	40	20		
UV-328	353	71	40	29	16.40	0.31
	353	282	40	23		
UV-327	358	57	40	32	17.14	0.71
	358	302	40	24		

[a] MQL: Method quantification limit, calculated as a signal-to-noise ratio of 10

Table S2: BZT concentrations in the sludge samples and information about the wastewater treatment plants

Sampling ID	Analyte concentration (ng/g, dry weight)										TOC (%)	Processing Volume (10^4 m^3/d)	WWTP Biotreatment Techniques [a]
	UV-P	UV-PS	UV-329	UV-350	UV-320	UV-234	UV-326	UV-328	UV-327	∑BZT			
BJ-1	79.4	n.d.[b]	315	n.d.	n.d.	187	144	142	15.4	883	35.5	40	AAO
BJ-2	18.9	n.d.	98.6	n.d.	n.d.	14.0	104	9.50	n.d.	245	18.5	1.0	SBR
BJ-3	44.1	n.d.	93.4	n.d.	n.d.	147	208	140	14.6	647	37.0	35	OD
BJ-4	34.2	n.d.	63.8	n.d.	n.d.	156	102	112	12.8	481	40.6	8.0	SBR
BJ-5	72.2	n.d.	103	n.d.	n.d.	142	115	97.2	13.3	543	39.1	60	AAO
BJ-6	119	n.d.	543	n.d.	n.d.	111	120	70.5	8.11	978	39.0	10	AO
BJ-7	96.4	n.d.	64.4	n.d.	n.d.	125	111	69.4	n.d.	466	37.4	4.0	AO
SH-1	48.8	n.d.	21.5	n.d.	n.d.	121	66.3	132	17.0	407	45.0	6.0	PASF
CQ-1	12.8	n.d.	110	n.d.	n.d.	93.8	82.7	28.6	n.d.	328	30.9	11	OD
CQ-2	n.d.	n.d.	0.57	n.d.	n.d.	n.d.	22.1	3.54	n.d.	26.2	39.6	3.0	OD
CQ-3	22.3	n.d.	80.3	n.d.	n.d.	152	94.5	64.1	n.d.	414	28.0	30	OD
CS-1	7.41	n.d.	39.8	n.d.	n.d.	26.6	20.0	30.8	n.d.	125	7.80	18	AO
CS-2	1.89	n.d.	17.7	n.d.	n.d.	15.4	23.4	30.6	3.27	92.3	7.62	2.0	AO
CS-3	5.66	n.d.	62.5	n.d.	n.d.	148	58.7	82.6	9.73	367	13.8	22	AAO
TA-1	30.4	n.d.	247	1.88	n.d.	139	72.8	130	10.9	632	25.7	7.0	AAO
TA-2	33.1	n.d.	220	12.2	n.d.	129	89.5	153	13.0	649	19.4	7.0	OD
TA-3	0.96	n.d.	11.7	n.d.	n.d.	11.6	28.6	15.1	n.d.	67.9	18.8	2.0	AAO
TA-4	n.d.	n.d.	1.80	n.d.	n.d.	10.6	12.1	n.d.	n.d.	24.5	8.80	2.0	AAO
JN-1	9.17	n.d.	34.1	n.d.	n.d.	64.5	87.8	41.4	133	370	17.8	30	AO

JN-2	7.97	n.d.	20.5	n.d.	n.d.	49.7	32.1	24.4	n.d.	135	13.9	20	OD
JN-3	19.1	n.d.	27.1	n.d.	n.d.	83.8	33.4	53.5	5.45	222	17.2	10	AAO
JN-4	69.7	n.d.	16.7	n.d.	n.d.	156	26.6	19.5	n.d.	288	22.5	3.0	SBR
LW-1	45.4	n.d.	30.8	42.7	n.d.	44.6	51.8	126	13.0	355	21.5	4.0	AO
LW-2	n.d.	n.d.	21.4	n.d.	n.d.	13.5	19.8	16.2	n.d.	70.9	20.0	3.0	AO
LW-3	9.3	n.d.	109	n.d.	n.d.	118	55.8	60.0	1.53	353	20.2	2.0	AO
DZ-1	11.4	n.d.	30.6	13.8	n.d.	126	58.7	163	11.0	414	32.6	6.0	AAO
DZ-2	3.40	n.d.	n.d.	n.d.	n.d.	0.96	4.00	n.d.	n.d.	8.36	10.4	2.0	AO
DZ-3	43.1	n.d.	31.2	33.8	n.d.	37.5	39.4	114	n.d.	300	16.2	2.0	AAO
QD-1	61.7	n.d.	757	n.d.	n.d.	140	116	70.9	n.d.	1.14×10^{3}	35.8	10	AAO
QD-2	3.16	n.d.	19.2	n.d.	n.d.	51.9	42.5	17.3	n.d.	134	34.8	3.0	OD
DY-1	n.d.	n.d.	4.87	n.d.	n.d.	28.4	n.d.	7.68	n.d.	41.0	30.7	2.0	AO
RZ-1	35.2	n.d.	95.8	n.d.	n.d.	225	136	98.7	n.d.	591	34.0	5.0	SBR
LY-1	21.3	n.d.	57.1	n.d.	n.d.	192	65.2	51.3	n.d.	387	29.6	10	OD
GS-1	32.2	n.d.	256	n.d.	n.d.	94.9	62.2	40.6	n.d.	486	40.2	16	AO
GS-2	2.52	n.d.	86.4	n.d.	n.d.	57.2	33.4	21.1	n.d.	201	37.9	3.0	OD
GS-3	60.3	n.d.	96.0	n.d.	n.d.	105	51.7	50.5	n.d.	363	43.3	4.0	OD
HF-1	31.3	n.d.	139	n.d.	n.d.	137	64.8	95.4	16.6	484	32.4	30	OD
HF-2	7.51	n.d.	50.0	n.d.	n.d.	101	61.9	80.3	21.1	322	28.1	18	OD
HF-3	5.98	n.d.	35.1	n.d.	n.d.	174	66.2	43.3	n.d.	324	25.8	6.0	SBR
GD-1	79.4	n.d.	232	n.d.	n.d.	114	54.4	86.7	15.1	582	28.8	10	OD
XA-1	85.9	n.d.	718	n.d.	n.d.	159	94.2	116	20.3	1.19×10^{3}	39.1	25	AAO
XA-2	5.24	n.d.	46.9	n.d.	n.d.	197	143	203	n.d.	595	29.9	8.0	OD
XA-3	17.1	n.d.	254	n.d.	n.d.	191	69.4	113	20.3	665	36.0	10	OD
HN-1	22.8	n.d.	107	n.d.	n.d.	235	90.5	102	15.9	573	34.4	7.0	OD

HN-2	31.2	n.d.	235	n.d.	n.d.	188	319	66.3	n.d.	839	27.0	9.0	AO
WH-1	12.4	n.d.	25.9	n.d.	n.d.	97.0	94.9	54.6	n.d.	285	13.6	15	AAO
WH-2	12.0	n.d.	69.1	n.d.	n.d.	25.1	15.6	16.1	n.d.	138	7.05	25	AO
HEB-1	82.1	n.d.	92.5	n.d.	n.d.	234	178	103	n.d.	690	35.5	20	OD
ZJ-1	24.0	n.d.	32.1	n.d.	n.d.	159	2.93×10^3	213	n.d.	3.36×10^3	16.8	3.0	AO
ZJ-2	22.3	n.d.	85.0	n.d.	n.d.	85.3	69.3	26.8	n.d.	289	25.5	20	AAO
ZJ-3	75.5	n.d.	257	n.d.	n.d.	118	88.7	50.3	n.d.	589	21.7	40	AO
YN-1	9.25	n.d.	143	n.d.	n.d.	111	46.0	45.6	n.d.	355	23.0	4.0	OD
YN-2	16.5	n.d.	184	n.d.	n.d.	109	78.2	47.3	n.d.	435	26.0	10	AAO
YN-3	n.d.	n.d.	43.6	n.d.	n.d.	99.3	45.0	28.7	n.d.	217	20.2	4.3	OD
YN-4	4.76	n.d.	53.9	n.d.	n.d.	93.1	64.7	42.3	n.d.	259	28.9	12	OD
YN-5	12.3	n.d.	210	n.d.	n.d.	145	69.6	48.6	n.d.	486	24.5	7.2	AO
YN-6	32.8	n.d.	274	n.d.	n.d.	168	91.8	54.0	n.d.	620	34.0	10	AAO
HB-1	28.6	n.d.	30.5	n.d.	n.d.	222	3.39×10^3	24.7×10^3	15.9	28.4×10^3	26.5	16	AO
JS-1	19.9	n.d.	209	n.d.	n.d.	99.0	69.6	71.5	11.4	480	28.7	13	CAST
FJ-1	30.0	n.d.	61.3	n.d.	n.d.	137	79.0	93.5	25.5	426	24.4	8.0	AO

[a] WWTP activated sludge biotreatment techniques. AAO: anaerobic-anoxic-oxic process, OD: oxidation ditch process, AO: anoxic/oxic process, SBR: sequencing batch reactor process, PASF: phosphorus and nitrogen removal combined with active sludge and biofilm process, CAST: cyclic activated sludge technology. PASF and CAST were treated as analogous AAO and SBR processes respectively in the statistics analysis. [b] Not detected. Nondetects were set as half MQL for each BZT analogue in the statistics analysis.

Figure S1: Principal component biplot of benzotriazole analogue concentrations in the sewage sludge samples.

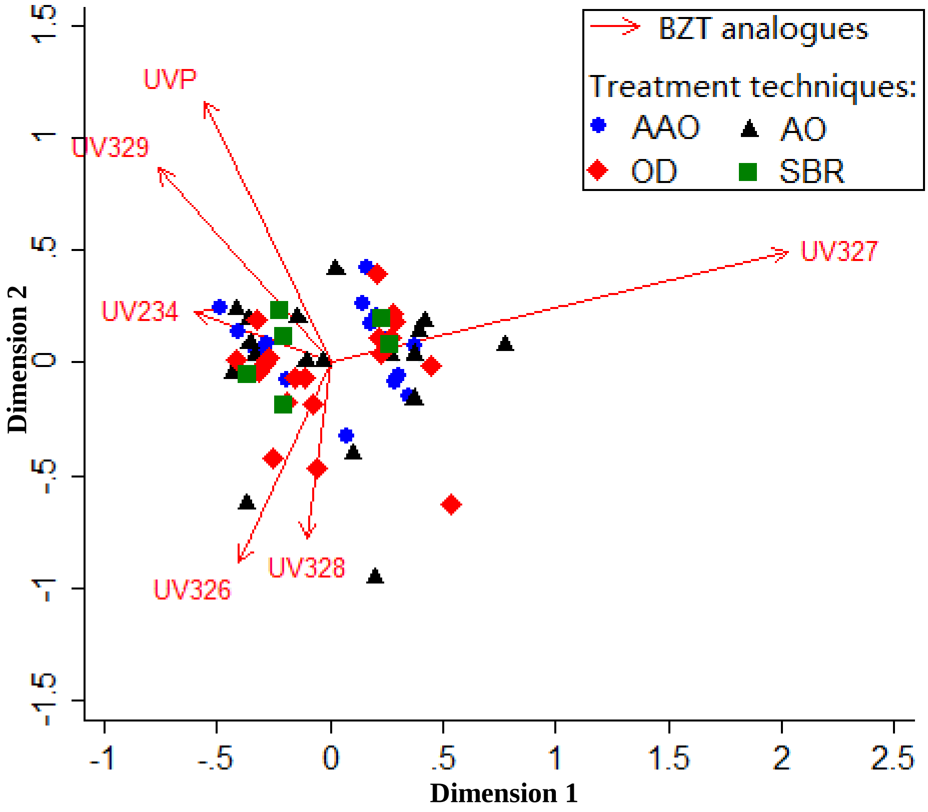
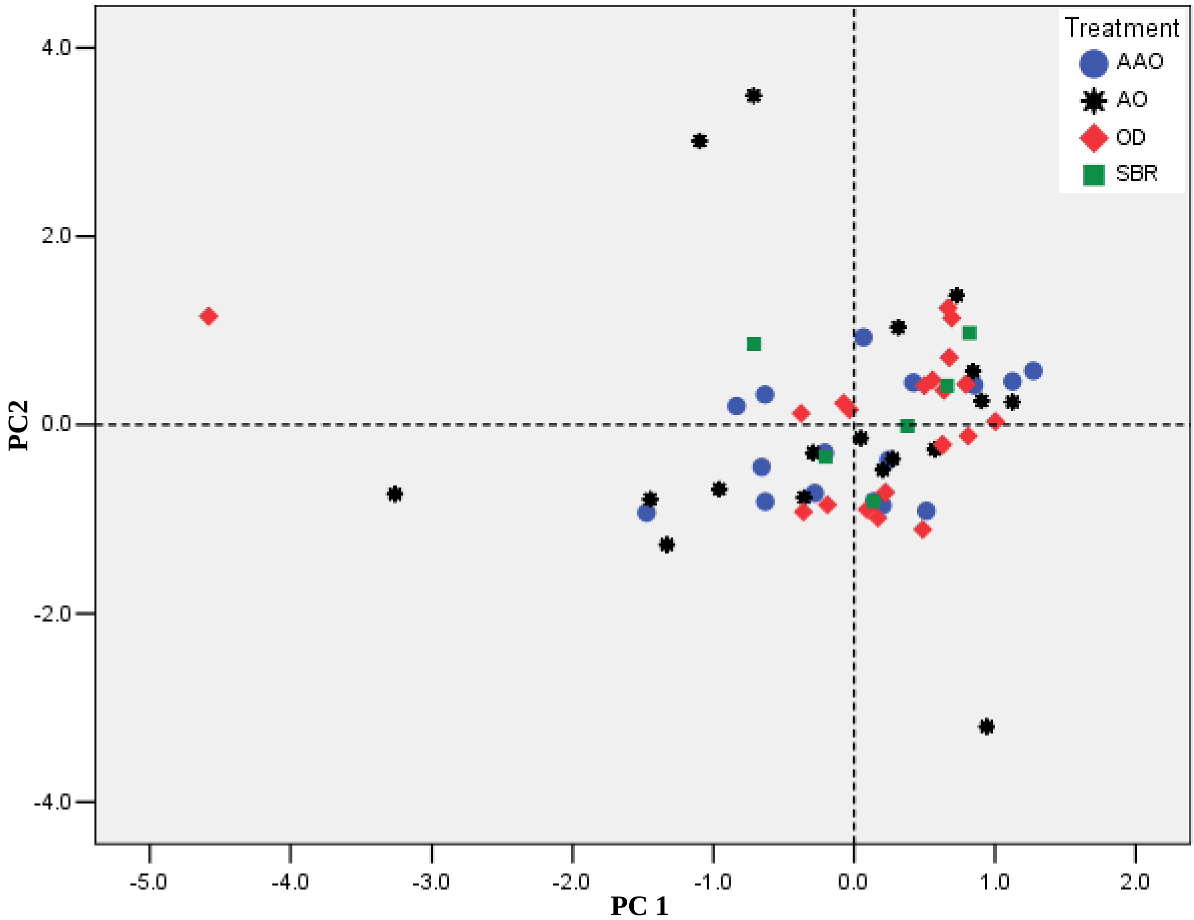
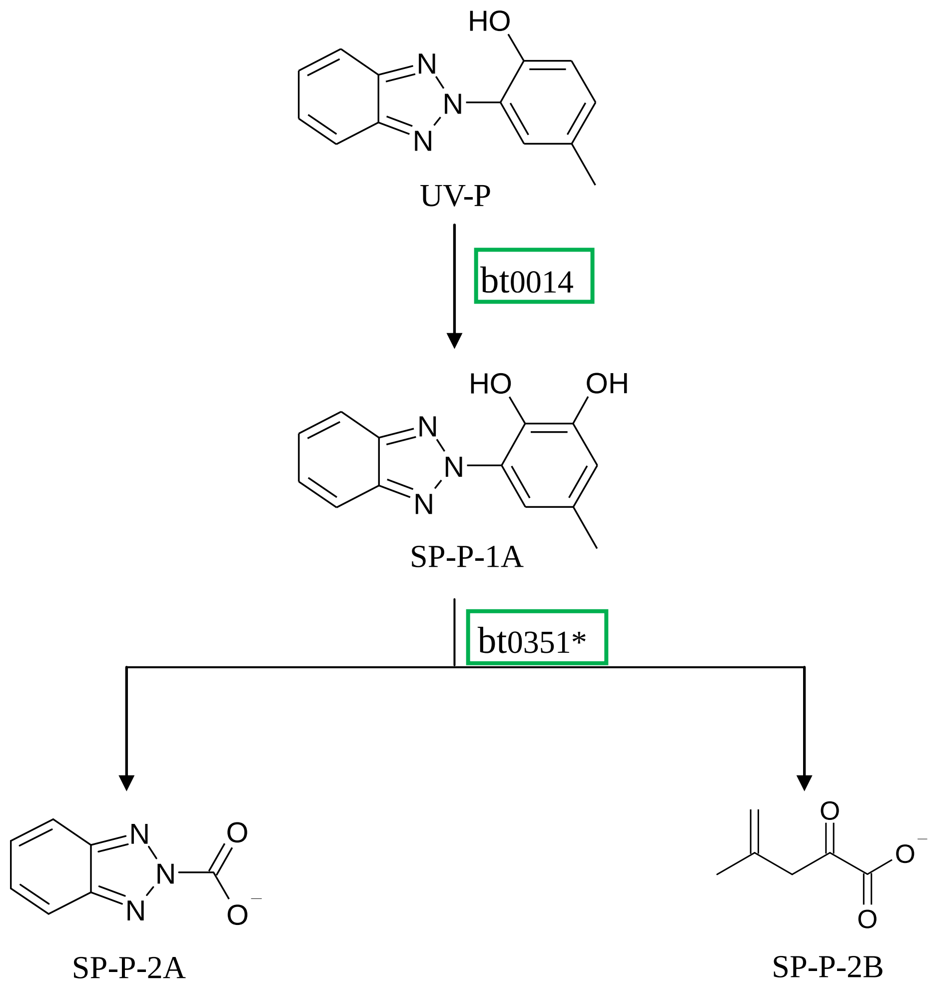


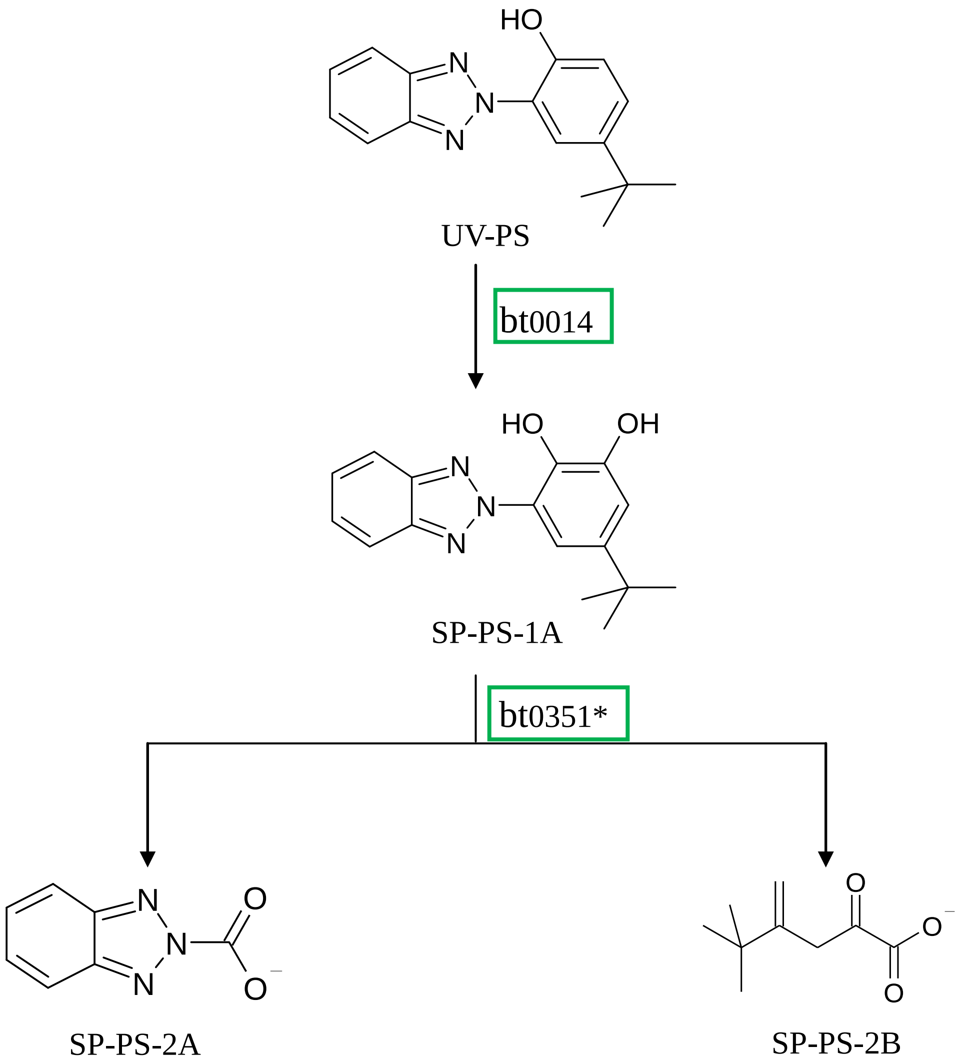
Figure S2: The score plots of benzotriazole analogue concentrations in the sewage sludge samples from the principal component analysis.



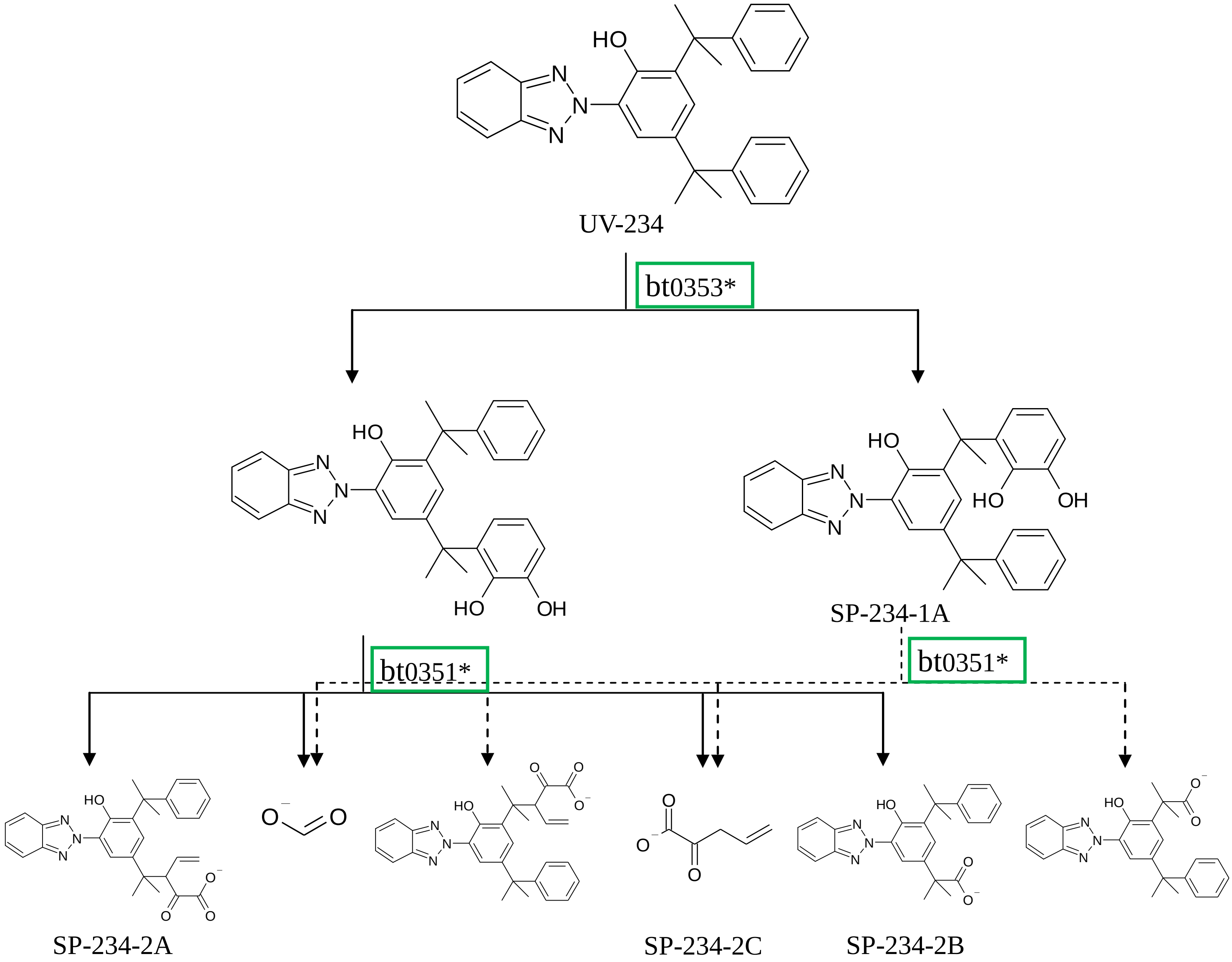
Scheme S1: Predicted UV-P biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes [1].



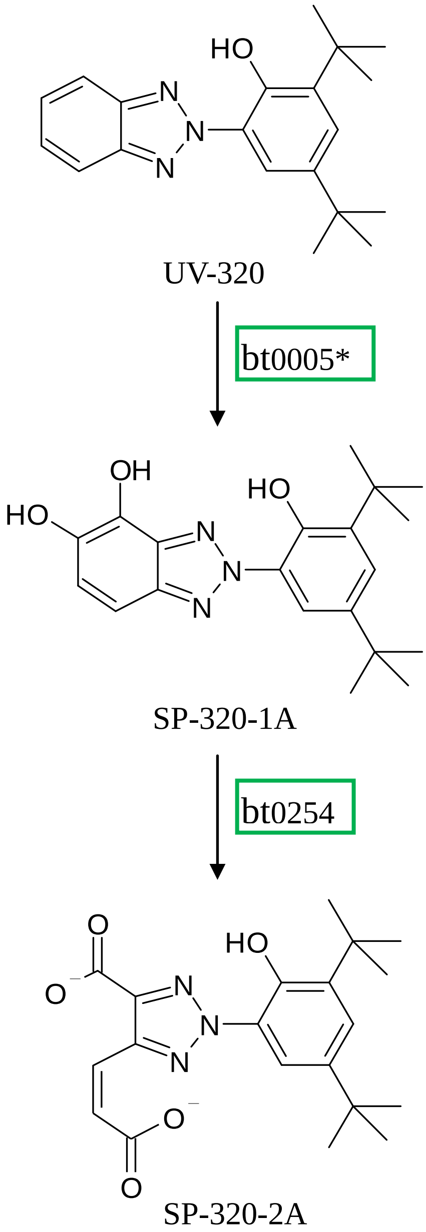
Scheme S2: Predicted UV-PS biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



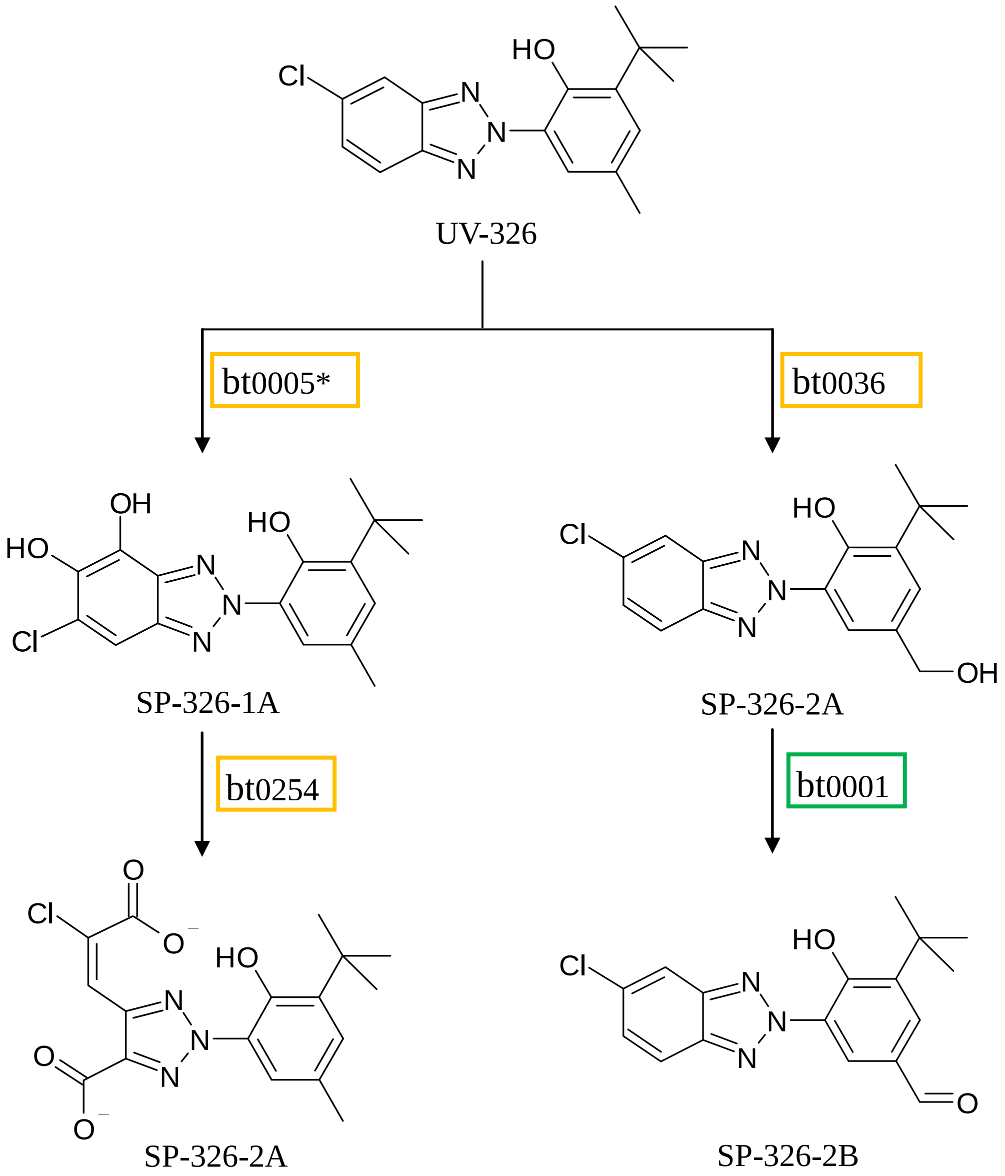
Scheme S3: Predicted UV-234 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



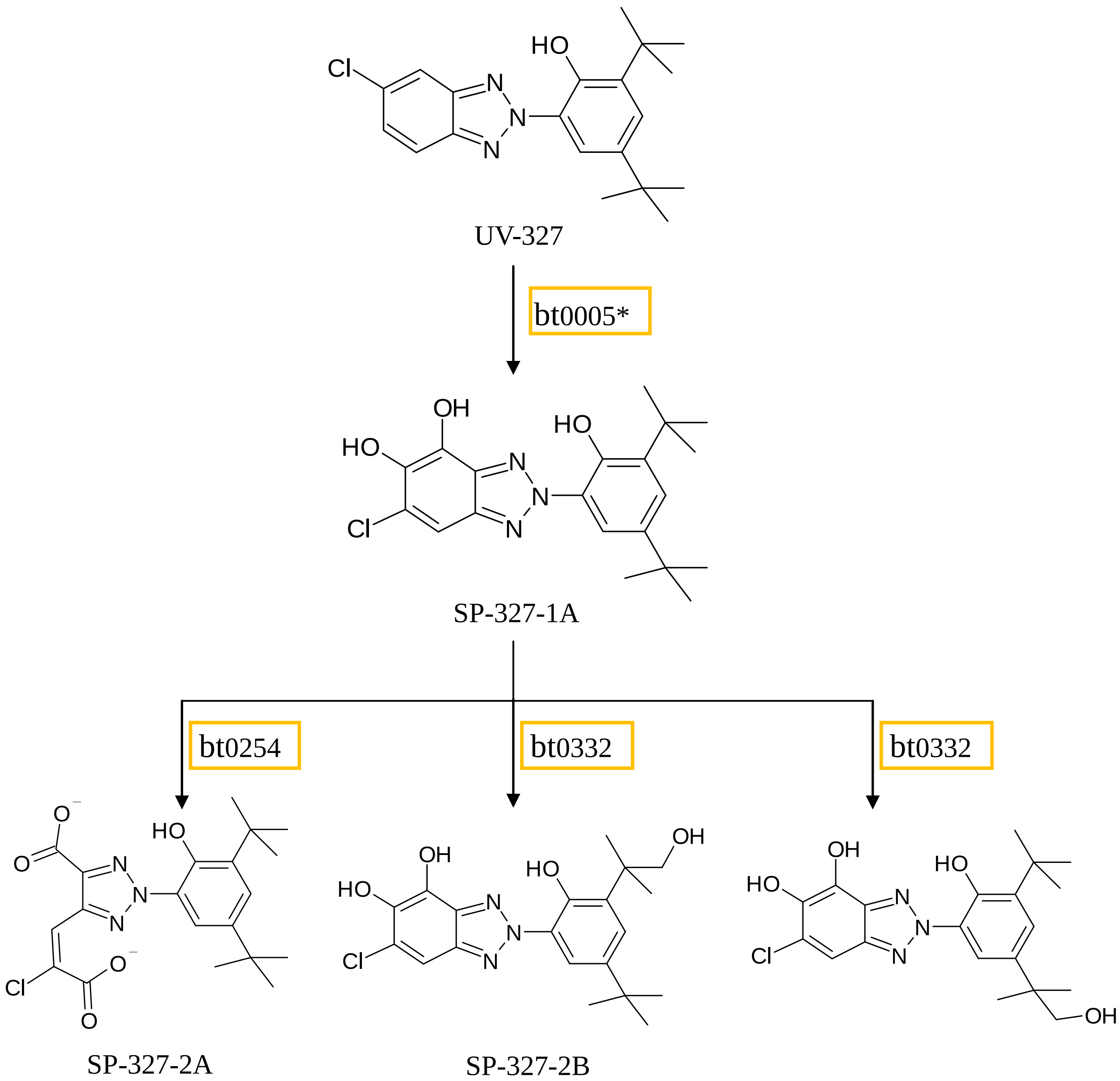
Scheme S4: Predicted UV-320 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



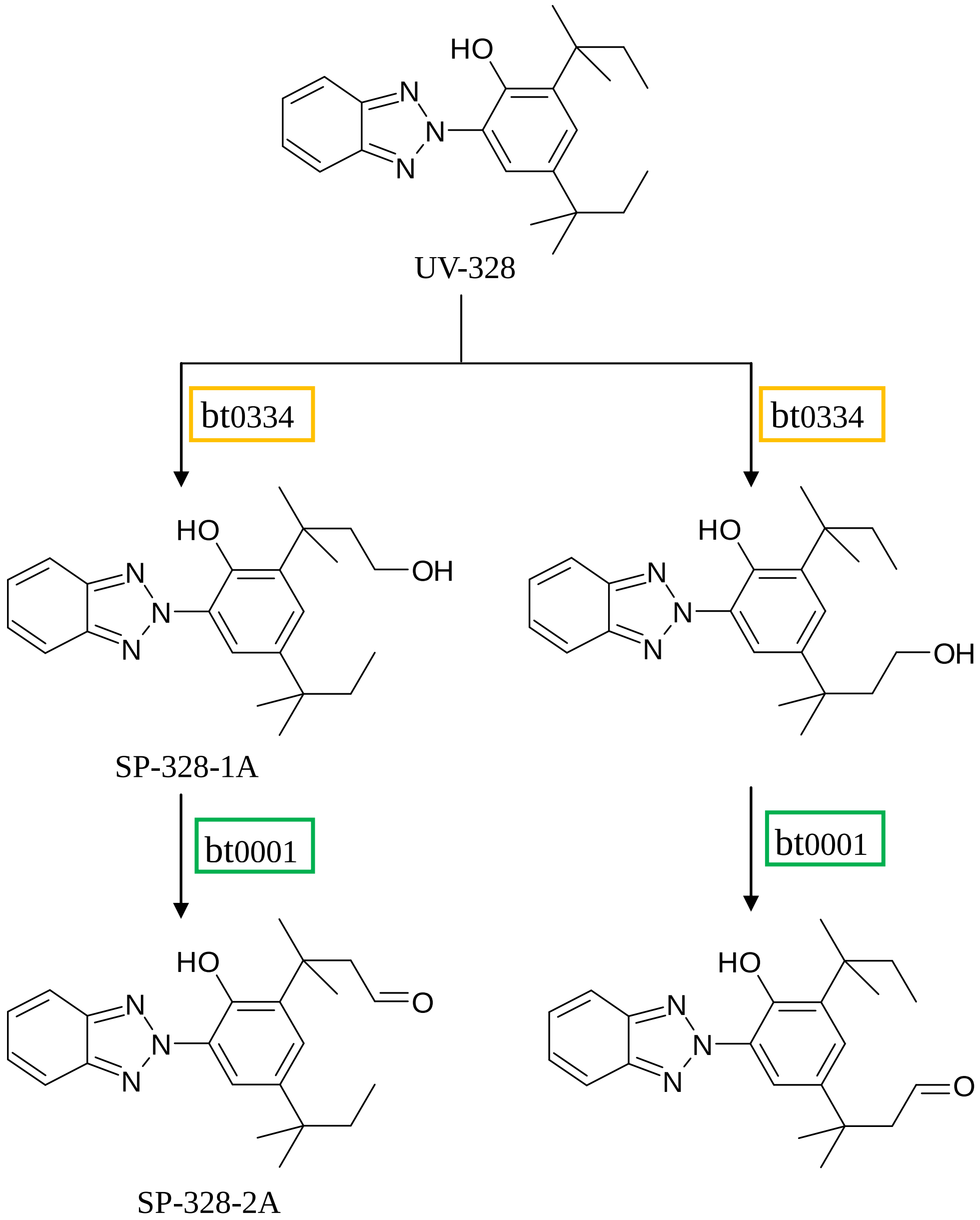
Scheme S5: Predicted UV-326 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



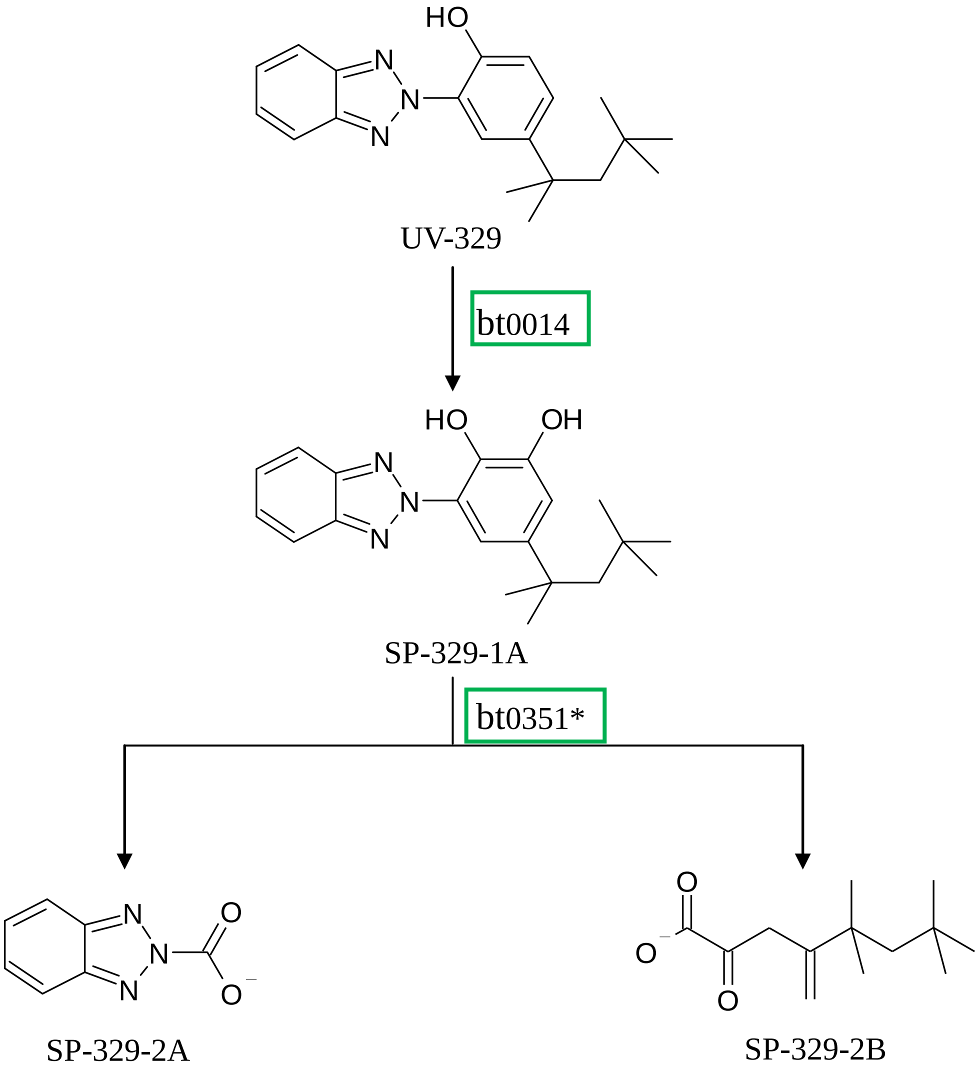
Scheme S6: Predicted UV-327 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



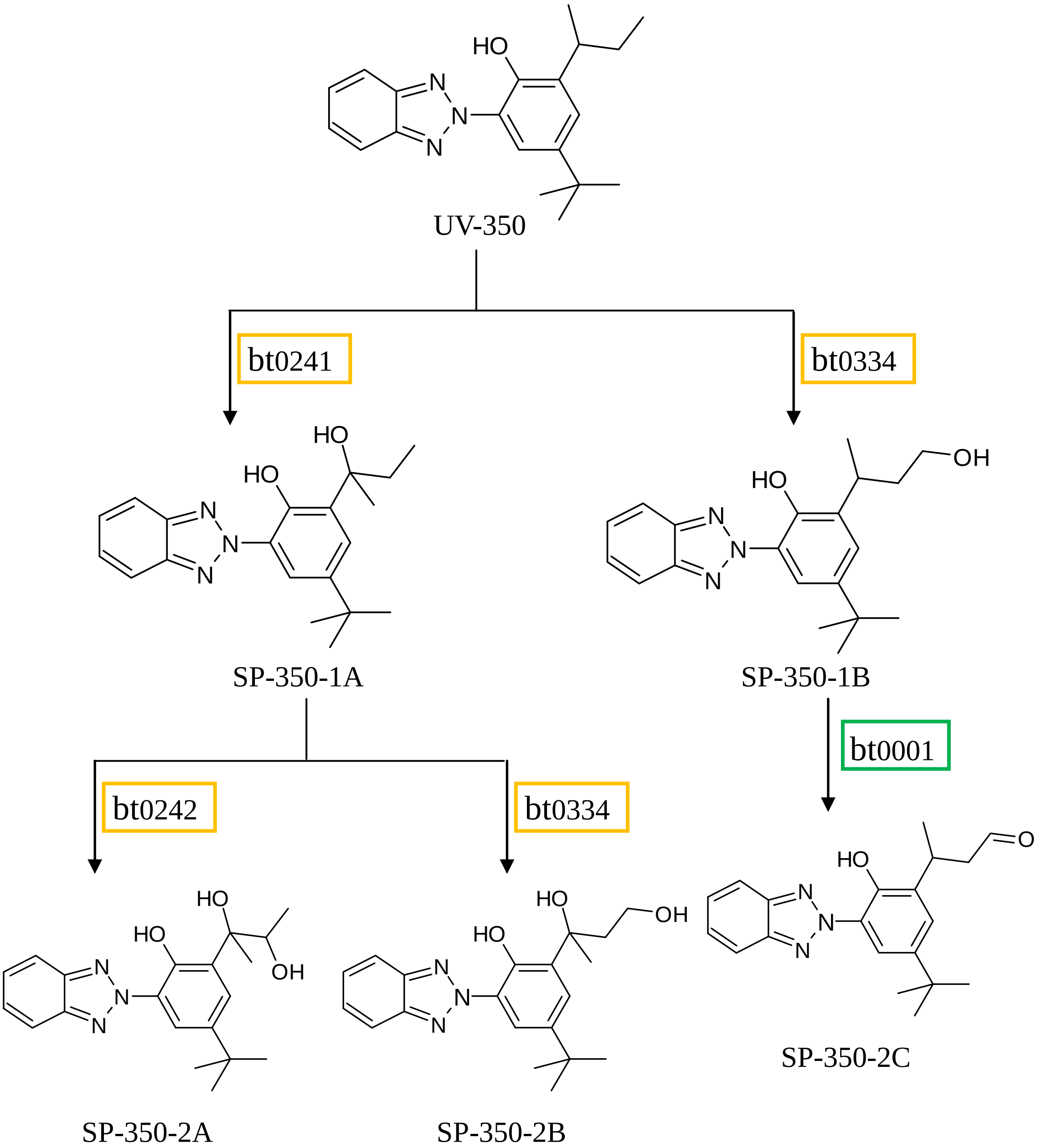
Scheme S7: Predicted UV-328 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



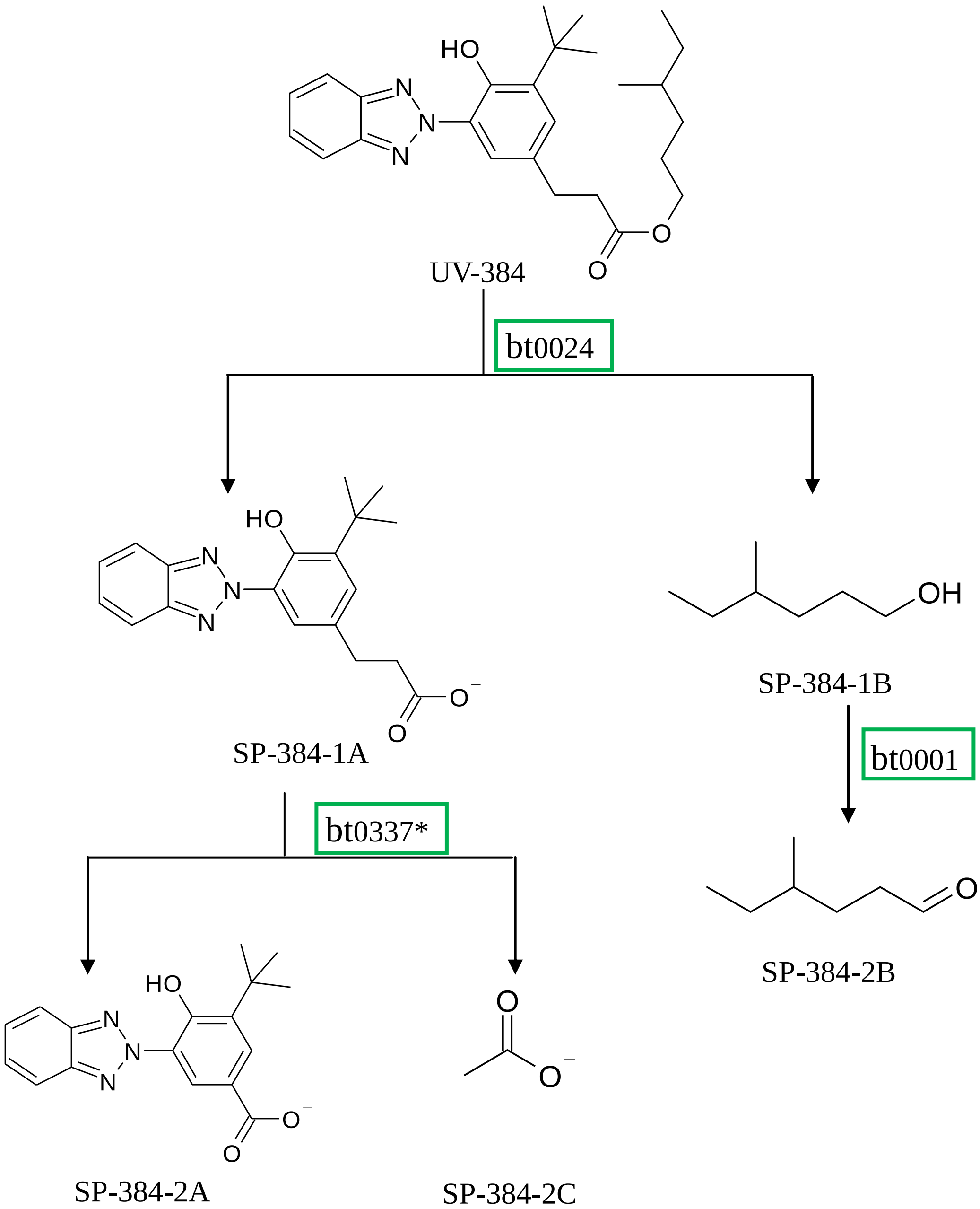
Scheme S8: Predicted UV-329 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



Scheme S9: Predicted UV-350 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



Scheme S10: Predicted UV-384 biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.



Scheme S11: Predicted UV-8M biotransformation routes by the UM-PPS framework to simplify combinatorial explosion routes.

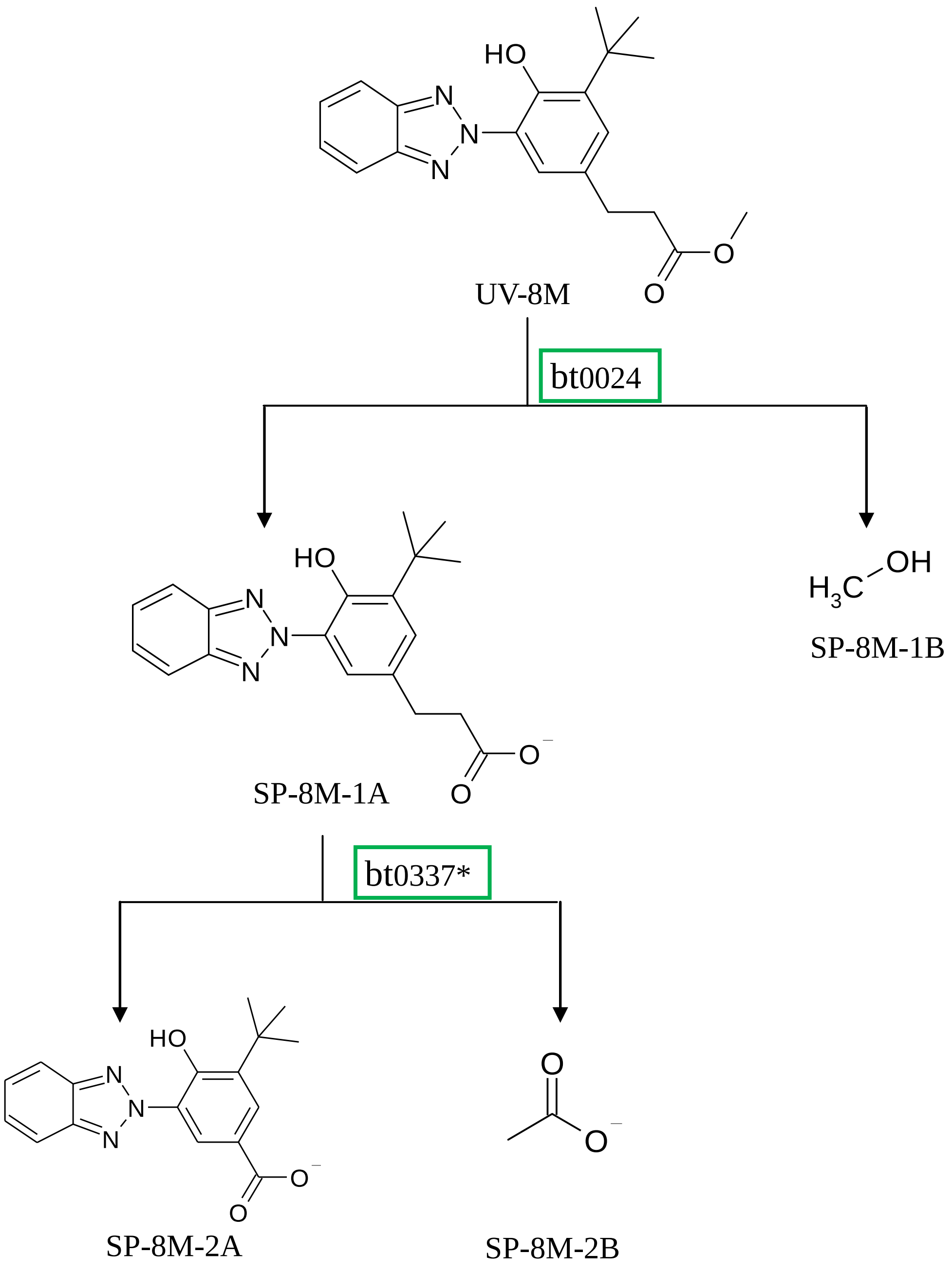


Table S3: Physicochemical parameters (Log Kow, Log Koa, half-lives in air, water and soil) calculated by the U.S. EPI Suite V4.1 [2] and predicted parameters for overall persistence and long-range transport potential (Pov, CTD and TE) by the Pov-LRTP Tool [3].

Chemical ID	Estimated physicochemical properties					Predicted total persistent and transport potential [a]		
	Log Kaw	Log Kow	$T_{1/2}$ in air (h)	$T_{1/2}$ in water (h)	$T_{1/2}$ in soil (h)	Pov (days)	CTD (Km)	TE (%)
UV-326	-11.3	5.55	17.2	1.44×10^3	2.88×10^3	173	1.38×10^3	6.10
UV-327	-11.0	6.91	19.5	1.44×10^3	2.88×10^3	173	2.73×10^3	12.1
UV-328	-10.6	7.25	16.3	1.44×10^3	2.88×10^3	173	2.80×10^3	12.4
UV-P	-11.6	4.31	8.43	900	1.80×10^3	108	145	0.64
UV-329	-10.7	6.21	8.03	1.44×10^3	2.88×10^3	173	2.32×10^3	10.3
UV-234	-13.3	7.67	11.8	1.44×10^3	2.88×10^3	173	2.84×10^3	12.6
UV-320	-10.8	6.27	19.1	1.44×10^3	2.88×10^3	173	2.37×10^3	10.5
UV-350	-10.8	6.31	14.5	900	1.80×10^3	108	2.41×10^3	10.7
UV-PS	-11.2	4.36	8.50	900	1.80×10^3	108	162	0.72
UV-8M	-13.7	4.94	15.9	900	1.80×10^3	108	531	2.35
UV-384	-13.0	7.81	10.3	1.44×10^3	2.88×10^3	173	2.84×10^3	12.6
SP-P-2A	-7.53	1.70	169	360	720	35.5	37.4	0.12
SP-P-1A	-15.6	2.52	2.43	900	1.80×10^3	94.8	93.3	0.01
SP-P-2B	-6.74	0.15	4.01	208	416	19.6	54.5	0.08
SP-8M-1A	-16.2	3.30	15.2	900	1.80×10^3	105	93.3	0.07
SP-8M-2A	-15.9	4.24	72.0	900	1.80×10^3	107	124	0.55
SP-8M-1B	-3.73	-0.77	272	208	416	18.8	2.57×10^3	6.28
SP-8M-2B	-5.39	-0.17	347	208	416	19.4	1.52×10^3	5.32
SP-384-1B	-3.02	2.24	22.5	360	720	32.2	443	0.11
SP-384-2B	-1.94	2.22	8.41	360	720	19.0	174	0.00
SP-326-1A	-19.3	4.59	13.0	1.44×10^3	2.88×10^3	173	264	1.17

SP-326-1B	-15.8	4.09	14.7	900	1.80×10^3	108	93.3	0.39
SP-326-2A	-20.6	2.83	10.5	900	1.80×10^3	100	93.3	0.02
SP-326-2B	-14.0	4.72	12.3	1.44×10^3	2.88×10^3	173	345	1.53
SP-234-1A	-21.2	6.71	3.76	1.44×10^3	2.88×10^3	173	2.66×10^3	11.8
SP-234-2A	-19.3	4.94	3.04	1.44×10^3	2.88×10^3	173	531	2.35
SP-234-2B	-17.3	4.02	14.3	900	1.80×10^3	108	93.3	0.34
SP-234-2C	-6.93	-0.40	6.63	208	416	19.5	58.5	0.15
SP-327-1A	-18.9	5.95	14.2	1.44×10^3	2.88×10^3	173	2.00×10^3	8.87
SP-327-2A	-20.3	4.20	11.3	1.44×10^3	2.88×10^3	172	149	0.50
SP-327-2B	-23.3	4.49	11.6	1.44×10^3	2.88×10^3	172	214	0.95
SP-328-1A	-15.0	5.79	12.8	1.44×10^3	2.88×10^3	173	1.77×10^3	7.82
SP-328-2A	-13.7	5.76	7.12	1.44×10^3	2.88×10^3	173	1.72×10^3	7.61
SP-329-1A	-14.7	5.73	2.81	1.44×10^3	2.88×10^3	173	1.67×10^3	7.40
SP-329-2A	-7.53	1.70	169	360	720	35.5	37.4	0.12
SP-329-2B	-5.88	3.37	3.92	900	1.80×10^3	105	93.3	0.03
SP-350-1A	-15.3	4.80	14.8	1.44×10^3	2.88×10^3	173	405	1.79
SP-350-1B	-15.3	4.84	11.7	900	1.80×10^3	108	438	1.94
SP-350-2A	-16.7	3.75	11.6	1.44×10^3	2.88×10^3	170	149	0.18
SP-350-2B	-16.7	3.75	11.6	1.44×10^3	2.88×10^3	170	149	0.18
SP-350-2C	-14.0	4.82	5.94	1.44×10^3	2.88×10^3	173	422	1.87
SP-PS-1A	-15.2	3.88	2.87	900	1.80×10^3	107	93.3	0.25
SP-PS-2A	-7.53	1.70	169	360	720	35.5	37.4	0.12
SP-PS-2B	-6.37	1.51	4.03	360	720	34.1	67.6	0.06
SP-320-1A	-18.8	5.31	10.5	1.44×10^3	2.88×10^3	173	996	4.41
SP-320-2A	-20.1	3.70	5.95	900	1.80×10^3	107	93.3	0.16

[a]: Pov: Overall persistence, CTD: characteristic travel distance, TE: transfer efficiency

Reference

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2. U.S. Envrionmental Protection Agency. Exposure Assessment Tools and Models, Estimation Program Interface (EPI) Suite, V 4.1; U.S. Environmental Protection Agency, Exposure Assessment Branch: Washington, DC, 2011.

3. Organization for Economic Co-operation and Development, Available online at http://www.oecd.org/LongAbstract/0,3425,en_2649_34379_40718985_119669_1_1_1,00.html (Accessed on July26, 2011).