Supplementary Information

Table S1: Carbon in "precursor", "product", "inorganic" (comprising CO, CO_2, and CH_4) and "lost" categories, each as a proportion of total carbon assessed at the end of each 6-hour simulation.

Precursor	Precursor carbon		Product carbon		Inorganic carbon		Lost carbon[1]	
	GECKO-A	MechGen	GECKO-A	MechGen	GECKO-A	MechGen	GECKO-A	MechGen
Propane	73%	72%	24%	25%	3%	3%	0%	0.1%
n-Butane	50%	50%	40%	35%	10%	13%	0.02%	3%
n-Octane	10%	8%	76%	63%	13%	13%	1.1%	16%
Cyclohexane	13%	14%	61%	70%	25%	9%	1.5%	7%
Hexanal	0.01%	0.01%	59%	61%	40%	31%	0.4%	8%
Trans-2-hexene	0%	0%	46%	37%	54%	60%	0.02%	3%
Isoprene (SAR)	0%	0%	33%	31%	67%	64%	0.6%	5%
Isoprene (MCM)	0%		26%		73%		0.1%	
α-Pinene	0%	0%	66%	49%	33%	12%	0.5%	39%
Camphene	0%	0%	71%	52%	28%	13%	0.9%	35%
2-Methyl furan	0%	0%	28%	56%	72%	38%	0.01%	6%

[1]"Lost carbon" in MechGen includes "lost radicals", which are tracked separately in that model.

Figure S1: simulation-mean product functional group abundances in GECKO-A (green, positive scale) and MechGen (purple, negative scale). Simulation-mean g:C ratios for double bonds (not depicted) are < 0.01 for all product mixtures except for isoprene (all types = 0.03) and 2-methylfuran (0.03 in GECKO-A, 0.08 in GECKO-A sensitivity run and in MechGen).

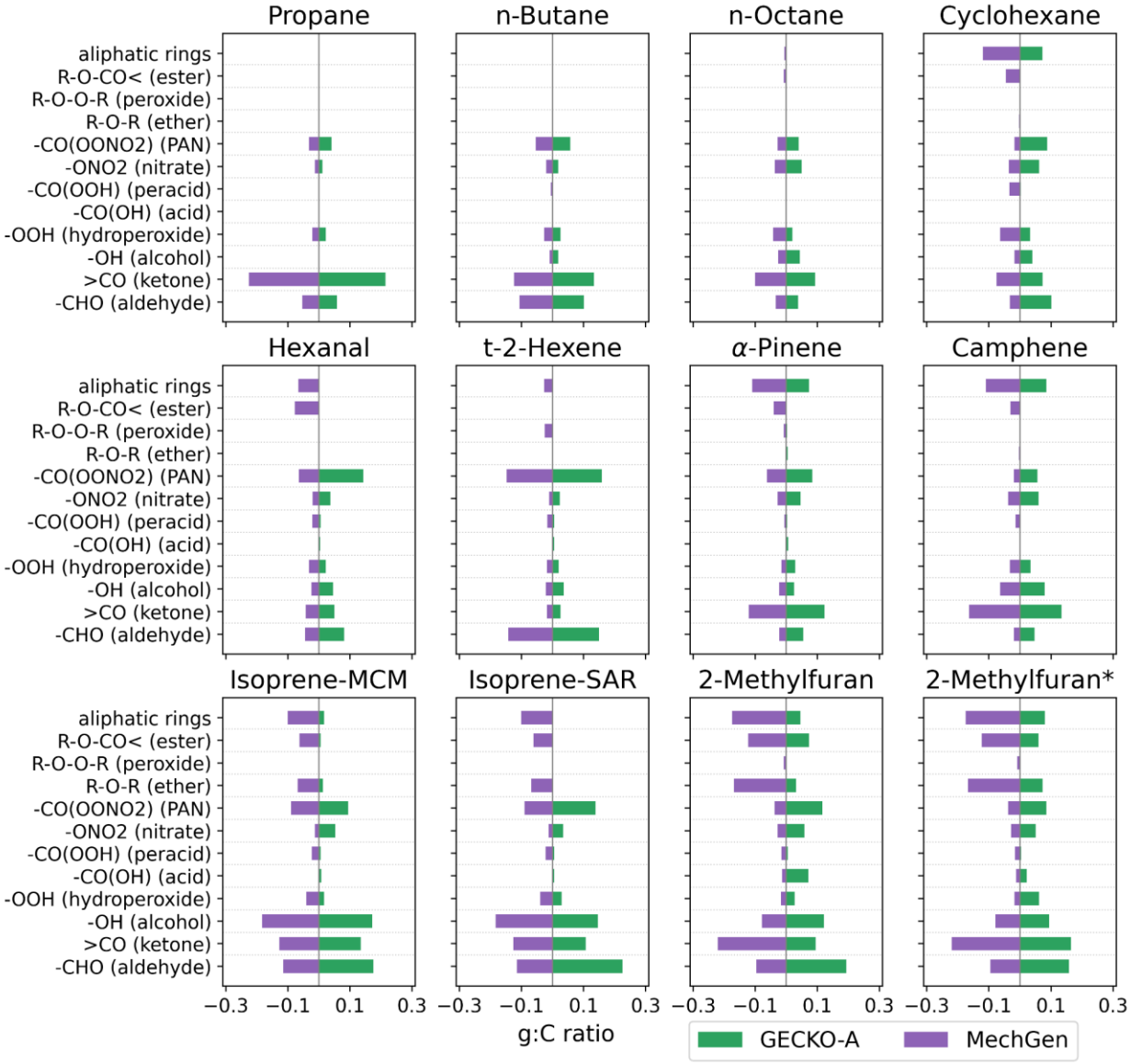

Table S2: Summary of diagnostic criteria[1] values in GECKO-A (GA) and MechGen (MG)

Precursor	Lifetime τ (h)	#species		#reactions		POHR(s^{-1})		log_{10}(Pvap)		log_{10}(H*)		O:C		$C:C_0$		$^3\Sigma$fn	
		GA	MG	GA	MG	GA	MG	GA	MG	GA	MG	GA	MG	GA	MG	GA	MG
propane	18.9	445	105	3085	245	11	10	-0.50	-0.39	1.73	1.75	0.56	0.53	0.96	0.96	0.35	0.35
n-butane	8.5	1329	358	9795	875	46	43	-0.91	-0.88	2.01	1.85	0.65	0.65	0.77	0.76	0.36	0.35
n-octane	2.6	10547	7133	78975	20020	211	191	-4.13	-4.42	3.39	3.79	0.57	0.52	0.75	0.77	0.29	0.29
cyclohexane	2.9	8425	1878	67673	5089	199	121	-4.47	-4.86	4.00	4.56	0.92	0.70	0.81	0.94	0.47	0.45
hexanal	0.7	7726	1484	61152	4059	236	171	-3.94	-4.10	2.62	2.73	1.07	0.80	0.71	0.80	0.39	0.39
t-2-hexene	0.2	6669	656	47278	1686	275	258	-1.44	-1.22	1.62	1.36	1.14	1.10	0.65	0.45	0.43	0.43
isoprene (MCM)	0.2	1611	1385	10860	3963	250	215	-2.60	-4.04	3.54	5.22	1.20	1.27	0.50	0.62	0.73	0.85
isoprene (SAR)	0.2	6507	1385	46795	3963	258	215	-2.36	-4.04	3.54	5.22	1.37	1.27	0.45	0.62	0.73	0.85
α-pinene	0.2	131771	8939	947079	23643	266	169	-5.71	-5.67	5.40	5.04	0.85	0.72	0.56	0.61	0.45	0.44
camphene	0.4	161704	8396	1155053	22253	284	174	-6.32	-6.25	6.01	5.98	0.80	0.65	0.53	0.52	0.50	0.50
2-methyl furan (original)	0.2	5657	1085	36927	2999	212	111	-4.76	-5.04	4.86	4.39	1.56	1.22	0.58	0.91	0.84	1.06
2-methyl furan (sensitivity)	0.2	5657	1085	36927	2999	246	111	-4.80	-5.04	4.76	4.39	1.37	1.22	0.61	0.91	0.85	1.06

[1]Diagnostic criteria are averaged over the duration of the 6 hours simulations, except for *log_{10}(Pvap)* and *log_{10}(H*)*, which are the distribution midpoints averaged at six 1-hour intervals(alkanes) or at five 1-lifetime intervals (all other species).

[2]Quoted ranges are the standard deviations of the means. Shaded values are statistically insignificant in the simulation mean.

[3]Σfn is the sum of the simulation-averaged individual functional group abundances (g:C values) shown in Figure S1.

Figure S2: graphical representation of Table 3, i.e. simulation-mean absolute differences between GECKO-A and MechGen bulk property metrics. Error bars represent one standard deviation about the mean.

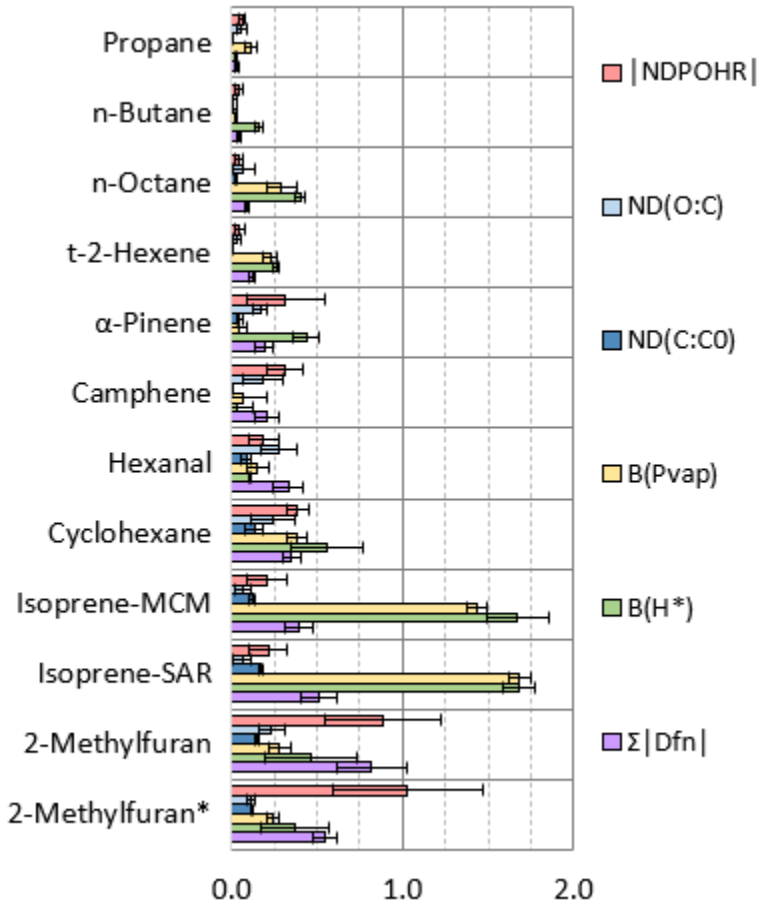

Table S3: Agreement range descriptors, scores and upper limits[1] for the simulation-mean inter-model comparison metrics.

Agreement descriptors	score	ND(C:C$_0$)	ND(O:C)	Σ|Dfn|	|NDPOHR|	*B(Pvap), B(H*)*	*δa*	*δc*
"very good"	0	—---------- statistically insignificant —----------						
"good"	1	<|0.04|	<|0.07|	<|0.20|	<|0.26|	<|0.42|	<|0.59|	<|0.13|
"moderate"	2	<|0.08|	<|0.14|	<|0.41|	<|0.51|	<|0.84|	<|1.19|	<|0.26|
"poor"	3	<|0.17|	<|0.28|	<|0.82|	<|1.03|	<|1.68|	<|2.38|	<|0.53|
"poorest"	4	—---------- maximum value —----------						

[1] *Values are rounded to 2 decimal places*

Figure S3: **As Figure 6, for the 2-methyl furan sensitivity study.** Left panel, original results; right panel, sensitivity results with reduced k(OH+maleic anhydride). Green lines, GECKO; purple lines, MechGen; solid and dash-dot lines, O:C; dashed and dotted lines, C:C_0. Notation on each plot gives the values of mND(C:C_0) and mND(O:C), in that order.

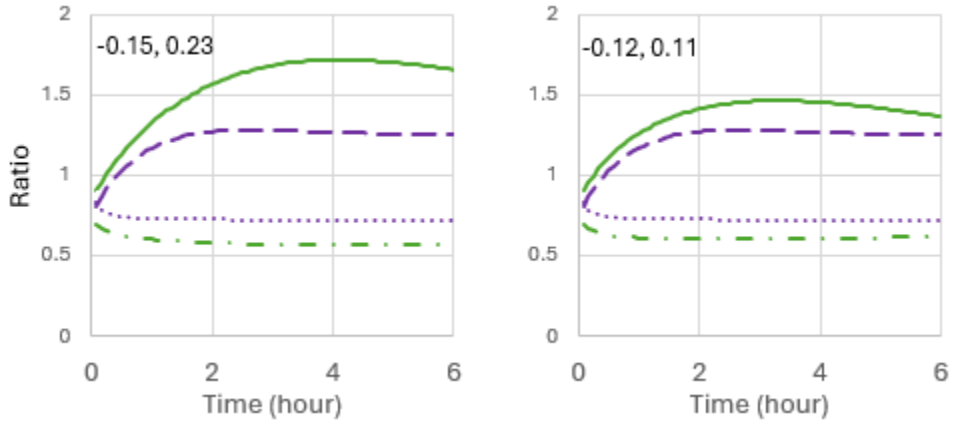

Figure S4: Sketch plot of major contributors to isoprene *Pvap* and *H distributions at 5 isoprene lifetimes**. Upper, GECKO-MCM; lower, MechGen; left, *Pvap*; right, *H**. Points are **stacked cumulatively** within each distribution `bin.Points with ≥0.5% carbon contribution are shown: points with ≥1.0% carbon contribution are labeled with functional group identities: A,` **A**cid; D, al**D**ehyde; E, **E**ther; G, peroxyacid; H, **H**ydroperoxide; J, ester; K, **K**etone; N, **N**itrate; O, hydr**O**xide; P, **P**AN; Q, peroxide; T, ring; U, **U**nsaturated. Selected label combinations: T + E = (usually) epoxide; T + J = lactone. Notable individual species: DK = methylglyoxal; TOOE = "iepox-b"; UD = methacrolein; UK = methyl vinyl ketone (MVK).

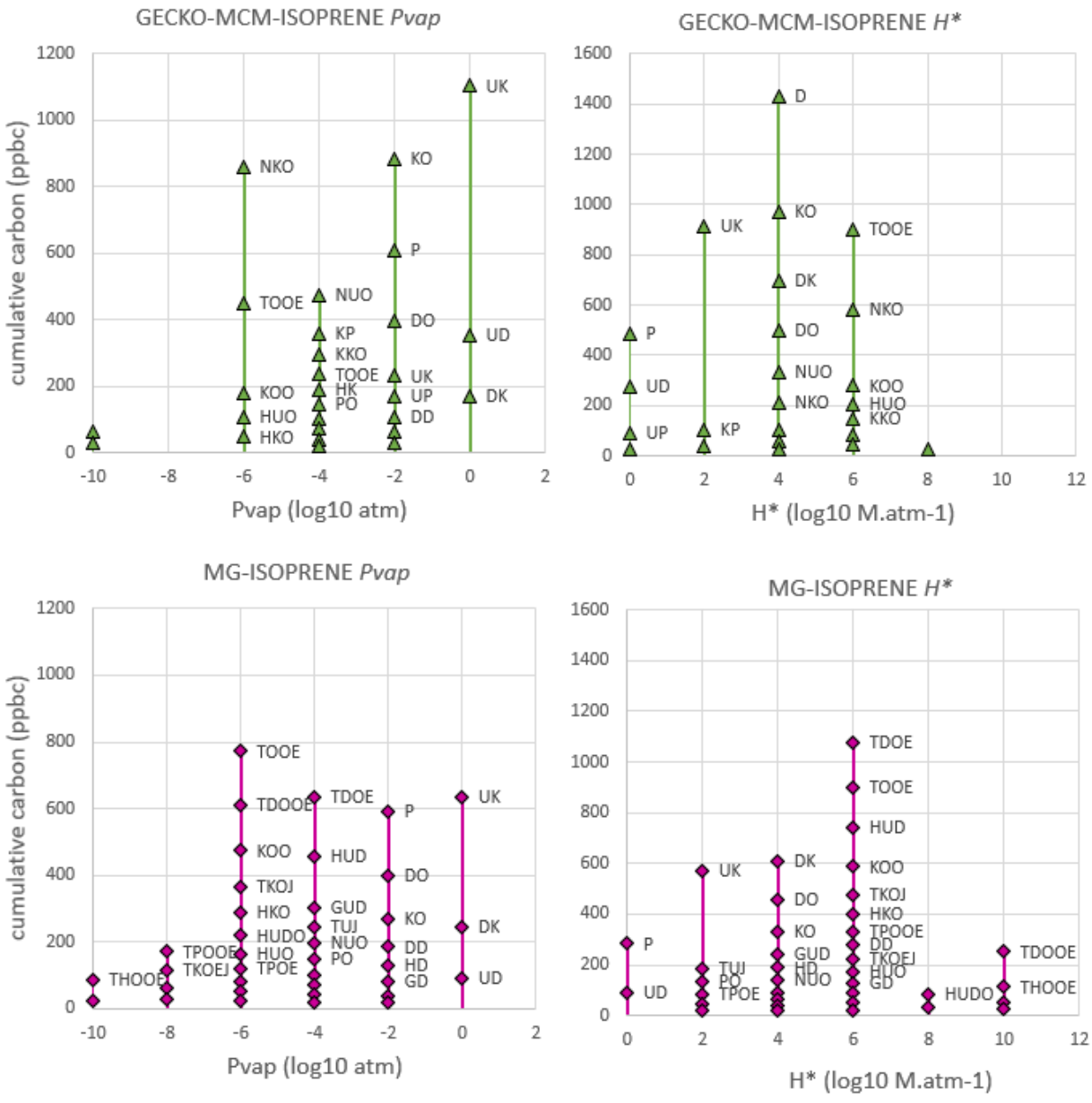

Figure S5. Sketch plot of major contributors to 2-methylfuran *Pvap* and *H distributions at 5 lifetimes**. Upper, GECKO-A; middle, GECKO-A* [sensitivity version]; lower, MechGen; left, *Pvap*; right, *H**. Points are stacked cumulatively within distribution bins. Points with ≥0.5% carbon contribution are shown; points with ≥1.0% carbon contribution are labeled with functional group identities: **A**, **A**cid; D, al**D**ehyde; E, **E**ther; G, peroxyacid; H, **H**ydroperoxide; J, ester; K, **K**etone; N, **N**itrate; O, hydr**O**xide; P, **P**AN; Q, peroxide; T, ring; U, **U**nsaturated. Selected combinations: T + E = epoxide; T + J = lactone. Notable individual species: TUKKE = maleic anhydride.

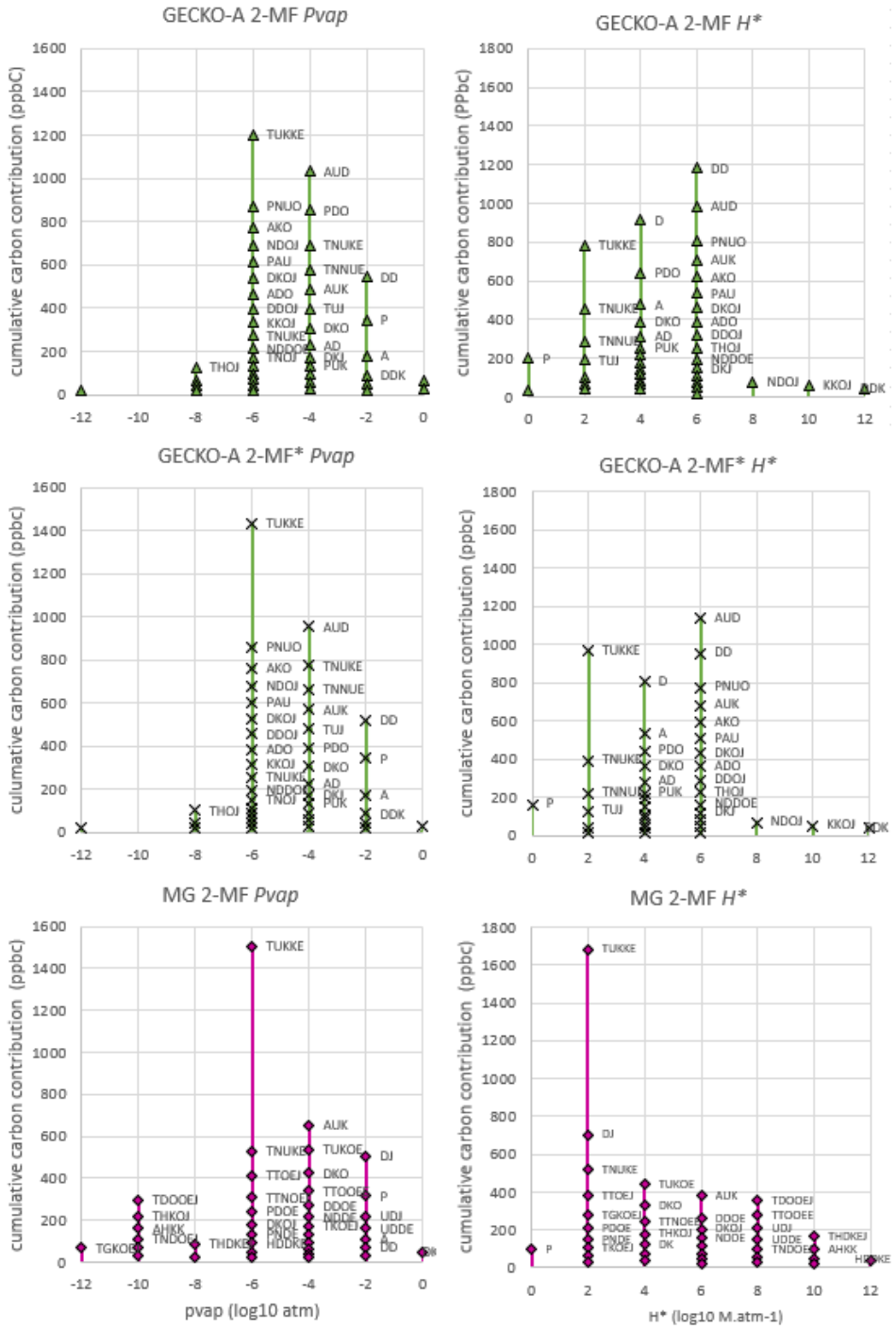

Figure S6: Normalized difference in product OH reactivity ("NDPOHR") by precursor lifetime. (Compare to Figure 2). Grey shading indicates agreement within ± 10%.

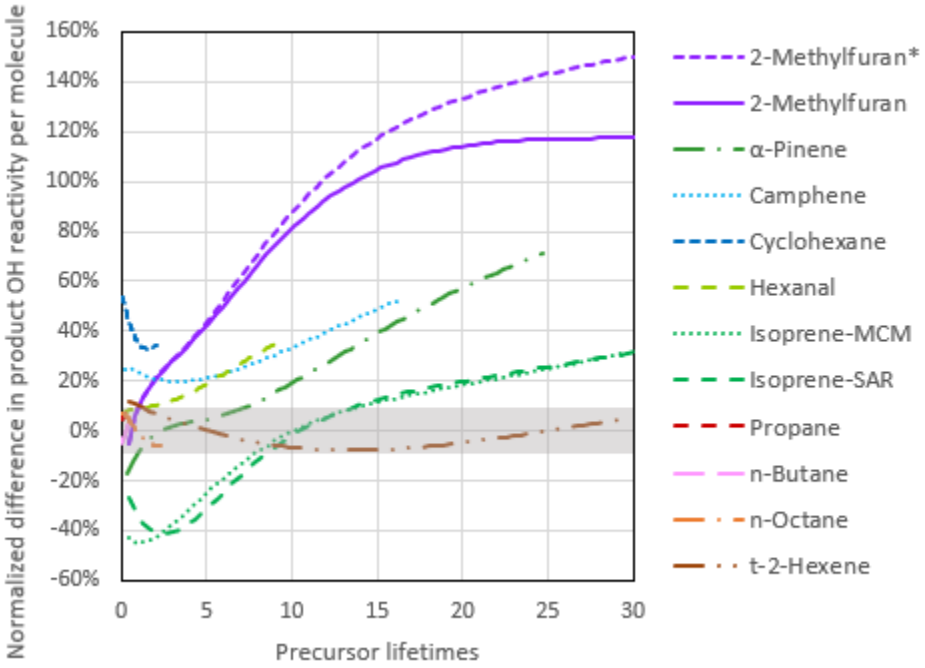

Table S4a: top 10 propane products in GECKO-A (GA) and MechGen (MG) by simulation-integrated molecular abundance.

[1]rank		[2]name		Canonical SMILES	kOH (molec s^{-1})		H*	Pvap	[4]Molecular abundance	
GA	MG	GA	MG	structure	GA	MG	(M atm^{-1})	(atm)	GA	MG
1	1	K03000	ACETONE	CC(=O)C	1.9E-13	1.9E-13	3.0E+01	4.8E-01	62%	66%
2	2	P03000	PPN	CCC(=O)OON(=O)=O	2.5E-13	6.5E-13	2.9E+00	1.3E-02	9%	6%
3	3	D03000	PROPALD	CCC=O	1.9E-11	2.0E-11	1.3E+01	4.9E-01	8%	6%
4	4	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	1.4E+01	2.0E-00	4%	5%
5	5	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	[3]-	4.1E+00	3.9E-02	4%	4%
6	6	H03001	ORG-0125	OOC(C)C	8.7E-12	8.1E-12	2.3E+02	1.6E-02	3%	3%
7	8	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	-	3%	2%
8	7	N03001	IC3-ONO2	CC(ON(=O)=O)C	2.9E-13	2.9E-13	6.2E-01	3.7E-02	2%	3%
9	9	H03000	ORG-0129	CCCOO	7.8E-12	8.1E-12	2.3E+02	8.1E-03	2%	1%
10	10	N03000	ORG-0050	CCCON(=O)=O	5.8E-13	6.3E-13	7.9E-01	2.2E-02	1%	1%
Others									2%	2%

[1]Ranks between 11 to 20 are enumerated if the species is found in the top 10 in another mechanism.
[2]Species "names" are assigned automatically by the mechanism generators and may vary between mechanisms.
[3]Null values indicate that the species is not found or the quantity is not assigned in the respective mechanism.
[4]Percent contributions are reported only for the top 10 species in each mechanism.

Table S4b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG), for propane.

rank		name		Canonical SMILES	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG	structure	GA	MG	GA	MG
1	1	C03000	PROPANE	CCC	1.1E-12	1.1E-12	69%	70%
2	2	D03000	PROPALD	CCC=O	1.9E-11	2.0E-11	15%	13%
3	3	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	7%	9%
4	4	H03001	ORG-0125	OOC(C)C	8.7E-12	8.1E-12	3%	3%
5	5	CH2O	CH2O	C=O	9.2E-12	9.2E-12	2%	2%
6	7	H03000	ORG-0129	CCCOO	7.8E-12	8.1E-12	1%	1%
7	6	K03000	ACETONE	CC(=O)C	1.9E-13	1.9E-13	1%	1%
8	9	H02000	ETOOH	CCOO	6.0E-12	6.0E-12	0.3%	0.4%
9	8	P03000	PPN	CCC(=O)OON(=O)=O	2.5E-13	6.5E-13	0.3%	0.4%
>20	10	CH3OOH	MEOOH	COO	5.5E-12	1.0E-11	-	0.2%
10	-	DD3000	-	O=CCC=O	4.2E-11	-	0.1%	-
Others							0.5%	0.5%

See footnotes for Table S4a

Table S5a: top 10 butane products by simulation-integrated molecular abundance in GECKO-A (GA) and MechGen (MG).

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		H*	Pvap	Molecular abundance	
GA	MG	GA	MG		GA	MG	($M\ atm^{-1}$)	(atm)	GA	MG
1	1	K04000	MEK	CCC(=O)C	1.1E-12	1.0E-12	2.0E+01	1.4E-01	40%	37%
2	2	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	1.4E+01	2.0E+00	15%	20%
3	3	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	-	4.1E+00	3.9E-02	14%	17%
4	4	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	-	9%	5%
5	5	N04001	2C4-ONO2	CCC(ON(=O)=O)C	8.6E-13	8.6E-13	4.4E-01	1.1E-02	4%	5%
6	6	H04001	ORG-0124	CC(OO)CC	1.1E-11	9.7E-12	1.8E+02	4.4E-03	3%	4%
8	8	DO4000	ORG-0006	OCCCC=O	3.3E-11	3.1E-11	3.3E+05	7.8E-04	1%	1%
9	7	H02000	ETOOH	CCOO	6.0E-12	6.0E-12	3.4E+02	3.1E-02	1%	1%
7	14	PO4000	PRD-3	OCCCC(=O)OON(=O)=O	6.8E-12	7.8E-12	5.6E+04	3.0E-05	1%	-
10	11	CH3OOH	MEOOH	COO	5.5E-12	1.0E-11	2.4E+02	-	1%	-
-	9	-	ORG-0572	OC1CCC(=O)O1	-	3.0E-12	4.2E+03	2.3E-05	-	1%
16	10	G02000	PAA	CC(=O)OO	3.2E-12	3.0E-14	8.4E+02	4.9E-02	-	1%
Others									11%	9%

See footnotes for Table S4a

Table S5b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG), for butane.

rank		name		Canonical SMILES	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG	structure	GA	MG	GA	MG
1	1	C04000	N-C4	CCCC	2.4E-12	2.4E-12	50%	50%
2	2	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	23%	27%
3	3	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6%	4%
4	4	K04000	MEK	CCC(=O)C	1.1E-12	1.0E-12	4%	4%
5	6	DO4000	ORG-0006	OCCCC=O	3.3E-11	3.1E-11	4%	3%
6	5	H04001	ORG-0124	CC(OO)CC	1.1E-11	9.7E-12	3%	3%
10	8	DK4000	ORG-0215	O=CCC(=O)C	2.2E-11	2.3E-11	1%	1%
7	>20	DD3000	ORG-0364	O=CCC=O	4.2E-11	4.4E-11	1%	-
8	>20	PD3000	PRD-12	O=CCC(=O)OON(=O)=O	2.1E-11	2.2E-11	1%	-
9	>20	DO3000	ORG-0238	OCCC=O	2.0E-11	2.8E-11	1%	-
12	7	D04000	1C4RCHO	CCCC=O	2.4E-11	2.4E-11	-	1%
15	9	H02000	ETOOH	CCOO	6.0E-12	6.0E-12	-	1%
Others							7%	6%

See footnotes for Table S4a

Table S6a: top 10 octane products by simulation-integrated molecular abundance in GECKO-A (GA) and MechGen (MG).

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		H*	Pvap	Molecular abundance	
GA	MG	GA	MG		GA	MG	($M\ atm^{-1}$)	(atm)	GA	MG
1	5	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	0.0E+00	6%	4%
2	1	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	-	4.1E+00	3.9E-02	5%	8%
4	2	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	1.4E+01	2.0E+00	5%	7%
3	3	P03000	PPN	CCC(=O)OON(=O)=O	2.5E-13	6.5E-13	2.9E+00	1.3E-02	5%	4%
5	7	N08002	ORG-0054	CCCCCC(ON(=O)=O)CC	3.6E-12	5.4E-12	1.8E-01	1.4E-04	4%	3%
6	20	KO8002	ORG-0203	CCC(CCC(=O)CC)O	1.5E-11	1.7E-11	1.6E+05	5.1E-05	4%	-
8	4	KK8007	ORG-0285	CCCC(=O)CCC(=O)C	9.2E-12	8.2E-12	2.5E+04	3.5E-04	3%	4%
7	6	N08003	ORG-0055	CCCCC(ON(=O)=O)CCC	5.0E-12	5.2E-12	1.8E-01	1.4E-04	3%	3%
9	14	KO8001	ORG-0201	CCCC(=O)CCC(O)C	1.9E-11	1.6E-11	1.6E+05	5.1E-05	3%	-
>20	8	HK800W	ORG-3306	CC(OO)CCC(=O)CCC	1.8E-11	1.7E-11	3.2E+05	3.9E-06	-	3%
>20	9	HK8009	ORG-3267	CCC(=O)CCC(OO)CC	1.9E-11	1.6E-11	3.2E+05	3.9E-06	-	3%
12	10	KK8000	ORG-0278	CCC(=O)CCC(=O)CC	7.6E-12	6.3E-12	2.5E+04	3.5E-04	-	3%
10	11	D03000	PROPALD	CCC=O	1.9E-11	2.0E-11	1.3E+01	4.9E-01	2%	-
Others									59%	58%

See footnotes for Table S4a

Table S6b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG), for octane.

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG		GA	MG	GA	MG
1	1	C08000	N-C8	CCCCCCCC	7.8E-12	8.5E-12	27%	29%
2	2	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	5%	7%
3	6	CH2O	CH2O	C=O	9.2E-12	9.2E-12	4%	2%
5	10	KO8001	ORG-0201	CCCC(=O)CCC(O)C	1.9E-11	1.6E-11	4%	2%
4	13	KO8002	ORG-0203	CCC(CCC(=O)CC)O	1.5E-11	1.7E-11	4%	-
6	3	D03000	PROPALD	CCC=O	1.9E-11	2.0E-11	3%	3%
7	17	KO8003	ORG-0962	CCCC(CCC(=O)C)O	2.3E-11	1.8E-11	3%	-
>20	4	HK800M	ORG-3306	CC(OO)CCC(=O)CCC	7.1E-11	1.7E-11	-	3%
>20	5	HK8002	ORG-3267	CCC(=O)CCC(OO)CC	1.9E-11	1.6E-11	-	3%
9	8	KK8007	ORG-0285	CCCC(=O)CCC(=O)C	9.2E-12	8.2E-12	2%	2%
10	9	DK4000	ORG-0215	O=CCC(=O)C	2.2E-11	2.3E-11	2%	2%
8	14	DK5000	ORG-0231	O=CCC(=O)CC	2.3E-11	2.4E-11	2%	-
>20	7	HK8005	ORG-3309	CCCC(CCC(=O)C)OO	2.7E-11	1.6E-11	-	2%
Others							44%	45%

See footnotes for Table S4a

Table S7a: top 10 cyclohexane products by simulation-integrated molecular abundance in GECKO-A (GA) and MechGen (MG).

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		H*	Pvap	Molecular abundance	
GA	MG	GA	MG		GA	MG	(M atm^{-1})	(atm)	GA	MG
1	1	TK6000	CC6-KET	O=C1CCCCC1	6.4E-12	6.4E-12	1.1E+02	5.2E-03	14%	20%
-	2	-	PRD-58	O=C(OO)CC1CCC(=O)O1	-	3.3E-12	2.3E+06	9.5E-07	-	11%
2	13	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	-	10%	-
3	3	TN6000	ORG-0051	O=N(=O)OC1CCCCC1	3.1E-12	5.5E-12	1.3E+00	6.0E-04	9%	8%
5	4	TH6000	ORG-0995	OOC1CCCCC1	1.8E-11	1.6E-11	4.2E+02	1.6E-04	3%	4%
4	>20	PP3000	PRD-822	O=C(CC(=O)OON(=O)=O)OON(=O)=O	7.7E-15	-	8.1E+01	4.9E-05	3%	-
6	>20	PD3000	PRD-202	O=CC(C(=O)OON(=O)=O)O	2.1E-11	2.2E-11	2.4E+03	1.2E-03	3%	-
>20	5	GH6003	PRD-2	O=CCCC(CC(=O)OO)OO	4.1E-11	3.5E-11	4.2E+09	8.6E-09	-	3%
-	6	-	PRD-66	OC1(CC(=O)OO)CCC(=O)O1	-	1.8E-12	1.4E+06	9.4E-09	-	3%
>20	7	PG6006	PRD-97	OOCOCC(=O)CCC(=O)OON(=O)=O	5.2E-12	2.8E-12	5.3E+07	7.8E-08	-	3%
-	8	-	GBUTYACT	O=C1CCCO1	-	2.9E-12	2.0E+01	1.1E-03	-	3%
7	>20	PP6003	PRD-536	O=C(OON(=O)=O)CCC(=O)CC(=O)OON(=O)=O	1.4E-12	2.8E-12	1.9E+05	2.0E-07	2%	-
9	-	PP4000	-	O=C(OON(=O)=O)CCC(=O)OON(=O)=O	2.1E-13	-	1.0E+03	1.7E-05	2%	-
8	-	DD6001	-	O=CCCC(CC=O)O	6.5E-11	-	5.5E+06	3.5E-06	2%	-
>20	9	GN6002	ORG-4898	OOC(CCCCCON(=O)=O)O	7.5E-12	6.1E-12	6.0E+04	8.3E-07	-	2%
>20	10	GH6000	ORG-4189	OOCCCCCC(=O)OO	1.5E-11	1.4E-11	2.0E+07	9.5E-08	-	2%
10	11	TN6002	ORG-0290	O=C1CCCC(C1)ON(=O)=O	3.8E-12	3.8E-12	5.0E+03	4.9E-05	1%	-
Others									51%	42%

See footnotes for Table S4a

Table S7b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG), for cyclohexane.

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG		GA	MG	GA	MG
1	1	T06000	CYCC6	C1CCCCC1	6.9E-12	6.7E-12	27%	38%
>20	3	GH6002	PRD-2	O=CCCC(CC(=O)OO)OO	2.4E-11	3.5E-11	-	8%
2	-	DD6001	-	O=CCCC(CC=O)O	6.5E-11	-	7%	-
4	2	TK6000	CC6-KET	O=C1CCCCC1	6.4E-12	6.4E-12	5%	9%
3	12	CH2O	CH2O	C=O	9.2E-12	9.2E-12	5%	-
5	4	TH6000	ORG-0995	OOC1CCCCC1	1.8E-11	1.6E-11	3%	5%
6	>20	PD3000	PRD-202	O=CCC(=O)OON(=O)=O	2.1E-11	2.2E-11	3%	-
7	>20	DD6002	PRD-14	O=CCCC(=O)CC=O	4.8E-11	4.7E-11	3%	-
8	>20	DD3000	ORG-0364	O=CCC=O	4.2E-11	4.4E-11	3%	-
>20	6	GD6001	ORG-4906	O=CCCC(CC(=O)OO)O	4.4E-11	3.5E-11	-	3%
10	5	TN6000	ORG-0051	O=N(=O)OC1CCCCC1	3.1E-12	5.5E-12	2%	3%
9	20	HD6000	PRD-1	OOCCCCCC=O	3.5E-11	3.4E-11	2%	-
-	7	-	PRD-58	O=C(OO)CC1CCC(=O)O1	-	3.3E-12	-	2%
>20	8	GD6004	PRD-15	O=CCCC(=O)CC(=O)OO	3.0E-11	2.5E-11	-	2%
>20	9	GH6001	ORG-4189	OOCCCCCC(=O)OO	2.6E-11	1.4E-11	-	2%
>20	10	GD3000	ORG-0541	OOC(=O)CC=O	2.5E-11	2.2E-11	-	1%
Others							41%	29%

See footnotes for Table S4a

Table S8a: top 10 hexanal products by simulation-integrated molecular abundance in GECKO-A (GA) and MechGen (MG).

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		H*	Pvap	Molecular abundance	
GA	MG	GA	MG		GA	MG	(M atm^{-1})	(atm)	GA	MG
1	2	P06000	PRD-1	CCCCCC(=O)OON(=O)=O	4.1E-12	6.8E-12	1.0E+00	5.3E-04	18%	13%
2	8	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	-	10%	3%
-	3	-	ORG-3354	CCC1CCC(=O)O1	-	4.0E-12	1.2E+01	2.6E-04	-	6%
3	7	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	-	4.1E+00	3.9E-02	5%	3%
-	4	-	ORG-0928	O=C1CCC(O1)(C)O	-	1.6E-12	3.2E+03	4.0E-05	-	4%
15	6	N05000	ORG-3613	CCCCCON(=O)=O	3.6E-12	3.2E-12	6.0E-01	2.1E-03	-	4%
>20	5	HD5001	PRD-5	CC(OO)CCC=O	3.5E-11	3.2E-11	5.0E+05	7.6E-05	-	4%
4	10	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	1.4E+01	2.0E+00	4%	2%
5	12	PK5000	PRD-281	CC(=O)CCC(=O)OON(=O)=O	1.4E-12	2.7E-12	6.7E+03	1.5E-04	3%	-
6	13	DO5000	ORG-0009	O=CCCC(O)C	3.7E-11	3.4E-11	2.5E+05	1.2E-03	2%	-
7	>20	PO5000	PRD-71	CC(CCC(=O)OON(=O)=O)O	1.1E-11	1.1E-11	4.3E+04	4.0E-05	2%	-
8	19	P03000	PPN	CCC(=O)OON(=O)=O	2.5E-13	6.5E-13	2.9E+00	1.3E-02	2%	-
9	>20	PP3000	PRD-615	O=C(CC(=O)OON(=O)=O)OON(=O)=O	7.7E-15	-	8.1E+01	4.9E-05	2%	-
10	14	PK4000	PRD-227	CC(=O)CC(=O)OON(=O)=O	2.1E-13	3.0E-13	5.5E+02	4.3E-04	2%	-
12	9	H05000	ORG-1038	CCCCCOO	1.1E-11	1.1E-11	1.3E+02	6.6E-04	-	2%
Others									49%	44%

See footnotes for Table S4a

Table S8b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG) for hexanal.

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG		GA	MG	GA	MG
1	1	D06000	1C6RCHO	CCCCCC=O	2.9E-11	2.9E-11	26%	31%
>20	2	HD5000	PRD-5	CC(OO)CCC=O	3.3E-11	3.2E-11	-	10%
2	9	CH2O	CH2O	C=O	9.2E-12	9.2E-12	7%	2%
3	5	DO5000	ORG-0009	O=CCCC(O)C	3.7E-11	3.4E-11	7%	3%
4	3	P06000	PRD-1	CCCCCC(=O)OON(=O)=O	4.1E-12	6.8E-12	6%	8%
5	6	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	5%	3%
-	4	-	ORG-3307	CC1CCC(=O)O1	-	2.7E-12	-	4%
6	>20	PD3000	PRD-175	O=CC(C(=O)OON(=O)=O)O	2.1E-11	2.2E-11	3%	-
10	8	DK5000	ORG-0217	O=CCCC(=O)C	2.6E-11	2.5E-11	2%	2%
7	>20	DD3000	ORG-0364	O=CCC=O	4.2E-11	4.4E-11	2%	-
8	11	DK4000	ORG-0215	O=CCC(=O)C	2.2E-11	2.3E-11	2%	-
9	>20	PO5000	PRD-71	CC(CCC(=O)OON(=O)=O)O	1.1E-11	1.1E-11	2%	-
14	7	H05000	ORG-1038	CCCCCOO	1.1E-11	1.1E-11	-	2%
-	10	-	ORG-3354	CCC1CCC(=O)O1	-	4.0E-12	-	2%
Others							38%	33%

See footnotes for Table S4a

Table S9a: top 10 trans-2-hexene products by simulation-integrated molecular abundance in GECKO-A (GA) and MechGen (MG).

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		H* ($M\ atm^{-1}$)	Pvap (atm)	Molecular abundance	
GA	MG	GA	MG		GA	MG			GA	MG
1	2	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	-	4.1E+00	3.9E-02	16%	20%
2	1	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	1.4E+01	2.0E+00	14%	20%
3	6	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	-	13%	6%
4	4	P04000	PBN	CCCC(=O)OON(=O)=O	1.3E-12	3.4E-12	2.3E+00	4.4E-03	12%	8%
5	3	P03000	PPN	CCC(=O)OON(=O)=O	2.5E-13	6.5E-13	2.9E+00	1.3E-02	9%	8%
6	7	D04000	1C4RCHO	CCCC=O	2.4E-11	2.4E-11	9.6E+00	1.4E-01	6%	6%
7	5	D03000	PROPALD	CCC=O	1.9E-11	2.0E-11	1.3E+01	4.9E-01	6%	7%
8	11	CH3OH	CH3OH	CO	9.3E-13	9.3E-13	-	-	3%	-
-	8	-	PRD-2	CCCCCC1OO1	-	2.4E-12	2.8E-02	4.5E-01	-	3%
-	9	-	PRD-1	CC1OO1	-	1.5E-13	4.8E-02	6.4E+00	-	3%
9	>20	PK4001	PRD-52	CC(=O)CC(=O)OON(=O)=O	2.1E-13	3.0E-13	5.5E+02	4.3E-04	2%	-
15	10	C03000	PROPANE	CCC	1.1E-12	1.1E-12	1.5E-03	6.7E+00	-	2%
10	13	NO6001	PRD-3	CCCC(C(O)C)ON(=O)=O	4.8E-12	5.4E-12	1.5E+03	2.7E-05	1%	-
Others									19%	16%

See footnotes for Table S4a

Table S9b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG), for t-2-hexene.

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG		GA	MG	GA	MG
1	1	D02000	ACETALD	CC=O	1.5E-11	1.5E-11	22%	31%
2	2	U06000	T-2-C6E	CCCC=CC	6.1E-11	6.1E-11	18%	19%
3	3	D04000	1C4RCHO	CCCC=O	2.4E-11	2.4E-11	15%	15%
5	4	D03000	PROPALD	CCC=O	1.9E-11	2.0E-11	11%	13%
4	5	CH2O	CH2O	C=O	9.2E-12	9.2E-12	13%	6%
6	6	P04000	PBN	CCCC(=O)OON(=O)=O	1.3E-12	3.4E-12	2%	3%
8	7	HO6001	PRD-4	CCCC(C(O)C)OO	3.1E-11	2.0E-11	1%	1%
7	8	HO6000	PRD-6	CC(C(CCC)O)OO	2.9E-11	2.2E-11	1%	1%
9	>20	DK4002	ORG-0215	CC(=O)CCOO	2.2E-11	2.3E-11	1%	-
10	>20	H03000	ORG-0129	CCCOO	7.8E-12	8.1E-12	1%	-
>20	9	GD2000	GLYACID	OOC(=O)C=O	1.6E-11	1.2E-11	-	1%
14	10	CH3OOH	MEOOH	COO	5.5E-12	1.0E-11	-	1%
Others							16%	8%

See footnotes for Table S4a

Table S10a: top 10 isoprene products by simulation-integrated molecular abundance in GECKO-MCM (GM), GECKO-SAR (GA) and MechGen (MG).

rank			name[1]			Canonical SMILES structure	kOH (molec s^{-1})			H*	Pvap	Molecular abundance		
GM	GA	MG	GM	GA	MG		GM	GA	MG	(M atm^{-1})	(atm)	GM	GA	MG
1	1	2	CH2O	CH2O	CH2O	C=O	9.2E-12	9.2E-12	9.2E-12	6.00E+03	-	26%	20%	11%
2	2	1	P02000	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	3.0E-14	-	4.10E+00	3.94E-02	14%	13%	14%
3	3	7	KO3000	KO3000	HOACET	CC(=O)CO	4.5E-12	4.5E-12	5.9E-12	1.50E+03	4.03E-03	7%	11%	3%
4	13	>20	C50066	NK4001	ORG-0583	OCC(C(=O)C)OON(=O)=O	1.3E-12	3.9E-12	3.3E-12	1.80E+05	5.49E-06	7%	-	-
5	6	5	MVK	UK4000	MVK	CC(=O)C=C	2.0E-11	2.0E-11	2.0E-11	4.10E+01	1.02E-01	6%	5%	4%
6	4	4	DO2000	DO2000	GLCLALD	OCC=O	1.0E-11	1.0E-11	1.1E-11	4.10E+04	1.01E-02	5%	7%	5%
7	5	3	PO2000	PO2000	HOPAN	OCC(=O)OON(=O)=O	4.2E-13	4.2E-13	8.7E-13	8.30E+02	3.17E-04	4%	5%	7%
8	7	9	DK3000	DK3000	MEGLYOX	O=CC(=O)C	1.3E-11	1.3E-11	1.2E-11	3.20E+04	1.49E-01	4%	3%	2%
11	8	11	DD2000	DD2000	GLYOXAL	O=CC=O	9.7E-12	9.7E-12	1.2E-11	3.60E+05	3.81E-03	-	3%	-
18	>20	6	KO3001	KO3001	DOHACT	OCC(=O)CO	5.8E-12	5.8E-12	4.4E-12	8.80E+06	4.74E-06	-	-	3%
-	-	8	-	-	ORG-2538	O=C1OCC(=O)C1(C)O	-	-	6.5E-13	1.90E+05	4.59E-07	-	-	3%
10	-	10	IEPOXB	-	PRD-26	OCC1OC1(C)CO	1.2E-11	-	8.6E-12	2.40E+06	7.50E-06	2%	-	2%
9	>20	>20	C50064	NK4000	ORG-0595	O=N(=O)OOCC(C(=O)C)O	2.2E-12	2.5E-12	2.1E-12	9.50E+04	5.49E-06	2%	-	-
12	9	16	MACR	UD4000	METHACRO	CC(=C)C=O	2.9E-11	2.9E-11	2.9E-11	6.50E+00	1.78E-01	-	2%	-
17	10	19	CH3OOH	CH3OOH	MEOOH	COO	5.5E-12	5.5E-12	1.0E-11	2.40E+02	-	-	2%	-
Others												23%	30%	44%

[1]Where a species has the same name in the two versions of GECKO-A, its loss reactions are assigned from lab data or are generated by the GECKO-A SARs.
For additional footnotes, see Table S4a

Table S10b: top 10 contributors to simulation-integrated TOHR in GECKO-MCM (GM), GECKO-SAR (GA), and MechGen (MG), for isoprene.

rank			name			Canonical SMILES	kOH (molec s^{-1})			TOHR contribution		
GM	GA	MG	GM	GA	MG	structure	GM	GA	MG	GM	GA	MG
1	1	1	ISOPRN	ISOPRE	ISOPRENE	C=CC(=C)C	9.99E-11	9.99E-11	9.99E-11	28%	27%	31%
2	2	2	CH2O	CH2O	CH2O	C=O	9.20E-12	9.20E-12	9.20E-12	20%	21%	7%
3	3	3	MVK	UK4000	MVK	CC(=O)C=C	2.01E-11	2.01E-11	2.01E-11	10%	7%	6%
>20	>20	4	C50075	HU5008	ORG-0163	CC(=CCOO)C=O	5.20E-11	7.89E-11	5.43E-11	-	-	5%
4	4	5	DO2000	DO2000	GLCLALD	OCC=O	1.02E-11	1.02E-11	1.10E-11	4%	6%	4%
5	5	8	DK3000	DK3000	MEGLYOX	O=CC(=O)C	1.31E-11	1.31E-11	1.19E-11	4%	5%	2%
6	6	7	MACR	UD4000	METHACRO	CC(=C)C=O	2.86E-11	2.86E-11	2.86E-11	3%	5%	2%
7	7	14	KO3000	KO3000	HOACET	CC(=O)CO	4.45E-12	4.45E-12	5.87E-12	3%	3%	-
-	>20	6	-	HU500F	ORG-5054	OOC(C(=C)CO)C=O	-	1.52E-10	1.02E-10	-	-	3%
9	10	16	ISPOO3	UD5002	ORG-0166	C=CC(C)(CO)OO	5.00E-11	1.31E-10	4.11E-11	2%	2%	-
8	-	13	IEPOXB	-	PRD-26	OCC1OC1(C)CO	1.16E-11	-	8.59E-12	2%	-	-
-	9	-	-	UD5003	-	CC(C(O))=CC(=O)	-	9.17E-11	-	-	2%	-
>20	>20	9	C50083	HU500D	ORG-0164	CC(=CC=O)COO	5.20E-11	1.03E-10	5.43E-11	-	-	2%
-	-	10	-	-	PRD-51	OCC1(CO)OC1C=O	-	-	3.97E-11	-	-	2%
10	8	11	DD2000	DD2000	GLYOXAL	O=CC=O	9.70E-12	9.70E-12	1.15E-11	1%	2%	-
Others										23%	20%	37%

[1]Where a species has the same name in the two versions of GECKO-A, its loss reactions are assigned from lab data or are generated by the GECKO-A SARs.
For additional footnotes, see Table S4a

Table S11a: top 10 α-pinene products by simulation-integrated molecular abundance in GECKO-A (GA) and MechGen (MG).

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		H*	Pvap	Molecular abundance	
GA	MG	GA	MG		GA	MG	(M atm^{-1})	(atm)	GA	MG
2	7	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	-	11%	3%
1	2	K03000	ACETONE	CC(=O)C	1.9E-13	1.9E-13	3.0E+01	4.8E-01	18%	17%
3	1	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	-	2.3E+02	3.9E-02	9%	18%
4	6	TP0001	PRD75	O=C(CC1CC(C1(C)C)C(=O)C)OON(=O)=O	4.6E-12	7.4E-12	7.9E+03	3.9E-06	4%	3%
-	3	-	PRD1	CC(=O)C1CC(C1(C)C)CC1OO1	-	5.2E-12	1.1E+02	2.3E-04	-	3%
>20	4	TE800v	ORG-4133	O=C1CC(C(O1)(C)C)C(=O)C	4.1E-12	2.6E-12	1.8E+03	4.4E-06	-	3%
7	5	TD0000	ORG-3908	O=CCC1CC(C1(C)C)C(=O)C	3.9E-11	2.7E-11	3.9E+04	1.2E-04	2%	3%
6	8	TP900O	PRD272	O=N(=O)OOC(=O)C1CC(C1(C)C)C(=O)C	3.1E-12	3.0E-12	9.6E+03	1.0E-05	2%	2%
5	>20	PP3000	PRD3143	O=C(CC(=O)OON(=O)=O)OON(=O)=O	7.7E-15	8.1E+01	8.1E+01	4.9E-05	2%	-
-	9	-	ORG-0667	O=C1OCC(=O)C1	-	4.4E-13	1.8E+03	2.8E-05	-	2%
8	11	TT000E	ORG-4299	O=N(=O)OC1CC2CC(C1(C)O)C2(C)C	6.5E-12	9.1E-12	8.4E+03	1.4E-06	1%	-
9	20	TT000G	ORG-4769	O=C1CC2CC(C1(C)O)C2(C)C	4.3E-12	7.1E-12	3.5E+03	1.6E-05	1%	-
10	>20	PP5001	PRD4418	O=C(CC(=O)OON(=O)=O)CC(=O)OON(=O)=O	1.5E-13	3.6E-13	2.3E+05	5.6E-07	1%	-
11	10	TD9000	ORG-4072	O=CC1CC(C1(C)C)C(=O)C	3.3E-11	3.4E-11	7.2E+04	3.5E-04	-	1%
Others									49%	44%

See footnotes for Table S4a

Table S11b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG), for α-pinene.

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG		GA	MG	GA	MG
1	1	APINEN	A-PINENE	CC1=CCC2CC1C2(C)C	5.3E-11	5.3E-11	22%	27%
3	2	TD0000	ORG-3908	O=CCC1CC(C1(C)C)C(=O)C	3.9E-11	2.7E-11	9%	9%
2	4	CH2O	CH2O	C=O	9.2E-12	9.2E-12	9%	3%
4	3	TD9000	ORG-4072	O=CC1CC(C1(C)C)C(=O)C	3.3E-11	3.4E-11	4%	5%
6	5	TP0001	PRD75	O=C(CC1CC(C1(C)C)C(=O)C)OON(=O)=O	4.6E-12	7.4E-12	2%	2%
5	>20	PD3002	PRD357	O=CCC(=O)OON(=O)=O	2.1E-11	2.2E-11	2%	-
-	6	-	PRD1	CC(=O)C1CC(C1(C)C)CC1OO1	-	5.2E-12	-	2%
8	7	TT000F	ORG-4063	OOC1CC2CC(C1(C)O)C2(C)C	2.7E-11	2.0E-11	1%	1%
7	>20	TH0000	PRD182	OOC(C1CC=C(C(=O)C1)C)(C)C	7.0E-11	9.6E-11	1%	-
9	>20	PD5000	PRD993	O=CCC(=O)CC(=O)OON(=O)=O	2.2E-11	2.3E-11	1%	-
10	-	PD2000	-	O=CC(=O)OON(=O)=O	1.3E-11	-	1%	-
11	8	TT000E	ORG-4299	O=N(=O)OC1CC2CC(C1(C)O)C2(C)C	6.5E-12	9.1E-12	-	1%
-	9	-	ORG-4283	O=CC1CC(O)C(=CC1(C)C)C	-	1.3E-10	-	1%
>20	10	TE800v	ORG-4133	O=C1CC(C(O1)(C)C)C(=O)C	4.1E-12	2.6E-12	-	1%
Others							46%	46%

See footnotes for Table S4a

Table S12a: top 10 camphene products by simulation-integrated molecular abundance in GECKO-A (GA) and MechGen (MG).

rank			name		Canonical SMILES structure	kOH (molec s^{-1})		H*	Pvap	Molecular abundance	
GA	GA'	MG	GA	MG		GA	MG	(M atm^{-1})	(atm)	GA	MG
1		1	K03000	ACETONE	CC(=O)C	1.9E-13	1.9E-13	3.0E+01	4.8E-01	30%	38%
2		4	CH2O	CH2O	C=O	9.2E-12	9.2E-12	6.0E+03	-	8%	3%
3		2	PO2000	HOPAN	OCC(=O)OON(=O)=O	4.2E-13	8.7E-13	8.3E+02	3.2E-04	5%	5%
4		3	TT000U	ORG-3925	OCC1(ON(=O)=O)C2CCC(C1(C)C)C2	6.0E-12	9.2E-12	8.7E+03	4.5E-07	3%	3%
-		5	-	ORG-0337	O=C1CCC(=O)O1	-	4.1E-13	2.6E+02	1.0E-02	-	3%
5		7	TN000C	ORG-3952	OCC(=O)C1CCC(C1)C(ON(=O)=O)(C)C	1.1E-11	1.2E-11	1.7E+05	4.3E-08	2%	2%
6		8	TT000V	ORG-3921	OCC1(OO)C2CCC(C1(C)C)C2	1.2E-11	2.0E-11	3.7E+06	6.2E-08	2%	2%
7		9	TT9002	ORG-4145	O=C1C2CCC(C1(C)C)C2	4.8E-12	9.1E-12	6.4E+01	1.5E-03	2%	2%
8		13	TN7000	ORG-4876	OCC(=O)C1CCC(C1)ON(=O)=O	8.4E-12	9.5E-12	3.5E+05	4.0E-07	2%	-
>20		10	GH5004	ORG-4956	OOCCC(=O)CC(=O)OO	1.7E-11	8.7E-12	6.1E+09	2.5E-08	-	2%
10		6	TK7000	ORG-4075	OCC(=O)C1CCC(=O)C1	9.1E-12	5.8E-12	9.4E+06	4.3E-06	1%	3%
9		12	TH000C	ORG-3943	OCC(=O)C1CCC(C1)C(OO)(C)C	1.6E-11	2.0E-11	5.9E+07	4.3E-09	1%	-
Others										43%	37%

See footnotes for Table S4a

Table S12b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA) and MechGen (MG), for camphene.

rank		name		Canonical SMILES structure	kOH (molec s^{-1})		TOHR contribution	
GA	MG	GA	MG		GA	MG	GA	MG
1	1	CMPHEN	CAMPHENE	C=C1C2CCC(C1(C)C)C2	5.3E-11	5.2E-11	34%	34%
2	4	CH2O	CH2O	C=O	9.2E-12	9.2E-12	4%	3%
3	2	TT000V	ORG-3921	OCC1(OO)C2CCC(C1(C)C)C2	1.2E-11	2.0E-11	4%	4%
5	3	TT000U	ORG-3925	OCC1(ON(=O)=O)C2CCC(C1(C)C)C2	6.0E-12	9.2E-12	3%	4%
4	6	TN000C	ORG-3952	OCC(=O)C1CCC(C1)C(ON(=O)=O)(C)C	1.1E-11	1.2E-11	3%	3%
6	5	TH000C	ORG-3943	OCC(=O)C1CCC(C1)C(OO)(C)C	1.6E-11	2.0E-11	3%	3%
9	7	TH7000	ORG-3987	OOC1CCC(C1)C(=O)CO	2.0E-11	1.9E-11	2%	2%
10	9	TK7000	ORG-4075	OCC(=O)C1CCC(=O)C1	9.1E-12	5.8E-12	2%	2%
7	11	TN7000	ORG-4876	OCC(=O)C1CCC(C1)ON(=O)=O	8.4E-12	9.5E-12	2%	-
8	>20	PD3000	PRD-2956	O=CCC(=O)OON(=O)=O	2.1E-11	2.2E-11	2%	-
12	8	TT9002	ORG-4145	O=C1C2CCC(C1(C)C)C2	4.8E-12	9.1E-12	-	2%
>20	10	GH5004	ORG-4956	OOCCC(=O)CC(=O)OO	1.7E-11	8.7E-12	-	2%
Others							42%	42%

See footnotes for Table S4a

Table S13a: top 10 2-methyl furan products by simulation-integrated molecular abundance in GECKO-A (GA), GECKO-A with amended k(OH + maleic anhydride) (GA*), and MechGen (MG).

rank			name		Canonical SMILES structure	kOH (molec s^{-1})			H*	Pvap	Molecular abundance		
GA	GA*	MG	GA	MG		GA	GA*	MG	(M atm^{-1})	(atm)	GA	GA*	MG
1	1	4	CH2O	CH2O	C=O	9.2E-12	9.2E-12	9.2E-12	6.0E+03	-	17%	16%	5%
2	3	3	P02000	PAN	CC(=O)OON(=O)=O	3.0E-14	3.0E-14	-	4.1E+00	3.9E-02	9%	8%	5%
3	4	7	A02000	ACETACID	CC(=O)O	6.9E-13	6.9E-13	7.5E-13	4.1E+03	1.8E-02	6%	6%	2%
4	5	15	DD2000	GLYOXAL	O=CC=O	9.7E-12	9.7E-12	1.2E-11	3.6E+05	3.8E-03	6%	4%	-
6	2	1	MALAHY	MAL-ANH	O=C1C=CC(=O)O1	1.7E-11	**3.9E-13**	3.9E-13	5.0E+01	2.3E-06	3%	15%	23%
5	6	2	ED3002	PRD-21	O=COC(=O)C	1.3E-13	1.3E-13	1.1E-13	2.5E+01	4.1E-02	3%	3%	12%
7	10	>20	PD3001	PRD-245	O=CC(C(=O)OON(=O)=O)O	1.3E-11	1.3E-11	1.6E-11	6.8E+03	1.1E-05	3%	1%	-
8	13	-	PP3000	-	OC(C(=O)OON(=O)=O)C(=O)OON(=O)=O	1.9E-13	1.9E-13	-	1.7E+02	4.1E-07	3%	-	-
-	-	5	-	ORG-2019	O=C1OC(=O)C(=O)O1	-	-	-	1.3E+01	2.3E-02	-	-	3%
-	-	6	-	PRD-168	O=C1OC2(C(C1O)O2)C	-	-	6.9E-13	5.3E+01	3.6E-06	-	-	3%
9	7	-	AK4000	-	OC(C(=O)O)C(=O)C	3.0E-12	3.0E-12	-	2.5E+05	2.5E-07	2%	2%	-
10	8	-	AU4000	-	O=CC=CC(=O)O	3.3E-11	3.3E-11	-	6.4E+06	3.0E-05	2%	2%	-
11	9	>20	CH3(OOH)	MEOOH	COO	5.6E-12	5.6E-12	1.0E-11	2.4E+2	-	-	2%	-
-	-	8	-	ORG-2145	O=C1OC(=O)C(O1)(C)O	-	-	2.6E-13	6.8E+01	1.3E-04	-	-	2%
-	-	9	-	PRD-228	CC(=O)OC(=O)OON(=O)=O	-	-	-	4.3E+01	2.1E-03	-	-	2%
-	-	10	-	PRD-312	O=N(=O)OC1(C)OC(=O)OC1=O	-	-	1.3E-13	6.1E-01	7.6E-05	-	-	1%
Others											45%	40%	42%

See footnotes for Table S4a

Table S13b: top 10 contributors to simulation-integrated TOHR in GECKO-A (GA), GECKO-A with amended k(OH + maleic anhydride) (GA*), and MechGen (MG), for 2-methyl furan.

rank			name		Canonical SMILES structure	kOH (molec s^{-1})			TOHR contribution		
GA	GA*	MG	GA	MG		GA	GA*	MG	GA	GA*	MG
1	1	1	FU0002	2M-FURAN	Cc1ccco1	7.3E-11	7.3E-11	7.0E-11	25%	23%	36%
4	2	13	MALAHY	MAL-ANH	O=C1C=CC(=O)O1	1.7E-11	**3.9E-13**	3.9E-13	4%	18%	-
2	3	2	CH2O	CH2O	C=O	9.2E-12	9.2E-12	9.2E-12	12%	11%	5%
3	4	-	AU4000	-	O=CC=CC(=O)O	3.3E-11	3.3E-11	-	5%	4%	-
5	5	12	DD2000	GLYOXAL	O=CC=O	9.7E-12	9.7E-12	1.2E-11	4%	3%	-
11	10	3	AU5000	4OX2PACD	CC(=O)C=CC(=O)O	2.9E-11	2.9E-11	3.6E-11	-	1%	4%
>20	>20	4	TE5005	HFON52M5	O=C1C=CC(O1)(C)O	4.6E-11	4.6E-11	4.0E-11	-	-	4%
8	7	5	UD5000	4OX2PEAL	O=CC=CC(=O)C	6.1E-11	6.1E-11	6.2E-11	3%	2%	3%
7	6	-	TE500A	-	CC1=CC(=O)OC1	5.5E-11	5.5E-11	-	3%	3%	-
6	12	>20	PD3001	PRD-245	O=CC(C(=O)OON(=O)=O)O	1.3E-11	1.3E-11	1.6E-11	3%	-	-
9	8	18	TE4000	HFON52	OC1C=CC(=O)O1	8.7E-11	8.7E-11	4.1E-11	2%	2%	-
10	9	>20	TE4001	PRD-17	O=N(=O)OC1C=CC(=O)O1	1.9E-11	1.9E-11	2.1E-11	2%	1%	-
>20	>20	6	TE5009	PRD-14	O=N(=O)OC1(C)C=CC(=O)O1	1.7E-11	1.7E-11	2.1E-11	-	-	2%
15	16	7	DK4000	ORG-0233	O=CC(C(=O)C)O	1.8E-11	1.8E-11	1.8E-11	-	-	2%
>20	>20	8	ED4004	ORG-1766	O=COC(C=O)(O)C	1.3E-11	1.3E-11	2.8E-11	-	-	2%
-	-	9	-	PRD-11	O=COC(=CC=O)C	-	-	3.3E-11	-	-	2%
-	-	10	-	PRD-83	O=CC1(O)OC(=O)OC1(C)O	-	-	2.8E-11	-	-	1%
Others									36%	31%	38%

See footnotes for Table S4a