

## **APPENDIX B**

### **Mapping of MEGAN3 Compounds to Chemical Mechanism Model Species**

## Appendix B. Mapping of MEGAN3 compounds to chemical mechanism model species

The table below provides a crosswalk between MEGAN3 compounds (abbreviated name (MEG3) and detailed name (compound name)) along with their properties (molecular weight (MW) and unique Chemical Abstracts Service (CAS) registry number) and model species of each condensed chemical mechanism supported in the MEGAN3 model (Carbon Bond mechanism version 6 (CB6), Carbon Bond 2005 chemical mechanism (CB05), Carbon-Bond Mechanism version Z (CBMZ), SAPRC-07 (S07), Regional Atmospheric Chemistry Mechanism (RACM), and Common Representative Intermediates version 2 Mechanism (CRIv2)).

No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRIv2-R5
1	78795	Isoprene	68.12	isoprene	ISOP	ISOP	ISOP	ISOP	ISO	C5H8
2	115184	Methylbutenol <2 methyl 3 ene 2 ol>	84.12	MBO_2m3e2ol	IOLE + PAR	IOLE + PAR	OLI + PAR	OLE2	OLI	TBUT2ENE
3	80568	pinene <alpha->	136.24	pinene_a	TERP	TERP	TERP	TERP	API	APINENE
4	127913	pinene <beta->	136.24	pinene_b	TERP	TERP	TERP	TERP	API	APINENE
5	123353	Myrcene	136.24	myrcene	TERP	TERP	TERP	TERP	LIM	BPINENE
6	673847	ocimene <allo>	136.24	ocimene_al	TERP	TERP	TERP	TERP	LIM	BPINENE
7	3338554	ocimene <cis beta>	136.24	ocimene_c_b	TERP	TERP	TERP	TERP	LIM	BPINENE
8	3779611	ocimene <trans beta>	136.24	ocimene_t_b	TERP	TERP	TERP	TERP	LIM	BPINENE
9	79925	Camphene	136.24	camphene	TERP	TERP	TERP	TERP	API	APINENE
10	464175	bornene <2->	136.24	bornene	TERP	TERP	TERP	TERP	API	APINENE
11	471841	fenchene <alpha->	136.24	fenchene_a	TERP	TERP	TERP	TERP	API	APINENE
12	508327	tricyclene	136.24	tricyclene	TERP	TERP	TERP	TERP	API	APINENE
13	13466789	carene <3->	136.24	carene_3	TERP	TERP	TERP	TERP	API	APINENE
14	33404670	fenchene <beta->	136.24	fenchene_b	TERP	TERP	TERP	TERP	API	APINENE
15	99832	phellandrene <alpha->	136.24	phellandrene_a	TERP	TERP	TERP	TERP	LIM	BPINENE
16	99854	terpinene <gamma->	136.24	terpinene_g	TERP	TERP	TERP	TERP	LIM	BPINENE
17	99865	terpinene <alpha->	136.24	terpinene_a	TERP	TERP	TERP	TERP	LIM	BPINENE
18	138863	limonene	136.24	limonene	TERP	TERP	TERP	TERP	LIM	BPINENE
19	555102	phellandrene <beta->	136.24	phellandrene_b	TERP	TERP	TERP	TERP	LIM	BPINENE
20	586629	Terpinolene	136.24	terpinolene	TERP	TERP	TERP	TERP	LIM	BPINENE
21	2867052	thujene <alpha->	136.24	thujene_a	TERP	TERP	TERP	TERP	API	APINENE

No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRiv2-R5
22	3387415	Sabinene	136.24	sabinene	TERP	TERP	TERP	TERP	API	APINENE
23	4080460	verbenene	134.22	verbenene	TERP	TERP	TERP	TERP	LIM	BPINENE
24	99876	cymene <para->	134.22	cymene_p	TERP	TERP	TERP	TERP	LIM	BPINENE
25	527844	cymene <ortho->	134.22	cymene_o	TERP	TERP	TERP	TERP	LIM	BPINENE
26	1124205	cymenene <meta->	132.21	meta-cymenene	TERP	TERP	TERP	TERP	LIM	BPINENE
27	1195320	cymenene <p->	132.21	p-cymenene	TERP	TERP	TERP	TERP	LIM	BPINENE
28	76222	camphor	152.24	camphor	TERP	TERP	TERP	TERP	API	APINENE
29	76493	bornyl acetate	196.29	bornyl_ACT	TERP	TERP	TERP	TERP	API	APINENE
30	89816	piperitone	152.24	piperitone	TERP	TERP	TERP	TERP	API	APINENE
31	98555	terpineol <alpha->	154.25	terpineol_a	TERP	TERP	TERP	TERP	API	APINENE
32	111875	octanol	128.21	octanol	TERP	TERP	TERP	TERP	API	APINENE
33	140670	estragole	148.20	estragole	TERP	TERP	TERP	TERP	LIM	BPINENE
34	464459	borneol	154.25	borneol	TERP	TERP	TERP	TERP	API	APINENE
35	471158	thujone <beta->	152.24	thujone_b	TERP	TERP	TERP	TERP	API	APINENE
36	546805	thujone <alpha->	152.24	thujone_a	TERP	TERP	TERP	TERP	API	APINENE
37	562743	terpineol <4->	154.25	terpineol_4	TERP	TERP	TERP	TERP	API	APINENE
38	564943	myrtenal	150.22	myrtenal	TERP	TERP	TERP	TERP	LIM	BPINENE
39	1195795	fenchone	152.24	fenchone	TERP	TERP	TERP	TERP	API	APINENE
40	3391864	octenol <1 ene 3 ol>	128.21	octenol_1e3ol	TERP	TERP	TERP	TERP	LIM	BPINENE
41	14901076	ionone <beta->	192.30	ionone_b	TERP	TERP	TERP	TERP	LIM	BPINENE
42	35628058	ipsenol	154.25	ipsenol	TERP	TERP	TERP	TERP	LIM	BPINENE
43	87445	caryophyllene <beta->	204.36	caryophyllene_b	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ
44	118650	caryophyllene <cis-iso>	204.36	caryophyllene_c_i	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ
45	483761	cadinene <delta->	204.36	cadinene_d	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ
46	483761	selinene <delta->	204.36	cadinene_d	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ
47	495614	bisabolene <beta->	204.36	bisabolene_b	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ
48	502614	farnescene <alpha->	204.36	farnescene_a	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ
49	514512	patchoulene-b	204.36	patchoulene_b	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ
50	515139	elemene <beta->	204.36	elemene_b	SEQ	SEQ	SEQ	SEQ	SEQ	SEQ

No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRlv2-R5
51	3790781	nerolidol <cis->	222.37	nerolidol_c	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
52	4602840	farnesol <E,E->	222.37	farnesol	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
53	6753986	humulene <alpha->	204.36	humulene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
54	10208807	muurolene <alpha->	204.36	muurolene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
55	13474594	bergamotene <alpha->	204.36	bergamotene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
56	15423571	germacrene B	204.36	germacrene_B	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
57	17066670	selinene <beta->	204.36	selinene_b	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
58	17334553	Calarene	204.36	calarene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
59	18794848	farnescene <beta->	204.36	farnescene_b	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
60	24048440	acoradiene <alpha->	204.36	acoradiene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
61	26259790	humulene <gamma->	204.36	humulene_g	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
62	30021740	muurolene <gamma->	204.36	muurolene_g	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
63	37839637	germacrene D	204.36	germacrene_D	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
64	39029419	cadinene <gamma->	204.36	cadinene_g	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
65	40716663	nerolidol <trans->	222.37	nerolidol_t	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
66	55123212	bergamotene <beta->	204.36	bergamotene_b	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
67	70332159	bisabolene <alpha->	204.36	bisabolene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
68	77532	cedrol <alpha->	222.37	cedrol	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
69	118569	homosalate	262.35	homosalate	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
70	118605	2-Ethyl-hexyl-salate	250.34	2ethyl_hexyl_salate	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
71	469614	cedrene <alpha->	204.36	cedrene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
72	470406	Thujopsene	204.36	thujopsene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
73	475207	longifolene	204.36	longifolene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
74	481345	cadinol <alpha->	222.37	cadinol_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
75	495603	zingiberene <alpha>	204.36	zingiberene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
76	1135666	isolongifolene	204.36	isolongifolene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
77	1137128	longicyclene	204.36	longicyclene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
78	3856255	copaene <alpha->	204.36	copaene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
79	5208593	bourbonene <beta->	204.36	bourbonene_b	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ

No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRlv2-R5
80	5989082	longipinene	204.36	longipinene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
81	13744155	cubebene <beta->	204.36	cubebene_b	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
82	14912448	ylangene <alpha->	204.36	ylangene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
83	17699148	cubebene <alpha->	204.36	cubebene_a	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
84	18252443	copaene <beta->	204.36	copaene_b	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
85	34424572	Kaur-16-ene	272.47	kaur_16_ene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
86	73464478	gurjunene <beta->	204.36	gurjunene_b	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
87	109119917	aromadendrene	204.36	aromadendrene	SESQ	SESQ	SESQ	SESQ	SESQ	SESQ
88	67541	Methanol	32.04	methanol	MEOH	MEOH	CH3OH	CH3OH	MOH	CH3OH
89	67641	Acetone	58.08	acetone	ACET	3 PAR	KET + 2 PAR	ACET	ACT	CH3COCH3
90	64175	Ethanol	46.07	ethanol	ETOH	ETOH	C2H5OH	ALK3	EOH	C2H5OH
91	75070	Acetaldehyde	44.05	acetaldehyde	ALD2	ALD2	ALD2	CCHO	ACD	CH3CHO
92	64186	formic acid	46.03	formic_acid	FACD	FACD	HCOOH	HCOOH	ORA1	HCOOH
93	64197	acetic acid	60.05	acetic_acid	AACD	AACD	RCOOH	AACD	ORA2	CH3CO2H
94	127173	pyruvic acid	88.06	pyruvic_acid						
95	74840	Ethane	30.07	ethane	ETHA	ETHA	ETH	ALK2	ETH	C2H6
96	74851	Ethene	28.05	ethene	ETH	ETH	OL2	ETHE	ETE	C2H4
97	74986	propane	44.10	propane	PRPA	1.5 PAR	1.5 PAR	ALK2	HC3	C3H8
98	106978	Butane	58.12	butane						
99	106989	Butene <1->	56.11	butene	OLE + 2 PAR	OLE + 2 PAR	OLT + 2 PAR	OLE1	OLT	C3H6
100	115071	Propene	42.08	propene	OLE + PAR	OLE + PAR	OLT + PAR	OLE1	OLT	C3H6
101	115117	2-Methylprop-1-ene	56.11	2_methylprop_1_ene	OLE + 2 PAR	OLE + 2 PAR	OLT + 2 PAR	OLE1	OLT	C3H6
102	590181	Butene <cis 2->	56.11	butene_c2	IOLE	IOLE	OLI + 2 PAR	OLE2	OLI	TBUT2ENE
103	624646	Butene <trans 2->	56.11	butene_t2	IOLE	IOLE	OLI + 2 PAR	OLE2	OLI	TBUT2ENE
104	50000	Formaldehyde	30.03	formaldehyde	FORM	FORM	HCHO	HCHO	HCHO	HCHO
105	110623	pentanal	86.13	pentanal						
106	110930	methyl heptenone <652>	126.20	met_heptenone	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
107	112312	decanal	156.27	decanal						
108	124130	octanal	128.21	octanal						

No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRIv2-R5
109	129196	nonanal	142.24	nonanal						
110	626960	oxopentanal	100.12	oxopentanal	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
111	2277192	nonenal	140.23	nonenal						
112	2548870	t-2-octenal	126.20	t-2-octenal						
113	3796701	geranyl acetone	194.32	geranyl_acetone	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
114	3879263	neryl acetone	194.32	neryl_acetone						
115	66251	hexanal	100.16	hexanal	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
116	71410	1-pentanol	88.15	1_pentanol						
117	71432	benzene	78.11	benzene						
118	74908	hydrogen cyanide	27.03	hydrogen_cyanide	HCN	HCN	HCN	HCN	HCN	HCN
119	78706	linalool	154.25	linalool	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
120	78820	Isobutyronitrile	69.11	isobutyronitrile						
121	78853	Methacrolein	70.09	methacrolein	ISPD	ISPD	ISOPRD	IPRD	MACR	UCARB10
122	78944	MethylVinylKetone	70.09	met_vinylketone	ISPD	ISPD	ISOPRD	IPRD	MVK	UCARB10
123	79209	methylacetate	74.08	met_acetate						
124	90028	Salicylaldehyde	122.12	salicylaldehyde						
125	90051	Guaiacol (Phenol, 2-methoxy-)	124.14	guaiacol						
126	93583	Methyl benzoate	136.15	met_benzoate						
127	94597	safrrole	162.19	safrrole						
128	96220	3-pentanone	86.13	3_pentanone						
129	97530	Eugenol (Phenol, 2-methoxy-4-(2-propenyl))	164.20	eugenol						
130	98862	acetophenone	120.15	acetophenone						
131	100514	benzyl-alcohol	108.14	benzyl_alcohol						
132	100527	benzaldehyde	106.12	benzaldehyde						
133	100663	anisole	108.14	anisole						
134	103366	ethyl cinnamate	176.22	ethyl_cinnamate						
135	104552	cinnamaldehyde	132.16	cinnamaldehyde						
136	108883	toluene	92.14	toluene						

No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRlv2-R5
137	108952	phenol	94.11	phenol						
138	109682	2-pentene	70.13	2_pentene						
139	111273	hexanol <1->	102.18	hexanol_1	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
140	119368	Methyl salicylate	152.15	met_salicylate	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
141	120514	benzyl benzoate	212.25	benzyl_benzoate						
142	122781	phenylacetaldehyde	120.15	phenylacetaldehyde						
143	140103	cinnamic acid	148.16	cinnamic_acid						
144	140114	benzyl-acetate	150.18	benzyl_acetate						
145	458355	coniferyl alcohol	180.20	coniferyl_alcohol						
146	470826	cineole <1,8>	154.25	cineole_1_8	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
147	488108	jasmone	164.25	jasmone						
148	501928	chavicol (Phenol, 4-(2-propenyl)-)	134.18	chavicol						
149	501984	p-coumaric acid	164.16	p_coumaric_acid						
150	505577	hexenal <trans- 2->	98.14	hexenal_t2	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
151	616444	3-methylthiophene	98.17	3_metthiophene						
152	821090	4-penten-1-ol	86.13	4_penten_1_ol						
153	928961	Hexenol <cis-3->	100.16	hexenol_c3	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
154	930278	3-methylfuran	82.10	3_metfuran						
155	1211296	Methyl jasmonate	224.30	met_jasmonate						
156	1330207	xylene	106.17	xylene						
157	1576950	z-2-penten-1-ol	86.13	z2_penten_1ol						
158	1629589	1-penten-3-one	84.12	1_penten_3_one						
159	3681718	hexenyl acetate <cis-3->	142.20	hexenyl_ACT_c3	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
160	3899341	3-penten-2-ol	86.13	3_penten_2_ol						
161	5989333	linalool oxide <cis->	170.25	linalool_OXD_c						
162	6789806	hexenal <cis-3->	98.14	hexenal_c3	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
163	16369123	8-heptadecene	238.46	8_heptadecene						
164	16491364	z-3-hexen-1-yl butyrate	170.25	z3_hexen_1yl_butyrate						
165	18936179	2-methylbutanenitrile	83.13	2_met_butanenitrile						

No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRlv2-R5
166	23007296	linalool oxide <trans->	170.25	linalool_OXD_t						
167	26049694	dimethyl-nonatriene	150.26	2met_nonatriene	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
168	57643024	z-2-penten-3-ol	86.13	z2_penten_3ol						
169	62235067	trimethyl tridecatetraene	218.38	3met_3DCTT						
170	74828	methane	16.04	methane	CH4	CH4	CH4	ALK1	CH4	CH4
171	74839	methyl bromide	94.94	met_bromide	CH3BR	CH3BR	CH3BR	CH3BR	CH3BR	CH3BR
172	74873	methyl chloride	50.49	met_chloride	CH3CL	CH3CL	CH3CL	CH3CL	CH3CL	CH3CL
173	74884	methyl iodide	141.94	met_iodide	CH3I	CH3I	CH3I	CH3I	CH3I	CH3I
174	74931	methyl mercaptan	48.11	met_mercaptan	TRS	TRS	TRS	TRS	TRS	DMS
175	75150	carbon disulfide	76.14	carbon_2s	TRS	TRS	TRS	TRS	TRS	DMS
176	75183	dimethyl sulfide	62.14	2met_s	TRS	TRS	TRS	TRS	TRS	DMS
177	78933	Butanone <2->	72.11	butanone_2	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
178	80262	terpinyl acetate <alpha->	196.29	terpinyl_ACT_a	ISPD	ISPD	ISOPRD	IPRD	0.5 MACR + 0.5 MVK	UCARB10
179	83341	Skatole	131.18	skatole						
180	91203	Naphthalene	128.17	naphthalene						
181	109660	pentane	72.15	pentane	5 PAR	5 PAR	5 PAR	ALK4	HC5	NC4H10
182	110430	heptanone	114.19	heptanone						
183	110543	hexane	86.18	hexane	6 PAR	6 PAR	6 PAR	ALK5	HC5	NC4H10
184	111717	heptanal	114.19	heptanal						
185	112414	dodecene <1->	168.32	dodecene_1						
186	120729	indole	117.15	indole						
187	124185	decane	142.28	decane	10 PAR	10 PAR	10 PAR	ALK5	HC8	NC4H10
188	142825	heptane	100.20	heptane	7 PAR	7 PAR	7 PAR	ALK5	HC8	NC4H10
189	463581	carbonyl sulfide	60.08	carbonyl_s	TRS	TRS	TRS	TRS	TRS	DMS
190	529168	santene	122.21	santene						
191	556821	Methylbutenol <3 methyl 2 ene 1 ol>	86.13	MBO_3m2e1ol						
192	624920	Dimethyl disulfide	94.20	2met_2s	TRS	TRS	TRS	TRS	TRS	DMS
193	763326	Methylbutenol <3 methyl 3 ene 1 ol>	86.13	MBO_3m3e1ol						
194	1120214	undecane	156.31	undecane	12 PAR	12 PAR	12 PAR	ALK5	HC8	NC4H10



No.	CAS	Compound Name	MW	MEG3	CB6	CB05	CBMZ	S07	RACM	CRlv2-R5
195	1120361	tetradecene <1->	196.38	tetradecene_1	14 PAR	14 PAR	14 PAR	ALK5	HC8	NC4H10
196	2179579	Diallyl disulfide	146.28	diallyl_2s	TRS	TRS	TRS	TRS	TRS	DMS
197	5905464	propenylpropyldisulfide	148.29	PPPP_2s	TRS	TRS	TRS	TRS	TRS	DMS
198	5905475	Methyl propenyl disulfide	120.24	met_propenyl_2s	TRS	TRS	TRS	TRS	TRS	DMS
199	7783064	Hydrogen sulfide	34.08	hydrogen_s	TRS	TRS	TRS	TRS	TRS	DMS
200	630080	carbon monoxide	28.01	carbon_monoxide	CO	CO	CO	CO	CO	CO
201	10102439	nitric oxide	30.01	nitric_OXD	NO	NO	NO	NO	NO	NO
202	68938001	TotalMT	136.24	totalMT						
203	1	TotalSQT	204.36	totalSQT						
204	7664417	ammonia	17.03	ammonia	NH3	NH3	NH3	NH3	NH3	NH3
205	10024972	nitrous oxide	44.01	nitrous_OXD	N2O	N2O	N2O	N2O	N2O	N2O