

APPENDIX EIGHT

Notebook Cross-Reference

The following notebook cross-reference has been included to facilitate access to the original spectroscopic data obtained for the compounds presented in this thesis. For each compound, both hardcopy and electronic characterization folders have been created that contain copies of the original ^1H NMR, ^{13}C NMR, and IR spectra. All notebooks and spectral data are stored in the Stoltz archives.

Table A8.1 Compounds Appearing in Chapter 3: Computational and Synthetic Validation of a Wolff/Cope Approach to the Synthesis of Ineleganolide

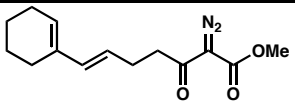
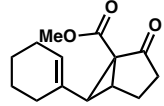
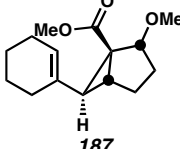
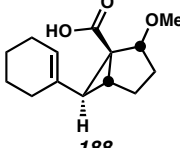
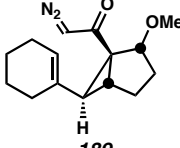
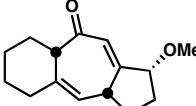
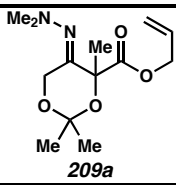
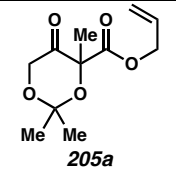
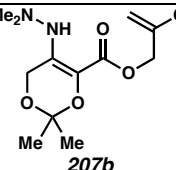
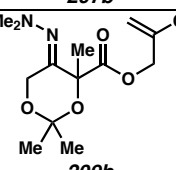
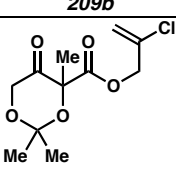
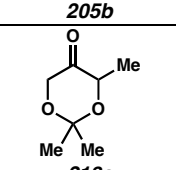
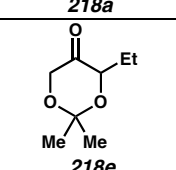
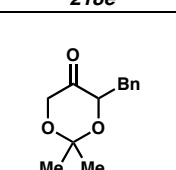
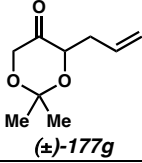
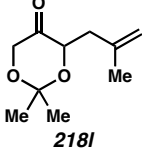
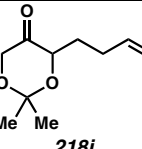
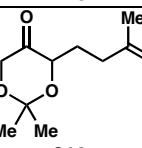
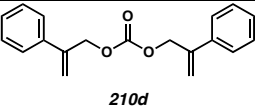
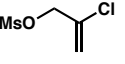
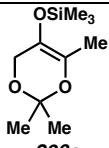
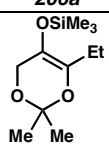
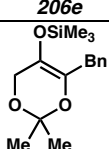
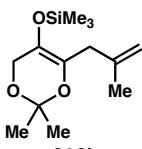
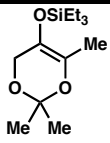
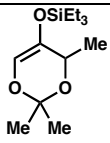
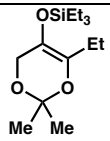
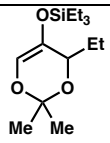
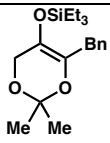
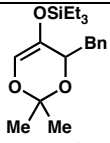
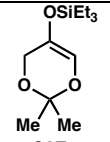
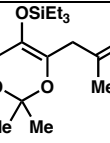
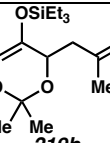
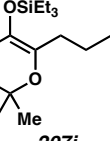
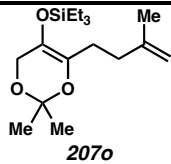
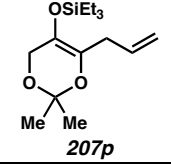
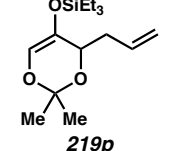
Compound	¹ H NMR	¹³ C NMR	IR	yield
 <p>185</p>	JLR-II-245h	JLR-II-245j	JLR-II-245j	JLR-III-067
 <p>186</p>	JLR-II-249i	JLR-II-249h	JLR-II-249h	JLR-III-085
 <p>187</p>	JLR-II-095h	JLR-II-095i	JLR-II-095e	JLR-III-057
 <p>188</p>	JLR-II-179d	JLR-II-179e	JLR-II-179h	JLR-II-299
 <p>189</p>	JLR-III-039g	JLR-III-039h	JLR-III-039b	JLR-II-171
 <p>191</p>	JLR-III-145c	JLR-III-145p2	JLR-III-145	JLR-III-159

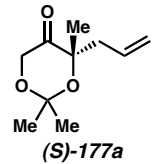
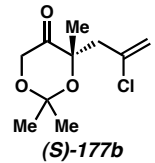
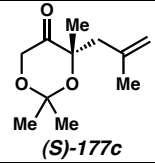
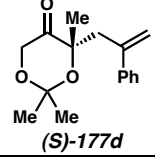
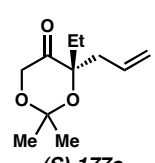
Table A8.2 Compounds Appearing in Chapter 4: Palladium-Catalyzed Enantioselective Alkylation

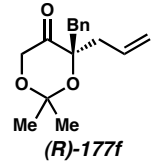
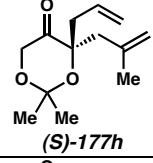
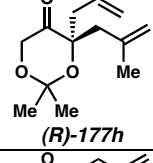
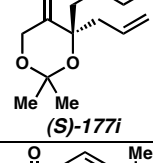
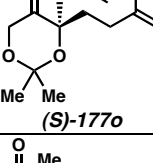
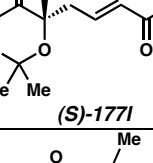
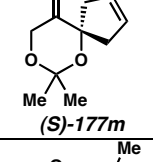
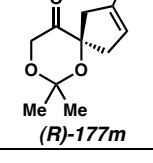
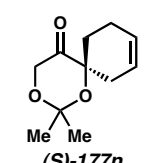
Compound	¹ H NMR	¹³ C NMR	IR	yield
 <p>209a</p>	JLR-VIII-087d	JLR-VIII-087e	JLR-VIII-087d2	JLR-VIII-081, 087
 <p>205a</p>	JLR-VII-277b	JLR-VII-277b2	JLR-VII-277b	
 <p>207b</p>	JLR-IX-283g	JLR-IX-283h	JLR-IX-283a	JLR-VIII-131
 <p>209b</p>	JLR-VIII-095g	JLR-VIII-095h		JLR-VIII-193
 <p>205b</p>	JLR-IX-061c	JLR-IX-061e	JLR-IX-061d	JLR-VIII-123
 <p>218a</p>	MS-II-241	MS-II-241	MS-II-241	MS-I-131
 <p>218e</p>	MS-I-277	MS-I-277	MS-I-277	MS-I-277
 <p>218f</p>	MS-I-259	MS-I-259	MS-I-259	MS-I-259

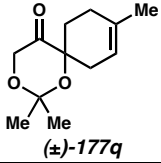
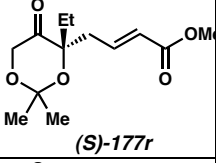
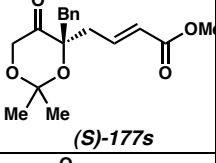
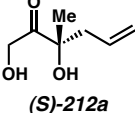
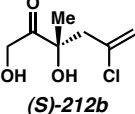
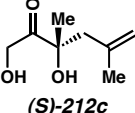
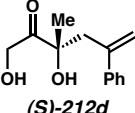
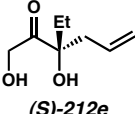
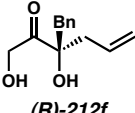
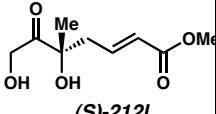
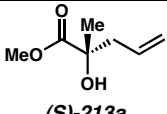
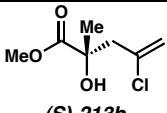
Compound	¹ H NMR	¹³ C NMR	IR	yield
 (±)-177g	JLR-XV-081a2	MS-II-105a	MS-II-105a	MS-II-105a
 218l	MS-I-293a	MS-I-293a	MS-I-293a	MS-I-293a
 218i	JLR-XV-203a2	JLR-XV-203a3	MS-III-55a	MS-III-55a
 218o	JLR-XV-215a2	JLR-XV-215a3	JLR-XV-215	JLR-XV-215
 210d	MS-III-51a	MS-III-51a	MS-III-51a	MS-III-51a
 210g	MS-II-291	MS-II-219		MS-II-219
 206a	MS-I-271a	MS-I-271a	MS-I-271a	MS-I-271a
 206e	MS-I-283a	MS-I-283a	MS-I-283a	MS-I-283a
 206f	MS-II-263a	MS-II-263a	MS-II-263a	MS-II-263a
 206h	MS-I-295a-2	MS-I-295a	MS-I-295a	MS-I-295a

Compound	¹ H NMR	¹³ C NMR	IR	yield
 207a	JLR-XV-291e2	MS-II-147a	MS-II-247a	MS-II-167a
 219a	MS-II-247b			MS-II-247
 207e	MS-II-199a	MS-II-199a	MS-II-199a	MS-II-199a
 219e	MS-II-199b			MS-II-199
 207f	MS-II-181a	MS-II-181a	MS-II-181a	MS-II-181a
 219f	MS-II-181b	MS-II-181b	MS-II-181b	MS-II-181b
 207g	JLR-XV-077b2	JLR-XV-077b	JLR-XV-077b	JLR-XV-077b
 207h	MS-I-225a	MS-I-225a	MS-I-225a	MS-I-225a
 219h	MS-II-225b	MS-II-225b	MS-II-225b	MS-II-225b
 207i	JLR-XV-205a4	JLR-XV-205a3	MS-III-79a	MS-III-79a

Compound	¹ H NMR	¹³ C NMR	IR	yield
 <p>207o</p>	JLR-XV-225a3	JLR-XV-225a2	JLR-XV-225a	JLR-XV-225a
 <p>207p</p>	MS-II-159a	MS-II-159a	MS-II-159c	MS-II-159a+c
 <p>219p</p>	MS-II-159d			MS-II-159

Compound	¹ H NMR	¹³ C NMR	IR	yield, rotation	<i>ee</i>
 <p>(S)-177a</p>	MS-I-245a	MS-I-245a	MS-I-245a	ketoester JLR-VII-243 TMS MS-I-245a TES MS-II-153a	TMS MS-I-245 TES MS-II-153
 <p>(S)-177b</p>	MS-II-89	MS-II-89	MS-II-89	TMS MS-I-125 TES MS-II-157	TMS JLR-XII-207 TES MS-II-157
 <p>(S)-177c</p>	MS-I-281a	MS-I-267a	MS-I-265a2	TMS MS-I-281a TES MS-II-205a	TMS MS-I-281 TES MS-II-205
 <p>(S)-177d</p>	MS-III-69a	MS-III-69a	MS-III-69a	MS-III-69a	MS-III-291
 <p>(S)-177e</p>	MS-I-289a	MS-I-289a	MS-I-289a	TMS MS-I-289a TES MS-II-227a	TMS MS-I-33 TES MS-II-275

Compound	¹ H NMR	¹³ C NMR	IR	yield, rotation	ee
 (R)-177f	MS-I-273a	MS-I-269a	MS-I-273a2	TMS MS-I-273a TES MS-II-189a	TMS MS-I-289 TES MS-II-195
 (S)-177h				MS-II-197a	MS-II-197a
 (R)-177h	MS-II-45a	MS-II-41a	MS-II-41a2	TMS MS-II-41a TES MS-II-257a	TMS MS-II-41 TES MS-II-261
 (S)-177i	MS-III-101a	MS-III-101a	MS-III-101a	MS-III-101a	MS-III-113
 (S)-177o	JLR-XV-231d2	JLR-XV-233a3	JLR-XV-233a	JLR-XV-233a	
 (S)-177l	MS-I-247a-2	MS-I-247a	MS-I-205a	MS-I-247a	MS-I-247a
 (S)-177m				MS-I-201	MS-I-201
 (R)-177m	MS-II-61a	MS-II-61a	MS-II-61a	MS-II-61a	MS-II-61a
 (S)-177n	MS-III-113a	MS-III-113a	MS-III-113a	MS-III-113a	MS-III-113a

Compound	¹ H NMR	¹³ C NMR	IR	yield, rotation	<i>ee</i>
 (±)-177q	JLR-XV-299a3	JLR-XV-299a4	JLR-XV-299a	JLR-XV-299a	
 (S)-177r	MS-II-33a	MS-II-33a	MS-II-33a	TMS MS-II-33a TES MS-II-263a	TMS MS-II-33 TES MS-II-263
 (S)-177s	MS-I-279a	MS-I-279a	MS-I-279a	MS-I-285a	MS-I-291a
 (S)-212a	MS-II-283a	MS-II-273a	MS-II-273a	MS-II-283a	MS-II-283a
 (S)-212b	MS-III-85a	MS-III-85a	MS-III-85a	MS-III-85a	MS-III-85a
 (S)-212c	MS-III-35a	MS-II-303a	MS-III-35a	MS-III-35a	MS-III-35a
 (S)-212d	MS-III-89a	MS-III-89a	MS-III-89a	MS-III-89a	MS-III-89a
 (S)-212e	MS-II-251a	MS-II-251a	MS-II-263a	MS-II-263a	MS-II-263a
 (R)-212f	MS-II-253a	MS-II-253a	MS-II-253a	MS-II-253a	MS-II-253a
 (S)-212l	MS-III-105a	MS-III-117a	MS-III-117a	MS-III-117a	MS-III-117a
 (S)-213a	MS-II-295a	MS-II-281a	MS-III-33a	MS-II-295a	MS-II-295a
 (S)-213b	MS-III-95a	MS-III-95a	MS-III-95a	MS-III-95a	MS-III-95a

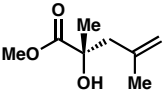
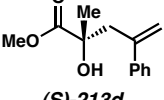
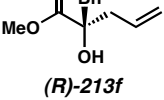
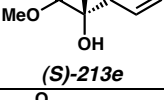
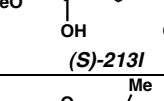
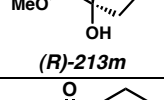
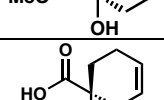
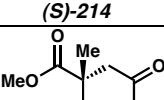
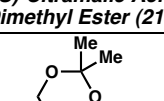
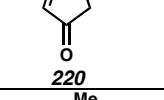
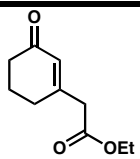
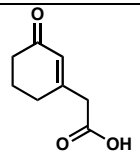
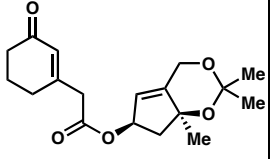
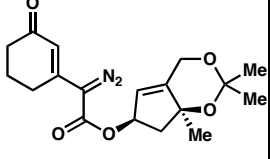
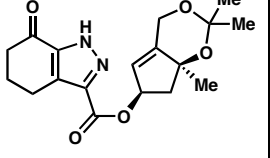
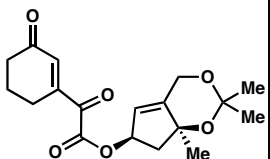
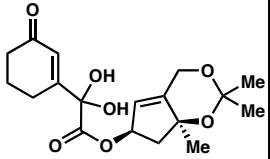
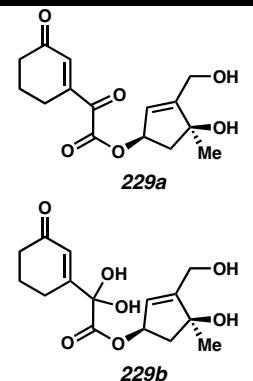
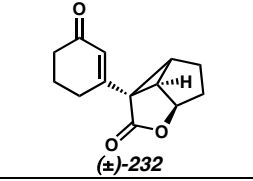
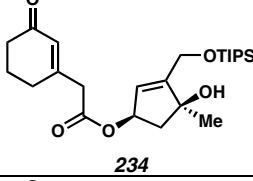
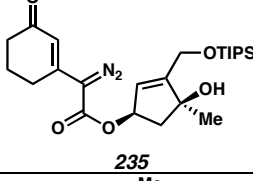
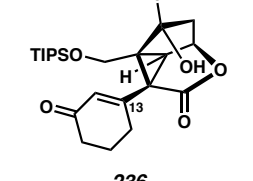
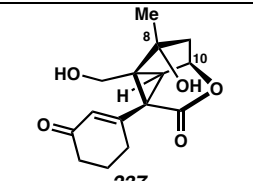
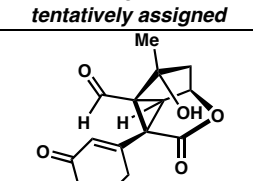
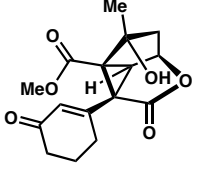
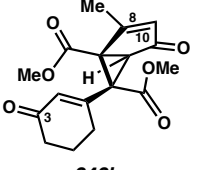
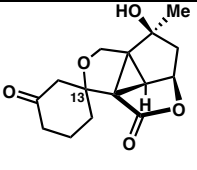
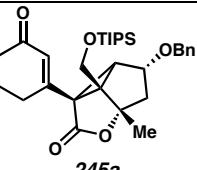
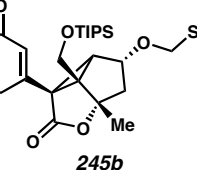
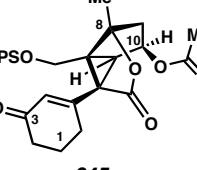
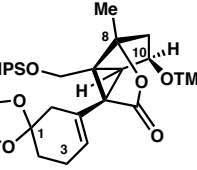
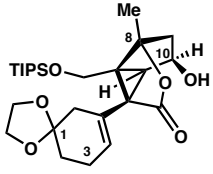
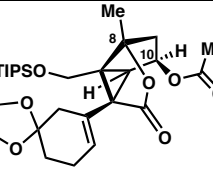
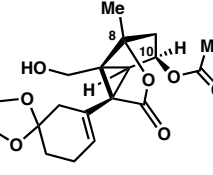
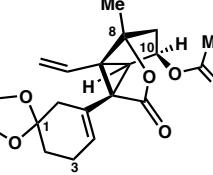
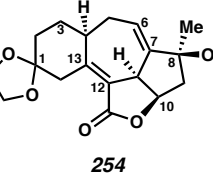
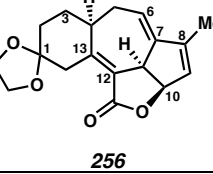
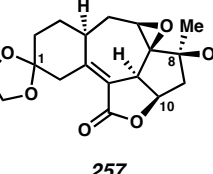
Compound	¹ H NMR	¹³ C NMR	IR	yield, rotation	<i>ee</i>
 (S)-213c	MS-III-45a	MS-III-39a	MS-III-39a	MS-III-45a	MS-III-45a
 (S)-213d	MS-III-99a	MS-III-99a	MS-III-99a	MS-III-99a	MS-III-99a
 (R)-213f	MS-II-271a	MS-II-209a	MS-II-271a2	MS-II-271a	MS-II-271a
 (S)-213e	MS-II-275a	MS-II-275a	MS-II-275a	MS-II-275a	MS-II-275a
 (S)-213l	MS-III-111a	MS-III-127a	MS-III-127a	MS-III-127a	MS-III-127a
 (R)-213m	MS-III-67a	MS-III-67a	MS-III-67a	MS-III-67a	MS-III-67a
 (S)-214	MS-III-143	MS-III-143	JLR-XV-213b	JLR-XV-213b	MS-III-147
 (S)-Citramalic Acid Dimethyl Ester (216)	JLR-XV-079a5	JLR-XV-079a6	JLR-XV-079a	JLR-XV-079a	
 220	JLR-XIV-241a4	JLR-XIV-241a5	JLR-XIV-241a	JLR-XIV-241	
 ent-176	JLR-XIV-265a2	JLR-XIV-265a3	JLR-XIV-265a2`	JLR-XIV-265	JLR-XIII-299, 199

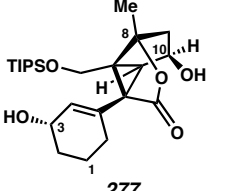
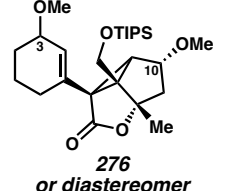
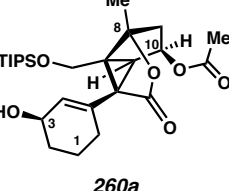
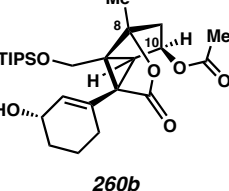
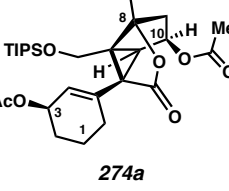
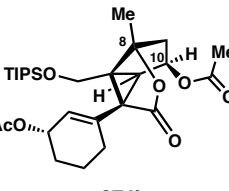
Table A8.3 Compounds Appearing in Chapter 5: Progress Toward an Enantioselective Synthesis of Ineleganolide

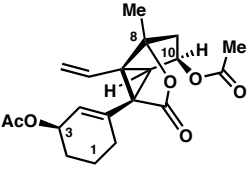
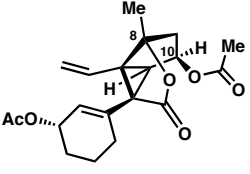
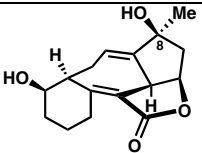
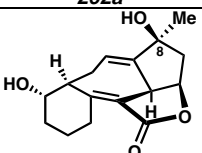
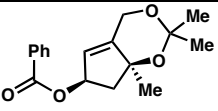
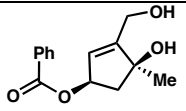
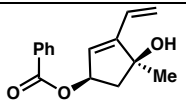
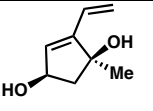
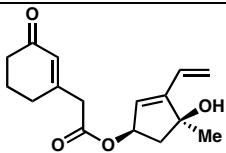
Compound	¹ H NMR	¹³ C NMR	IR and HRMS	yield
 <p>222b</p>				With TEMPOBF ₄ : ACJ-IV-119
 <p>174b</p>	ACJ-V-065a	ACJ-V-065a	ACJ-V-065a	ACJ-IV-097
 <p>224</p>	JLR-XII-285r	JLR-XII-285t3	IR: JLR-XII-285t HRMS: JLR-VIII-293	JLR-XVI-035
 <p>173</p>	JLR-XII-291h	JLR-XII-291h	JLR-XII-291h	JLR-IX-127
 <p>225</p>	JLR-XII-235h_a_1H	JLR-XII-235h_i_13C	IR: JLR-XII-235j HRMS: JLR-XII-235	yield: JLR-X-033 recrystallization: JLR-X-219
 <p>228a</p>	JLR-XIII-049c	JLR-XIII-049c	JLR-XIII-049d	JLR-XIII-049
 <p>228b</p>				

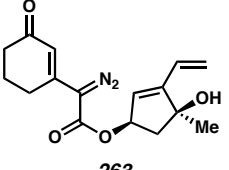
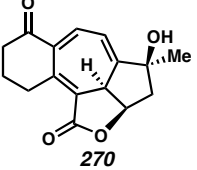
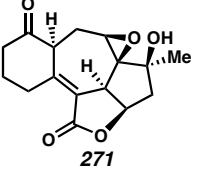
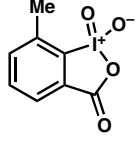
Compound	¹ H NMR	¹³ C NMR	IR and HRMS	yield
 <p>229a</p> <p>229b</p>	JLR-XIII-049h	JLR-XIII-049h [supports assignment as 229a]	JLR-XIII-049_diol	JLR-XIII-049
 <p>(±)-232</p>	JLR-XIII-143h2	JLR-XIII-143j5	JLR-XIII-143h	JLR-XIII-143
 <p>234</p>	JLR-XIII-255b2	JLR-XIII-255b5	IR: JLR-XIII-255b6 HRMS: JLR-XIV-285c2	ACJ-IV-213
 <p>235</p>	JLR-XIII-271b	JLR-XIV-129a3_13C	IR: JLR-XIII-271c HRMS: JLR-XIV-129a	JLR-XV-103
 <p>236</p>	JLR-XIV-169b2	JLR-XIV-303a6	IR: JLR-XIV-191a HRMS: JLR-XIV-143e	JLR-XV-113
 <p>237 <i>tentatively assigned</i></p>	JLR-XV-101a2		IR: n/a HRMS: JLR-XV-269e #4	JLR-XV-101
 <p>241a <i>tentatively assigned</i></p>	JLR-XV-293b2	JLR-XV-293b4	IR: n/a HRMS: JLR-XV-269d	JLR-XV-293

Compound	¹ H NMR	¹³ C NMR	IR and HRMS	yield
 <p>241b tentatively assigned</p>	JLR-XV-257		HRMS: JLR-XV-257	JLR-XV-257
 <p>242b tentatively assigned</p>	JLR-XV-175d2			JLR-XV-175
 <p>240 mixture of C(13) diastereomers</p>	JLR-XVI-231f	JLR-XVI-231f	JLR-XVI-231e	JLR-XVI-231
 <p>245a</p>	JLR-XVII-239d	JLR-XVII-239d	JLR-XVII-239d	JLR-XVII-187
 <p>245b</p>	JLR-XVII-221d	JLR-XVII-221d3	JLR-XVII-221d2	JLR-XVII-221
 <p>245c</p>	CDCl ₃ : JLR-XVII-209a C ₆ D ₆ : JLR-XVII-209a2	JLR-XVII-209a3	IR: JLR-XVII-209a HRMS: JLR-XVII-209a3	yield: JLR-XVII-251 rotation: JLR-XVII-213
 <p>250a C(10) TMS ether tentatively assigned</p>	CDCl ₃ : JLR-XVII-121d C ₆ D ₆ : JLR-XVII-121d2	JLR-XVII-121d3	IR: JLR-XVII-121d5 HRMS: TEST4.d	JLR-XVII-121

Compound	¹ H NMR	¹³ C NMR	IR and HRMS	yield
 272 C(10) alcohol tentatively assigned	JLR-XVII-267b2	JLR-XVII-267b3	IR: JLR-XVII-267b_5 HRMS: JLR-XVII-267	JLR-XVII-267
 250b	JLR-XVII-253c3	JLR-XVII-253c4	IR: JLR-XVII-253c HRMS: JLR-XVII-253c	yield: JLR-XVII-259 rotation: JLR-XVII-253c
 251	JLR-XVIII-035g	JLR-XVIII-035g3	JLR-XVIII-035g	rotation: JLR-XVIII-035
 253	JLR-XVII-281c	JLR-XVII-281c	JLR-XVII-281c	yield: JLR-XVIII-135 rotation: JLR-XVII-281
Unknown 273	JLR-XVIII-173b	JLR-XVIII-173b3	JLR-XVIII-173b2	procedure: JLR-XVIII-173
 254	JLR-XVIII-055f	JLR-XVIII-187e	IR: JLR-XVIII-187e HRMS: JLR-XVIII-047d	JLR-XVIII-187
 256	JLR-XVIII-233e	JLR-XVIII-233e	IR: JLR-XVIII-233e HRMS: JLR-XVIII-233e_7	rotation: JLR-XVIII-233
 257	JLR-XVIII-221c	JLR-XVIII-221c	IR: JLR-XVIII-221c HRMS: JLR-XVIII-221c_2_1	JLR-XVIII-221

Compound	¹ H NMR	¹³ C NMR	IR and HRMS	yield
 277 <i>or diastereomer at C(10) and / or C(3)</i>	JLR-XVII-151b3	JLR-XVII-151b4	IR: JLR-XVII-151b HRMS: JLR-XVII-151b	yield: JLR-XVII-163 rotation: JLR-XVII-151
 276 <i>or diastereomer at C(10) and / or C(3)</i>	JLR-XVII-165b	JLR-XVII-165b6	IR: JLR-XVII-165b_4 HRMS: JLR-XVII-165b	JLR-XVII-163, 165
 260a	JLR-XVIII-291a2	JLR-XVIII-291a3	JLR-XVIII-291a	yield: JLR-IXX-059 rotation: JLR-XVIII-291
 260b	JLR-XVIII-291b2	JLR-XVIII-291b2	IR: JLR-XVIII-291b HRMS: JLR-XVIII-291b_2	yield: JLR-IXX-059 rotation: JLR-XVIII-291
 274a	JLR-XVIII-105d6	JLR-XVIII-105d7	IR: JLR-XVIII-105d_2 HRMS: JLR-XVIII-105d_secon	three-step yield: JLR-XVIII-235 one-step yield: JLR-XVIII-297 rotation: JLR-XVIII-105
 274b	JLR-XVIII-299a	JLR-XVIII-117c2	IR: JLR-XVIII-117c_1 HRMS: JLR-XVIII-117c-secon	three-step yield: JLR-XVIII-235 one-step yield: JLR-XVIII-299 rotation: JLR-XVIII-117

Compound	¹ H NMR	¹³ C NMR	IR and HRMS	yield
 <p>261a</p>	JLR-XVIII-139g	JLR-XVIII-139g3 (saved as 239g3)	IR: JLR-XVIII-139 HRMS: JLR-XVIII-139g	yield: JLR-IXX-113
 <p>261b</p>	JLR-XVIII-189d2	JLR-XVIII-189d2	JLR-XVIII-189	JLR-IXX-067
 <p>262a</p>	JLR-IXX-079b	JLR-IXX-079b	JLR-IXX-079b	yield: JLR-IXX-131 rotation: JLR-IXX-079
 <p>262b</p>	JLR-IXX-043b	JLR-IXX-043b	JLR-IXX-043b	yield: JLR-IXX-121
 <p>266</p>	JLR-XIII-061a2	JLR-XIII-061a4	JLR-XIII-061a	yield: ACJ-V-255 rotation: JLR-XIII-061a
 <p>267</p>	JLR-XIII-061f	JLR-XIII-061f	JLR-XIII-061f	JLR-XIII-061
 <p>268</p>	JLR-XIII-041	JLR-XIII-041	JLR-XIII-041	yield: ACJ-VI-177, 179 rotation: JLR-XIII-069
 <p>269</p>	JLR-XIII-069b2	JLR-XIII-069b2	JLR-XIII-069b2	ACJ-V-109
 <p>275</p>	JLR-XIV-177b	JLR-XIV-177b2	IR: JLR-XIII-235g HRMS: JLR-XIII-235	ACJ-VI-195

Compound	¹ H NMR	¹³ C NMR	IR and HRMS	yield
 263	CDCl ₃ : JLR-XIV-182c2 C ₆ D ₆ : JLR-XVII-083a3	JLR-XVII-083a4	JLR-XVII-083a5	ACJ-VI-199
 270	ACJV-259	ACJV-259	ACJV-259	ACJ-V-267, 275, 289
 271	ACJVI-165-A-1H	ACJVI-165-A-13C	ACJVI-165-A	ACJ-VI-223, 165
 280	JLR-IXX-189a	JLR-IXX-189a4	JLR-IXX-115	JLR-IXX-189a