# **Supplementary Materials**

# Immunomodulatory Polyketides from a *Phoma*-like Fungus Isolated from a Soft Coral

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PCM/MeCN optimized MMFF conformers

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EI-GYW-1	7158 A20-c1#	9 RT: 1.78	
T: + C E:	I Full ms [ 4	9.50-1000.50	]
m/z = 47	.50-1002.50		
m / 7	Intensity	Relative T	'h

n/z = 47.50	0-1002.50	e e a a	123	100		
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Compositio
163.1098	2923124.0	13.21	163.1117	-1.92	4.5	C11 H15 O1
164.1178	3007200.0	13.59	164.1196	-1.78	4.0	C11 H16 O1
165.0896	419175.0	1.89	165.0910	-1.39	4.5	C10 H13 O2
165.1261	17093120.0	77.27	165.1274	-1.28	3.5	C11 H17 O1
166.0977	321448.0	1.45	166.0988	-1.17	4.0	C10 H14 O2
167.1059	607760.0	2.75	167.1067	-0.75	3.5	C10 H15 O2
170.0934	239456.0	1.08	170.0937	-0.35	3.0	C 9 H 14 O 3
172.1241	491313.0	2.22	172.1247	-0.54	6.0	C 13 H 16
173.0953	233377.0	1.05	173.0961	-0.83	6.5	C12 H13 O1
173.1319	1056410.0	4.78	173.1325	-0.60	5.5	C 13 H 17
174.1394	688260.0	3.11	174.1403	-0.89	5.0	C13 H18
175.1119	652048.0	2.95	175.1117	0.15	5.5	C12 H15 O1
175.1481	11233792.0	50.78	175.1481	-0.06	4.5	C 13 H 19
176.1185	359810.0	1.63	176.1196	-1.08	5.0	C <sub>12</sub> H <sub>16</sub> O <sub>1</sub>
176.1539	3428505.0	15.50	176.1560	-2.02	4.0	C <sub>13</sub> H <sub>20</sub>
177.1275	3010668.0	13.61	177.1274	0.08	4.5	C <sub>12</sub> H <sub>17</sub> O <sub>1</sub>
177.1611	819806.0	3.71	177.1638	-2.71	3.5	C <sub>13</sub> H <sub>21</sub>
178.1341	2270197.0	10.26	178.1352	-1.07	4.0	C <sub>12</sub> H <sub>18</sub> O <sub>1</sub>
179.1068	252361.0	1.14	179.1067	0.11	4.5	C <sub>11</sub> H <sub>15</sub> O <sub>2</sub>
179.1428	1909926.0	8.63	179.1430	-0.24	3.5	C <sub>12</sub> H <sub>19</sub> O <sub>1</sub>
182.1300	861065.0	3.89	182.1301	-0.13	3.0	C <sub>11</sub> H <sub>18</sub> O <sub>2</sub>
187.1476	5729625.0	25.90	187.1481	-0.58	5.5	C14 H19
189.1276	358669.0	1.62	189.1274	0.22	5.5	C <sub>13</sub> H <sub>17</sub> O <sub>1</sub>
190.1346	2145476.0	9.70	190.1352	-0.60	5.0	C13 H18 O1
191.1417	1123851.0	5.08	191.1430	-1.32	4.5	C13 H19 O1
192.1481	285741.0	1.29	192.1509	-2.77	4.0	C13 H20 O1
193.1217	302355.0	1.37	193.1223	-0.57	4.5	C12 H17 O2
193.1582	2239648.0	10.12	193.1587	-0.46	3.5	C <sub>13</sub> H <sub>21</sub> O <sub>1</sub>
195.1380	1460179.0	6.60	195.1380	0.09	3.5	C <sub>12</sub> H <sub>19</sub> O <sub>2</sub>
196.1442	677045.0	3.06	196.1458	-1.62	3.0	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>
202.1724	287694.0	1.30	202.1716	0.77	5.0	C15 H22
203.1435	1333439.0	6.03	203.1430	0.43	5.5	C14 H19 O1
204.1493	482337.0	2.18	204.1509	-1.55	5.0	C14 H20 O1
205.1595	1537759.0	6.95	205.1587	0.86	4.5	C14 H21 O1
206.1640	335142.0	1.52	206.1665	-2.52	4.0	C14 H22 O1
207.1382	377279.0	1.71	207.1380	0.23	4.5	C13 H19 O2
208.1463	926663.0	4.19	208.1458	0.55	4.0	C <sub>13</sub> H <sub>20</sub> O <sub>2</sub>
209.1531	463309.0	2.09	209.1536	-0.54	3.5	C <sub>13</sub> H <sub>21</sub> O <sub>2</sub>
215.1424	1173230.0	5.30	215.1430	-0.68	6.5	C15 H19 O1
217.1584	570956.0	2.58	217.1587	-0.24	5.5	C15 H21 O1
218.1647	355158.0	1.61	218.1665	-1.79	5.0	C15 H22 O1
221.1530	633854.0	2.87	221.1536	-0.56	4.5	C14 H21 O2
223.1679	229229.0	1.04	223.1693	-1.35	3.5	C14 H23 O2
230.1659	548417.0	2.48	230.1665	-0.60	6.0	C16 H 22 O1
233.1529	1267709.0	5.73	233.1536	-0.71	5.5	C15 H21 O2
236.1751	350461.0	1.58	236.1771	-1.96	4.0	C15 H 24 U 2
248.1762	1389907.0	6.28	248.1771	-0.85	5.0	C16 H 24 U 2
266.1870	977425.0	4.42	266.1876	-0.66	4.0	C16 H 26 U 3

Figure S1. HREIMS spectrum of 1



Figure S2. FTIR spectrum of 1



Figure S3. <sup>1</sup>H NMR spectrum of 1 in *Pyridine-d*<sub>5</sub> at 400 MHz



**Figure S4.** <sup>13</sup>C and NMR DEPT spectra of **1** in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S5. HSQC spectrum of 1 in *Pyridine-d*<sub>5</sub>



**Figure S6.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **1** in *Pyridine-d*<sub>5</sub>



Figure S7. HMBC spectrum of 1 in *Pyridine-d*<sub>5</sub>



Figure S8. NOESY spectrum of 1 in *Pyridine-d*<sub>5</sub>

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EI-G	YW-17160	) A2-c1#	17 RT:	3.5	6
T: +	c EI Fu	11 ms [	49.50-	100	0.50]
m/z=	47.50-	1002.50			

m/z	Intensity	Relative	Theo.	Delta	RDB	Composition
126 0077	1207410 0	0 00	126 0003	-0.57	A O	C + H 12 O 1
136.0877	1307410.0	14.09	137.0061	0.19	3.5	Co H12 01
137.0963	22//85/.0	7 01	130,10301	_0.19	3.0	Co Hay On
138.1035	1262245.0	7.01	130.1039	-0.30	3.0	Co H 11 O 1
139.0761	10/3287.0	0.04	141 0010	0.70	2.5	Collin Oc
141.0915	1333922.0	8.25	141.0910	0.40	6.5	C 13 H 13 O 2
143.0858	504086.0	5.12	143.0055	0.31	2.0	Ca Hao Oo
144.0790	877679.0	10 55	144.0701	0.00	5.5	C 11 H 12 O 3
145.1012	1705408.0	10.55	145.1012	0.02	5.5	Cir His Os
147.0802	882178.0	5.46	147.0804	-0.23	J.J 4 E	Cio Hillol
147.1168	2176245.0	13.47	147.1100	-0.02	4.5	C11 H15
148.0881	/0085/.0	4.34	148.0883	-0.17	5.0	C10 H12 O1
149.0961	3681020.0	22.78	149.0961	0.01	4.0	C10 H13 01
149.1328	3477182.0	21.52	149.1325	0.32	3.0	C11 H17
151.1114	1620036.0	10.02	151.1117	-0.31	3.0	C10 H15 01
152.0834	11//466.0	1.29	152.0832	0.19	4.0	C 9 H 12 U 2
152.1199	4027641.0	24.92	152.1196	0.34	3.0	C10 H16 01
157.1013	421765.0	2.61	157.1012	0.13	0.0	C12 H13
164.1187	3728994.0	23.07	164.1196	-0.87	4.0	C11 H16 O1
165.1268	15808768.0	97.82	165.1274	-0.58	3.5	C11 H17 01
170.0947	552499.0	3.42	170.0937	0.94	3.0	C9H14O3
172.1248	1121612.0	6.94	172.1247	0.12	6.0	C13 H16
173.0963	448122.0	2.77	173.0961	0.17	6.5	C12 H13 O1
173.1325	1604323.0	9.93	173.1325	0.01	5.5	C13 H17
174.1394	850246.0	5.26	174.1403	-0.90	5.0	C13 H18
175.1119	1094531.0	6.77	175.1117	0.20	5.5	C <sub>12</sub> H <sub>15</sub> O <sub>1</sub>
175.1483	9457408.0	58.52	175.1481	0.19	4.5	C13 H19
177.1274	7694308.0	47.61	177.1274	0.03	4.5	C <sub>12</sub> H <sub>17</sub> O <sub>1</sub>
179.1425	936407.0	5.79	179.1430	-0.54	3.5	C12 H19 O1
187.1482	8422400.0	52.11	187.1481	0.10	5.5	C14 H19
189.1270	668618.0	4.14	189.1274	-0.41	5.5	C13 H17 O1
190.1351	4152888.0	25.70	190.1352	-0.15	5.0	C13 H18 O1
193.1584	2865493.0	17.73	193.1587	-0.32	3.5	C <sub>13</sub> H <sub>21</sub> O <sub>1</sub>
202.1355	447793.0	2.77	202.1352	0.24	6.0	C14 H18 O1
202.1722	734303.0	4.54	202.1716	0.56	5.0	C15 H22
203.1433	835344.0	5.17	203.1430	0.21	5.5	C14 H19 O1
205.1592	1393440.0	8.62	205.1587	0.49	4.5	C14 H21 O1
221.1536	530443.0	3.28	221.1536	-0.06	4.5	C14 H21 O2
230.1667	2290213.0	14.17	230.1665	0.18	6.0	C16 H22 O1
233.1534	1894695.0	11.72	233.1536	-0.24	5.5	C15 H21 O2
248.1769	2371656.0	14.67	248.1771	-0.21	5.0	C16 H24 O2
308.1982	558864.0	3.46	308.1982	0.00	5.0	C18 H28 O4

Figure S9. HREIMS spectrum of 2



Figure S10. FTIR spectrum of 2



Figure S11. <sup>1</sup>H NMR spectrum of 2 in CDCl<sub>3</sub> at 400 MHz



Figure S12.  $^{13}$ C and NMR DEPT spectra of 2 in CDCl<sub>3</sub> at 100 MHz



Figure S13. HSQC spectrum of 2 in CDCl<sub>3</sub>



Figure S14. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 2 in CDCl<sub>3</sub>



Figure S15. HMBC spectrum of 2 in CDCl<sub>3</sub>



Figure S16. NOESY spectrum of 2 in CDCl<sub>3</sub>



**Figure S17.** <sup>1</sup>H NMR spectrum of **2** in *Pyridine-d*<sub>5</sub> at 600 MHz



Figure S18. <sup>13</sup>C and NMR DEPT spectra of 2 in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S19. HSQC spectrum of 2 in *Pyridine-d*<sub>5</sub>



**Figure S20.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **2** in *Pyridine-d*<sub>5</sub>



Figure S21. HMBC spectrum of 2 in *Pyridine-d*<sub>5</sub>





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EI-GYW-171	161_A6-c1#1	3-17 RT: 2	.67-3.56	AV: 5		
T: + c EI	Full ms [	49.50-1000	.50]			
m/z = 47.5	0-1002.50	Del en includ	mb e e	Dolta	DDB	Compositio
m/z	Intensity	Relative	Mass	(mmu)	equiv.	Composiere
60.0205	432127.0	5.71	60.0206	-0.05	1.0	C2 H4 O2
93.0694	1544724.4	20.40	93.0699	-0.46	3.5	C7 H9
98.0730	3187629.0	42.10	98.0726	0.39	2.0	C 6 H 10 O 1
103.0545	297438.2	3.93	103.0542	0.23	5.5	C 8 H 7
105.0693	2099195.2	27.72	105.0699	-0.55	4.5	C 8 H 9
110.0732	2500401.0	33.02	110.0726	0.56	3.0	C7H10O1
117.0694	653039.8	8.62	117.0699	-0.51	5.5	C 9 H 9
118.0769	317712.6	4.20	118.0777	-0.83	5.0	C9H10
123.0813	1245173.6	16.44	123.0804	0.87	3.5	C 8 H 11 O 1
129.0702	489965.2	6.47	129.0699	0.34	6.5	C10H9
136.0878	324532.0	4.29	136.0883	-0.45	4.0	C 9 H 12 O 1
143.0854	608642.2	8.04	143.0855	-0.14	6.5	C11 H11
151.0956	208085.6	2.75	151.0965	-0.86	-0.5	C 6 H 15 O 4
152.0830	213075.6	2.81	152.0832	-0.13	4.0	C9H12O2
156.0927	113225.0	1.50	156.0934	-0.60	7.0	C12 H12
161.0966	801827.0	10.59	161.0961	0.46	5.5	C11 H13 O1
167.1059	3817270.2	50.41	167.1067	-0.77	3.5	C10H15O2
169.1018	114813.8	1.52	169.1012	0.66	7.5	C 13 H 13
170.0938	473145.4	6.25	170.0937	0.06	3.0	C 9 H 14 O 3
188.1191	367556.8	4.85	188.1196	-0.43	6.0	C13H16O1
205.1220	137400.2	1.81	205.1223	-0.34	5.5	C13 H17 O2
219.1380	161551.0	2.13	219.1380	0.06	5.5	C14 H19 O2
227.1277	224370.6	2.96	227.1278	-0.10	3.5	C12 H19 O4
228.1505	377002.8	4.98	228.1509	-0.32	7.0	C16 H20 O1
231.1382	296679.0	3.92	231.1380	0.21	6.5	C15 H19 O2
306.1821	196542.6	2.60	306.1826	-0.42	6.0	C18 H26 O4
324,1925	85932.8	1.13	324.1931	-0.63	5.0	C18 H28 O5

Figure S23. HREIMS spectrum of 3



Figure S24. FTIR spectrum of 3



**Figure S25.** <sup>1</sup>H NMR spectrum of **3** in *Pyridine-d*<sub>5</sub> at 400 MHz



**Figure S26.** <sup>13</sup>C and NMR DEPT spectra of **3** in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S27. HSQC spectrum of 3 in *Pyridine-d*<sub>5</sub>



**Figure S28.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **3** in *Pyridine-d*<sub>5</sub>



Figure S29. HMBC spectrum of 3 in *Pyridine-d*<sub>5</sub>



Figure S30 NOESY spectrum of 3 in Pyridine-d<sub>5</sub>

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Figure S31. <sup>1</sup>H NMR spectrum of 3 in CDCl<sub>3</sub> at 500 MHz



Figure S32. <sup>13</sup>C and NMR DEPT spectra of 3 in CDCl<sub>3</sub> at 125 MHz



Figure S33. HSQC spectrum of 3 in CDCl<sub>3</sub>



Figure S34. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 3 in CDCl<sub>3</sub>



Figure S35. HMBC spectrum of 3 in CDCl<sub>3</sub>



Figure S36. NOESY spectrum of 3 in CDCl<sub>3</sub>

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20170313\_EI\_GYW\_17155\_A10-c1#14 RT: 2.93 T: + c EI Full ms [ 49.50-1000.50] m/z= 48.97-305.15

1/2- 40.2	1 - 202 + 12					
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composit
53.8829	64807.0	2.56	54.0100	-127.10	3.0	C3H2O1
65.0682	84032.0	3.32	65.0386	29.60	3.5	C5H5
77.0376	247335.0	9.78	77.0386	-1.00	4.5	C6H5
78.0450	73103.0	2.89	78.0464	-1.40	4.0	C6H6
79.0534	213582.0	8.44	79.0542	-0.78	3.5	C 6 H 7
81.0689	94523.0	3.74	81.0699	-1.02	2.5	С 6 Н 9
91.0539	667827.0	26.40	91.0542	-0.35	4.5	C7 H7
92.0598	82496.0	3.26	92.0621	-2.25	4.0	C7 H8
93.0697	173903.0	6.87	93.0699	-0.18	3.5	C7H9
94.0772	66695.0	2.64	94.0777	-0.46	3.0	C7 H10
95.0490	80060.0	3.16	95.0491	-0.12	3.5	C6H7O1
95.0854	71369.0	2.82	95.0855	-0.10	2.5	C7H11
97.0641	164027.0	6.48	97.0648	-0.64	2.5	C 6 H 9 O 1
103.0542	119827.0	4.74	103.0542	-0.01	5.5	C 8 H 7
104.0619	96871.0	3.83	104.0621	-0.19	5.0	C 8 H 8
105.0700	1771137.0	70.01	105.0699	0.15	4.5	C 8 H 9
106.0762	304681.0	12.04	106.0777	-1.52	4.0	C 8 H 10
107.0858	172300.0	6.81	107.0855	0.32	3.5	C 8 H 11
108.0932	63622.0	2.51	108.0934	-0.20	3.0	C 8 H 12
115.0539	215930.0	8.54	115.0542	-0.28	6.5	C 9 H 7
116.0608	78897.0	3.12	116.0621	-1.27	6.0	C 9 H 8
117.0698	276041.0	10.91	117.0699	-0.11	5.5	C 9 H 9
118.0771	133675.0	5.28	118.0777	-0.58	5.0	C 9 H 10
119.0856	2529713.0	100.00	119.0855	0.09	4.5	C 9 H 11
120.0924	1076952.0	42.57	120.0934	-0.95	4.0	C9H12
121.0641	97200.0	3.84	121.0648	-0.69	4.5	C 8 H 9 O 1
121.0990	208183.0	8.23	121.1012	-2.14	3.5	C 9 H 13
128.0616	105057.0	4.15	128.0621	-0.48	7.0	C10 H8
129.0693	111355.0	4.40	129.0699	-0.57	6.5	C 10 H 9
131.0854	147325.0	5.82	131.0855	-0.15	5.5	C 10 H 11
132.0926	168591.0	6.66	132.0934	-0.73	5.0	C 10 H 12
133.1007	207634.0	8.21	133.1012	-0.52	4.5	C10 H13
134.1072	118488.0	4.68	134.1090	-1.76	4.0	C 10 H 14
145.0995	72444.0	2.86	145.1012	-1.68	5.5	C 11 H 13
147.1144	93710.0	3.70	147.1168	-2.41	4.5	C 11 H 15
149.1302	87127.0	3.44	149.1325	-2.26	3.5	C11 H17
159.1152	302662.0	11.96	159.1168	-1.59	5.5	C <sub>12</sub> H <sub>15</sub>
161.1313	535074.0	21.15	161.1325	-1.15	4.5	C <sub>12</sub> H <sub>17</sub>
162.1359	70403.0	2.78	162.1403	-4.45	4.0	C <sub>12</sub> H <sub>18</sub>
174.1404	163544.0	6.46	174.1403	0.14	5.0	C 13 H 18
175.1475	656547.0	25.95	175.1481	-0.60	4.5	C 13 H 19
176.1554	939370.0	3713	176.1560	-0.60	4.0	C <sub>13</sub> H <sub>20</sub>
177.1264	558096.0	22.06	177.1274	-1.04	4.5	C12 H17 O1
177.1584	124918.0	4.94	177.1638	-5.36	3.5	C13 H21
178.1325	148181.0	5.86	178.1352	-2.74	4.0	C <sub>12</sub> H <sub>18</sub> O <sub>1</sub>
220.1467	133785.0	5.29	220.1458	0.92	5.0	C14 H20 O2
238.1563	123536.0	4.88	238.1563	-0.09	4.0	C14 H22 O3

Figure S37. HREIMS spectrum of 4



Figure S38. FTIR spectrum of 4



**Figure S39.** <sup>1</sup>H NMR spectrum of **4** in *Pyridine-d*<sub>5</sub> at 500 MHz



Figure S40. <sup>13</sup>C and NMR DEPT spectra of 4 in *Pyridine-d*<sub>5</sub> at 125 MHz



Figure S41. HSQC spectrum of 4 in *Pyridine-d*<sub>5</sub>



**Figure S42.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **4** in *Pyridine-d*<sub>5</sub>



Figure S43. HMBC spectrum of 4 in *Pyridine-d*<sub>5</sub>



Figure S44. NOESY spectrum of 4 in *Pyridine-d*<sub>5</sub>

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T: + C EI	Full ms [ 4	49.50-1000	.50]			
m/z= 48.9	7-302.95				1202220	
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
170.1097	33248.0	0.66	170.1090	0.65	7.0	C 13 H 14
171.1163	123536.0	2.44	171.1168	-0.53	6.5	C13H15
172.1238	133719.0	2.64	172.1247	-0.83	6.0	C13H16
173.0957	82606.0	1.63	173.0961	-0.39	6.5	C <sub>12</sub> H <sub>13</sub> O <sub>1</sub>
173.1323	4782749.0	94.50	173.1325	-0.17	5.5	C13H17
174.1035	54800.0	1.08	174.1039	-0.41	6.0	C12 H14 O1
174.1373	1002071.0	19.80	174.1403	-2.97	5.0	C13H18
175.1114	486945.0	9.62	175.1117	-0.35	5.5	C12 H15 O1
176.1187	470617.0	9.30	176.1196	-0.89	5.0	C <sub>12</sub> H <sub>16</sub> O <sub>1</sub>
177.0928	28091.0	0.56	177.0910	1.83	5.5	C11 H13 O2
177.1267	601659.0	11.89	177.1274	-0.68	4.5	C12 H17 O1
178.0989	101216.0	2.00	178.0988	0.11	5.0	C <sub>11</sub> H <sub>14</sub> O <sub>2</sub>
179.1053	101875.0	2.01	179.1067	-1.33	4.5	C <sub>11</sub> H <sub>15</sub> O <sub>2</sub>
181.1211	120726.0	2.39	181.1223	-1.22	3.5	C <sub>11</sub> H <sub>17</sub> O <sub>2</sub>
183.1156	42510.0	0.84	183.1168	-1.20	7.5	C <sub>14</sub> H <sub>15</sub>
187.1101	36101.0	0.71	187.1117	-1.60	6.5	C <sub>13</sub> H <sub>15</sub> O <sub>1</sub>
189.1249	43014.0	0.85	189.1274	-2.44	5.5	C <sub>13</sub> H <sub>17</sub> O <sub>1</sub>
190.1342	57192.0	1.13	190.1352	-1.05	5.0	C13 H18 O1
191.1416	975472.0	19.27	191.1430	-1.41	4.5	C <sub>13</sub> H <sub>19</sub> O <sub>1</sub>
192.1132	68670.0	1.36	192.1145	-1.33	5.0	C <sub>12</sub> H <sub>16</sub> O <sub>2</sub>
193.1209	47799.0	0.94	193.1223	-1.44	4.5	C <sub>12</sub> H <sub>17</sub> O <sub>2</sub>
194.1286	39810.0	0.79	194.1301	-1.56	4.0	C12 H18 O2
195.1385	26511.0	0.52	195.1380	0.58	3.5	C12 H19 O2
201.1271	290569.0	5.74	201.1274	-0.25	6.5	C14 H17 O1
207.1370	57367.0	1.13	207.1380	-0.97	4.5	C13 H19 O2
216.1498	325991.0	6.44	216.1509	-1.09	6.0	C <sub>15</sub> H <sub>20</sub> O <sub>1</sub>
217.1559	80938.0	1.60	217.1587	-2.84	5.5	C <sub>15</sub> H <sub>21</sub> O <sub>1</sub>
219.1372	228681.0	4.52	219.1380	-0.73	5.5	C14 H19 O2
234.1612	646715.0	12.78	234.1614	-0.22	5.0	C <sub>15</sub> H <sub>22</sub> O <sub>2</sub>
237.1487	137998.0	2.73	237.1485	0.14	4.5	C <sub>14</sub> H <sub>21</sub> O <sub>3</sub>
252.1703	149937.0	2.96	252.1720	-1.70	4.0	C 15 H 24 O 3

Figure S45. HREIMS spectrum of 5





Figure S47. <sup>1</sup>H NMR spectrum of 5 in CDCl<sub>3</sub> at 400 MHz



Figure S48.  $^{13}$ C and NMR DEPT spectra of 5 in CDCl<sub>3</sub> at 100 MHz



Figure S49. HSQC spectrum of 5 in CDCl<sub>3</sub>



Figure S50. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 5 in CDCl<sub>3</sub>







Figure S52. NOESY spectrum of 5 in CDCl<sub>3</sub>

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**Figure S53.** <sup>1</sup>H NMR spectrum of **5** in *Pyridine-d*<sub>5</sub> at 500 MHz


**Figure S54.** <sup>13</sup>C and NMR DEPT spectra of **5** in *Pyridine-d*<sub>5</sub> at 125 MHz



Figure S55. HSQC spectrum of 5 in Pyridine-d<sub>5</sub>



**Figure S56.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **5** in *Pyridine-d*<sub>5</sub>



Figure S57. HMBC spectrum of 5 in *Pyridine-d*<sub>5</sub>







Figure S59. HRESIMS spectrum of 6



Figure S60. FTIR spectrum of 6





Figure S61. <sup>1</sup>H NMR spectrum of 6 in CDCl<sub>3</sub> at 500 MHz



Figure S62. <sup>13</sup>C and NMR DEPT spectra of 6 in CDCl<sub>3</sub> at 125 MHz



Figure S63. HSQC spectrum of 6 in CDCl<sub>3</sub>



Figure S64. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 6 in CDCl<sub>3</sub>



Figure S65. HMBC spectrum of 6 in CDCl<sub>3</sub>



Figure S66. NOESY spectrum of 6 in CDCl<sub>3</sub>



**Figure S67.** <sup>1</sup>H NMR spectrum of **6** in *Pyridine-d*<sub>5</sub> at 400 MHz



Figure S68. <sup>13</sup>C and NMR DEPT spectra of 6 in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S69. HSQC spectrum of 6 in *Pyridine-d*<sub>5</sub>



**Figure S70.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **6** in *Pyridine-d*<sub>5</sub>



Figure S71. HMBC spectrum of 6 in *Pyridine-d*<sub>5</sub>







Figure S73. HRESIMS spectrum of 7



Figure S74. FTIR spectrum of 7



**Figure S75.** <sup>1</sup>H NMR spectrum of **7** in MeOD at 500 MHz



Figure S76.  $^{13}$ C and NMR DEPT spectra of 7 in MeOD at 100 MHz



Figure S77. HSQC spectrum of 7 in MeOD



Figure S78. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 7 in MeOD



Figure S79. HMBC spectrum of 7 in MeOD



Figure S80. NOESY spectrum of 7 in MeOD



**Figure S81.** <sup>1</sup>H NMR spectrum of **7** in *Pyridine-d*<sub>5</sub> at 500 MHz



**Figure S82.** <sup>13</sup>C and NMR DEPT spectra of **7** in *Pyridine-d*<sub>5</sub> at 125 MHz



Figure S83. HSQC spectrum of 7 in *Pyridine-d*<sub>5</sub>



**Figure S84.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **7** in *Pyridine-d*<sub>5</sub>



Figure S85. HMBC spectrum of 7 in *Pyridine-d*<sub>5</sub>



Figure S86. NOESY spectrum of 7 in *Pyridine-d*<sub>5</sub>

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EI-GYW-17159 A21-c1#16-19 RT: 3.34-4.00 AV: 4 T: + c EI Full ms [ 49.50-1000.50] m/z= 47.50-1002.50

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
55.0186	299687.5	27.20	55.0178	0.76	2.5	C 3 H 3 O 1
65.0378	83582.5	7.58	65.0386	-0.74	3.5	C 5 H 5
67.0536	183751.0	16.67	67.0542	-0.58	2.5	C 5 H 7
71.0516	168744.3	15.31	71.0491	2.48	1.5	C4 H7 O1
77.0384	244998.0	22.23	77.0386	-0.19	4.5	C 6 H 5
78.0458	60955.5	5.53	78.0464	-0.64	4.0	C 6 H 6
79.0541	329118.3	29.87	79.0542	-0.12	3.5	C 6 H 7
80.0611	64949.8	5.89	80.0621	-0.96	3.0	СбНа
84.0574	149448.3	13.56	84.0570	0.45	2.0	C 5 H 8 O 1
91.0540	517582.5	46.97	91.0542	-0.26	4.5	C 7 H 7
92.0600	82940.3	7.53	92.0621	-2.01	4.0	C 7 H 8
93.0693	344705.5	31.28	93.0699	-0.59	3.5	C 7 H 9
94.0763	368566.3	33.45	94.0777	-1.43	3.0	C7H10
97.0657	285103.8	25.87	97.0648	0.92	2.5	C 6 H 9 O 1
98.0717	218277.0	19.81	98.0726	-0.92	2.0	C 6 H 10 O 1
101.0589	226617.5	20.56	101.0597	-0.85	1.5	C 5 H 9 O 2
103.0538	71879.3	6.52	103.0542	-0.43	5.5	C 8 H 7
105.0692	438098.3	39.76	105.0699	-0.65	4.5	C 8 H 9
106.0768	201406.8	18.28	106.0777	-0.90	4.0	C 8 H 10
108.0795	84706.3	7.69	108.0781	1.38	-1.0	C4H12O3
111.0787	115502.5	10.48	111.0804	-1.71	2.5	C7H11O1
115.0537	119552.3	10.85	115.0542	-0.48	6.5	C 9 H 7
117.0693	182236.8	16.54	117.0699	-0.57	5.5	C 9 H 9
118.0766	85519.0	7.76	118.0777	-1.14	5.0	C 9 H 10
119.0848	868817.3	78.84	119.0855	-0.73	4.5	C 9 H 11
120.0908	181446.5	16.47	120.0934	-2.59	4.0	C 9 H 12
121.0869	220873.0	20.04	121.0859	1.00	-0.5	C 5 H 13 O 3
129.0699	137131.3	12.44	129.0699	0.04	6.5	C10 H9
130.0772	62217.5	5.65	130.0777	-0.53	6.0	C10 H10
131.0834	247005.3	22.41	131.0855	-2.12	5.5	C10 H11
132.0918	139128.3	12.63	132.0934	-1.57	5.0	C <sub>10</sub> H <sub>12</sub>
137.0936	83746.5	7.60	137.0961	-2.48	3.5	C 9 H 13 O 1
142.0768	72861.3	6.61	142.0777	-0.95	7.0	C11 H10
143.0846	176541.5	16.02	143.0855	-0.93	6.5	C 11 H 11
144.0919	107317.3	9.74	144.0934	-1.47	6.0	C11 H12
147.1037	175131.3	15.89	147.1016	2.16	0.5	C7 H15 O3
149.0586	196830.3	17.86	149.0597	-1.08	5.5	C 9 H 9 O 2
157.1010	166605.5	15.12	157.1012	-0.14	6.5	C 12 H 13
171.1157	154222.0	14.00	171.1168	-1.09	6.5	C 13 H 15
172.1222	83862.0	7.61	172.1247	-2.47	6.0	C13 H16
173.1298	1101970.0	100.00	173.1325	-2.68	5.5	C13 H17
174.1384	983931.3	89.29	174.1403	-1.94	5.0	C13 H18
175.1340	276688.0	25.11	175.1329	1.16	0.5	C 9 H 19 O 3
215.1416	478638.8	43.43	215.1430	-1.41	6.5	C 15 H 19 O 1
230.1653	63155.8	5.73	230.1665	-1.20	6.0	C16 H22 O1
233.1529	497370.0	45.13	233.1536	-0.75	5.5	C15 H21 O2
248.1761	114285.3	10.37	248.1771	-0.95	5.0	C16 H24 O2
251.1633	472938.3	42.92	251.1642	-0.91	4.5	C 15 H 23 O 3
266.1879	65196.8	5.92	266.1876	0.22	4.0	C16 H26 O3

Figure S87. HREIMS spectrum of 8



Figure S88. FTIR spectrum of 8



Figure S89. <sup>1</sup>H NMR spectrum of 8 in CDCl<sub>3</sub> at 600 MHz



Figure S90. <sup>13</sup>C and NMR DEPT spectra of 8 in CDCl<sub>3</sub> at 125 MHz



Figure S91. HSQC spectrum of 8 in CDCl<sub>3</sub>



Figure S92. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 8 in CDCl<sub>3</sub>



Figure S93. HMBC spectrum of 8 in CDCl<sub>3</sub>



Figure S94. NOESY spectrum of 8 in CDCl<sub>3</sub>



**Figure S95.** <sup>1</sup>H NMR spectrum of **8** in *Pyridine-d*<sub>5</sub> at 500 MHz



Figure S96. <sup>13</sup>C and NMR DEPT spectra of 8 in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S97. HSQC spectrum of 8 in *Pyridine-d*<sub>5</sub>



**Figure S98.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **8** in *Pyridine-d*<sub>5</sub>



Figure S99. HMBC spectrum of 8 in *Pyridine-d*<sub>5</sub>







Figure S101. HRESIMS spectrum of 9



Figure S102. FTIR spectrum of 9



Figure S103. <sup>1</sup>H NMR spectrum of 9 in CDCl<sub>3</sub> at 600 MHz



-17.0

Figure S104. <sup>13</sup>C and NMR DEPT spectra of 9 in CDCl<sub>3</sub> at 100 MHz



Figure S105. HSQC spectrum of 9 in CDCl<sub>3</sub>



Figure S106. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 9 in CDCl<sub>3</sub>



Figure S107. HMBC spectrum of 9 in CDCl<sub>3</sub>



Figure S108. NOESY spectrum of 9 in CDCl<sub>3</sub>

## D:\data\2017-HR\EI-17178-GTW\_A12-c1

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EI-17178-GTW\_A12-c1#10 RT: 4.13 T: + c EI Full ms [ 49.50-800.50] m/z= 116.5837-310.8237

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Compositio
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	154 0625	134144 0	5 87	154 0624	0.03	4 0	Ce H10 03
$\begin{array}{c} 137, 1021 \\ 157, 1021 \\ 159, 1166 \\ 631758, 0 \\ 27, 3332246, 0 \\ 14, 54 \\ 159, 0864 \\ -1, 11 \\ 6, 5 \\ C_{11}H_{13} \\ 0, 0863 \\ 149692, 0 \\ 6, 55 \\ 160, 0883 \\ -1, 95 \\ 64, 0820, 0 \\ 28, 22 \\ 161, 0961 \\ -0, 43 \\ 5, 5 \\ C_{11}H_{12} \\ 0, 1142 \\ 0, 11$	155 0721	220747 0	9.66	155 0703	1 79	3.5	Ce H11 03
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	157 1021	730440 0	31 97	157 1012	0.94	6.5	C12 H13
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	159 0793	332246 0	14 54	159.0804	-1 11	6.5	C11 H11 O1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	159 1166	631758 0	27 65	159 1168	-0.24	5.5	C12 H15
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	160 0863	149692 0	6 55	160 0883	-1 95	6.0	C11 H12 O1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	161 0957	644832 0	28 22	161 0961	-0.43	5.5	C11 H12 O1
163.0751282680.012.37163.0754 $0.72$ 5.5 $C10 B11 02$ 163.01110.154.5 $C11 H19 01$ 164.0831123576.05.41164.08320.165.0 $C10 H12 02$ 164.1197403301.017.65164.11960.154.0 $C11 H16 01$ 165.0917391159.017.12165.0910 $0.72$ 4.5 $C10 H12 02$ 165.1284821283.035.94165.1274 $0.99$ 3.5 $C11 H17 01$ 167.0709266683.011.67167.0703 $0.59$ 4.5 $C9 H10 03$ 169.08416350.07.16169.0859 $-0.52$ 3.5 $C9 H12 03$ 169.1010128009.05.60169.1012 $-0.13$ 7.5 $C13 H13$ 171.1178416761.018.24171.1168 $0.96$ $6.5$ $C13 H13$ 173.095231815.013.65173.0961 $-0.93$ $6.5$ $C12 H13 01$ 176.010452291.09.94174.1039 $-1.03$ $6.0$ $C12 H14 01$ 177.1265250686.010.97177.1274 $-0.89$ $4.5$ $C12 H13 02$ 177.1265250686.010.97177.1274 $-0.89$ $4.5$ $C11 H13 02$ 179.1055843640.036.22179.1067 $-1.5$ $5.5$ $C13 H13 02$ 179.1055843640.036.22179.1067 $-1.5$ $5.5$ $C13 H13 02$ 181.1214194246.08.50181.1223 $-0.95$ $3.5$ $C13 H13 02$ 185	161,1319	189106.0	8.28	161,1325	-0.63	4.5	C12 H17
163.1119751384.032.88163.11170.154.5C11 H18 01164.0833123576.05.41164.08320.165.0C10 H12 02164.119740301.017.65164.11960.154.0C11 H16 01165.0917391159.017.12165.09100.724.5C10 H12 02165.1284821283.035.94165.12740.993.5C11 H17 01167.0709266683.011.67167.07030.594.5C9 H103168.0789729187.031.91166.07810.854.0C9 H13 03169.0101128009.05.60169.1012-0.137.5C13 H13171.1174416761.018.24171.11680.966.5C13 H15173.0952311815.013.65173.0961-0.936.5C12 H13 01174.1029227108.09.94174.1039-1.036.0C12 H13 01177.1265250686.010.97177.1274-0.894.5C12 H13 01177.1265250686.010.97177.1274-0.894.5C11 H13 02177.1265250686.010.97177.1274-0.894.5C11 H13 02181.0848259134.011.34181.0859-1.144.5C10 H13 03181.1214194246.08.50181.1223-0.955.5C13 H13 01186.1036133181.05.83186.1039-0.277.0C13 H14 01187.112882786.0<	163.0761	282680.0	12.37	163.0754	0.72	5.5	C10 H11 O2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	163,1119	751384.0	32.88	163.1117	0.15	4.5	C11 H15 O1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	164.0833	123576.0	5.41	164.0832	0.16	5.0	C10 H12 O2
165.0917391159.017.12165.09100.724.5C10H13 O2165.1284821283.035.94165.12740.993.5C1 H13 O1167.0709266683.011.67167.07030.594.5C9 H11 O3168.0789729187.031.91166.07810.854.0C H12 O3169.0854163505.07.16169.0859 $-0.52$ 3.5C H13 O3169.1010128009.05.60169.1012 $-0.13$ 7.5C13 H13171.1178416761.018.24171.11680.966.5C13 H15173.0952311815.013.65173.0961 $-0.93$ 6.5C12 H13 O1174.1029227108.09.94174.1039 $-1.03$ 6.0C12 H14 O1175.1111816541.036.61175.1117 $-0.67$ 5.5C12 H13 O1177.1265250686.010.97177.1274 $-0.89$ 4.5C11 H13 O2177.1265250686.010.97177.1274 $-0.89$ 4.5C11 H13 O2177.1265250686.013.91177.1274 $-0.89$ 4.5C11 H13 O2178.0976137517.06.02178.0988 $-1.23$ 5.0C11 H14 O2179.1055843640.036.92177.1674 $-1.95$ 5.5C11 H13 O3181.1214194246.08.50181.1223 $-0.95$ 3.5C11 H13 O3181.1214194246.08.50181.11711.196.5C13 H13 O1	164,1197	403301.0	17.65	164.1196	0.15	4.0	C11 H16 O1
165.1284821283.035.94165.1274 $0.99$ $3.5$ $C_{11}$ $H_{17}$ $O_{1}$ 167.0709266683.0 $11.67$ $167.0703$ $0.59$ $4.5$ $C_{9}H_{12}O_{3}$ 168.0789729187.0 $31.91$ $168.0781$ $0.85$ $4.0$ $C_{9}H_{12}O_{3}$ 169.0854 $163505.0$ $7.16$ $169.0821$ $-0.13$ $7.5$ $C_{13}H_{13}$ 171.1178 $416761.0$ $18.24$ $171.1168$ $0.96$ $6.5$ $C_{13}H_{13}$ 173.0952 $311815.0$ $13.65$ $173.0961$ $-0.93$ $6.0$ $C_{12}H_{14}O_1$ 174.1029 $227108.0$ $9.94$ $174.1039$ $-1.03$ $6.0$ $C_{12}H_{14}O_1$ 175.1111 $836541.0$ $36.61$ $175.117$ $-0.67$ $5.5$ $C_{11}H_{13}O_2$ 177.1265 $250686.0$ $10.97$ $177.1274$ $-0.89$ $4.5$ $C_{12}H_{17}O_1$ 178.0976 $137517.0$ $6.02$ $178.0986$ $-1.23$ $5.0$ $C_{11}H_{14}O_2$ 179.1055 $843640.0$ $36.92$ $179.1067$ $-1.15$ $4.5$ $C_{11}H_{14}O_2$ 179.1055 $843640.0$ $36.92$ $179.1067$ $-1.15$ $4.5$ $C_{11}H_{10}O_2$ 181.0848 $259134.0$ $11.34$ $181.022$ $-0.95$ $3.5$ $C_{13}H_{13}O_1$ 186.1036 $133181.0$ $5.83$ $186.1039$ $-0.27$ $7.0$ $C_{13}H_{14}O_1$ 187.1129 $862786.0$ $37.76$ $187.117$ $1.95$ $5.5$ $C_{13}H_{10}O_1$ 189.129	165.0917	391159.0	17.12	165.0910	0.72	4.5	C10 H13 O2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	165.1284	821283.0	35.94	165.1274	0.99	3.5	C11 H17 O1
168.0789729187.031.91168.07810.854.0C $_9$ H $_{12}$ O $_3$ 169.0854163505.07.16169.0859 $-0.52$ 3.5C $_9$ H $_{13}$ O $_3$ 169.1010128009.05.60169.1012 $-0.13$ 7.5C $_13$ H $_{13}$ 171.1178416761.018.24171.11680.966.5C $_{12}$ H $_{13}$ O $_1$ 173.0952311815.013.65173.0961 $-0.93$ 6.5C $_{12}$ H $_{14}$ O $_1$ 174.1029227108.09.94174.1039 $-1.03$ 6.5C $_{12}$ H $_{14}$ O $_1$ 175.1111836541.036.61175.1117 $-0.67$ 5.5C $_{11}$ H $_{14}$ O $_2$ 177.1265250686.010.97177.1274 $-0.89$ 4.5C $_{12}$ H $_{14}$ O $_2$ 178.0976137517.06.02178.0988 $-1.23$ 5.0C $_{11}$ H $_{14}$ O $_2$ 179.1055843640.036.92179.1067 $-1.15$ 4.5C $_{11}$ H $_{14}$ O $_2$ 181.0848259134.011.34181.0859 $-1.14$ 4.5C $_{10}$ H $_{13}$ O $_3$ 185.0950224409.09.82185.0961 $-1.06$ 6.0C $_{13}$ H $_{14}$ O $_1$ 187.1129962786.037.76187.1171.196.5C $_{11}$ H $_{12}$ O $_2$ 189.0917117344.05.14189.09100.656.5C $_{12}$ H $_{13}$ O $_2$ 189.1293354860.015.53189.12741.955.5C $_{11}$ H $_{12}$ O $_2$ 193.0876162477.07.11193.0859	167.0709	266683.0	11.67	167.0703	0.59	4.5	C9H11O3
169.0854163505.07.16169.0859 $-0.52$ $3.5$ $C9$ H13 O3169.1010128009.0 $5.60$ 169.1012 $-0.13$ $7.5$ $C_{13}$ H13171.1178416761.018.24171.1168 $0.96$ $6.5$ $C_{12}$ H13 O1173.0952311815.013.65173.0961 $-0.93$ $6.5$ $C_{12}$ H13 O1174.1029227108.0 $9.94$ 174.1039 $-1.03$ $6.0$ $C_{12}$ H14 O1175.1111836541.0 $36.61$ 175.1117 $-0.67$ $5.5$ $C_{11}$ H15 O1177.0901 $451293.0$ $19.75$ $177.0910$ $-0.99$ $4.5$ $C_{11}$ H15 O2177.1265250686.0 $10.97$ $177.1274$ $-0.89$ $4.5$ $C_{12}$ H17 O1178.0976137517.0 $6.02$ $178.0986$ $-1.23$ $5.0$ $C_{11}$ H14 O2179.1055843640.0 $36.92$ $179.1067$ $-1.15$ $4.5$ $C_{11}$ H15 O2181.024194246.0 $8.50$ $181.1223$ $-0.95$ $3.5$ $C_{11}$ H15 O2185.0950224409.0 $9.82$ $186.0039$ $-0.27$ $7.0$ $C_{13}$ H14 O1186.1036133181.0 $5.83$ $186.1039$ $-0.27$ $7.0$ $C_{13}$ H14 O1187.1129 $862786.0$ $37.76$ $187.117$ $1.96$ $6.0$ $C_{13}$ H16 O1189.0917 $117344.0$ $5.44$ $189.0910$ $0.65$ $C_{12}$ H13 O2193.0876 $162477.0$ $7.11$ $193.0859$ $1.71$ $5.5$	168.0789	729187.0	31,91	168.0781	0.85	4.0	C9H12O3
169.1010128009.05.60169.1012 $-0.13$ $7.5$ $C_{13}H_{13}$ 171.1178416761.018.24171.1168 $0.96$ $6.5$ $C_{13}H_{13}$ 173.0952311815.013.65173.0961 $-0.93$ $6.5$ $C_{12}H_{13}$ O1174.1029227108.0 $9.94$ 174.1039 $-1.067$ $5.5$ $C_{12}H_{14}$ O1175.1111836541.0 $36.61$ $175.1117$ $-0.67$ $5.5$ $C_{12}H_{15}$ O1177.0901 $451293.0$ $19.75$ $177.0910$ $-0.90$ $5.5$ $C_{11}H_{13}$ O2177.1265250686.0 $10.97$ $177.1274$ $-0.89$ $4.5$ $C_{12}H_{17}O1$ 178.0976137517.0 $6.02$ $179.1067$ $-1.15$ $4.5$ $C_{11}H_{15}O2$ 181.0848259134.0 $11.34$ $181.0859$ $-1.14$ $4.5$ $C_{10}H_{13}O3$ 181.1214194246.0 $8.50$ $181.1223$ $-0.95$ $3.5$ $C_{11}H_{17}O2$ 185.0950224409.0 $9.82$ $185.0961$ $-1.08$ $7.5$ $C_{13}H_{13}O1$ 186.1036133181.0 $5.83$ $186.1039$ $-0.27$ $7.0$ $C_{13}H_{14}O1$ 187.1129 $862786.0$ $37.76$ $187.1117$ $1.19$ $6.5$ $C_{12}H_{15}O2$ 189.1293 $354860.0$ $15.53$ $189.1274$ $1.95$ $5.5$ $C_{13}H_{15}O2$ 193.0876 $162477.0$ $7.11$ $193.0859$ $1.71$ $5.5$ $C_{11}H_{15}O3$ 203.1067 $316670.0$ $13.82$ $2$	169.0854	163505.0	7.16	169.0859	-0.52	3.5	C 9 H 13 O 3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	169,1010	128009.0	5.60	169.1012	-0.13	7.5	C13 H13
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	171,1178	416761.0	18.24	171.1168	0.96	6.5	C13 H15
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	173.0952	311815.0	13.65	173.0961	-0.93	6.5	C12 H13 O1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	174.1029	227108.0	9,94	174.1039	-1.03	6.0	C12 H14 O1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	175.1111	836541.0	36.61	175.1117	-0.67	5.5	C12 H15 O1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	177.0901	451293.0	19.75	177.0910	-0.90	5.5	C11 H13 O2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	177.1265	250686.0	10.97	177.1274	-0.89	4.5	C12 H17 O1
179.1055843640.036.92179.1067 $-1.15$ $4.5$ $C11$ $H15$ $O2$ 181.0848259134.011.34181.0859 $-1.14$ $4.5$ $C10$ $H13$ $O3$ 181.1214194246.0 $8.50$ 181.1223 $-0.95$ $3.5$ $C11$ $H17$ $O2$ 185.0950224409.0 $9.82$ 185.0961 $-1.08$ $7.5$ $C13$ $H13$ $O1$ 186.1036133181.0 $5.83$ 186.1039 $-0.27$ $7.0$ $C13$ $H16$ $O1$ 187.1129862786.0 $37.76$ 187.1117 $1.19$ $6.5$ $C13$ $H16$ $O1$ 188.1176193057.0 $8.45$ 188.1196 $-1.96$ $6.0$ $C13$ $H16$ $O1$ 189.0917117344.0 $5.14$ 189.0910 $0.65$ $6.5$ $C12$ $H13$ $O2$ 189.1293354860.015.53189.1274 $1.95$ $5.5$ $C13$ $H1.02$ 191.1082273300.011.96191.1067 $1.59$ $5.5$ $C12$ $H15$ $O2$ 193.0876162477.0 $7.11$ 193.0859 $1.71$ $5.5$ $C11$ $H16$ $O1$ 201.195137453.0 $6.02$ 200.1196 $-0.09$ $7.0$ $C14$ $H16$ $O1$ 203.1067315670.013.82203.1067 $0.06$ $6.5$ $C13$ $H16$ $O2$ 205.1212543742.023.80205.1223 $-1.09$ $5.5$ $C13$ $H16$ $O2$ 207.1365	178.0976	137517.0	6.02	178.0988	-1.23	5.0	C11 H14 O2
181.0848259134.011.34181.0859 $-1.14$ 4.5C10 H13 O3181.1214194246.08.50181.1223 $-0.95$ $3.5$ C11 H17 O2185.0950224409.09.82185.0961 $-1.08$ $7.5$ C13 H13 O1186.1036133181.0 $5.83$ 186.1039 $-0.27$ $7.0$ C13 H14 O1187.1129862786.0 $37.76$ 187.1117 $1.19$ $6.5$ C13 H15 O1188.1176193057.0 $8.45$ 188.1196 $-1.96$ $6.0$ C13 H16 O1189.0917117344.0 $5.14$ 189.0910 $0.65$ $6.5$ C12 H13 O2189.1293354860.015.53189.1274 $1.95$ $5.5$ C13 H17 O1191.1082273300.011.96191.1067 $1.59$ $5.5$ C12 H13 O3194.1311219527.0 $9.61$ 194.1301 $0.99$ $4.0$ C12 H18 O2193.0876162477.0 $7.11$ 193.0859 $1.71$ $5.5$ C11 H15 O3200.1195137453.0 $6.02$ 200.1196 $-0.09$ $7.0$ C14 H16 O1203.1067315670.013.82203.1067 $0.06$ $6.5$ C13 H17 O2207.1365168837.0 $7.39$ 207.1380 $-1.47$ $4.5$ C13 H19 O2217.1215662082.028.98217.1223 $-0.83$ $6.5$ C14 H17 O2221.1523270666.011.85221.1536 $-1.26$ $4.5$ C14 H21 O2235.1345327716.014.34235.1329 <t< td=""><td>179.1055</td><td>843640.0</td><td>36,92</td><td>179.1067</td><td>-1.15</td><td>4.5</td><td>C11 H15 O2</td></t<>	179.1055	843640.0	36,92	179.1067	-1.15	4.5	C11 H15 O2
181.1214194246.08.50181.1223 $-0.95$ 3.5 $C_{11} H_{17} O_2$ 185.0950224409.09.82185.0961 $-1.08$ $7.5$ $C_{13} H_{13} O_1$ 186.1036133181.05.83186.1039 $-0.27$ $7.0$ $C_{13} H_{14} O_1$ 187.1129862786.037.76187.1117 $1.19$ $6.5$ $C_{13} H_{16} O_1$ 188.1176193057.08.45188.1196 $-1.96$ $6.0$ $C_{13} H_{16} O_1$ 189.0917117344.05.14189.0910 $0.65$ $6.5$ $C_{12} H_{13} O_2$ 189.1293354860.015.53189.1274 $1.95$ $5.5$ $C_{11} H_{15} O_2$ 193.0876162477.07.11193.0859 $1.71$ $5.5$ $C_{11} H_{15} O_2$ 193.0876162477.07.11193.0859 $1.71$ $5.5$ $C_{11} H_{15} O_2$ 195.1031136778.0 $5.99$ 195.1016 $1.53$ $4.5$ $C_{11} H_{15} O_3$ 200.1195137453.0 $6.02$ 200.1196 $-0.09$ $7.0$ $C_{14} H_{16} O_1$ 203.1067315670.0 $13.82$ 203.1067 $0.06$ $6.5$ $C_{13} H_{17} O_2$ 207.1365168837.0 $7.39$ $207.1380$ $-1.47$ $4.5$ $C_{14} H_{17} O_2$ 217.1215 $662082.0$ $28.98$ $21.1172$ $-0.43$ $5.5$ $C_{14} H_{17} O_2$ 211.1523 $270666.0$ $11.85$ $221.1536$ $-1.26$ $4.5$ $C_{14} H_{19} O_3$ 245.1173380365.0 $16.65$ <	181.0848	259134.0	11.34	181.0859	-1.14	4.5	C10 H13 O3
185.0950224409.09.82185.0951 $-1.08$ 7.5C13 H13 O1186.1036133181.05.83186.1039 $-0.27$ 7.0C13 H14 O1187.1129862786.037.76187.11171.196.5C13 H15 O1188.1176193057.08.45188.1196 $-1.96$ 6.0C13 H16 O1189.0917117344.05.14189.09100.656.5C12 H13 O2189.1293354860.015.53189.12741.955.5C13 H17 O1191.1082273300.011.96191.10671.595.5C1 H13 O3194.1311219527.09.61194.13010.994.0C12 H18 O2195.1031136778.05.99195.10161.534.5C11 H15 O3200.1195137453.06.02200.1196 $-0.09$ 7.0C14 H16 O1203.1067315670.013.82203.10670.066.5C13 H17 O2207.136516887.07.39207.1380 $-1.47$ 4.5C14 H17 O2217.1215662082.028.98217.1223 $-0.83$ 6.5C14 H17 O2225.1345327716.014.34235.13291.595.5C15 H17 O3245.1173380365.016.65245.11720.087.5C15 H17 O3249.1483342300.014.98249.1485 $-0.19$ 5.5C14 H19 O3264.1347218081.09.54264.1356 $-0.88$ 6.0C15 H20 O4277.152 <td>181,1214</td> <td>194246.0</td> <td>8.50</td> <td>181,1223</td> <td>-0.95</td> <td>3.5</td> <td>C11 H17 O2</td>	181,1214	194246.0	8.50	181,1223	-0.95	3.5	C11 H17 O2
186.1036133181.05.83186.1039 $-0.27$ $7.0$ $C_{13}$ H <sub>14</sub> O <sub>1</sub> 187.1129862786.037.76187.11171.19 $6.5$ $C_{13}$ H <sub>15</sub> O <sub>1</sub> 188.1176193057.08.45188.1196 $-1.96$ $6.0$ $C_{13}$ H <sub>16</sub> O <sub>1</sub> 189.0917117344.05.14189.0910 $0.65$ $6.5$ $C_{12}$ H <sub>13</sub> O <sub>2</sub> 189.1293354860.015.53189.12741.95 $5.5$ $C_{13}$ H <sub>17</sub> O <sub>1</sub> 191.1082273300.011.96191.10671.59 $5.5$ $C_{12}$ H <sub>15</sub> O <sub>2</sub> 193.0876162477.07.11193.08591.71 $5.5$ $C_{11}$ H <sub>18</sub> O <sub>2</sub> 195.1031136778.0 $5.99$ 195.10161.53 $4.5$ $C_{11}$ H <sub>16</sub> O <sub>1</sub> 203.1067315670.013.82203.1067 $0.06$ $6.5$ $C_{13}$ H <sub>16</sub> O <sub>2</sub> 205.1212543742.023.80205.1223 $-1.09$ $5.5$ $C_{13}$ H <sub>17</sub> O <sub>2</sub> 207.1365168837.0 $7.39$ 207.1380 $-1.47$ $4.5$ $C_{13}$ H <sub>19</sub> O <sub>2</sub> 217.1215662082.028.98217.1223 $-0.83$ $6.5$ $C_{14}$ H <sub>17</sub> O <sub>2</sub> 221.1168188111.0 $8.23$ 221.1172 $-0.43$ $5.5$ $C_{14}$ H <sub>19</sub> O <sub>3</sub> 245.1173380365.016.65245.1172 $0.08$ $7.5$ $C_{15}$ H <sub>17</sub> O <sub>3</sub> 249.1483342300.014.98249.1485 $-0.19$ $5.5$ $C_{14}$ H <sub>19</sub> O <sub>3</sub> 249.1483342300.014.98249.1485 $-0$	185.0950	224409.0	9.82	185.0961	-1.08	7.5	C13 H13 O1
187.1129862786.037.76187.11171.196.5C13 H15 01188.1176193057.08.45188.1196 $-1.96$ 6.0C13 H16 01189.0917117344.05.14189.09100.656.5C12 H13 02189.1293354860.015.53189.12741.955.5C13 H17.01191.1082273300.011.96191.10671.595.5C12 H15 02193.0876162477.07.11193.08591.715.5C11 H13 03194.1311219527.09.61194.13010.994.0C12 H16 02195.1031136778.05.99195.10161.534.5C11 H15 03200.1195137453.06.02200.1196 $-0.09$ 7.0C14 H16 01203.1067315670.013.82203.10670.066.5C13 H17 02207.1365168837.07.39207.1380 $-1.47$ 4.5C13 H19 02217.1215662082.028.98217.1223 $-0.83$ 6.5C14 H17 02221.1168188111.08.23221.1172 $-0.43$ 5.5C13 H17 03221.1523270666.011.85221.1536 $-1.26$ $4.5$ C14 H21 02235.1345327716.014.34235.13291.595.5C14 H19 03245.1173380365.016.65245.11720.087.5C15 H17 03249.1483342300.014.98249.1485 $-0.19$ 5.5C15 H21 03261.1486	186,1036	133181.0	5.83	186.1039	-0.27	7.0	C13 H14 O1
$188.1176$ $193057.0$ $8.45$ $188.1196$ $-1.96$ $6.0$ $C_{13}H_{16}O_{1}$ $189.0917$ $117344.0$ $5.14$ $189.0910$ $0.65$ $6.5$ $C_{12}H_{13}O_{2}$ $189.1293$ $354860.0$ $15.53$ $189.1274$ $1.95$ $5.5$ $C_{13}H_{12}O_{1}$ $191.1082$ $273300.0$ $11.96$ $191.1067$ $1.59$ $5.5$ $C_{12}H_{15}O_{2}$ $193.0876$ $162477.0$ $7.11$ $193.0859$ $1.71$ $5.5$ $C_{11}H_{13}O_{3}$ $194.1311$ $219527.0$ $9.61$ $194.1301$ $0.99$ $4.0$ $C_{12}H_{18}O_{2}$ $195.1031$ $136778.0$ $5.99$ $195.1016$ $1.53$ $4.5$ $C_{11}H_{15}O_{3}$ $200.1195$ $137453.0$ $6.02$ $200.1196$ $-0.09$ $7.0$ $C_{14}H_{16}O_{1}$ $203.1067$ $315670.0$ $13.82$ $203.1067$ $0.06$ $6.5$ $C_{13}H_{17}O_{2}$ $207.1365$ $16837.0$ $7.39$ $207.1380$ $-1.47$ $4.5$ $C_{13}H_{19}O_{2}$ $217.1215$ $662082.0$ $28.98$ $217.1223$ $-0.83$ $6.5$ $C_{14}H_{17}O_{2}$ $221.1168$ $188111.0$ $8.23$ $221.1172$ $-0.43$ $5.5$ $C_{14}H_{19}O_{3}$ $245.1173$ $380365.0$ $16.65$ $245.1172$ $0.08$ $7.5$ $C_{15}H_{17}O_{3}$ $245.1173$ $380365.0$ $16.65$ $245.1172$ $0.08$ $7.5$ $C_{15}H_{19}O_{3}$ $249.1483$ $342300.0$ $14.98$ $249.1485$ $-0.19$ <t< td=""><td>187,1129</td><td>862786.0</td><td>37.76</td><td>187,1117</td><td>1.19</td><td>6.5</td><td>C13H15O1</td></t<>	187,1129	862786.0	37.76	187,1117	1.19	6.5	C13H15O1
189.0917       117344.0       5.14       189.0910       0.65       6.5       C12 H13 O2         189.1293       354860.0       15.53       189.1274       1.95       5.5       C13 H17,O1         191.1082       273300.0       11.96       191.1067       1.59       5.5       C12 H13 O2         193.0876       162477.0       7.11       193.0859       1.71       5.5       C11 H13 O3         194.1311       219527.0       9.61       194.1301       0.99       4.0       C12 H18 O2         195.1031       136778.0       5.99       195.1016       1.53       4.5       C11 H15 O3         200.1195       137453.0       6.02       200.1196       -0.09       7.0       C14 H16 O1         203.1067       315670.0       13.82       203.1067       0.06       6.5       C13 H15 O2         207.1365       168837.0       7.39       207.1380       -1.47       4.5       C13 H19 O2         217.1215       662082.0       28.98       217.1223       -0.83       6.5       C14 H17 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65       24	188,1176	193057.0	8,45	188,1196	-1.96	6.0	C13 H16 O1
189.1293       354860.0       15.53       189.1274       1.95       5.5       C13 H17 O1         191.1082       273300.0       11.96       191.1067       1.59       5.5       C12 H15 O2         193.0876       162477.0       7.11       193.0859       1.71       5.5       C11 H13 O3         194.1311       219527.0       9.61       194.1301       0.99       4.0       C12 H18 O2         195.1031       136778.0       5.99       195.1016       1.53       4.5       C11 H15 O3         200.1195       137453.0       6.02       200.1196       -0.09       7.0       C14 H16 O1         203.1067       315670.0       13.82       203.1067       0.06       6.5       C13 H17 O2         205.1212       543742.0       23.80       205.1223       -1.09       5.5       C13 H17 O2         207.1365       168837.0       7.39       207.1380       -1.47       4.5       C13 H19 O2         217.1215       662082.0       28.98       217.1223       -0.83       6.5       C14 H17 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65	189.0917	117344.0	5.14	189.0910	0.65	6.5	C12 H13 O2
191.1082273300.011.96191.10671.595.5C12 H15 O2193.0876162477.07.11193.08591.715.5C11 H13 O3194.1311219527.09.61194.13010.994.0C12 H18 O2195.1031136778.05.99195.10161.534.5C11 H15 O3200.1195137453.06.02200.1196-0.097.0C14 H16 O1203.1067315670.013.82203.10670.066.5C13 H15 O2205.1212543742.023.80205.1223-1.095.5C13 H17 O2207.1365168837.07.39207.1380-1.474.5C13 H19 O2217.1215662082.028.98217.1223-0.836.5C14 H17 O2221.1168188111.08.23221.1172-0.435.5C13 H17 O3221.1523270666.011.85221.1536-1.264.5C14 H21 O2235.1345327716.014.34235.13291.595.5C14 H19 O3245.1173380365.016.65245.11720.087.5C15 H17 O3249.1483342300.014.98249.1485-0.195.5C16 H21 O3264.1347218081.09.54264.1356-0.886.0C15 H20 O4278.15322284894.0100.00278.15131.976.0C16 H22 O4296.1623124379.05.44296.16180.455.0C16 H24 O5	189.1293	354860.0	15.53	189.1274	1.95	5.5	C13 H17 O1
193.0876162477.07.11193.08591.715.5C11 H13 O3194.1311219527.09.61194.13010.994.0C12 H18 O2195.1031136778.05.99195.10161.534.5C11 H15 O3200.1195137453.06.02200.1196-0.097.0C14 H16 O1203.1067315670.013.82203.10670.066.5C13 H15 O2205.1212543742.023.80205.1223-1.095.5C13 H17 O2207.1365168837.07.39207.1380-1.474.5C13 H19 O2217.1215662082.028.98217.1223-0.836.5C14 H17 O2221.1168188111.08.23221.1172-0.435.5C13 H17 O3221.1523270666.011.85221.1536-1.264.5C14 H21 O2235.1345327716.014.34235.13291.595.5C15 H17 O3249.1483342300.014.98249.1485-0.195.5C15 H21 O3261.1486184738.08.09261.14850.126.5C16 H21 O3264.1347218081.09.54264.1356-0.886.0C15 H20 O4278.15322284894.0100.00278.15131.976.0C16 H22 O4296.1623124379.05.44296.16180.455.0C16 H24 O5	191.1082	273300.0	11.96	191.1067	1.59	5.5	C12 H15 O2
194.1311219527.09.61194.13010.994.0C12 H18 O2195.1031136778.05.99195.10161.534.5C11 H15 O3200.1195137453.06.02200.1196-0.097.0C14 H16 O1203.1067315670.013.82203.10670.066.5C13 H15 O2205.1212543742.023.80205.1223-1.095.5C13 H17 O2207.1365168837.07.39207.1380-1.474.5C13 H19 O2217.1215662082.028.98217.1223-0.836.5C14 H17 O2221.1168188111.08.23221.1172-0.435.5C13 H17 O3221.1523270666.011.85221.1536-1.264.5C14 H21 O2235.1345327716.014.34235.13291.595.5C14 H19 O3245.1173380365.016.65245.11720.087.5C15 H17 O3249.1483342300.014.98249.1485-0.195.5C16 H21 O3261.1486184738.08.09261.14850.126.5C16 H21 O3264.1347218081.09.54264.1356-0.886.0C15 H20 O4278.15322284894.0100.00278.15131.976.0C16 H22 O4296.1623124379.05.44296.16180.455.0C16 H24 O5	193.0876	162477.0	7.11	193.0859	1.71	5.5	C11 H13 O3
195.1031136778.05.99195.10161.534.5C11 H15 O3200.1195137453.06.02200.1196-0.097.0C14 H16 O1203.1067315670.013.82203.10670.066.5C13 H15 O2205.1212543742.023.80205.1223-1.095.5C13 H17 O2207.1365168837.07.39207.1380-1.474.5C13 H19 O2217.1215662082.028.98217.1223-0.836.5C14 H17 O2221.1168188111.08.23221.1172-0.435.5C13 H17 O3221.1523270666.011.85221.1536-1.264.5C14 H21 O2235.1345327716.014.34235.13291.595.5C14 H19 O3245.1173380365.016.65245.11720.087.5C15 H17 O3249.1483342300.014.98249.1485-0.195.5C16 H21 O3261.1486184738.08.09261.14850.126.5C16 H21 O3264.1347218081.09.54264.1356-0.886.0C15 H20 O4278.15322284894.0100.00278.15131.976.0C16 H22 O4296.1623124379.05.44296.16180.455.0C16 H24 O5	194.1311	219527.0	9.61	194.1301	0.99	4.0	C12 H18 O2
200.1195       137453.0       6.02       200.1196       -0.09       7.0       C14 H16 O1         203.1067       315670.0       13.82       203.1067       0.06       6.5       C13 H15 O2         205.1212       543742.0       23.80       205.1223       -1.09       5.5       C13 H17 O2         207.1365       168837.0       7.39       207.1380       -1.47       4.5       C13 H19 O2         217.1215       662082.0       28.98       217.1223       -0.83       6.5       C14 H17 O2         221.1168       188111.0       8.23       221.1172       -0.43       5.5       C13 H17 O3         221.1523       270666.0       11.85       221.1536       -1.26       4.5       C14 H21 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       <	195.1031	136778.0	5.99	195.1016	1.53	4.5	C11 H15 O3
203.1067       315670.0       13.82       203.1067       0.06       6.5       C13 H15 O2         205.1212       543742.0       23.80       205.1223       -1.09       5.5       C13 H17 O2         207.1365       168837.0       7.39       207.1380       -1.47       4.5       C13 H19 O2         217.1215       662082.0       28.98       217.1223       -0.83       6.5       C14 H17 O2         221.1168       188111.0       8.23       221.1172       -0.43       5.5       C13 H17 O3         221.1523       270666.0       11.85       221.1536       -1.26       4.5       C14 H21 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C15 H17 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00	200.1195	137453.0	6.02	200.1196	-0.09	7.0	C14 H16 O1
205.1212       543742.0       23.80       205.1223       -1.09       5.5       C13 H17 O2         207.1365       168837.0       7.39       207.1380       -1.47       4.5       C13 H19 O2         217.1215       662082.0       28.98       217.1223       -0.83       6.5       C14 H17 O2         221.1168       188111.0       8.23       221.1172       -0.43       5.5       C13 H17 O3         221.1523       270666.0       11.85       221.1536       -1.26       4.5       C14 H21 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C15 H17 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44	203.1067	315670.0	13.82	203.1067	0.06	6.5	C13 H15 O2
207.1365       168837.0       7.39       207.1380       -1.47       4.5       C13 H19 O2         217.1215       662082.0       28.98       217.1223       -0.83       6.5       C14 H17 O2         221.1168       188111.0       8.23       221.1172       -0.43       5.5       C13 H17 O3         221.1523       270666.0       11.85       221.1536       -1.26       4.5       C14 H21 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	205.1212	543742.0	23.80	205.1223	-1.09	5.5	C13 H17 O2
217.1215       662082.0       28.98       217.1223       -0.83       6.5       C14 H17 O2         221.1168       188111.0       8.23       221.1172       -0.43       5.5       C13 H17 O3         221.1523       270666.0       11.85       221.1536       -1.26       4.5       C14 H21 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	207.1365	168837.0	7.39	207.1380	-1.47	4.5	C13 H19 O2
221.1168       188111.0       8.23       221.1172       -0.43       5.5       C13 H17 O3         221.1523       270666.0       11.85       221.1536       -1.26       4.5       C14 H21 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	217.1215	662082.0	28.98	217.1223	-0.83	6.5	C14 H17 O2
221.1523       270666.0       11.85       221.1536       -1.26       4.5       C14 H21 O2         235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	221.1168	188111.0	8.23	221.1172	-0.43	5.5	C13 H17 O3
235.1345       327716.0       14.34       235.1329       1.59       5.5       C14 H19 O3         245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C16 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	221.1523	270666.0	11.85	221.1536	-1.26	4.5	C14 H21 O2
245.1173       380365.0       16.65       245.1172       0.08       7.5       C15 H17 O3         249.1483       342300.0       14.98       249.1485       -0.19       5.5       C15 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	235.1345	327716.0	14.34	235.1329	1.59	5.5	C14 H19 O3
249.1483       342300.0       14.98       249.1485       -0.19       5.5       C15 H21 O3         261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	245.1173	380365.0	16.65	245.1172	0.08	7.5	C15 H17 O3
261.1486       184738.0       8.09       261.1485       0.12       6.5       C16 H21 O3         264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	249.1483	342300.0	14.98	249.1485	-0.19	5.5	C15 H21 O3
264.1347       218081.0       9.54       264.1356       -0.88       6.0       C15 H20 O4         278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	261.1486	184738.0	8.09	261.1485	0.12	6.5	C16 H21 O3
278.1532       2284894.0       100.00       278.1513       1.97       6.0       C16 H22 O4         296.1623       124379.0       5.44       296.1618       0.45       5.0       C16 H24 O5	264.1347	218081.0	9.54	264.1356	-0.88	6.0	C15 H20 O4
296,1623 124379.0 5.44 296,1618 0.45 5.0 C16 H24 O5	278,1532	2284894.0	100.00	278.1513	1.97	6.0	C16 H22 O4
	296.1623	124379.0	5.44	296.1618	0.45	5.0	C16 H24 O5

Figure S109. HREIMS spectrum of 10



Figure S110. FTIR spectrum of 10



**Figure S111.** <sup>1</sup>H NMR spectrum of **10** in CDCl<sub>3</sub> at 600 MHz



Figure S112.  $^{13}$ C and NMR DEPT spectra of 10 in CDCl<sub>3</sub> at 100 MHz



Figure S113. HSQC spectrum of 10 in CDCl<sub>3</sub>



Figure S114. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 10 in CDCl<sub>3</sub>



Figure S115. HMBC spectrum of 10 in CDCl<sub>3</sub>

zw-syz-al2 NOESY



Figure S116. NOESY spectrum of 10 in CDCl<sub>3</sub>



Figure S117. ESIMS spectrum of 11

Elemen	tal Compo	sition	Report									Page 1
Single I Tolerance Element Number	Mass Analy e = 10.0 PP prediction: ( of isotope pe	<b>ysis</b> M / D Off eaks use	BE: min ed for i-F	= -1.5, i IT = 3	max = 50	).0						
Monoisoto 28 formula Elements	opic Mass, Ev a(e) evaluate Used:	ven Elect d with 2 i	ron lons results wit	thin limit	s (up to 5	0 clo	sest re	sults for eac	h mass)			
SIPI	11. 1-40 0	. 14	140. 1-1	01. 0	•	Q-	Tof micr	0			10:31:	34,23-Mar-2017
AN7						-	YA019			00.400		TOPNO FR
Q17-0395	HR1 102 (1.891	<ol> <li>AM (Ce</li> </ol>	n,4, 80.00,	Ar,5000.	0,383.16,1	.00);	Sm (SG	, 2x3.00); Sb	(1,40.00); Cm	(99:108)		1.12e+004
100						3	41.1521					
100												
0/												
70												
												mlz
0	340.9	00	341.0	00	341.1	00		341.200	341.300	)	341.400	117.84
Minimum: Maximum:		5.0	10.0	-1.5 50.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	F	ormula					
341.1521	341.1517 341.1498	0.4	1.2 7.3	11.5 2.5	rı∕a n∕a	C	22 H22 16 H27	02 Na 04 Na CI				

Figure S118. HRESIMS spectrum of 11



Figure S119. FTIR spectrum of 11



Figure S120. <sup>1</sup>H NMR spectrum of 11 in *Pyridine-d*<sub>5</sub> at 400 MHz



Figure S121. <sup>13</sup>C and NMR DEPT spectra of 11 in *Pyridine-d*<sub>5</sub> at 100 MHz


Figure S122. HSQC spectrum of 11 in *Pyridine-d*<sub>5</sub>



**Figure S123.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **11** in *Pyridine-d*<sub>5</sub>



Figure S124. HMBC spectrum of 11 in Pyridine-d<sub>5</sub>



Figure S125. NOESY spectrum of 11 in Pyridine-d<sub>5</sub>







Figure S127. HRESIMS spectrum of 12



Figure S128. FTIR spectrum of 12



**Figure S129.** <sup>1</sup>H NMR spectrum of **12** in *Pyridine-d*<sub>5</sub> at 400 MHz





Figure S130. <sup>13</sup>C and NMR DEPT spectra of 12 in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S131. HSQC spectrum of 12 in Pyridine-d<sub>5</sub>



**Figure S132.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **12** in *Pyridine-d*<sub>5</sub>



Figure S133. HMBC spectrum of 12 in Pyridine-d<sub>5</sub>







Figure S135. ESIMS spectrum of 13

Elemen	ital Comp	position	Report						5	42 .	Pa 1 5 -Pa	ge 1
Single Tolerand Element Number	Mass Ana ce = 10.0 P prediction of isotope	alysis PM / [ Off peaks us	DBE: min sed for i-F	= -1.5, IT = 3	max = 5(	0.0				8	4 E 40.	
Vono soti 20 formul Elements C: 1-30	opic Mass, la(e) evalua Used: H: 1-40	Even Elected with 2	tron lons results wit Na: 1-1	thin limi CI: 0-	ts (up to 5	0 closest re	sults for	each mas	ss)			
SIPI						Q-Tof micr	0				10:52:24,23-Ma	r-2017
A7 Q17-0395	HR 37 (0.685	i) AM (Cen	,4, 80.00, Ar	r,5000.0	,383.16,1.0	YA019 0); Sm (SG, 2	x3.00); S	b (1,40.00	); Cm (6:40)		TOF MS	SES+
100 .								311.138	7		0.02	01004
%												
				310.8	8661							m/7
3	10.600	310.700	310.80	00	310.900	311.000	31	1.100	311.200	311.300	311,400	111/2
Minimum: Maorimum:		5.0	10.0	-1.5 50.0								
Masss	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula						
311.1387	311.1390 311.1412	-0.3 -2.5	-1.0 -8.0	2.5 11.5	n∕a n∕a	C15 H25 C21 H20	03 Na 0 Na	01				

Figure S136. HRESIMS spectrum of 13



Figure S137. FTIR spectrum of 13



Figure S138. <sup>1</sup>H NMR spectrum of 13 in *Pyridine-d*<sub>5</sub> at 400 MHz



Figure S139. <sup>13</sup>C and NMR DEPT spectra of 13 in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S140. HSQC spectrum of 13 in *Pyridine-d*<sub>5</sub>



Figure S141. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 13 in *Pyridine-d*<sub>5</sub>



Figure S142. HMBC spectrum of 13 in *Pyridine-d*<sub>5</sub>



Figure S143. NOESY spectrum of 13 in *Pyridine-d*<sub>5</sub>

	3/14/2017 10:32:46 AM								
D:\data\\EI-GYW	V-17157_A14-c1		G1 1.11						
D:Wata\_WEI-GYW EI-GYW-17: T: + c EI m/z= 47.5 m/z 191.1423 192.1134 195.1143 199.1092 201.1246 208.1448 215.1404 216.1508 218.1638 219.1398	V-17157_A14-c1 157_A14-c1# Full ms [ 4 0-1002.50 Intensity 3337866.0 8383.0 5157.0 10797.0 147677.0 36957.0 10622.0 136155.0 4235.0 76900.0	13 RT: 2.6 19.50-1000 Relative 60.74 0.15 0.09 0.20 2.69 0.67 0.19 2.48 0.08 1.40	3/14/ 7 .50] Theo. Mass 191.1430 192.1145 195.1168 199.1117 201.1274 208.1458 215.1430 216.1509 218.1665 219.1380 230.1458	Delta (mmu) -0.71 -1.08 -2.48 -2.58 -2.76 -0.96 -2.65 -0.11 -2.75 1.84	RDB equiv. 4.5 5.0 8.5 7.5 6.5 4.0 6.5 6.0 5.0 4.0 6.5 6.0 5.0	Composition C 13 H 19 O1 C 12 H 16 O2 C 15 H 15 C 14 H 15 O1 C 14 H 17 O1 C 13 H 20 O2 C 15 H 19 O1 D C 15 H 20 O1 D C 15 H 22 O1 5 C 14 H 19 O2 O C 14 H 20 O2			
219.1398 220.1470 233.1555 234.1599 237.1486 252 1696	8317.0 11126.0 99417.0 39942.0 145175.0	0.15 0.20 1.81 0.73 2.64	220.1458 233.1536 234.1614 237.1485 252.1720	1.18 1.8 -1.5 0.0 -2.4	3 5. 7 5. 4 5. 9 4. 5 4.	0 C14 H20 02 5 C15 H21 02 0 C15 H22 02 5 C14 H21 03 0 C15 H24 03			

Figure S144. HREIMS spectrum of 14



Figure S145. FTIR spectrum of 14



Figure S146. <sup>1</sup>H NMR spectrum of 14 in *Pyridine-d*<sub>5</sub> at 400 MHz



Figure S147. <sup>13</sup>C and NMR DEPT spectra of 14 in *Pyridine-d*<sub>5</sub> at 100 MHz



Figure S148. HSQC spectrum of 14 in *Pyridine-d*<sub>5</sub>



**Figure S149.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **14** in *Pyridine-d*<sub>5</sub>







Figure S151. NOESY spectrum of 14 in *Pyridine-d*<sub>5</sub>



Figure S152. <sup>1</sup>H NMR spectrum of 14 in CDCl<sub>3</sub> at 500 MHz



Figure S153. <sup>13</sup>C and NMR DEPT spectra of 14 in CDCl<sub>3</sub> at 125 MHz



Figure S154. HSQC spectrum of 14 in CDCl<sub>3</sub>



Figure S155. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 14 in CDCl<sub>3</sub>



Figure S156. HMBC spectrum of 14 in CDCl<sub>3</sub>



Figure S157. NOESY spectrum of 14 in CDCl<sub>3</sub>

0170312_1	7031310265	4-c1#12 F	T: 2.45		- Carlos	
': + C EI 1	Full ms [ 4	49.50-100	0.50]			
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB	Composition
175.1471	718600.0	26.96	175.1481	-0.98	4.5	C12 H10
176.1177	218300.0	8.19	176,1196	-1.88	5.0	Ciallico
176.1515	103854.0	3.90	176,1560	-4 49	1.0	
177.1272	395963.0	14.86	177 1274	-0.10	4.0	C 13 H 20
178.0975	44777.0	1.68	178 0988	-1 20	4.0	C 12 H 17 01
178.1318	74290.0	2.79	178 1352	-1.29	5.0	C11 H14 02
179.1062	103727.0	3.89	179 1067	-0.40	4.0	C 12 H 18 O 1
179.1429	124605.0	-4 68	179.1007	-0.49	4.5	C11 H15 O2
180,1151	1627766 0	61 09	19.1430	-0.13	3.5	C12 H19 O1
181.1201	330511 0	12 40	100.1145	0.66	4.0	C11 H16 O2
185.0947	42440 0	1 50	101.1223	-2.19	3.5	C11 H17 O2
185,1319	214846 0	9.00	185.0961	-1.41	7.5	C13 H13 O1
186,1028	47444 0	1 70	105.1325	-0.55	6.5	C14 H17
186,1388	97631 0	1.78	186.1039	-1.10	7.0	C13 H14 O1
187,1112	117544 0	3.00	100.1403	-1.53	6.0	C14 H18
187.1463	51432 0	1.41	107.1117	-0.54	6.5	C13 H15 O1
188.1187	95777 0	3.50	107.1481	-1.80	5.5	C14 H19
189.1274	646062 0	24.24	100.1196	-0.84	6.00	C13 H16 O1
190.1345	411989 0	15 /6	109.1274	-0.03	5.5	C13 H17 O1
191,1063	41932 0	1 57	190.1352	-0.67	5.00	C13 H18 O1
191.1435	2665067.0	100.00	191 1430	-0.39	5.50	C12 H15 O2
192.1473	551148.0	20.68	192 1509	-3 53	4.50	C 13 H 19 O 1
193.1221	46530.0	1.75	193,1223	-0.24	4.00	
193.1553	80564.0	3.02	193,1587	-3 39	3.50	C12 Hay Or
195.1375	69617.0	2.61	195.1380	-0.47	3.50	C12 H10 O2
199.1110	42618.0	1.60	199.1117	-0.79	7.50	C14 H15 O1
201.1266	177383.0	6.66	201.1274	-0.81	6.50	C14 H17 O1
202.1332	86101.0	3.23	202.1352	-2.04	6.00	C14 H18 O1
203.1059	42085.0	1.58	203.1067	-0.72	6.5 0	C13 H15 O2
203.1429	584597.0	21.94	203.1430	-0.14	5.5 0	C14 H19 O1
204.1488	144797.0	5.43	204.1509	-2.05	5.00	C14 H20 O1
205.1218	183148.0	6.87	205.1223	-0.55	5.5 C	C13 H17 O2
206.1283	62454.0	2.34	206.1301	-1.83	5.00	C13 H18 O2
207.1378	240854.0	9.04	207.1380	-0.19	4.5 C	C13 H19 O2
208.1429	51051.0	1.92	208.1458	-2.89	4.00	13 H20 O2
209.1545	117696.0	4.42	209.1536	0.90	3.50	13 H21 O2
210.1231	45082.0	1.69	210.1250	-1.96	4.00	12 H 18 O 3
215.1251	103524 0	3.0/	215.1274	-2.32	6.50	15 11701
216.1485	75941 0	2 85	216,1509	-2.33	6.00	15 H 20 Q 1
219,1377	178526.0	6.70	219.1380	-0.26	5.5 0	14 H19 O2
220.1433	55216.0	2.07	220.1458	-2.52	5.0 C	14 H 20 O 2
221.1538	197778.0	7.42	221.1536	0.19	4.5 C	14 H21 O2
228.1509	153711.0	5.77	228.1509	0.04	7.0 C	16 H 20 O1
229.1572	60245.0	2.26	229.1587	-1.50	6.5 C	16 H21 O1
230.1662	83535.0	3.13	230.1665	-0.32	6.0 C	16 H 22 O 1
231.1377	86304.0	3.24	231.1380	-0.23	6.5 C	15 H 19 O2
232.1446	49831.0	1.87	232.1458	-1.13	6.0 C	15 H 20 O 2
234.1607	57756.0	2.17	234.1614	-0.77	5.0 C	15 H 22 O 2
244.1451	69185.0	2.60	244.1458	-0.70	7.0C	16 H 20 O 2
264 1722	13/304.0	5.15	246.1614	-0.38	6.0C	16 H 22 O 2
202 2022	110839.0	4.16	204.1720	1.22	0.00	16 11 24 03

Figure S158. HREIMS spectrum of 15



Figure S159. FTIR spectrum of 15





Figure S160. <sup>1</sup>H NMR spectrum of 15 in CDCl<sub>3</sub> at 500 MHz



Figure S161. <sup>13</sup>C and NMR DEPT spectra of 15 in CDCl<sub>3</sub> at 100 MHz



Figure S162. HSQC spectrum of 15 in CDCl<sub>3</sub>



Figure S163. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 15 in CDCl<sub>3</sub>



Figure S164. HMBC spectrum of 15 in CDCl<sub>3</sub>





Elemer	ntal Comp	osition	Repo	rt						Page 1
Single Tolerand Element Number	Mass Ana ce = 10.0 Pl t prediction: of isotope p	<b>lysis</b> PM / [ Off peaks us	DBE: mi sed for i	n = -1.5, i -FIT = 3	max = 50	0.0				
Monoisol 14 formu Elements C: 1-40 SIPI A22	topic Mass, E la(e) evaluat s Used: H: 1-50	even Elec ed with 1 O: 1-4	tron lons results Na: 1-	s within limit: 1	s (up to 5	Q-Tof YAC	st results for e micro 019	each mass)	•	14:42:28,14-Mar-2017
100	HR1 28 (0.519	9) AM (Cer	n,4, 80.00	, Ar,5000.0	,308.05,1.	00); Sm (	Mn, 2x3.00); Si 3(	b (1,40.00 ); Cm (2 03.1576	?7:61)	TOF MS ES+ 2.05e+004
%										
0				302	.9385					
0	302.700	302.8	800	302.900	303	3.000	303.100	303.200	303.300	303.400 m/z
Minimum: Maximum:		5.0	10.0	-1.5 50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formu	la			
303.1576	303.1572	0.4	1.3	4.5	n∕a	C16	H24 04 Na			

Figure S166. HRESIMS spectrum of 16



Figure S168. <sup>1</sup>H NMR spectrum of 16 in CDCl<sub>3</sub> at 500 MHz



Figure S169. <sup>13</sup>C and NMR DEPT spectra of 16 in CDCl<sub>3</sub> at 125 MHz



Figure S170. HSQC spectrum of 16 in CDCl<sub>3</sub>



Figure S171. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 16 in CDCl<sub>3</sub>



Figure S172. HMBC spectrum of 16 in CDCl<sub>3</sub>



Figure S173. NOESY spectrum of 16 in CDCl<sub>3</sub>



**Figure S174.** Structures and populations of the low-energy B97D/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (1R,4R,6S,9S,10S)-1.



Figure S175. Structures and populations of the low-energy B97D/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (1R,4S,6S,9S,10S)-5.



Figure S176. Structures and populations of the low-energy B97D/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (1R,4S,6S,9S,10S)-6.



Figure S177. Structures and populations of the low-energy CAM-B3LYP/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (1R,4S,6R,7R,8R,9R,10S)-9.



Figure S178. Structures and populations of the low-energy B97D/TZVP PCM/MeCN conformers ( $\geq 1\%$ ) of (1R,4S,6R,7S,10S)-14.

## Analysis of splenocytes proliferation, apoptosis and T cell subtypes

Splenocytes  $(2 \times 10^6 \text{ cell/ml})$  from C57BL/6 mice were incubated with compounds for 24 h. The cells were collected and washed with PBS, and then samples were immediately detected by a FACScan flow cytometer (BD, USA) for apoptosis.

To investigate the effects of compounds on the differentiation of T cell subtypes. The cells were collected and stained with PE-CD3, FITC-CD4 and Percp/cy5.5-CD8, respectively. The percentage of CD3+T, CD4+T, and CD8+T cells was analyzed by flow cytometry.



## **Supplementary Data**

**Figure S179.** Effects of the compounds **1-16** on the Cell Viability by CCK-8 assay. Splenocytes were incubated with compounds for 24 h. The values are presented as means $\pm$ S.D. (n=3). \*P<0.05 and \*\*P<0.01.



**Figure S180.** Effects of compounds **1-16** on the apoptosis of splenocytes by Annexin V-FITC/PI staining. Splenocytes were incubated with compounds  $(3\mu M)$  for 24 h. The apoptosis of splenocytes was analyzed by flow cytometry. The values are presented as means±S.D. (n=3). \*P<0.05 and \*\*P<0.01.



Figure S181. Effects of compounds 1-16 on the proliferation of CD3+T. Splenocytes

were incubated with compounds ( $3\mu$ M) for 24 h using Con A as a positive control ( $5\mu$ g/mL). The cells were collected and stained with PE-CD3. The percentage of CD3+T was analyzed by flow cytometry. The values are presented as means±S.D. (n=3). Significant differences with Con A group were designated as \*P<0.05 and \*\*P<0.01.



**Figure S182.** Effects of compounds **1-16** on the proliferation of CD3+T. Con A-stimulated ( $5\mu$ g/mL) splenocytes were incubated with compounds for 24 h. The cells were collected and stained with PE-CD3. The percentage of CD3+T was analyzed by flow cytometry. The values are presented as means±S.D. (n=3). Significant differences with Con A group were designated as \*P<0.05 and \*\*P<0.01.



**Figure S183**. Effects of compounds **1-16** on the differentiation of T cell subtypes. Con A-stimulated splenocytes were incubated with compounds for 24 h. The cells were collected and stained with FITC-CD4 and Percp/cy5.5-CD8. The percentage of CD4+T and CD8+T cells was analyzed by flow cytometry. The values are presented as means $\pm$ S.D. (n=3). Significant differences with Con A group were designated as \*P<0.05 and \*\*P<0.01.

	3		5		6	
	$\delta$ H (mult., J in Hz)	$\delta C$	$\delta H$ (mult., J in Hz)	$\delta C$	δH (mult., J in Hz)	$\delta C$
1	1.78 ddd 10.9, 10.7, 2.43	43.2	1.75 ov	43.4	1.29 ov	46.2
2	α 1.43 ov β 1 29 ov	23.1	α 1.46 ov β 1 34 ov	23.2	1.48 ov	20.9
3	α 1.52 ddd 13.8, 13.5, 4.2 β 1.65 ddd 13.8, 3.2, 3.1	39.5	α 1.55 ddd 13.5 13.2, 4.2 β 1.66 ov	39.5	α 1.38 ov β 1.79-1.68 ov	39.3
4	-	70.1	-	70.1	-	69.8
5	α 1.25 ov β 1.73 ddd 13.3, 3.0, 3.0	45.3	α 1.25 ov β 1.72 ov	45.4	α 1.79-1.68 ov β 1.21 ov	69.8
6	2.23 dddd 13.0, 11.7, 5.2, 3.0	33.7	2.21 ov	33.8	2.38 dddd 13.0, 11.5, 5.7, 2.5	35.0
7	5.35 ov	130.7	5.37-5.35 ov	130.9	5.38 dd 10.2, 2.5	131.1
8	5.35 ov	133.7	5.37-5.35 ov	133.7	5.62 dd 10.1, 2.9	130.9
9	-	73.9	-	73.8	-	84.9
10	-	57.0	-	57.1	-	37.65
11	1.23 s	31.7	1.23 s	31.7	1.25 s	31.8
12	1.11 s	27.3	1.13 s	27.4	1.42 s	26.0
13	1.32 s	11.9	1.31 s	12.5	0.98 s	14.6
14	-	211.4	-	213.0	1.79-1.68 ov	26.6
15	a 2.75 (dt, 18.5, 6.0) b 3.19 (dt,18.5, 6.0)	40.7	2.26 s	30.7	a 2.73 ddd 19.8, 9.5, 7.3 b 2.64 ddd 19.8, 9.2, 3.3	27.4
16	a 4.31 (dt, 11.1, 6.0) b 4.36 (dt, 11.1, 6.0)	59.7				172.4
17		171.1				
18	2.01 s	21.0				

**Table S1.** <sup>1</sup>H and <sup>13</sup>C NMR Data for compounds **3**, **5** and **6** (in CDCl<sub>3</sub>, J in Hz)

500 MHz for <sup>1</sup>H NMR and 100 MHz for <sup>13</sup>C NMR

**Table S2.** <sup>1</sup>H and <sup>13</sup>C NMR Data for compounds **7**, **8** and **14** (in CDCl<sub>3</sub>, *J* in Hz)

	$7^{\rm a}$		<b>8</b> <sup>a</sup>	<b>14</b> <sup>b</sup>			
	$\delta$ H (mult., J in Hz)	δC	$\delta$ H (mult., J in Hz)	$\delta C$	$\delta$ H (mult., J in Hz)	$\delta C$	
1	1.84-1.73 ov	42.9	2.09 ov	39.8	1.74-1.62 ov	41.2	
r	α 1.84-1.73 ov	26.2	α 2.13 ov	22.0	α 1.08 m	22.1	
2	β 1.58 ov	20.2	β 1.29 ov	22.0	β 1.74-1.62 ov	22.1	
2	α 1.51 ov	20.7	α 1.70 ov	20.4	α 1.31 m	28.0	
3	β 1.84-1.73 ov	39.7	β 2.47 ov	39.4	β 1.74-1.62 ov	38.0	
4		70.4		69.7		69.0	
5	α 1.51 dd 15.0, 10.0	156	α 1.73 ov	61.2	α 1.13 ov	12 6	
3	β 1.84-1.73 ov 45.6		β 1.32 dd 13.2, 13.2	01.2	β 2.28 ddd 13.8, 3.6, 3.6	43.0	
6	2.44 dddd 13.1, 10.4, 2.8, 2.5	36.2	2.24 m	34.1	1.74-1.62 ov	36.9	

7	5.44 dd 10.2, 2.5	132.2	5.49 dd 9.8, 1.8	134.3	3.85 ddd 8.4, 2.1, 1.4	73.6
8	5.58 dd 10.1, 3.0	132.4	5.35 dd 9.8, 2.6	131.8	5.57 d 1.4	128.3
9		86.5		77.4		138.4
10		43.4		42.9		57.6
11	1.26 s	31.6	1.22 s	31.7	1.26 s	31.8
12	1.66 s	27.7	1.26 s	18.6	1.57 t 1.7	19.7
13	0.91 s	15.4	0.99 s	15.1	1.13 s	15.7
14	4.03 dd 8.6, 1.7	68.9	4.09 dd 12.7, 4.0	75.4		211.6
15	α 2.72 dd 19.4, 1.6	40.4	$\alpha2.00$ dddd 12.6, 12.6, 12.6, 5.6	31.0	2 07 s	25.6
15	β 3.27 dd 19.4, 8.5	40.4	$\beta$ 1.70 dddd 12.4, 4.1, 2.8, 1.3	51.0	2.07 5	25.0
16		1743	α 3.85 ddd 11.9, 5.5, 1.3	61.2		
10		174.5	$\beta$ 3.73 ddd 12.3, 12.1, 2.9	01.2		

<sup>a</sup>500 MHz for <sup>1</sup>H NMR and 100 MHz for <sup>13</sup>C NMR; <sup>b</sup>400 MHz for <sup>1</sup>H NMR and 100 MHz for <sup>13</sup>C NMR

**Table S3.** <sup>1</sup>H and <sup>13</sup>C NMR Data for compounds **16** (in C<sub>5</sub>D<sub>5</sub>N, *J* in Hz)

$\begin{array}{c c c c c c c c c c c c c c c c c c c $			
1 $1.55, \text{ ov}$ $48.8$ $2\alpha$ $1.60, \text{ ov}$ $29.6$ $2\beta$ $1.02, \text{ ov}$ $36.1$ $3\alpha$ $1.03, \text{ ov}$ $36.1$ $3\beta$ $1.66, \text{ ov}$ $36.1$ $4$ $1.36, \text{ m}$ $33.2$ $5\alpha$ $0.81, \text{ ov}$ $40.3$ $5\beta$ $2.67, \text{ ov}$ $40.3$ $6$ $3.10, \text{ ov}$ $44.8$ $7$ $3.97, \text{ dd} (9.6, 1.0)$ $75.2$ $8$ $4.51, \text{ d} (1.0)$ $90.1$ $9$ - $79.5$ $10$ - $50.0$ $11$ $0.89, \text{ d} (6.5)$ $23.3$ $12$ $1.45, \text{ s}$ $25.4$ $13$ $1.17, \text{ s}$ $12.1$ $14$ - $187.9$ $15$ $5.35, \text{ d} (8.5)$ $99.6$ $16$ $10.43, \text{ d} (8.5)$ $189.1$		$\delta_{ m H}$	$\delta_{ m C}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1	1.55, ov	48.8
2β1.02, ov29.0 $3α$ 1.03, ov36.1 $3β$ 1.66, ov36.1 $4$ 1.36, m33.2 $5α$ 0.81, ov40.3 $5β$ 2.67, ov40.3 $6$ 3.10, ov44.8 $7$ 3.97, dd (9.6, 1.0)75.2 $8$ 4.51, d (1.0)90.1 $9$ -79.5 $10$ -50.0 $11$ 0.89, d (6.5)23.3 $12$ 1.45, s25.4 $13$ 1.17, s12.1 $14$ -187.9 $15$ 5.35, d (8.5)99.6 $16$ 10.43, d (8.5)189.1	2α	1.60, ov	20.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2β	1.02, ov	29.0
3β1.66, ov $30.1$ 41.36, m $33.2$ 5α0.81, ov $40.3$ 5β2.67, ov $40.3$ 63.10, ov $44.8$ 73.97, dd (9.6, 1.0) $75.2$ 8 $4.51$ , d (1.0) $90.1$ 9- $79.5$ 10- $50.0$ 110.89, d (6.5) $23.3$ 121.45, s $25.4$ 131.17, s $12.1$ 14- $187.9$ 15 $5.35$ , d (8.5) $99.6$ 1610.43, d (8.5) $189.1$	3α	1.03, ov	26.1
$\begin{array}{cccccccc} 4 & 1.36, m & 33.2 \\ 5\alpha & 0.81, ov & 40.3 \\ 5\beta & 2.67, ov & 40.3 \\ 6 & 3.10, ov & 44.8 \\ 7 & 3.97, dd (9.6, 1.0) & 75.2 \\ 8 & 4.51, d (1.0) & 90.1 \\ 9 & - & 79.5 \\ 10 & - & 79.5 \\ 10 & - & 50.0 \\ 11 & 0.89, d (6.5) & 23.3 \\ 12 & 1.45, s & 25.4 \\ 13 & 1.17, s & 12.1 \\ 14 & - & 187.9 \\ 15 & 5.35, d (8.5) & 99.6 \\ 16 & 10.43, d (8.5) & 189.1 \\ \end{array}$	3β	1.66, ov	50.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	4	1.36, m	33.2
5β2.67, ov40.563.10, ov44.873.97, dd (9.6, 1.0)75.284.51, d (1.0)90.19-79.510-50.0110.89, d (6.5)23.3121.45, s25.4131.17, s12.114-187.9155.35, d (8.5)99.61610.43, d (8.5)189.1	5α	0.81, ov	40.2
6       3.10, ov       44.8         7       3.97, dd (9.6, 1.0)       75.2         8       4.51, d (1.0)       90.1         9       -       79.5         10       -       50.0         11       0.89, d (6.5)       23.3         12       1.45, s       25.4         13       1.17, s       12.1         14       -       187.9         15       5.35, d (8.5)       99.6         16       10.43, d (8.5)       189.1	5β	2.67, ov	40.5
7 $3.97, dd (9.6, 1.0)$ $75.2$ 8 $4.51, d (1.0)$ $90.1$ 9- $79.5$ 10- $50.0$ 11 $0.89, d (6.5)$ $23.3$ 12 $1.45, s$ $25.4$ 13 $1.17, s$ $12.1$ 14- $187.9$ 15 $5.35, d (8.5)$ $99.6$ 16 $10.43, d (8.5)$ $189.1$	6	3.10, ov	44.8
8       4.51, d (1.0)       90.1         9       -       79.5         10       -       50.0         11       0.89, d (6.5)       23.3         12       1.45, s       25.4         13       1.17, s       12.1         14       -       187.9         15       5.35, d (8.5)       99.6         16       10.43, d (8.5)       189.1	7	3.97, dd (9.6, 1.0)	75.2
9       -       79.5         10       -       50.0         11       0.89, d (6.5)       23.3         12       1.45, s       25.4         13       1.17, s       12.1         14       -       187.9         15       5.35, d (8.5)       99.6         16       10.43, d (8.5)       189.1	8	4.51, d (1.0)	90.1
10       -       50.0         11       0.89, d (6.5)       23.3         12       1.45, s       25.4         13       1.17, s       12.1         14       -       187.9         15       5.35, d (8.5)       99.6         16       10.43, d (8.5)       189.1	9	-	79.5
110.89, d (6.5)23.3121.45, s25.4131.17, s12.114-187.9155.35, d (8.5)99.61610.43, d (8.5)189.1	10	-	50.0
12       1.45, s       25.4         13       1.17, s       12.1         14       -       187.9         15       5.35, d (8.5)       99.6         16       10.43, d (8.5)       189.1	11	0.89, d (6.5)	23.3
13       1.17, s       12.1         14       -       187.9         15       5.35, d (8.5)       99.6         16       10.43, d (8.5)       189.1	12	1.45, s	25.4
14-187.9155.35, d (8.5)99.61610.43, d (8.5)189.1	13	1.17, s	12.1
155.35, d (8.5)99.61610.43, d (8.5)189.1	14	-	187.9
16 10.43, d (8.5) 189.1	15	5.35, d (8.5)	99.6
	16	10.43, d (8.5)	189.1

500 MHz for <sup>1</sup>H NMR and 125 MHz for <sup>13</sup>C NMR

**Table S4.** Boltzmann populations and optical rotations of the low-energy conformers of (1R,4R,6S,9S,10S)-1 computed at various levels for the B3LYP/6-31G(d) in vacuo optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	PBE0/TZVP

Conf. A	44.68 %	30.37	15.40	30.56
Conf. B	32.73 %	-57.02	-67.64	-57.03
Conf. C	8.50 %	-32.57	-41.80	-33.08
Conf. D	6.68 %	53.31	41.60	53.43
Conf. E	2.74 %	16.03	0.04	13.74
Conf. F	2.71 %	-75.04	-55.67	-73.31
Average	N/A	-6.01	-17.89	-5.98

**Table S5.** Boltzmann populations and optical rotations of the low-energy conformers of (1R,4R,6S,9S,10S)-1 computed at various levels for the B97D/TZVP PCM/MeCN optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	34.44 %	76.32	52.94	59.55	76.58
Conf. B	28.83 %	-32.86	-50.04	-45.43	-34.08
Conf. C	14.32 %	-93.46	-67.81	-79.93	-90.64
Conf. D	5.65 %	26.35	5.68	13.44	23.98
Conf. E	3.65 %	-140.44	-114.12	-129.99	-138.11
Conf. F	2.25 %	-76.04	-43.75	-56.34	-72.62
Conf. G	1.82 %	90.82	75.47	80.66	92.11
Conf. H	1.76 %	-27.77	-40.89	-38.21	-28.31
Conf I	1.50 %	-20.61	-30.88	-27.53	-21.25
Conf J	1.09 %	37.61	14.00	20.99	35.20
Average	N/A	-0.69	-10.90	-9.10	-0.53

**Table S6.** Boltzmann populations and optical rotations of the low-energy conformers of (1R, 4R, 6S, 9S, 10S)-1 computed at various levels for the CAM-B3LYP/TZVP PCM/MeCN optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	40.64 %	70.33	47.08	53.69	70.27
Conf. B	25.45 %	-44.11	-61.48	-56.57	-45.39
Conf. C	8.92 %	86.01	69.89	75.37	86.72
Conf. D	8.68 %	22.43	2.69	10.31	19.83
Conf. E	5.86 %	-24.94	-36.87	-32.64	-25.99
Conf. F	1.99 %	-85.30	-63.12	-73.18	-82.92
Conf. G	1.02 %	-34.53	-47.23	-44.60	-35.39
Conf. H	0.99 %	-70.96	-41.68	-52.90	-68.12
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Conf I	0.97 %	14.56	-6.84	-0.51	13.14
Average	N/A	24.23	5.90	11.31	23.68

**Table S7.** Boltzmann populations and optical rotations of the low-energy conformers of (1R,4S,6S,9S,10S)-5 computed at various levels for the B3LYP/6-31G(d) in vacuo optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	PBE0/TZVP
Conf. A	45.52 %	-26.25	-38.94	-26.28
Conf. B	32.60 %	-51.33	-59.16	-50.64
Conf. C	6.68 %	5.31	-5.83	4.77
Conf. D	6.15 %	-60.75	-65.38	-59.71
Conf. E	5.10 %	-15.46	-22.81	-15.52
Conf. F	1.48 %	-97.93	-82.33	-96.59
Conf G	1.29 %	-75.58	-63.60	-74.60
Conf H	1.18 %	-25.21	-29.56	-24.92
Average	N/A	-35.57	-44.97	-35.30

**Table S8.** Boltzmann populations and optical rotations of the low-energy conformers of (1R,4S,6S,9S,10S)-5 computed at various levels for the B97D/TZVP PCM/MeCN optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	30.27 %	-3.00	-17.24	-12.69	-2.86
Conf. B	28.51 %	-3.88	-18.96	-13.54	-3.33
Conf. C	26.23 %	20.35	-0.88	5.19	20.05
Conf. D	5.24 %	-92.37	-73.01	-85.62	-89.88
Conf. E	4.71 %	-68.77	-54.68	-66.78	-66.85
Conf. F	1.87 %	15.28	7.40	10.82	16.02
Conf. G	1.67 %	14.16	5.45	9.67	15.27
Conf. H	1.50 %	36.59	22.25	27.07	36.98
Average	N/A	-3.68	-16.69	-13.20	-3.30

**Table S9** Boltzmann populations and optical rotations of the low-energy conformers of (1R,4S,6S,9S,10S)-5 computed at various levels for the CAM-B3LYP/TZVP PCM/MeCN optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	35.05 %	7.45	-12.94	-7.17	6.94
Conf. B	33.51 %	-18.61	-32.27	-27.40	-18.13
Conf. C	9.21 %	-19.13	-31.52	-27.80	-18.95
Conf. D	7.61 %	29.81	14.60	19.78	29.69
Conf. E	7.37 %	5.70	-3.34	0.99	6.42
Conf. F	2.56 %	-97.40	-77.80	-89.97	-95.74
Conf. G	2.52 %	-72.65	-58.96	-70.33	-71.70
Conf. H	2.17 %	5.13	-2.67	0.60	5.60
Average	N/A	-6.92	-20.93	-16.75	-6.80

**Table S10** Boltzmann populations and optical rotations of the low-energy conformers of (1R,4S,6R,7S,10S)-**14** computed at various levels for the B3LYP/6-31G(d) in vacuo optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	PBE0/TZVP
Conf. A	42.06 %	-103.56	-66.97	-100.65
Conf. B	36.46 %	-125.02	-88.01	-122.65
Conf. C	4.20 %	-143.02	-106.64	-140.85
Conf. D	3.44 %	-127.68	-89.73	-124.95
Conf. E	3.05 %	-58.35	-31.21	-57.45
Conf. F	2.43 %	-83.47	-53.66	-82.97
Conf G	2.41 %	-122.41	-86.48	-119.67
Conf H	2.13 %	-160.04	-137.19	-161.84
Conf I	1.61 %	-151.48	-127.42	-152.55
Average	N/A	-114.68	-78.88	-112.30

**Table S11** Boltzmann populations and optical rotations of the low-energy conformers of (1R, 4S, 6R, 7S, 10S)-**14** computed at various levels for the B97D/TZVP PCM/MeCN optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	23.15 %	-137.81	-91.95	-98.75	-134.02

Conf. B	21.13 %	-117.30	-73.82	-80.32	-113.52
Conf. C	19.55 %	-135.13	-90.75	-96.65	-131.63
Conf. D	8.43 %	-107.35	-69.95	-74.52	-106.00
Conf. E	6.56 %	-86.49	-51.38	-55.66	-85.14
Conf. F	5.55 %	-107.95	-70.85	-74.99	-106.75
Conf. G	4.45 %	-157.15	-112.01	-119.32	-153.58
Conf. H	3.49 %	-137.49	-94.42	-101.54	-133.88
Conf I	3.46 %	-155.27	-110.99	-117.70	-151.87
Conf J	1.01 %	-133.73	-111.16	-115.32	-135.41
Average	N/A	-126.41	-83.76	-89.80	-123.29

**Table S12** Boltzmann populations and optical rotations of the low-energy conformers of (1R, 4S, 6R, 7S, 10S)-**14** computed at various levels for the CAM-B3LYP/TZVP PCM/MeCN optimized MMFF conformers.

Conformer	Boltzmann population	B3LYP/TZVP	BH&HLYP/TZVP	CAM-B3LYP/TZVP	PBE0/TZVP
Conf. A	25.45 %	-125.73	-79.86	-87.63	-121.82
Conf. B	24.61 %	-145.44	-97.63	-105.22	-141.59
Conf. C	9.05 %	-165.77	-117.76	-126.41	-161.95
Conf. D	8.62 %	-145.66	-99.94	-108.58	-141.86
Conf. E	8.03 %	-95.98	-57.55	-63.62	-94.29
Conf. F	7.17 %	-119.19	-77.74	-84.15	-117.46
Conf. G	6.07 %	-146.26	-97.30	-105.64	-142.17
Conf. H	2.51 %	-165.14	-116.74	-125.77	-161.23
Conf I	2.30 %	-117.03	-75.55	-82.25	-115.22
Conf J	1.63 %	-131.94	-107.36	-112.74	-133.14
Conf K	1.60 %	-150.49	-123.46	-128.81	-151.74
Average	N/A	-135.90	-90.80	-98.41	-132.57