

**A** Decision Tree confusion matrix: full GC-TOF data

Genotype predictions from Decision Tree models

True sample classes

	Ag	Gr	Li	So	De1	De2	S18	S22	S36	SF19	SF30	SF34
Ag	<b>50</b>	2	1	1	3	0	1	0	0	0	0	0
Gr	0	<b>55</b>	1	1	3	0	0	0	0	0	0	0
Li	3	3	<b>48</b>	3	3	0	0	0	0	0	0	0
So	2	1	0	<b>54</b>	1	0	2	0	0	0	0	0
De1	8	1	1	1	<b>38</b>	11	0	0	0	0	0	0
De2	3	9	1	4	9	<b>34</b>	0	0	0	0	0	0
S18	2	0	1	3	0	0	<b>33</b>	11	10	0	0	0
S22	1	0	1	0	0	0	8	<b>40</b>	8	1	1	0
S36	0	0	0	2	1	0	6	5	<b>44</b>	1	0	1
SF19	0	0	0	0	0	0	0	1	0	<b>51</b>	1	7
SF30	0	0	0	0	0	0	0	2	0	4	<b>47</b>	7
SF34	0	0	0	1	0	0	0	0	3	1	3	<b>52</b>

**B** Decision Tree confusion matrix: GC-TOF data with out-of-range metabolites omitted

Genotype predictions from Decision Tree models

True sample classes

	Ag	Gr	Li	So	De1	De2	S18	S22	S36	SF19	SF30	SF34
Ag	<b>48</b>	1	4	0	0	0	2	0	2	0	0	3
Gr	1	<b>50</b>	1	0	2	1	1	3	0	0	0	1
Li	2	2	<b>47</b>	2	1	2	0	3	0	1	0	0
So	4	0	1	<b>47</b>	0	0	0	0	4	0	0	0
De1	2	0	2	0	<b>42</b>	1	1	2	6	2	0	2
De2	0	3	0	0	9	<b>36</b>	0	2	2	1	0	7
S18	1	0	1	0	1	3	<b>30</b>	8	0	4	6	6
S22	0	3	1	0	2	4	3	<b>29</b>	2	5	8	3
S36	1	2	3	1	1	2	2	4	<b>27</b>	4	4	9
SF19	0	0	0	0	4	1	4	7	2	<b>34</b>	2	8
SF30	2	0	0	4	0	1	8	5	2	6	<b>27</b>	8
SF34	1	0	1	1	0	1	4	2	1	3	1	<b>45</b>