

| $\begin{gathered} \text { PCC C } \\ 0.6 \end{gathered}$ | 0.057 | 0.072 | bASA | PCC |
| :---: | :---: | :---: | :---: | :---: |
|  | 0.146 | 0.079 | bRSA | . 4 |
| 0.5 | 0.092 | -0.063 | UASA | 0.3 |
| 0.4 | 0.142 | -0.037 | uRSA | 0.2 |
|  | 0.195 | 0.064 | dASA |  |
| 0.3 | 0.237 | -0.086 | dRSA |  |
| 0.2 | 0.388 | 0.233 | IR-dASA |  |
|  | 0.312 | 0.024 | IR-dRSA |  |
|  | 0.067 | 0.072 | NHB |  |
| PCC | 0.214 | 0.097 | IR-NHB |  |
| 0.4 | 0.071 | 0.051 | CFAA |  |
| 0.3 | 0.357 | 0.135 | CFNA |  |
|  | 0.407 | 0.075 | IR-CFAA |  |
| 0.2 | 0.292 | 0.244 | IR-CFNA |  |
| 0.1 | 0.331 | 0.002 | ENDES |  |
| 0.0 | 0.340 | 0.319 | IR-ENDES |  |
|  | -0.041 | 0.056 | JSD |  |
|  | 0.247 | 0.330 | Nonenergy |  |
|  | MPD48 | MPR79 |  |  |

S7 Fig. PCC values of individual and integrative feature groups for independent
testing. (A) PCC values of energy feature groups for MPD48. (B) PCC values of energy feature groups for MPR79. (C) PCC values of nonenergy feature groups for MPD48 and MPR79. The last row in each figure shows the performance of integrative feature groups.

