**Supplementary File 9-** **Comparison of KeyAlloSite and SCA methods**

**Supplementary File 9**. Comparison of KeyAlloSite and SCA methods

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| Proteins | Known key allo-residues | SCAa | KeyAlloSiteb |
| BCR-ABL1 | L359 | N | L359 |
| Tar | Y149, Q152 | Y149, Q152 | Y149, Q152 |
| PDZ3 | A347, L353 | A347, L353 | A347, L353 |
| AurA | T288, T287, S342 | N | T288, T287 |
| CALB | A225c | N (32.8%)c | A225 (38.5%)c |
| CMs | L40, L41, R44, D50, D83, L92, Q93, H95 | D83 | R44, L40 |
| aSCA: Known key allo-residues contained in sectors predicted by SCA. "N" indicates that sectors do not contain known allo-key residues. bKeyAlloSite: The known key allo-residues predicted by KeyAlloSite. cA225: Since CALB contains many key allo-residues, only a typical key allo-residue A225 that has a great impact on enzyme activity is listed here. "N" means that A225 is not included in sectors, and the numbers in brackets represent the proportion of known key allo-residues predicted by SCA and KeyAlloSite. |