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| --- | --- | --- |
|  | Description | Formula |
| 1 | Hydroxyhexamide | C15H22N2O4S |
| 2 | Nummularine B | C32H41N5O6 |
| 3 | Penicilloic acid | C16H20N2O5S |
| 4 | LysoPC(17:0) | C25H52NO7P |
| 5 | 2-acetyl-1-alkyl-sn-glycero-3-phosphocholine | C26H54NO7P |
| 6 | (2E)-3-phenyl-1-[2,3,4,6-tetrahydroxy-5-(3-methylbut-2-en-1-yl)phenyl]prop-2-en-1-one | C20H20O5 |
| 7 | 1-(2-Furanylmethyl)-1H-pyrrole | C9H9NO |

**Supplementary Table 1. Seven selected metabolites in HT29 cells**