

Supplemental Data for:

Propofol Inhibits SIRT2 Deacetylase Through a Conformation-Specific, Allosteric Site*

Brian P. Weiser^{1,2}, Roderic G. Eckenhoff¹

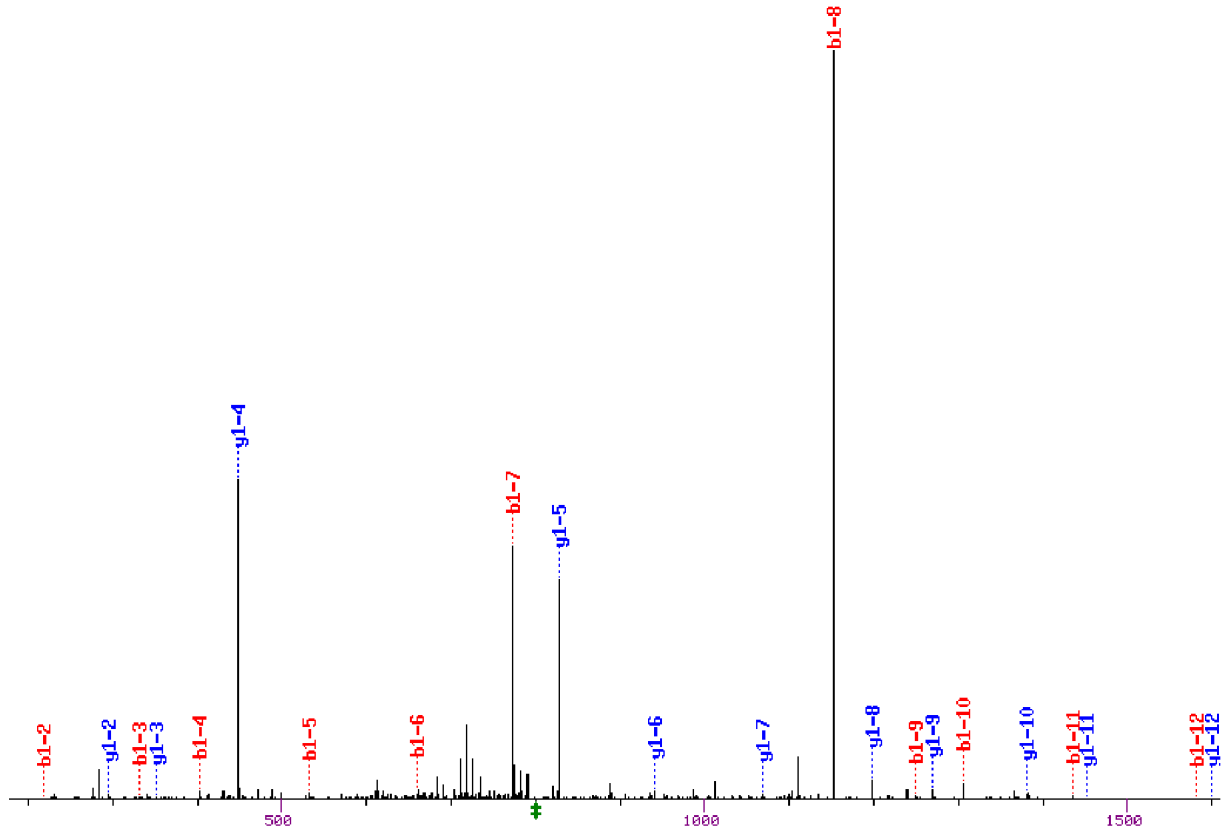
From the ¹Department of Anesthesiology & Critical Care and ²Department of Pharmacology,
University of Pennsylvania Perelman School of Medicine, Philadelphia, PA 19104

*Running title: *Inhibition of SIRT2 by propofol*

To whom correspondence should be addressed: Roderic G. Eckenhoff, Department of
Anesthesiology & Critical Care, University of Pennsylvania Perelman School of Medicine, 3620
Hamilton Walk, Philadelphia, PA 19104, Tel.: (215) 662-3705; Fax: (215) 349-5078; E-mail:
roderic.eckenhoff@uphs.upenn.edu

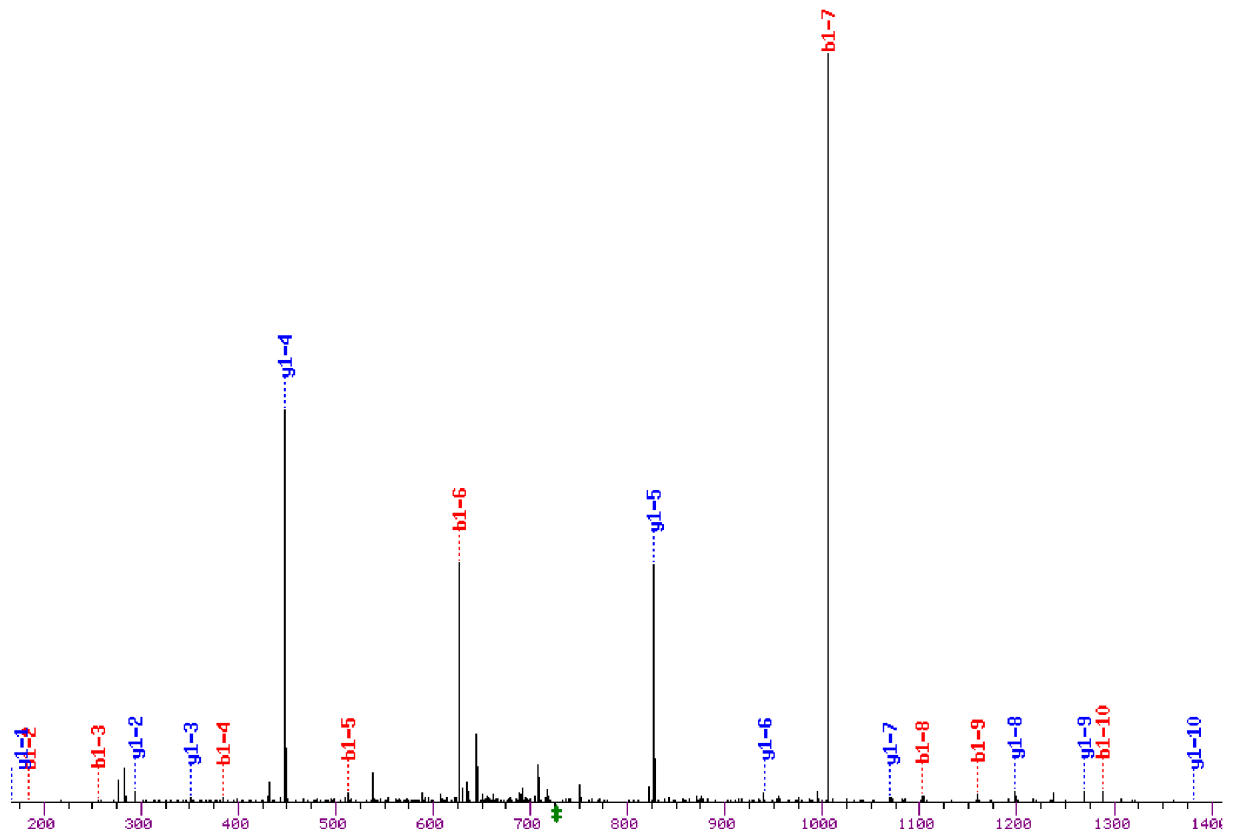
Fig. S1. Mass spectra of SIRT2 peptides photolabeled by AziPm. For all spectra, hypothetical fragment ions are listed in the tables, and their predicted positions are indicated on the spectra. Fragment ions that were identified on the spectra are colored in the ion tables. Only +1 fragment ions are shown. #Indicates a 216.0762 Da modification was detected; amino acid numbering is according to full-length rat SIRT2.

Peptide: $^{131}\text{F.FALAKELY}^{\#}\text{PGQF.K}^{144}$



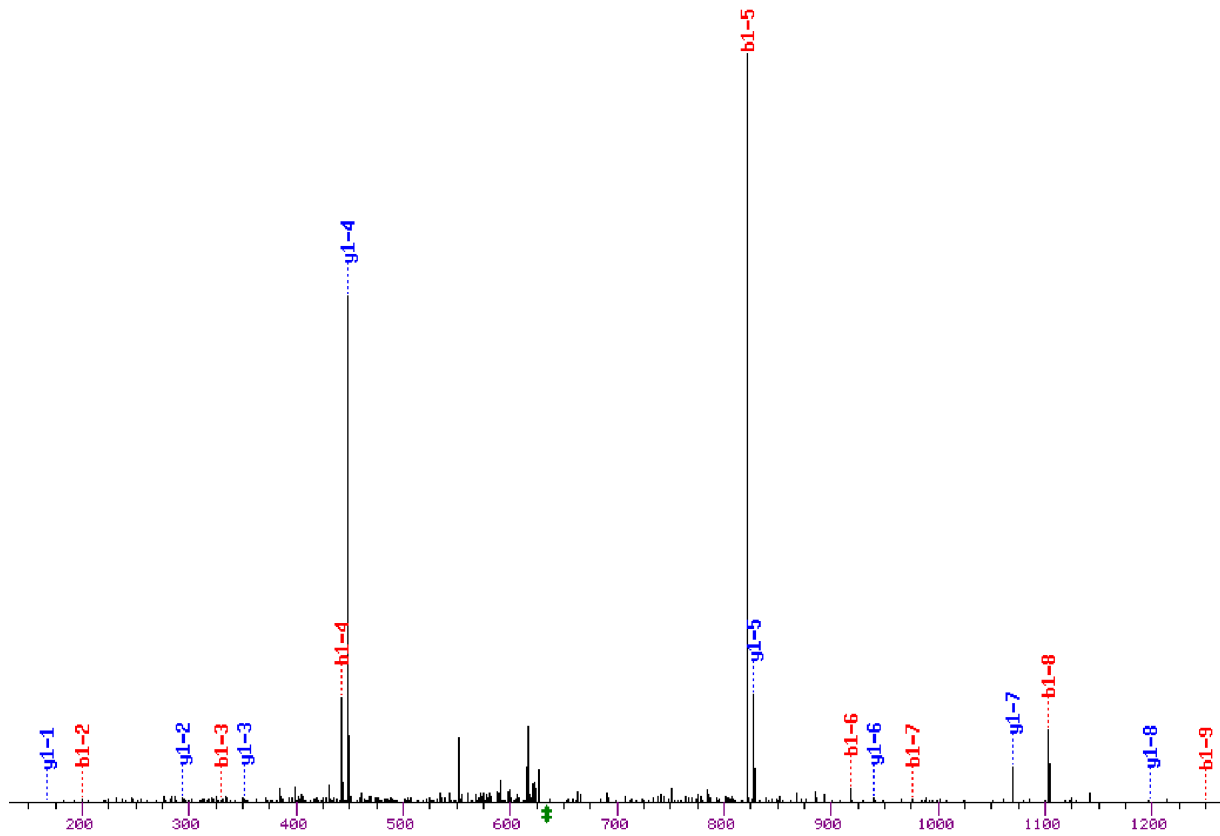
Sequence	#	b	y	#
F	1	148.1	1599.8	12
A	2	219.1	1452.7	11
L	3	332.2	1381.7	10
A	4	403.2	1268.6	9
K	5	531.3	1197.6	8
E	6	660.4	1069.5	7
L	7	773.5	940.4	6
Y#	8	1152.6	827.4	5
P	9	1249.6	448.2	4
G	10	1306.7	351.2	3
Q	11	1434.7	294.1	2
F	12	1581.8	166.1	1

Peptide: ¹³²F.ALAKELY#PGQF.K¹⁴⁴



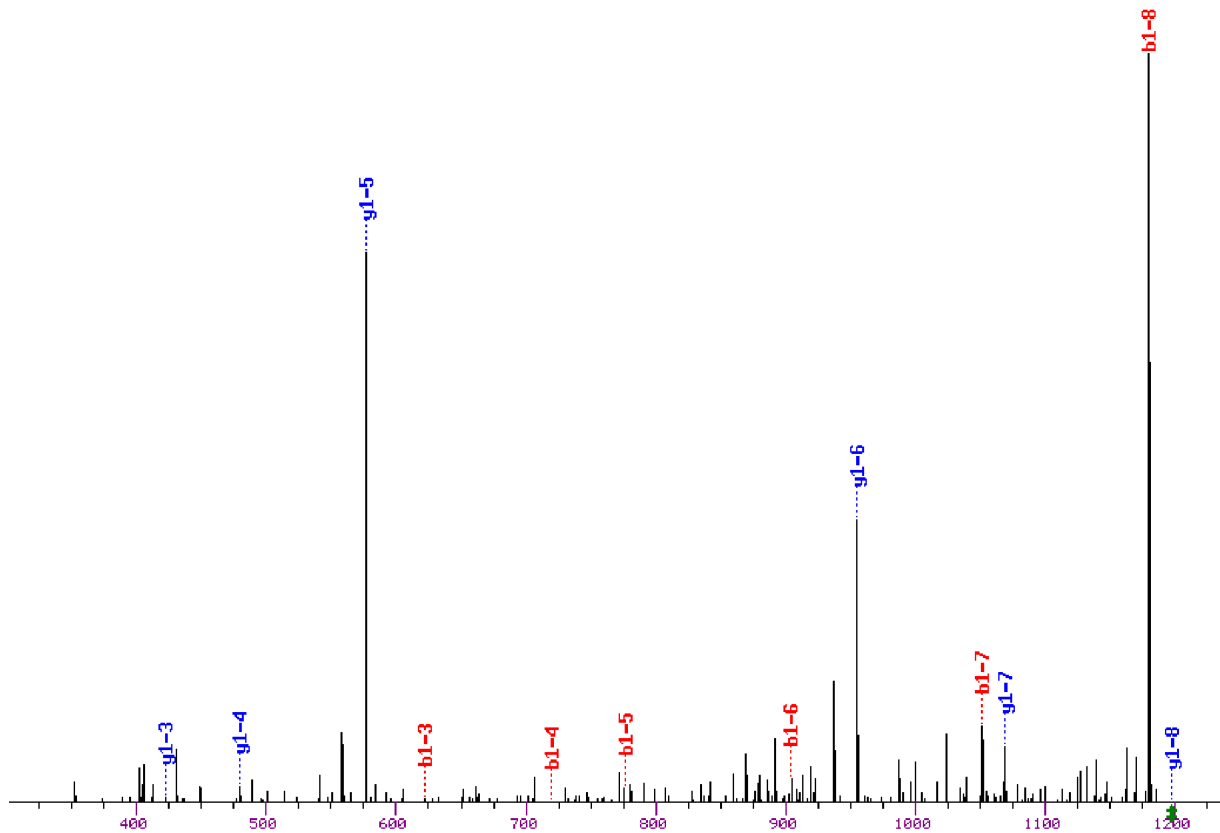
Sequence	#	b	y	#
A	1	72.0	1452.7	11
L	2	185.1	1381.7	10
A	3	256.2	1268.6	9
K	4	384.3	1197.6	8
E	5	513.3	1069.5	7
L	6	626.4	940.4	6
Y#	7	1005.5	827.4	5
P	8	1102.6	448.2	4
G	9	1159.6	351.2	3
Q	10	1287.7	294.1	2
F	11	1434.7	166.1	1

Peptide: ¹³⁴L.AKELY#PGQF.K¹⁴⁴



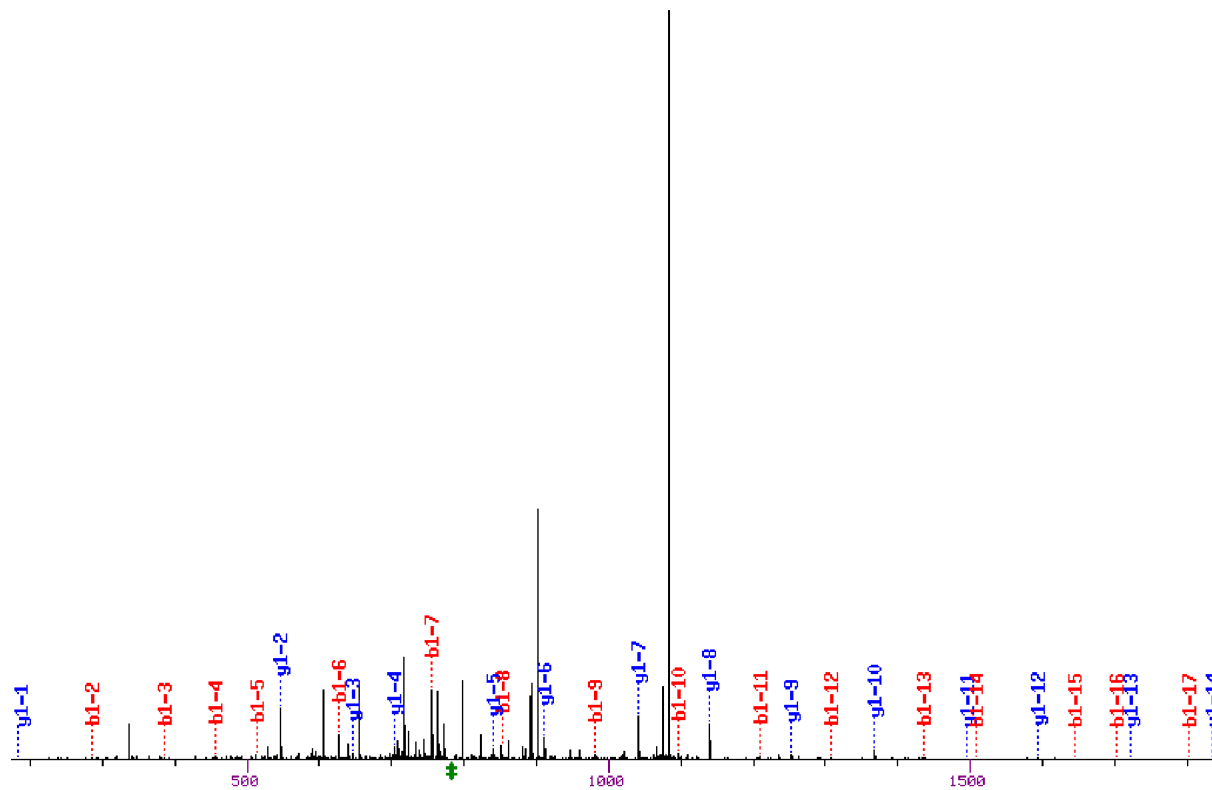
Sequence	#	b	y	#
A	1	72.0	1268.6	9
K	2	200.1	1197.6	8
E	3	329.2	1069.5	7
L	4	442.3	940.4	6
Y#	5	821.4	827.4	5
P	6	918.5	448.2	4
G	7	975.5	351.2	3
Q	8	1103.5	294.1	2
F	9	1250.6	166.1	1

Peptide: $^{136}\text{K}.\text{ELY}\#\text{PGQFK}.\text{P}^{145}$



Sequence	#	b	y	#
E	1	130.1	1197.6	8
L	2	243.1	1068.5	7
Y#	3	622.3	955.5	6
P	4	719.3	576.3	5
G	5	776.3	479.3	4
Q	6	904.4	422.2	3
F	7	1051.5	294.2	2
K	8	1179.6	147.1	1

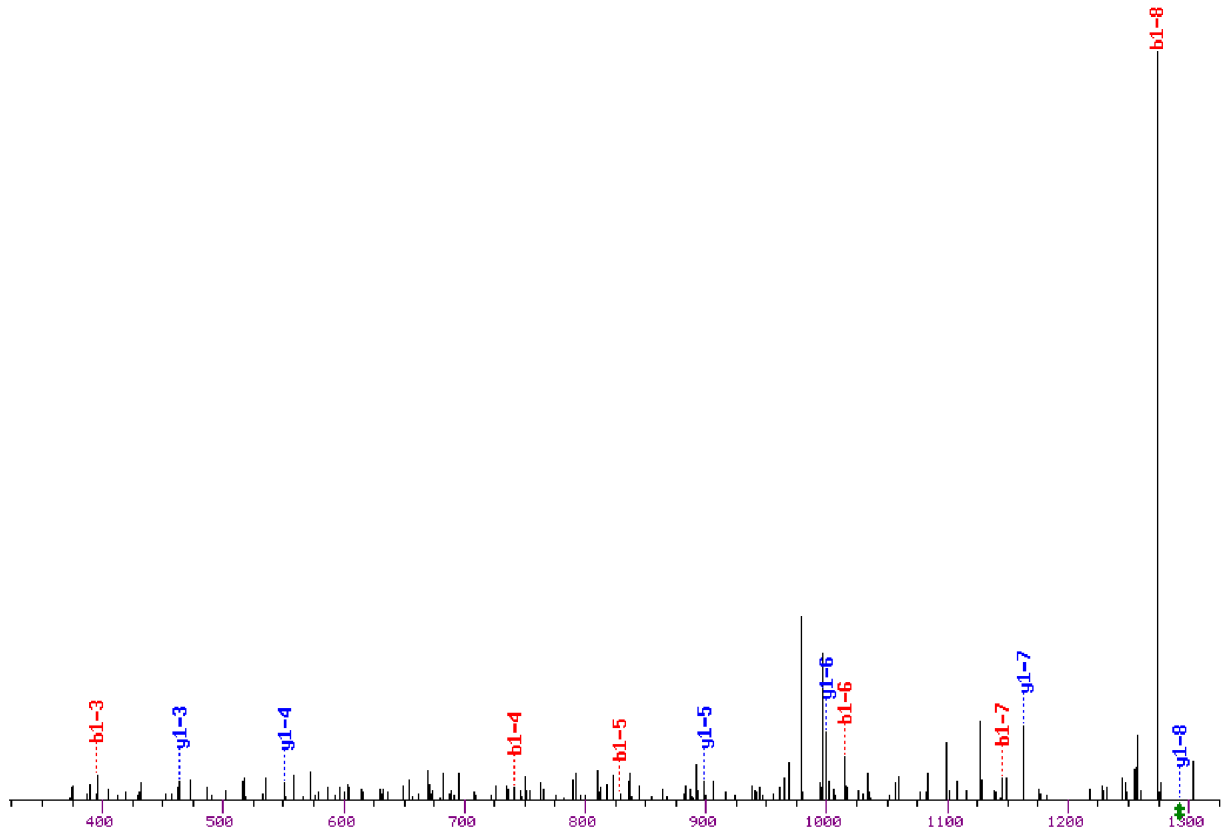
Peptide: ¹⁷²L.ERVAGLEPQDLVEAHGTF#Y.T¹⁹²



Sequence	#	b	y	#
E	1	130.1	2347.1	19
R	2	286.2	2218.1	18
V	3	385.2	2062.0	17
A	4	456.3	1962.9	16
G	5	513.3	1891.9	15
L	6	626.4	1834.9	14
E	7	755.4	1721.8	13
P	8	852.5	1592.7	12
Q	9	980.5	1495.7	11
D	10	1095.5	1367.6	10
L	11	1208.6	1252.6	9
V	12	1307.7	1139.5	8
E	13	1436.7	1040.4	7
A	14	1507.8	911.4	6
H	15	1644.8	840.4	5
G	16	1701.9	703.3	4
T	17	1802.9	646.3	3
F#	18	2166.0	545.2	2
Y	19	2329.2	182.0	1

note: the peaks at $m/z = 902.0$ and 1083.5 are b17 and b18 +2 fragment ions, respectively

Peptide: ²⁰²K.EYTM#SWMK.E²¹¹



Sequence	#	b	y	#
E	1	130.1	1291.5	8
Y	2	293.1	1162.5	7
T	3	394.2	999.4	6
M#	4	741.3	898.4	5
S	5	828.3	551.3	4
W	6	1014.4	464.2	3
M	7	1145.4	278.2	2
K	8	1273.5	147.1	1