The NISTmAb Disulfide Library V21.1
Readme File, March 8, 2021

I Description of the library peptide entry name
Example:
SCDKTHTCPPCPAPELLGGPSVFLFPPKPK_S-S_SFNRGEC/7_2(7,C,CAM)(10,C,CAM)_H-L_NCE24

sequence	SCDKTHTCPPCPAPELLGGPSVFLFPPKPK_S-S_SFNRGEC
charge state	7+
modification	2(7,C,CAM)(10,C,CAM)
disulfide bond name	H-L; Interchain disulfide bond between heavy and light chain
Normalized collision energy	NCE24

II Description of the comment fields of the reference spectra

Spec	Selected “best” spectra
Pep	Tryptic, N/C-terminal Semitryptic
Miscleav	Number of missed tryptic cleavages in peptides
Parent	m/z of the peptide precursor
MS1ab	Absolute intensity of full MS scan ion clusters
Inst	Instrument
Frag	Fragmentation methods, HCD and HCID (High resolution CID)
NCE	Normalized collision energy
Scan	three parts, (1) runid; (2) MS1 ion cluster number; and (3) MS2 scan number
IsolationMZ	Sampled m/z
MS2RT	Sampled retention time
Mz_diff	mass error ppm between observed and theoretical m/z values
Protein	IgG1 heavy chain or light chain
DSB	Name of disulfide bonds corresponding to its locating regions, VH, CH1, CH2, CH3, VL, CL, H-L, and Hinge
Cys	the location of cysteine in protein
Nreps	Number of replicates used to create consensus spectra
Score	library score of selected spectra
Assigned_PK	Number of assigned peaks
Assigned_AB	Percentage of assigned abundances
Unassigned_AB	Percentage of unassigned abundances
IntactDSB_AB	Percentage of fragments with intact SS bonds
Run	Name of LC-MS/MS runs

Note

1. The fragment intensity in the msp files is provided in percent. Hence, the largest one is 100.00. The intensity data may be renormalized when spectra in txt format are processed into a library. For example, the largest intensity in each spectrum in the NIST library is 999.00.

2. Some significant instrumental noise peaks were removed.