Degradation of chemical warfare agents by nickel doped titanium dioxide powders: Enhanced surface activity

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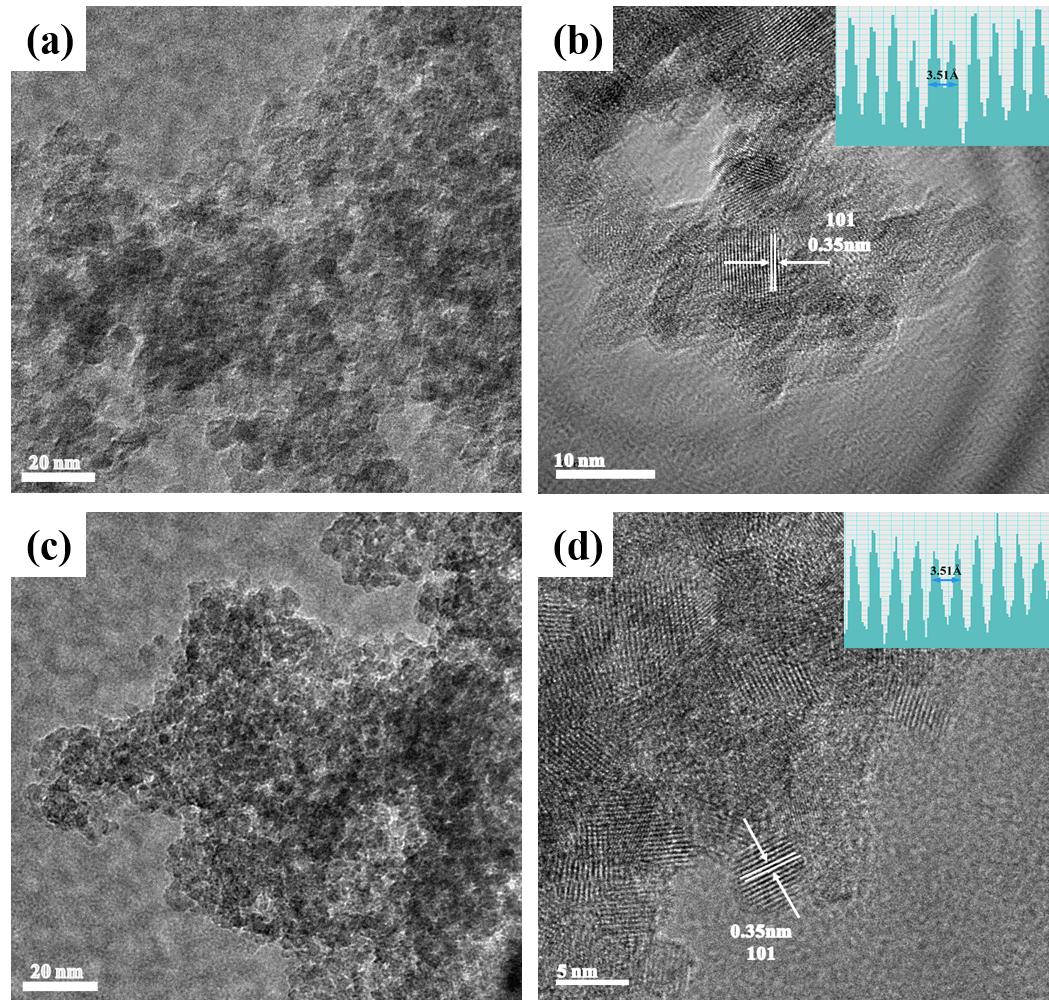
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**High-resolution XPS spectroscopy**



***Fig. S1*** *High-resolution XPS spectroscopy of (c) Ni 2p, and, (d) O 1s and (e) Ti 2p of TN2.*

**TEM images of TN1 and TN2**



**Fig. S2** Low-resolution TEM images of TN1 (a) and TN3 (c). High-resolution TEM images of TN1 (b) and TN3 (d). The inset on the upper right corner is the corresponding lattice distance of (101) facet.

**N2 sorption curves**





**Fig. S3** Pore size distribution curves of TN1 (a) and TN3 (b) calculated from desorption branch of the nitrogen isotherm. The inset on the upper right corner is the nitrogen adsorption-desorption isotherms.

**Stability test of the catalyst**

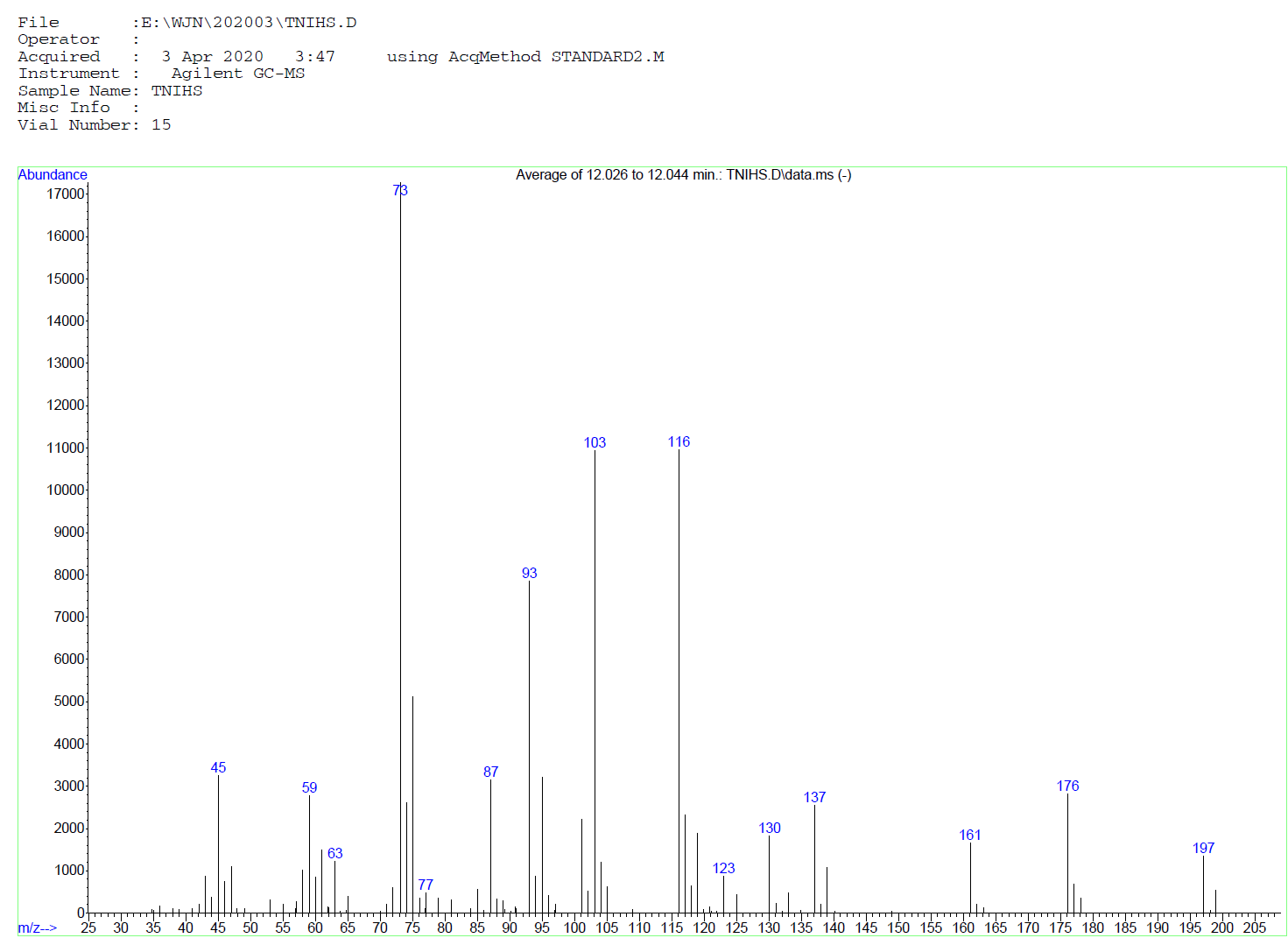


**Fig. S4** Recyclability of TN2 for the degradation of (a) HD, (b) GD and (c)VX.

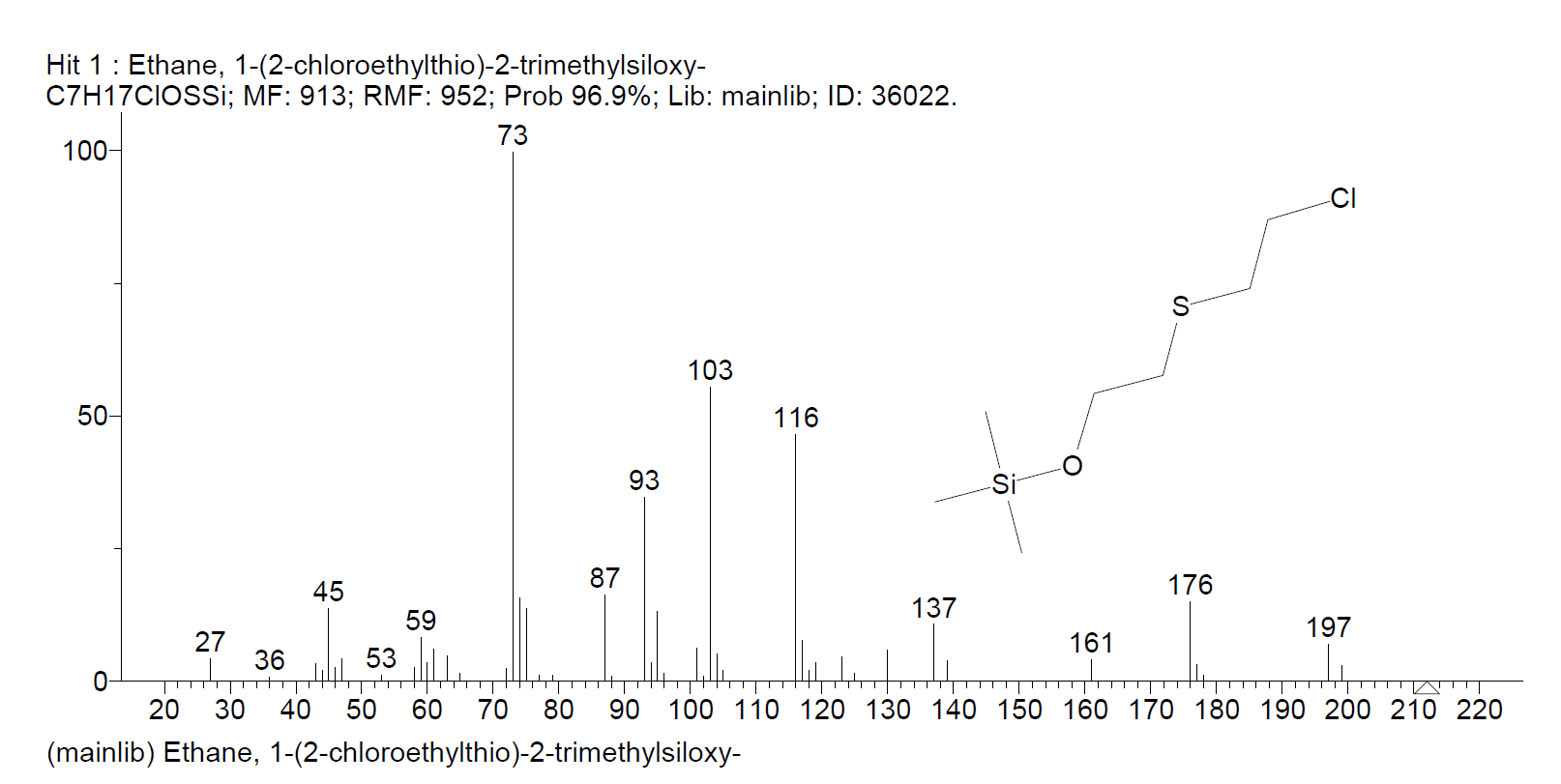
**Degradation of HD by different ratios of TN2**



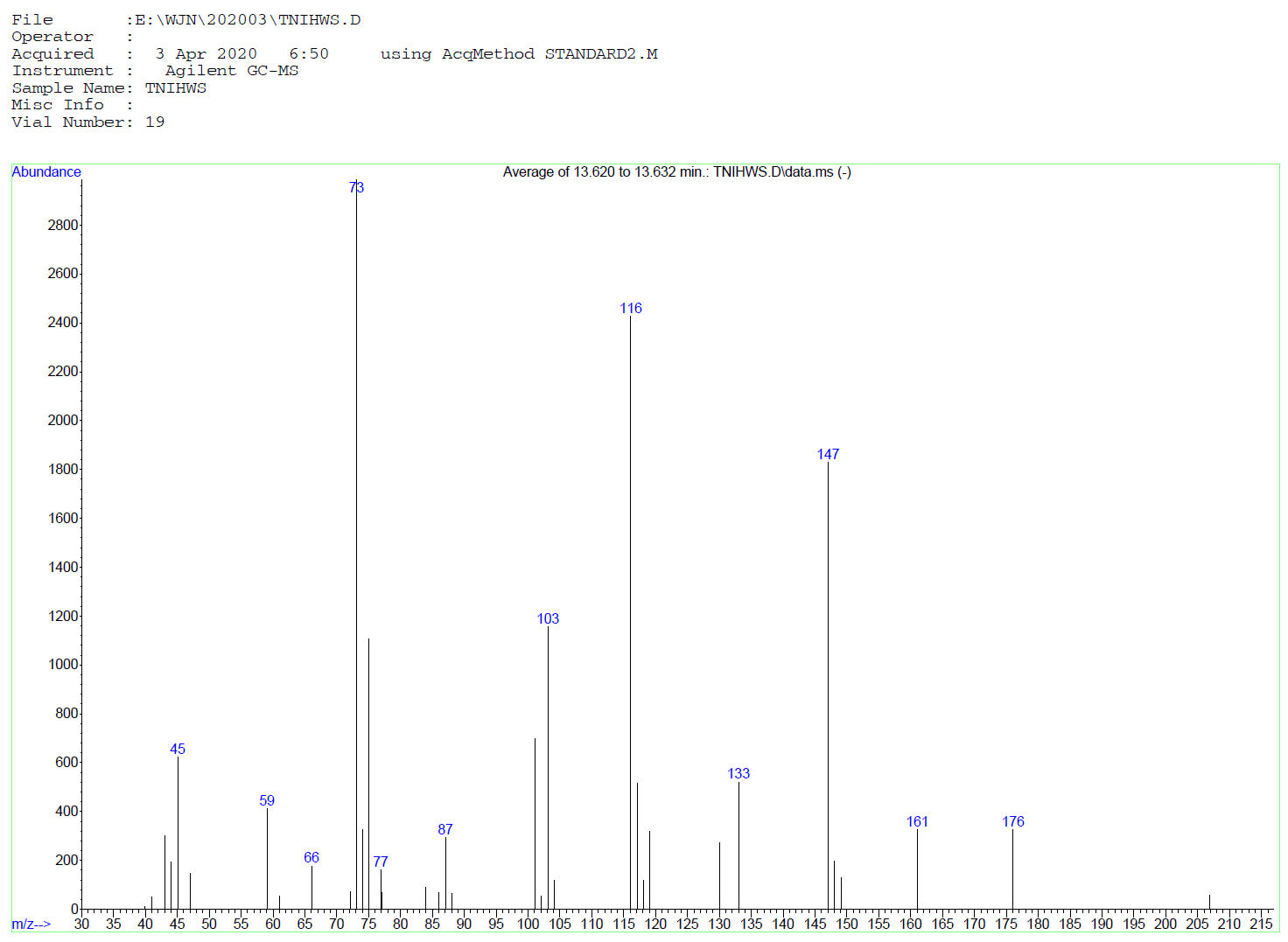
**Fig. S5** Degradation of HD in 1 hour by different ratios of TN2.



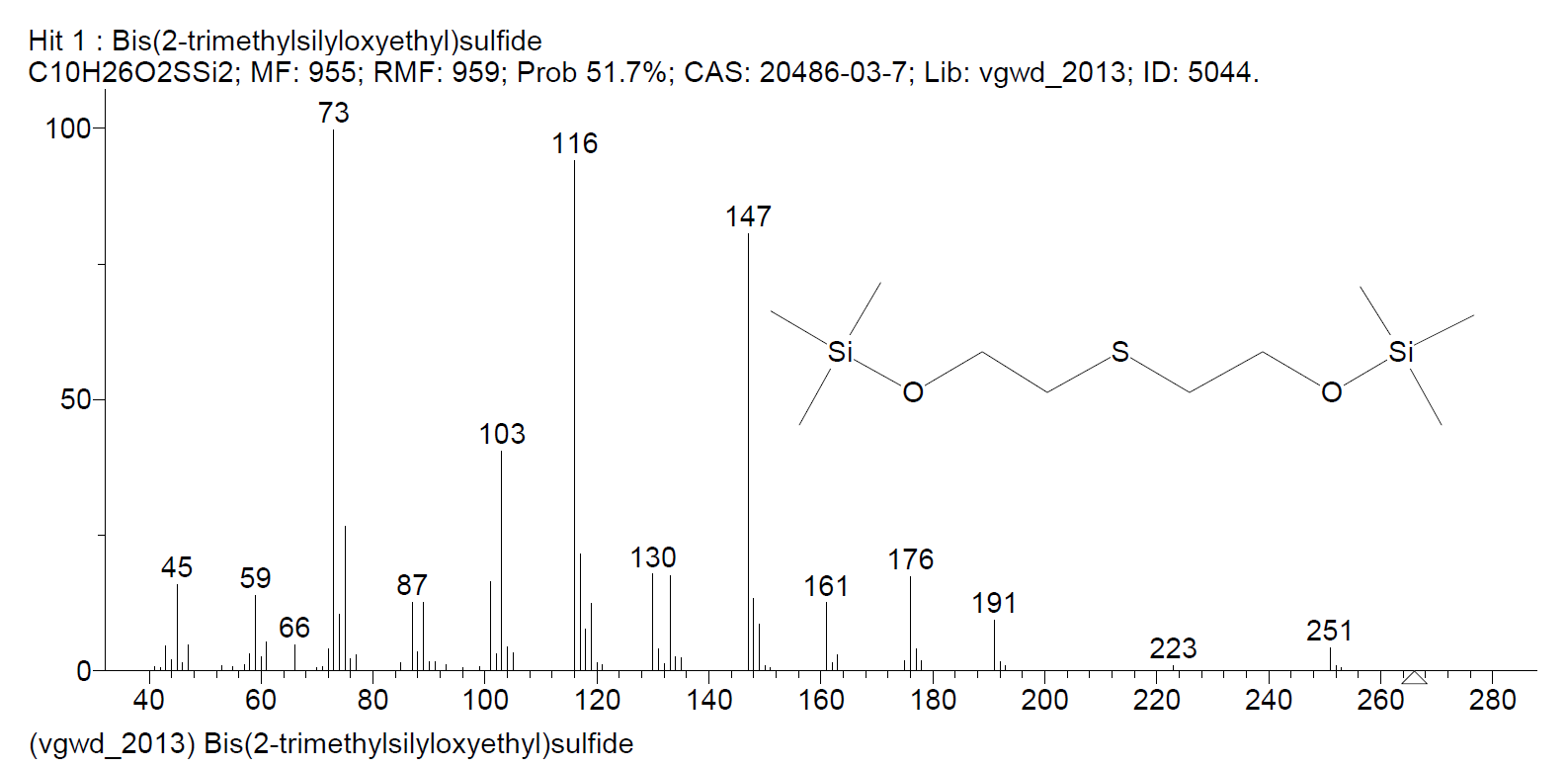
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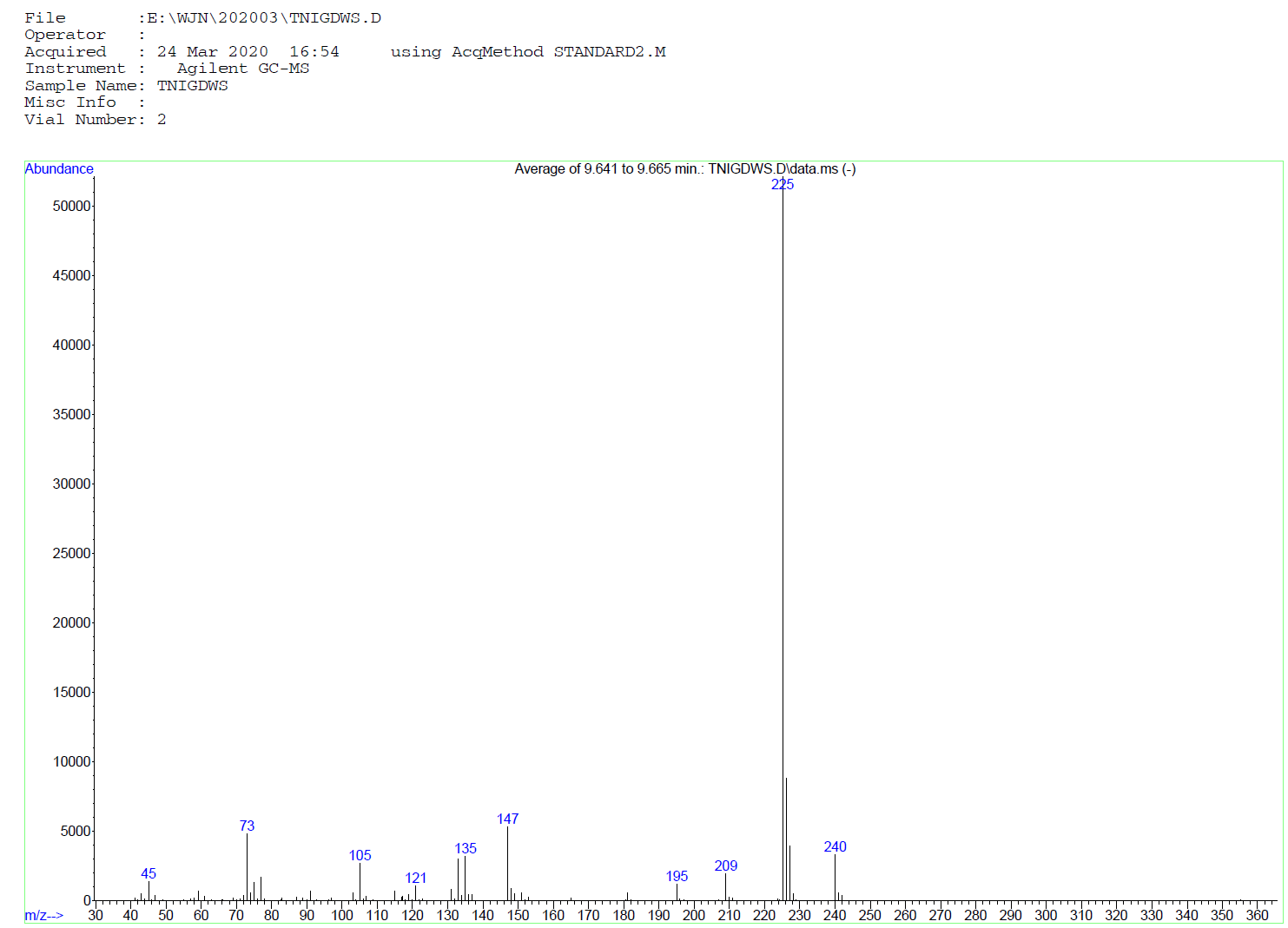
**Fig. S6** Mass spectrometry of silylated product C4H9ClOS **(2)** of HD detected by GC/MS (Agilent 7890A GC & Agilent 5975C MSD) and the corresponding reference spectrum.



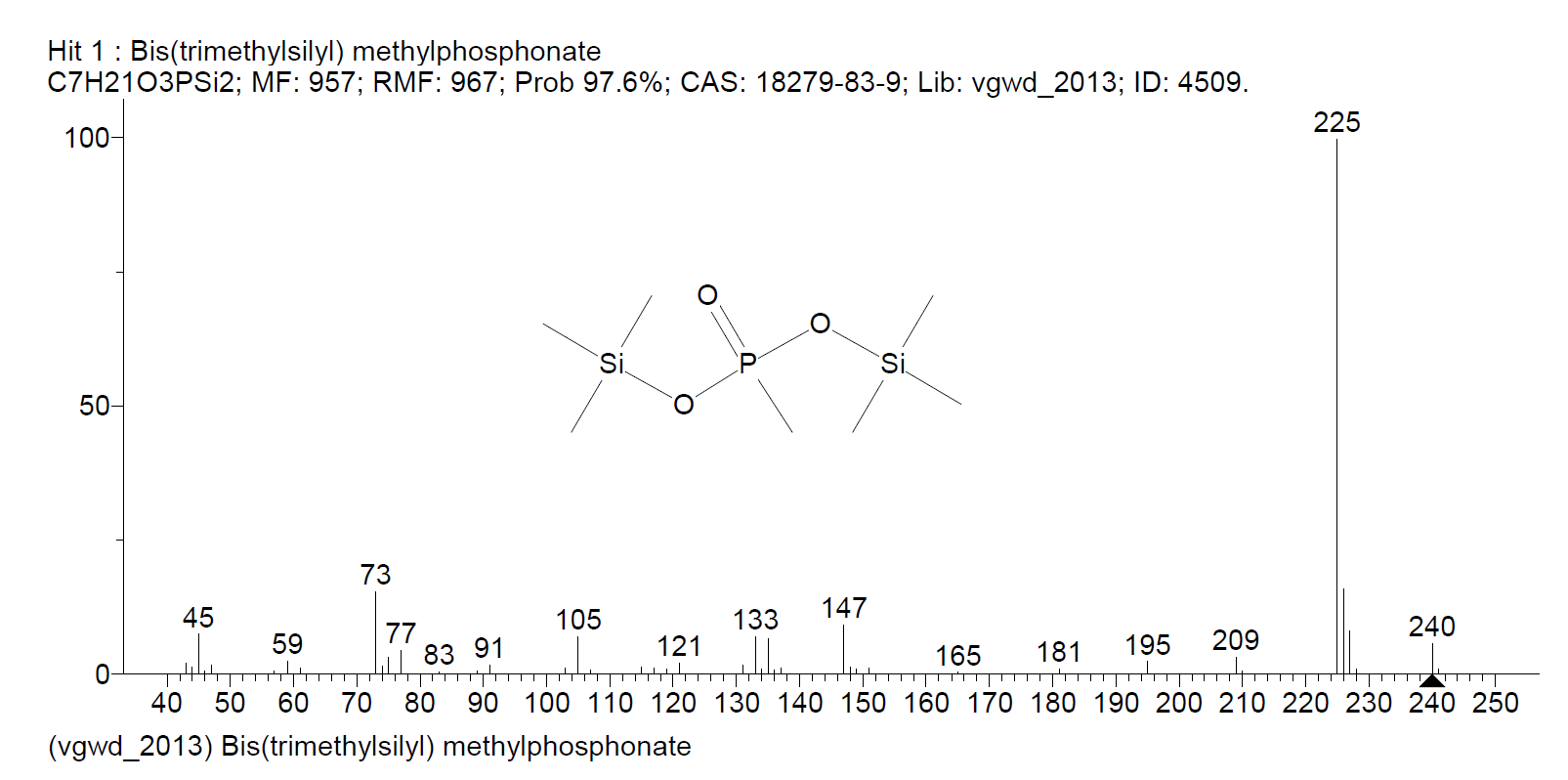
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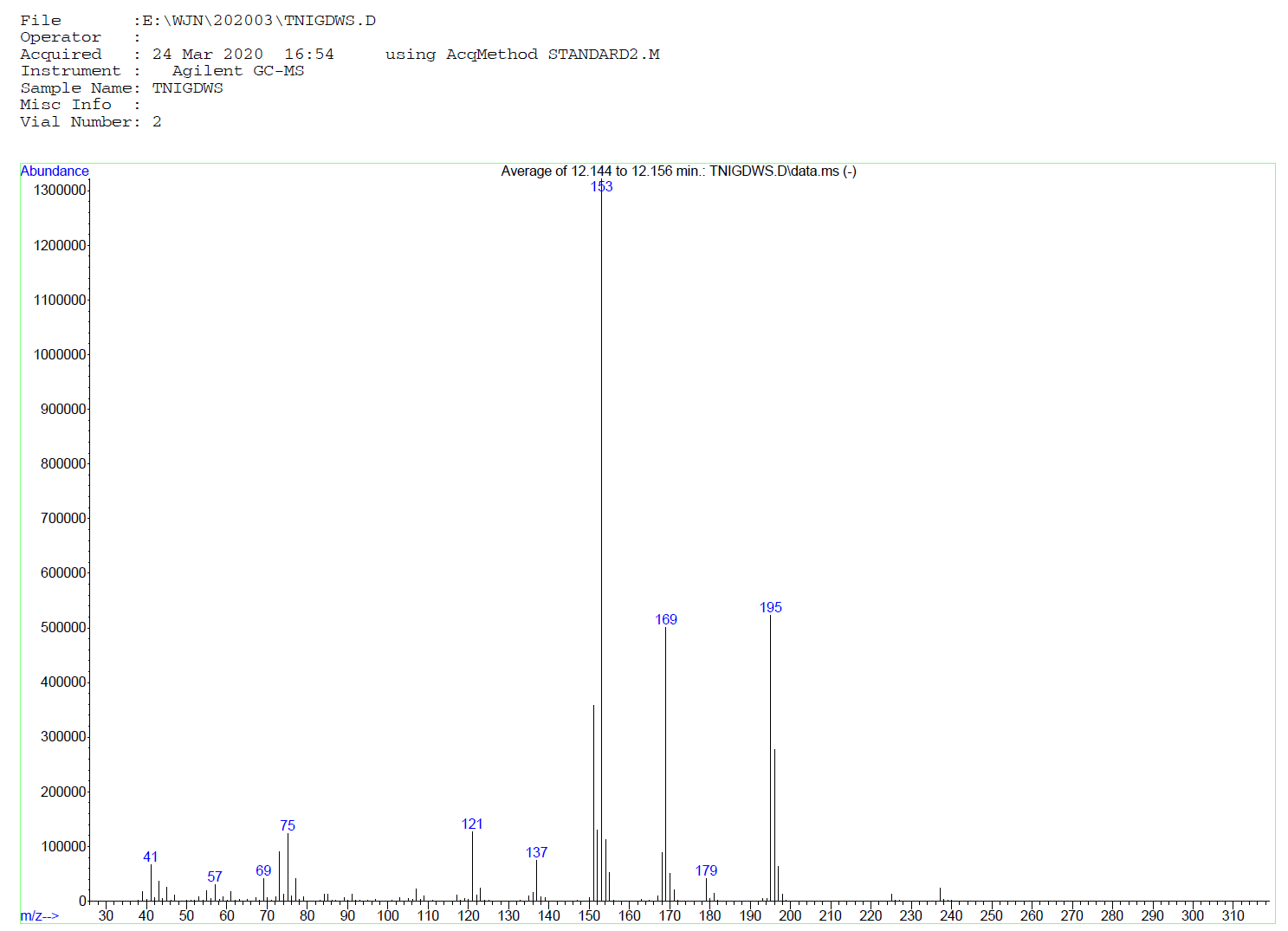
**Fig. S7** Mass spectrometry of silylated product C4H10O2S of HD detected by GC/MS (Agilent 7890A GC & Agilent 5975C MSD) and the corresponding reference spectrum.



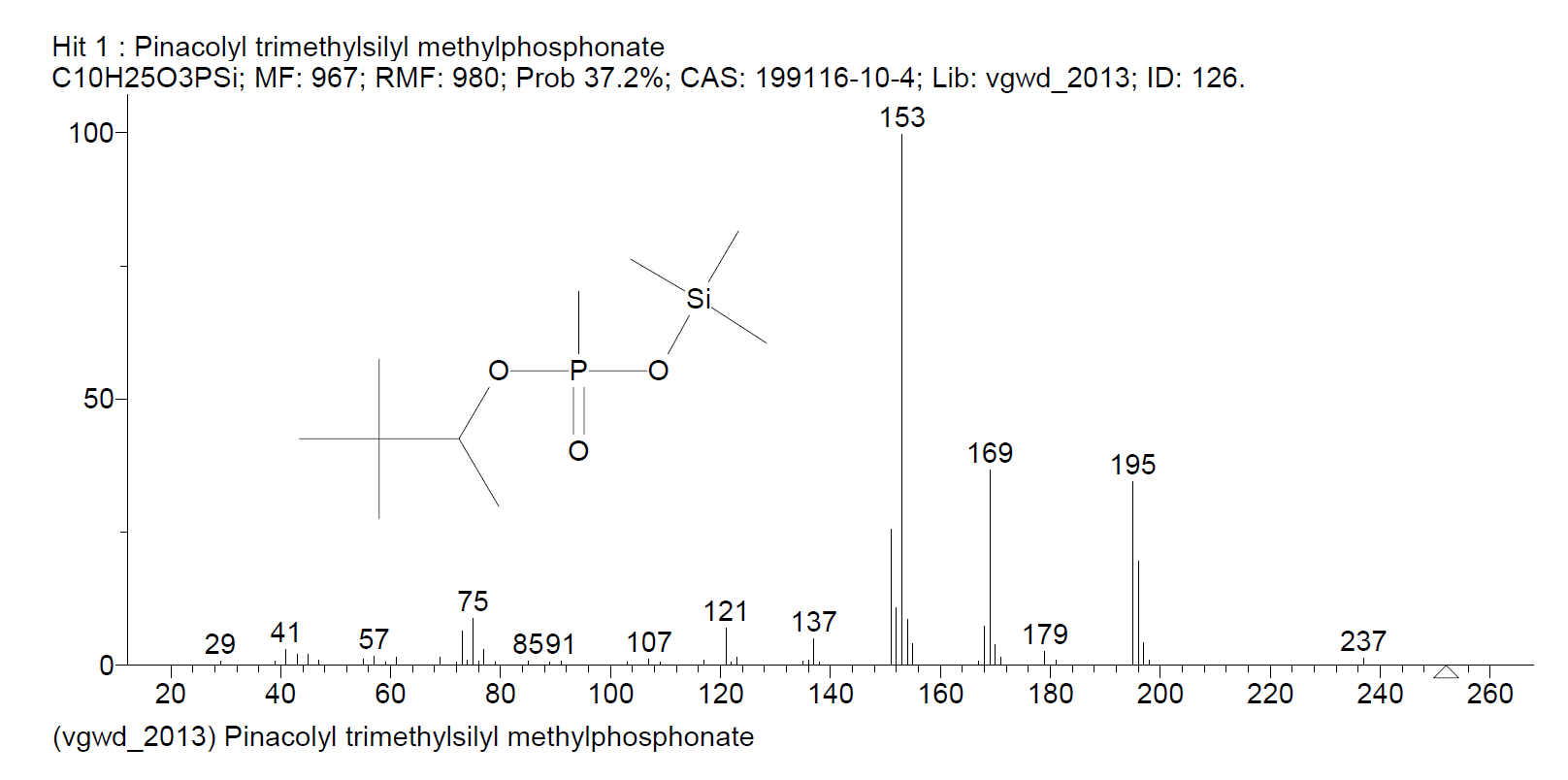
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**Fig. S8** Mass spectrometry of silylated product CH5O3P of GD detected by GC/MS (Agilent 7890A GC & Agilent 5975C MSD) and the corresponding reference spectrum.



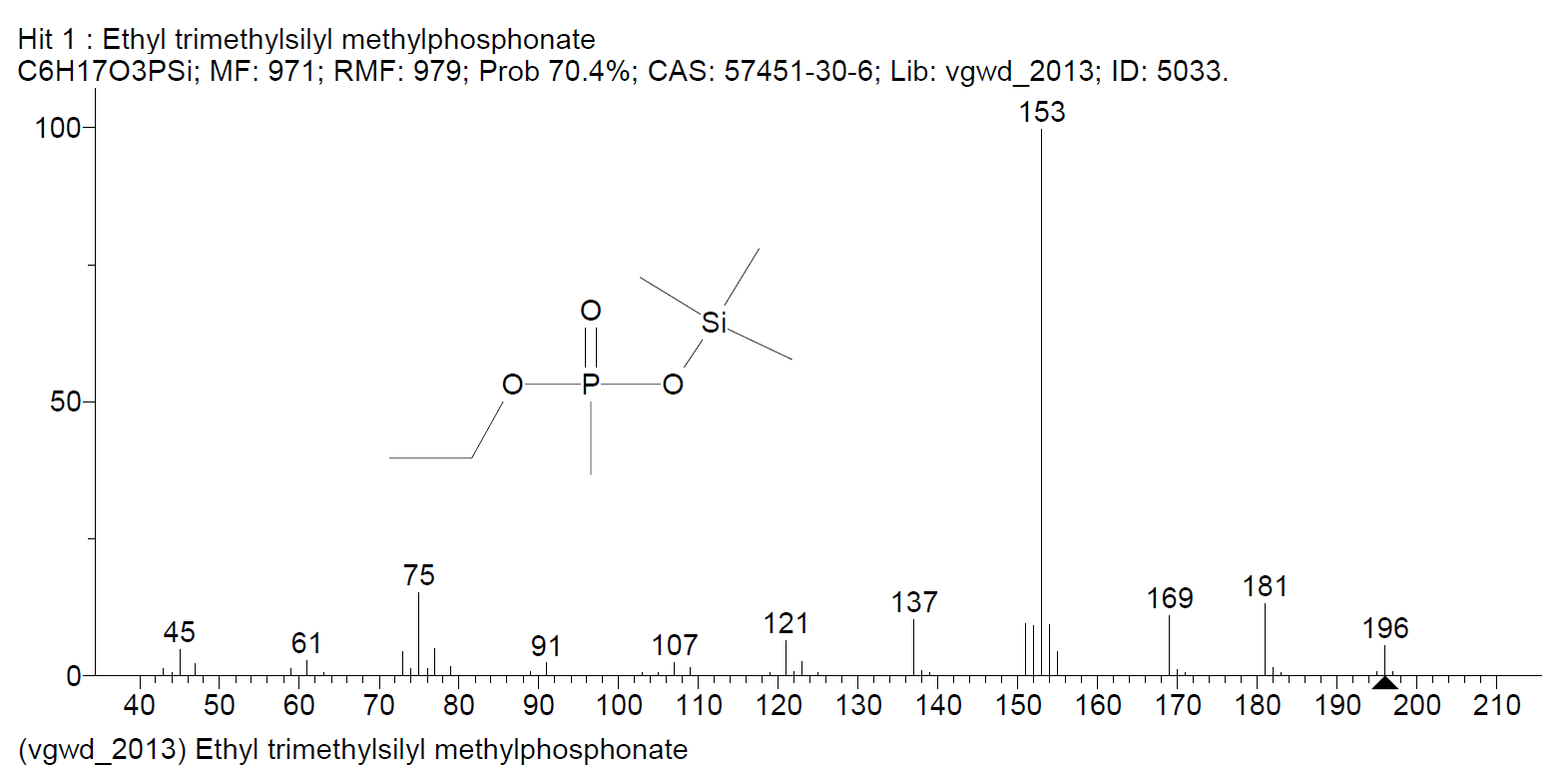
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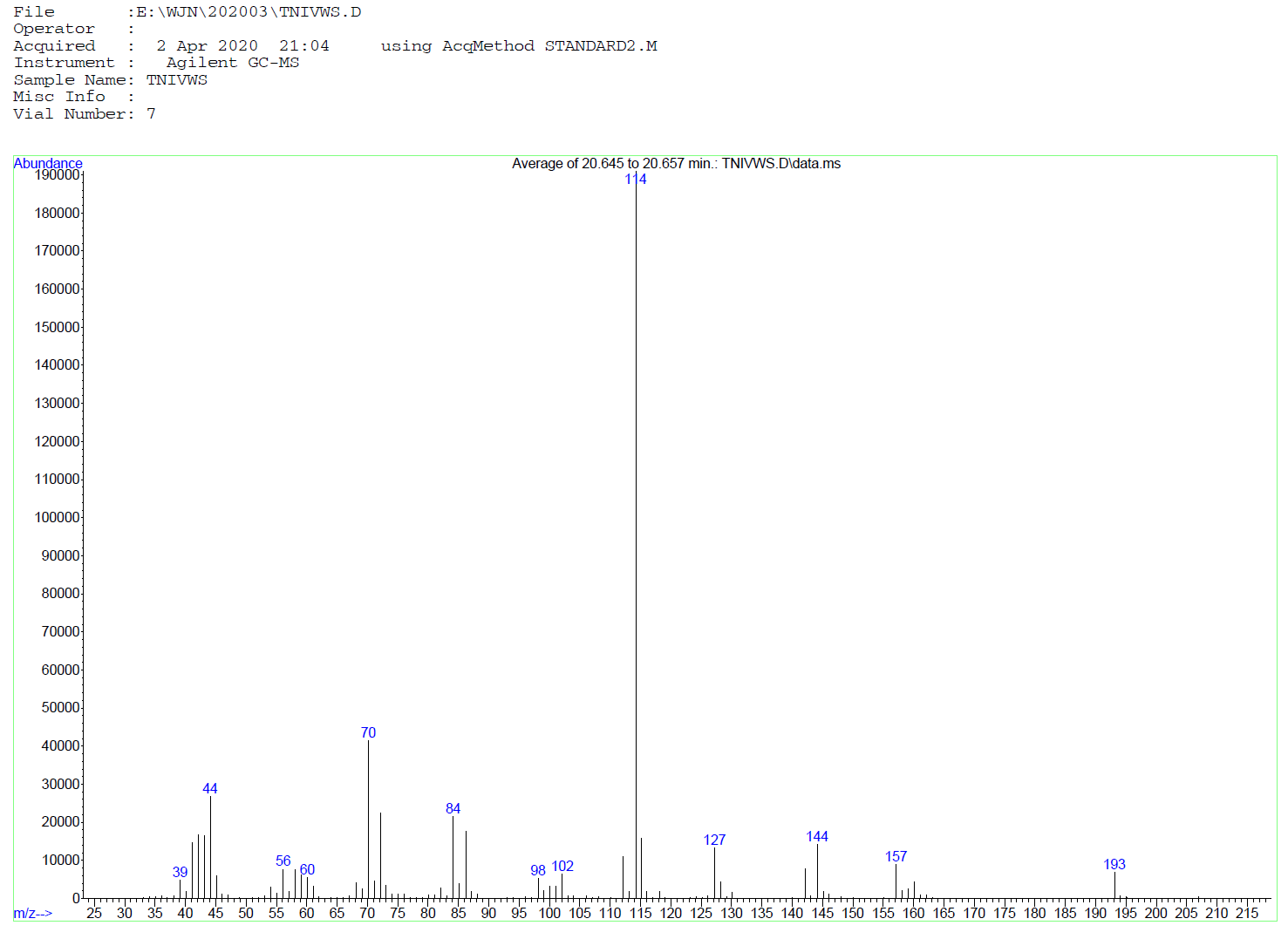
**Fig. S9** Mass spectrometry of silylated product C7H17O3P of GD detected by GC/MS (Agilent 7890A GC & Agilent 5975C MSD) and the corresponding reference spectrum.



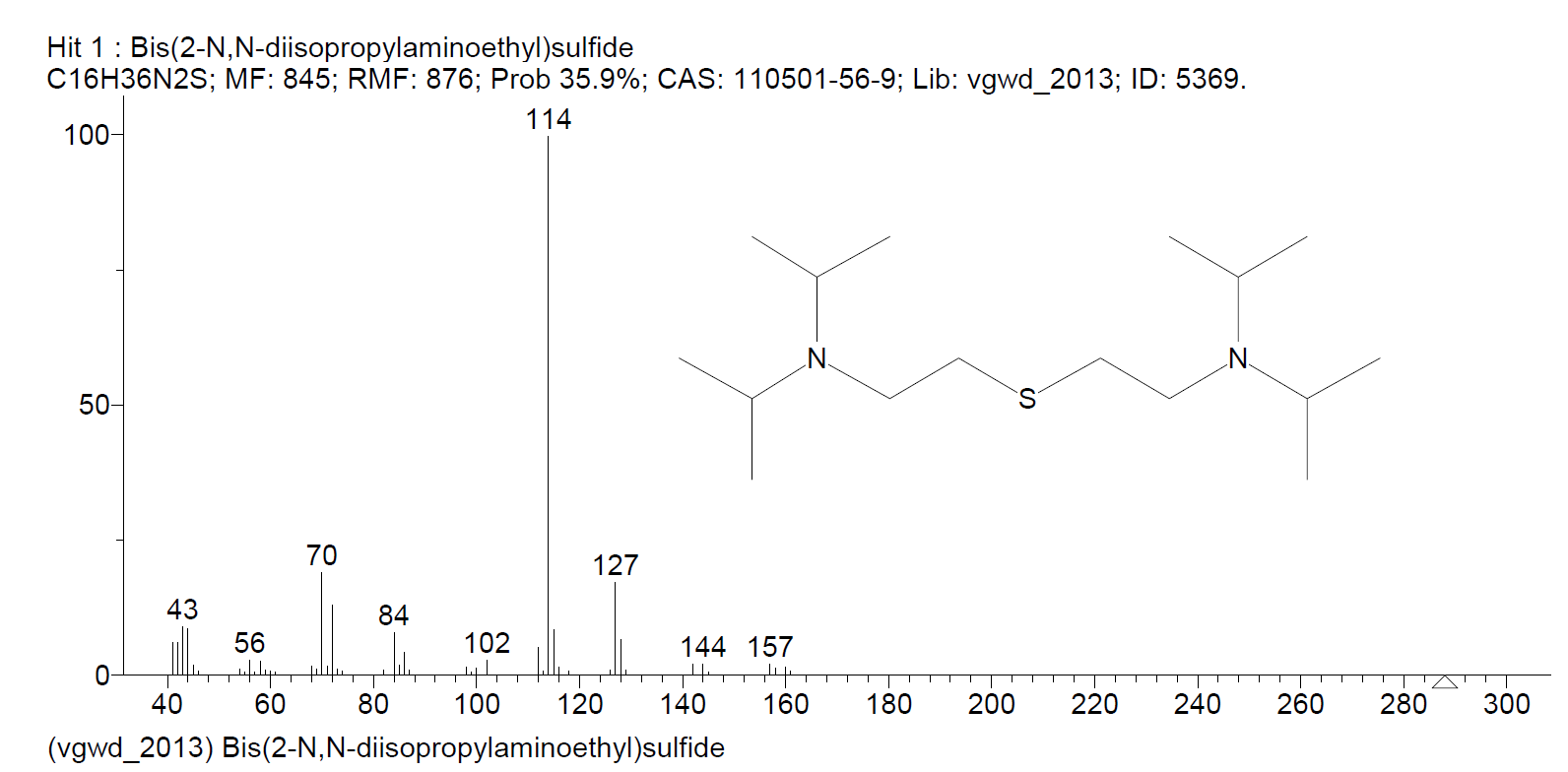
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**Fig. S10** Mass spectrometry of silylated product C3H9O3P of VX detected by GC/MS (Agilent 7890A GC & Agilent 5975C MSD) and the corresponding reference spectrum.

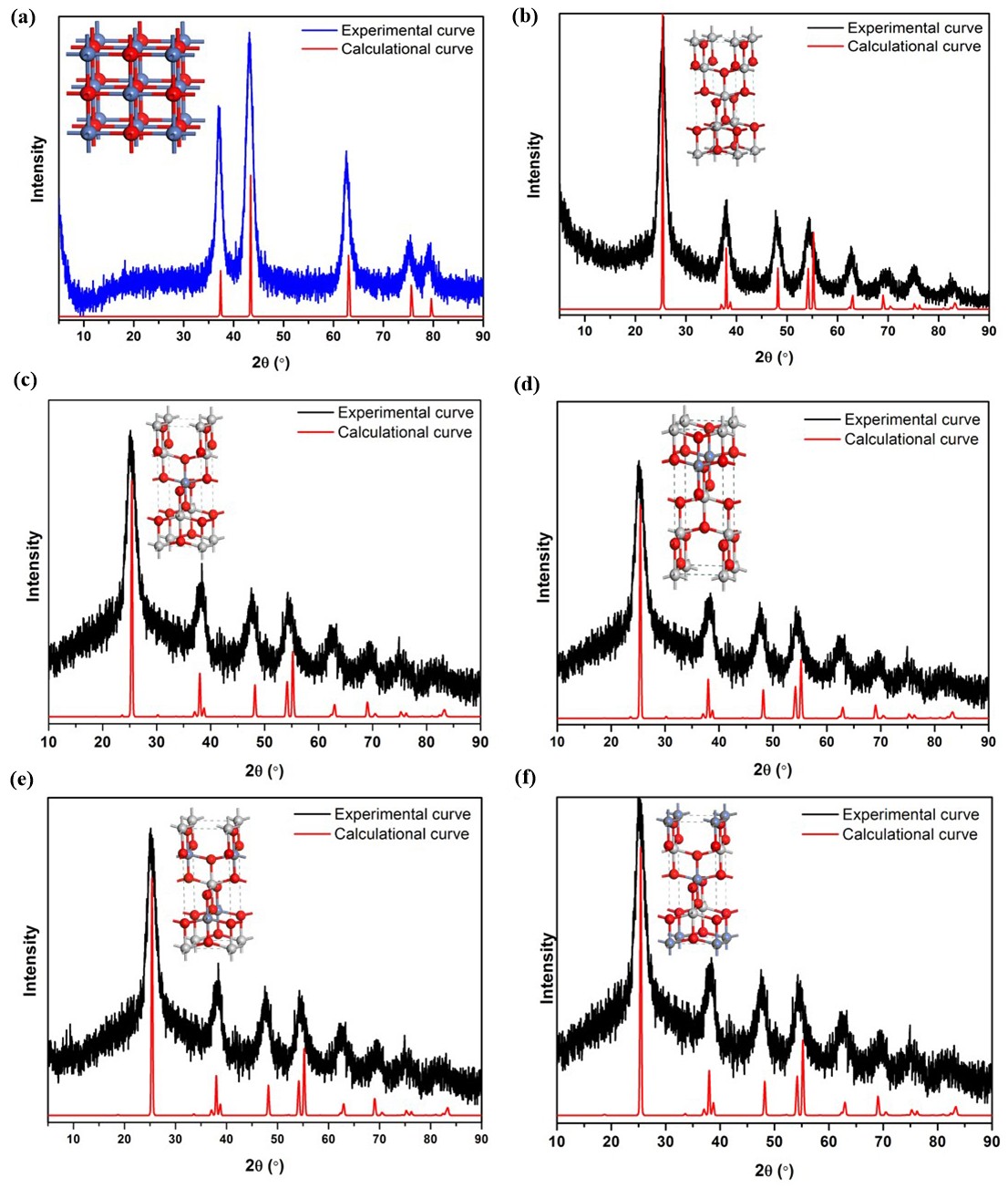


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**Fig. S11** Mass spectrometry of silylated product C16H36N2S of VX detected by GC/MS (Agilent 7890A GC & Agilent 5975C MSD) and the corresponding reference spectrum.

**XRD spectra of the computational model of anatase TiO2**



**Fig. S12.** The calculational and experimental XRD spectra of the NiO crystal (a)、anatase TiO2 (b) and the different structures of Ni2+ dopped anatase TiO2 (c-f).

**Surface structures of TiO2 (101) surface with HD/GD molecule**



**Fig. S13.** The optimal surface structures of the anatase TiO2 (101) surface with and without doping of Ni2+ and HD/GD molecule. The calculated interaction energies between the surface structures (TiO2-OH, TiO2-OH-Ni-1) and HD are 6.52, 7.18 kcal/mol, respectively. The calculated interaction energies between the surface structures (TiO2-OH, TiO2-OH-Ni-1) and GD are 7.90, 8.41 kcal/mol, respectively.