Electronic supporting information for

Quantitative detection of C-deuterated drugs by CARS microscopy and Raman microspectroscopy

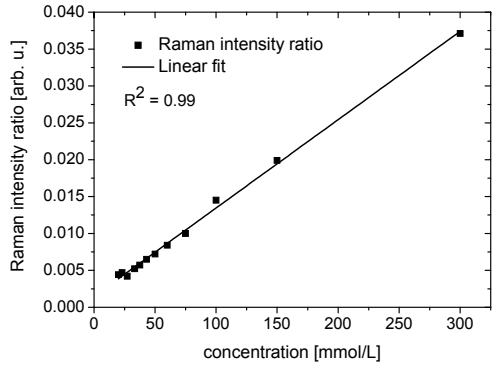


Fig. S1 Concentration-dependent Raman measurements of d_9-etacrynic acid. The intensity ratio between the Raman band at 2230 cm^{-1} and the band of the solvent DMSO at 1045 cm^{-1} is plotted against the concentration.

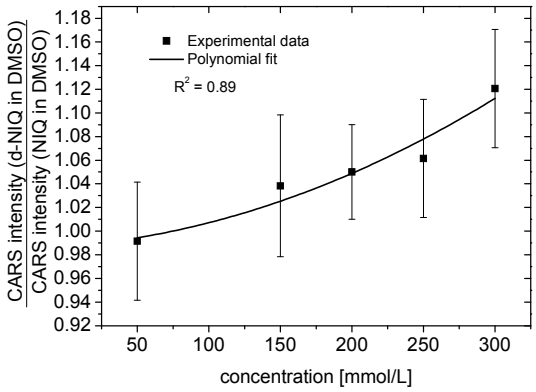


Fig. S2 Concentration-dependent CARS measurements of d_5-NIQ dissolved in a 15 µM β-carotene solution in DMSO *vs.* dissolved undeuterated NIQ. The intensity ratio between the two channels is plotted against the concentration of dissolved d_5-NIQ.

Table S1. DFT calculated harmonic wavenumbers of C-D stretching vibrations in the region ~2100-2300 cm^{-1} (compounds A-C in Fig. 1).

Compound **A**

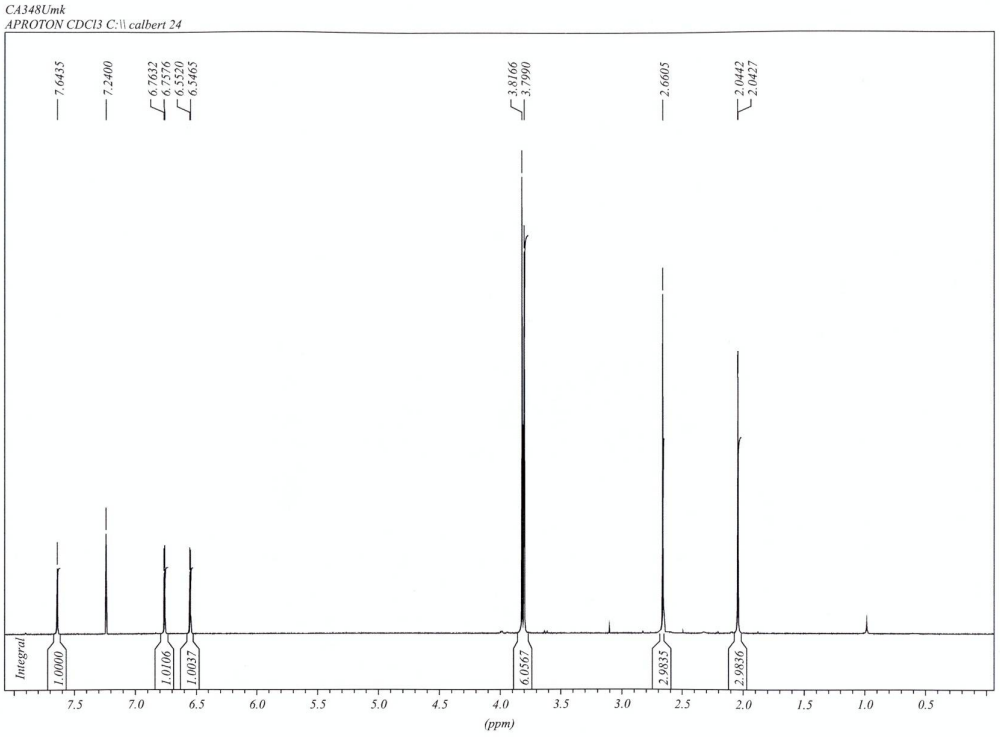
Wavenumber [cm^{-1}] (intensity %)	**Molecular subunit**
2295 (3)	Benzene ring
2298 (89)	Benzene ring
2307 (100)	Benzene ring
2316 (53)	Benzene ring
2326 (96)	Benzene ring

Compound **B**

Wavenumber [cm^{-1}] (intensity %)	**Molecule part**
2129 (7)	CD_2 (acid part)
2131 (12)	CD_3 group
2154 (17)	aliphat. CD_2
2203 (39)	CD_2 (acid part)
2207 (61)	aliphat. CD_2
2243 (24)	CD_3 group
2250 (100)	CD_3 group
2250 (18)	olefin. CD_2
2355 (36)	olefin. CD_2

Compound **C**

Wavenumber [cm^{-1}] (intensity %)	**Molecule part**
2126 (5)	CD_3 (hexane part)
2131 (5)	Hexane part
2132 (8)	CD_3 (butene part)
2134 (0)	Hexane part
2142 (9)	Hexane part
2144 (1)	Hexane part
2146 (1)	CD_2 (acid part)
2154 (11)	aliphat. CD_2 (butene part)
2156 (13)	Hexane part
2186 (100)	Hexane part
2197 (1)	Hexane part
2206 (38)	aliphat. CD_2 (butene part)
2211 (27)	Hexane part
2218 (3)	Hexane part
2230 (22)	CD_2 (acid part)
2238 (17)	Hexane part
2243 (15)	aliphat. (butene part)
2244 (54)	CD_3 (hexane part)
2246 (11)	Hexane part
2250 (64)	Butene part
2250 (13)	Butene part
2355 (23)	olefin. CD_2



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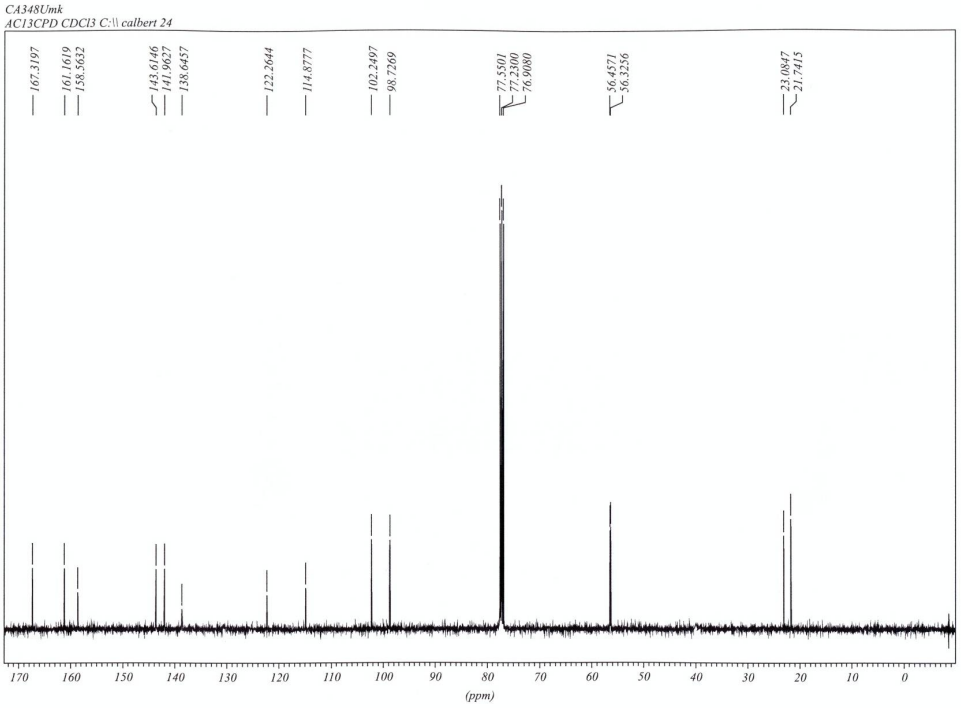

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