

Supporting information

Assessing CaDPA Levels, Metabolic Activity, and Spore Detection through Deuterium Labeling

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Supporting information

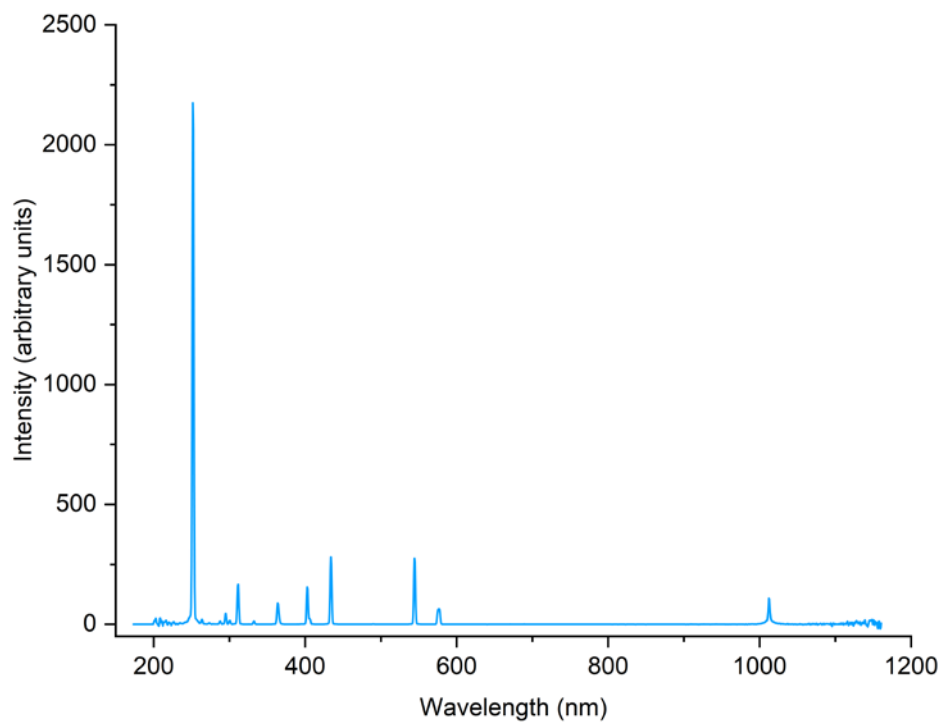


Fig. S1: Emission profile of Hg-lamp used for UV-decontamination. The most intense emission line is situated at 253.7 nm.

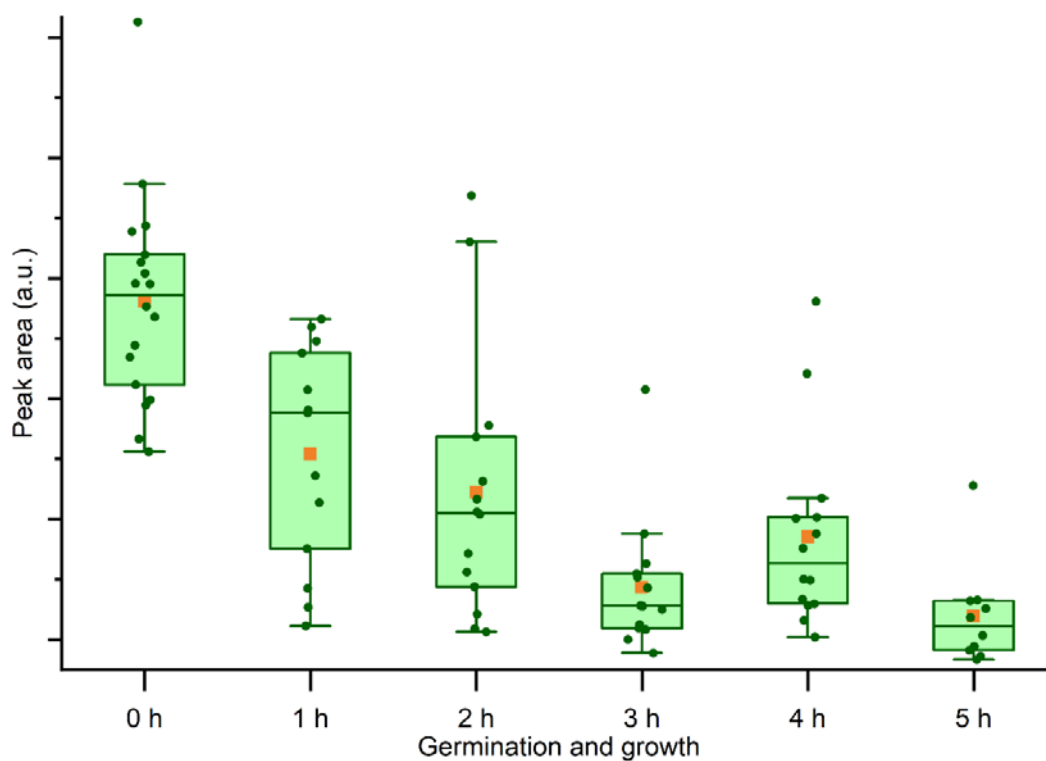


Fig. S2: Area of 2183 cm⁻¹ Raman peak upon growth of deuterated spores in non-deuterated TSA. The loss of Intensity of the peak indicating the germination and growth of the spores to cell and subsequent division.

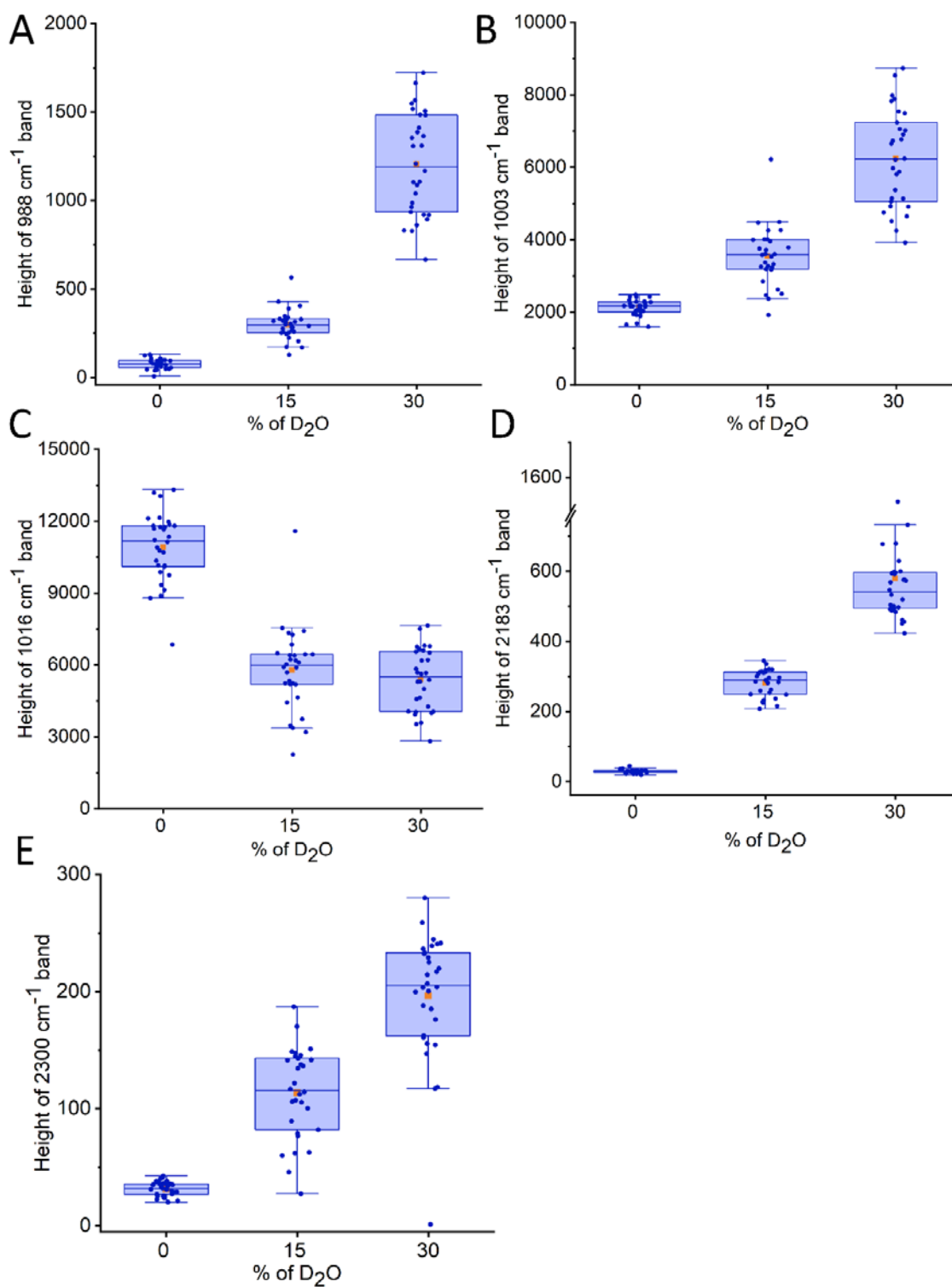


Fig. S3: Differences in the peak intensity of various Raman peaks in spore spectra, depending on the deuterium content of the growth media. The height reported here is the maximum height of the indicated Raman peaks. For each measurement, data are collected from 30 spores. The orange square represents the mean.

Supporting information

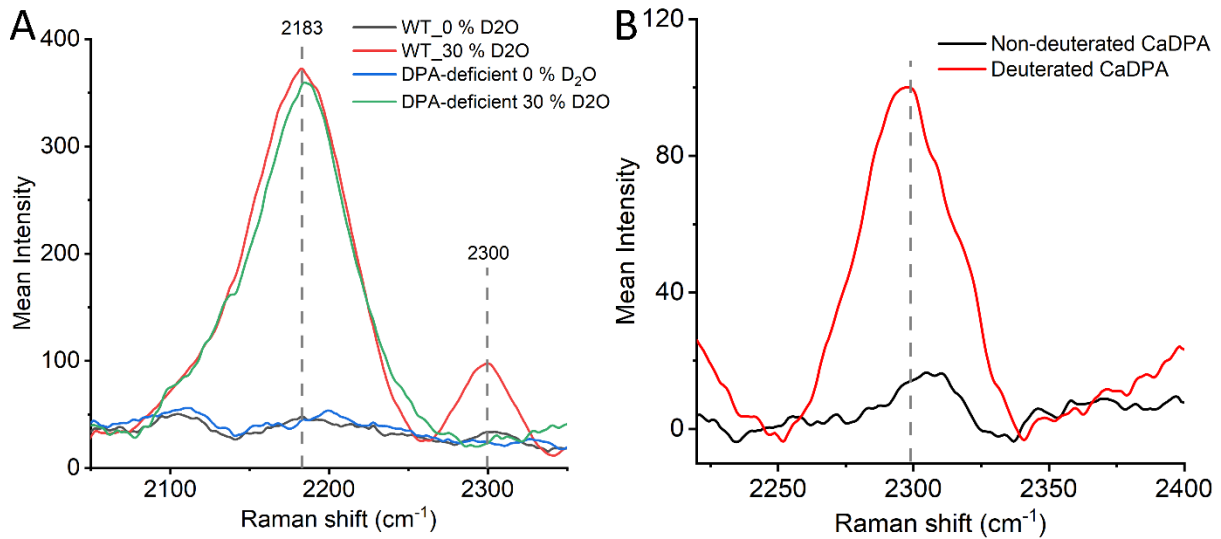


Fig. S4: Comparison of spores' Raman spectra (2200 cm⁻¹ region, C-D stretching) between WT and DPA deficient mutants of *B. Subtilis* prepared in non-deuterated and 30 % deuterium infused TSA (A). Raman spectra of CaDPA in its native spore environment is obtained by subtraction of DPA-deficient spectra from WT, shows the presence of 2300 cm⁻¹ peak in deuterated CaDPA (B).

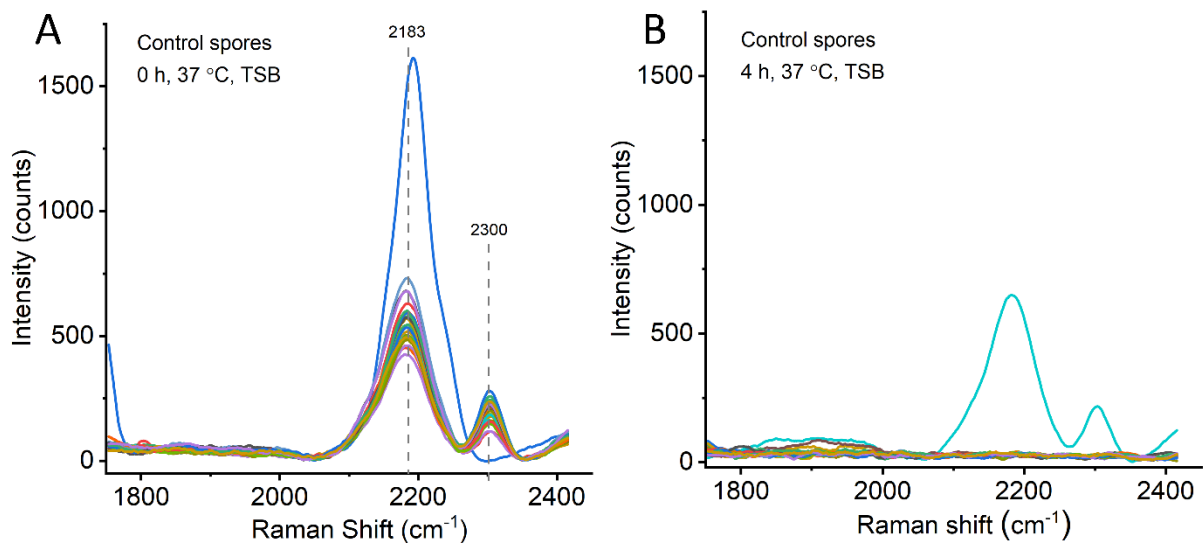


Fig S5: Raman spectra of control deuterium labelled spores of *B. cereus*, prepared using 30 % infused D₂O in TSA (A). After 4 hours of growth in non-deuterated TSA, resulting in loss of Raman intensity of the peaks associated with C-D bond vibration, indicating germination and subsequent cell division (B). (n = 30)

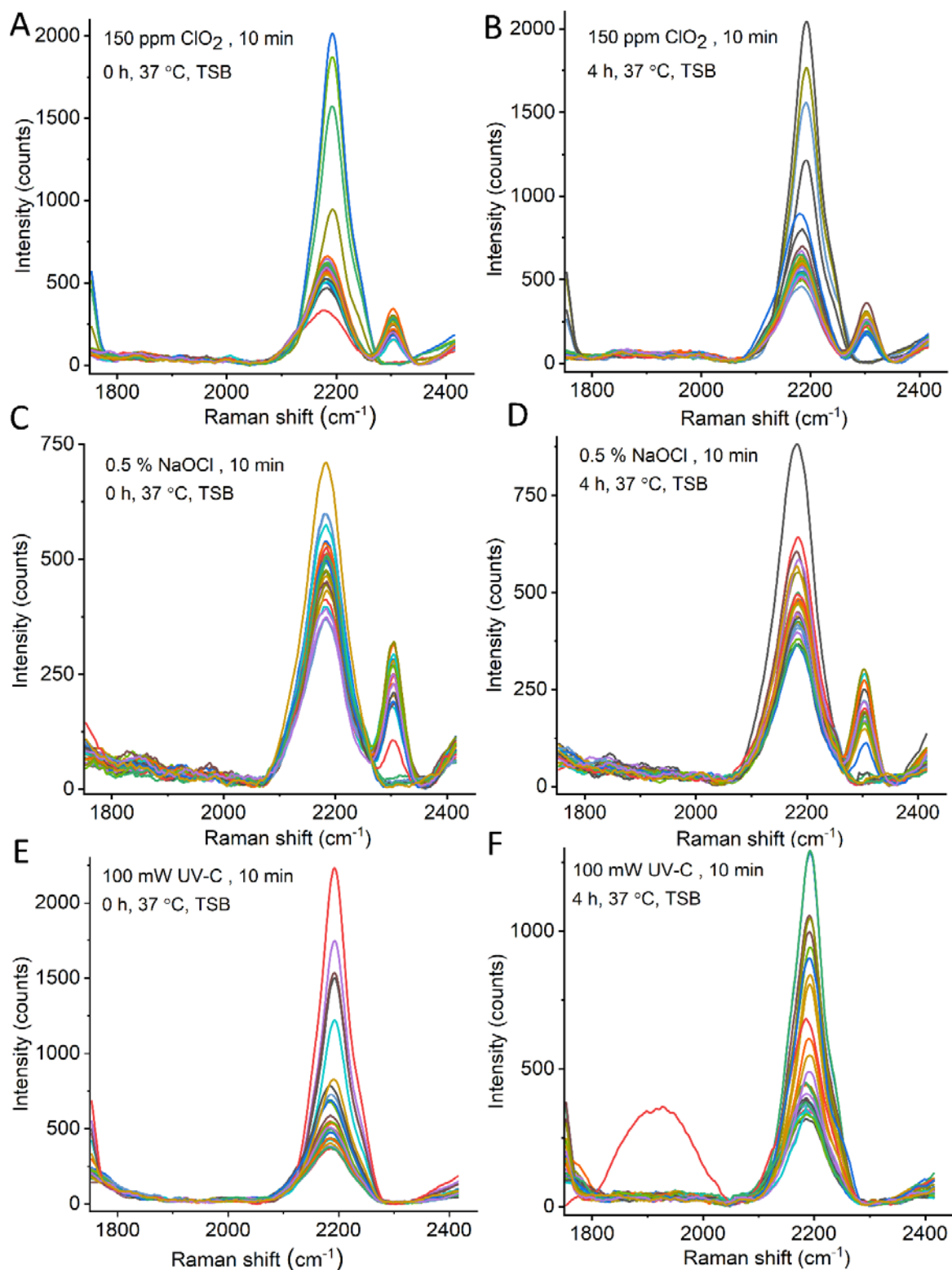


Fig S6: Raman spectra of deuterium labelled spores of *B. cereus*, after decontamination with different decontaminant *viz.* Chlorine dioxide (A), Sodium hypochlorite (C) and Ultraviolet-C radiation (E). After decontamination the spores are grown for 4 hours at 37 °C in non-deuterated TSA to check their viability. Figure B, D, and F represent Raman spectra of spores after 4 h of growth which are decontaminated in Chlorine dioxide (B), Sodium hypochlorite (D) and Ultraviolet-C radiation (F) respectively. (n = 30)

Table S1: DFT calculated Raman fingerprint for DPA and H-D substituted isotopologues.

Substituted H-atoms: none		Substituted H-atoms: 1-5		Substituted H-atoms: 4	
Raman shift (cm ⁻¹)	Intensity	Raman shift (cm ⁻¹)	Intensity	Raman shift (cm ⁻¹)	Intensity
43.8	1.0	43.1	1.1	43.8	1.0
48.8	0.0	48.3	0.0	48.5	0.0
133.3	0.5	129.3	0.4	133.2	0.5
148.4	2.8	142.6	2.4	146.5	2.4
163.6	6.3	150.5	4.8	163.6	6.3
254.7	0.3	245.2	0.3	252.8	0.3
351.8	7.3	348.6	7.2	351.7	7.3
383.5	2.3	369.3	2.3	380.9	2.4
426.4	0.1	382.3	0.0	397.7	0.0
459.6	1.2	392.7	1.8	459.6	1.2
461.9	2.3	438.3	1.9	461.1	2.4
556.3	1.0	450.8	2.2	550.3	0.9
581.0	4.5	501.7	2.9	574.3	3.4
610.9	6.5	536.6	1.0	610.9	6.5
631.7	0.6	584.5	0.9	625.5	1.4
642.1	0.4	592.4	0.2	641.9	0.4
716.3	0.8	592.7	1.1	684.4	1.2
721.7	41.3	669.8	31.4	715.1	41.2
757.6	0.5	687.5	0.5	723.7	0.5
808.9	2.5	750.8	3.9	808.9	2.5
865.9	0.9	785.4	0.3	812.4	1.7
873.3	6.1	801.1	1.1	825.2	0.8
970.8	0.2	826.0	1.9	942.3	9.7
989.4	86.0	840.0	0.5	966.3	0.1
1021.1	0.1	875.7	1.0	970.8	0.2
1071.4	2.6	876.9	8.5	979.0	84.8
1096.2	6.8	973.9	95.2	1052.4	4.9
1106.2	1.6	975.6	1.5	1093.4	15.8
1147.4	8.3	972.7	35.9	1094.4	1.4
1186.4	16.7	982.9	0.1	1169.1	9.1
1198.8	159.6	1096.7	30.3	1182.1	158.6
1287.4	7.4	1212.4	31.2	1266.6	8.6
1345.2	15.1	1263.4	6.9	1311.5	8.1
1367.7	96.0	1297.6	121.1	1350.5	85.8
1418.0	3.8	1360.9	59.7	1402.2	6.3
1453.1	38.0	1369.9	38.8	1407.0	35.7
1573.8	119.8	1534.9	131.9	1547.4	128.4
1581.5	166.3	1535.2	176.7	1557.4	172.7
1712.4	31.0	1688.8	28.3	1694.7	30.1
1718.4	274.5	1694.4	277.6	1700.7	276.1
3042.4	173.4	2247.3	71.4	2253.7	114.8
3063.3	108.0	2264.9	41.8	3063.1	299.1
3066.1	387.4	2272.3	158.3	3063.3	108.1
3547.0	146.7	2580.4	71.0	3547.0	146.7
3547.1	282.3	2580.6	140.7	3547.1	282.4

Supporting information

Substituted H-atoms: 3		Substituted H-atoms: 3,4		Substituted H-atoms: 3,5	
Raman shift (cm ⁻¹)	Intensity	Raman shift (cm ⁻¹)	Intensity	Raman shift (cm ⁻¹)	Intensity
43.8	1.0	43.8	1.0	43.8	1.0
48.7	0.0	48.5	0.0	48.6	0.0
133.1	0.5	133.0	0.5	132.9	0.5
147.6	2.7	145.8	2.3	147.4	2.5
157.9	5.6	157.8	5.6	152.0	4.9
252.8	0.3	250.9	0.3	250.9	0.3
351.0	7.3	350.9	7.4	350.2	7.4
379.5	2.3	377.3	2.3	376.0	2.3
419.0	0.1	392.4	0.0	413.8	0.2
450.6	0.6	449.3	0.6	440.7	0.2
460.6	2.3	459.9	2.5	459.4	2.4
549.1	1.2	544.3	1.1	542.7	1.4
580.6	4.5	574.2	3.3	579.3	4.3
606.7	7.8	605.4	7.8	606.3	8.2
629.4	0.5	622.8	1.3	613.3	0.3
640.0	0.4	639.4	0.4	626.3	0.5
661.1	0.3	640.4	0.3	638.2	0.4
719.6	0.5	700.4	1.6	719.3	0.5
721.5	40.6	714.9	40.6	721.2	39.8
803.5	2.7	790.5	1.8	752.6	2.9
846.6	1.5	805.6	0.2	826.7	1.3
858.8	0.9	810.9	2.0	840.2	0.4
872.7	7.6	858.2	0.7	848.1	1.7
905.2	0.1	869.8	5.3	865.5	5.4
967.1	89.9	951.5	7.0	905.1	2.8
996.9	0.1	968.3	0.2	973.9	94.2
1077.1	3.2	967.2	89.8	980.0	0.2
1086.3	3.5	1071.1	2.6	1084.1	0.3
1113.2	2.9	1093.0	9.8	1085.7	4.4
1163.9	25.5	1138.7	17.6	1160.6	25.2
1186.0	156.5	1181.4	153.5	1183.8	158.9
1273.4	6.9	1265.5	8.5	1273.0	6.7
1324.2	9.1	1295.0	3.1	1321.9	6.6
1347.5	72.3	1343.3	61.7	1330.5	32.6
1384.8	32.3	1381.0	47.2	1376.1	57.4
1423.2	32.9	1399.7	20.3	1402.7	41.3
1551.3	125.4	1540.1	132.9	1542.0	169.8
1555.3	164.8	1548.3	170.6	1545.8	126.8
1694.7	31.0	1694.6	30.2	1694.6	30.8
1700.6	275.5	1700.6	276.9	1700.5	276.6
2265.6	75.6	2249.9	79.9	2265.1	41.3
3043.9	206.0	2269.2	113.0	2266.0	110.0
3064.8	261.4	3063.2	203.6	3045.6	266.1
3547.0	146.8	3547.0	146.8	3547.0	146.9
3547.1	282.1	3547.1	282.3	3547.1	282.0

Supporting information

Substituted H-atoms: 3,4,5		Substituted H-atoms: 1		Substituted H-atoms: 1,2	
Raman shift (cm ⁻¹)	Intensity	Raman shift (cm ⁻¹)	Intensity	Raman shift (cm ⁻¹)	Intensity
43.8	1.0	43.4	1.1	43.1	1.1
48.4	0.0	48.7	0.0	48.7	0.0
132.8	0.5	131.5	0.5	129.7	0.4
145.6	2.2	146.8	3.0	145.4	3.1
152.0	4.9	162.8	6.2	161.8	6.2
249.0	0.3	252.6	0.4	250.5	0.4
350.2	7.4	351.0	7.2	350.3	7.2
374.0	2.3	381.2	2.3	379.0	2.3
387.3	0.0	405.0	1.8	401.2	3.3
440.7	0.2	432.9	1.1	408.0	0.3
458.8	2.5	457.7	2.1	453.4	2.0
538.7	1.2	493.1	1.3	454.9	2.1
573.9	3.1	554.9	0.9	516.1	1.2
593.5	0.6	593.1	1.6	553.2	0.7
606.3	8.2	597.7	5.4	588.2	0.9
619.6	1.2	635.1	0.9	598.4	2.1
637.4	0.4	703.2	34.7	683.0	31.3
698.8	1.6	712.3	0.5	707.8	0.1
714.8	40.0	757.4	0.6	757.2	0.7
752.6	2.9	808.4	2.8	807.9	3.1
801.4	0.9	857.8	7.8	841.2	5.3
801.5	0.0	865.9	0.9	865.9	0.9
826.3	1.4	970.8	0.2	970.8	0.2
840.2	0.4	976.8	63.0	971.6	63.9
875.7	1.0	980.1	38.6	979.8	55.8
891.1	8.9	1010.7	0.1	982.0	0.5
973.9	94.2	1062.1	5.6	1010.7	0.1
980.3	1.8	1090.8	5.5	1064.7	11.7
1078.7	0.4	1117.1	15.9	1114.4	23.3
1113.7	23.0	1136.8	10.0	1120.2	0.1
1177.8	157.1	1178.5	68.0	1138.6	5.1
1263.3	8.0	1260.4	55.1	1242.4	44.6
1286.0	2.5	1306.6	53.0	1303.2	9.3
1324.0	24.1	1346.1	90.1	1317.6	196.7
1375.9	60.7	1402.3	3.7	1401.4	3.9
1380.4	40.2	1437.5	37.2	1436.7	36.4
1534.9	132.1	1557.7	119.8	1557.7	119.8
1535.3	175.1	1565.3	167.4	1565.2	168.6
1694.6	30.1	1690.7	65.6	1689.0	29.2
1700.5	277.8	1699.0	238.6	1694.8	273.7
2247.3	71.4	2580.5	106.1	2580.4	70.9
2264.9	41.8	3042.4	173.3	2580.6	141.2
2272.3	158.0	3063.3	107.9	3042.4	173.2
3547.0	146.9	3066.1	387.5	3063.3	107.8
547.1	282.2	3547.1	214.5	3066.1	387.6