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Studies on the formation of formaldehyde during 2-ethylhexyl 4-(dimethylamino)benzoate demethylation in the presence of reactive oxygen and chlorine species

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I. Selected quantum-chemical calculations results

Table S1 Bond lengths of optimized 2-ethylhexyl 4-(dimethylamino)benzoate (ODPABA) molecule (atoms numbering according to Fig. 3a)

| No. | Atom1 | Atom2 | Cyclicity | Length [Å] |
|-----|-------|-------|-----------|------------|
| 1   | H1    | C36   | acyclic   | 1.0905     |
| 2   | H2    | C36   | acyclic   | 1.1005     |
| 3   | H3    | C36   | acyclic   | 1.0964     |
| 4   | H4    | C47   | acyclic   | 1.0906     |
| 5   | H5    | C47   | acyclic   | 1.1004     |
| 6   | H6    | C47   | acyclic   | 1.0963     |
| 7   | H7    | C34   | acyclic   | 1.0827     |
| 8   | H8    | C33   | acyclic   | 1.0852     |
| 9   | H9    | C30   | acyclic   | 1.0828     |
| 10  | H10   | C31   | acyclic   | 1.0843     |
| 11  | H11   | C43   | acyclic   | 1.0949     |
| 12  | H12   | C43   | acyclic   | 1.0963     |
| 13  | H13   | C39   | acyclic   | 1.1003     |
| 14  | H14   | C41   | acyclic   | 1.0957     |
| 15  | H15   | C41   | acyclic   | 1.1000     |
| 16  | H16   | C45   | acyclic   | 1.0967     |
| 17  | H17   | C45   | acyclic   | 1.0954     |
| 18  | H18   | C45   | acyclic   | 1.0953     |
| 19  | H19   | C42   | acyclic   | 1.0998     |
| 20  | H20   | C40   | acyclic   | 1.0993     |
| 21  | H21   | C40   | acyclic   | 1.0988     |
| 22  | H22   | C42   | acyclic   | 1.0983     |
| 23  | H23   | C46   | acyclic   | 1.0965     |
| 24  | H24   | C44   | acyclic   | 1.0990     |
| 25  | H25   | C44   | acyclic   | 1.0990     |
| 26  | H26   | C46   | acyclic   | 1.0954     |
| 27  | H27   | C46   | acyclic   | 1.0966     |
| 28  | C28   | C32   | acyclic   | 1.4795     |
| 29  | C28   | O37   | acyclic   | 1.3580     |
| 30  | C28   | O38   | acyclic   | 1.2212     |
| 31  | C29   | C34   | cyclic    | 1.4194     |
| No. | Atom1 | Atom2 | Cyclicity | Length [Å] |
|-----|-------|-------|-----------|------------|
| 32  | C29   | C30   | cyclic    | 1.4188     |
| 33  | C29   | N35   | acyclic   | 1.3810     |
| 34  | C30   | C31   | cyclic    | 1.3888     |
| 35  | C31   | C32   | cyclic    | 1.4039     |
| 36  | C32   | C33   | cyclic    | 1.4038     |
| 37  | C33   | C34   | cyclic    | 1.3872     |
| 38  | N35   | C47   | acyclic   | 1.4554     |
| 39  | N35   | C36   | acyclic   | 1.4552     |
| 40  | O37   | C43   | acyclic   | 1.4451     |
| 41  | C39   | C40   | acyclic   | 1.5538     |
| 42  | C39   | C41   | acyclic   | 1.5428     |
| 43  | C39   | C43   | acyclic   | 1.5292     |
| 44  | C40   | C42   | acyclic   | 1.5366     |
| 45  | C41   | C45   | acyclic   | 1.5332     |
| 46  | C42   | C44   | acyclic   | 1.5342     |
| 47  | C44   | C46   | acyclic   | 1.5331     |

Table S2 Bond angles of optimized 2-ethylhexyl 4-(dimethylamino)benzoate (ODPABA) molecule (atoms numbering according to Fig. 3a)

| No. | Atom1 | Atom2 | Atom3 | Angle [°] |
|-----|-------|-------|-------|-----------|
| 1   | C32   | C28   | O37   | 112.81    |
| 2   | C32   | C28   | O38   | 124.66    |
| 3   | O37   | C28   | O38   | 122.53    |
| 4   | C34   | C29   | C30   | 117.36    |
| 5   | C34   | C29   | N35   | 121.31    |
| 6   | C30   | C29   | N35   | 121.34    |
| 7   | H9    | C30   | C29   | 120.41    |
| 8   | H9    | C30   | C31   | 118.56    |
| 9   | C29   | C30   | C31   | 121.03    |
| 10  | H10   | C31   | C30   | 119.31    |
| 11  | H10   | C31   | C32   | 119.49    |
| 12  | C30   | C31   | C32   | 121.20    |
| 13  | C28   | C32   | C31   | 123.21    |
| 14  | C28   | C32   | C33   | 118.69    |
| 15  | C31   | C32   | C33   | 118.10    |
| 16  | H8    | C33   | C32   | 118.57    |
| 17  | H8    | C33   | C34   | 120.04    |
| 18  | C32   | C33   | C34   | 121.39    |
| 19  | H7    | C34   | C29   | 120.45    |
| 20  | H7    | C34   | C33   | 118.64    |
| 21  | C29   | C34   | C33   | 120.91    |
| 22  | C29   | N35   | C47   | 119.96    |
| 23  | C29   | N35   | C36   | 119.97    |
| 24  | C47   | N35   | C36   | 118.78    |
| No. | Atom1 | Atom2 | Atom3 | Angle [°] |
|-----|-------|-------|-------|-----------|
| 25  | H1    | C36   | H2    | 108.21    |
| 26  | H1    | C36   | H3    | 107.64    |
| 27  | H1    | C36   | N35   | 109.09    |
| 28  | H2    | C36   | H3    | 108.15    |
| 29  | H2    | C36   | N35   | 112.39    |
| 30  | H3    | C36   | N35   | 111.21    |
| 31  | C28   | O37   | C43   | 116.24    |
| 32  | H13   | C39   | C40   | 108.42    |
| 33  | H13   | C39   | C41   | 108.02    |
| 34  | H13   | C39   | C43   | 106.94    |
| 35  | C40   | C39   | C41   | 113.18    |
| 36  | C40   | C39   | C43   | 108.98    |
| 37  | C41   | C39   | C43   | 111.06    |
| 38  | H20   | C40   | H21   | 105.44    |
| 39  | H20   | C40   | C39   | 109.69    |
| 40  | H20   | C40   | C42   | 107.96    |
| 41  | H21   | C40   | C39   | 109.47    |
| 42  | H21   | C40   | C42   | 109.38    |
| 43  | C39   | C40   | C42   | 114.49    |
| 44  | H14   | C41   | H15   | 106.27    |
| 45  | H14   | C41   | C39   | 108.52    |
| 46  | H14   | C41   | C45   | 109.05    |
| 47  | H15   | C41   | C39   | 108.44    |
| 48  | H15   | C41   | C45   | 109.36    |
| 49  | C39   | C41   | C45   | 114.86    |
| 50  | H19   | C42   | H22   | 105.98    |
| 51  | H19   | C42   | C40   | 108.95    |
| 52  | H19   | C42   | C44   | 109.17    |
| 53  | H22   | C42   | C40   | 109.81    |
| 54  | H22   | C42   | C44   | 109.25    |
| 55  | C40   | C42   | C44   | 113.41    |
| 56  | H11   | C43   | H12   | 107.66    |
| 57  | H11   | C43   | O37   | 108.42    |
| 58  | H11   | C43   | C39   | 111.19    |
| 59  | H12   | C43   | O37   | 108.95    |
| 60  | H12   | C43   | C39   | 111.56    |
| 61  | O37   | C43   | C39   | 108.97    |
| 62  | H24   | C44   | H25   | 106.04    |
| 63  | H24   | C44   | C42   | 109.20    |
| 64  | H24   | C44   | C46   | 109.43    |
| 65  | H25   | C44   | C42   | 109.21    |
| 66  | H25   | C44   | C46   | 109.42    |
| 67  | C42   | C44   | C46   | 113.28    |
| 68  | H16   | C45   | H17   | 107.59    |
| No. | Atom1 | Atom2 | Atom3 | Angle [°] |
|-----|-------|-------|-------|-----------|
| 69  | H16   | C45   | H18   | 107.68    |
| 70  | H16   | C45   | C41   | 111.23    |
| 71  | H17   | C45   | H18   | 107.37    |
| 72  | H17   | C45   | C41   | 110.71    |
| 73  | H18   | C45   | C41   | 112.06    |
| 74  | H23   | C46   | H26   | 107.66    |
| 75  | H23   | C46   | H27   | 107.53    |
| 76  | H23   | C46   | C44   | 111.16    |
| 77  | H26   | C46   | H27   | 107.67    |
| 78  | H26   | C46   | C44   | 111.43    |
| 79  | H27   | C46   | C44   | 111.20    |
| 80  | H4    | C47   | H5    | 108.23    |
| 81  | H4    | C47   | H6    | 107.64    |
| 82  | H4    | C47   | N35   | 109.08    |
| 83  | H5    | C47   | H6    | 108.14    |
| 84  | H5    | C47   | N35   | 112.42    |
| 85  | H6    | C47   | N35   | 111.17    |

**Table S3** Dihedral angles of optimized 2-ethylhexyl 4-(dimethylamino)benzoate (ODPABA) molecule (atoms numbering according to Fig. 3a)

| No. | Atom1 | Atom2 | Atom3 | Atom4 | Dihedral angle [°] |
|-----|-------|-------|-------|-------|--------------------|
| 1   | O37   | C28   | C32   | C31   | -0.85              |
| 2   | O37   | C28   | C32   | C33   | 179.13             |
| 3   | O38   | C28   | C32   | C31   | 179.05             |
| 4   | O38   | C28   | C32   | C33   | -0.96              |
| 5   | C32   | C28   | O37   | C43   | 178.72             |
| 6   | O38   | C28   | O37   | C43   | -1.19              |
| 7   | C30   | C29   | C34   | H7    | -179.07            |
| 8   | C30   | C29   | C34   | C33   | 1.01               |
| 9   | N35   | C29   | C34   | H7    | 1.27               |
| 10  | N35   | C29   | C34   | C33   | -178.66            |
| 11  | C34   | C29   | C30   | H9    | 179.15             |
| 12  | C34   | C29   | C30   | C31   | -0.98              |
| 13  | N35   | C29   | C30   | H9    | -1.19              |
| 14  | N35   | C29   | C30   | C31   | 178.68             |
| 15  | C34   | C29   | N35   | C47   | -6.59              |
| 16  | C34   | C29   | N35   | C36   | -173.48            |
| 17  | C30   | C29   | N35   | C47   | 173.76             |
| 18  | C30   | C29   | N35   | C36   | 6.87               |
| 19  | H9    | C30   | C31   | H10   | 0.17               |
| 20  | H9    | C30   | C31   | C32   | -179.74            |
| 21  | C29   | C30   | C31   | H10   | -179.71            |
| 22  | C29   | C30   | C31   | C32   | 0.38               |
| 23  | H10   | C31   | C32   | C28   | 0.30               |
|    |     |     |     |     |     |
|----|-----|-----|-----|-----|-----|
| 24 | H10 | C31 | C32 | C33 | -179.69 |
| 25 | C30 | C31 | C32 | C28 | -179.79 |
| 26 | C30 | C31 | C32 | C33 | 0.22   |
| 27 | C28 | C32 | C33 | H8  | -0.37  |
| 28 | C28 | C32 | C33 | C34 | 179.82 |
| 29 | C31 | C32 | C33 | H8  | 179.62 |
| 30 | C31 | C32 | C33 | C34 | -0.19  |
| 31 | H8  | C33 | C34 | H7  | -0.17  |
| 32 | H8  | C33 | C34 | C29 | 179.76 |
| 33 | C32 | C33 | C34 | H7  | 179.63 |
| 34 | C32 | C33 | C34 | C29 | -0.44  |
| 35 | C29 | N35 | C47 | H4  | 177.95 |
| 36 | C29 | N35 | C47 | H5  | -62.00 |
| 37 | C29 | N35 | C47 | H6  | 59.40  |
| 38 | C36 | N35 | C47 | H4  | -15.00 |
| 39 | C36 | N35 | C47 | H5  | 105.05 |
| 40 | C36 | N35 | C47 | H6  | -133.55|
| 41 | C29 | N35 | C36 | H1  | -178.47|
| 42 | C29 | N35 | C36 | H2  | 61.52  |
| 43 | C29 | N35 | C36 | H3  | -59.90 |
| 44 | C47 | N35 | C36 | H1  | 14.48  |
| 45 | C47 | N35 | C36 | H2  | -105.53|
| 46 | C47 | N35 | C36 | H3  | 133.06 |
| 47 | C28 | O37 | C43 | H11 | -60.19 |
| 48 | C28 | O37 | C43 | H12 | 56.72  |
| 49 | C28 | O37 | C43 | C39 | 178.65 |
| 50 | H13 | C39 | C40 | H20 | 104.57 |
| 51 | H13 | C39 | C40 | H21 | -140.19|
| 52 | H13 | C39 | C40 | C42 | -16.96 |
| 53 | C41 | C39 | C40 | H20 | -135.61|
| 54 | C41 | C39 | C40 | H21 | -20.36 |
| 55 | C41 | C39 | C40 | C42 | 102.86 |
| 56 | C43 | C39 | C40 | H20 | -11.50 |
| 57 | C43 | C39 | C40 | H21 | 103.75 |
| 58 | C43 | C39 | C40 | C42 | -133.03|
| 59 | H13 | C39 | C41 | H14 | -64.90 |
| 60 | H13 | C39 | C41 | H15 | -179.93|
| 61 | H13 | C39 | C41 | C45 | 57.41  |
| 62 | C40 | C39 | C41 | H14 | 175.05 |
| 63 | C40 | C39 | C41 | H15 | 60.02  |
| 64 | C40 | C39 | C41 | C45 | -62.64 |
| 65 | C43 | C39 | C41 | H14 | 52.08  |
| 66 | C43 | C39 | C41 | H15 | -62.95 |
| 67 | C43 | C39 | C41 | C45 | 174.40 |
| 68 | H13 | C39 | C43 | H11 | -63.28 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   |   |   |   |   |   |
| 69 | H13 | C39 | C43 | H12 | 176.51 |
| 70 | H13 | C39 | C43 | O37 | 56.17  |
| 71 | C40 | C39 | C43 | H11 | 53.72  |
| 72 | C40 | C39 | C43 | H12 | -66.48 |
| 73 | C40 | C39 | C43 | O37 | 173.18 |
| 74 | C41 | C39 | C43 | H11 | 179.07 |
| 75 | C41 | C39 | C43 | H12 | 58.87  |
| 76 | C41 | C39 | C43 | O37 | -61.48 |
| 77 | H20 | C40 | C42 | H19 | -63.45 |
| 78 | H20 | C40 | C42 | H22 | -179.12 |
| 79 | H20 | C40 | C42 | C44 | 58.35  |
| 80 | H21 | C40 | C42 | H19 | -177.71 |
| 81 | H21 | C40 | C42 | H22 | 66.63  |
| 82 | H21 | C40 | C42 | C44 | -55.91 |
| 83 | C39 | C40 | C42 | H19 | 59.02  |
| 84 | C39 | C40 | C42 | H22 | -56.65 |
| 85 | C39 | C40 | C42 | C44 | -179.18 |
| 86 | H14 | C41 | C45 | H16 | 63.87  |
| 87 | H14 | C41 | C45 | H17 | -55.69 |
| 88 | H14 | C41 | C45 | H18 | -175.53 |
| 89 | H15 | C41 | C45 | H16 | 179.69 |
| 90 | H15 | C41 | C45 | H17 | 60.12  |
| 91 | H15 | C41 | C45 | H18 | -59.72 |
| 92 | C39 | C41 | C45 | H16 | -58.15 |
| 93 | C39 | C41 | C45 | H17 | -177.72 |
| 94 | C39 | C41 | C45 | H18 | 62.44  |
| 95 | H19 | C42 | C44 | H24 | 64.75  |
| 96 | H19 | C42 | C44 | H25 | -179.70 |
| 97 | H19 | C42 | C44 | C46 | -57.47 |
| 98 | H22 | C42 | C44 | H24 | -179.77 |
| 99 | H22 | C42 | C44 | H25 | -64.23 |
|100 | H22 | C42 | C44 | C46 | 58.00  |
|101 | C40 | C42 | C44 | H24 | -56.92 |
|102 | C40 | C42 | C44 | H25 | 58.62  |
|103 | C40 | C42 | C44 | C46 | -179.15 |
|104 | H24 | C44 | C46 | H23 | -62.22 |
|105 | H24 | C44 | C46 | H26 | 57.87  |
|106 | H24 | C44 | C46 | H27 | 178.00 |
|107 | H25 | C44 | C46 | H23 | -178.02 |
|108 | H25 | C44 | C46 | H26 | -57.93 |
|109 | H25 | C44 | C46 | H27 | 62.20  |
|110 | C42 | C44 | C46 | H23 | 59.87  |
|111 | C42 | C44 | C46 | H26 | 179.97 |
|112 | C42 | C44 | C46 | H27 | -59.90 |
Table S4 List of frequencies, reduced masses, force constants and IR intensities, calculated for optimized ODPABA molecule

| No | Frequencies [cm\(^{-1}\)] | Reduced mass [AMU] | Force constants [mDyne/Å] | IR intensity [km/mol] |
|----|---------------------------|-------------------|---------------------------|----------------------|
| 1  | 15.1631                   | 3.8713            | 0.0005                    | 0.6975               |
| 2  | 20.5029                   | 3.2435            | 0.0008                    | 1.0581               |
| 3  | 34.0201                   | 2.7473            | 0.0019                    | 4.5793               |
| 4  | 38.7171                   | 3.5672            | 0.0032                    | 1.3155               |
| 5  | 42.2815                   | 2.5833            | 0.0027                    | 1.0839               |
| 6  | 67.9098                   | 4.2676            | 0.0116                    | 2.1992               |
| 7  | 71.9738                   | 1.7523            | 0.0053                    | 0.1883               |
| 8  | 81.2458                   | 2.4840            | 0.0097                    | 0.1178               |
| 9  | 88.1116                   | 3.1223            | 0.0143                    | 1.2784               |
| 10 | 105.4334                  | 2.5937            | 0.0170                    | 0.9067               |
| 11 | 120.6005                  | 2.5202            | 0.0218                    | 0.3225               |
| 12 | 126.0891                  | 2.3628            | 0.0221                    | 0.1304               |
| 13 | 166.0810                  | 2.8863            | 0.0469                    | 0.2039               |
| 14 | 179.1672                  | 2.2347            | 0.0423                    | 0.4852               |
| 15 | 190.4113                  | 1.9476            | 0.0416                    | 1.3255               |
| 16 | 195.2767                  | 1.9041            | 0.0428                    | 1.0174               |
| 17 | 215.6932                  | 2.3957            | 0.0657                    | 8.2620               |
| 18 | 234.9577                  | 1.8200            | 0.0592                    | 4.7826               |
| 19 | 249.3847                  | 1.4127            | 0.0518                    | 2.0713               |
| 20 | 251.1058                  | 1.4840            | 0.0551                    | 0.7425               |
| 21 | 270.6109                  | 1.7595            | 0.0759                    | 0.6332               |
| 22 | 300.7940                  | 5.3882            | 0.2872                    | 10.7097              |
| 23 | 314.3866                  | 3.9226            | 0.2284                    | 1.0634               |
| 24 | 320.3445                  | 3.8179            | 0.2308                    | 2.8299               |
| 25 | 370.1971                  | 2.3769            | 0.1919                    | 0.4085               |
| 26 | 390.4327                  | 2.7715            | 0.2489                    | 0.6180               |
| 27 | 432.6829                  | 3.0523            | 0.3367                    | 0.0017               |
| 28 | 452.3379                  | 2.8283            | 0.3410                    | 0.5617               |
| 29 | 469.8858                  | 3.7137            | 0.4831                    | 5.4074               |
| 30 | 496.4195                  | 3.1197            | 0.4530                    | 7.0583               |
| 31 | 513.5783                  | 2.5833            | 0.4015                    | 20.0392              |
| 32 | 520.1591                  | 3.1007            | 0.4943                    | 17.4713              |
| 33 | 561.3670                  | 4.3118            | 0.8006                    | 3.6309               |
| 34 | 609.5726                  | 4.4345            | 0.9708                    | 13.9151              |
| 35 | 644.4602                  | 7.1576            | 1.7515                    | 4.1636               |
| 36 | 704.6661                  | 3.2381            | 0.9473                    | 32.3723              |
| 37 | 729.6401                  | 1.0802            | 0.3388                    | 7.0232               |
| 38 | 758.2935                  | 5.1088            | 1.7308                    | 5.4754               |
| 39 | 773.6519                  | 5.3342            | 1.8811                    | 71.2879              |
| 40 | 780.0289                  | 1.1912            | 0.4270                    | 4.4539               |
| 41 | 782.7223                  | 1.4799            | 0.5342                    | 6.7163               |
| No | Frequencies [cm⁻¹] | Reduced mass [AMU] | Force constants [mDyne/Å] | IR intensity [km/mol] |
|----|-------------------|------------------|--------------------------|---------------------|
| 42 | 808.5866          | 1.2607           | 0.4856                   | 0.6037              |
| 43 | 825.1791          | 1.7710           | 0.7105                   | 6.6252              |
| 44 | 835.9577          | 2.1484           | 0.8846                   | 58.8164             |
| 45 | 864.5351          | 5.4850           | 2.4154                   | 10.4753             |
| 46 | 899.9372          | 1.8128           | 0.8650                   | 2.5986              |
| 47 | 928.0165          | 1.3052           | 0.6623                   | 4.4040              |
| 48 | 956.4867          | 3.3574           | 1.8097                   | 1.0167              |
| 49 | 962.6871          | 3.2190           | 1.7577                   | 67.6974             |
| 50 | 968.2586          | 1.3818           | 0.7633                   | 3.5246              |
| 51 | 972.2200          | 1.3300           | 0.7407                   | 1.1339              |
| 52 | 980.3835          | 1.3403           | 0.7590                   | 0.0449              |
| 53 | 996.0501          | 2.4799           | 1.4496                   | 58.5877             |
| 54 | 1009.2700         | 3.0134           | 1.8085                   | 7.0886              |
| 55 | 1022.1680         | 3.3227           | 2.0454                   | 15.0862             |
| 56 | 1044.4160         | 2.7069           | 1.7397                   | 7.0240              |
| 57 | 1061.8900         | 2.1364           | 1.4194                   | 0.3610              |
| 58 | 1067.1490         | 1.6378           | 1.0989                   | 4.2590              |
| 59 | 1080.2050         | 1.5535           | 1.0680                   | 43.6374             |
| 60 | 1087.2950         | 1.7576           | 1.2242                   | 3.7757              |
| 61 | 1133.6790         | 3.8501           | 2.9154                   | 330.8127            |
| 62 | 1135.4920         | 1.2380           | 0.9405                   | 0.6717              |
| 63 | 1137.9450         | 1.3321           | 1.0163                   | 52.2656             |
| 64 | 1146.5660         | 2.3258           | 1.8008                   | 67.7831             |
| 65 | 1152.4730         | 1.4849           | 1.1620                   | 0.3338              |
| 66 | 1162.6880         | 2.3420           | 1.8653                   | 12.0823             |
| 67 | 1186.6570         | 1.9314           | 1.6024                   | 9.2230              |
| 68 | 1197.2580         | 1.5944           | 1.3465                   | 4.7476              |
| 69 | 1198.7450         | 1.3454           | 1.1391                   | 905.0415            |
| 70 | 1242.7870         | 1.3610           | 1.2386                   | 0.4867              |
| 71 | 1255.1630         | 1.2009           | 1.1147                   | 8.6813              |
| 72 | 1267.1390         | 2.8335           | 2.6805                   | 51.7245             |
| 73 | 1268.5880         | 1.2666           | 1.9209                   | 1.6701              |
| 74 | 1295.4690         | 2.5841           | 2.5551                   | 987.2576            |
| 75 | 1299.6740         | 1.2580           | 1.2520                   | 1.4721              |
| 76 | 1313.4920         | 1.1577           | 1.1768                   | 18.9608             |
| 77 | 1324.7030         | 1.0967           | 1.1339                   | 12.3443             |
| 78 | 1333.0200         | 1.2157           | 1.2728                   | 36.3769             |
| 79 | 1342.2420         | 1.5131           | 1.6062                   | 103.5930            |
| 80 | 1346.5510         | 1.2592           | 1.3453                   | 3.2104              |
| 81 | 1373.7960         | 1.4866           | 1.6530                   | 0.5913              |
| 82 | 1374.8940         | 5.1324           | 5.7162                   | 19.7524             |
| 83 | 1390.4600         | 1.5747           | 1.7937                   | 31.8408             |
| 84 | 1395.3410         | 2.8879           | 3.3128                   | 403.2864            |
| No | Frequencies [cm⁻¹] | Reduced mass [AMU] | Force constants [mDyne/Å] | IR intensity [km/mol] |
|----|---------------------|-------------------|--------------------------|----------------------|
| 85 | 1402.0890           | 1.4918            | 1.7279                   | 4.8766               |
| 86 | 1410.3020           | 1.2545            | 1.4700                   | 3.5627               |
| 87 | 1411.8690           | 1.4154            | 1.6623                   | 22.6769              |
| 88 | 1415.3590           | 1.3574            | 1.6021                   | 7.0071               |
| 89 | 1450.3570           | 1.2573            | 1.5583                   | 4.5610               |
| 90 | 1469.3680           | 2.2861            | 2.9081                   | 20.7738              |
| 91 | 1478.0940           | 1.0667            | 1.3731                   | 0.1962               |
| 92 | 1483.8320           | 1.0385            | 1.3711                   | 0.6324               |
| 93 | 1485.0500           | 1.0724            | 1.3934                   | 2.0033               |
| 94 | 1486.9630           | 1.2170            | 1.5854                   | 55.9909              |
| 95 | 1488.3190           | 1.0638            | 1.3884                   | 0.3907               |
| 96 | 1489.6450           | 1.0460            | 1.3675                   | 20.1267              |
| 97 | 1495.9160           | 1.0405            | 1.3718                   | 8.9571               |
| 98 | 1498.4840           | 1.0732            | 1.4198                   | 10.5941              |
| 99 | 1499.8980           | 1.0814            | 1.4334                   | 5.7480               |
| 100| 1501.9700           | 1.0620            | 1.4116                   | 3.4284               |
| 101| 1507.5870           | 1.0768            | 1.4420                   | 19.1450              |
| 102| 1509.8610           | 1.0766            | 1.4461                   | 8.0158               |
| 103| 1510.4330           | 1.1304            | 1.5195                   | 3.3381               |
| 104| 1526.5790           | 1.1242            | 1.5436                   | 79.3379              |
| 105| 1560.2640           | 2.5834            | 3.7055                   | 268.4185             |
| 106| 1582.7860           | 6.1504            | 9.0782                   | 27.2050              |
| 107| 1639.3640           | 5.5818            | 8.8384                   | 1031.4300            |
| 108| 1689.0450           | 11.2117           | 18.8453                  | 588.8097             |
| 109| 2981.2800           | 1.0837            | 5.6751                   | 3.6772               |
| 110| 3003.0290           | 1.0607            | 5.6360                   | 4.1502               |
| 111| 3003.8060           | 1.0612            | 5.6412                   | 2.6860               |
| 112| 3005.9180           | 1.0400            | 5.5367                   | 112.8523             |
| 113| 3009.9400           | 1.0666            | 5.6932                   | 18.9500              |
| 114| 3011.8760           | 1.0674            | 5.7050                   | 144.1304             |
| 115| 3012.6810           | 1.0436            | 5.5807                   | 90.6296              |
| 116| 3023.6780           | 1.0364            | 5.5826                   | 50.4438              |
| 117| 3029.9520           | 1.0411            | 5.6312                   | 40.1115              |
| 118| 3033.5520           | 1.0894            | 5.9068                   | 32.6502              |
| 119| 3038.4690           | 1.0972            | 5.9685                   | 18.8009              |
| 120| 3041.8270           | 1.0623            | 5.7909                   | 30.1728              |
| 121| 3062.4820           | 1.1037            | 6.0991                   | 102.0408             |
| 122| 3063.7610           | 1.1018            | 6.0936                   | 36.9144              |
| 123| 3064.6450           | 1.1016            | 6.0959                   | 48.2166              |
| 124| 3065.2680           | 1.0959            | 6.0668                   | 27.2018              |
| 125| 3089.7940           | 1.1029            | 6.2035                   | 96.2116              |
| 126| 3094.8410           | 1.1022            | 6.2198                   | 35.8778              |
| 127| 3094.9350           | 1.1024            | 6.2213                   | 57.4240              |
| No | Frequencies [cm\(^{-1}\)] | Reduced mass [AMU] | Force constants [mDyne/Å] | IR intensity [km/mol] |
|----|--------------------------|-------------------|---------------------------|---------------------|
| 128 | 3095.5280                | 1.1089            | 6.2606                    | 62.7141             |
| 129 | 3104.1350                | 1.1017            | 6.2544                    | 70.3538             |
| 130 | 3145.1660                | 1.0989            | 6.4046                    | 3.0332              |
| 131 | 3156.8310                | 1.0962            | 6.4362                    | 23.1319             |
| 132 | 3158.3950                | 1.0925            | 6.4212                    | 1.3056              |
| 133 | 3180.4530                | 1.0906            | 6.4959                    | 0.1561              |
| 134 | 3203.6130                | 1.0919            | 6.6024                    | 2.1513              |
| 135 | 3204.0860                | 1.0933            | 6.6130                    | 3.1831              |

II. Supplementary experimental results

**Fig. S1** UV spectra of ODPABA aqueous solution used in photodegradation experiments (green plot) and provided by the manufacturer emission spectra of Heraeus TQ 150W medium pressure mercury lamp used in the study (black plot)

**Fig. S2** Mass spectra of 2-ethylhexyl 4-aminobenzoate identified in ODPABA/UV reaction mixture (retention time, \(t_R=18.02\) min.)
Fig. S3 Mass spectra of 2-ethyl-1-hexanol identified in ODPABA/UV reaction mixture (retention time, $t_R=4.17$ min.)

Fig. S4 Mass spectra of ODPABA identified in ODPABA/H$_2$O$_2$ reaction mixture (retention time, $t_R=19.44$ min.)

Fig. S5 Mass spectra of 2-ethylhexyl 4-(methylamino)benzoate identified in ODPABA/H$_2$O$_2$ reaction mixture (retention time, $t_R=19.11$ min.)

Fig. S6 Mass spectra of dichlorinated 2-ethylhexyl 4-(methylamino)benzoate identified in ODPABA/NaOCl reaction mixture (retention time, $t_R=20.38$ min.)
Fig. S7 Mass spectra of dichlorinated 2-ethylhexyl 4-aminobenzoate identified in ODPABA/NaOCl reaction mixture (retention time, $t_R$=19.79 min.)

III. Resonance structures

Selected resonance structures of potential ODPABA demethylation transitional product are presented below (Fig. S7).

Fig. S7 The selected resonance structures of the radical formed through hydrogen abstraction from ODPABA ($R=\text{CH}_2\text{CH(C}_2\text{H}_5\text{)}\text{C}_4\text{H}_9-n$)