Electronic Supplementary Information for

Intertwined Chemistry of Hydroxyl Hydrogen-bond Donors, Epoxides and Isocyanates in the Organocatalytic Synthesis of Oxazolidinones versus Isocyanurates: Rational Catalytic Investigation and Mechanistic Understanding

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Summary

S1. General information

All reagents (isocyanates and epoxides), hydrogen bond donors (HBDs), nucleophiles (TBAI, TBAB, TBAC, DMAP, L-Carnitine hydrochloride, DABCO, PPY, DBU, TBD) were purchased from commercial sources except for 2-(phenoxymethyl)oxirane,[1] 2-((allyloxy)methyl)oxirane,[2] 2-((benzyloxy)methyl)oxirane,[3] glycerol carbonate and ascorbic acid derivatives (**AA1**, **AA2**, **AA3**)[4] that were synthesized according to published procedures. Dry reaction solvents were obtained from a solvent purification system (MBRAUN MB-SPS). $CDCl_3$, DMSO-d_6 were purchased from Cambridge Isotope Laboratories. NMR spectra were measured on an automated Bruker (600 MHz for ^1H; 125 MHz for ^{13}C). Mass spectrometry experiments were carried out using a Bruker data analysis Esquire-LC mass spectrometer (APCI mode).

S2. ^{1}H NMR methods for the calculations of conversions and selectivities

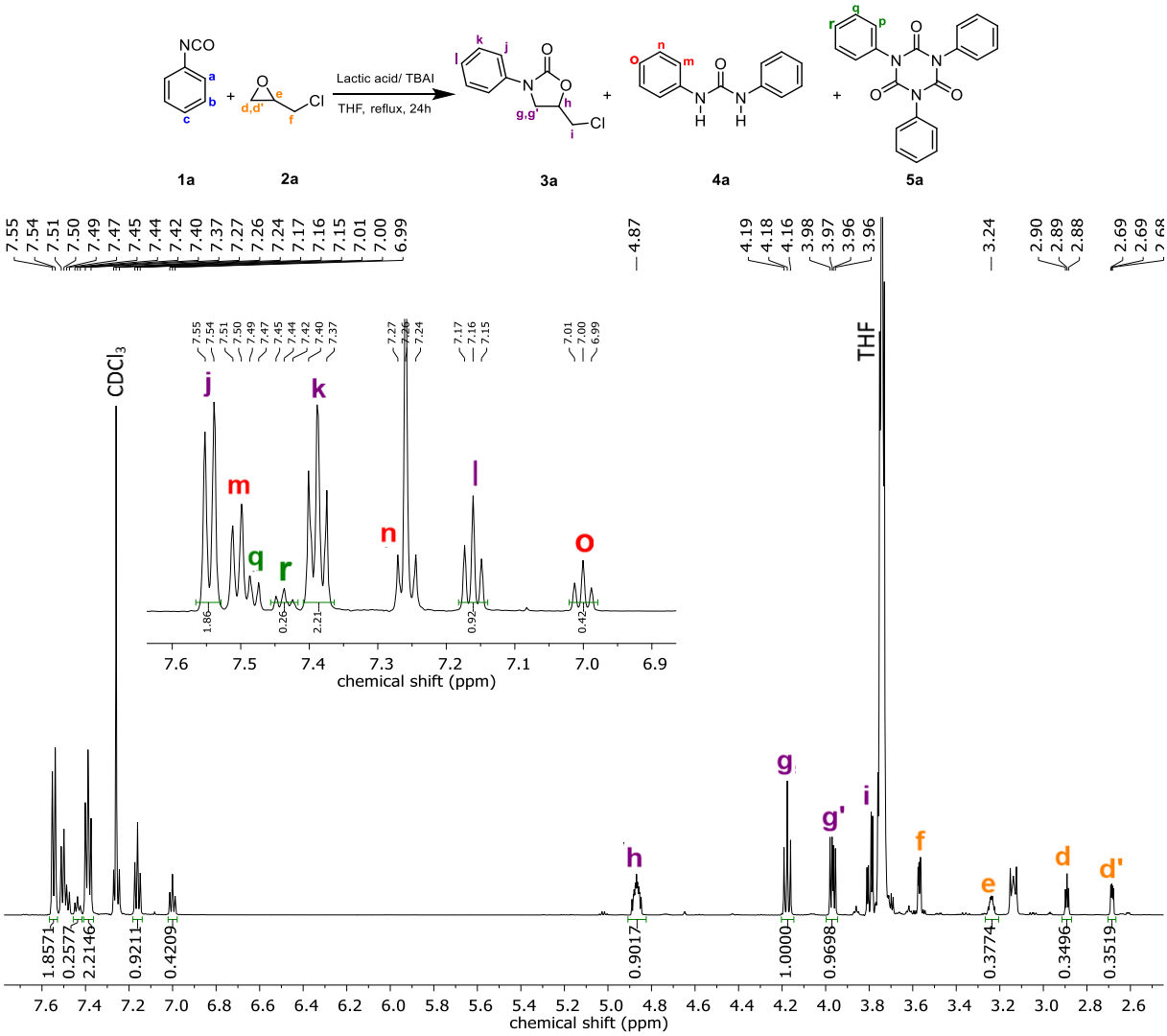


Figure S1. Cycloaddition reaction of phenyl isocyanate (**1a**) to epichlorohydrin (**2a**) using 4 mol% lactic acid and 8 mol% TBAI in 3 mL THF under reflux for 24 h.

Conversion of 2a

$$= \left[\frac{Ig}{Ig + Id} \right] \times 100$$

$$= \left[\frac{1.0000}{(1.0000 + 0.3496)} \right] \times 100$$

$$= 74\%$$

Selectivity 3a:4a:5a

Ratio of **3a**

$$= \left[\frac{Il}{Il + \left(\frac{Io}{2}\right) + \left(\frac{Ir}{3}\right)} \right] \times 100$$

$$= \left[\frac{0.9211}{0.9211 + \left(\frac{0.4209}{2}\right) + \left(\frac{0.2577}{3}\right)} \right] \times 100$$

$$= 76\%$$

Ratio of **4a**

$$= \left[\frac{\left(\frac{Io}{2}\right)}{Il + \left(\frac{Io}{2}\right) + \left(\frac{Ir}{3}\right)} \right] \times 100$$

$$= \left[\frac{\left(\frac{0.4209}{2}\right)}{0.9211 + \left(\frac{0.4209}{2}\right) + \left(\frac{0.2577}{3}\right)} \right] \times 100$$

$$= 17\%$$

Ratio of **5a**

$$= \left[\frac{\left(\frac{Ir}{2}\right)}{Il + \left(\frac{Io}{2}\right) + \left(\frac{Ir}{3}\right)} \right] \times 100$$

$$= \left[\frac{\left(\frac{0.2577}{3}\right)}{0.9211 + \left(\frac{0.4209}{2}\right) + \left(\frac{0.2577}{3}\right)} \right] \times 100$$

$$= 7\%$$

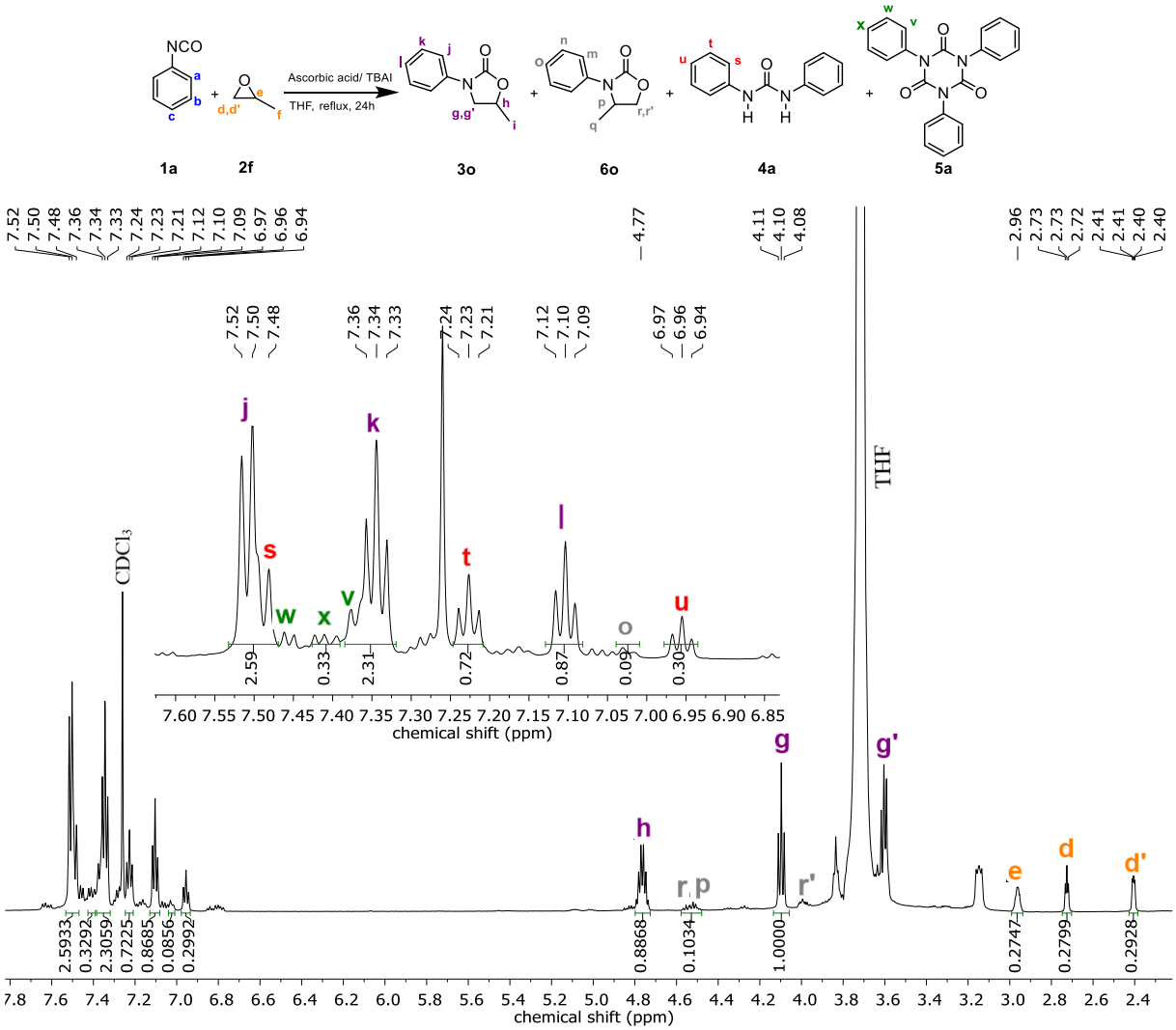


Figure S2. Cycloaddition reaction of phenyl isocyanate (**1a**) to propylene oxide (**2f**) using 4 mol% ascorbic acid and 8 mol% TBAI in 3 mL THF under reflux for 24 h.

Conversion of 2f

$$= \left[\frac{Ig}{Ig + Id} \right] \times 100$$

$$= \left[\frac{1.0000}{(1.0000 + 0.2799)} \right] \times 100$$

$$= 78\%$$

Ratio of 3o:6o

Ratio of **3o**

$$= \left[\frac{Ig}{Ig + \left(\frac{I(r+p)}{2} \right)} \right] \times 100$$

$$= \left[\frac{1.0000}{1.0000 + \left(\frac{0.1034}{2} \right)} \right] \times 100$$

$$= 95\%$$

Ratio of **6o**

$$= \left[\frac{\left(\frac{I(r+p)}{2} \right)}{Ig + \left(\frac{I(r+p)}{2} \right)} \right] \times 100$$

$$= \left[\frac{\left(\frac{0.1034}{2} \right)}{1.0000 + \left(\frac{0.1034}{2} \right)} \right] \times 100$$

$$= 5\%$$

Selectivity of (3o+6o):(4a+5a)

Ratio of **3o**

$$= \left[\frac{Il}{Il + Io + \left(\frac{Iu}{2} \right) + \left(\frac{Ix}{3} \right)} \right] \times 100$$

$$= \left[\frac{0.8685}{0.8685 + 0.0856 + \left(\frac{0.2992}{2} \right) + \left(\frac{0.3292}{3} \right)} \right] \times 100$$

$$= 72\%$$

Ratio of **6o**

$$= \left[\frac{Io}{Il + Io + \left(\frac{Iu}{2}\right) + \left(\frac{Ix}{3}\right)} \right] \times 100$$

$$= \left[\frac{0.0856}{0.8685 + 0.0856 + \left(\frac{0.2992}{2}\right) + \left(\frac{0.3292}{3}\right)} \right] \times 100$$

$$= 7\%$$

Ratio of **4a**

$$= \left[\frac{\left(\frac{Iu}{2}\right)}{Il + Io + \left(\frac{Iu}{2}\right) + \left(\frac{Ix}{3}\right)} \right] \times 100$$

$$= \left[\frac{\left(\frac{0.2992}{2}\right)}{0.8685 + 0.0856 + \left(\frac{0.2992}{2}\right) + \left(\frac{0.3292}{3}\right)} \right] \times 100$$

$$= 12\%$$

Ratio of **5a**

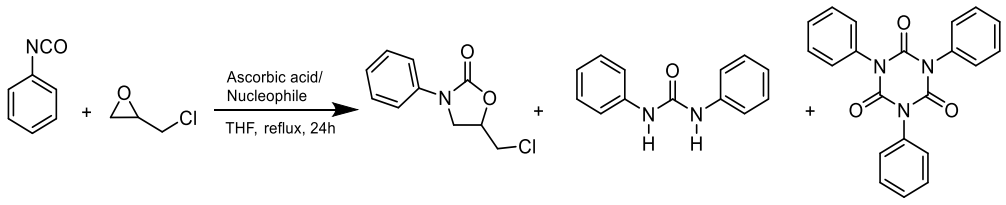
$$= \left[\frac{\left(\frac{Ix}{3}\right)}{Il + Io + \left(\frac{Iu}{2}\right) + \left(\frac{Ix}{3}\right)} \right] \times 100$$

$$= \left[\frac{\left(\frac{0.3292}{3}\right)}{0.8685 + 0.0856 + \left(\frac{0.2992}{2}\right) + \left(\frac{0.3292}{3}\right)} \right] \times 100$$

$$= 9\%$$

S3. Supplementary catalysis results

Table S1. Screening of various nucleophiles for the cycloaddition reaction of phenyl isocyanate (**1a**) and epichlorohydrin (**2a**).[a]



Entry	Nucleophile	Conversion of **2a** (%)[b]	Conversion of **1a** (%)[b]	Ratio of **3a** : **4a** : **5a**[b]	TOF (h^{-1})
1	TBAI	96	100	93 : 7 : 0	1
2	TBAB	68	100	80 : 19 : 0	0.71
3	TBAC	45	100	64 : 36 : 0	0.47
4	DMAP	30	100	42 : 24 : 34	0.31
5	L-Carnitine hydrochloride	25	100	46 : 23 : 31	0.26
6	DABCO	24	100	38 : 36 : 26	0.25
7	PPY	23	100	42 : 29 : 29	0.24
8	DBU	9	100	16 : 27 : 57	0.09
9	TBD	0	100	0 : 39 : 61	0

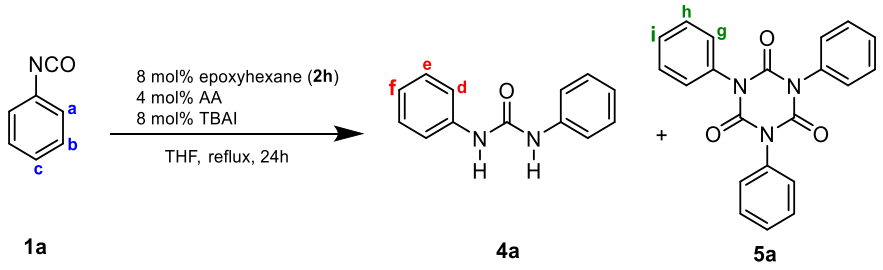
[a] Reaction condition: phenyl isocyanate (**1a**, 2 mmol), epichlorohydrin (**2a**, 2 mmol), ascorbic acid (4 mol%) and nucleophiles (8 mol%) in THF (3 mL) under reflux for 24 h. [b] Conversion and selectivity determined by ^{1}H NMR.

Table S2. Supplementary catalytic results for the cycloaddition of phenyl isocyanate **1a** to epoxides at 67 °C for 24 h catalyzed by HBDs in the presence of in the absence of TBAI.[a]

Entry	HBD	TBAI added (Y/N)	Epoxide	Conversion of **1a** (%)[b]	Conversion of **2** (%)[b]	Ratio of **3o** : **4a** : **5a** (%)[b]
1[c]	L-Ascorbic acid	N	**2a**	25	0	0 : 100 : 0
2[c]	L-Ascorbic acid	N	**2f**	0	0	-
3	Pentaerythritol	N	**2a**	38	0	0 : 100 : 0
4	*meso*-Erythritol	N	**2a**	53	0	0 : 100 : 0
5	Pentaerythritol	N	**2f**	27	0	0 : 100 : 0
6	*meso*-Erythritol	N	**2f**	33	0	0 : 100 : 0
7	Pentaerythritol	Y	**2f**	100	5	1:3[d]
8	*meso*-Erythritol	Y	**2f**	100	6	≈1:2[d]
9	-	Y	**2f**	100	19	41 : 23 : 36

[a] Reaction condition: phenyl isocyanate (2 mmol), epoxide (2 mmol), HBDs (4 mol%) and TBAI (8 mol%, only where indicated by "Y") in THF (3 mL) under reflux for 24 h. [b] Determined by ^{1}H NMR of the reaction mixture. [c] Data taken from Table 4. [d] The oxazolidinone product was formed in very minor amounts along with traces of propylene carbonate and therefore only the **4a** : **5a** ratio is provided.

S4. Study of ^{1}H NMR shifts of 4a in different mixtures



1a 4a 5a

Scheme S1. Cycloaddition reaction of phenyl isocyanate (**1a**, 2 mmol), 1-epoxyhexane (**2h**, 8 mol%) ascorbic acid (4 mol%) and TBAI (8 mol%) in 3 THF (3 mL) under reflux for 24 h.

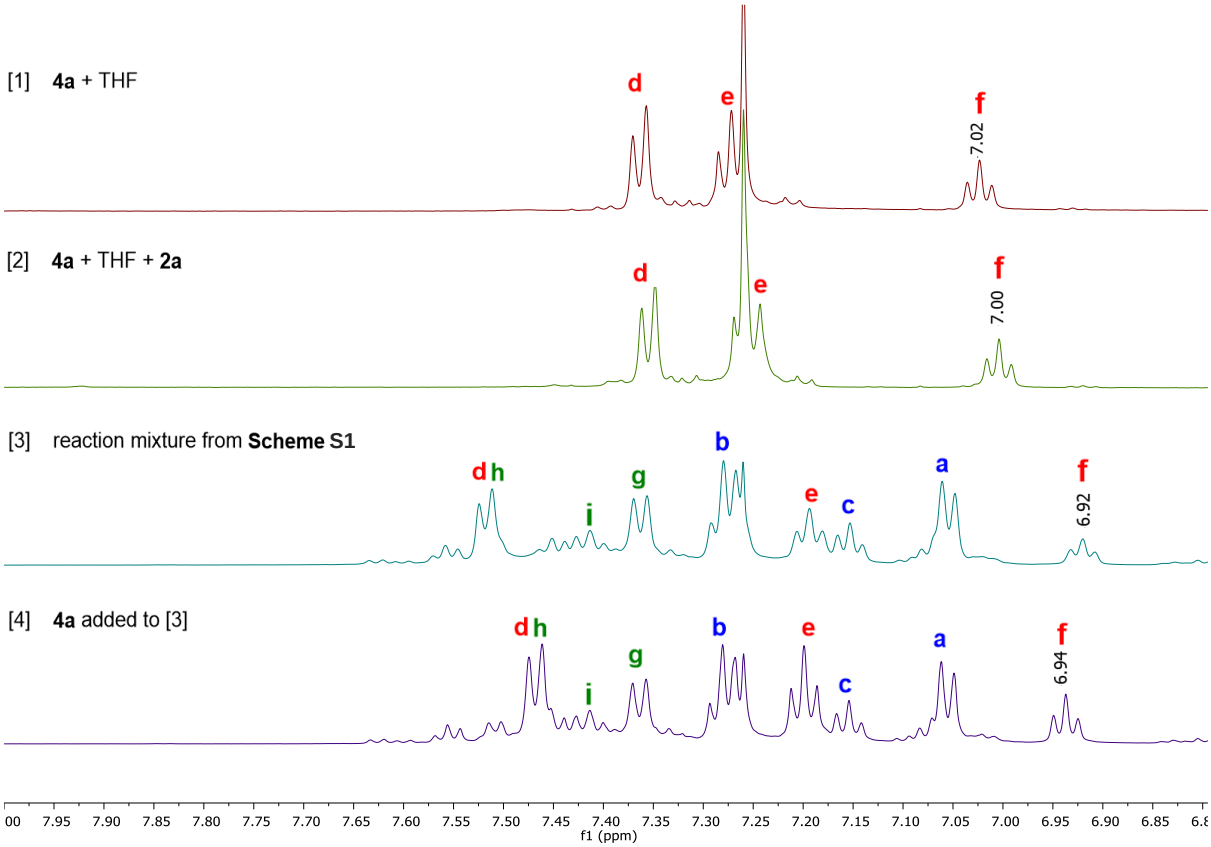


Figure S3. Comparison of ^{1}H NMR (600 MHz, $CDCl_3$) spectra for different mixtures containing urea **4a**. [1] solution of **4a** (0.15 M) in THF. [2] Mixture between **4a** (0.15 M) and **2a** (0.15 M) in THF. [3] Reaction mixture from **Scheme S1** (**1a** (2 mmol, 0.67 M), **2h** (8 mol%) ascorbic acid (4 mol%) and TBAI (8 mol%) in THF (3 mL) under reflux for 24 h. [4] **4a** (0.15 M) was added to the reaction mixture in [3].

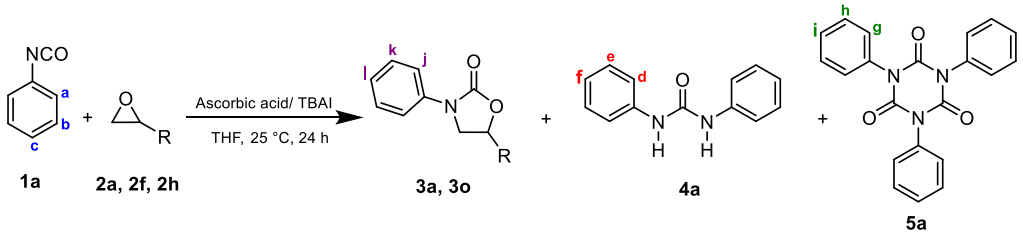
S5. Mechanistic experiments at 25 °C

The results of the set of mechanistic experiments carried out at room temperature are displayed in Table S3 whereas the ^{1}H NMR signals relative to the aromatic protons region of the compounds formed during the catalytic reactions listed in Table S3 are provided in Figure S4 for epoxide **2h**. The ^{1}H NMR peaks were generally assigned using the pure isolated or commercial compounds as standards. To note, the position of the ^{1}H NMR signals assigned to **4a** in Figure S4 was found to change slightly from trace to trace. In Figure S3, it is possible to observe that the position of the ^{1}H NMR signals of **4a** is affected by its chemical environment and depends on the compounds present in the mixture; for instance the position of the aromatic protons denoted with "f" (See Scheme of Table S3) was found to vary between about 6.90 and 7.00 ppm in different mixtures.

Stirring **1a** at room temperature in THF (Table S3, entry 1) did not lead to the formation of new products as detected by ^{1}H NMR with the only proton signals found in the aromatic region corresponding to those of pure **1a** (Figure S4, trace 1). The addition of a catalytic amount of TBAI (8 mol%, Table S3, entry 2), led to the formation of small amounts of cyclic isocyanurate trimer **5a** as supported by the appearance of new aromatic signals in the 7.35-7.50 ppm spectral region (Figure S4, trace 2).[5] Importantly, the addition of one equivalent of epoxide **2h** to **1a** in the presence of TBAI (Table S3, entry 3) led to a much higher (81%) degree of conversion of **1a** to **5a** without formation of **3q** (Figure S4, trace 3). This observation indicates that the presence of epoxide accelerates the formation of the cyclic isocyanurate trimer and might play a role in the mechanism of such process. This result was confirmed also with other epoxides, albeit with slightly different selectivities. When the epoxide substrate was changed to **2a** (Table S3, entry 4) or **2f** (Table S3, entry 5) the conversion of **1a** became quantitative and trimer **5a** was still the main product but the formation of low amounts of oxazolidinones and urea **4a** was also observed. We subsequently investigated the effect of the presence of ascorbic acid in the reaction mixture. In the presence of one equivalent of epoxide **2f** and of a catalytic amount of ascorbic acid (4 mol%), but in the absence of TBAI, no new reaction products were formed (Table S3, entry 6 and Figure S4, trace 4). However, when TBAI (8 mol%) was added (Table S3, entry 7) the conversion of **1a** sharply increased to a level comparable to that observed without adding ascorbic acid (Table S3, entry 3). Nevertheless, the product formed was mostly diphenyl urea **4a** (Figure S4, trace 5). Importantly, stirring **5a** in THF at room temperature for one day in the presence of ascorbic acid (4 mol%) or ascorbic acid and TBAI (4 mol% and 8 mol% respectively) did not lead to the formation of **4a** suggesting that the latter was not formed by decomposition of **5a** catalyzed by ascorbic acid but, likely, via a dimeric isocyanurate that subsequently underwent decarbonylation. When the experiment in Table S3, entry 7 was carried out with different epoxides, i.e. **2a** (Table S3, entry 8) or **2h** (Table S3, entry 9) different mixtures of products were formed with oxazolidinone **3a** being the main product for **2a** and cyclic trimer **5a** being the main product for epoxide **2h**. To note, comparison of the corresponding reactions carried out without ascorbic acid (Table S3, entries 3-5) and with ascorbic acid (Table S3, entries 7-9) shows that the presence of ascorbic acids inhibits **1a** conversion at room temperature and leads to a decrease of selectivity for **5a** in favor of oxazolidinones and **4a**. Importantly, when **1a** was stirred in the presence of catalytic amounts of ascorbic acid and TBAI (Table S3, entry 10), but in the absence of epoxide, no new products were formed (Figure S4, trace 6). Overall, these results show the importance of the presence of epoxide in any process involving the conversion of **1a** at room temperature with the ultimate

reaction outcome being strongly dependent on the identity of the epoxide and on the presence of absence of ascorbic acid. Prompted by these results, we investigated whether catalytic amounts of epoxide were sufficient for the formation of isocyanurates. The reaction in Table S3, entry 11, compared to the same reaction carried out without epoxide (Table S3, entry 10), shows that by adding just 4 mol% **2h** low but significant conversion of **1a** to a mixture of **4a** and **5a** was observed (Figure S4, trace 7) suggesting that the epoxide plays a catalytic role for the formation of both byproducts. This was further confirmed when using identical catalytic amounts (4 mol%) of epoxides **2a** and **2f** (Table S3, entries 12, 13) that led to much higher **1a** conversion compared to **2h** to afford mixtures of **4a** and **5a**. Increasing the loading of epoxide **2h** to 8 mol% (Table S3, entry 14) led, as expected, to higher conversion of **1a** to a mixture of **4a** and **5a** (Figure S4, trace 8). Finally, we observed that in the presence of catalytic amounts of epoxide **2h** (4 mol%) and TBAI (8 mol%), but in the absence of ascorbic acid, only trimer **5a** was obtained with moderate **1a** conversion (Table S3, entry 15 and Figure S4, trace 9). The latter result shows, once more, that the absence of ascorbic acid favors the formation of **5a**.

Table S3. Mechanistic experiments for the cycloaddition of **1a** to epoxides at 25 °C.[a]



Entry	Amount of **1a** (mmol)	Amount of **2** (mmol, mol%)	Loading of *L*-Ascorbic acid (mol %)	Loading of TBAI (mol%)	Conversion of **1a** (%)[b]	Ratio **3** : **4a**: **5a** (%)[b]
1	4	-	-	-	0	-
2	4	-	-	8	12	0 : 0 : 100
3	4	4, 100 (**2h**)	-	8	81	0 : 0 : 100
4	4	4, 100 (**2a**)	-	8	100	24 : 13 : 63
5	4	4, 100 (**2f**)	-	8	100	11 : 28 : 61
6	4	4, 100 (**2h**)	4	-	0	-
7	4	4, 100 (**2h**)	4	8	70	0 : 100 : 0
8[c]	4	4, 100 (**2a**)	4	8	39	59: 25 : 16
9	4	4, 100 (**2f**)	4	8	77[d]	27 : 24 : 49
10	4	-	4	8	0	-
11	4	0.16, 4 (**2h**)	4	8	19	0 : 68 : 32
12	4	0.16, 4 (**2a**)	4	8	63[d]	0 : 54 : 46
13	4	0.16, 4 (**2f**)	4	8	82[d]	0 : 42 : 58
14	4	0.32, 8 (**2h**)	4	8	30	0 : 63 : 37
15	4	0.16, 4 (**2h**)	-	8	54	0 : 0 : 100

[a] Reaction condition: 3 mL of THF at room temperature (25 °C) for 24 h; amounts of catalytic components and substrates as indicated in the Table. [b] Conversion and selectivity determined by ^{1}H NMR. [c] Taken from Table 2, Entry 6. [d] The aromatic region of the ^{1}H NMR of the reaction mixture includes also signals from a minor species at 7.10, 7.30, 7.55 ppm attributable to the dimeric cyclooligomer of phenyl isocyanate (1,3-diphenylene uretedione) according to ref. [6].

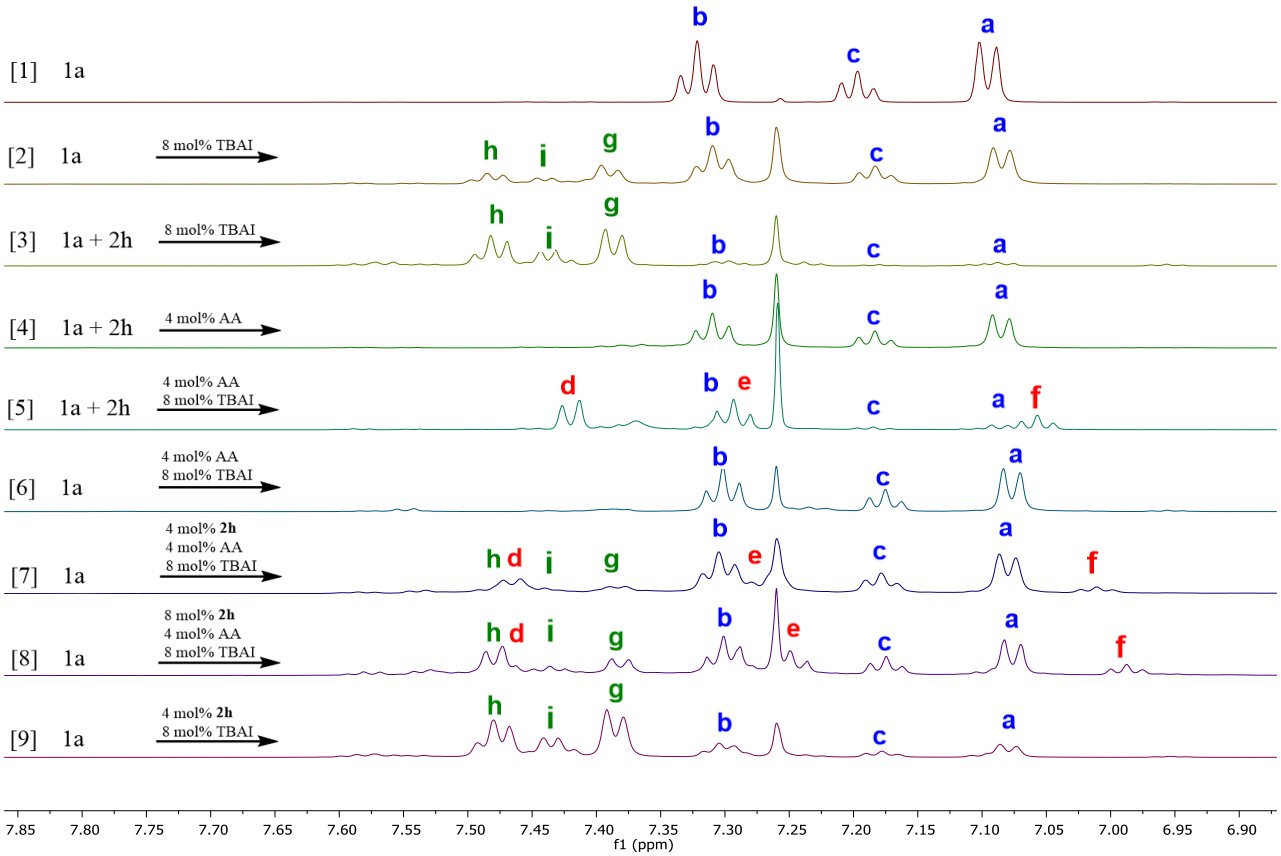


Figure S4. ^{1}H NMR ($CDCl_3$) analysis of the reaction products formed in several solutions of phenyl isocyanate (**1a**) and one or more reactants chosen among **2h**, ascorbic acid and TBAI (25 °C, 24 h, THF) as described in Table S3.

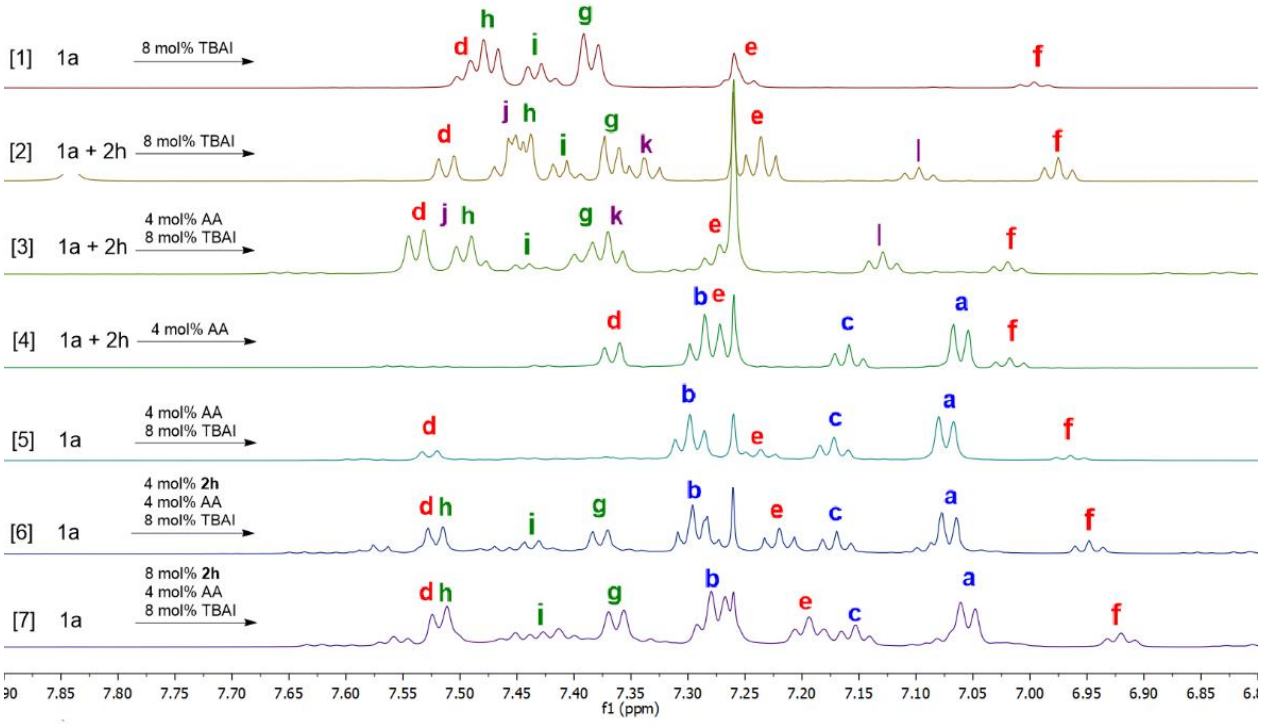
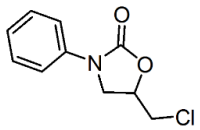


Figure S5. ^{1}H NMR ($CDCl_3$) analysis of the reaction products formed in several solutions of phenyl isocyanate (**1a**) and one or more reactants chosen among **2h**, ascorbic acid and TBAI (in THF under reflux (67 °C), 24 h) as described in Table 3.

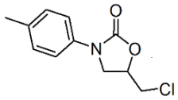
S6. Spectral data (^{1}H NMR, ^{13}C NMR) and APCI-MS data of oxazolidinones (3a-3r)

5-butyl-3phenyloxazolidin-2-one (3a)



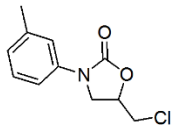
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.55 (d, 2H), 7.39 (t, 2H), 7.17 (t, 1H), 4.89-4.85 (m, 1H), 4.18 (t, 1H), 3.97 (dd, 1H), 3.83-3.71 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.98, 129.30, 124.57, 118.53, 71.00, 48.37, 44.64; APCI-MS: Exact mass calculated for $C_{10}H_{11}ClNO_2^+$ $[M+H]^+$ 212.0473, found 212.0483.

5-(chloromethyl)-3-*p*-tolyloxazolidin-2-one (3b)



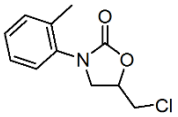
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (d, 2H), 7.18 (d, 2H), 4.89-4.79 (m, 1H), 4.13 (t, 1H), 3.92 (dd, 1H), 3.79-3.71 (m, 2H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.15, 135.42, 134.28, 129.77, 118.65, 70.98, 48.47, 44.71, 20.86; APCI-MS: Exact mass calculated for $C_{11}H_{13}ClNO_2^+$ $[M+H]^+$ 226.0629, found 226.0632.

5-(chloromethyl)-3-*m*-tolyloxazolidin-2-one (3c)



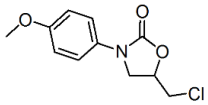
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 (s, 1H), 7.25-7.19 (m, 2H), 6.91 (d, 1H), 4.83-4.74 (m, 1H), 4.09 (t, 1H), 3.88 (dd, 1H), 3.75-3.64 (m, 2H), 2.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.06, 139.31, 137.91, 129.11, 125.44, 119.32, 115.69, 70.99, 48.51, 44.66, 21.76; APCI-MS: Exact mass calculated for $C_{11}H_{13}ClNO_2^+$ $[M+H]^+$ 226.0629, found 226.0633.

5-(chloromethyl)-3-*o*-tolyloxazolidin-2-one (3d)



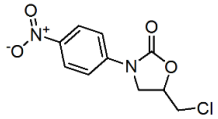
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.21 (m, 4H), 4.97-4.93 (m, 1H), 4.09 (t, 1H), 3.92-3.78 (m, 3H), 2.35 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.47, 136.14, 135.66, 131.60, 128.59, 127.21, 126.75, 71.75, 50.65, 44.99, 18.01; APCI-MS: Exact mass calculated for $C_{11}H_{13}ClNO_2^+$ $[M+H]^+$ 226.0629, found 226.0631.

5-(chloromethyl)-3-(4-methoxyphenol)oxazolidin-2-one (3e)



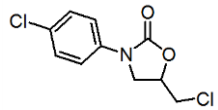
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 (d, 2H), 6.92 (d, 2H), 4.88-4.81 (m, 1H), 4.13 (t, 1H), 3.92 (dd, 1H), 3.80 (s, 3H), 3.78-3.72 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 156.84, 154.37, 131.10, 120.66, 114.56, 70.98, 55.68, 48.92, 44.70; APCI-MS: Exact mass calculated for $C_{11}H_{13}ClNO_3^+$ $[M+H]^+$ 242.0578, found 242.0579.

5-(chloromethyl)-3-(4-nitrophenyl)oxazolidin-2-one (3f)



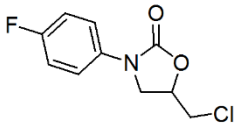
^{1}H NMR (600 MHz, DMSO-d_6) δ 8.29 (d, 2H), 7.83 (d, 2H), 5.11-5.03 (m, 1H), 4.30 (t, 1H), 4.09-3.96 (m, 2H), 3.92 (dd, 1H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 124.81, 117.60, 71.60, 47.32, 45.93, 39.52; APCI-MS: Exact mass calculated for $C_{10}H_{10}ClN_2O_4^+$ $[M+H]^+$ 257.0324, found 257.0328.

5-(chloromethyl)-3-(4-chlorophenyl)oxazolidin-2-one (3g)



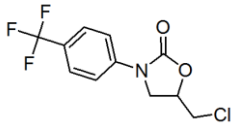
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (d, 2H), 7.35 (d, 2H), 4.88 (q, 1H), 4.15 (t, 1H), 3.94 (dd, 1H), 3.84-3.71 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.87, 136.58, 129.87, 129.34, 119.64, 70.98, 48.29, 44.60; APCI-MS: Exact mass calculated for $C_{10}H_{10}Cl_2NO_2^+$ $[M+H]^+$ 246.0083, found 246.0089.

5-(chloromethyl)-3-(4-fluorophenyl)oxazolidin-2-one (3h)



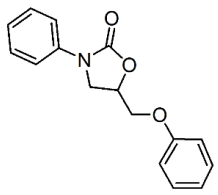
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54-7.47 (m, 2H), 7.08 (t, 2H), 4.91-4.83 (m, 1H), 4.15 (t, 1H), 3.94 (dd, 1H), 3.81-3.74 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.16, 134.05, 120.45, 120.39, 116.12, 115.97, 70.96, 48.63, 44.64; APCI-MS: Exact mass calculated for $C_{11}H_{10}ClFNO_2^+$ $[M+H]^+$ 230.0379, found 230.0380.

5-(chloromethyl)-3-(4-(trifluoromethyl)phenyl)oxazolidin-2-one (3i)



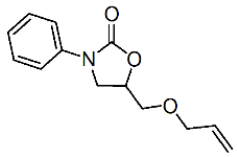
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71-7.59 (m, 4H), 4.92 (dq, 1H), 4.19 (t, 1H), 3.98 (dd, 1H), 3.79-3.78 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.77, 140.91, 126.50, 126.47, 126.45, 126.42, 126.34, 126.12, 123.21, 117.92, 71.09, 47.95, 44.66; APCI-MS: Exact mass calculated for $C_{11}H_{10}ClF_3NO_2^+$ $[M+H]^+$ 280.0347, found 280.0347.

5-(phenoxymethyl)-3-phenyloxazolidin-2-one (3j)



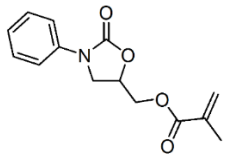
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, 2H), 7.39 (t, 2H), 7.30 (t, 2H), 7.16 (t, 1H), 7.00 (t, 1H), 6.91 (d, 2H), 4.97 (dq, 1H), 4.26-4.14 (m, 3H), 4.06 (dd, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.15, 138.28, 129.76, 129.22, 124.30, 121.88, 118.44, 114.77, 70.51, 68.06, 47.52; APCI-MS: Exact mass calculated for $C_{16}H_{16}NO_3^+$ $[M+H]^+$ 270.1125, found 270.1127.

5-(allyloxymethyl)-3-phenyloxazolidin-2-one (3k)



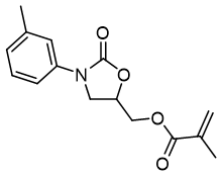
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.55 (d, 2H), 7.37 (t, 2H), 7.13 (t, 1H), 5.92-5.85 (m, 1H), 5.30 (d, 1H), 5.20 (d, 1H), 4.79-4.74 (m, 1H), 4.08-4.05 (m, 3H), 3.94 (dd, 1H), 3.70-3.69 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.44, 129.17, 124.14, 118.36, 117.90, 72.82, 71.39, 70.22, 47.46; APCI-MS: Exact mass calculated for $C_{13}H_{16}NO_3^+$ $[M+H]^+$ 234.1125, found 234.1132.

(2-oxo-3-phenyloxazolidin-5-yl)methylmethacrylate (3l)



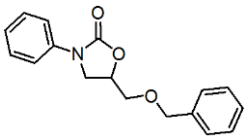
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, 2H), 7.38 (t, 2H), 7.15 (t, 1H), 6.12 (s, 1H), 5.59 (s, 1H), 4.91 (dq, 1H), 4.47-4.35 (m, 2H), 4.17 (t, 1H), 3.87 (dd, 1H), 1.91 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.98, 138.09, 135.51, 129.28, 127.07, 124.45, 118.42, 70.17, 64.71, 47.29, 18.31; APCI-MS: Exact mass calculated for $C_{14}H_{16}NO_4^+$ $[M+H]^+$ 262.1074, found 262.1076.

(2-oxo-3-(m-tolyl)oxazolidin-5-yl)methyl methacrylate (3m)



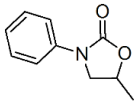
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.31 (d, 1H), 7.26 (t, 1H), 6.97 (d, 1H), 6.12 (s, 1H), 5.60 (s, 1H), 4.90 (m, 1H), 4.47 – 4.34 (m, 2H), 4.16 (t, 1H), 3.86 (dd, 1H), 2.37 (s, 3H), 1.92 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.91, 154.36, 139.16, 137.99, 135.47, 129.00, 126.94, 125.21, 119.12, 115.52, 70.11, 64.67, 47.32, 21.67, 18.24; APCI-MS: Exact mass calculated for $C_{15}H_{18}NO_4^+$ $[M+H]^+$ 276.1231, found 276.1130.

5-(benzyloxymethyl)-3-phenyloxazolidin-2-one (3n)



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, 2H), 7.39-7.26 (m, 7H), 7.14 (t, 1H), 4.77 (dq, 1H), 4.66-4.57 (m, 2H), 4.06 (t, 1H), 3.96-3.89 (m, 1H), 3.73 (d, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.42, 137.51, 129.17, 128.67, 128.13, 127.92, 124.16, 118.40, 73.94, 71.41, 70.26, 47.49; APCI-MS: Exact mass calculated for $C_{17}H_{18}NO_3^+$ $[M+H]^+$ 284.1281, found 284.1292.

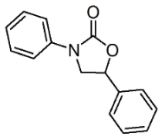
5-methyl-3-phenyloxazolidin-2-one (3o)



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.52 (d, 2H), 7.36 (t, 2H), 7.13 (t, 1H), 4.77 (h, 1H), 4.10 (t, 1H), 3.61 (t, 1H), 1.52 (d, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.51, 129.13, 124.05, 118.32,

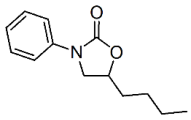
69.64, 52.01, 20.80; APCI-MS: Exact mass calculated for $C_{10}H_{12}NO_2^+$ $[M+H]^+$ 178.0863, found 178.0868.

3, 5-diphenyloxazolidin-2-one (3p)



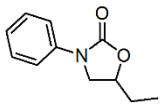
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (d, 2H), 7.43 (d, 4H), 7.38 (t, 3H), 7.15 (t, 1H), 5.63 (t, 1H), 4.38 (t, 1H), 3.96 (t, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.24, 129.21, 129.15, 125.79, 124.29, 118.44, 74.15, 52.81; APCI-MS: Exact mass calculated for $C_{15}H_{14}NO_2^+$ $[M+H]^+$ 240.1019, found 240.1021

5-butyl-3-phenyloxazolidin-2-one (3q)



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, 2H), 7.36 (t, 2H), 7.12 (t, 1H), 4.62 (p, 1H), 4.06 (t, 1H), 3.64 (t, 1H), 1.89-1.81 (m, 1H), 1.75-1.69 (m, 1H), 1.55-1.46 (m, 1H), 1.46-1.36 (m, 3H), 0.94 (t, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.53, 129.10, 123.99, 118.27, 73.19, 50.60, 34.80, 26.72, 22.46, 13.97; APCI-MS: Exact mass calculated for $C_{13}H_{18}NO_2^+$ $[M+H]^+$ 220.1332, found 220.1337.

5-ethyl-3-phenyloxazolidin-2-one (3r)



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, 2H), 7.37 (t, 2H), 7.13 (t, 1H), 4.58 (p, 1H), 4.07 (t, 1H), 3.66 (t, 1H), 1.90-1.84 (m, 1H), 1.82-1.76 (m, 1H), 1.07 (t, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.54, 129.15, 124.05, 118.31, 74.24, 50.22, 28.16, 8.86; APCI-MS: Exact mass calculated for $C_{11}H_{14}NO_2^+$ $[M+H]^+$ 192.1019, found 192.1022.

S7. Copies of ^{1}H NMR, ^{13}C NMR spectra of oxazolidinones 3a-3r

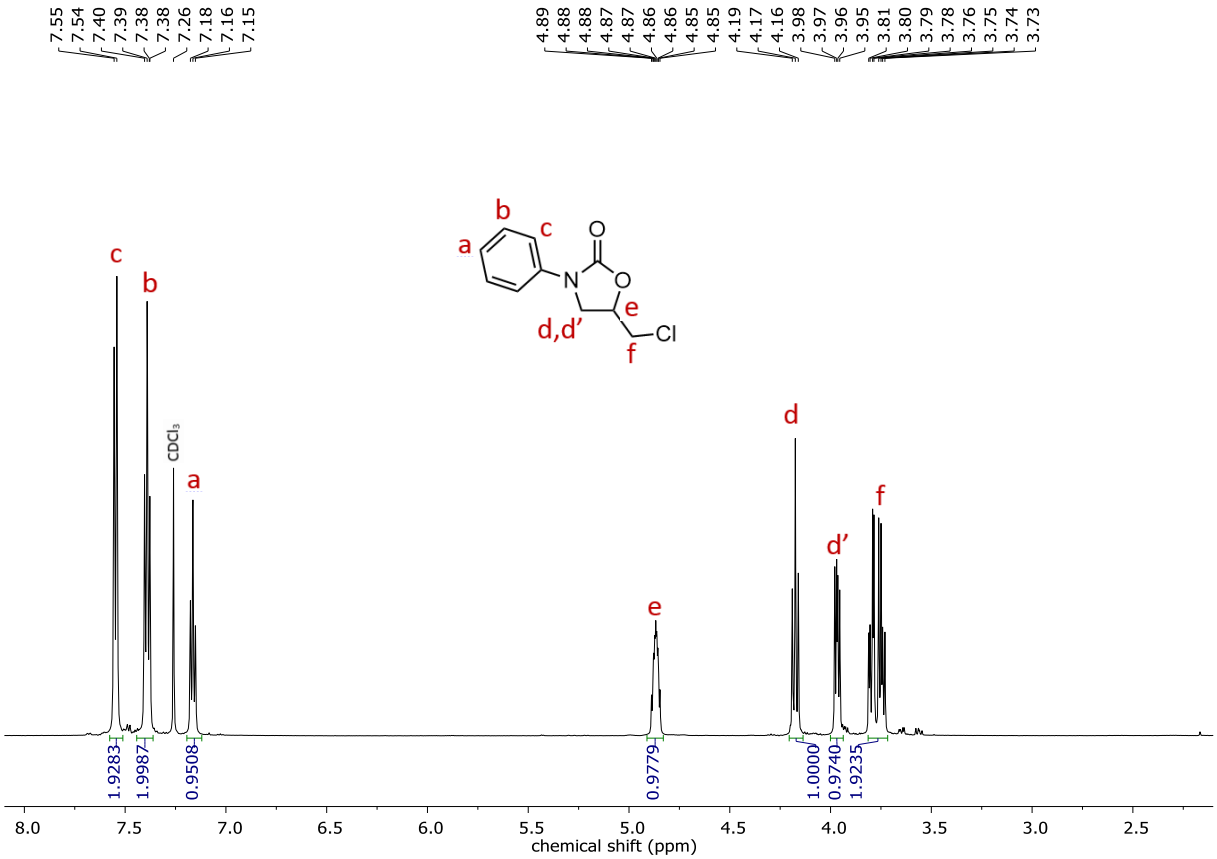


Figure S6. ^{1}H NMR ($CDCl_3$) of 5-butyl-3phenyloxazolidin-2-one (**3a**).

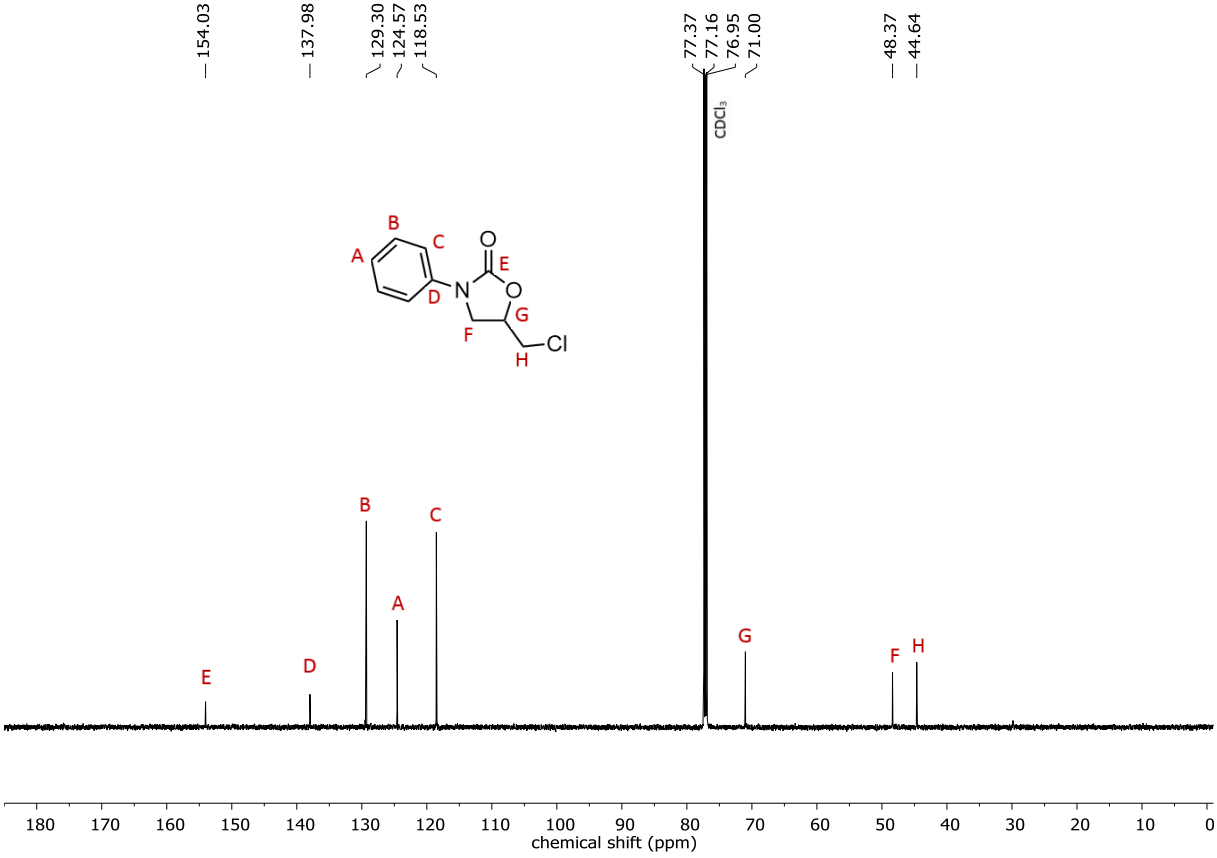


Figure S7. ^{13}C NMR ($CDCl_3$) of 5-butyl-3phenyloxazolidin-2-one (**3a**).

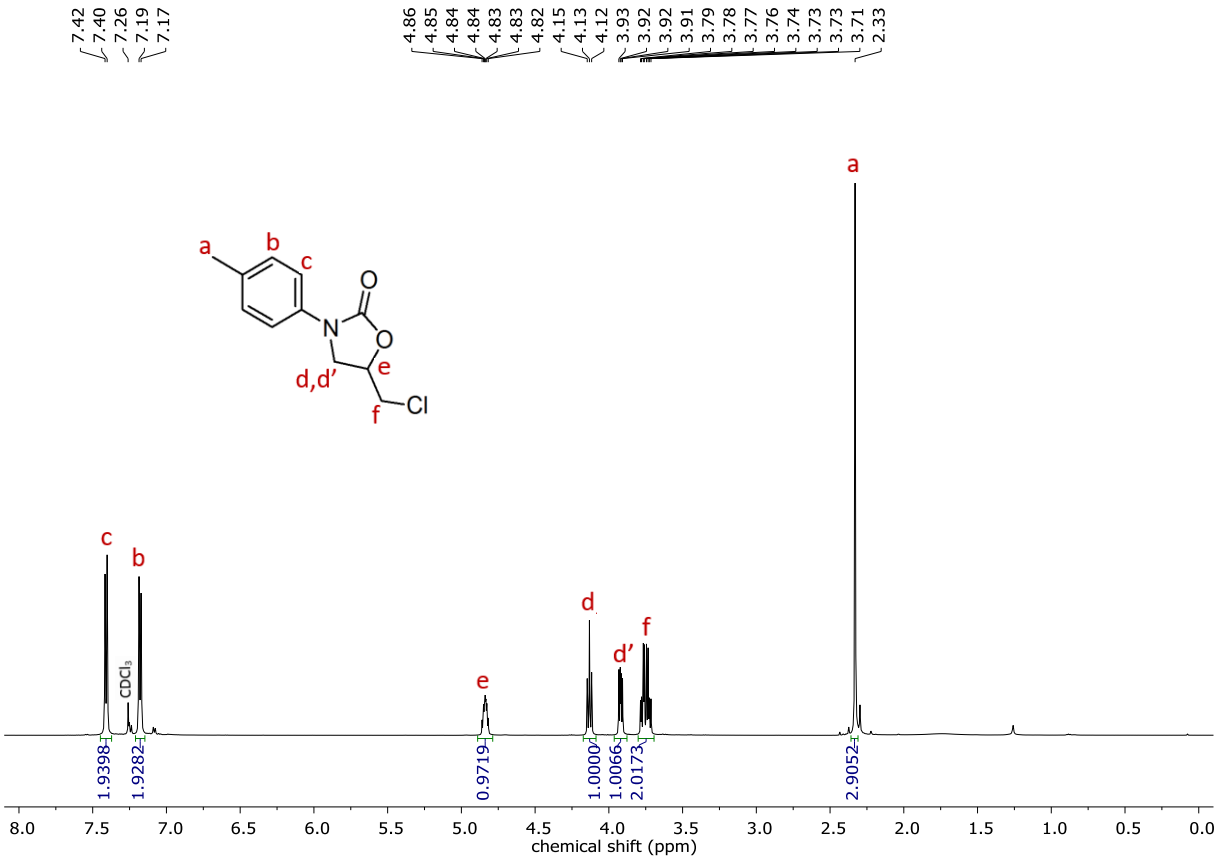


Figure S8. ^{1}H NMR ($CDCl_3$) of 5-(chloromethyl)-3-*p*-tolyloxazolidin-2-one (**3b**).

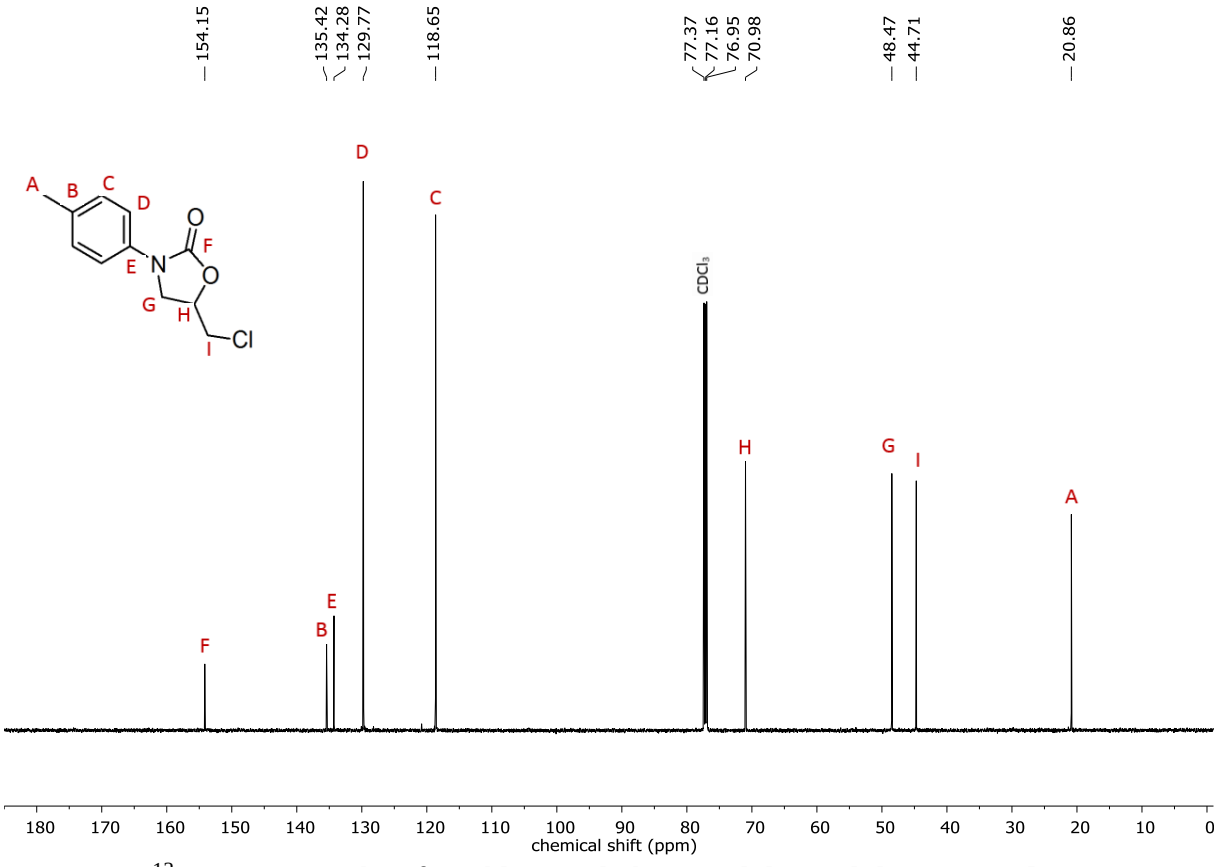


Figure S9. ^{13}C NMR ($CDCl_3$) of 5-(chloromethyl)-3-*p*-tolyloxazolidin-2-one (**3b**).

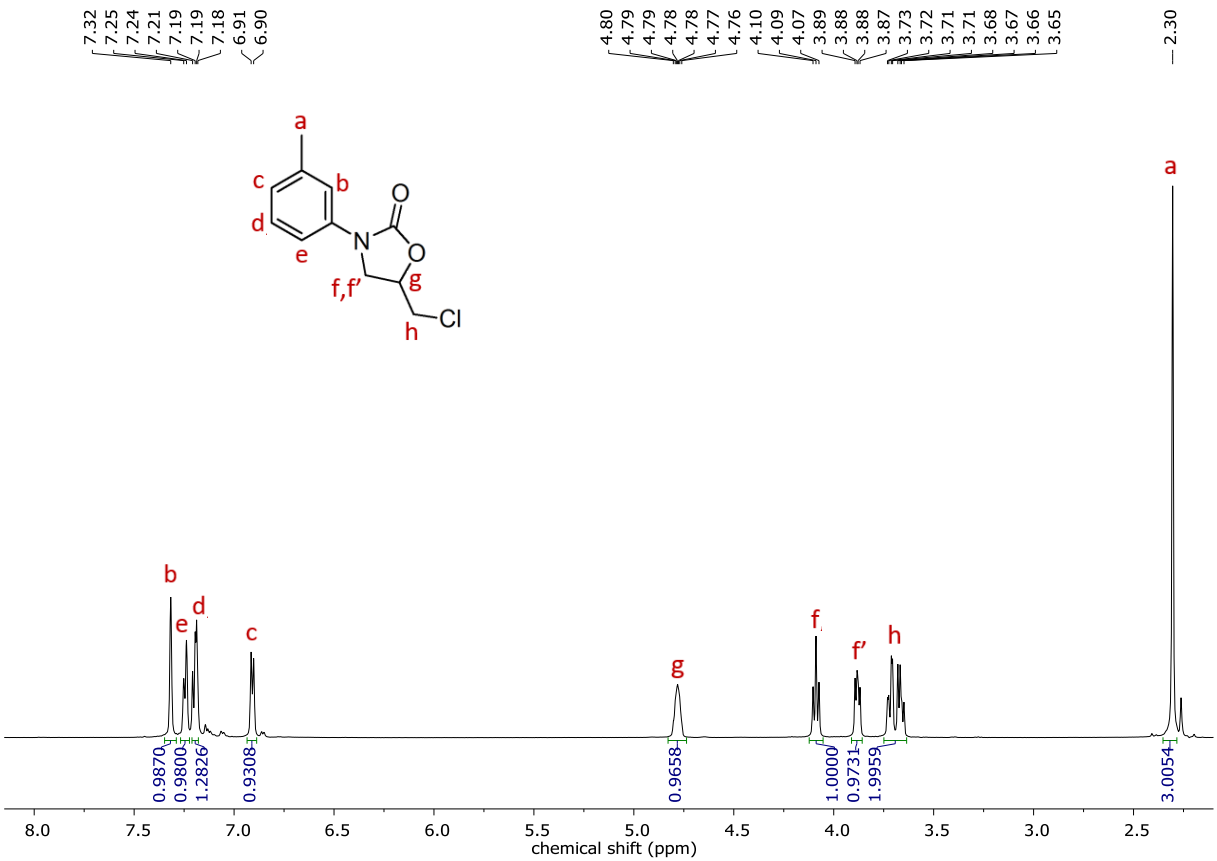


Figure S10. ^{1}H NMR ($CDCl_3$) of 5-(chloromethyl)-3-*m*-tolyloxazolidin-2-one (**3c**).

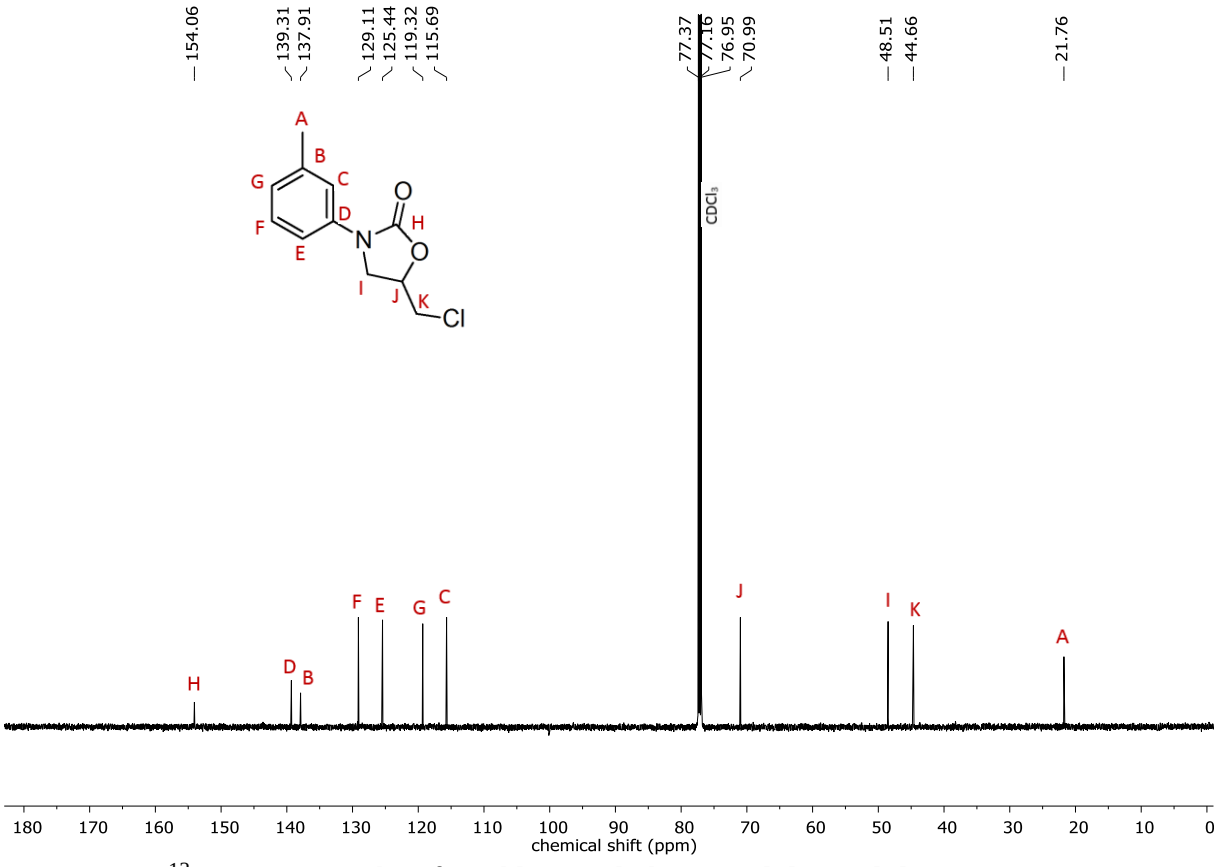


Figure S11. ^{13}C NMR ($CDCl_3$) of 5-(chloromethyl)-3-*m*-tolyloxazolidin-2-one (**3c**).

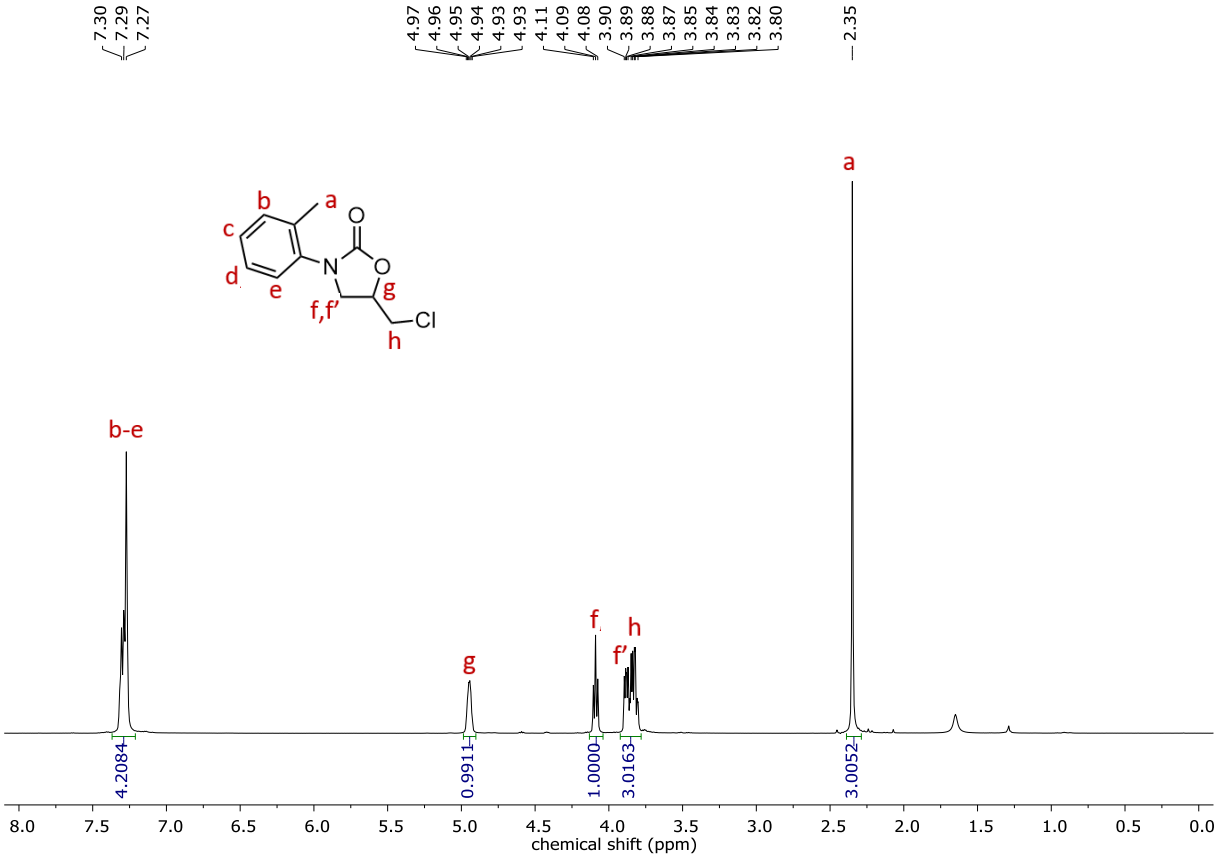


Figure S12. ^{1}H NMR ($CDCl_3$) of 5-(chloromethyl)-3-*o*-tolyloxazolidin-2-one (**3d**).

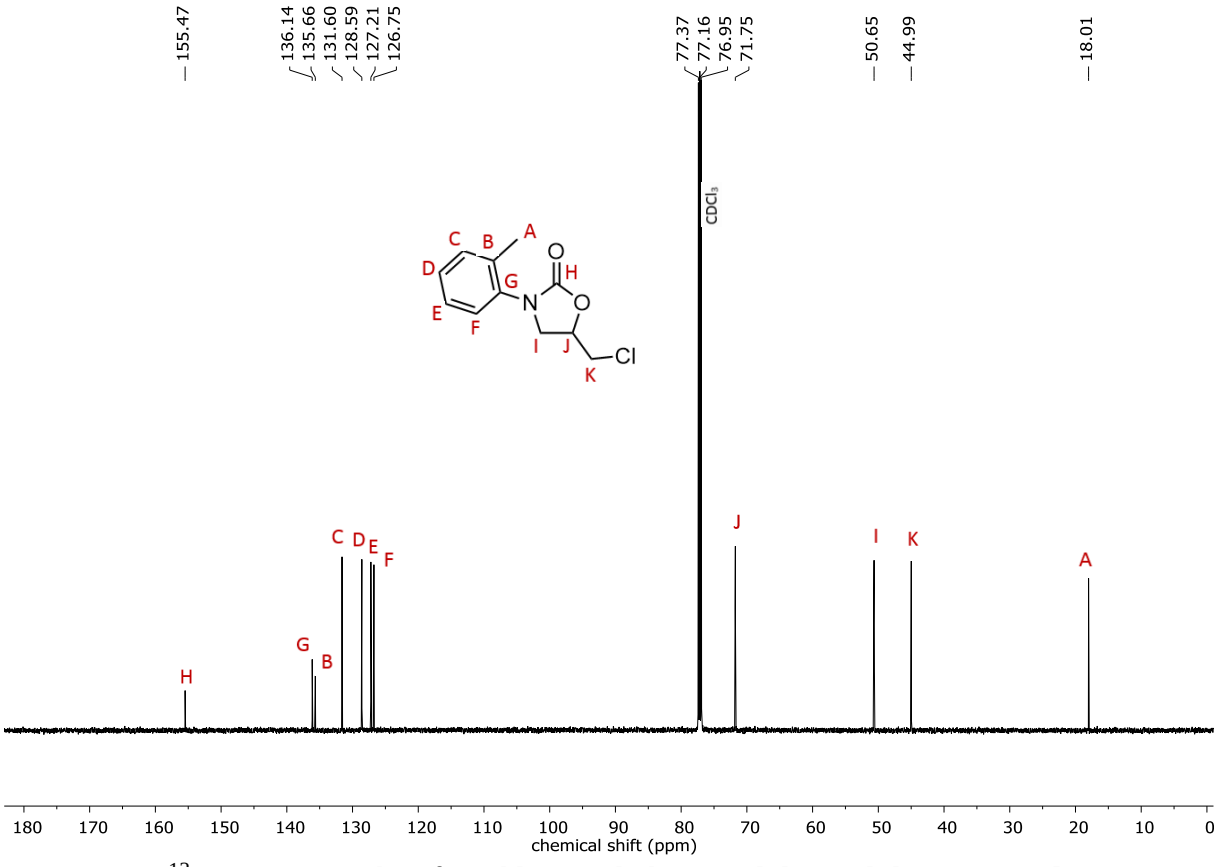


Figure S13. ^{13}C NMR ($CDCl_3$) of 5-(chloromethyl)-3-*o*-tolyloxazolidin-2-one (**3d**).

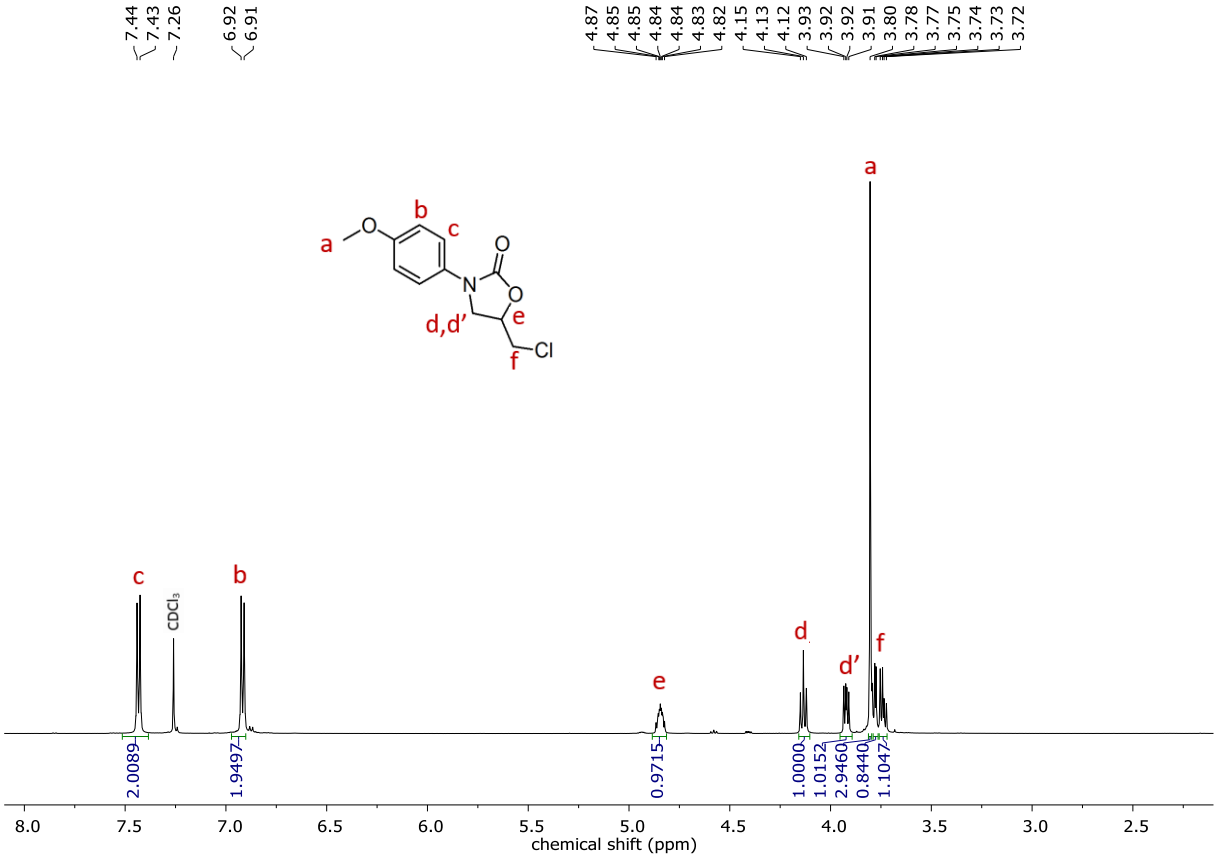


Figure S14. ^{1}H NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-methoxyphenol)oxazolidin-2-one (**3e**).

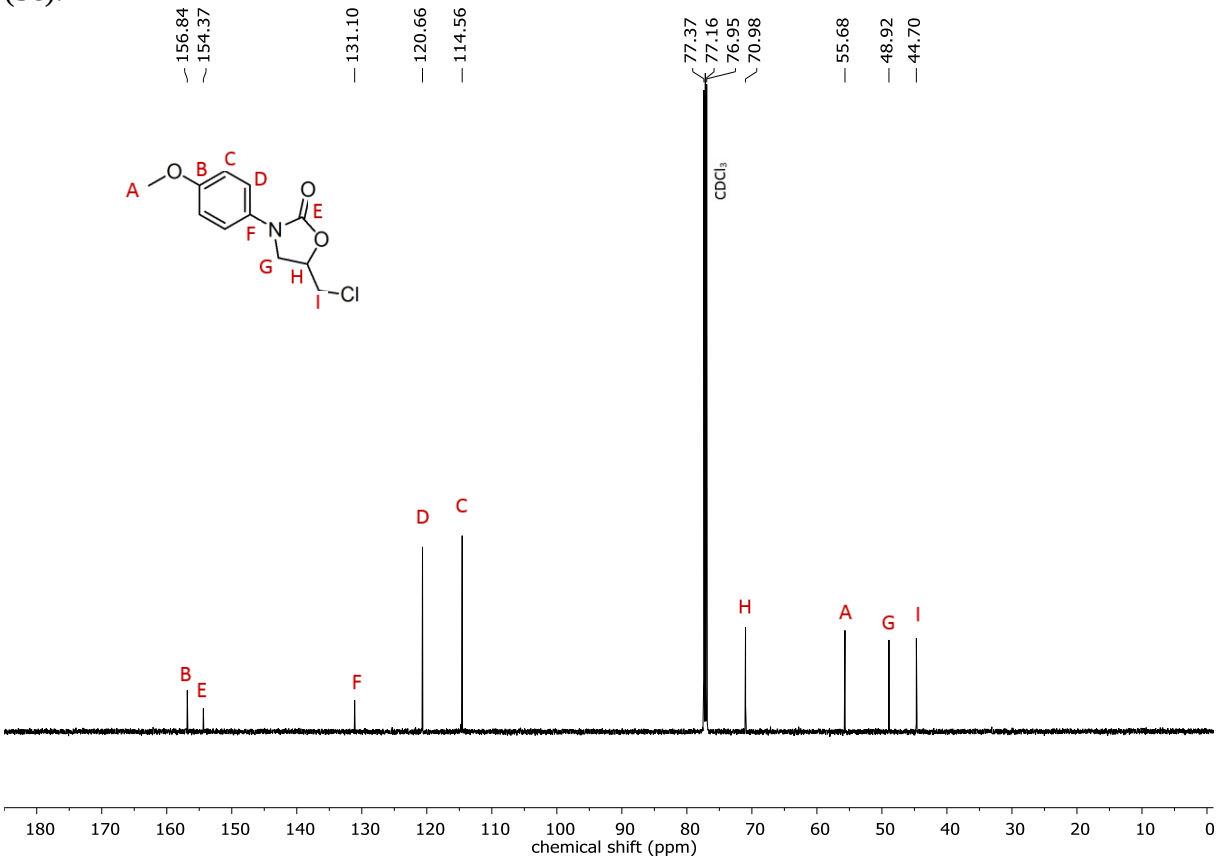


Figure S15. ^{13}C NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-methoxyphenol)oxazolidin-2-one (**3e**).

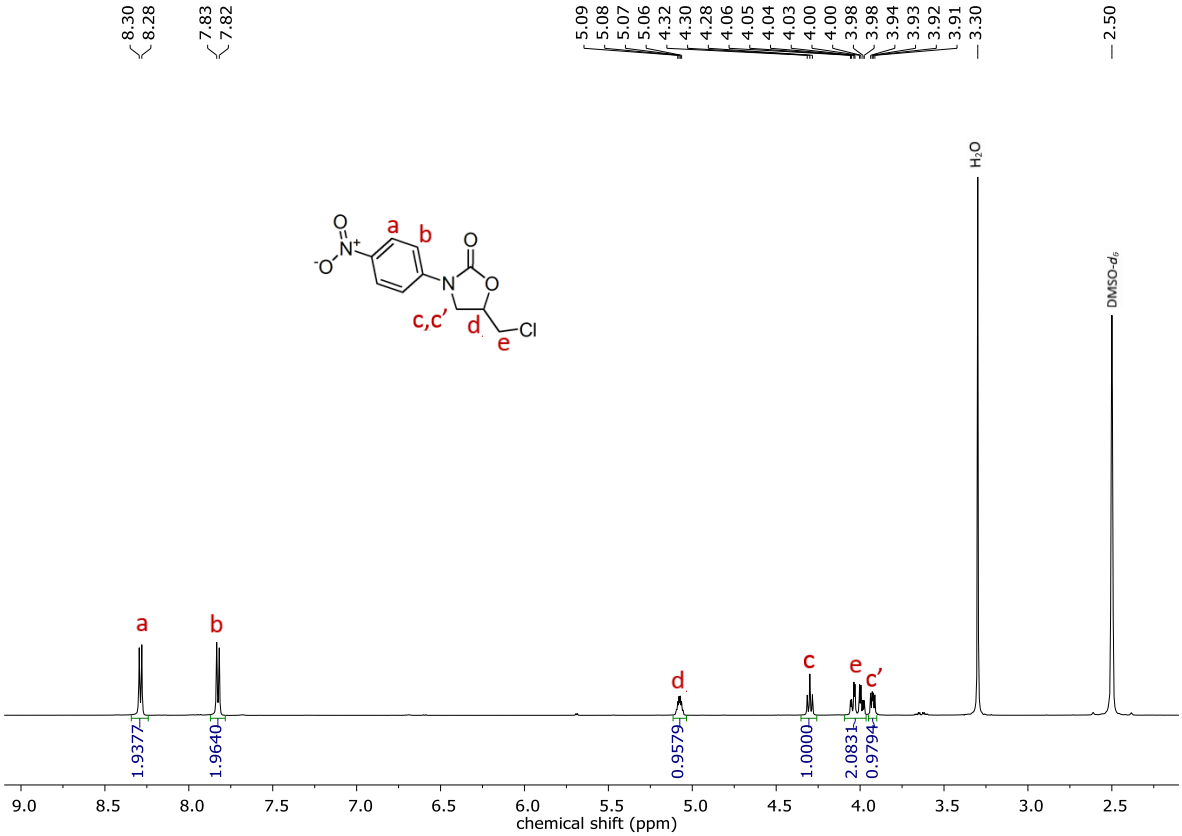


Figure S16. ^{1}H NMR (DMSO-d_6) of 5-(chloromethyl)-3-(4-nitrophenyl)oxazolidin-2-one (**3f**).

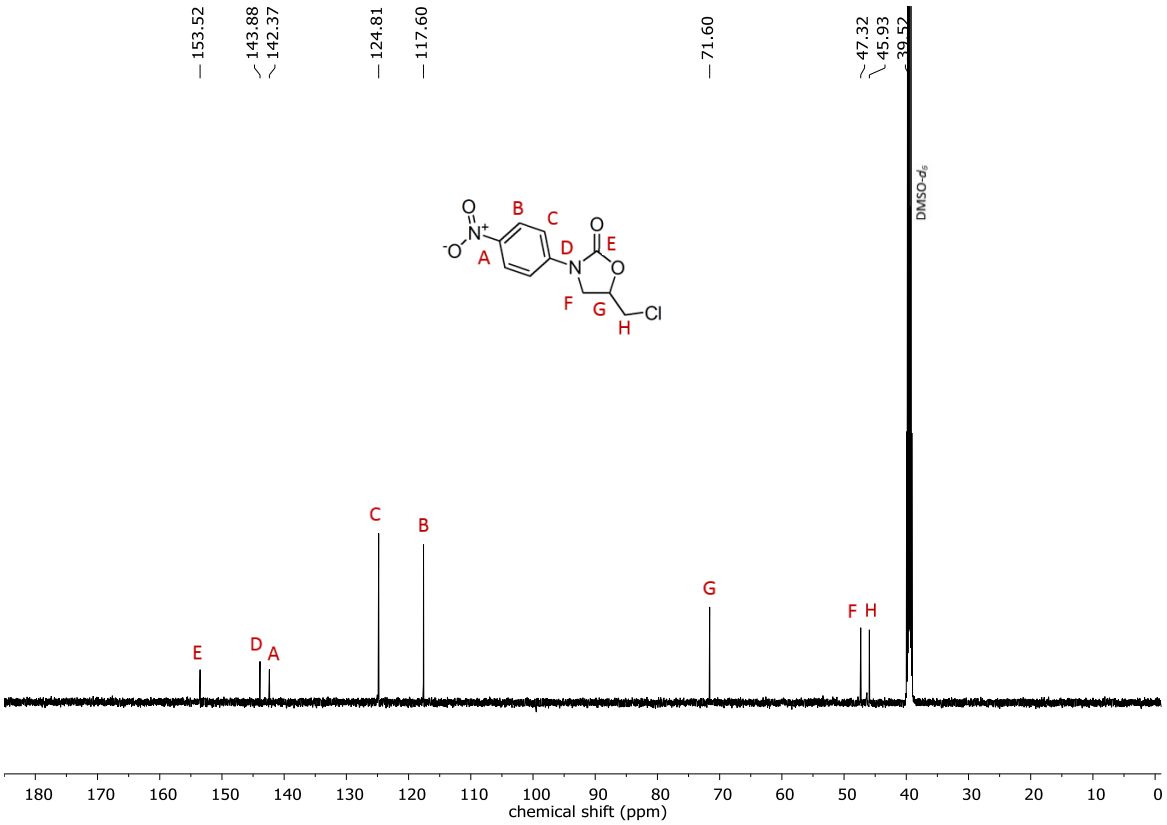


Figure S17. ^{13}C NMR (DMSO-d_6) of 5-(chloromethyl)-3-(4-nitrophenyl)oxazolidin-2-one (**3f**).

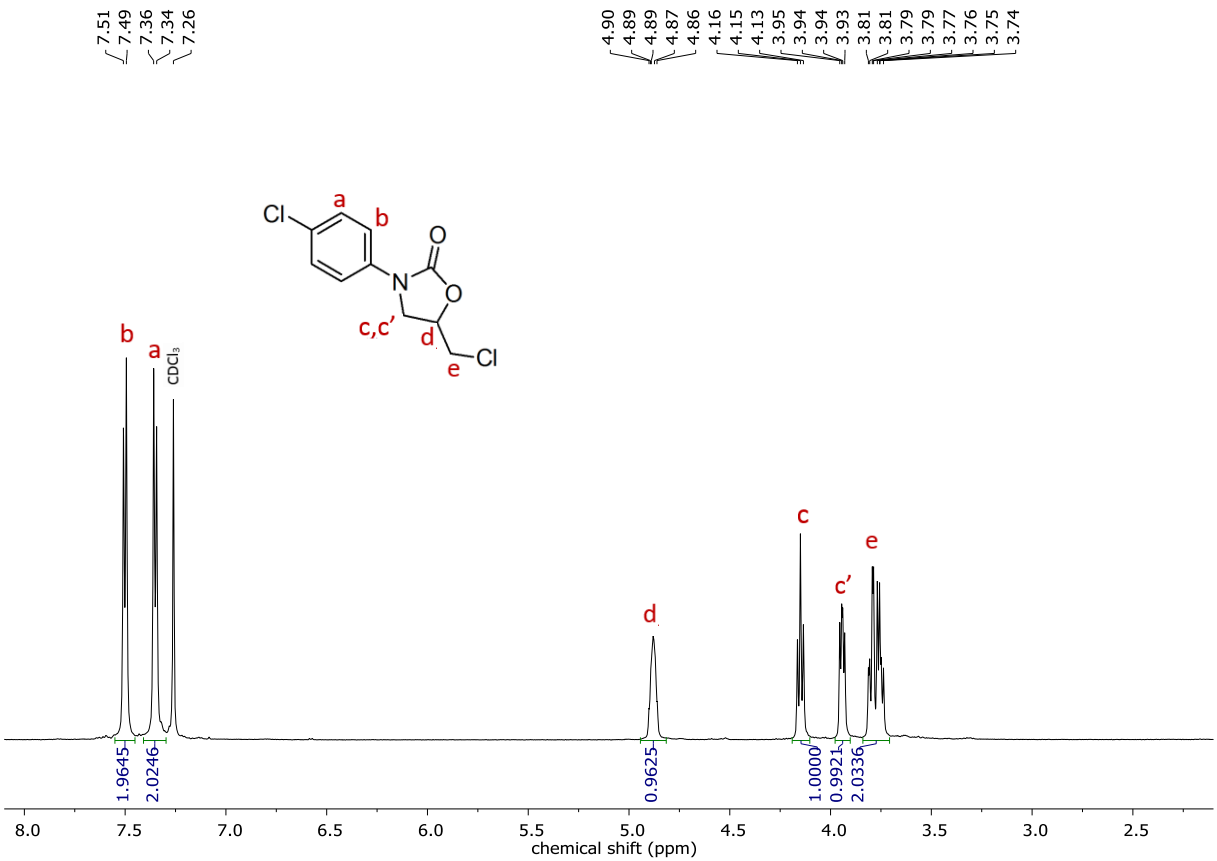


Figure S18. ^{1}H NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-chlorophenyl)oxazolidin-2-one (**3g**).

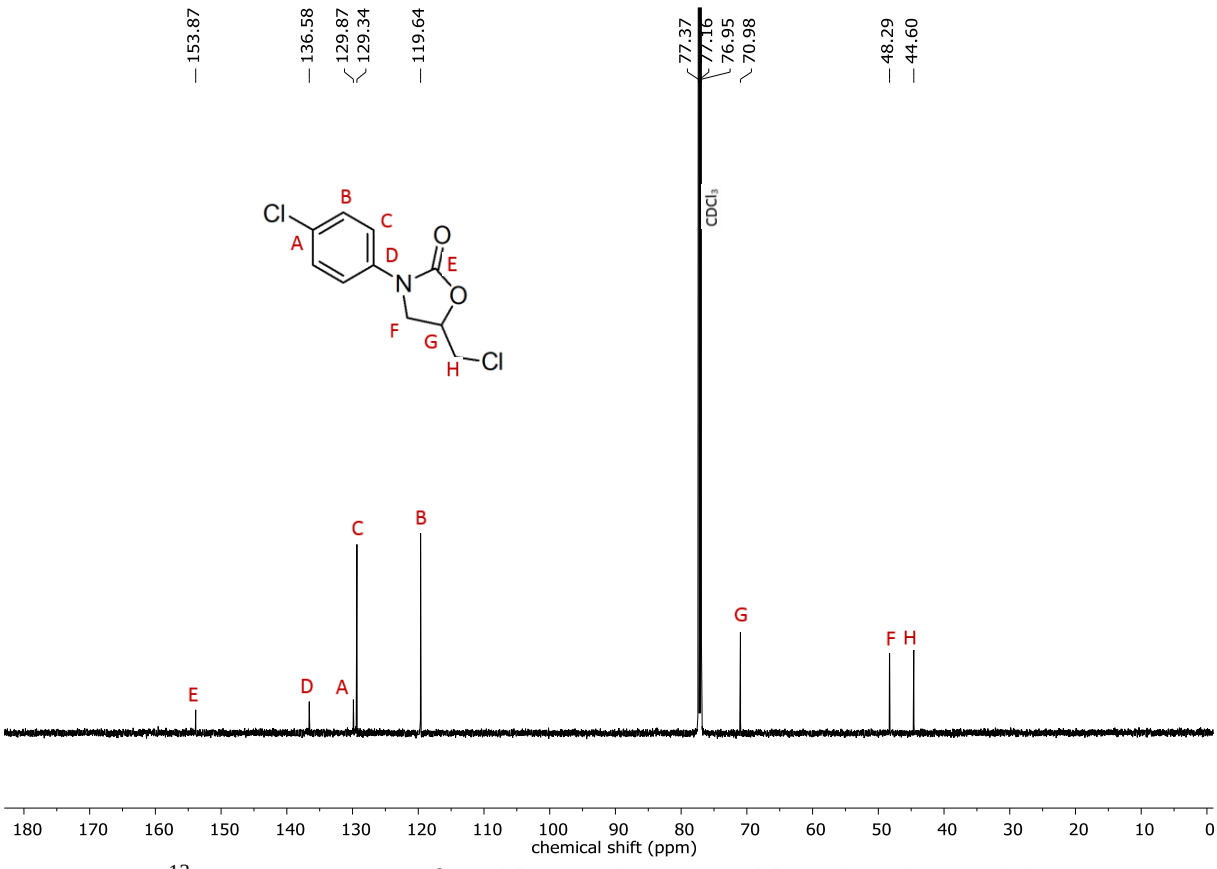


Figure S19. ^{13}C NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-chlorophenyl)oxazolidin-2-one (**3g**).

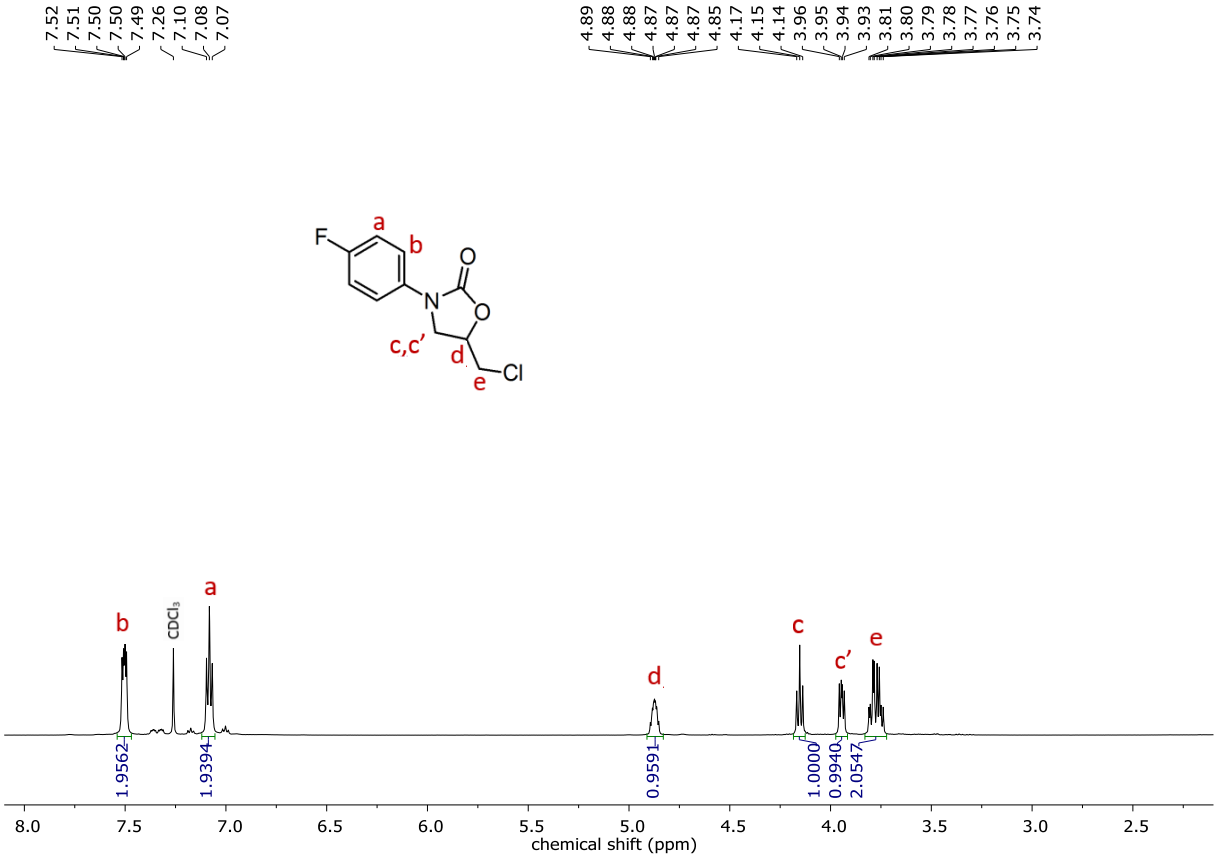


Figure S20. ^{1}H NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-fluorophenyl)oxazolidin-2-one (**3h**).

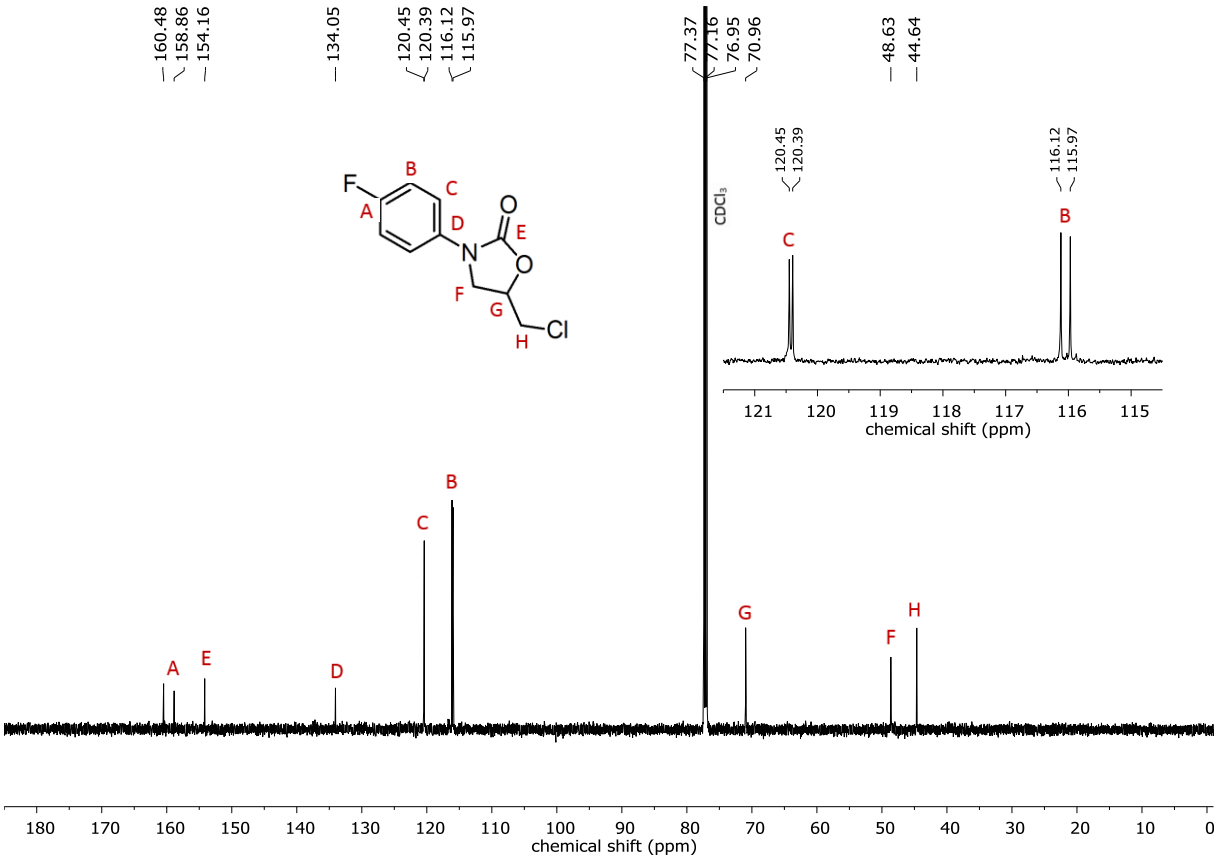


Figure S21. ^{13}C NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-fluorophenyl)oxazolidin-2-one (**3h**).

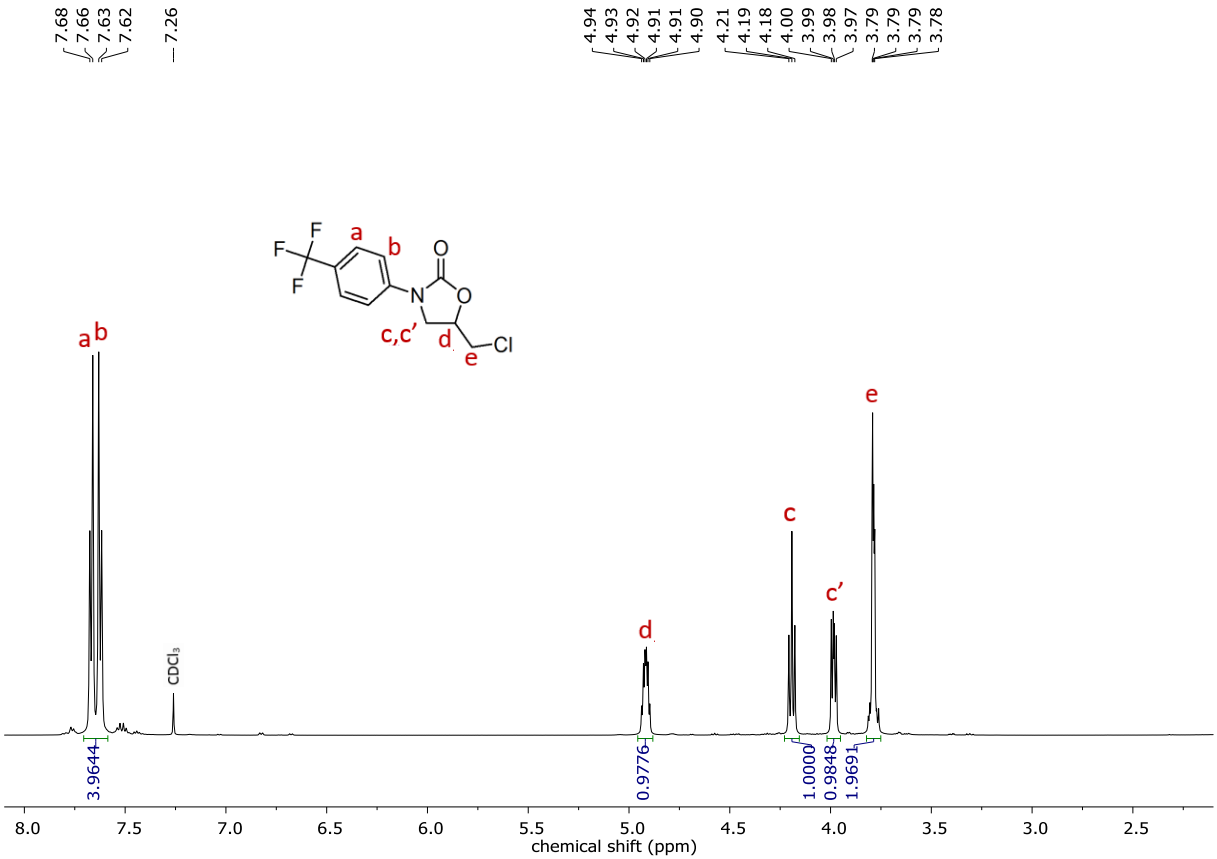


Figure S22. ^{1}H NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-(trifluoromethyl)phenyl)oxazolidin-2-one (**3i**).

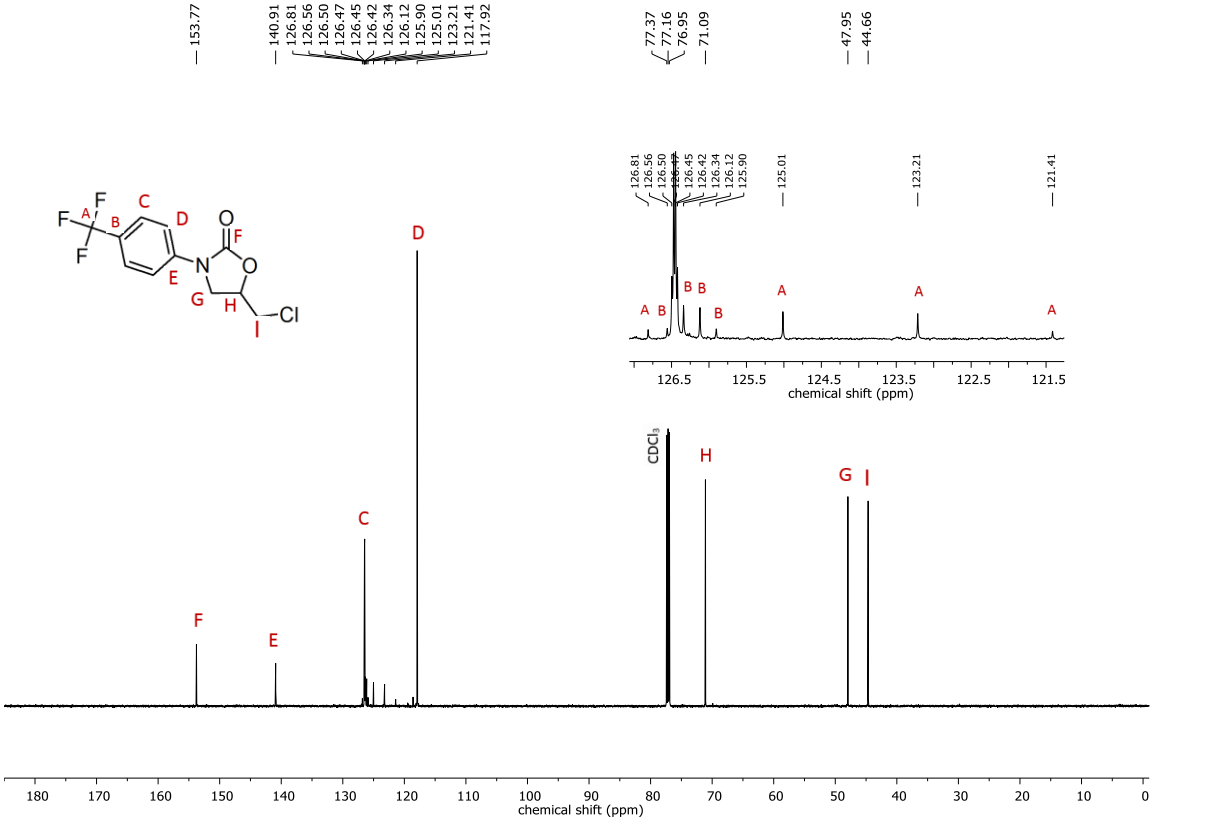


Figure S23. ^{13}C NMR ($CDCl_3$) of 5-(chloromethyl)-3-(4-(trifluoromethyl)phenyl)oxazolidin-2-one (**3i**).

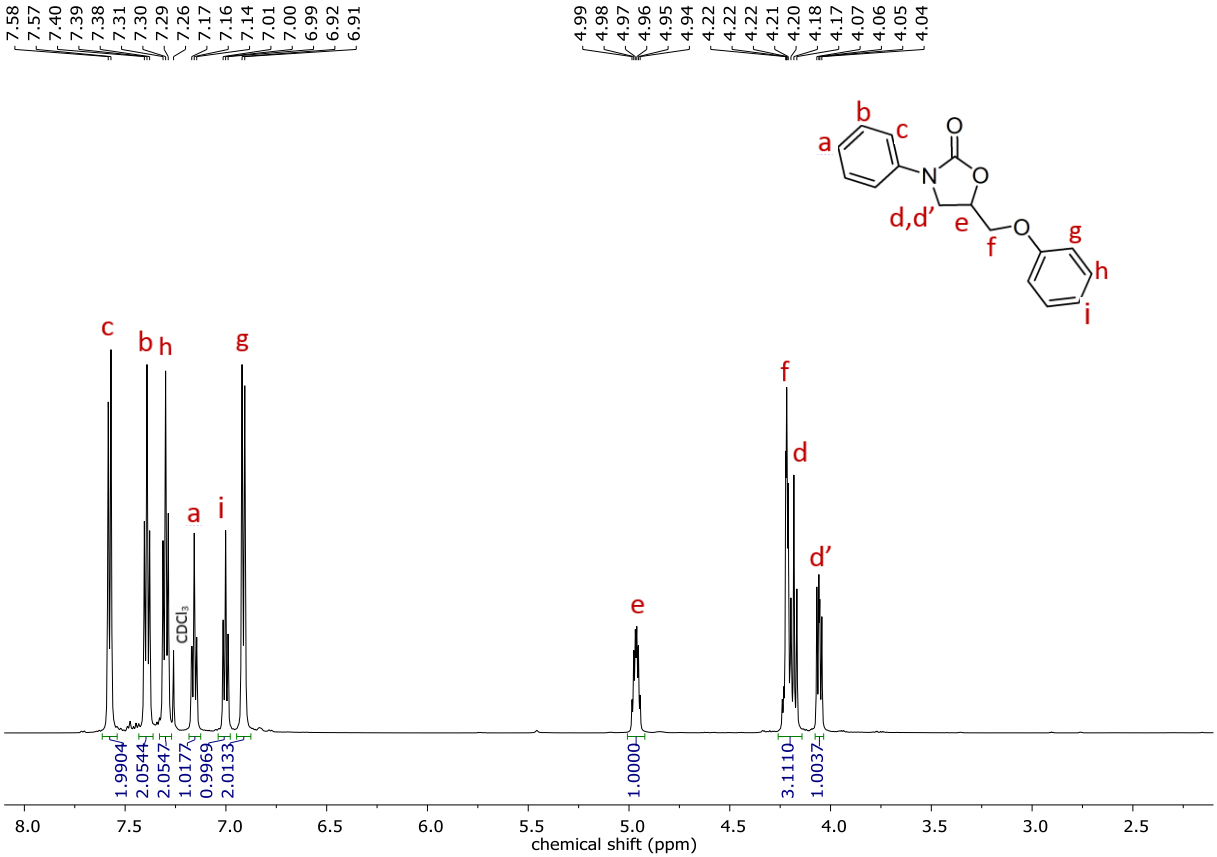


Figure S24. ^{1}H NMR ($CDCl_3$) of 5-(phenoxymethyl)-3-phenyloxazolidin-2-one (**3j**).

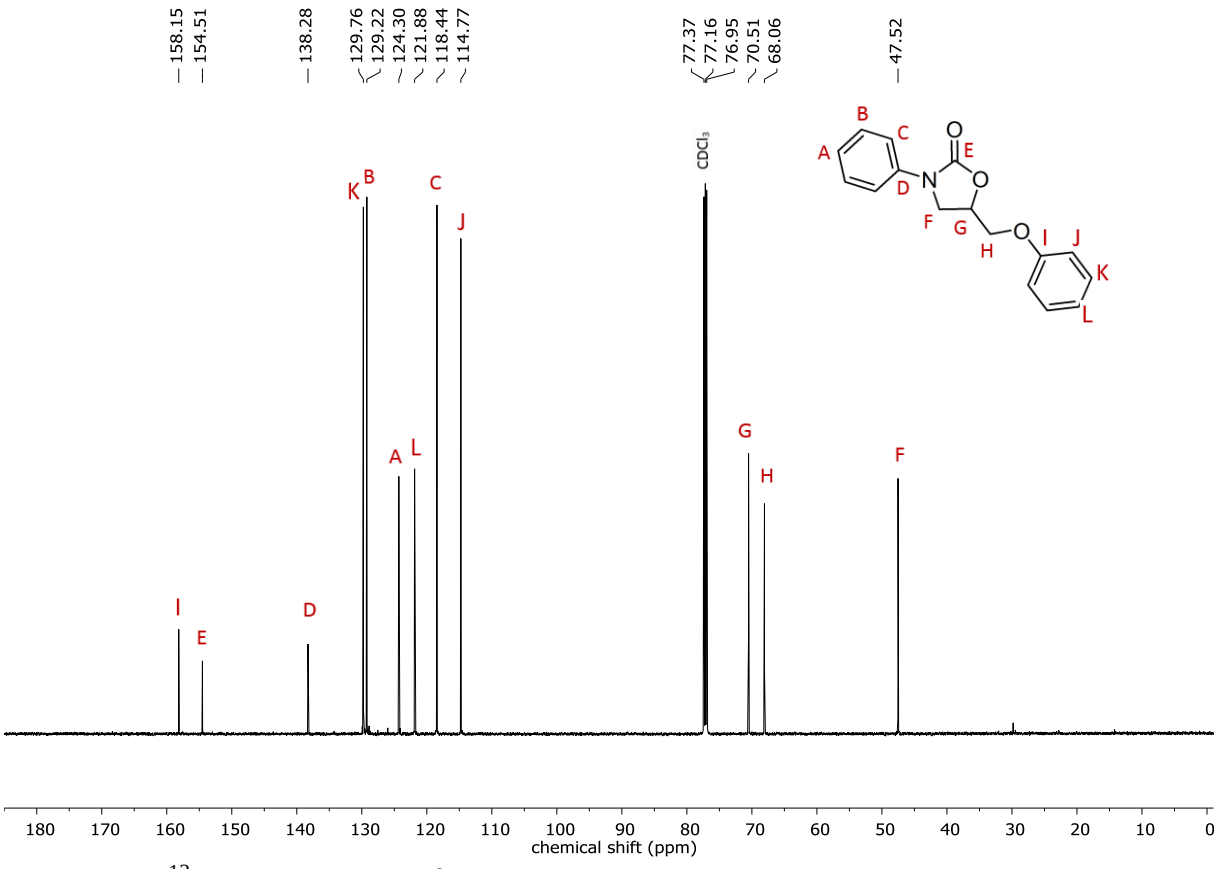


Figure S25. ^{13}C NMR ($CDCl_3$) of 5-(phenoxymethyl)-3-phenyloxazolidin-2-one (**3j**).

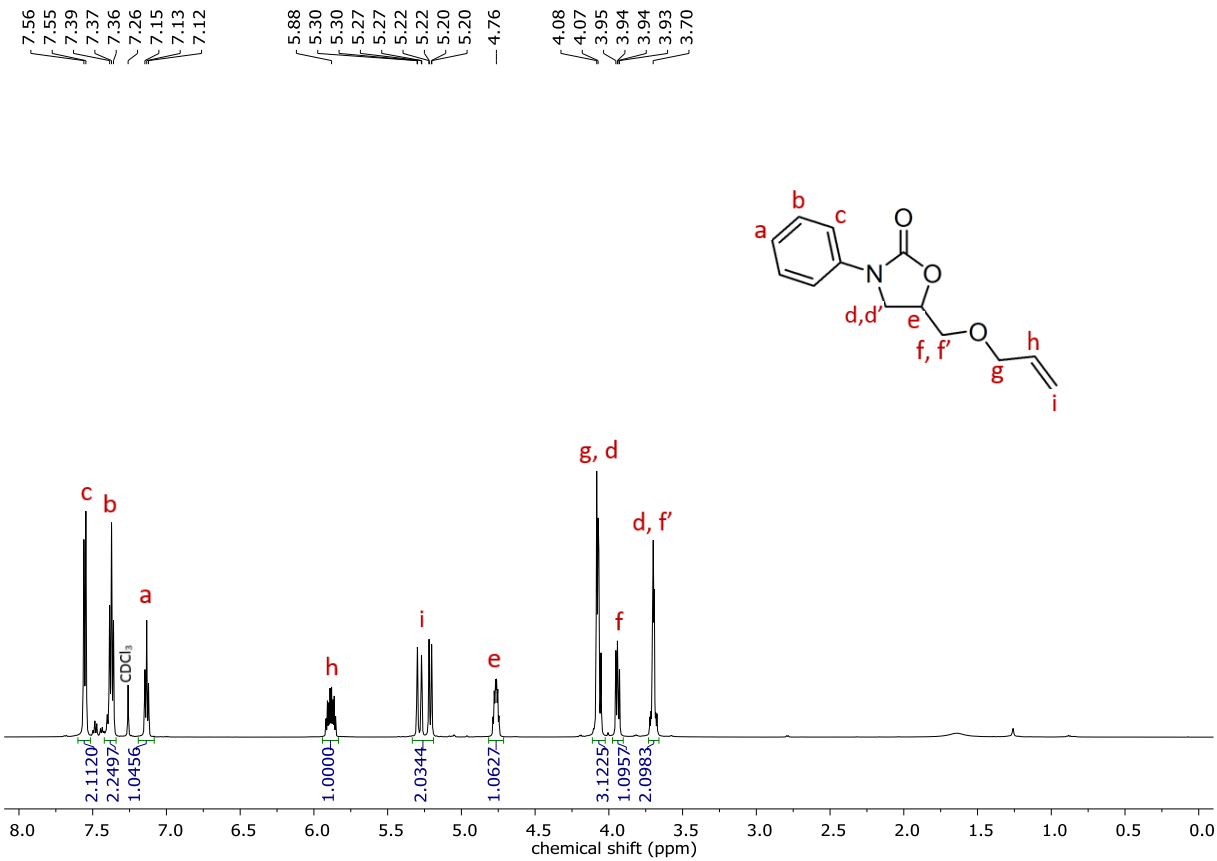


Figure S26. ^{1}H NMR ($CDCl_3$) of 5-(allyloxymethyl)-3-phenyloxazolidin-2-one (**3k**).

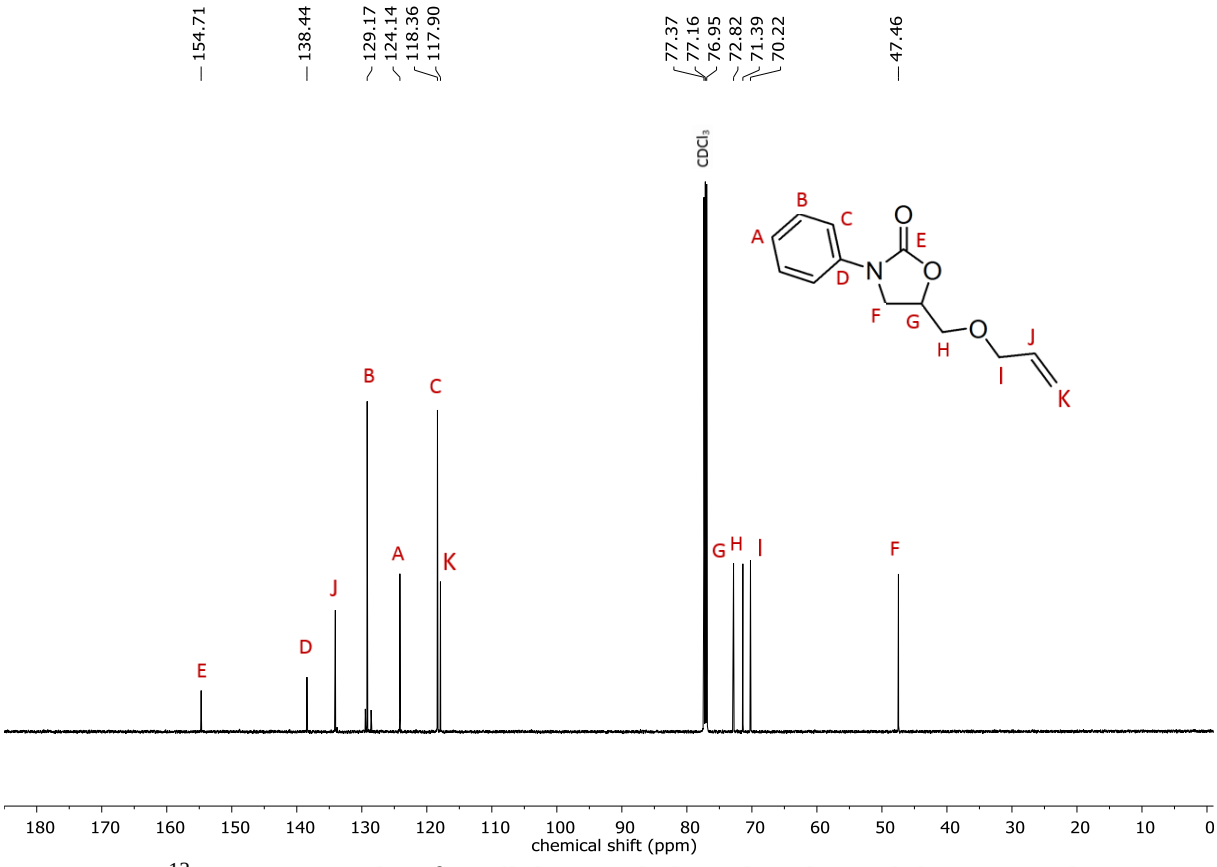


Figure S27. ^{13}C NMR ($CDCl_3$) of 5-(allyloxymethyl)-3-phenyloxazolidin-2-one (**3k**).

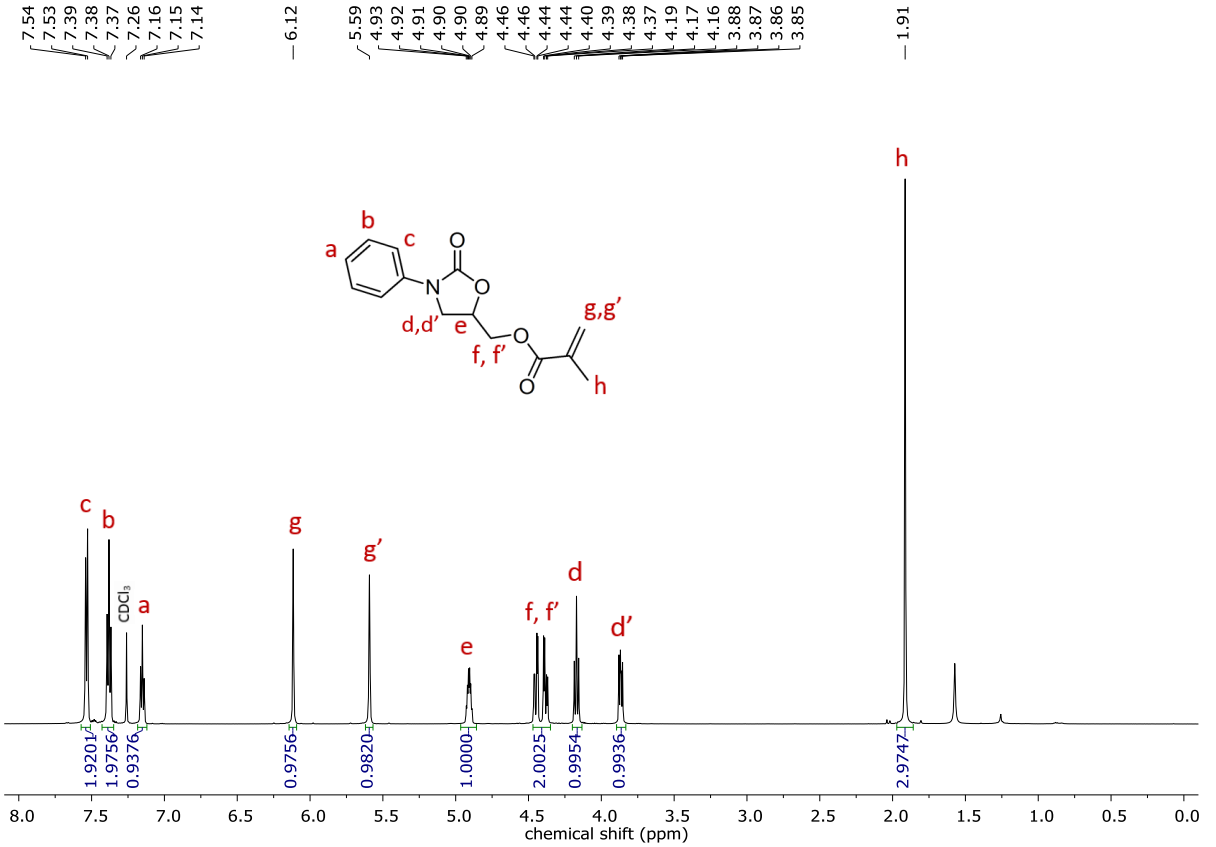


Figure S28. ^{1}H NMR ($CDCl_3$) of (2-oxo-3-phenyloxazolidin-5-yl)methylmethacrylate (**3l**).

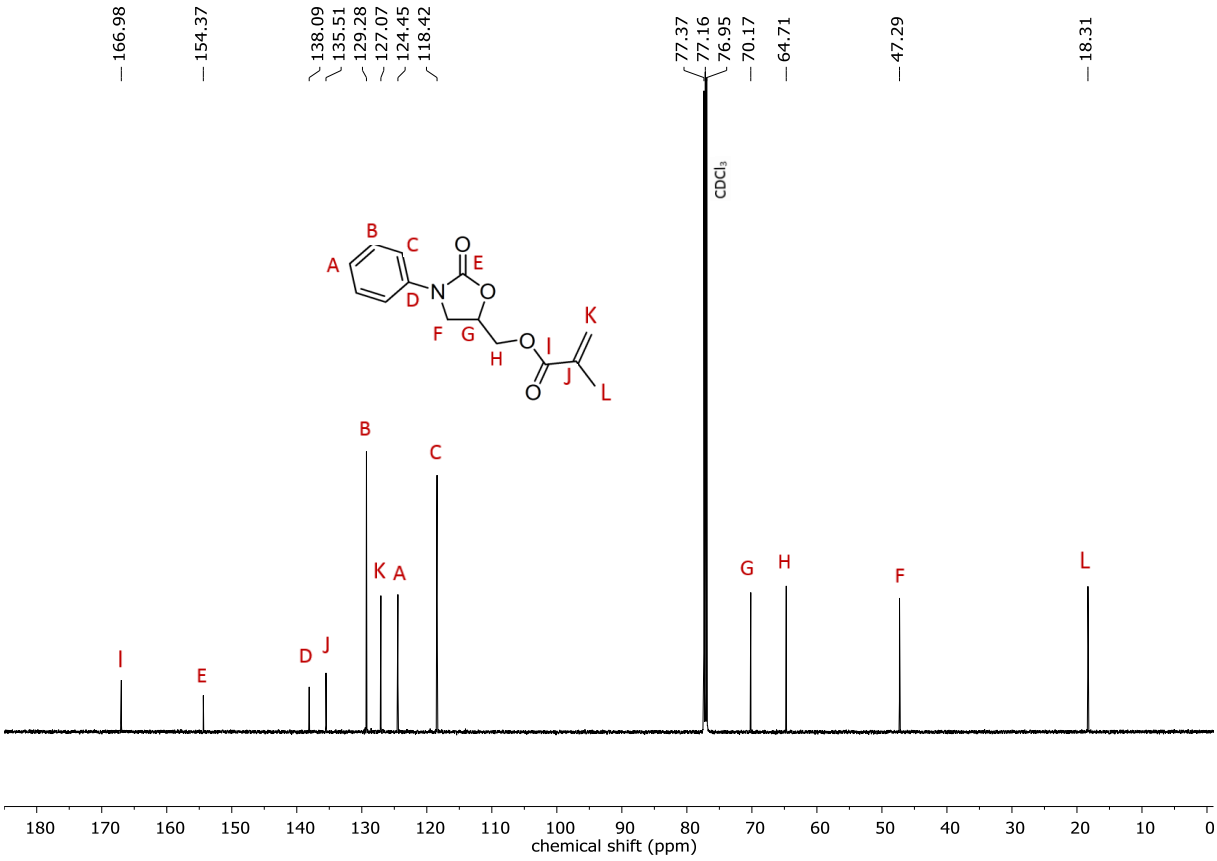


Figure S29. ^{13}C NMR ($CDCl_3$) of (2-oxo-3-phenyloxazolidin-5-yl)methylmethacrylate (**3l**).

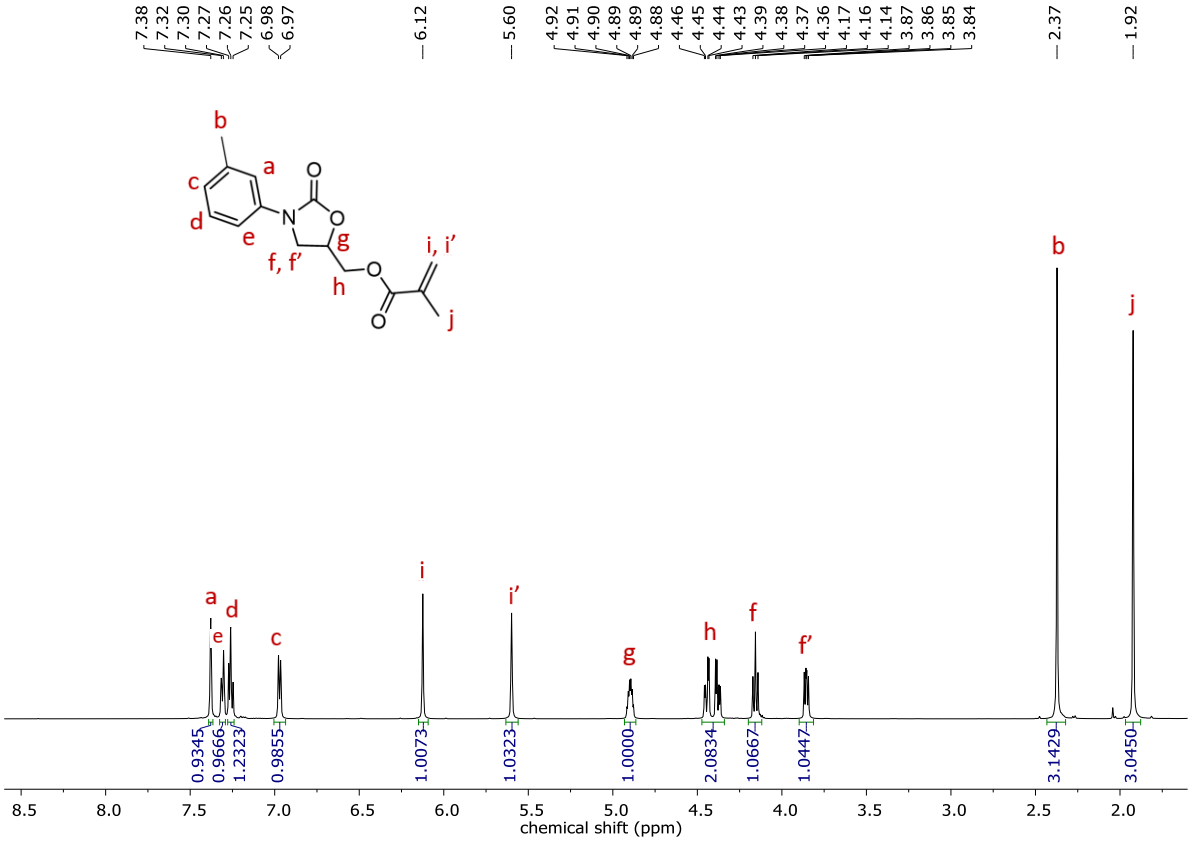


Figure S30. ^{1}H NMR ($CDCl_3$) of (2-oxo-3-(m-tolyl)oxazolidin-5-yl)methyl methacrylate (**3m**).

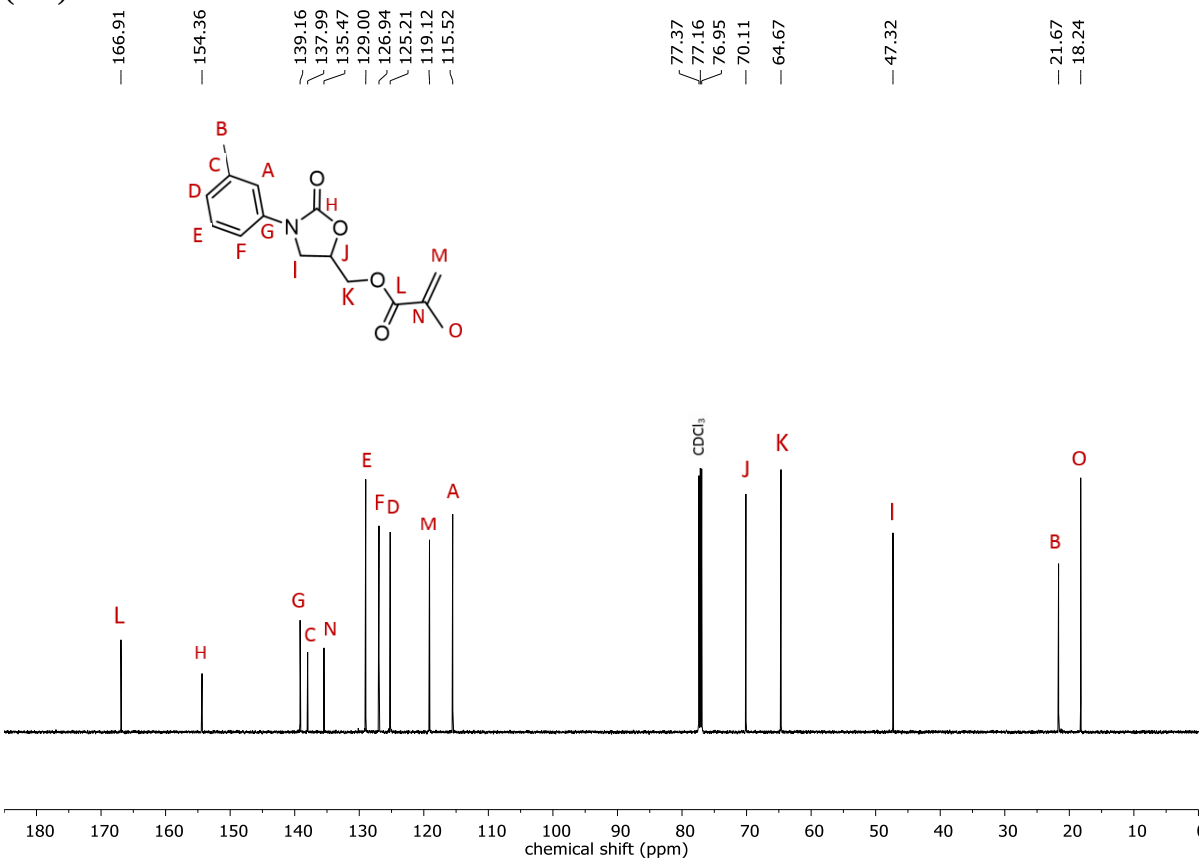


Figure S31. ^{13}C NMR ($CDCl_3$) of (2-oxo-3-(m-tolyl)oxazolidin-5-yl)methyl methacrylate (**3m**).

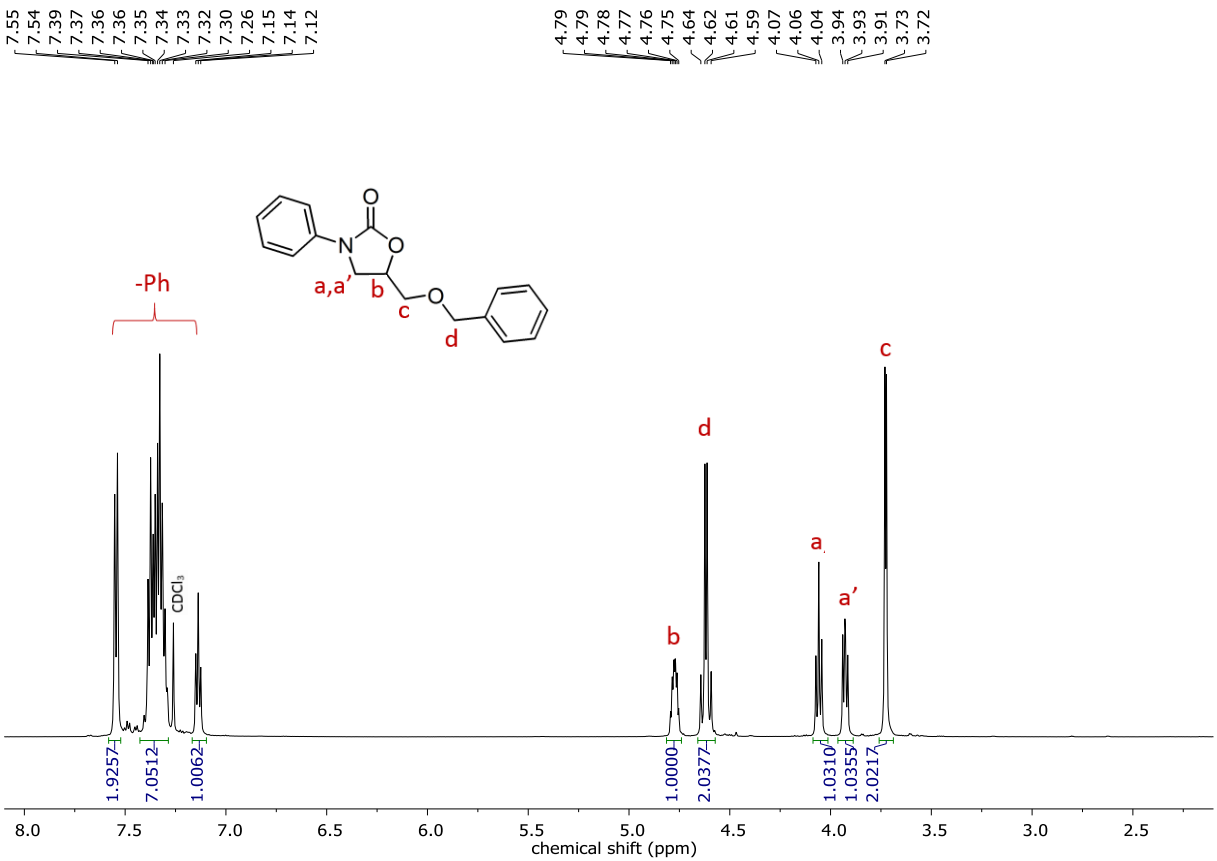


Figure S32. ^{1}H NMR ($CDCl_3$) of 5-(benzyloxymethyl)-3-phenyloxazolidin-2-one (**3n**).

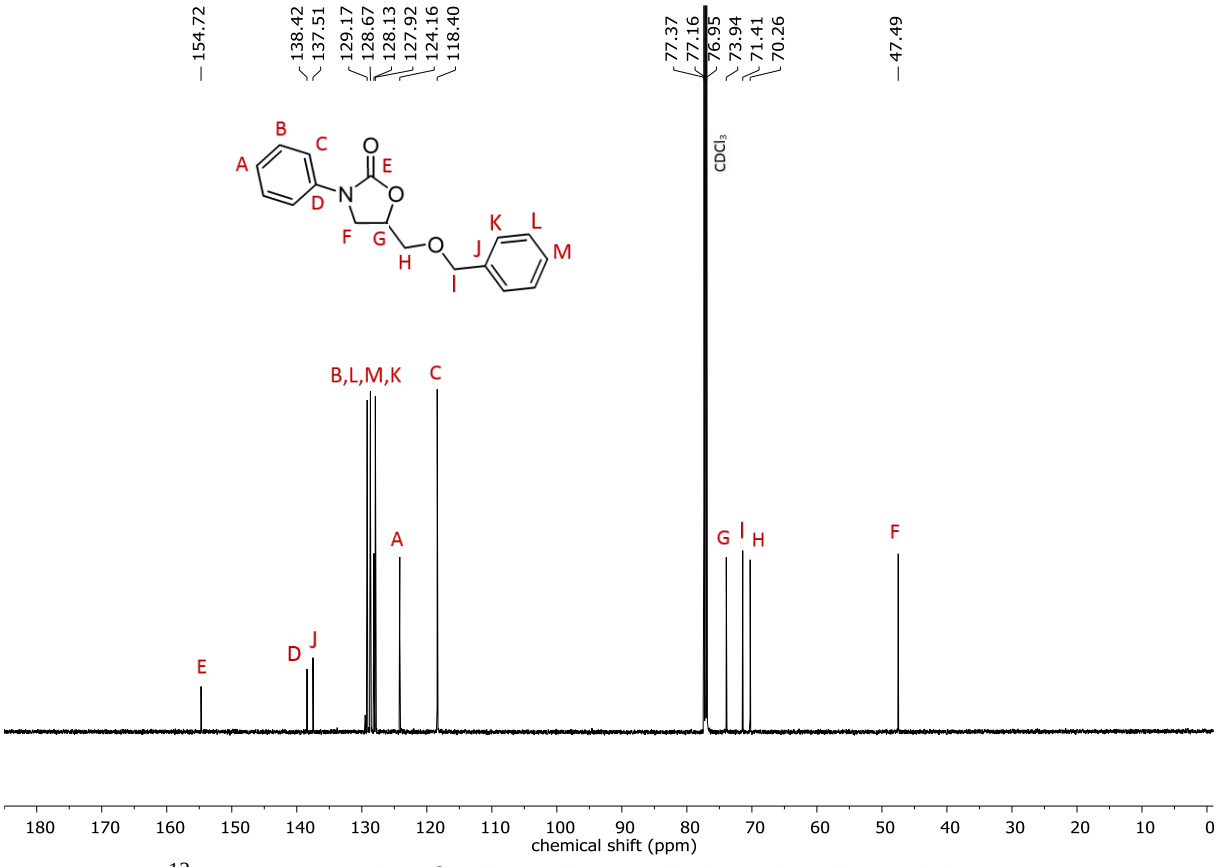


Figure S33. ^{13}C NMR ($CDCl_3$) of 5-(benzyloxymethyl)-3-phenyloxazolidin-2-one (**3n**).

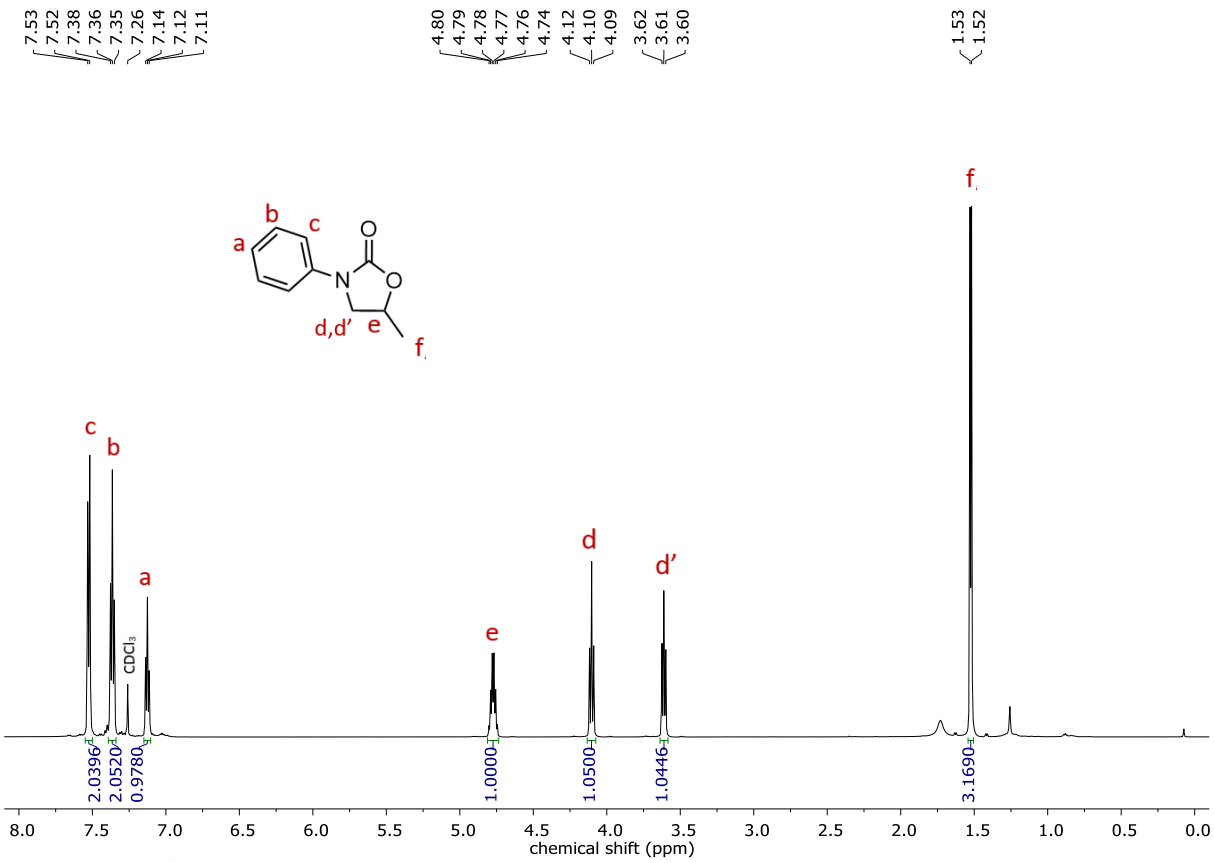


Figure S34. ^{1}H NMR ($CDCl_3$) of 5-methyl-3-phenyloxazolidin-2-one (**3o**).

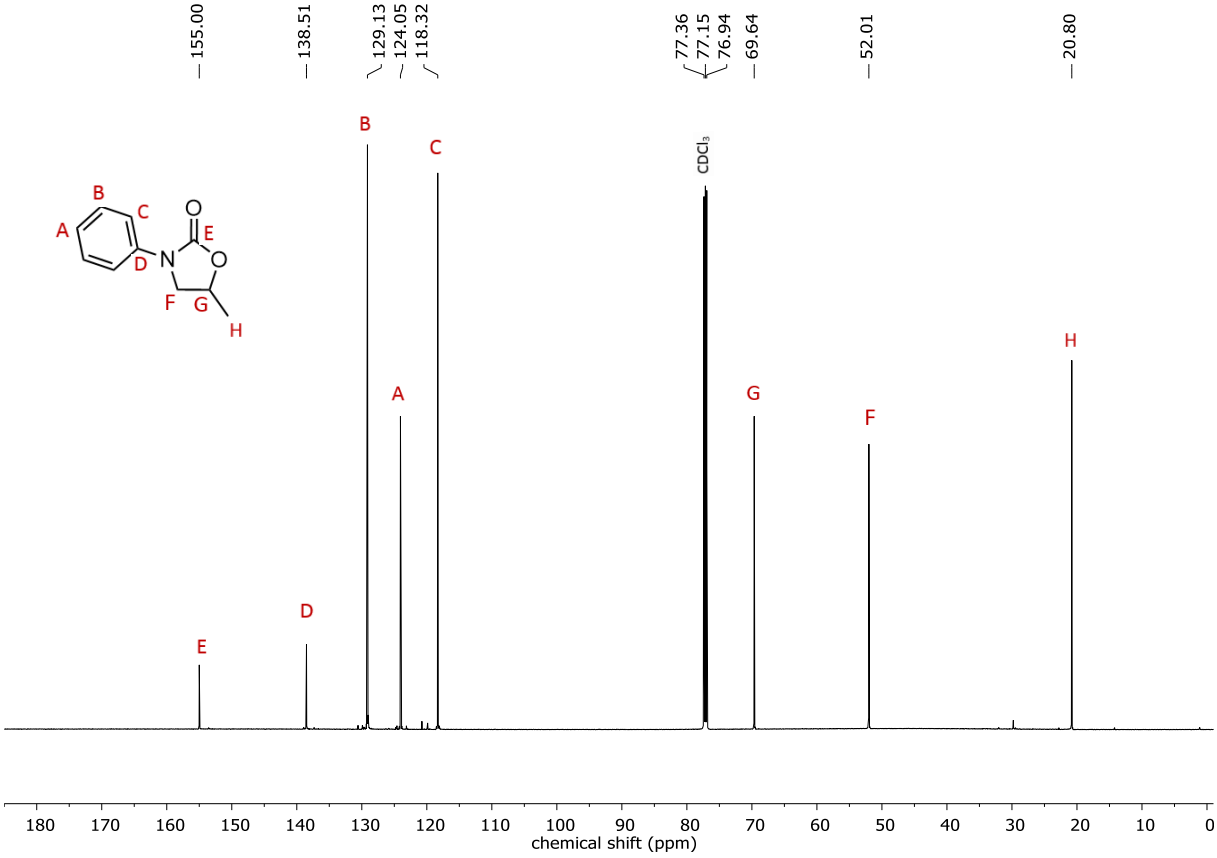


Figure S35. ^{13}C NMR ($CDCl_3$) of 5-methyl-3-phenyloxazolidin-2-one (**3o**).

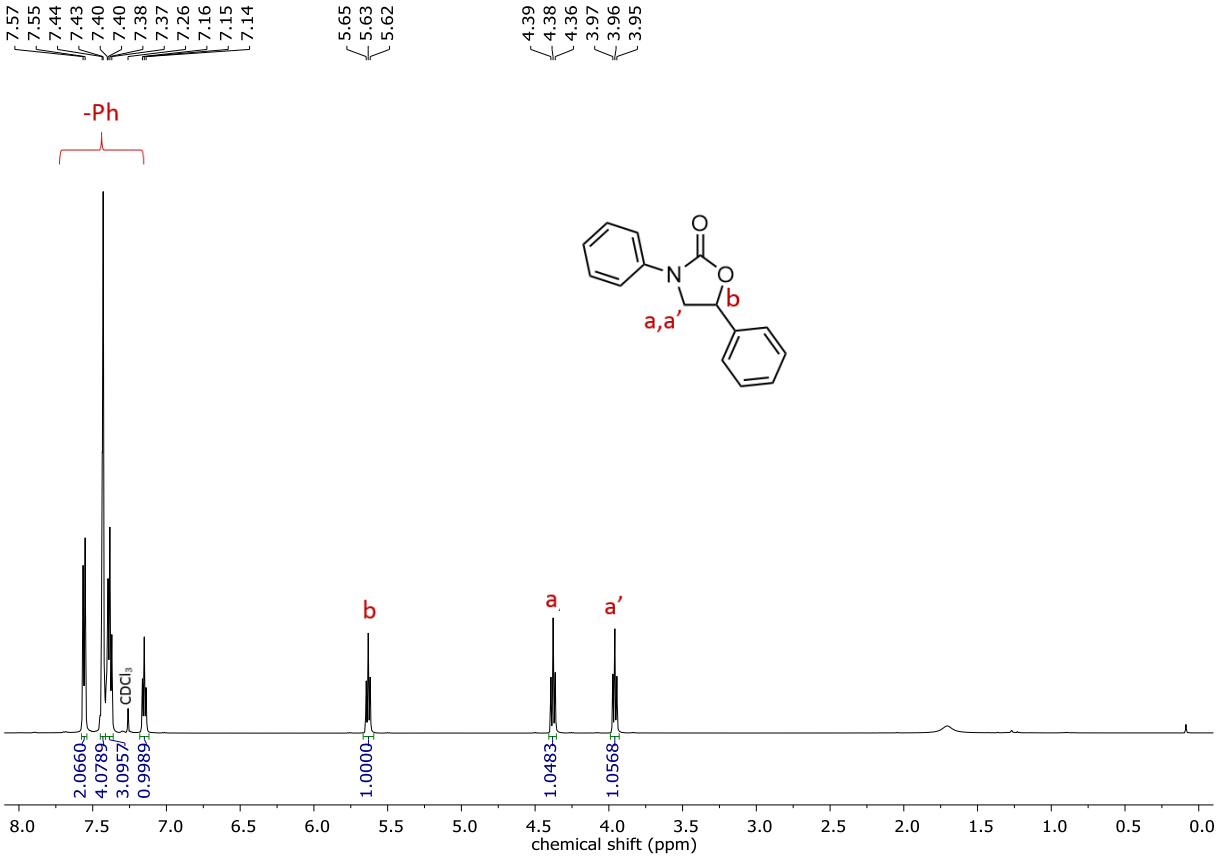


Figure S36. ^{1}H NMR ($CDCl_3$) of 3, 5-diphenyloxazolidin-2-one (**3p**).

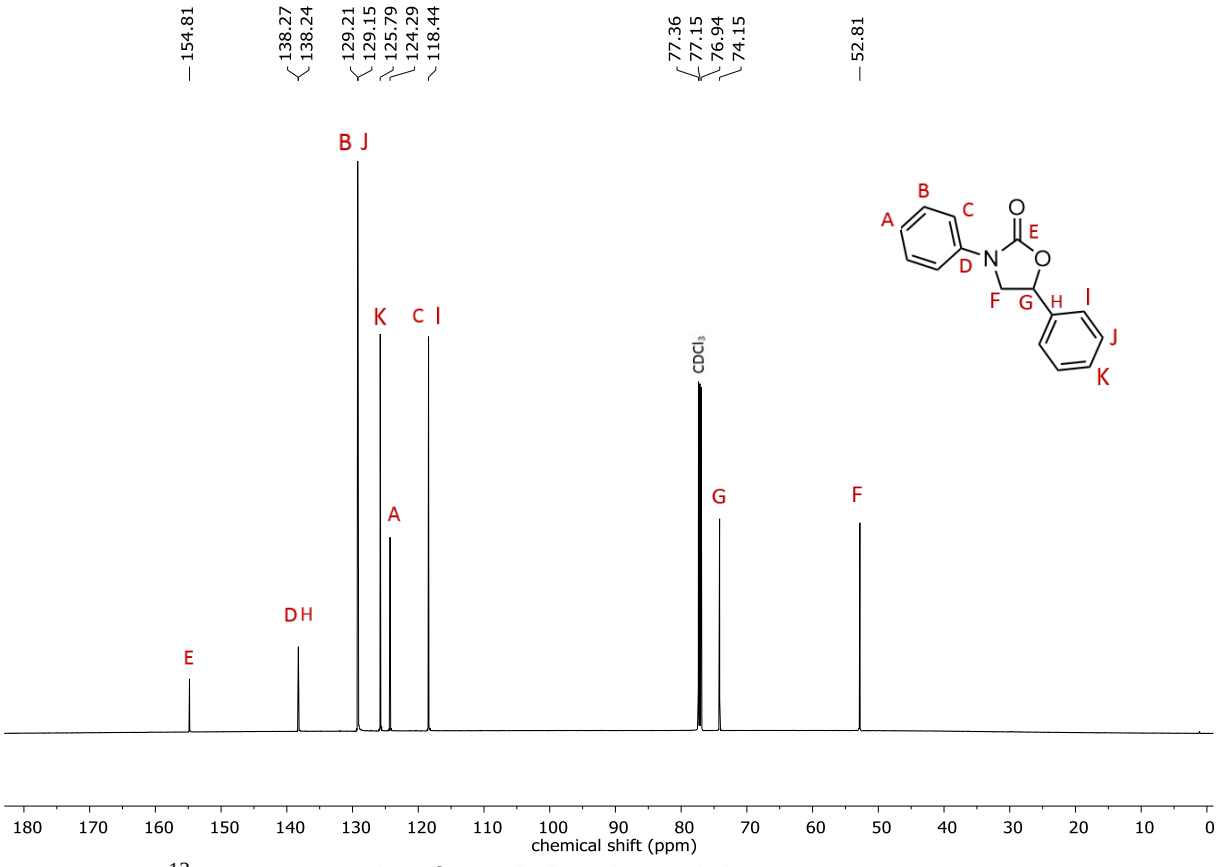


Figure S37. ^{13}C NMR ($CDCl_3$) of 3, 5-diphenyloxazolidin-2-one (**3p**).

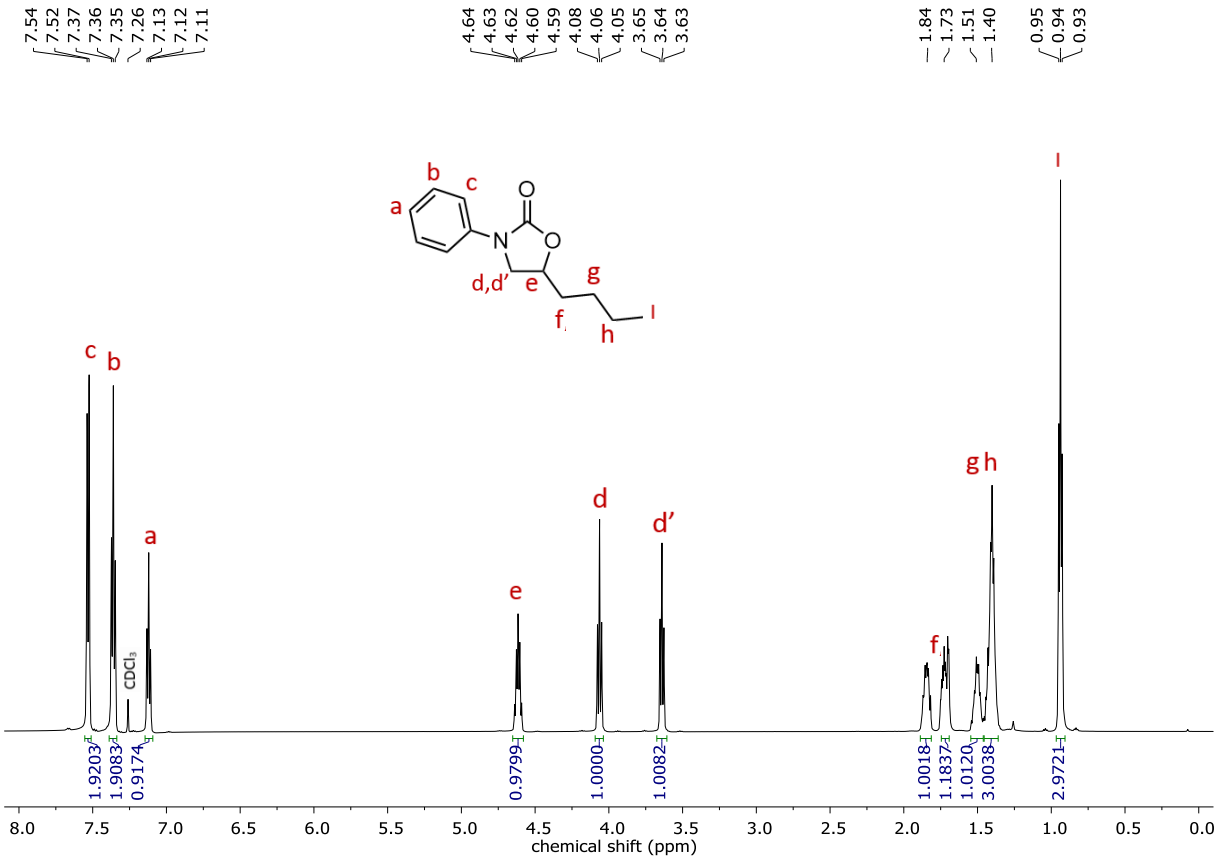


Figure S38. ^{1}H NMR ($CDCl_3$) of 5-butyl-3-phenyloxazolidin-2-one (**3q**).

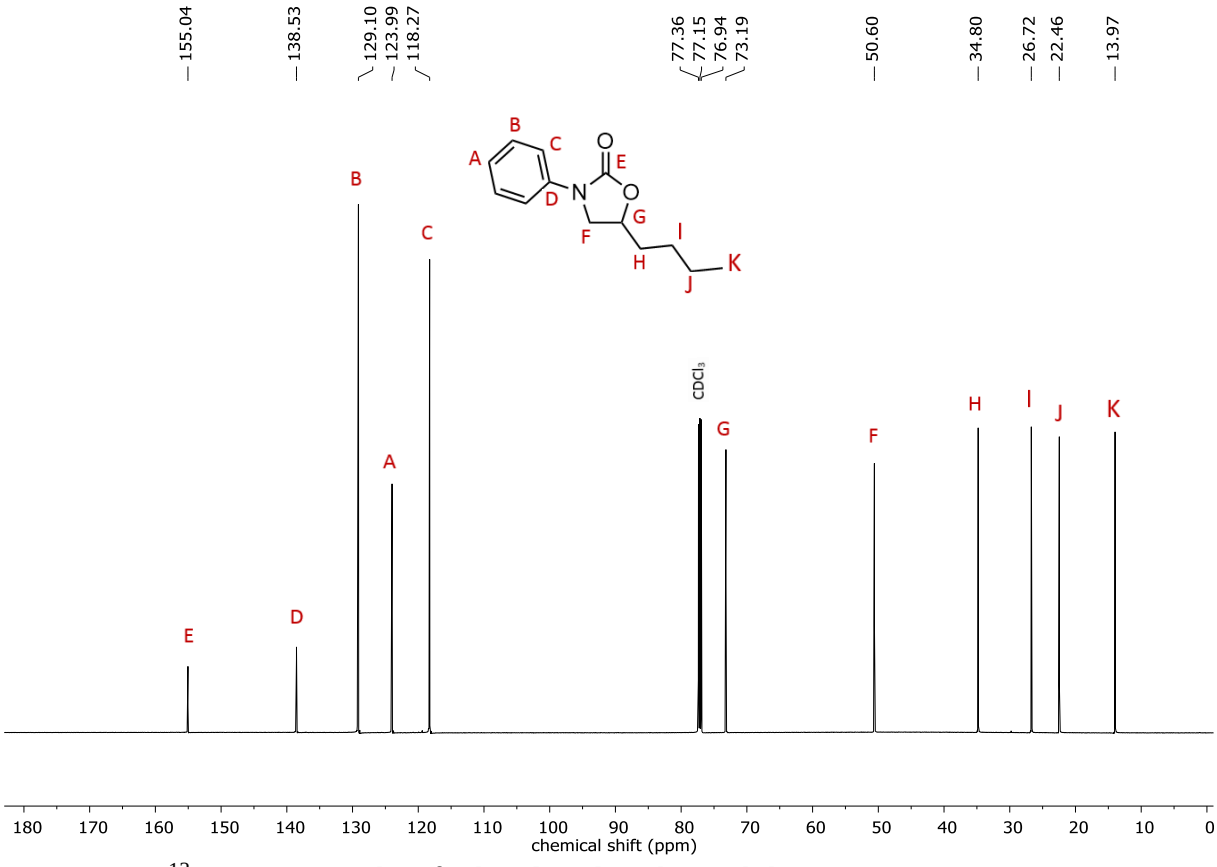


Figure S39. ^{13}C NMR ($CDCl_3$) of 5-butyl-3-phenyloxazolidin-2-one (**3q**).

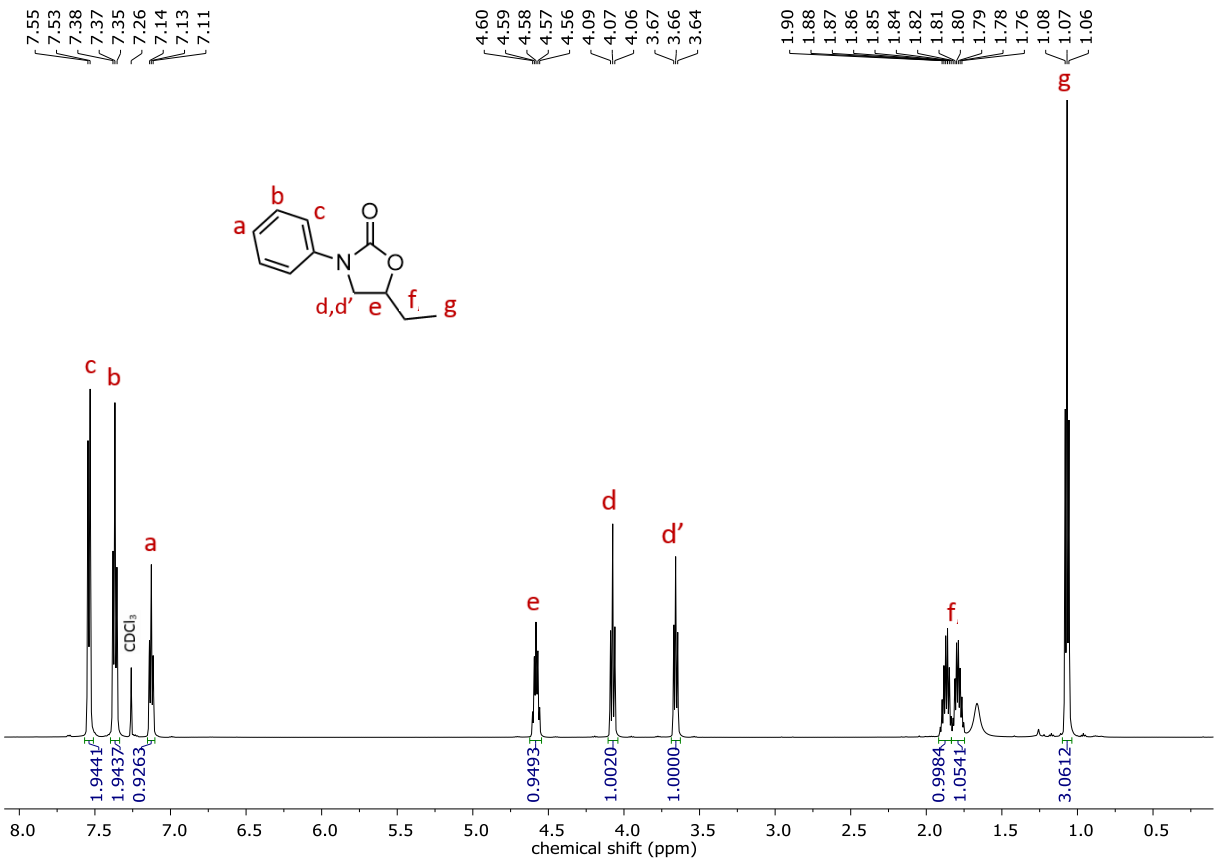


Figure S40. ^{1}H NMR ($CDCl_3$) of 5-ethyl-3-phenyloxazolidin-2-one (**3r**).

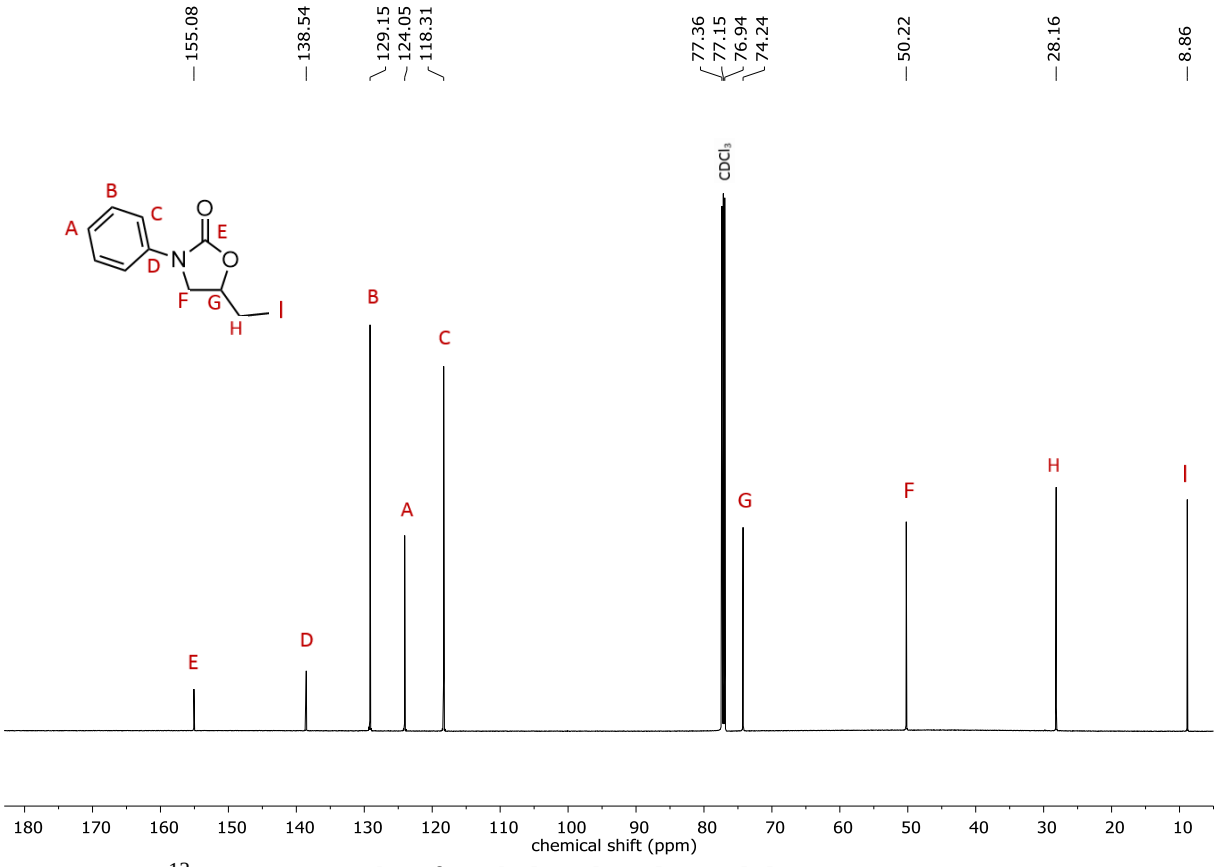
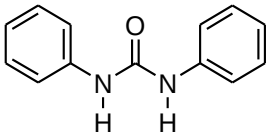


Figure S41. ^{13}C NMR ($CDCl_3$) of 5-ethyl-3-phenyloxazolidin-2-one (**3r**)

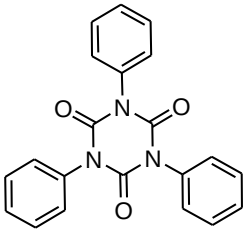
S8. ^{1}H NMR, ^{13}C NMR and APCI-MS data for 4a and 5a

1,3-Diphenylurea (4a)



^{1}H NMR (600 MHz, DMSO-d_6) δ 8.64 (s, 2H), 7.45 (d, 4H), 7.27 (t, 4H), 6.96 (t, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 152.48, 139.66, 128.73, 121.75, 118.14; APCI-MS: Exact mass calculated for $C_{13}H_{13}N_2O^+$ $[M+H]^+$ 213.1028, found 213.1023.

1,3,5-Triphenyl-1,3,5-triazinane-2,4,6-trione (5a)



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 (t, 6H), 7.44 (t, 3H), 7.40 (d, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.84, 133.78, 129.49, 129.33, 128.57; APCI-MS: Exact mass calculated for $C_{21}H_{16}N_3O_3^+$ $[M+H]^+$ 358.1192, found 358.1190.

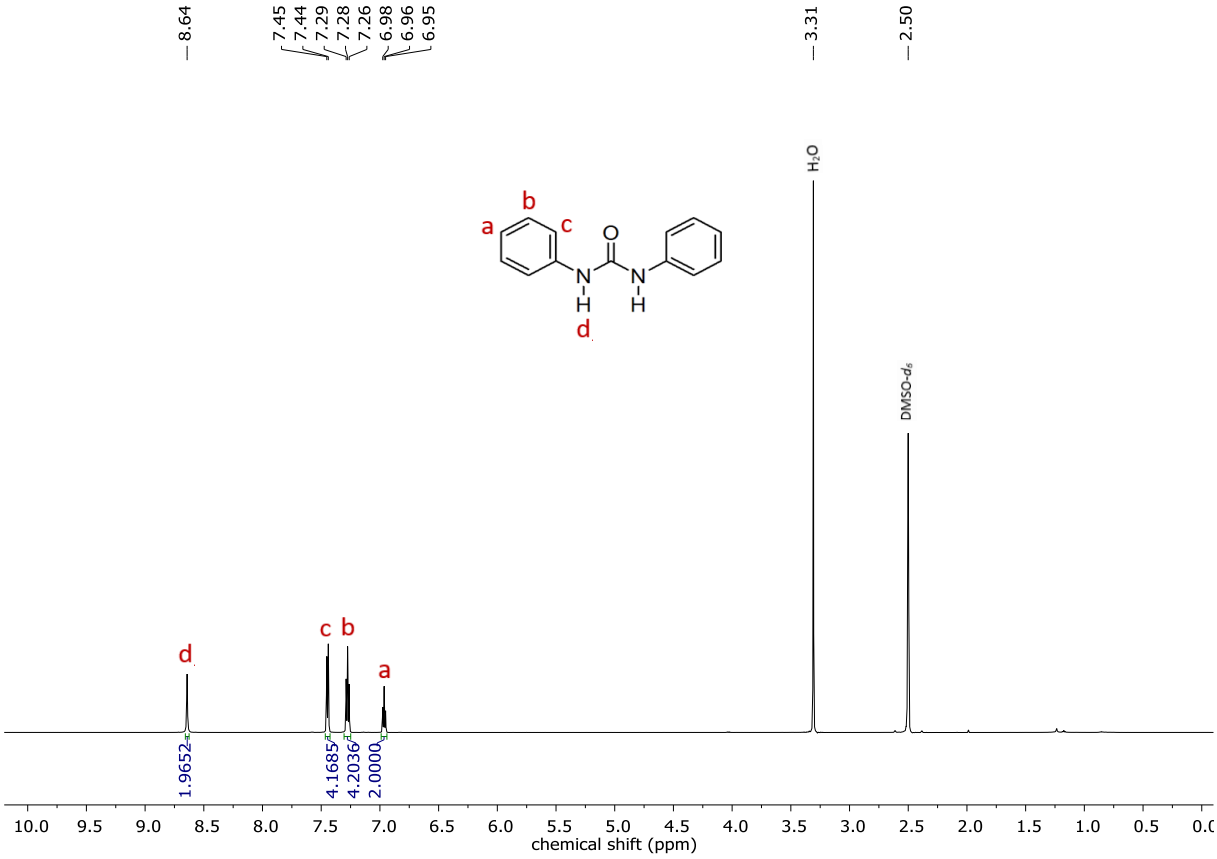


Figure S42. ^{1}H NMR (DMSO-d_6) of 1,3-Diphenylurea.

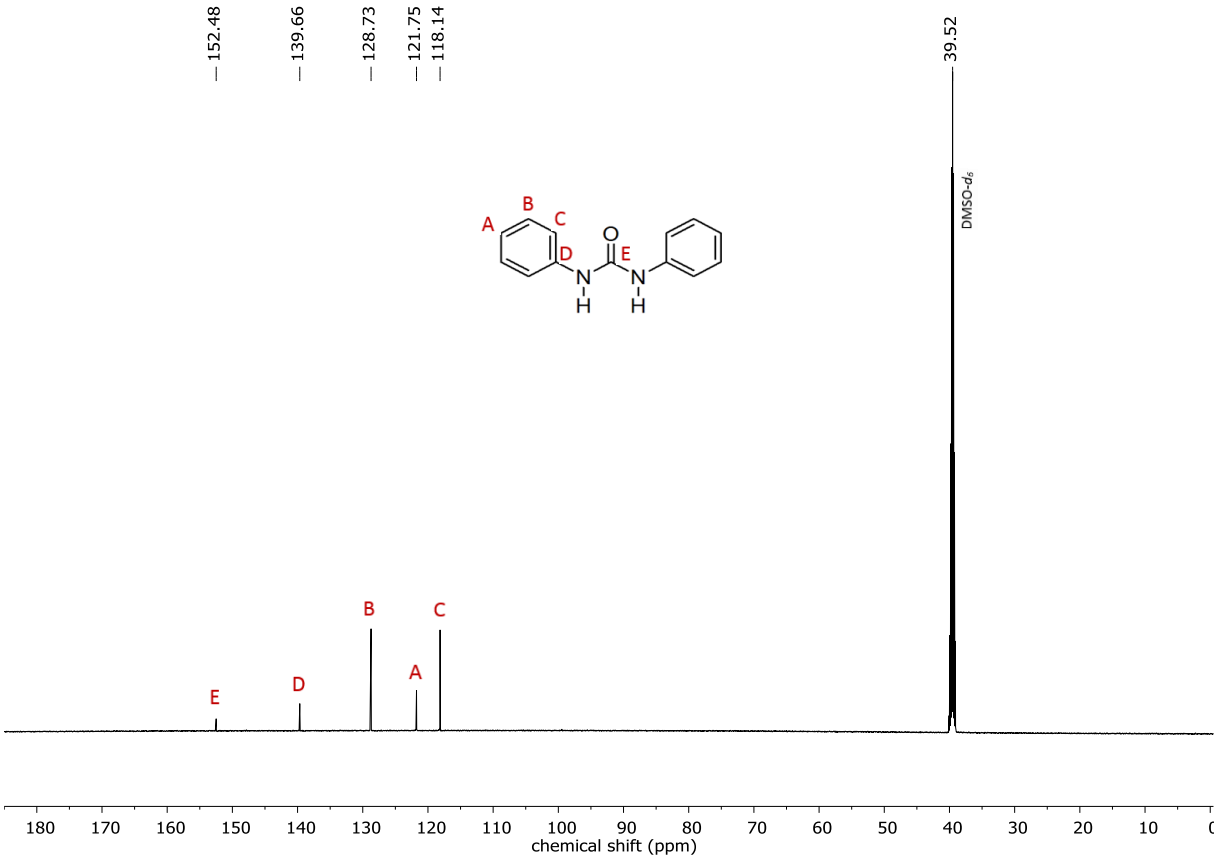


Figure S43. ^{13}C NMR (DMSO-d_6) of 1,3-Diphenylurea.

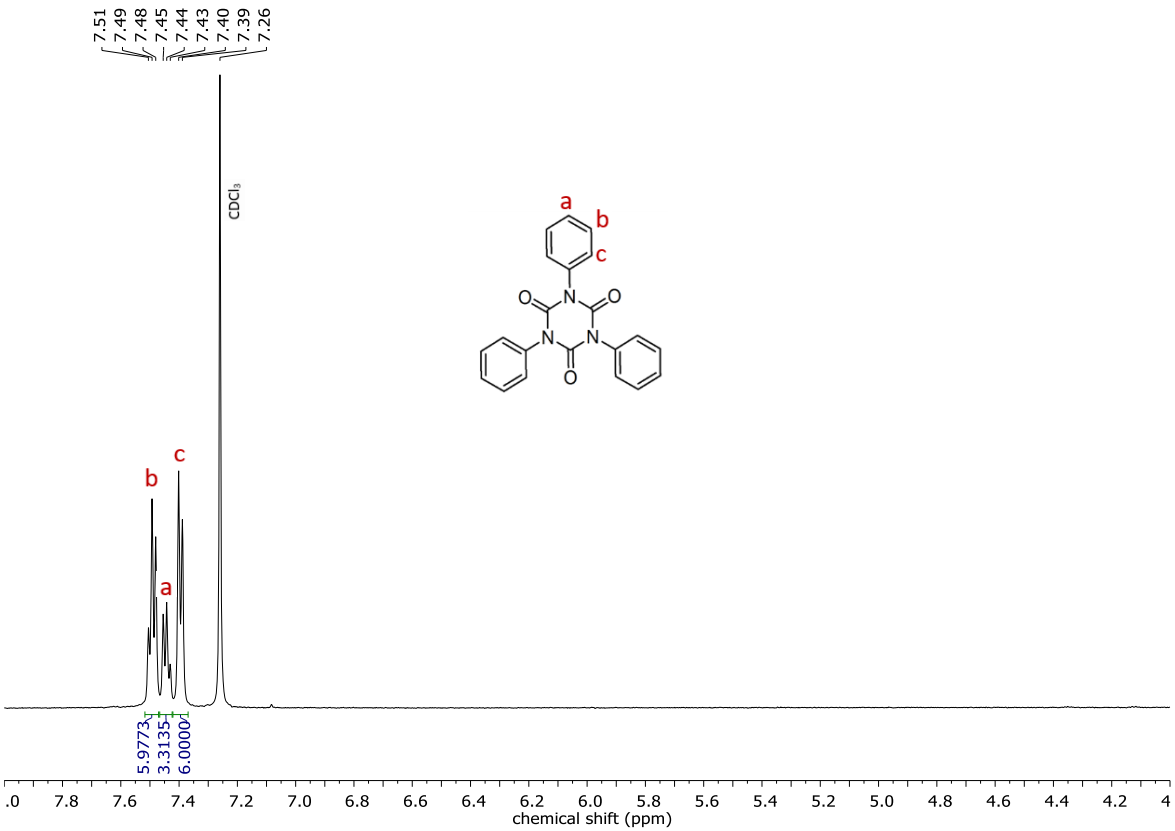


Figure S44. ^{1}H NMR ($CDCl_3$) of 1,3,5-Triphenyl-1,3,5-triazinane-2,4,6-trione.

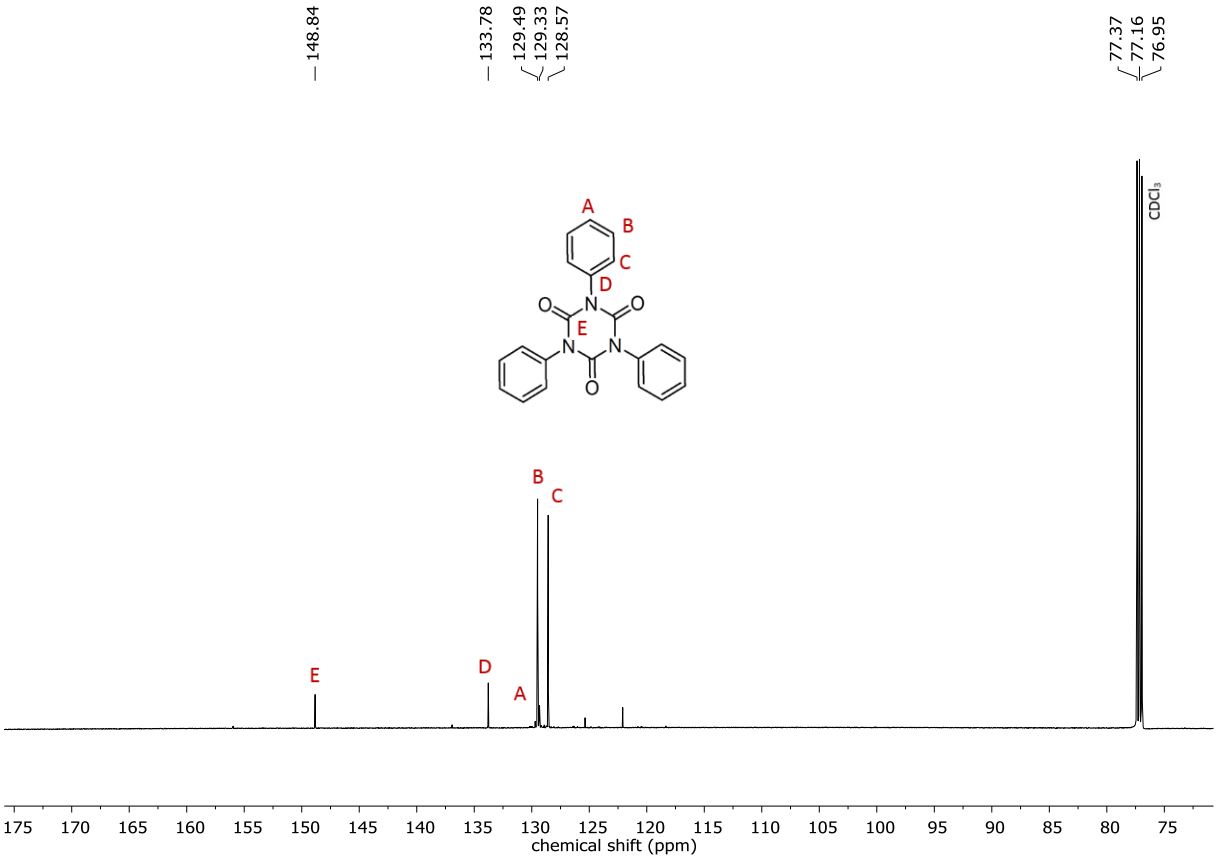


Figure S45. ^{13}C NMR ($CDCl_3$) of 1,3,5-Triphenyl-1,3,5-triazinane-2,4,6-trione.

S9. Computational data and details

DFT static calculations were performed with the Gausian09 set of programs,[7] using the BP86 functional of Becke and Perdew,[8-10] including corrections due to dispersion through the Grimme's method (GD3 keyword in Gaussian).[11, 12] The electronic configuration of the molecular systems was described with the double-ζ basis set with polarization of Ahlrichs for main-group atoms (Def2SVP keyword in Gaussian),[13, 14] using the SDD ECP on I.[15-17] The geometry optimizations were performed without symmetry constraints, and analytical frequency calculations performed the characterization of the located stationary points. These frequencies were used to calculate unscaled zero-point energies (ZPEs), as well. Energies were obtained by single-point calculations on the optimized geometries with the M06-2X functional[18, 19] and the triple-ζ basis set Def2TZVP, using the SDD ECP on I and by estimating solvent effects with the polarizable continuous solvation model (PCM) as implemented in Gaussian09 for THF.[20, 21] The reported free energies in this work include energies obtained at the M06-2X/Def2TZVP~sdd level of theory corrected with zero-point energies, thermal corrections and entropy effects achieved at the BP86/Def2SVP~sdd level. They were evaluated at 298.15 and 353.15 K, and 300 atm, following the suggestion by Martin et al.,[22] and more recently proved in Ru-based olefin metathesis,[23] and olefin polymerization to reduce the overestimation of the entropic contribution when calculated at p = 1 atm,[24, 25] in particular, the expected values for the dissociative steps in the condensed phase.

Possible mechanistic pathways for isocyanate cyclo-oligomerization

Plausible mechanistic pathways for the formation of **1a** cyclo-oligomers **4a** and **5a** are shown in Figure S46 starting from linear dimer **CC** (See Figure 3). From **CC**, two possible processes, either ring closure to generate an uretdione (**CCdimer**, via **TS-CCdimer**) or the insertion of a third isocyanate molecule to generate the linear trimer **CCC** (via **TS-CCC**) can take place. The former product is likely decomposed by traces of moisture to **4a** as observed experimentally.[26, 27] Independent of temperature, formation of **CCC** was kinetically disfavoured compared to **CCdimer** by just 2.1 kcal/mol (2.8 kcal/mol at 67 °C), albeit, thermodynamically favoured by 10.2 kcal/mol at 25 °C (8.6 kcal/mol at 67 °C). From **CCC**, the formation of the six-membered isocyanurate (**CCCtrimer**) was favored by 1.7 kcal/mol (1.4 kcal/mol at 67 °C) over formation of dimeric isocyanurate (**CCCdimer**). Given the small differences in calculated energy barriers for the formation of **4a** and **5a** it is expected that the process of isocyanate oligomerization in the presence of PO should lead to the formation of both compounds as indeed experimentally observed (Table S3, entry 9).

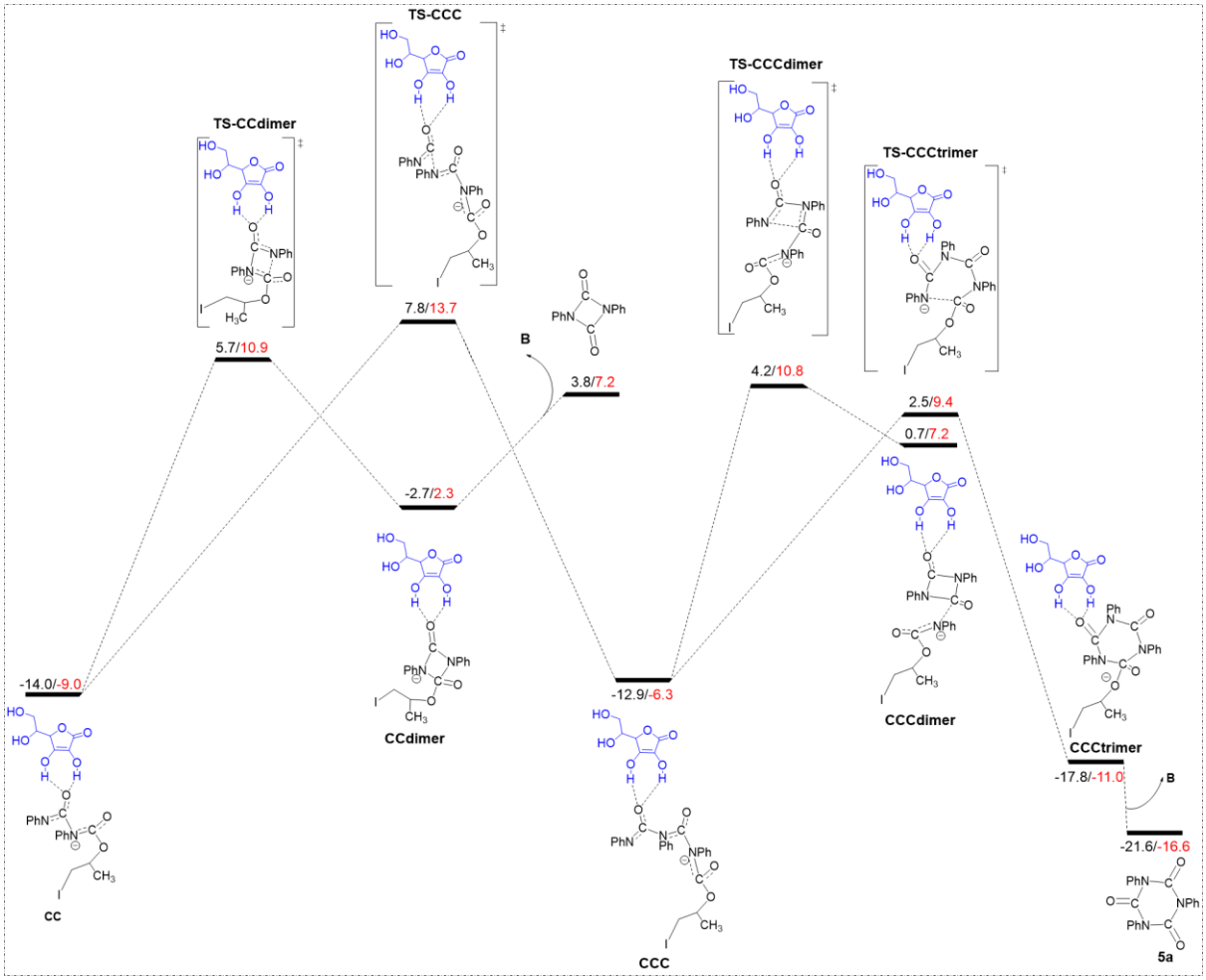


Figure S46. Calculated pathways for isocyanate cyclo-oligomerization starting from intermediate **CC** (See Figure 3 of the main text). Free energies at 25 °C (in black) and at 67 °C (in red) in solution (THF as the solvent) are given in kcal/mol.

Table S4. Computed free energy surface for the cycloaddition of isocyanate (**1a**) to PO catalyzed by ascorbic acid, *meso*-erythritol and pentaerythritol. Free energies at 25 °C and 67 °C in solution (THF as the solvent) are given in kcal/mol relative to the corresponding starting materials.

HBD	T (°C)	**A_0**	**A**	**TS-AB**	**B**	**TS-BC**	**C**	**TS-CD**	**D**	**D0**	**TS-CC**	**CC**
L-Ascorbic acid	25 °C	2.0	1.6	15.6	3.4	19.9	-2.9	6.9	-35.6	-36.1	3.7	-14.0
	67 °C	3.3	3.0	17.2	5.3	23.4	-2.0	10.2	-34.5	-33.5	12.2	-9.0
meso-erythritol	25 °C	0.2	0.6	25.4	19.7	24.8	-1.4	13.5	-38.3	-35.0	11.5	-6.0
	67 °C	0.2	4.3	29.8	24.0	32.8	6.6	21.5	-30.2	-28.5	23.4	5.7
penta-erythritol	25 °C	-1.2	-0.5	5.0	23.4	28.7	4.8	12.2	-37.8	-38.0	12.6	-6.9
	67 °C	2.6	4.3	7.6	27.0	36.3	14.6	17.5	-28.3	-32.2	21.6	2.1

Table S5. Computed free energy surface (selection of energetically demanding transition states) for the cycloaddition of isocyanate (**1a**) to epichlorohydrin (**2a**) catalyzed by ascorbic acid, *meso*-erythritol and pentaerythritol. Free energies at 67 ºC in solution (THF as the solvent) are given in kcal/mol relative to the corresponding starting HBD. The transition states names follow the notation used in Figure 3 of the main text; the "**(2a)**" suffix indicate that the energy barriers refer to the use of **2a** as the epoxide.

HBD	**TS-BC(2a)**	**TS-CC(2a)**	**TS-CD(2a)**
L-Ascorbic acid	21.9	11.6	10.9
meso-erythritol	32.5	23.4	19.2
pentaerythritol	29.0	19.3	17.9

Table S6. The xyz coordinates for all the DFT optimized structures (absolute energies in a.u.) using propylene oxide as the substrate.

HBD = Ascorbic acid

Ascorbic Acid	
Zero-point correction= 0.145479 (Hartree/Particle) Thermal correction to Energy= 0.157599 Thermal correction to Enthalpy= 0.158543 Thermal correction to Gibbs Free Energy= 0.106946 Sum of electronic and zero-point Energies= -684.160545 Sum of electronic and thermal Energies= -684.148424 Sum of electronic and thermal Enthalpies= -684.147480 Sum of electronic and thermal Free Energies= -684.199077	20 ACIDASCORBIC SCF Done: -684.306023558 A.U. O 0.817660 2.384533 -0.399043 O 3.074632 0.472565 0.654800 H 3.488694 -0.402982 0.832704 C 0.920047 1.034129 -0.391262 O 2.032832 -2.204417 0.151553 C 1.879952 0.195196 0.080110 O 0.192017 -1.163831 -0.744779 C 1.426202 -1.189909 -0.136678 O -1.283074 0.181460 1.351183 H -0.746806 0.911359 1.712739 O -3.830390 -0.202639 0.342214 H -3.523506 -0.230860 1.271667 C -0.245520 0.205450 -0.872469 H -0.474220 0.402881 -1.945253 C -1.521008 0.437174 -0.030329 H -1.837873 1.495935 -0.200530 C -2.679108 -0.484149 -0.427888 H -2.935281 -0.321761 -1.496742 H -2.328409 -1.540044 -0.320285 H 1.644606 2.756756 -0.030628

A0	
Zero-point correction= 0.231353 (Hartree/Particle) Thermal correction to Energy= 0.248453 Thermal correction to Enthalpy= 0.249397 Thermal correction to Gibbs Free Energy= 0.186030 Sum of electronic and zero-point Energies= -877.074230 Sum of electronic and thermal Energies= -877.057130 Sum of electronic and thermal Enthalpies= -877.056185 Sum of electronic and thermal Free Energies= -877.119553	30 Yso-AminusI SCF Done: -877.940238687 A.U. O -0.417942 -1.191034 -0.787522 O -1.449783 1.610024 0.321642 H -2.125031 0.924472 0.169763 C 0.207458 -0.012471 -0.548192 O 0.970664 3.236935 0.369156 C -0.228243 1.170029 -0.069253 O 2.040332 1.407553 -0.443491 C 0.925553 2.088272 0.004461 O 2.270898 -0.957767 1.352723 H 1.402840 -1.340835 1.531947 O 4.767593 -1.798782 0.391719 H 4.495141 -1.840160 1.319460 C 1.684453 0.066532 -0.816544 H 1.893814 -0.050771 -1.889768 C 2.522343 -0.974338 -0.052076 H 2.270588 -1.960017 -0.470199 C 4.024856 -0.747730 -0.211370 H 4.293213 -0.744937 -1.272167 H 4.289326 0.226799 0.218008 H -1.382401 -1.116626 -0.642135

	O -3.112988 -0.591325 -0.321628 C -4.293541 -0.641560 -1.165561 H -4.724128 0.334350 -1.380122 C -4.344292 -1.167811 0.207602 H -4.267278 -2.248837 0.322811 C -4.996076 -0.424439 1.341518 H -6.025900 -0.776054 1.469587 H -4.459575 -0.601111 2.279156 H -5.016801 0.652052 1.149118 H -4.209058 -1.322035 -2.009756

A	
Zero-point correction= 0.230130 (Hartree/Particle) Thermal correction to Energy= 0.250164 Thermal correction to Enthalpy= 0.251108 Thermal correction to Gibbs Free Energy= 0.175680 Sum of electronic and zero-point Energies= -888.656473 Sum of electronic and thermal Energies= -888.636440 Sum of electronic and thermal Enthalpies= -888.635496 Sum of electronic and thermal Free Energies= -888.710924	31 Yso-A SCF Done: -888.886603751 A.U. O 1.571519 0.134353 -1.909554 O 1.301911 2.488844 0.278324 H 0.475415 2.206787 -0.206381 C 2.414330 0.649978 -0.997149 O 3.961345 2.523934 1.511706 C 2.297109 1.635584 -0.045247 O 4.472363 0.797602 0.111967 C 3.607115 1.755075 0.645323 O 2.953322 -1.507272 0.921591 H 2.209372 -0.870942 0.888820 O 4.792510 -3.457698 0.409993 H 4.139450 -3.350330 1.132110 C 3.764480 -0.005032 -0.840371 H 4.326832 -0.011397 -1.803775 C 3.626776 -1.457514 -0.332234 H 3.056865 -2.018239 -1.116455 C 4.973110 -2.146644 -0.099290 H 5.524479 -2.228098 -1.061603 H 5.571681 -1.496695 0.586022 H 0.658165 0.543187 -1.783199 O -0.625164 1.219589 -1.044422 C -2.115073 1.040837 -1.039359 H -2.662109 1.902698 -0.623884 C -1.287408 0.227304 -0.151564 H -1.092454 -0.811641 -0.478936 I -4.907234 -0.505133 0.156653 C -1.192349 0.481135 1.325455 H -2.007946 -0.091663 1.815176 H -0.210322 0.158242 1.729290 H -1.334604 1.555508 1.555429 H -2.522408 0.605462 -1.965444

TS-AB	
Zero-point correction= 0.228416 (Hartree/Particle) Thermal correction to Energy= 0.247977 Thermal correction to Enthalpy= 0.248921 Thermal correction to Gibbs Free Energy= 0.175234 Sum of electronic and zero-point Energies= -888.650754 Sum of electronic and thermal Energies= -888.631194 Sum of electronic and thermal Enthalpies= -888.630249 Sum of electronic and thermal Free Energies= -888.703936	31 Yso-AB SCF Done: -888.879170496 A.U. O 1.362056 -1.015830 -0.256335 O 1.234457 2.113390 0.414699 H 0.425289 1.533716 0.593485 C 2.240813 -0.016627 -0.405300 O 3.875382 3.074584 -0.466270 C 2.202689 1.326533 -0.095874 O 4.303932 0.906932 -1.030394 C 3.493779 1.924440 -0.513635 O 4.482309 -0.708184 1.351743 H 3.670109 -0.180334 1.506087 O 6.473806 -2.391688 0.576535 H 6.275135 -1.952694 1.429400 C 3.621938 -0.348924 -0.915747 H 3.576313 -0.832890 -1.920202 C 4.371650 -1.286583 0.053845 H 3.784701 -2.239545 0.093875 C 5.804756 -1.592073 -0.387411 H 5.792152 -2.154122 -1.346974

	H 6.319823 -0.615958 -0.566263 H 0.491253 -0.628618 0.135282 O -0.647348 0.311417 0.578075 C -1.735333 0.432802 -0.352720 H -1.905913 1.460829 -0.735050 C -2.383949 0.072805 0.907489 H -2.472382 -0.999404 1.134608 I -5.157259 -0.469506 -0.314192 C -2.770118 1.073998 1.954191 H -3.839030 0.941128 2.210749 H -2.166826 0.920641 2.874114 H -2.619489 2.110585 1.593303 H -1.750532 -0.322676 -1.163679

B	
Zero-point correction= 0.230699 (Hartree/Particle) Thermal correction to Energy= 0.249366 Thermal correction to Enthalpy= 0.250311 Thermal correction to Gibbs Free Energy= 0.179839 Sum of electronic and zero-point Energies= -888.671177 Sum of electronic and thermal Energies= -888.652510 Sum of electronic and thermal Enthalpies= -888.651566 Sum of electronic and thermal Free Energies= -888.722038	31 Yso-B SCF Done: -888.901876263 A.U. O 1.157144 -0.762740 0.719434 O 1.034969 2.369457 0.984733 H 0.397641 1.775979 1.474742 C 1.833592 0.181509 0.100977 O 3.360824 3.253397 -0.647874 C 1.826230 1.558573 0.222511 O 3.642433 1.042187 -1.146682 C 2.961380 2.109048 -0.520295 O 3.811479 -1.342677 1.158994 H 2.843360 -1.363499 1.378102 O 6.066230 -2.236660 -0.028384 H 5.668815 -2.291107 0.867807 C 2.950330 -0.183858 -0.864475 H 2.532621 -0.563013 -1.829213 C 3.847346 -1.302541 -0.266900 H 3.467086 -2.272833 -0.680134 C 5.326350 -1.182862 -0.634612 H 5.456793 -1.243587 -1.737090 H 5.677289 -0.172875 -0.311780 H 0.050526 -0.130553 1.410914 O -0.725302 0.467387 1.828155 C -1.722477 0.688728 0.853260 H -2.443164 1.433293 1.254070 C -2.436765 -0.639607 0.567292 I -4.515632 -0.186194 -0.361726 H -1.312319 1.102755 -0.102477 C -1.691400 -1.590943 -0.342512 H -2.185665 -2.579655 -0.417884 H -1.581055 -1.162133 -1.360032 H -0.656525 -1.711437 0.058211 H -2.736633 -1.104169 1.527798

TS-BC	
Zero-point correction= 0.332638 (Hartree/Particle) Thermal correction to Energy= 0.359023 Thermal correction to Enthalpy= 0.359967 Thermal correction to Gibbs Free Energy= 0.273041 Sum of electronic and zero-point Energies= -1288.043676 Sum of electronic and thermal Energies= -1288.017291 Sum of electronic and thermal Enthalpies= -1288.016347 Sum of electronic and thermal Free Energies= -1288.103272	45 Yso-BC SCF Done: -1288.37631364 A.U. O -1.161256 -0.749166 -1.501888 O -0.506224 -3.209089 0.349806 H 0.170523 -2.457987 0.257863 C -1.950813 -1.683879 -0.960233 O -3.199871 -4.397390 0.852174 C -1.677796 -2.744768 -0.128887 O -4.000461 -2.671198 -0.409523 C -2.963105 -3.400325 0.200450 O -3.566389 -0.250792 1.067004 H -2.619587 -0.489142 1.205486 O -5.623555 1.310009 0.339086 H -5.102022 1.189466 1.161927 C -3.445738 -1.515489 -1.044832 H -3.805367 -1.468527 -2.100939 C -3.861187 -0.212046 -0.326589

	H -3.288961 0.607725 -0.831478 C -5.350482 0.122026 -0.397307 H -5.653441 0.292741 -1.453107 H -5.923299 -0.756736 -0.008464 H -0.218004 -0.839970 -1.051650 O 0.916590 -1.035923 -0.109445 C 2.204421 -0.867216 -0.656345 H 2.606413 -1.864902 -0.972511 C 2.203503 0.076824 -1.866821 H 3.219867 0.194320 -2.296057 H 1.534009 -0.331215 -2.651671 H 1.814004 1.069651 -1.565404 C 3.039338 -0.364499 0.526532 H 2.961280 -1.054970 1.386160 H 2.757185 0.665279 0.816747 I 5.273596 -0.251164 0.127828 O -0.760480 -0.276653 1.650186 C -0.121794 0.452994 0.949961 N 0.288338 1.532576 0.469381 C -0.517798 2.672512 0.311404 C 0.080805 3.876330 -0.130166 C -1.920750 2.646268 0.523726 C -0.708043 5.014476 -0.364698 H 1.169267 3.892824 -0.295253 C -2.703673 3.778008 0.258887 H -2.405864 1.725991 0.882059 C -2.103731 4.973244 -0.182505 H -0.225089 5.943906 -0.709717 H -3.796370 3.697083 0.382014 H -2.719310 5.862962 -0.391191

C	
Zero-point correction= 0.333769 (Hartree/Particle) Thermal correction to Energy= 0.360407 Thermal correction to Enthalpy= 0.361351 Thermal correction to Gibbs Free Energy= 0.272519 Sum of electronic and zero-point Energies= -1288.057054 Sum of electronic and thermal Energies= -1288.030416 Sum of electronic and thermal Enthalpies= -1288.029472 Sum of electronic and thermal Free Energies= -1288.118304	45 Yso-C SCF Done: -1288.39082315 A.U. O -2.641701 -1.703072 -1.714640 O -2.180008 -2.370178 1.373241 H -1.310487 -2.023837 0.915329 C -3.337306 -1.435471 -0.604257 O -4.562681 -1.115602 2.654239 C -3.168023 -1.715966 0.731906 O -5.156447 -0.494403 0.539781 C -4.304277 -1.113364 1.466922 O -3.293579 1.524407 -0.149874 H -2.475369 1.007670 0.011173 O -4.776101 3.176291 -1.633418 H -4.020164 3.262284 -1.011075 C -4.527856 -0.521417 -0.745495 H -5.251926 -0.903311 -1.504615 C -4.081275 0.903993 -1.155356 H -3.510904 0.798482 -2.112928 C -5.253112 1.866549 -1.367082 H -5.868543 1.532475 -2.231905 H -5.895591 1.823444 -0.451496 H -1.749397 -2.174366 -1.546673 C 0.350446 -1.698708 -0.892977 O -0.180560 -2.581525 -1.594343 O 1.656161 -1.349299 -1.276561 C 2.601403 -0.948963 -0.261072 H 2.186612 -0.128239 0.364158 C 2.972902 -2.141674 0.616311 H 3.724411 -1.856802 1.379621 H 2.064405 -2.501042 1.139140 H 3.379427 -2.966733 -0.005249 C 3.735856 -0.388000 -1.117402 H 3.371658 0.435562 -1.758818 H 4.219321 -1.170742 -1.733286 I 5.385006 0.524712 0.084621 N -0.221520 -1.138140 0.180096 C -0.213475 0.203098 0.512098

	C -0.770844 0.585236 1.770953 C 0.208064 1.250411 -0.365574 C -0.862734 1.933591 2.138335 H -1.170867 -0.210312 2.418894 C 0.113696 2.595255 0.022320 H 0.597655 0.985921 -1.360973 C -0.412661 2.953727 1.276899 H -1.316734 2.192142 3.108898 H 0.443055 3.379392 -0.680197 H -0.496767 4.012539 1.567819

TS-CD	
Zero-point correction= 0.334129 (Hartree/Particle) Thermal correction to Energy= 0.360565 Thermal correction to Enthalpy= 0.361509 Thermal correction to Gibbs Free Energy= 0.271810 Sum of electronic and zero-point Energies= -1288.053986 Sum of electronic and thermal Energies= -1288.027549 Sum of electronic and thermal Enthalpies= -1288.026605 Sum of electronic and thermal Free Energies= -1288.116304	45 Yso-CD SCF Done: -1288.38811410 A.U. O 2.378906 -1.341599 0.183646 O 2.550975 1.851213 -0.100688 H 1.737639 1.451938 0.333215 C 3.289124 -0.522443 -0.347218 O 5.106921 2.233266 -1.505897 C 3.384398 0.849117 -0.454152 O 5.316863 -0.036341 -1.425754 C 4.646833 1.164762 -1.162282 O 5.681018 -0.858900 1.311223 H 4.929967 -0.230588 1.370676 O 7.451601 -2.877529 0.924886 H 7.374476 -2.179480 1.608119 C 4.575368 -1.125060 -0.861175 H 4.377418 -1.884612 -1.654132 C 5.374396 -1.792188 0.278238 H 4.735005 -2.622689 0.672377 C 6.721071 -2.359215 -0.177238 H 6.556893 -3.189364 -0.898967 H 7.270480 -1.543225 -0.708796 H 1.578551 -0.782553 0.509510 O 0.579496 0.370036 0.812608 C -0.679149 0.189121 0.745716 O -1.066624 -1.124718 0.746693 C -3.322798 -0.416302 0.007770 H -2.949359 -0.183043 -0.998592 H -3.931916 0.358324 0.484218 C -2.494744 -1.371086 0.867439 H -2.590270 -2.398426 0.463310 I -5.294557 -1.794673 -0.720801 C -2.920376 -1.348995 2.335460 H -3.982929 -1.654849 2.423103 H -2.294683 -2.047507 2.925577 H -2.802787 -0.324593 2.742746 N -1.668394 1.059168 0.712462 C -1.556943 2.421335 0.475662 C -0.540961 3.013834 -0.325930 C -2.560289 3.274119 1.012954 C -0.526173 4.398177 -0.551179 H 0.247737 2.385400 -0.761554 C -2.542649 4.655239 0.773056 H -3.352376 2.817778 1.628036 C -1.522391 5.231287 -0.008143 H 0.283357 4.828621 -1.163287 H -3.333912 5.291199 1.204319 H -1.504537 6.317542 -0.192263

TS-CD+AscorbicAcid	
Zero-point correction= 0.499735 (Hartree/Particle) Thermal correction to Energy= 0.538021 Thermal correction to Enthalpy= 0.538965 Thermal correction to Gibbs Free Energy= 0.422522 Sum of electronic and zero-point Energies= -1972.067002 Sum of electronic and thermal Energies= -1972.028716	65 Yso-CD+ACID SCF Done: -1972.56673699 A.U. O -2.254176 0.454814 0.385955 O -1.349500 3.470141 0.521549 H -0.645285 2.785745 0.527225 C -2.945682 1.603189 0.257377

Sum of electronic and thermal Enthalpies= -1972.027772 Sum of electronic and thermal Free Energies= -1972.144215	O -3.838276 4.939049 0.060019 C -2.547270 2.896214 0.325475 O -4.826835 2.911064 -0.078137 C -3.734414 3.743907 0.098999 O -4.379129 1.560306 -2.444207 H -4.676729 2.474679 -2.321562 O -6.827247 -0.219719 -0.351034 H -6.498248 -1.131626 -0.466373 C -4.422274 1.538850 -0.007640 H -4.966410 1.046954 0.818063 C -4.825594 0.840304 -1.319447 H -4.314157 -0.136085 -1.343576 C -6.342841 0.591284 -1.389707 H -6.860455 1.563707 -1.316987 H -6.560909 0.179681 -2.395545 H -1.274139 0.626281 0.459728 O 0.249156 1.242252 0.555414 C 1.402257 0.940467 0.175374 O 1.585053 -0.402213 -0.160606 C 3.987325 0.086424 -0.236663 H 4.144143 0.105753 0.837688 H 4.526298 0.802972 -0.842555 C 2.853783 -0.738455 -0.819030 H 2.989605 -1.792068 -0.546071 I 6.004198 -1.581919 -0.534009 C 2.703819 -0.592978 -2.325610 H 3.618231 -0.950273 -2.821034 H 1.854634 -1.193762 -2.683922 H 2.538005 0.460122 -2.598917 N 2.489881 1.638426 0.026223 C 2.681115 2.961215 0.429927 C 2.015804 3.545004 1.529517 C 3.632494 3.736758 -0.264326 C 2.291604 4.860952 1.904135 H 1.273029 2.965796 2.078518 C 3.906298 5.048535 0.121963 H 4.150444 3.292689 -1.117487 C 3.236777 5.621133 1.208476 H 1.755426 5.296432 2.751689 H 4.647378 5.629767 -0.433931 H 3.446894 6.650976 1.508083 O -0.586216 -1.851596 -1.100816 O 0.946475 -2.584517 1.564232 H 1.183800 -1.746188 1.129056 C -0.817802 -2.771642 -0.150281 O -0.677714 -4.764707 2.675196 C -0.172276 -3.082388 0.996322 O -1.997037 -4.490367 0.860484 C -0.912983 -4.179381 1.655478 O -3.394917 -1.985018 1.031449 H -2.936755 -1.130737 0.899734 O -5.738748 -2.756622 0.142054 H -5.423698 -2.239518 0.906320 C -2.070086 -3.594622 -0.244103 H -2.097060 -4.184214 -1.180542 C -3.344499 -2.731036 -0.162926 H -3.325866 -2.059985 -1.042991 C -4.628133 -3.568556 -0.193912 H -4.796415 -3.988317 -1.198201 H -4.527879 -4.406191 0.520005 H 0.152771 -1.263896 -0.836315

D	
Zero-point correction= 0.339335 (Hartree/Particle) Thermal correction to Energy= 0.365310 Thermal correction to Enthalpy= 0.366254 Thermal correction to Gibbs Free Energy= 0.278839 Sum of electronic and zero-point Energies= -1288.107441 Sum of electronic and thermal Energies= -1288.081466	45 Yso-D SCF Done: -1288.44677581 A.U. O 2.738240 -0.066896 -2.377044 O 2.405056 2.591718 -0.660249 H 1.609811 2.262507 -1.156092 C 3.443313 0.438570 -1.348995

Sum of electronic and thermal Enthalpies= -1288.080522 Sum of electronic and thermal Free Energies= -1288.167937	O 4.539251 2.339240 1.367980 C 3.284916 1.559540 -0.579512 O 5.071610 0.377413 0.330542 C 4.310485 1.538407 0.486884 O 2.819735 -1.490281 0.683600 H 2.025032 -1.284511 0.140156 O 4.288619 -3.755693 1.089700 H 3.422344 -3.438221 1.424059 C 4.519219 -0.414290 -0.729585 H 5.332159 -0.662146 -1.452748 C 3.915908 -1.733997 -0.191568 H 3.587678 -2.320285 -1.084596 C 4.909902 -2.572751 0.615947 H 5.770618 -2.863612 -0.025016 H 5.303971 -1.931650 1.443026 H 1.811323 0.321056 -2.327939 O 0.457522 1.019438 -1.617997 C -0.056698 0.311506 -0.731102 O 0.281604 -1.000191 -0.579303 C -1.283806 -0.445059 1.101787 H -2.380612 -0.567617 1.245201 H -0.767916 -0.286987 2.076564 C -0.733121 -1.632917 0.305927 H -1.541228 -2.007863 -0.364525 I -4.591198 -1.578553 -0.213633 C -0.111442 -2.754196 1.107748 H -0.911401 -3.242328 1.701142 H 0.332573 -3.516777 0.437187 H 0.677020 -2.381187 1.792224 N -0.981824 0.669174 0.191472 C -1.551900 1.973388 0.327657 C -0.716693 3.097753 0.481703 C -2.955126 2.102222 0.333858 C -1.298832 4.368640 0.622272 H 0.377259 2.977393 0.494605 C -3.519992 3.377680 0.492366 H -3.589070 1.205636 0.198967 C -2.698144 4.511628 0.631407 H -0.648060 5.250045 0.737525 H -4.616802 3.480683 0.494891 H -3.149443 5.510208 0.749015

D0 (without iodide)	
Zero-point correction= 0.337996 (Hartree/Particle) Thermal correction to Energy= 0.362630 Thermal correction to Enthalpy= 0.363574 Thermal correction to Gibbs Free Energy= 0.279599 Sum of electronic and zero-point Energies= -1276.501345 Sum of electronic and thermal Energies= -1276.476711 Sum of electronic and thermal Enthalpies= -1276.475767 Sum of electronic and thermal Free Energies= -1276.559743	44 Yso-DminusI SCF Done: -1276.83934137 A.U. O -1.526578 1.410683 0.294587 O -0.487838 -1.629295 0.445777 H 0.103071 -0.920051 0.796108 C -2.036835 0.241759 -0.140126 O -2.614182 -3.112801 -0.911888 C -1.609817 -1.056669 -0.062596 O -3.657638 -1.098624 -1.166484 C -2.620339 -1.916809 -0.727673 O -4.529242 -0.148020 1.396651 H -3.622232 -0.228537 1.751285 O -6.853539 1.116878 0.647176 H -6.661064 0.579664 1.442616 C -3.415638 0.252296 -0.752781 H -3.454935 0.919522 -1.645684 C -4.489504 0.708992 0.261142 H -4.233491 1.759319 0.553110 C -5.907338 0.689529 -0.315701 H -5.967056 1.384386 -1.181197 H -6.107393 -0.343786 -0.692465 H -0.601185 1.260928 0.633648 O 0.996876 0.624081 0.868932 C 1.931434 1.218456 0.322770 O 1.860273 2.542327 0.052300 C 4.042530 1.815296 -0.441600

	H 4.655489 1.551571 -1.326212 H 4.725658 2.079688 0.398588 C 3.033348 2.946469 -0.720706 H 2.725013 2.930736 -1.790688 C 3.468148 4.337216 -0.303207 H 4.355590 4.648379 -0.891637 H 2.657272 5.069780 -0.483094 H 3.730036 4.355955 0.774233 N 3.148357 0.715906 -0.071828 C 3.578374 -0.637362 0.051500 C 4.927143 -0.909901 0.367007 C 2.679521 -1.700156 -0.178587 C 5.364904 -2.240758 0.467486 H 5.638075 -0.089362 0.544995 C 3.126772 -3.024260 -0.056240 H 1.632337 -1.508184 -0.446538 C 4.467288 -3.302711 0.264450 H 6.418618 -2.444654 0.714373 H 2.409893 -3.842421 -0.226023 H 4.812819 -4.344430 0.350153

1a	
Zero-point correction= 0.101111 (Hartree/Particle) Thermal correction to Energy= 0.108365 Thermal correction to Enthalpy= 0.109309 Thermal correction to Gibbs Free Energy= 0.068640 Sum of electronic and zero-point Energies= -399.359623 Sum of electronic and thermal Energies= -399.352369 Sum of electronic and thermal Enthalpies= -399.351425 Sum of electronic and thermal Free Energies= -399.392094	14 YsoREACTANT SCF Done: -399.460733955 A.U. O 3.700167 -0.280521 -0.000023 C 2.568280 0.068045 -0.000059 N 1.454473 0.559213 -0.000036 C 0.095895 0.245111 -0.000011 C -0.844414 1.299672 0.000023 C -0.355548 -1.096700 -0.000017 C -2.217944 1.011912 0.000054 H -0.479211 2.337435 0.000026 C -1.731126 -1.370018 0.000013 H 0.380672 -1.915744 -0.000046 C -2.668411 -0.320370 0.000047 H -2.943905 1.840254 0.000081 H -2.073598 -2.417005 0.000008 H -3.746999 -0.541175 0.000069

Product-1a	
Zero-point correction= 0.190466 (Hartree/Particle) Thermal correction to Energy= 0.201510 Thermal correction to Enthalpy= 0.202454 Thermal correction to Gibbs Free Energy= 0.152901 Sum of electronic and zero-point Energies= -592.318126 Sum of electronic and thermal Energies= -592.307081 Sum of electronic and thermal Enthalpies= -592.306137 Sum of electronic and thermal Free Energies= -592.355691	24 YsoPROD SCF Done: -592.508591600 A.U. O -0.917620 2.292805 0.204431 C -1.265554 1.133452 0.259129 O -2.576230 0.757428 0.429355 C -1.282091 -1.211677 0.446603 H -1.106746 -1.589640 1.480266 H -1.050965 -2.031730 -0.265451 C -2.716727 -0.670788 0.247842 H -3.400021 -1.032793 1.043439 C -3.296898 -0.957430 -1.134359 H -3.482475 -2.044163 -1.261627 H -4.253860 -0.415915 -1.269279 H -2.591102 -0.624887 -1.923859 N -0.479932 -0.025603 0.174384 C 0.929063 -0.068326 0.057389 C 1.684927 1.078540 -0.295681 C 1.607336 -1.291904 0.283190 C 3.078699 0.985265 -0.416011 H 1.170463 2.032942 -0.459526 C 3.004097 -1.365162 0.154827 H 1.054252 -2.198280 0.567326 C 3.751771 -0.229993 -0.195240 H 3.647868 1.887825 -0.690539 H 3.508581 -2.327655 0.336141 H 4.846599 -0.290207 -0.294006

oxazolidinone	
Zero-point correction= 0.082461 (Hartree/Particle) Thermal correction to Energy= 0.086943 Thermal correction to Enthalpy= 0.087887 Thermal correction to Gibbs Free Energy= 0.056041 Sum of electronic and zero-point Energies= -192.886681 Sum of electronic and thermal Energies= -192.882200 Sum of electronic and thermal Enthalpies= -192.881255 Sum of electronic and thermal Free Energies= -192.913101	10 EPO SCF Done: -192.969142232 A.U. O 0.828026 0.790395 -0.248225 C -0.154040 0.043547 0.489409 C 1.053233 -0.612981 -0.058224 H -0.162614 0.263727 1.578954 H 0.961422 -1.244690 -0.965528 H 1.891973 -0.884264 0.614611 C -1.516148 -0.104257 -0.148588 H -2.095983 -0.915347 0.341054 H -2.097421 0.836700 -0.050340 H -1.419856 -0.337140 -1.228537

iodide	
Zero-point correction= 0.000000 (Hartree/Particle) Thermal correction to Energy= 0.001416 Thermal correction to Enthalpy= 0.002360 Thermal correction to Gibbs Free Energy= -0.016848 Sum of electronic and zero-point Energies= -11.555583 Sum of electronic and thermal Energies= -11.554167 Sum of electronic and thermal Enthalpies= -11.553223 Sum of electronic and thermal Free Energies= -11.572431	1 I- SCF Done: -11.5555831350 A.U. I 0.000000 0.000000 0.000000

C+C	
Zero-point correction= 0.436595 (Hartree/Particle) Thermal correction to Energy= 0.472342 Thermal correction to Enthalpy= 0.473286 Thermal correction to Gibbs Free Energy= 0.361993 Sum of electronic and zero-point Energies= -1687.449175 Sum of electronic and thermal Energies= -1687.413428 Sum of electronic and thermal Enthalpies= -1687.412484 Sum of electronic and thermal Free Energies= -1687.523777	59 Yso-C+C SCF Done: -1687.88576986 A.U. O -0.237755 2.245793 0.550373 O -0.380165 1.733970 -2.613881 H 0.063079 0.941605 -2.098611 C -1.100670 2.618196 -0.407620 O -2.843536 3.170565 -3.385858 C -1.181367 2.394506 -1.762262 O -3.025942 3.720566 -1.180741 C -2.395990 3.087631 -2.260221 O -3.691570 1.336989 0.241445 H -2.920840 0.769142 0.035842 O -5.202926 2.243613 2.282829 H -5.102534 1.389558 1.806166 C -2.337570 3.371043 0.023591 H -2.067981 4.301968 0.578708 C -3.229170 2.495718 0.925566 H -2.601946 2.213869 1.806008 C -4.498530 3.160073 1.452038 H -4.239719 4.055543 2.058778 H -5.106015 3.500023 0.576609 H 0.607065 1.796830 0.178274 C 1.671632 -0.117730 -0.629445 O 1.943272 0.999455 -0.113490 O 2.568315 -1.171377 -0.441109 C 3.685743 -0.943494 0.443769 H 3.363050 -0.280259 1.275481 C 4.115958 -2.314048 0.953263 H 4.980870 -2.226819 1.640159 H 3.276545 -2.791338 1.497168 H 4.399116 -2.970798 0.104499 C 4.724595 -0.203484 -0.399819 H 4.312216 0.761541 -0.745830 H 5.087667 -0.819473 -1.245180 I 6.564420 0.368070 0.751501 N 0.592903 -0.352713 -1.365995 C 0.029261 -1.572575 -1.731859 C -1.024912 -1.510291 -2.690917 C 0.321457 -2.843334 -1.157124 C -1.751366 -2.653630 -3.046340 H -1.266040 -0.526371 -3.124360 C -0.419595 -3.979837 -1.518389

	H 1.121827 -2.923817 -0.411016 C -1.461453 -3.902349 -2.460789 H -2.567427 -2.564533 -3.782397 H -0.181166 -4.946367 -1.042776 H -2.042049 -4.798783 -2.731061 C -5.779230 -3.254974 0.877944 O -6.829247 -3.812436 0.859321 N -4.678116 -2.756453 0.785666 C -3.746712 -1.884885 1.350009 C -2.516271 -1.681499 0.688545 C -4.025273 -1.198807 2.556352 C -1.577248 -0.790497 1.235923 H -2.313153 -2.205109 -0.257035 C -3.070789 -0.327237 3.100215 H -4.997600 -1.348281 3.052145 C -1.843202 -0.122571 2.444929 H -0.649267 -0.580405 0.685665 H -3.310511 0.227873 4.020109 H -1.102334 0.588236 2.840138

TS-CCisomer	
Zero-point correction= 0.437200 (Hartree/Particle) Thermal correction to Energy= 0.471805 Thermal correction to Enthalpy= 0.472749 Thermal correction to Gibbs Free Energy= 0.364228 Sum of electronic and zero-point Energies= -1687.424954 Sum of electronic and thermal Energies= -1687.390349 Sum of electronic and thermal Enthalpies= -1687.389404 Sum of electronic and thermal Free Energies= -1687.497926	59 Yso-C--C SCF Done: -1687.86215387 A.U. O -1.746199 -0.034177 -1.877320 O -0.285650 1.064591 0.747533 H 0.297542 0.837524 -0.041140 C -2.207581 0.478461 -0.733498 O -2.529473 1.911190 2.436426 C -1.588297 0.956901 0.394415 O -3.886723 1.152473 0.758887 C -2.622064 1.401750 1.339954 O -4.127238 2.749283 -1.482504 H -4.104325 2.931775 -0.517121 O -6.633242 2.138271 -2.312871 H -6.056616 2.933149 -2.248681 C -3.698101 0.540248 -0.530301 H -4.109912 -0.497682 -0.500091 C -4.459035 1.361795 -1.582449 H -4.130182 1.031270 -2.591894 C -5.986152 1.212903 -1.458733 H -6.298480 0.183313 -1.744124 H -6.264123 1.358237 -0.381460 H -0.721902 -0.110059 -1.806897 C 1.681189 -0.925838 -1.143437 O 0.741599 -0.099434 -1.384745 O 1.379220 -2.279877 -0.990141 C 0.013116 -2.678669 -0.763582 H -0.675219 -2.104858 -1.418926 C -0.048639 -4.165293 -1.095306 H -1.072792 -4.560351 -0.946257 H 0.248062 -4.323580 -2.151030 H 0.653146 -4.732321 -0.448879 C -0.285572 -2.332162 0.697938 H -0.162380 -1.249575 0.893585 H 0.331476 -2.929909 1.396627 I -2.404701 -2.741454 1.281764 N 2.946955 -0.596533 -1.059511 C 3.971147 -1.434721 -0.618181 C 3.871454 -2.252082 0.541236 C 5.215048 -1.399532 -1.302203 C 4.965012 -3.011751 0.980097 H 2.920452 -2.275537 1.092716 C 6.304781 -2.161818 -0.854722 H 5.298931 -0.746594 -2.183115 C 6.190220 -2.977817 0.286144 H 4.861339 -3.636045 1.883733 H 7.259175 -2.116841 -1.406003 H 7.047234 -3.575974 0.636031 C 3.452832 1.577313 -1.032267

	O 4.319140 1.605599 -1.852946 N 2.653069 1.959163 -0.151161 C 2.644226 3.253091 0.403050 C 1.602771 3.592952 1.301404 C 3.638861 4.222370 0.107472 C 1.564038 4.869408 1.883400 H 0.825707 2.843605 1.515545 C 3.589396 5.493578 0.699961 H 4.448977 3.965600 -0.593730 C 2.553117 5.827795 1.592027 H 0.742613 5.115838 2.576249 H 4.371399 6.233317 0.458906 H 2.516753 6.827722 2.054140

TS-CC	
Zero-point correction= 0.437353 (Hartree/Particle) Thermal correction to Energy= 0.471512 Thermal correction to Enthalpy= 0.472456 Thermal correction to Gibbs Free Energy= 0.365815 Sum of electronic and zero-point Energies= -1687.432558 Sum of electronic and thermal Energies= -1687.398399 Sum of electronic and thermal Enthalpies= -1687.397455 Sum of electronic and thermal Free Energies= -1687.504096	59 Yso-C--CmodFll SCF Done: -1687.86991076 A.U. O 2.596063 -1.003922 -1.819532 O 1.059963 1.786582 -1.398393 H 0.455072 1.002874 -1.563465 C 3.011665 0.269310 -1.745189 O 3.239010 3.719599 -1.257858 C 2.359997 1.458654 -1.549489 O 4.635345 1.961986 -1.670657 C 3.377142 2.529576 -1.461103 O 4.630759 0.475547 0.741633 H 3.671507 0.262060 0.844538 O 7.154088 -0.406230 0.845163 H 6.459215 -0.138931 1.487973 C 4.495951 0.537303 -1.711309 H 5.016222 0.142991 -2.617222 C 5.133956 -0.096658 -0.449919 H 4.918909 -1.195158 -0.502460 C 6.651015 0.108461 -0.377017 H 7.150304 -0.422579 -1.217976 H 6.851671 1.203327 -0.494999 H 1.734420 -1.145507 -1.261909 C -0.629352 -1.182415 -0.967226 O -0.720083 -0.198354 -1.713558 O -1.689049 -2.031795 -0.786511 C -2.980012 -1.557320 -1.247794 H -2.844410 -1.028627 -2.215089 C -3.859776 -2.790351 -1.398726 H -4.871789 -2.505783 -1.748265 H -3.409721 -3.487195 -2.133311 H -3.953904 -3.320396 -0.428163 C -3.430877 -0.553831 -0.181534 H -2.687610 0.255531 -0.054533 H -3.628774 -1.046168 0.790086 I -5.333477 0.478430 -0.725158 N 0.505490 -1.480052 -0.267052 C 0.670158 -2.654828 0.520218 C -0.286950 -3.102426 1.463163 C 1.911984 -3.325211 0.435004 C -0.014221 -4.216962 2.270103 H -1.232622 -2.553733 1.560978 C 2.178461 -4.437305 1.250135 H 2.661909 -2.950609 -0.278245 C 1.215566 -4.894610 2.166829 H -0.769228 -4.554385 2.999565 H 3.152078 -4.947694 1.168865 H 1.424940 -5.767437 2.806283 C 0.773649 0.006283 0.959891 O 1.946977 0.016728 1.249803 N -0.404243 0.435042 1.160340 C -0.692261 1.687387 1.719305 C -1.907721 1.834316 2.433702 C 0.140503 2.823201 1.542249 C -2.269586 3.075050 2.980376

	H -2.556677 0.951930 2.550280 C -0.235960 4.058922 2.088408 H 1.049072 2.736992 0.928703 C -1.434647 4.195788 2.815407 H -3.217327 3.167305 3.536609 H 0.417516 4.932420 1.929894 H -1.721946 5.171936 3.238593

TS-CC+AcidAscorbic	
Zero-point correction= 0.585026 (Hartree/Particle) Thermal correction to Energy= 0.631961 Thermal correction to Enthalpy= 0.632905 Thermal correction to Gibbs Free Energy= 0.499986 Sum of electronic and zero-point Energies= -2371.644306 Sum of electronic and thermal Energies= -2371.597371 Sum of electronic and thermal Enthalpies= -2371.596427 Sum of electronic and thermal Free Energies= -2371.729346	79 Yso-C--Cmod+AcidF SCF Done: -2372.22933170 A.U. O -3.709741 1.801279 1.155731 O -1.995952 2.149578 -1.511582 H -1.507206 2.363546 -0.655768 C -4.048926 1.837178 -0.141249 O -3.950544 1.657492 -3.625782 C -3.311881 1.961088 -1.289573 O -5.509378 1.565468 -1.959558 C -4.209628 1.726812 -2.440825 O -5.160244 -0.880386 -0.368084 H -4.210580 -0.632112 -0.429223 O -7.747469 -1.417656 0.165683 H -6.966524 -1.976741 -0.033312 C -5.484489 1.564821 -0.523642 H -6.173663 2.361700 -0.153296 C -5.956752 0.217212 0.053533 H -5.908296 0.333986 1.167226 C -7.389731 -0.145029 -0.348942 H -8.100823 0.605279 0.062104 H -7.450972 -0.101844 -1.465048 H -2.774554 1.378846 1.255436 C -0.447423 1.577141 1.442860 O -0.521149 2.534735 0.652914 O 0.582767 1.493227 2.335088 C 1.643394 2.486203 2.226020 H 1.181846 3.476461 2.026249 C 2.371994 2.462097 3.562224 H 3.178774 3.220743 3.576960 H 1.661052 2.680632 4.383382 H 2.820870 1.463214 3.740747 C 2.478039 2.058034 1.016420 H 1.858240 2.048401 0.101397 H 2.952224 1.071654 1.173592 I 4.127023 3.480690 0.554373 N -1.359321 0.563852 1.446964 C -1.435936 -0.524123 2.348161 C -0.361270 -1.060787 3.110653 C -2.693855 -1.187272 2.401703 C -0.561449 -2.197897 3.914205 H 0.628875 -0.597303 3.049412 C -2.871932 -2.327272 3.196492 H -3.518391 -0.812862 1.778884 C -1.810852 -2.837269 3.967119 H 0.289851 -2.600623 4.486155 H -3.853420 -2.827211 3.202775 H -1.951114 -3.738301 4.584202 C -1.241764 -0.284015 -0.446675 O -2.310143 -0.773386 -0.651696 N -0.011422 -0.095937 -0.717927 C 0.483552 -0.024337 -2.038363 C 1.889903 0.024060 -2.204249 C -0.350720 0.040790 -3.180808 C 2.454994 0.080392 -3.490443 H 2.530328 0.037813 -1.309948 C 0.227692 0.111326 -4.456230 H -1.443416 0.082524 -3.068894 C 1.626344 0.114571 -4.624478 H 3.551965 0.090628 -3.593417 H -0.434554 0.170868 -5.334613

	H 2.065161 0.159748 -5.633516 O 1.943046 -1.028997 0.843524 O -0.410384 -3.168457 0.697640 H -0.616965 -2.404584 1.281864 C 1.943517 -2.363768 0.650417 O 1.014334 -5.701410 0.227287 C 0.933250 -3.280038 0.574772 O 2.922987 -4.455247 0.270634 C 1.538303 -4.614939 0.332795 O 2.966902 -2.836902 -2.077463 H 2.338081 -2.086535 -2.157512 O 5.612394 -2.829365 -2.622765 H 4.791252 -2.827567 -3.162872 C 3.246197 -3.062488 0.350818 H 4.000279 -2.908913 1.159755 C 3.848928 -2.583135 -0.991661 H 4.057663 -1.489911 -0.888573 C 5.159591 -3.287271 -1.360434 H 5.941392 -3.060080 -0.603269 H 4.974283 -4.390126 -1.341439 H 1.117358 -0.615597 0.399257

CC	
Zero-point correction= 0.438677 (Hartree/Particle) Thermal correction to Energy= 0.472884 Thermal correction to Enthalpy= 0.473828 Thermal correction to Gibbs Free Energy= 0.367960 Sum of electronic and zero-point Energies= -1687.462002 Sum of electronic and thermal Energies= -1687.427795 Sum of electronic and thermal Enthalpies= -1687.426851 Sum of electronic and thermal Free Energies= -1687.532719	59 Yso-CC SCF Done: -1687.90067877 A.U. O -1.491289 -0.480916 -1.498237 O -0.004870 0.393940 1.171941 H -0.325573 1.243282 0.581589 C -1.442349 -1.017650 -0.270310 O -0.818549 -1.721479 3.091933 C -0.808053 -0.648522 0.891362 O -2.033332 -2.584700 1.365917 C -1.168060 -1.642380 1.931697 O -4.241691 -0.829243 0.623508 H -3.864273 0.010520 0.280540 O -6.081156 -2.712555 0.031288 H -6.099807 -1.799586 0.393288 C -2.306244 -2.218475 0.007190 H -2.026056 -3.069185 -0.659716 C -3.805501 -1.910899 -0.193541 H -3.943331 -1.674230 -1.278105 C -4.718946 -3.081817 0.180018 H -4.514001 -3.949696 -0.484503 H -4.468645 -3.386704 1.226542 H -0.682115 0.099437 -1.641106 C 1.705345 1.077593 -1.189590 O 0.921317 0.454197 -1.918060 O 2.919331 0.565226 -0.817351 C 3.118442 -0.848698 -1.078970 H 2.655654 -1.095972 -2.057974 C 4.624435 -1.068750 -1.100762 H 4.853323 -2.136918 -1.285508 H 5.087731 -0.458433 -1.901228 H 5.071678 -0.770643 -0.129947 C 2.369079 -1.584217 0.032940 H 1.310380 -1.274712 0.076012 H 2.843825 -1.453101 1.023659 I 2.271804 -3.783536 -0.312781 N 1.494188 2.331612 -0.718366 C 2.300577 2.979935 0.264735 C 2.570280 2.352291 1.499887 C 2.759197 4.288961 0.013705 C 3.333343 3.028797 2.463346 H 2.141082 1.357656 1.693197 C 3.507660 4.962147 0.993989 H 2.496637 4.757590 -0.946220 C 3.807523 4.331457 2.214972 H 3.541749 2.539907 3.428890 H 3.863006 5.987170 0.798756

	H 4.400290 4.859398 2.979669 C 0.154340 2.974940 -1.026221 O 0.144736 3.929253 -1.805853 N -0.784678 2.364504 -0.293721 C -2.141051 2.675646 -0.358764 C -2.980435 2.102348 0.641020 C -2.750741 3.502650 -1.343949 C -4.364487 2.338610 0.648837 H -2.511386 1.484049 1.423084 C -4.137470 3.719740 -1.329359 H -2.111852 3.969628 -2.105217 C -4.958609 3.143638 -0.342508 H -4.983812 1.880890 1.437691 H -4.586527 4.357407 -2.110038 H -6.045754 3.322967 -0.340394

TS-CCC	
Zero-point correction= 0.540285 (Hartree/Particle) Thermal correction to Energy= 0.583791 Thermal correction to Enthalpy= 0.584735 Thermal correction to Gibbs Free Energy= 0.451101 Sum of electronic and zero-point Energies= -2086.689129 Sum of electronic and thermal Energies= -2086.645623 Sum of electronic and thermal Enthalpies= -2086.644679 Sum of electronic and thermal Free Energies= -2086.778313	73 Yso-CC--C SCF Done: -2087.22941405 A.U. O -1.343172 -1.824936 0.731392 O -0.996437 -1.490711 -2.442923 H -0.863600 -0.673036 -1.894598 C -1.551727 -2.655134 -0.302967 O -1.783855 -4.131246 -3.458337 C -1.406408 -2.512292 -1.660529 O -2.148724 -4.698710 -1.275045 C -1.771789 -3.792688 -2.295826 O 0.028453 -5.250038 0.305815 H -0.228615 -5.490546 -0.612129 O -0.973507 -6.990647 2.103239 H -0.144841 -6.853950 1.589193 C -2.072613 -4.036970 -0.000548 H -3.100810 -3.974097 0.433049 C -1.194567 -4.880644 0.942982 H -0.915836 -4.255768 1.819479 C -1.899151 -6.162381 1.428341 H -2.727392 -5.909536 2.127928 H -2.358468 -6.672878 0.540986 H -1.062015 -0.924906 0.382215 C -0.668891 1.641134 -0.222512 O -0.950298 0.452198 -0.501806 O -1.434967 2.370864 0.643446 C -2.653237 1.763407 1.153524 H -2.524804 0.661892 1.171319 C -2.859170 2.317159 2.557493 H -3.782354 1.901441 3.006717 H -1.999700 2.039576 3.198910 H -2.939897 3.423806 2.536925 C -3.730202 2.130051 0.129703 H -3.489925 1.708932 -0.863620 H -3.886600 3.223460 0.063964 I -5.738148 1.279530 0.601217 N 0.362235 2.314868 -0.753535 C 0.680567 3.684761 -0.516395 C 0.909455 4.520825 -1.632460 C 0.817673 4.204342 0.788718 C 1.260674 5.865777 -1.438948 H 0.806706 4.086549 -2.638739 C 1.155825 5.555158 0.968437 H 0.677500 3.535261 1.647883 C 1.377708 6.392552 -0.139901 H 1.439073 6.509800 -2.315505 H 1.262451 5.953564 1.990827 H 1.648741 7.450331 0.008933 C 1.220652 1.562856 -1.789288 O 0.801054 1.598001 -2.949817 N 2.315245 1.083471 -1.215401 C 3.219192 0.353863 -2.005120 C 2.815030 -0.715391 -2.848165

	C 4.602443 0.657442 -1.926134 C 3.763700 -1.443963 -3.581241 H 1.746354 -0.968120 -2.919007 C 5.545607 -0.074455 -2.666085 H 4.914551 1.489172 -1.277309 C 5.134457 -1.132048 -3.498136 H 3.424655 -2.270316 -4.228378 H 6.615058 0.188243 -2.594609 H 5.874663 -1.707923 -4.077806 C 2.602640 0.681300 1.059649 O 1.543573 1.018626 1.501980 N 3.761382 0.243462 0.990138 C 4.600096 -0.200222 2.015959 C 5.864444 -0.733788 1.665120 C 4.244795 -0.132727 3.388508 C 6.746698 -1.182559 2.659031 H 6.123435 -0.787701 0.596775 C 5.135683 -0.583399 4.374381 H 3.260651 0.275389 3.668761 C 6.391819 -1.109964 4.019321 H 7.725652 -1.597223 2.366641 H 4.842581 -0.524401 5.435924 H 7.087231 -1.463906 4.797297

CCC	
Zero-point correction= 0.543518 (Hartree/Particle) Thermal correction to Energy= 0.585401 Thermal correction to Enthalpy= 0.586345 Thermal correction to Gibbs Free Energy= 0.464027 Sum of electronic and zero-point Energies= -2086.839376 Sum of electronic and thermal Energies= -2086.797493 Sum of electronic and thermal Enthalpies= -2086.796549 Sum of electronic and thermal Free Energies= -2086.918868	73 Yso-CCC SCF Done: -2087.38289433 A.U. O -2.984436 0.923210 1.418556 O -1.729965 0.641491 -1.567784 H -0.969950 0.585386 -0.929445 C -3.302468 1.409204 0.225056 O -3.632573 2.170555 -3.171636 C -2.792751 1.305027 -1.046345 O -4.699102 2.645175 -1.213007 C -3.684798 2.042417 -1.964823 O -6.136071 0.433079 -0.056546 H -5.448419 -0.255704 0.069180 O -8.179261 1.746997 1.095513 H -8.052696 0.868868 0.674148 C -4.533962 2.287861 0.161973 H -4.370211 3.216339 0.763215 C -5.792563 1.585930 0.704557 H -5.575785 1.314545 1.767606 C -7.041022 2.472402 0.657294 H -6.906146 3.352565 1.323544 H -7.151198 2.849531 -0.390224 H -2.136752 0.324059 1.472446 C 1.426125 -0.471228 -0.710538 O 0.683554 0.467179 -0.423239 O 2.775483 -0.408098 -0.607904 C 3.338649 0.795593 -0.003149 H 2.624908 1.165030 0.761178 C 4.642469 0.358519 0.642158 H 5.124240 1.215714 1.150556 H 4.428475 -0.420945 1.399102 H 5.338952 -0.050857 -0.118908 C 3.447124 1.804649 -1.145617 H 2.451463 2.014769 -1.577695 H 4.160106 1.474770 -1.925936 I 4.182540 3.795937 -0.461758 N 1.029705 -1.702319 -1.206950 C 2.025111 -2.652882 -1.644656 C 2.544051 -2.584447 -2.946648 C 2.451114 -3.643541 -0.742790 C 3.515429 -3.516223 -3.349553 H 2.175107 -1.804882 -3.629815 C 3.416128 -4.575324 -1.155312 H 2.007583 -3.628011 0.266612 C 3.951947 -4.511432 -2.455621

	H 3.927305 -3.470688 -4.370572 H 3.757583 -5.354306 -0.454561 H 4.711135 -5.243432 -2.775928 C -0.301648 -2.249109 -1.055367 O -0.725713 -3.011631 -1.909672 N -0.984820 -1.887099 0.101144 C -2.392395 -2.117402 0.175209 C -3.227773 -1.917129 -0.944152 C -2.961767 -2.524036 1.402262 C -4.608546 -2.135141 -0.833255 H -2.794540 -1.559174 -1.885490 C -4.346625 -2.716229 1.509732 H -2.314145 -2.672265 2.278072 C -5.180796 -2.530355 0.392824 H -5.249175 -1.961877 -1.712127 H -4.776588 -3.017988 2.478156 H -6.268743 -2.678082 0.476781 C -0.315826 -1.362130 1.316290 O -0.938984 -0.450980 1.930446 N 0.831790 -1.954617 1.588970 C 1.743612 -1.415077 2.490196 C 2.814546 -2.255776 2.912249 C 1.751160 -0.067253 2.964469 C 3.833035 -1.785289 3.753089 H 2.823673 -3.296242 2.550743 C 2.786374 0.399394 3.788711 H 0.927885 0.596633 2.669797 C 3.834018 -0.448461 4.197232 H 4.644151 -2.468426 4.056907 H 2.770408 1.450535 4.123430 H 4.638872 -0.073300 4.849564

TS-CCCtrimer	
Zero-point correction= 0.560608 (Hartree/Particle) Thermal correction to Energy= 0.600943 Thermal correction to Enthalpy= 0.601887 Thermal correction to Gibbs Free Energy= 0.482141 Sum of electronic and zero-point Energies= -2086.611702 Sum of electronic and thermal Energies= -2086.571366 Sum of electronic and thermal Enthalpies= -2086.570422 Sum of electronic and thermal Free Energies= -2086.690168	73 Yso-CCC--TRIMER SCF Done: -2087.17230949 A.U. O -1.537053 -1.450009 -1.680585 O -0.259717 -2.461841 1.009022 H -0.227689 -1.487633 1.062272 C -1.921239 -2.372521 -0.806381 O -2.216266 -4.501210 1.915692 C -1.397482 -2.825274 0.357235 O -3.374135 -3.974156 0.046299 C -2.307734 -3.842358 0.914815 O -4.472454 -1.317709 0.307516 H -3.706679 -0.732156 0.464957 O -6.762491 -1.546550 -1.089244 H -6.490163 -1.009780 -0.326394 C -3.266744 -3.015118 -1.000253 H -3.322149 -3.537214 -1.974068 C -4.400433 -1.972933 -0.935099 H -4.203241 -1.256337 -1.756978 C -5.789532 -2.564964 -1.158416 H -5.850099 -3.030306 -2.156741 H -5.959672 -3.356165 -0.401541 H -0.677133 -0.995217 -1.431912 C 0.989572 0.463516 -0.082938 O 0.656287 -0.173234 -1.089552 O 2.272250 0.467565 0.365195 C 3.234611 -0.368360 -0.311984 H 2.993655 -0.385185 -1.383872 C 4.596908 0.255715 -0.058631 H 4.800049 0.304716 1.023179 H 5.388161 -0.337899 -0.538199 H 4.622683 1.275892 -0.465192 C 3.061868 -1.771724 0.270275 H 2.034544 -2.140162 0.173825 H 3.390388 -1.828672 1.315629 I 4.276720 -3.302989 -0.793260 N 0.078736 0.582102 1.007295

	C 0.461914 0.939176 2.352423 C -0.096599 0.213572 3.415522 C 1.336442 2.004085 2.619983 C 0.214931 0.553013 4.734681 H -0.772118 -0.614894 3.199355 C 1.654168 2.323464 3.942071 H 1.765935 2.568760 1.794424 C 1.094113 1.605356 5.003464 H -0.226828 -0.020403 5.553795 H 2.341823 3.149968 4.141084 H 1.344004 1.864398 6.035956 C -1.279946 0.916108 0.654406 O -2.194965 0.225142 1.080229 N -1.453245 2.034975 -0.102583 C -2.812253 2.374264 -0.445596 C -3.498137 1.591744 -1.379307 C -3.447828 3.460903 0.164130 C -4.832550 1.876995 -1.682407 H -2.981841 0.750585 -1.846380 C -4.774220 3.754808 -0.157941 H -2.893905 4.071227 0.876849 C -5.472048 2.960937 -1.074397 H -5.379287 1.237266 -2.379799 H -5.268314 4.606841 0.317036 H -6.515591 3.184948 -1.311996 C -0.400115 3.003258 -0.527551 O -0.783440 4.142271 -0.759322 N 0.807066 2.460666 -0.639143 C 1.893453 3.243681 -1.031724 C 2.772652 2.746956 -2.017458 C 2.185746 4.504299 -0.463661 C 3.905099 3.466872 -2.403976 H 2.531007 1.791876 -2.488505 C 3.318279 5.219142 -0.855689 H 1.499485 4.922600 0.273709 C 4.190735 4.707266 -1.823338 H 4.565807 3.057952 -3.174616 H 3.521241 6.193364 -0.400010 H 5.075944 5.272440 -2.127651

CCCtrimer	
Zero-point correction= 0.544774 (Hartree/Particle) Thermal correction to Energy= 0.585948 Thermal correction to Enthalpy= 0.586893 Thermal correction to Gibbs Free Energy= 0.466241 Sum of electronic and zero-point Energies= -2086.849942 Sum of electronic and thermal Energies= -2086.808768 Sum of electronic and thermal Enthalpies= -2086.807824 Sum of electronic and thermal Free Energies= -2086.928476	73 Yso-CCCtrimer SCF Done: -2087.39471621 A.U. O -1.369872 1.618585 0.308131 O -1.760413 -0.979200 2.044695 H -0.863128 -0.765677 1.612104 C -2.456417 1.094251 0.874616 O -4.672210 -1.010102 2.569199 C -2.630135 -0.016780 1.667833 O -4.734692 0.947318 1.402462 C -4.069976 -0.138132 1.973458 O -3.427588 3.184937 2.683967 H -2.867305 2.392897 2.829627 O -5.109409 5.155382 1.877152 H -4.660299 4.968105 2.727545 C -3.788945 1.780186 0.710813 H -4.070075 1.821119 -0.367820 C -3.783839 3.200677 1.301409 H -3.035073 3.788847 0.712747 C -5.146862 3.893191 1.225665 H -5.425556 4.064224 0.162954 H -5.903946 3.203718 1.674421 H -0.578799 0.948617 0.471347 C 0.779416 -0.812192 -0.332024 O 0.343993 -0.170634 0.743384 O 2.204692 -0.977257 -0.370071 C 2.976790 -0.245713 0.597549 H 2.413432 0.660764 0.902353 C 3.252057 -1.117215 1.820377

	H 3.868475 -0.578407 2.568474 H 2.285286 -1.396040 2.282738 H 3.771991 -2.051081 1.522381 C 4.207559 0.163673 -0.211122 H 3.920829 0.703455 -1.130794 H 4.867527 -0.693133 -0.448545 I 5.518576 1.616423 0.878372 N 0.422390 -0.133519 -1.621240 C 1.321830 0.868859 -2.105890 C 1.446980 2.107029 -1.446242 C 2.140384 0.576766 -3.213447 C 2.422013 3.026995 -1.868852 H 0.778684 2.338909 -0.606288 C 3.098908 1.507128 -3.645882 H 2.025766 -0.399882 -3.706282 C 3.251447 2.729870 -2.964816 H 2.534223 3.983876 -1.335231 H 3.744037 1.270142 -4.507261 H 4.019222 3.450914 -3.287505 C -0.863959 -0.175552 -2.120302 O -1.288131 0.621146 -2.951133 N -1.637310 -1.256864 -1.600690 C -3.061756 -1.274914 -1.815957 C -3.903366 -1.619798 -0.737707 C -3.630939 -0.929429 -3.058191 C -5.296086 -1.564899 -0.880012 H -3.463978 -1.936657 0.215991 C -5.030054 -0.882157 -3.194158 H -2.978700 -0.670664 -3.900293 C -5.868353 -1.186541 -2.108279 H -5.924001 -1.797292 -0.005974 H -5.464753 -0.596885 -4.166281 H -6.963651 -1.130977 -2.217721 C -1.065561 -2.387978 -0.933508 O -1.680223 -3.440767 -0.811104 N 0.227202 -2.200488 -0.470512 C 0.801210 -3.221897 0.357555 C 0.186449 -3.584812 1.572771 C 2.008444 -3.832504 -0.032312 C 0.793956 -4.544530 2.398687 H -0.762157 -3.107890 1.858786 C 2.613273 -4.787420 0.800801 H 2.468558 -3.524827 -0.981171 C 2.009325 -5.143771 2.020257 H 0.312751 -4.822123 3.350295 H 3.563258 -5.255837 0.495779 H 2.484947 -5.892118 2.675018

TS-CCCisomer	
Zero-point correction= 0.542881 (Hartree/Particle) Thermal correction to Energy= 0.584766 Thermal correction to Enthalpy= 0.585710 Thermal correction to Gibbs Free Energy= 0.463381 Sum of electronic and zero-point Energies= -2086.836549 Sum of electronic and thermal Energies= -2086.794664 Sum of electronic and thermal Enthalpies= -2086.793720 Sum of electronic and thermal Free Energies= -2086.916049	73 Yso-CC--Cisomer SCF Done: -2087.37943012 A.U. O 0.614129 2.038950 1.880976 O 1.860776 1.884581 -0.967317 H 1.082127 1.256199 -1.045464 C 0.722105 2.965444 0.928384 O 1.367317 4.677649 -2.050306 C 1.296804 2.948730 -0.314123 O 0.261865 5.020164 -0.080646 C 1.025943 4.246316 -0.967904 O -1.855089 3.111859 -0.354592 H -1.370429 2.228118 -0.397290 O -3.917189 4.494872 0.617332 H -3.766549 3.841993 -0.101885 C -0.133982 4.197405 1.024364 H -0.002269 4.765556 1.973491 C -1.623586 3.754282 0.885247 H -1.832741 3.067671 1.740250 C -2.603215 4.933860 0.922292 H -2.610922 5.389946 1.936995

	H -2.236925 5.705993 0.199031 H 1.015713 1.169771 1.570259 C 1.339509 -1.169238 0.389236 O 1.674335 -0.261035 1.161093 O 2.239694 -2.076068 -0.086375 C 3.634606 -1.820503 0.248761 H 3.687021 -1.469317 1.301114 C 4.353889 -3.149254 0.064365 H 5.431286 -3.038600 0.295566 H 3.919869 -3.913717 0.738998 H 4.247739 -3.504073 -0.981551 C 4.087620 -0.691072 -0.682167 H 3.466106 0.221264 -0.568801 H 4.116436 -1.017392 -1.739919 I 6.157807 -0.004731 -0.214804 N 0.077926 -1.353642 -0.088228 C -0.445670 -2.552418 -0.651568 C -1.394685 -2.442539 -1.688779 C -0.146507 -3.816229 -0.102290 C -2.050500 -3.588169 -2.160356 H -1.644733 -1.450265 -2.092025 C -0.790157 -4.958887 -0.598039 H 0.555961 -3.888185 0.739293 C -1.749364 -4.852253 -1.622453 H -2.813038 -3.477018 -2.947240 H -0.563334 -5.941094 -0.153078 H -2.270246 -5.751110 -1.989422 C -0.882227 -0.194325 0.042022 O -0.574004 0.802911 -0.678583 N -1.942634 -0.363477 0.774241 C -2.080453 -1.486922 1.589853 C -3.141986 -2.399368 1.365425 C -1.178684 -1.745022 2.655415 C -3.273033 -3.548514 2.157741 H -3.824714 -2.205254 0.525090 C -1.319428 -2.896395 3.445227 H -0.364950 -1.025107 2.834958 C -2.362220 -3.809817 3.199613 H -4.091202 -4.258063 1.950266 H -0.604836 -3.082494 4.264716 H -2.467851 -4.715318 3.818857 C -4.182291 1.168081 1.322410 O -3.769550 1.663337 2.311886 N -4.830251 0.665360 0.411620 C -4.630822 0.158282 -0.868429 C -3.671436 0.711964 -1.748145 C -5.420465 -0.934191 -1.297702 C -3.502090 0.165604 -3.027945 H -3.063858 1.560005 -1.406638 C -5.236843 -1.475673 -2.580140 H -6.164350 -1.354065 -0.603589 C -4.277983 -0.930575 -3.453175 H -2.741142 0.601399 -3.694897 H -5.848647 -2.335715 -2.897882 H -4.133936 -1.357460 -4.458583

TS-CCdimer	
Zero-point correction= 0.438712 (Hartree/Particle) Thermal correction to Energy= 0.472157 Thermal correction to Enthalpy= 0.473101 Thermal correction to Gibbs Free Energy= 0.369731 Sum of electronic and zero-point Energies= -1687.438228 Sum of electronic and thermal Energies= -1687.404784 Sum of electronic and thermal Enthalpies= -1687.403840 Sum of electronic and thermal Free Energies= -1687.507209	59 Yso-CC--DIMER SCF Done: -1687.87694059 A.U. O -1.113814 0.342629 -1.434994 O -0.132481 -2.653692 -1.227999 H 0.170354 -2.121630 -0.411825 C -1.715599 -0.827937 -1.735016 O -2.413826 -4.176625 -2.408186 C -1.291345 -2.128062 -1.655755 O -3.448117 -2.149924 -2.563769 C -2.374890 -2.980748 -2.215562 O -4.029661 -1.498812 0.081233 H -3.161310 -1.478312 0.542052

	O -6.346275 -0.158126 -0.119129 H -5.950189 -0.782020 0.528469 C -3.168125 -0.817358 -2.117915 H -3.373244 -0.096980 -2.944448 C -4.077103 -0.478114 -0.905044 H -3.733452 0.504298 -0.492404 C -5.558459 -0.365703 -1.279568 H -5.712152 0.494840 -1.967065 H -5.840060 -1.299378 -1.828803 H -0.118154 0.221022 -1.391903 C 1.945117 -0.013391 -0.059173 O 1.543579 0.225191 -1.201709 O 1.967927 0.921835 0.935489 C 0.962222 1.971067 0.866152 H 0.080167 1.581122 0.316510 C 0.593425 2.306162 2.303042 H -0.180035 3.098528 2.329768 H 0.189639 1.399261 2.794359 H 1.485451 2.654821 2.863764 C 1.612265 3.090510 0.055009 H 1.884684 2.725407 -0.951895 H 2.488010 3.525701 0.574358 I 0.229698 4.805827 -0.327189 N 2.671111 -1.167274 0.341159 C 3.874650 -1.571143 -0.262248 C 4.507960 -2.783113 0.115636 C 4.488892 -0.759913 -1.251351 C 5.715829 -3.160720 -0.489189 H 4.044642 -3.399777 0.896335 C 5.696760 -1.156271 -1.843302 H 4.003465 0.171526 -1.575247 C 6.324709 -2.358178 -1.470965 H 6.189134 -4.107572 -0.180509 H 6.149226 -0.511544 -2.614857 H 7.272652 -2.665238 -1.940708 C 1.854868 -1.894922 1.304214 O 2.317202 -2.710658 2.102785 N 0.586049 -1.437637 1.081339 C -0.425838 -1.480689 2.033088 C -1.554687 -0.636898 1.807132 C -0.417491 -2.268824 3.220690 C -2.612752 -0.568859 2.727743 H -1.547008 -0.003369 0.905409 C -1.485221 -2.193215 4.128643 H 0.440997 -2.929276 3.402011 C -2.589945 -1.351202 3.897607 H -3.467088 0.096145 2.519928 H -1.455120 -2.815151 5.039611 H -3.422439 -1.306269 4.617658

CCdimer	
Zero-point correction= 0.439801 (Hartree/Particle) Thermal correction to Energy= 0.473789 Thermal correction to Enthalpy= 0.474733 Thermal correction to Gibbs Free Energy= 0.368811 Sum of electronic and zero-point Energies= -1687.449745 Sum of electronic and thermal Energies= -1687.415758 Sum of electronic and thermal Enthalpies= -1687.414814 Sum of electronic and thermal Free Energies= -1687.520735	59 Yso-CCdimer SCF Done: -1687.88954647 A.U. O -1.132323 1.247096 -1.477479 O -1.139832 -1.875669 -2.026464 H -0.328446 -1.422805 -1.641581 C -2.100068 0.410458 -1.887868 O -3.912516 -2.377845 -2.950868 C -2.114666 -0.944170 -2.109022 O -4.250993 -0.146440 -2.618813 C -3.467093 -1.308073 -2.590791 O -4.271830 0.294619 0.165696 H -3.393101 0.008005 0.487743 O -5.983245 2.333719 0.465021 H -5.670499 1.576891 1.010246 C -3.498126 0.940648 -2.070618 H -3.520141 1.800468 -2.782986 C -4.106632 1.391419 -0.722327 H -3.413159 2.153909 -0.289222

	C -5.502607 2.006958 -0.830195 H -5.465206 2.937038 -1.439668 H -6.161414 1.274417 -1.361509 H -0.317978 0.675650 -1.215033 C 0.730835 -0.788872 0.430697 O 0.721765 -0.383968 -0.803903 O 1.606505 -0.085866 1.318929 C 2.020487 1.237330 0.945592 H 1.247914 1.726635 0.312059 C 2.214760 2.011694 2.244223 H 2.560592 3.045552 2.047151 H 1.251689 2.049590 2.791373 H 2.961798 1.500055 2.885989 C 3.276001 1.036914 0.094891 H 3.016421 0.481388 -0.823470 H 4.083848 0.534489 0.660769 I 4.171046 2.951991 -0.668079 N 0.921467 -2.260575 0.692405 C 1.906350 -3.157330 0.316059 C 1.858969 -4.505725 0.757224 C 2.977627 -2.730043 -0.508184 C 2.876649 -5.393782 0.381927 H 1.016795 -4.827274 1.386841 C 3.987530 -3.634556 -0.865973 H 2.989705 -1.694561 -0.871850 C 3.950150 -4.970563 -0.425493 H 2.828457 -6.439145 0.729324 H 4.813486 -3.287940 -1.508732 H 4.745337 -5.676392 -0.713418 C -0.296645 -2.373640 1.370785 O -0.851504 -3.292665 1.948042 N -0.623368 -1.020705 1.159793 C -1.496453 -0.183863 1.834526 C -1.439992 1.223205 1.649903 C -2.488626 -0.724048 2.701675 C -2.356983 2.057503 2.305498 H -0.718526 1.650224 0.943609 C -3.397177 0.130513 3.341348 H -2.533974 -1.813901 2.835684 C -3.346430 1.524035 3.149791 H -2.310253 3.143781 2.127824 H -4.171490 -0.308042 3.991684 H -4.079390 2.185464 3.636701

TS-CCCdimer	
Zero-point correction= 0.542738 (Hartree/Particle) Thermal correction to Energy= 0.584295 Thermal correction to Enthalpy= 0.585239 Thermal correction to Gibbs Free Energy= 0.463165 Sum of electronic and zero-point Energies= -2086.819680 Sum of electronic and thermal Energies= -2086.778124 Sum of electronic and thermal Enthalpies= -2086.777179 Sum of electronic and thermal Free Energies= -2086.899253	73 Yso-CCC--DIMER SCF Done: -2087.36241821 A.U. C 1.676788 0.499314 -0.174039 O 0.895453 0.058406 0.671003 O 1.732594 1.834743 -0.481279 C 0.793175 2.692645 0.221130 H 0.626891 2.276123 1.236972 C 1.435434 4.071118 0.280399 H 0.762429 4.785310 0.794649 H 2.392888 4.019265 0.834974 H 1.642573 4.447227 -0.742711 C -0.509329 2.613745 -0.578558 H -0.865920 1.570849 -0.676937 H -0.422259 3.105747 -1.566705 I -2.204849 3.623510 0.454898 N 2.566872 -0.226092 -0.927133 C 3.621642 0.450615 -1.632552 C 3.718954 0.349156 -3.032192 C 4.576693 1.191740 -0.910188 C 4.762721 1.001318 -3.707837 H 2.983086 -0.256799 -3.578710 C 5.611043 1.851614 -1.591863 H 4.501664 1.231114 0.187143 C 5.708165 1.758425 -2.992318

	H 4.838246 0.915136 -4.803722 H 6.353840 2.432438 -1.021670 H 6.525499 2.269729 -3.526125 C 2.625336 -1.734260 -0.958577 O 3.391631 -2.236738 -1.763027 N 1.403768 -2.381387 -0.497970 C 0.303690 -2.698703 -1.293913 C -0.685061 -3.608725 -0.843065 C 0.147192 -2.088186 -2.565285 C -1.814426 -3.865187 -1.633492 H -0.580233 -4.075700 0.144645 C -0.978917 -2.369425 -3.348997 H 0.907762 -1.378827 -2.921811 C -1.975513 -3.252330 -2.889239 H -2.588495 -4.547602 -1.247518 H -1.085164 -1.879984 -4.331191 H -2.866817 -3.459592 -3.502170 C 1.597011 -2.479614 0.901558 O 0.732134 -2.807345 1.738137 N 2.886146 -2.093714 1.031567 C 3.431406 -1.398585 2.090408 C 4.761325 -0.910653 1.935228 C 2.741412 -1.083244 3.298942 C 5.365726 -0.127712 2.929043 H 5.293092 -1.158999 1.003210 C 3.362459 -0.304167 4.285264 H 1.718352 -1.460633 3.432842 C 4.673114 0.185467 4.115088 H 6.394471 0.240737 2.776210 H 2.807081 -0.070420 5.209665 H 5.149143 0.797586 4.898113 O -1.513237 -0.445435 -0.157497 O -1.829344 -2.641759 2.184174 H -0.856411 -2.601805 1.909064 C -2.529999 -1.223707 0.259901 O -4.612286 -3.503261 1.868148 C -2.664748 -2.152010 1.255490 O -4.711028 -2.046152 0.120977 C -4.056401 -2.669375 1.184943 O -4.625546 0.761614 0.897676 H -3.750620 0.977450 1.274724 O -6.300813 1.744317 -0.998068 H -6.103054 1.977620 -0.065420 C -3.824806 -1.103140 -0.494974 H -3.670488 -1.395061 -1.562427 C -4.417881 0.318319 -0.443434 H -3.703802 0.995376 -0.975417 C -5.788371 0.426284 -1.117033 H -5.696038 0.182466 -2.197616 H -6.458852 -0.337495 -0.650837 H -0.672819 -0.530504 0.372931

CCCdimer	
Zero-point correction= 0.544867 (Hartree/Particle) Thermal correction to Energy= 0.586208 Thermal correction to Enthalpy= 0.587152 Thermal correction to Gibbs Free Energy= 0.466451 Sum of electronic and zero-point Energies= -2086.836894 Sum of electronic and thermal Energies= -2086.795552 Sum of electronic and thermal Enthalpies= -2086.794608 Sum of electronic and thermal Free Energies= -2086.915310	73 Yso-CCC-dimer SCF Done: -2087.38176021 A.U. O -1.464706 -1.135263 -1.581336 O -0.422023 -0.550580 1.305520 H -0.302006 0.380103 0.942994 C -2.069199 -1.219622 -0.399527 O -2.855711 -1.106422 3.005480 C -1.653784 -0.967125 0.877955 O -3.878092 -1.621213 1.029579 C -2.782818 -1.205755 1.799314 O -4.304080 0.730992 -0.672521 H -3.457668 1.149459 -1.002677 O -6.668171 0.046684 -1.723412 H -6.204675 0.875857 -1.465282 C -3.527403 -1.594587 -0.361346 H -3.681835 -2.613400 -0.791963

	C -4.410136 -0.598942 -1.147835 H -4.084330 -0.666028 -2.215947 C -5.903728 -0.944671 -1.060526 H -6.098955 -1.928252 -1.542792 H -6.168445 -1.037801 0.022716 H -0.530126 -0.765569 -1.484253 C 1.826155 0.125215 -0.601187 O 0.958472 -0.199338 -1.422999 O 2.839280 -0.733526 -0.248662 C 2.653730 -2.129564 -0.598811 H 2.083735 -2.185308 -1.550139 C 4.044556 -2.728156 -0.751228 H 3.971620 -3.808040 -0.988660 H 4.592654 -2.217882 -1.567885 H 4.621598 -2.607097 0.188867 C 1.814373 -2.710104 0.540108 H 0.895523 -2.112650 0.704709 H 2.389909 -2.785127 1.482981 I 1.099371 -4.776871 0.103538 N 1.945241 1.325891 0.021987 C 2.805041 1.467022 1.160937 C 2.459120 0.832160 2.370870 C 3.940479 2.292912 1.092033 C 3.268940 1.008795 3.503982 H 1.549277 0.214179 2.416010 C 4.742806 2.470479 2.230990 H 4.170211 2.796143 0.142841 C 4.412478 1.826094 3.437373 H 2.994358 0.513499 4.449060 H 5.630216 3.121830 2.177312 H 5.042591 1.968658 4.330383 C 0.997545 2.570594 -0.192787 O 1.492569 3.639727 0.180074 N -0.472360 2.049461 0.374927 C -1.130141 2.464477 1.556052 C -2.494668 2.166191 1.773677 C -0.371732 3.091756 2.572998 C -3.089730 2.503743 2.998551 H -3.075395 1.628097 1.012133 C -0.988303 3.425889 3.788185 H 0.686599 3.320643 2.386097 C -2.347295 3.137236 4.010579 H -4.145148 2.236843 3.165740 H -0.390734 3.915100 4.575218 H -2.819619 3.386963 4.974345 C -0.934346 2.086800 -0.955027 O -2.030546 1.875203 -1.477564 N 0.275396 2.437520 -1.518778 C 0.772494 2.416804 -2.814765 C 2.081414 2.905743 -3.047901 C 0.006383 1.905971 -3.890969 C 2.617205 2.864939 -4.343427 H 2.644958 3.327317 -2.202444 C 0.557949 1.883992 -5.179689 H -1.003838 1.523216 -3.689139 C 1.863227 2.356519 -5.417796 H 3.637924 3.244153 -4.516547 H -0.041291 1.480205 -6.012366 H 2.288706 2.329994 -6.433737

TS-CCdimer+AcidAscorbic	
Zero-point correction= 0.586066 (Hartree/Particle) Thermal correction to Energy= 0.633035 Thermal correction to Enthalpy= 0.633980 Thermal correction to Gibbs Free Energy= 0.499621 Sum of electronic and zero-point Energies= -2371.634101 Sum of electronic and thermal Energies= -2371.587132 Sum of electronic and thermal Enthalpies= -2371.586187 Sum of electronic and thermal Free Energies= -2371.720546	79 Yso-CC--DIMER+ACIDsn2Fallfprovarll SCF Done: -2372.22016700 A.U. O 3.156200 0.476898 0.766061 O 1.875505 -2.061886 2.034681 H 1.274137 -1.739784 1.276890 C 3.693346 -0.729092 1.059111 O 4.224961 -3.929865 2.329738

	C 3.143337 -1.838882 1.635678 O 5.406877 -2.286312 1.275780 C 4.232845 -2.836944 1.808581 O 4.459089 -2.420901 -1.321352 H 3.498177 -2.218722 -1.378393 O 6.596655 -1.752900 -2.812256 H 5.845447 -2.379257 -2.908900 C 5.090395 -1.052465 0.617825 H 5.820026 -0.267931 0.926305 C 5.171561 -1.260460 -0.921367 H 4.761212 -0.341107 -1.410258 C 6.603374 -1.480901 -1.421862 H 7.213470 -0.568223 -1.245054 H 7.048562 -2.313514 -0.820850 H 2.310504 0.587724 1.282551 C -0.162774 0.545615 1.304661 O 0.751959 0.971369 2.002342 O -0.565294 1.268515 0.152886 C 0.425051 2.158373 -0.469212 H 1.429431 1.727572 -0.283043 C 0.116963 2.177005 -1.958780 H 0.811087 2.864492 -2.480292 H 0.246176 1.161846 -2.384558 H -0.922945 2.518570 -2.142824 C 0.273346 3.490192 0.262839 H 0.432842 3.351539 1.347327 H -0.708192 3.963567 0.062388 I 1.801779 4.986325 -0.351770 N -1.073885 -0.466064 1.570184 C -1.576829 -0.740867 2.883233 C -2.940987 -1.070510 3.005840 C -0.736200 -0.729571 4.014785 C -3.472879 -1.356010 4.272557 H -3.562683 -1.111908 2.102413 C -1.285729 -1.000071 5.278898 H 0.336846 -0.536277 3.883553 C -2.651637 -1.308827 5.413591 H -4.542382 -1.602620 4.363817 H -0.631311 -0.987754 6.165416 H -3.074607 -1.522719 6.408422 C -0.973147 -1.534121 0.550505 O -1.879014 -2.346991 0.385107 N 0.244397 -1.342690 -0.025164 C 0.570396 -1.796219 -1.299329 C 1.703870 -1.185273 -1.911782 C -0.144776 -2.774646 -2.044430 C 2.103225 -1.530382 -3.214092 H 2.230596 -0.402373 -1.341211 C 0.267370 -3.110579 -3.342850 H -1.017305 -3.252424 -1.579498 C 1.388883 -2.501693 -3.939120 H 2.987327 -1.042799 -3.657041 H -0.300055 -3.872780 -3.902784 H 1.702254 -2.781263 -4.957262 O -2.322665 -0.027163 -1.548523 O -3.190349 1.976591 0.761257 H -2.230756 1.896969 0.549100 C -3.428479 0.041167 -0.780312 O -5.860461 0.984511 1.537960 C -3.816284 0.912937 0.199323 O -5.521127 -0.655438 -0.010907 C -5.152728 0.491473 0.686738 O -5.623096 0.291971 -2.734019 H -5.015315 0.973035 -2.381909 O -6.743855 -1.894794 -3.915665 H -6.868879 -0.934473 -4.060986 C -4.503951 -0.993474 -0.972224 H -4.084339 -1.996398 -0.728638 C -5.078080 -0.984851 -2.398715 H -4.234692 -1.251931 -3.084857 C -6.219047 -1.983961 -2.599865

	H -5.840600 -3.018117 -2.450763 H -6.990416 -1.783389 -1.815793 H -1.577190 0.415894 -1.070660

TS-BC (with epichlorohydrin as a substrate)	
Zero-point correction= 0.296629 (Hartree/Particle) Thermal correction to Energy= 0.332242 Thermal correction to Enthalpy= 0.333360 Thermal correction to Gibbs Free Energy= 0.222324 Sum of electronic and zero-point Energies= -1708.298090 Sum of electronic and thermal Energies= -1708.262477 Sum of electronic and thermal Enthalpies= -1708.261359 Sum of electronic and thermal Free Energies= -1708.372395	42 ClYso-BC SCF Done: -1708.59471848 A.U. O -1.953584 -1.869369 -1.221463 O -1.092093 -1.304433 1.798782 H -0.437088 -1.157796 1.054825 C -2.650935 -1.793843 -0.078419 O -3.674623 -1.380657 3.237543 C -2.295976 -1.526555 1.221097 O -4.617103 -1.757427 1.194087 C -3.526342 -1.524589 2.040915 O -4.200984 0.670520 -0.309986 H -3.223566 0.739810 -0.398907 O -6.542413 0.798775 -1.627121 H -5.896396 1.443609 -1.262870 C -4.154817 -1.784539 -0.160862 H -4.558724 -2.694274 -0.666055 C -4.639591 -0.529270 -0.929561 H -4.235347 -0.618817 -1.969444 C -6.165295 -0.411197 -0.988749 H -6.590754 -1.262300 -1.565282 H -6.551148 -0.480679 0.059039 H -1.021018 -1.488731 -1.050528 O 0.265524 -0.821600 -0.424389 C 1.510923 -1.235318 -0.753879 H 1.539716 -2.321354 -1.007324 Cl 2.097032 -0.432259 -2.365100 C 2.478154 -0.885928 0.378102 H 2.094959 -1.316493 1.323449 H 2.592919 0.208753 0.465936 I 4.529687 -1.754231 0.180974 O -1.373943 1.069747 -0.702279 C -0.228010 1.129229 -0.354378 N 0.824474 1.689951 0.032306 C 0.961234 3.074379 0.214412 C 2.230204 3.564680 0.608740 C -0.098466 3.999890 0.027882 C 2.433661 4.937628 0.811634 H 3.049077 2.842178 0.747498 C 0.115503 5.371161 0.233857 H -1.089476 3.629878 -0.277630 C 1.379187 5.851274 0.626488 H 3.429491 5.298215 1.117803 H -0.720049 6.075248 0.086157 H 1.540271 6.929288 0.787208

TS-CD (with epichlorohydrin as a substrate)	
Zero-point correction= 0.298342 (Hartree/Particle) Thermal correction to Energy= 0.333185 Thermal correction to Enthalpy= 0.334303 Thermal correction to Gibbs Free Energy= 0.224240 Sum of electronic and zero-point Energies= -1708.304117 Sum of electronic and thermal Energies= -1708.269274 Sum of electronic and thermal Enthalpies= -1708.268156 Sum of electronic and thermal Free Energies= -1708.378219	42 ClYso-CD SCF Done: -1708.60245890 A.U. O 2.490091 -0.987810 0.823494 O 2.472262 2.050153 -0.171516 H 1.727742 1.730764 0.418094 C 3.276981 -0.305360 -0.008440 O 4.844376 2.165009 -1.922282 C 3.275637 0.996775 -0.451617 O 5.125866 -0.050036 -1.429382 C 4.436997 1.185811 -1.334240 O 6.116792 -0.593703 1.083294 H 6.335775 0.073282 0.395347 O 7.470484 -2.904557 0.653592 H 7.580446 -2.080438 1.179558 C 4.437700 -1.032432 -0.636480 H 4.068729 -1.847735 -1.304560

	C 5.430290 -1.630215 0.376524 H 4.854898 -2.202103 1.136714 C 6.473975 -2.546997 -0.286099 H 5.988992 -3.475239 -0.663230 H 6.897415 -2.008170 -1.174699 H 1.697721 -0.399678 1.093181 O 0.608490 0.746351 1.182041 C -0.596018 0.450591 0.928205 O -0.887383 -0.912125 0.996212 C -3.023981 -0.404851 -0.087817 H -2.536228 -0.217241 -1.052664 H -3.811644 0.280883 0.234687 C -2.251273 -1.231664 0.931000 H -2.289598 -2.314765 0.721009 I -4.693250 -2.088384 -1.074107 Cl -3.050627 -1.047083 2.589557 N -1.640816 1.187526 0.643261 C -1.662629 2.546048 0.352310 C -0.647606 3.208753 -0.388513 C -2.796746 3.293456 0.766271 C -0.765666 4.575734 -0.681969 H 0.237312 2.651646 -0.727622 C -2.908358 4.656919 0.459264 H -3.577407 2.771994 1.342259 C -1.892127 5.309423 -0.264815 H 0.039224 5.070887 -1.249427 H -3.797149 5.218134 0.792335 H -1.978459 6.381634 -0.503748

TS-CC (with epichlorohydrin as a substrate)	
Zero-point correction= 0.401702 (Hartree/Particle) Thermal correction to Energy= 0.447099 Thermal correction to Enthalpy= 0.448217 Thermal correction to Gibbs Free Energy= 0.316947 Sum of electronic and zero-point Energies= -2107.678123 Sum of electronic and thermal Energies= -2107.632726 Sum of electronic and thermal Enthalpies= -2107.631607 Sum of electronic and thermal Free Energies= -2107.762877	56 ClYso-C--C SCF Done: -2108.07982439 A.U. O 2.426021 -1.128540 -1.808090 O 0.871283 1.708556 -1.707818 H 0.280576 0.904451 -1.697522 C 2.826350 0.153868 -1.718563 O 3.051071 3.631364 -1.488824 C 2.168444 1.356001 -1.672356 O 4.454084 1.839646 -1.601532 C 3.189846 2.428635 -1.569994 O 4.369075 0.337349 0.855368 H 3.512661 -0.124885 1.045687 O 6.934183 -0.443059 0.999600 H 6.218100 -0.203706 1.630691 C 4.307903 0.414727 -1.608857 H 4.852327 0.000273 -2.493025 C 4.929825 -0.197887 -0.334504 H 4.760166 -1.301788 -0.392560 C 6.437709 0.066839 -0.226094 H 6.975381 -0.431918 -1.062787 H 6.597098 1.169876 -0.327625 H 1.536310 -1.300611 -1.336422 C -0.866389 -1.295667 -0.904713 O -0.896608 -0.326373 -1.669186 O -2.051903 -1.929931 -0.556335 C -3.233228 -1.200357 -0.873466 H -3.157941 -0.744255 -1.880224 Cl -4.583469 -2.401570 -0.906168 C -3.393442 -0.155139 0.223459 H -2.458043 0.439364 0.279899 H -3.611617 -0.630592 1.197617 I -5.013726 1.308586 -0.149092 N 0.265788 -1.762041 -0.312077 C 0.427517 -3.039014 0.299792 C -0.568068 -3.738963 1.025878 C 1.730474 -3.591665 0.232016 C -0.265315 -4.969060 1.632639 H -1.578291 -3.321503 1.106554 C 2.024208 -4.815436 0.850834

	H 2.503968 -3.036091 -0.317587 C 1.027015 -5.516867 1.551581 H -1.056230 -5.502034 2.186067 H 3.045685 -5.223895 0.782284 H 1.256017 -6.480521 2.034768 C 0.892941 -0.407570 0.907385 O 1.960874 -0.808872 1.327884 N -0.023938 0.465802 0.945831 C 0.181936 1.772644 1.423739 C -0.944168 2.516325 1.849992 C 1.455095 2.395300 1.429778 C -0.800120 3.845680 2.276572 H -1.936547 2.039099 1.834131 C 1.585383 3.729340 1.837534 H 2.338839 1.841486 1.079932 C 0.464315 4.462568 2.269786 H -1.690395 4.408575 2.602812 H 2.578231 4.203750 1.791108 H 0.573202 5.513309 2.583483

TS-CC+AcidAscorbic (with epichlorohydrin as a substrate)	
Zero-point correction= 0.548685 (Hartree/Particle) Thermal correction to Energy= 0.611726 Thermal correction to Enthalpy= 0.612844 Thermal correction to Gibbs Free Energy= 0.443364 Sum of electronic and zero-point Energies= -2791.888366 Sum of electronic and thermal Energies= -2791.825325 Sum of electronic and thermal Enthalpies= -2791.824207 Sum of electronic and thermal Free Energies= -2791.993687	76 ClYso-C--C+ACID SCF Done: -2792.43705098 A.U. O -3.729015 -1.872416 -1.070820 O -2.070594 -2.070926 1.651683 H -1.566986 -2.333250 0.823018 C -4.094259 -1.840266 0.220397 O -4.074324 -1.485622 3.692427 C -3.382441 -1.900750 1.388932 O -5.595366 -1.484905 1.989368 C -4.307018 -1.614543 2.507414 O -5.220721 0.879457 0.283987 H -4.271570 0.639213 0.377522 O -7.800483 1.375222 -0.327747 H -7.028485 1.949915 -0.139011 C -5.538908 -1.556437 0.556236 H -6.215832 -2.374889 0.211588 C -6.004744 -0.241565 -0.097628 H -5.933994 -0.413678 -1.202896 C -7.447147 0.132598 0.257670 H -8.146214 -0.641548 -0.128941 H -7.530635 0.145238 1.373060 H -2.797542 -1.456603 -1.176555 C -0.452027 -1.628653 -1.293532 O -0.539839 -2.559033 -0.476230 O 0.638188 -1.553479 -2.130721 C 1.676864 -2.509453 -1.901186 H 1.245551 -3.512815 -1.713693 Cl 2.620228 -2.581150 -3.436726 C 2.499618 -2.005277 -0.723139 H 1.827695 -1.898557 0.150124 H 2.983688 -1.040853 -0.959869 I 4.076358 -3.406456 -0.059420 N -1.366442 -0.628154 -1.383982 C -1.431018 0.408099 -2.350694 C -0.350631 0.890227 -3.139526 C -2.687467 1.067213 -2.450003 C -0.543779 1.979033 -4.008821 H 0.636856 0.424602 -3.056680 C -2.857452 2.159786 -3.310748 H -3.517146 0.731765 -1.812077 C -1.789747 2.620233 -4.102590 H 0.310804 2.341479 -4.602013 H -3.837156 2.661273 -3.352219 H -1.923220 3.484647 -4.771351 C -1.303866 0.304693 0.433532 O -2.380588 0.789911 0.610377 N -0.075861 0.152856 0.748913

	C 0.375808 0.218320 2.086359 C 1.776848 0.230894 2.297673 C -0.492713 0.225634 3.204414 C 2.301627 0.304738 3.599823 H 2.444561 0.162868 1.425828 C 0.045794 0.285736 4.497869 H -1.579400 0.140202 3.063618 C 1.437617 0.342837 4.707176 H 3.394385 0.339858 3.736185 H -0.642367 0.282000 5.358131 H 1.844495 0.400305 5.728863 O 1.903817 1.041372 -0.813027 O -0.479249 3.151421 -0.835413 H -0.668663 2.347275 -1.368192 C 1.884442 2.385525 -0.710779 O 0.908191 5.731760 -0.536614 C 0.861880 3.290905 -0.707769 O 2.833341 4.511549 -0.475122 C 1.447326 4.647861 -0.558788 O 2.865070 3.081941 1.986724 H 2.227679 2.344314 2.105429 O 5.503497 3.141995 2.564719 H 4.677296 3.180633 3.095246 C 3.174547 3.120999 -0.447945 H 3.940885 2.916846 -1.233491 C 3.763514 2.751935 0.935519 H 3.983916 1.656006 0.921132 C 5.062908 3.495307 1.264863 H 5.856254 3.216707 0.537606 H 4.868866 4.591530 1.157608 H 1.072694 0.644534 -0.365984

HBD = *meso*-erythritol

***meso*-erythritol**	
Zero-point correction= 0.147934 (Hartree/Particle) Thermal correction to Energy= 0.160289 Thermal correction to Enthalpy= 0.161407 Thermal correction to Gibbs Free Energy= 0.112404 Sum of electronic and zero-point Energies= -458.844998 Sum of electronic and thermal Energies= -458.832643 Sum of electronic and thermal Enthalpies= -458.831525 Sum of electronic and thermal Free Energies= -458.880528	18 mesoerythritol SCF Done: -458.992931972 A.U. C 1.788979 0.772416 -0.211482 H 2.204339 1.722257 0.199720 H 1.740504 0.875122 -1.322400 C 0.359648 0.609071 0.317769 H 0.429444 0.402741 1.421084 C -0.359641 -0.609061 -0.317880 H -0.429422 -0.402670 -1.421191 C -1.788990 -0.772378 0.211418 H -2.204312 -1.722225 -0.199850 H -1.740294 -0.875385 1.322320 O 2.567864 -0.365304 0.191298 H 3.409494 -0.352839 -0.299534 O 0.297066 -1.830550 -0.036477 H 1.259823 -1.619037 0.012770 O -0.297114 1.830544 0.036317 H -1.259864 1.619035 -0.012709 O -2.567849 0.365289 -0.191017 H -3.409427 0.352883 0.299881

A0	
Zero-point correction= 0.232591 (Hartree/Particle) Thermal correction to Energy= 0.252704 Thermal correction to Enthalpy= 0.253822 Thermal correction to Gibbs Free Energy= 0.182448 Sum of electronic and zero-point Energies= -651.748524	28 mesoerythritol SCF Done: -651.981114355 A.U. C 0.109552 0.716872 0.123691 H -0.330877 1.602946 -0.396070 H 0.170561 0.967795 1.210486

Sum of electronic and thermal Energies= -651.728410 Sum of electronic and thermal Enthalpies= -651.727292 Sum of electronic and thermal Free Energies= -651.798666	C 1.537532 0.530998 -0.402953 H 1.461327 0.201776 -1.475871 C 2.286167 -0.597170 0.352098 H 2.363450 -0.270994 1.425858 C 3.712626 -0.793558 -0.173637 H 4.149545 -1.685566 0.333823 H 3.653155 -1.019118 -1.265859 O -0.647488 -0.471235 -0.112229 H -1.470694 -0.435838 0.443864 O 1.646944 -1.850576 0.210745 H 0.678860 -1.651946 0.150159 O 2.174094 1.788928 -0.269395 H 3.140626 1.601142 -0.208544 O 4.477424 0.394068 0.089993 H 5.312621 0.339724 -0.408746 O -3.143836 -0.135736 0.886320 C -3.765419 -0.038948 -0.427675 C -3.533423 1.167343 0.393072 H -3.041512 -0.226550 -1.245972 H -4.379793 1.630305 0.935313 H -2.699570 1.850568 0.143751 C -5.122109 -0.679695 -0.571627 H -5.626335 -0.307237 -1.487898 H -5.025448 -1.781484 -0.660086 H -5.762575 -0.454164 0.304505

A	
Zero-point correction= 0.232329 (Hartree/Particle) Thermal correction to Energy= 0.255379 Thermal correction to Enthalpy= 0.256497 Thermal correction to Gibbs Free Energy= 0.173773 Sum of electronic and zero-point Energies= -663.323002 Sum of electronic and thermal Energies= -663.299952 Sum of electronic and thermal Enthalpies= -663.298833 Sum of electronic and thermal Free Energies= -663.381558	29 mesoerythritol-A SCF Done: -663.555330657 A.U. C -2.848599 0.820830 0.027531 H -2.492182 1.710053 0.603299 H -2.920900 1.136363 -1.042955 C -4.259903 0.473675 0.515767 H -4.167818 0.099657 1.572684 C -4.879534 -0.683827 -0.309413 H -5.002255 -0.296596 -1.359585 C -6.269709 -1.078002 0.202861 H -6.600852 -1.985818 -0.355317 H -6.173640 -1.357639 1.279806 O -1.998861 -0.306107 0.201452 H -1.159891 -0.135942 -0.335021 O -4.100792 -1.859796 -0.250815 H -3.159542 -1.543624 -0.150824 O -5.032605 1.662089 0.434183 H -5.969658 1.368265 0.362423 O -7.183470 0.018751 0.014427 H -7.972638 -0.150900 0.559398 O 0.202530 0.367735 -1.075403 C 1.424233 -0.388024 -0.762727 H 1.267593 -1.357404 -0.256629 C 1.132633 0.859183 -0.048131 H 0.719359 0.759480 0.975706 I 4.964430 -0.322943 0.201391 H 2.196734 -0.382670 -1.550926 C 1.869192 2.136664 -0.343559 H 2.133331 2.187345 -1.418636 H 1.263739 3.028047 -0.074311 H 2.819527 2.132995 0.232417

TS-AB	
Zero-point correction= 0.229656 (Hartree/Particle) Thermal correction to Energy= 0.251982 Thermal correction to Enthalpy= 0.253100 Thermal correction to Gibbs Free Energy= 0.172916 Sum of electronic and zero-point Energies= -663.307424 Sum of electronic and thermal Energies= -663.285098 Sum of electronic and thermal Enthalpies= -663.283980	29 mesoerythritol-AB SCF Done: -663.537080060 A.U. C 1.946833 0.245621 0.087384 H 1.243966 1.113332 0.001072 H 1.907823 -0.086234 1.156316 C 3.365261 0.761068 -0.191634 H 3.405319 1.059354 -1.275950

Sum of electronic and thermal Free Energies= -663.364164	C 4.418662 -0.361729 -0.005601 H 4.413294 -0.622440 1.090738 C 5.834667 0.108151 -0.360177 H 6.515627 -0.775733 -0.318479 H 5.819715 0.474714 -1.415133 O 1.631664 -0.798395 -0.813526 H 0.852585 -1.361765 -0.379434 O 4.159826 -1.473529 -0.832788 H 3.157037 -1.473496 -0.940066 O 3.603030 1.864554 0.672633 H 4.580907 1.927241 0.759347 O 6.255764 1.138367 0.556139 H 7.005841 1.608365 0.150230 O -0.272145 -2.065605 0.251802 C -1.455569 -1.753038 -0.435934 H -1.334706 -1.322703 -1.459220 C -1.652163 -0.758112 0.633264 H -1.082606 0.178234 0.524544 I -4.011813 0.635581 -0.257189 H -2.221118 -2.567622 -0.460169 C -2.118111 -1.145753 2.010823 H -1.253708 -1.502156 2.610132 H -2.574148 -0.277823 2.524543 H -2.872313 -1.957456 1.959737

B	
Zero-point correction= 0.228809 (Hartree/Particle) Thermal correction to Energy= 0.251048 Thermal correction to Enthalpy= 0.252166 Thermal correction to Gibbs Free Energy= 0.174223 Sum of electronic and zero-point Energies= -663.317035 Sum of electronic and thermal Energies= -663.294795 Sum of electronic and thermal Enthalpies= -663.293677 Sum of electronic and thermal Free Energies= -663.371620	29 mesoerythritol-B SCF Done: -663.545843332 A.U. O -0.045737 2.261115 0.228088 C -0.650186 1.070440 0.613933 H -0.064331 0.154599 0.332258 C -0.965821 1.028504 2.112333 H -1.517466 0.107890 2.396437 H -0.015485 1.075037 2.684701 H -1.575223 1.915660 2.391424 C -1.863916 1.181323 -0.291117 H -1.610175 1.109593 -1.363194 H -2.492672 2.061074 -0.059873 I -3.501299 -0.609771 -0.125535 C 2.886916 1.747100 -0.428336 H 3.577660 2.591084 -0.696279 H 2.567425 1.926424 0.629996 C 3.718577 0.450143 -0.437771 H 4.086851 0.280542 -1.488437 C 2.826227 -0.769029 -0.097702 H 2.446699 -0.612554 0.950933 C 3.595694 -2.093092 -0.122730 H 2.861744 -2.923482 0.010472 H 4.054913 -2.204565 -1.135321 O 1.774123 1.665889 -1.290041 H 0.890923 1.990282 -0.661346 O 1.781379 -0.907941 -1.035600 H 1.580342 0.057323 -1.298656 O 4.800063 0.611390 0.476026 H 5.028890 -0.296208 0.778040 O 4.595595 -2.103429 0.917949 H 5.220413 -2.823329 0.719159

TS-BC	
Zero-point correction= 0.334127 (Hartree/Particle) Thermal correction to Energy= 0.367368 Thermal correction to Enthalpy= 0.368486 Thermal correction to Gibbs Free Energy= 0.267389 Sum of electronic and zero-point Energies= -1062.712496 Sum of electronic and thermal Energies= -1062.679255 Sum of electronic and thermal Enthalpies= -1062.678137 Sum of electronic and thermal Free Energies= -1062.779234	43 mesoerythritol-BC SCF Done: -1063.04662284 A.U. O 0.342600 -1.345420 -0.406307 C -0.775908 -1.293712 0.419150 H -0.997240 -2.289405 0.898852 C -0.683349 -0.246933 1.538037 H -1.570324 -0.274930 2.205746 H 0.233970 -0.452051 2.128677

	H -0.597153 0.772968 1.113383 C -1.830682 -1.029540 -0.646367 H -1.921736 -1.861553 -1.366672 H -1.671237 -0.061924 -1.153645 I -4.063709 -0.790377 0.111798 O 2.090899 -0.451376 -2.682107 C 1.341760 0.368693 -2.252784 N 0.589619 1.305387 -2.058806 C 0.179794 2.162607 -1.038082 C -1.166301 2.586023 -0.992291 C 1.099721 2.605461 -0.058687 C -1.599920 3.416875 0.052400 H -1.869642 2.231517 -1.760425 C 0.650060 3.440995 0.973936 H 2.153929 2.278855 -0.104579 C -0.696851 3.845091 1.041553 H -2.659063 3.715375 0.100629 H 1.366751 3.766030 1.745261 H -1.044050 4.485504 1.868012 C 3.057293 -2.692182 -0.321442 H 3.739566 -3.574212 -0.387793 H 2.723538 -2.467568 -1.365416 C 3.881229 -1.449162 0.152726 H 4.742162 -1.767649 0.784328 C 3.032981 -0.488523 1.023491 H 2.136411 -0.182596 0.424700 C 3.811001 0.768647 1.426790 H 3.169642 1.368550 2.110450 H 4.711757 0.455448 2.018040 O 1.941936 -2.998915 0.482210 H 1.167609 -2.343984 0.076180 O 2.643998 -1.159333 2.214622 H 2.239094 -2.003083 1.850459 O 4.463183 -0.778299 -0.992569 H 3.741758 -0.720564 -1.660792 O 4.164147 1.581765 0.310974 H 4.474405 0.924136 -0.364213

C	
Zero-point correction= 0.340055 (Hartree/Particle) Thermal correction to Energy= 0.372655 Thermal correction to Enthalpy= 0.373773 Thermal correction to Gibbs Free Energy= 0.267421 Sum of electronic and zero-point Energies= -1062.768248 Sum of electronic and thermal Energies= -1062.735648 Sum of electronic and thermal Enthalpies= -1062.734530 Sum of electronic and thermal Free Energies= -1062.840882	43 mesoerythritol-C SCF Done: -1063.10830273 A.U. O -0.231292 0.385210 0.478170 C 1.116797 0.973347 0.584939 H 1.146069 1.855963 -0.081856 C 1.379409 1.375824 2.026291 H 2.371998 1.871835 2.065879 H 0.601768 2.080953 2.382106 H 1.385536 0.483130 2.687575 C 2.037677 -0.145120 0.059565 H 2.368203 0.033984 -0.984991 H 2.951499 -0.239338 0.677388 I 4.497766 2.440585 -0.285119 O -1.143698 -1.680392 0.365659 C -0.146797 -0.953647 0.338618 N 1.171972 -1.332290 0.161985 C 1.657183 -2.639199 -0.059066 C 3.014405 -2.808708 -0.435024 C 0.839248 -3.788402 0.094679 C 3.534002 -4.095484 -0.646414 H 3.672281 -1.937987 -0.567572 C 1.378789 -5.064351 -0.123258 H -0.213233 -3.663785 0.375890 C 2.725301 -5.233889 -0.493211 H 4.591457 -4.199982 -0.937978 H 0.726113 -5.943924 0.001579 H 3.138312 -6.241135 -0.661140 C -3.564376 0.638253 0.192608 H -2.893854 1.461220 0.534702 H -3.276040 0.406999 -0.862443

	C -5.010028 1.146787 0.197132 H -5.310812 1.287136 1.272567 C -5.985329 0.100040 -0.401065 H -5.709604 -0.006409 -1.487217 C -7.444312 0.566964 -0.338104 H -8.094427 -0.275446 -0.675216 H -7.691499 0.779868 0.730144 O -3.475614 -0.506610 1.036177 H -2.611898 -0.966183 0.829164 O -5.943712 -1.130361 0.292113 H -5.012621 -1.196377 0.646396 O -5.027791 2.366583 -0.527088 H -5.953557 2.478613 -0.842166 O -7.616409 1.729812 -1.169130 H -8.454760 2.157452 -0.918750

TS-CD	
Zero-point correction= 0.336763 (Hartree/Particle) Thermal correction to Energy= 0.368442 Thermal correction to Enthalpy= 0.369561 Thermal correction to Gibbs Free Energy= 0.271030 Sum of electronic and zero-point Energies= -1062.720707 Sum of electronic and thermal Energies= -1062.689028 Sum of electronic and thermal Enthalpies= -1062.687910 Sum of electronic and thermal Free Energies= -1062.786441	43 mesoerythritol-CD180 SCF Done: -1063.05747068 A.U. O -0.099396 0.013797 -0.440204 C 1.201802 -0.252045 0.146247 H 1.891648 0.346841 -0.479118 C 1.236671 0.234092 1.593641 H 2.261124 0.118170 2.001849 H 0.932019 1.298488 1.653028 H 0.535399 -0.367869 2.208402 C 1.527207 -1.731447 0.001238 H 1.487094 -2.198203 -0.990178 H 1.643560 -2.381268 0.873517 I 4.226482 -1.628163 -0.136522 O -0.521446 -2.098052 0.208835 C -1.008857 -0.981126 -0.168102 N -2.266487 -0.601789 -0.334136 C -3.364341 -1.448568 -0.179902 C -4.646165 -0.824833 -0.185442 C -3.320396 -2.865325 -0.032536 C -5.820904 -1.576991 -0.058228 H -4.679163 0.272281 -0.282165 C -4.506756 -3.606436 0.090243 H -2.342705 -3.364876 -0.008108 C -5.765838 -2.978145 0.079029 H -6.795885 -1.060466 -0.063957 H -4.442439 -4.702710 0.200770 H -6.690235 -3.570202 0.179283 C -2.084557 2.343463 0.866051 H -2.795576 2.642296 1.675021 H -1.504343 1.474715 1.249764 C -1.072216 3.491609 0.650759 H -1.629544 4.461370 0.538910 C -0.292213 3.315327 -0.677789 H 0.190450 2.307341 -0.662232 C 0.811891 4.358009 -0.855234 H 1.219290 4.254209 -1.888700 H 0.364470 5.379163 -0.765342 O -2.781196 1.983788 -0.320943 H -2.571712 0.970119 -0.446235 O -1.164731 3.471594 -1.781028 H -1.938947 2.891028 -1.524901 O -0.231581 3.520836 1.805858 H 0.652846 3.825581 1.495410 O 1.827107 4.131104 0.139697 H 2.472472 4.859082 0.092042

D	
Zero-point correction= 0.340499 (Hartree/Particle) Thermal correction to Energy= 0.372880 Thermal correction to Enthalpy= 0.373998	43 mesoerythritol-D SCF Done: -1063.10907457 A.U. O -0.267763 -0.393977 -1.663763

Thermal correction to Gibbs Free Energy= 0.270769 Sum of electronic and zero-point Energies= -1062.768576 Sum of electronic and thermal Energies= -1062.736195 Sum of electronic and thermal Enthalpies= -1062.735077 Sum of electronic and thermal Free Energies= -1062.838305	C 0.431671 0.632283 -0.863990 H 0.725593 1.446841 -1.552769 C -0.487106 1.146375 0.231736 H 0.049269 1.955801 0.769716 H -1.430606 1.553393 -0.184036 H -0.732880 0.333465 0.948461 C 1.668663 -0.128259 -0.353604 H 2.570843 0.070761 -0.969910 H 1.913382 0.161583 0.686284 I 3.055975 3.146765 0.144942 O -0.460321 -2.653590 -1.656027 C 0.129332 -1.655723 -1.280900 N 1.237529 -1.531797 -0.455008 C 1.990838 -2.593819 0.087178 C 3.228527 -2.306197 0.717577 C 1.546657 -3.940495 0.029513 C 3.995226 -3.341511 1.275182 H 3.601626 -1.273710 0.773269 C 2.329425 -4.958985 0.591975 H 0.595036 -4.168947 -0.465693 C 3.556240 -4.674826 1.219209 H 4.953358 -3.091822 1.758858 H 1.966138 -5.998405 0.536734 H 4.162314 -5.483067 1.658374 C -3.363386 -1.104802 -0.852138 H -3.591048 -2.146234 -1.178027 H -2.551340 -1.173399 -0.091448 C -4.602456 -0.510046 -0.171531 H -5.391704 -0.367142 -0.961357 C -4.302239 0.893400 0.414715 H -3.521747 0.750693 1.210140 C -5.530491 1.527101 1.076024 H -5.265897 2.569988 1.370695 H -6.345768 1.584076 0.314198 O -2.982725 -0.278612 -1.955594 H -1.998385 -0.351072 -2.041121 O -3.880991 1.808672 -0.581468 H -3.450384 1.244481 -1.282361 O -5.008154 -1.433301 0.826172 H -5.497448 -0.905836 1.498900 O -5.916761 0.737891 2.215445 H -6.801386 1.028917 2.500408

D0 (without iodide)	
Zero-point correction= 0.340597 (Hartree/Particle) Thermal correction to Energy= 0.369892 Thermal correction to Enthalpy= 0.371010 Thermal correction to Gibbs Free Energy= 0.280014 Sum of electronic and zero-point Energies= -1051.183950 Sum of electronic and thermal Energies= -1051.154655 Sum of electronic and thermal Enthalpies= -1051.153537 Sum of electronic and thermal Free Energies= -1051.244533	42 mesoerythritol-DminusI SCF Done: -1051.52454651 A.U. O -0.363111 1.443387 1.145869 C -0.504328 2.253540 -0.057490 H -0.342122 3.306131 0.249817 C 0.516007 1.819127 -1.101393 H 0.440156 2.468021 -1.998279 H 1.551254 1.885873 -0.707672 H 0.322611 0.771253 -1.412788 C -1.973014 1.998308 -0.462622 H -2.668369 2.772337 -0.065208 H -2.088503 1.955312 -1.565067 O -1.239401 -0.499354 1.927687 C -1.304406 0.426369 1.148418 N -2.232257 0.696245 0.147980 C -3.387440 -0.073489 -0.140781 C -4.399634 0.479528 -0.961747 C -3.547343 -1.389218 0.360023 C -5.544924 -0.270366 -1.276010 H -4.309516 1.501219 -1.357156 C -4.699620 -2.120299 0.037628 H -2.772634 -1.822628 1.003874 C -5.704999 -1.573728 -0.780003 H -6.320729 0.179173 -1.915846 H -4.807322 -3.142028 0.435063

	H -6.604102 -2.158758 -1.027487 C 2.106562 -0.769964 1.226330 H 1.888033 -1.621044 1.910677 H 1.322268 -0.778302 0.433496 C 3.468274 -1.000781 0.562066 H 4.255180 -0.884798 1.357864 C 3.759983 0.065622 -0.525399 H 3.012484 -0.108687 -1.345235 C 5.160777 -0.088470 -1.127760 H 5.335364 0.759141 -1.832207 H 5.905631 -0.000703 -0.300203 O 2.132198 0.478440 1.929974 H 1.216209 0.838532 1.911028 O 3.678613 1.394263 -0.024815 H 3.148011 1.323543 0.816403 O 3.440168 -2.306839 0.018635 H 4.148165 -2.328894 -0.666991 O 5.243816 -1.357642 -1.794602 H 6.180091 -1.543509 -1.989491

TS-CC	
Zero-point correction= 0.438106 (Hartree/Particle) Thermal correction to Energy= 0.481964 Thermal correction to Enthalpy= 0.483082 Thermal correction to Gibbs Free Energy= 0.353456 Sum of electronic and zero-point Energies= -1462.077825 Sum of electronic and thermal Energies= -1462.033966 Sum of electronic and thermal Enthalpies= -1462.032848 Sum of electronic and thermal Free Energies= -1462.162474	57 mesoerythritol-C--CFllall SCF Done: -1462.51593037 A.U. C -1.949864 -0.422671 1.718181 O -0.836810 -0.325830 2.279435 O -2.320721 -1.670489 1.158247 C -1.236833 -2.546728 0.819803 H -0.456714 -2.498738 1.611249 C -1.811937 -3.952331 0.699356 H -1.022442 -4.675339 0.411552 H -2.249946 -4.263745 1.668698 H -2.614846 -3.974946 -0.067150 C -0.668645 -1.972583 -0.483768 H -0.378929 -0.912370 -0.353705 H -1.377133 -2.083673 -1.327228 I 1.214914 -2.972035 -1.155475 N -2.850356 0.544316 1.605302 C -4.020166 0.443187 0.847751 C -4.054041 -0.028977 -0.494662 C -5.222006 0.967639 1.390794 C -5.241509 0.001217 -1.239194 H -3.123076 -0.404166 -0.940599 C -6.409384 0.991100 0.642641 H -5.186707 1.360301 2.418877 C -6.431941 0.503941 -0.677700 H -5.237217 -0.368000 -2.279115 H -7.329302 1.399747 1.094722 H -7.363578 0.523959 -1.266771 C -1.844517 2.293462 0.726590 O -2.432924 3.210126 1.210760 N -1.025120 1.679618 -0.002368 C -0.287353 2.259229 -1.044762 C 0.802985 1.526000 -1.576566 C -0.594660 3.527308 -1.603972 C 1.557769 2.047278 -2.637190 H 1.069276 0.569509 -1.102115 C 0.164957 4.034808 -2.669348 H -1.434509 4.107200 -1.189378 C 1.244395 3.300732 -3.196641 H 2.408065 1.462925 -3.025951 H -0.090163 5.021023 -3.092647 H 1.838112 3.705074 -4.032473 C 1.991964 1.202566 1.612330 H 1.337097 2.059998 1.330603 H 2.098390 1.217866 2.725589 C 3.380077 1.431442 1.004069 H 3.264286 1.448744 -0.113088 C 4.359607 0.274754 1.333203 H 4.511966 0.292235 2.449065

	C 5.729157 0.478379 0.673461 H 6.338975 -0.439863 0.849345 H 5.566293 0.572019 -0.427166 O 1.469970 -0.032465 1.147201 H 0.566936 -0.175854 1.585136 O 3.905357 -0.976697 0.863488 H 2.910045 -0.946631 0.936685 O 3.846850 2.676970 1.507429 H 4.826432 2.648335 1.423321 O 6.374080 1.647031 1.217424 H 7.071822 1.917049 0.594046

TS-CC+*meso*-erythritol	
Zero-point correction= 0.587613 (Hartree/Particle) Thermal correction to Energy= 0.645971 Thermal correction to Enthalpy= 0.647090 Thermal correction to Gibbs Free Energy= 0.481319 Sum of electronic and zero-point Energies= -1920.951636 Sum of electronic and thermal Energies= -1920.893278 Sum of electronic and thermal Enthalpies= -1920.892159 Sum of electronic and thermal Free Energies= -1921.057930	75 mesoerythritolD-C--C SCF Done: -1921.53924879 A.U. C -0.887103 -0.946694 -0.402399 O -0.678323 0.093465 -1.086306 O -1.972740 -1.774341 -0.760396 C -3.029294 -1.213032 -1.551203 H -2.792229 -0.149439 -1.771373 C -3.150762 -2.009083 -2.846597 H -3.982616 -1.631570 -3.475116 H -2.203700 -1.921254 -3.415164 H -3.328555 -3.082420 -2.624274 C -4.215698 -1.306896 -0.594500 H -4.016398 -0.703409 0.311282 H -4.459176 -2.354483 -0.334267 I -6.136325 -0.463213 -1.428968 N -0.144345 -1.400577 0.585981 C -0.566273 -2.353460 1.502436 C -1.805827 -2.237792 2.197791 C 0.287341 -3.435751 1.852039 C -2.173590 -3.173753 3.173501 H -2.454626 -1.378091 1.969916 C -0.089349 -4.365313 2.834145 H 1.249100 -3.525483 1.324645 C -1.323865 -4.250072 3.501091 H -3.137754 -3.055388 3.697697 H 0.592849 -5.197421 3.080012 H -1.616489 -4.981973 4.271767 C 2.170958 -0.773609 0.409384 O 2.520458 -1.823262 -0.065745 N 2.095400 0.367154 0.829013 C 2.910368 1.375479 1.337335 C 2.330438 2.634394 1.619096 C 4.292297 1.163565 1.576374 C 3.133031 3.667957 2.126131 H 1.252546 2.753073 1.418508 C 5.078196 2.210042 2.082442 H 4.739173 0.182493 1.347852 C 4.506812 3.466231 2.360246 H 2.676363 4.648041 2.341818 H 6.152966 2.037510 2.258269 H 5.130008 4.283988 2.757177 C -1.349609 3.007553 -0.239295 H -0.799154 3.973554 -0.342478 H -1.540898 2.620109 -1.266158 C -2.706595 3.296968 0.421041 H -2.511359 3.637113 1.476142 C -3.562729 2.011246 0.520916 H -3.758367 1.669310 -0.529343 C -4.917366 2.247051 1.196543 H -5.437662 1.264055 1.281652 H -4.726798 2.629797 2.229016 O -0.599628 2.068223 0.523390 H -0.398255 1.282904 -0.106569 O -2.920850 1.007335 1.294799 H -1.939470 1.176213 1.186469 O -3.339789 4.303775 -0.354303

	H -4.304685 4.214349 -0.179063 O -5.685586 3.176782 0.415190 H -6.499324 3.388315 0.906006 C 9.244927 -0.358948 -1.400332 H 9.996799 -1.183650 -1.407351 H 9.339564 0.177936 -0.425730 C 7.847692 -0.988110 -1.457567 H 7.715582 -1.434942 -2.481705 C 6.727092 0.072204 -1.292242 H 6.876239 0.550205 -0.285309 C 5.329751 -0.556832 -1.299559 H 4.578662 0.262251 -1.209226 H 5.170741 -1.054805 -2.286583 O 9.425026 0.526971 -2.519315 H 10.185372 1.104319 -2.326518 O 6.742069 1.023260 -2.343735 H 7.689169 1.150709 -2.580527 O 7.835486 -1.963717 -0.433857 H 6.881801 -2.090929 -0.194929 O 5.231853 -1.483334 -0.215635 H 4.299509 -1.818083 -0.179796

CC	
Zero-point correction= 0.442561 (Hartree/Particle) Thermal correction to Energy= 0.485064 Thermal correction to Enthalpy= 0.486183 Thermal correction to Gibbs Free Energy= 0.363017 Sum of electronic and zero-point Energies= -1462.117256 Sum of electronic and thermal Energies= -1462.074753 Sum of electronic and thermal Enthalpies= -1462.073634 Sum of electronic and thermal Free Energies= -1462.196800	57 mesoerythritol-CC SCF Done: -1462.55981694 A.U. C -0.395299 -0.282111 0.486909 O -0.420384 0.903478 0.145094 O -1.534984 -1.073052 0.461886 C -2.718124 -0.483833 -0.128175 H -2.421473 0.180038 -0.969175 C -3.565403 -1.648458 -0.622398 H -4.486190 -1.280796 -1.116258 H -2.981531 -2.245099 -1.350625 H -3.849158 -2.310452 0.221902 C -3.339510 0.365145 0.982317 H -2.639231 1.163301 1.288922 H -3.651632 -0.252572 1.846609 I -5.180004 1.458290 0.333467 N 0.685044 -1.007275 0.886577 C 0.593119 -2.436476 1.024401 C 0.352809 -2.991224 2.293709 C 0.776314 -3.265704 -0.098106 C 0.277646 -4.386673 2.443497 H 0.228046 -2.313882 3.152426 C 0.700291 -4.659216 0.060297 H 0.982594 -2.803839 -1.078882 C 0.449611 -5.223076 1.325730 H 0.086779 -4.822367 3.437970 H 0.844331 -5.312250 -0.816006 H 0.393208 -6.317993 1.442282 C 2.075519 -0.413635 0.924596 O 2.937531 -1.135735 0.346992 N 2.111072 0.718455 1.579364 C 3.262957 1.490574 1.670843 C 3.118146 2.754692 2.316303 C 4.568341 1.153383 1.193634 C 4.197166 3.633107 2.473290 H 2.110440 3.013408 2.678535 C 5.643200 2.042722 1.354440 H 4.717007 0.184250 0.700833 C 5.475849 3.286015 1.991999 H 4.040615 4.604382 2.973572 H 6.636976 1.754441 0.969804 H 6.327353 3.976514 2.109553 C -0.214710 0.005644 -2.969180 H -0.859819 -0.822155 -2.579725 H -0.292905 -0.014898 -4.078526 C 1.226138 -0.284464 -2.536095 H 1.268224 -0.130546 -1.432459

	C 2.280580 0.659067 -3.161301 H 2.431618 0.286756 -4.211287 C 3.604375 0.526190 -2.367876 H 4.435586 0.989204 -2.947321 H 3.477975 1.127126 -1.437306 O -0.665532 1.288389 -2.527802 H -0.578071 1.290928 -1.532784 O 1.908688 2.028977 -3.162489 H 0.937675 2.060242 -2.980736 O 1.520633 -1.636775 -2.877131 H 2.495692 -1.699697 -2.671744 O 3.938888 -0.830159 -2.060666 H 3.620492 -0.982651 -1.114980

TS-BC (with epichlorohydrin as a substrate)	
Zero-point correction= 0.298130 (Hartree/Particle) Thermal correction to Energy= 0.330534 Thermal correction to Enthalpy= 0.331653 Thermal correction to Gibbs Free Energy= 0.228277 Sum of electronic and zero-point Energies= -1482.974071 Sum of electronic and thermal Energies= -1482.941667 Sum of electronic and thermal Enthalpies= -1482.940548 Sum of electronic and thermal Free Energies= -1483.043924	40 Clmesoerythritol-BC SCF Done: -1483.27220095 A.U. O 0.179896 -0.070559 1.457112 C 1.447098 -0.250122 1.166427 H 2.101411 0.653985 1.253268 Cl 2.370864 -1.434787 2.466858 C 1.561208 -0.931712 -0.201299 H 0.974301 -0.353235 -0.942664 H 1.222968 -1.983639 -0.148395 I 3.620885 -1.011587 -1.103296 O -0.937757 -2.557775 1.811727 C -1.345301 -1.705653 1.100512 N -1.989044 -1.018158 0.280870 C -3.250390 -1.292864 -0.271997 C -3.758271 -0.379404 -1.227135 C -4.024657 -2.423328 0.089284 C -5.017639 -0.599229 -1.804742 H -3.132375 0.485970 -1.498175 C -5.283413 -2.629290 -0.496362 H -3.629616 -3.134925 0.832121 C -5.788980 -1.720868 -1.445207 H -5.401368 0.118030 -2.548796 H -5.876672 -3.512371 -0.206499 H -6.777826 -1.887441 -1.901785 C -1.853525 2.241074 1.585610 H -2.253253 1.276026 1.200016 H -2.691929 2.788718 2.075656 C -1.321995 3.108877 0.427797 H -2.164875 3.487659 -0.196151 C -0.322051 2.367111 -0.495934 H 0.548566 2.079289 0.141070 C 0.201326 3.280063 -1.617280 H 0.851047 2.666816 -2.281842 H -0.682309 3.594376 -2.240065 O -0.819050 2.060742 2.537276 O -0.912579 1.230681 -1.109331 H -1.044616 0.526697 -0.421684 O -0.670420 4.241867 1.038995 H -0.263027 3.806309 1.834976 O 0.947175 4.379753 -1.133182 H 0.493371 4.631389 -0.290158 H -0.320683 1.223361 2.232291

TS-CD (with epichlorohydrin as a substrate)	
Zero-point correction= 0.300163 (Hartree/Particle) Thermal correction to Energy= 0.331728 Thermal correction to Enthalpy= 0.332847 Thermal correction to Gibbs Free Energy= 0.232601 Sum of electronic and zero-point Energies= -1482.969275 Sum of electronic and thermal Energies= -1482.937709 Sum of electronic and thermal Enthalpies= -1482.936591 Sum of electronic and thermal Free Energies= -1483.036837	40 Clmesoerythritol-CD SCF Done: -1483.26943772 A.U. O -0.173735 -0.127830 -0.522429 C 1.078751 -0.378873 0.034726 H 1.806442 0.204793 -0.553453 Cl 1.156262 0.311361 1.753515 C 1.346182 -1.872030 0.081859 H 1.342981 -2.429156 -0.862755

	H 1.549028 -2.395079 1.019464 I 4.124623 -1.836522 -0.212355 O -0.609112 -2.174508 0.311751 C -1.108099 -1.098140 -0.164446 N -2.340869 -0.721611 -0.397729 C -3.472183 -1.505348 -0.176066 C -4.720268 -0.902130 -0.498024 C -3.486090 -2.831223 0.341930 C -5.926680 -1.590192 -0.315474 H -4.703441 0.126189 -0.893476 C -4.702590 -3.509850 0.519500 H -2.532638 -3.310735 0.602730 C -5.930056 -2.902964 0.195320 H -6.877733 -1.095017 -0.573943 H -4.688604 -4.536720 0.922759 H -6.878416 -3.445406 0.340409 C -2.155267 2.519083 0.133417 H -3.127731 2.885655 0.548133 H -1.708040 1.839225 0.898319 C -1.229307 3.733658 -0.024176 H -1.612575 4.338356 -0.893329 C 0.213935 3.298048 -0.381053 H 0.596810 2.709651 0.493440 C 1.151995 4.490133 -0.591317 H 2.132171 4.099373 -0.954079 H 0.722795 5.136662 -1.395873 O -2.321454 1.863046 -1.117405 H -2.396820 0.864634 -0.910656 O 0.264682 2.554542 -1.585177 H -0.603342 2.066349 -1.623272 O -1.279569 4.465925 1.193583 H -0.424608 4.950702 1.249997 O 1.299473 5.208892 0.647942 H 1.724113 6.062731 0.451441

TS-CC (with epichlorohydrin as a substrate)	
Zero-point correction= 0.401429 (Hartree/Particle) Thermal correction to Energy= 0.445019 Thermal correction to Enthalpy= 0.446138 Thermal correction to Gibbs Free Energy= 0.313962 Sum of electronic and zero-point Energies= -1882.326620 Sum of electronic and thermal Energies= -1882.283030 Sum of electronic and thermal Enthalpies= -1882.281912 Sum of electronic and thermal Free Energies= -1882.414087	54 Clmesoerythritol-C--C SCF Done: -1882.72804958 A.U. C -1.855998 0.424587 -1.204528 O -0.754378 0.268067 -1.773291 O -2.082394 1.678663 -0.526597 C -1.018793 2.584877 -0.555973 H -0.383557 2.430321 -1.451856 Cl -1.716173 4.271558 -0.675620 C -0.231386 2.388042 0.733710 H 0.104003 1.333838 0.787274 H -0.832310 2.664260 1.620393 I 1.660992 3.552468 0.846962 N -2.852075 -0.432836 -1.154662 C -4.062171 -0.303971 -0.474966 C -4.236197 0.329905 0.787639 C -5.190518 -0.955499 -1.046281 C -5.486145 0.326339 1.425072 H -3.376583 0.826093 1.256425 C -6.435069 -0.954266 -0.401243 H -5.046233 -1.472651 -2.006605 C -6.597558 -0.308855 0.839555 H -5.591785 0.827214 2.402591 H -7.290987 -1.466078 -0.873138 H -7.576264 -0.305413 1.346704 C -2.135158 -2.498496 -0.933722 O -2.872421 -3.114764 -1.641894 N -1.221467 -2.263234 -0.110493 C -0.526473 -3.217204 0.640678 C 0.593402 -2.778412 1.390662 C -0.890309 -4.588482 0.694841 C 1.327781 -3.686378 2.166158 H 0.879676 -1.718518 1.308223 C -0.151866 -5.485886 1.481753

	H -1.755039 -4.937782 0.108249 C 0.961160 -5.044908 2.222535 H 2.204349 -3.326604 2.730246 H -0.448426 -6.547939 1.512352 H 1.540339 -5.755581 2.834049 C 2.036059 -1.381483 -1.277184 H 1.406142 -2.297813 -1.202560 H 2.141737 -1.139072 -2.363334 C 3.425230 -1.706537 -0.721109 H 3.309528 -1.907546 0.378931 C 4.403396 -0.512435 -0.863240 H 4.561255 -0.363015 -1.967930 C 5.770272 -0.808963 -0.233870 H 6.381226 0.124360 -0.272981 H 5.603763 -1.060037 0.841418 O 1.474064 -0.293830 -0.549181 H 0.597421 -0.062629 -0.997806 O 3.941968 0.654794 -0.217583 H 2.948951 0.633229 -0.287819 O 3.890517 -2.850320 -1.424118 H 4.869784 -2.840602 -1.330146 O 6.414775 -1.886678 -0.939699 H 7.115141 -2.242123 -0.364054

HBD = pentaerythritol

pentaerythritol	
Zero-point correction= 0.176944 (Hartree/Particle) Thermal correction to Energy= 0.190330 Thermal correction to Enthalpy= 0.191448 Thermal correction to Gibbs Free Energy= 0.140784 Sum of electronic and zero-point Energies= -498.108730 Sum of electronic and thermal Energies= -498.095344 Sum of electronic and thermal Enthalpies= -498.094226 Sum of electronic and thermal Free Energies= -498.144890	21 pentaerythritol SCF Done: -498.285674121 A.U. C -0.352657 0.265488 -0.014501 C -1.828031 0.734541 -0.038289 H -2.001516 1.419299 0.821161 H -2.005846 1.336484 -0.965589 C 0.567103 1.512134 -0.062401 H 0.342445 2.175893 0.802082 H 0.349299 2.100306 -0.989944 C -0.096183 -0.532259 1.289864 H -0.806814 -1.382876 1.342711 H -0.311730 0.126128 2.168263 O -2.774442 -0.315823 0.104713 H -2.781024 -0.832205 -0.722404 O 1.957613 1.183978 0.020210 H 2.092529 0.511982 -0.697667 O 1.230464 -1.070381 1.365796 H 1.817112 -0.282025 1.231490 C -0.071717 -0.631574 -1.248282 H -0.770831 -1.506619 -1.234728 H -0.280666 -0.059119 -2.180532 O 1.284518 -1.076240 -1.328391 H 1.460725 -1.469499 -0.431819

A	
Zero-point correction= 0.261737 (Hartree/Particle) Thermal correction to Energy= 0.285673 Thermal correction to Enthalpy= 0.286792 Thermal correction to Gibbs Free Energy= 0.202690 Sum of electronic and zero-point Energies= -702.589743 Sum of electronic and thermal Energies= -702.565807 Sum of electronic and thermal Enthalpies= -702.564689 Sum of electronic and thermal Free Energies= -702.648791	32 pentaerythritol-A SCF Done: -702.851480700 A.U. C 3.077240 -0.194532 0.138207 C 1.675433 0.398650 0.386199 H 0.912572 -0.290127 -0.065516 H 1.478477 0.397649 1.489746 C 3.134166 -1.628817 0.716368 H 2.366482 -2.267823 0.226808 H 2.884582 -1.598827 1.806932 C 3.342523 -0.229650 -1.389174

	H 3.255603 0.797627 -1.796958 H 2.552335 -0.848967 -1.881289 O 1.610190 1.695798 -0.164429 H 0.773033 2.127648 0.175977 O 4.406124 -2.262721 0.503405 H 5.063110 -1.583268 0.815160 O 4.655508 -0.720411 -1.720949 H 4.717117 -1.578083 -1.224797 C 4.135355 0.697238 0.837412 H 4.029119 1.739372 0.458316 H 3.934533 0.721659 1.931897 O 5.480832 0.209108 0.671846 H 5.555296 0.065623 -0.309621 O -0.724329 2.662978 0.767250 C -1.620457 1.535207 1.056867 H -1.191133 0.525465 0.932685 H -2.266631 1.663620 1.942849 C -1.837530 2.353109 -0.139359 H -2.645011 3.109964 -0.086565 I -4.018862 -0.932422 0.003369 C -1.503669 1.843125 -1.517603 H -0.563828 1.256780 -1.492209 H -2.328318 1.178638 -1.853863 H -1.372613 2.677425 -2.238596

TS-AB	
Zero-point correction= 0.261948 (Hartree/Particle) Thermal correction to Energy= 0.284769 Thermal correction to Enthalpy= 0.285887 Thermal correction to Gibbs Free Energy= 0.206141 Sum of electronic and zero-point Energies= -702.584980 Sum of electronic and thermal Energies= -702.562158 Sum of electronic and thermal Enthalpies= -702.561040 Sum of electronic and thermal Free Energies= -702.640787	32 pentaerythritol-AB SCF Done: -702.846927373 A.U. C 3.160675 0.102495 0.490930 C 2.059623 -0.530374 1.424144 H 2.457489 -0.569258 2.464422 H 1.186991 0.168767 1.464217 C 4.452913 0.314564 1.319357 H 4.809515 -0.666688 1.705870 H 4.212680 0.947860 2.212014 C 3.453822 -0.838421 -0.707811 H 2.527731 -0.996600 -1.297820 H 3.769698 -1.835102 -0.323162 O 1.658595 -1.837927 1.088185 H 1.084790 -1.750088 0.275181 O 5.533857 0.890588 0.570053 H 5.109300 1.668333 0.115477 O 4.437129 -0.291286 -1.611755 H 5.199298 -0.050279 -1.024415 C 2.650470 1.466408 -0.040192 H 1.702881 1.301543 -0.609267 H 2.405262 2.139022 0.812128 O 3.620810 2.155605 -0.848135 H 3.893254 1.466109 -1.512763 O 0.133737 -1.263946 -1.070471 C -0.863241 -0.234526 -0.739070 H -0.829297 0.158022 0.292845 H -1.039201 0.520761 -1.524245 C -1.288021 -1.620685 -0.944145 H -1.754179 -1.858994 -1.919786 I -4.228815 0.628740 0.117467 C -1.680318 -2.501460 0.212594 H -1.061616 -2.264969 1.102219 H -2.744901 -2.297203 0.456306 H -1.551055 -3.576734 -0.032802

B	
Zero-point correction= 0.259572 (Hartree/Particle) Thermal correction to Energy= 0.282626 Thermal correction to Enthalpy= 0.283744 Thermal correction to Gibbs Free Energy= 0.205607 Sum of electronic and zero-point Energies= -702.578765	32 pentaerythritol-B SCF Done: -702.838336320 A.U. C -2.874076 -0.260932 0.409475 C -1.569797 -0.168226 1.269258 H -1.817331 -0.592461 2.278088

Sum of electronic and thermal Energies= -702.555711 Sum of electronic and thermal Enthalpies= -702.554592 Sum of electronic and thermal Free Energies= -702.632729	H -0.823886 -0.881225 0.817353 C -3.502971 -1.660085 0.583662 H -3.765323 -1.830837 1.653274 H -2.750241 -2.441237 0.304213 C -3.858597 0.822955 0.905563 H -3.377600 1.816427 0.804203 H -4.052357 0.665645 1.997304 O -1.072550 1.117865 1.432771 H -0.628478 1.437793 0.507520 O -4.715125 -1.830012 -0.176809 H -4.476033 -1.451008 -1.071386 O -5.100862 0.849185 0.170697 H -5.380005 -0.103484 0.151581 C -2.530998 -0.032758 -1.083569 H -1.979263 0.928423 -1.207951 H -1.841961 -0.835789 -1.427334 O -3.701018 -0.104312 -1.942139 H -4.338626 0.523685 -1.513269 O 0.007131 1.797095 -0.726879 C 0.962492 0.860796 -1.029233 H 0.608019 -0.212550 -1.060729 H 1.486498 1.035985 -2.014958 C 1.974804 1.017560 0.107114 H 1.494079 0.774421 1.075881 I 3.615969 -0.735261 0.009267 C 2.728269 2.333040 0.132465 H 1.956067 3.130762 0.139449 H 3.375253 2.434802 1.026204 H 3.349458 2.456830 -0.780106

TS-BC	
Zero-point correction= 0.362383 (Hartree/Particle) Thermal correction to Energy= 0.396838 Thermal correction to Enthalpy= 0.397956 Thermal correction to Gibbs Free Energy= 0.292119 Sum of electronic and zero-point Energies= -1101.954855 Sum of electronic and thermal Energies= -1101.920400 Sum of electronic and thermal Enthalpies= -1101.919281 Sum of electronic and thermal Free Energies= -1102.025119	46 pentaerythritol-BC SCF Done: -1102.31723744 A.U. O 0.853257 -0.280895 0.505833 C 2.181339 -0.400668 0.908459 H 2.405440 0.280716 1.774603 C 2.584153 -1.826936 1.310810 H 3.620193 -1.865297 1.707226 H 1.881897 -2.185524 2.091440 H 2.517412 -2.512343 0.440927 C 2.874434 0.135116 -0.337993 H 2.618411 1.190750 -0.537327 H 2.700840 -0.509825 -1.218869 I 5.239512 0.244288 -0.231389 O 0.793088 -2.159955 -1.437185 C -0.026652 -1.986030 -0.589928 N -0.998497 -2.212041 0.149062 C -2.369880 -2.246884 0.004966 C -3.167094 -2.623026 1.117800 C -3.028017 -1.883825 -1.204603 C -4.566390 -2.625786 1.024412 H -2.656538 -2.891079 2.055015 C -4.427426 -1.877321 -1.279277 H -2.424798 -1.576493 -2.072925 C -5.209931 -2.247600 -0.169199 H -5.165029 -2.910839 1.905377 H -4.913865 -1.562371 -2.216471 H -6.309055 -2.224764 -0.229417 H 0.258776 0.955341 1.172363 C -2.429101 1.760186 0.524165 C -1.568299 1.240637 1.714322 H -2.063547 1.572628 2.664207 H -1.611151 0.120772 1.701189 C -3.849941 1.163516 0.622969 H -4.334858 1.504019 1.566351 H -3.791944 0.052710 0.666082 C -2.500665 3.301107 0.581216 H -1.468775 3.709621 0.555307 H -2.956321 3.611537 1.556755

	O -0.248818 1.701984 1.676633 O -4.709300 1.579227 -0.459092 H -4.156710 1.391816 -1.266509 O -3.235514 3.870092 -0.521839 H -4.069002 3.328009 -0.541811 C -1.743883 1.322773 -0.793274 H -0.712565 1.739639 -0.821470 H -1.635179 0.223257 -0.806329 O -2.491357 1.689681 -1.974618 H -2.645035 2.662128 -1.852425

C	
Zero-point correction= 0.366171 (Hartree/Particle) Thermal correction to Energy= 0.400147 Thermal correction to Enthalpy= 0.401265 Thermal correction to Gibbs Free Energy= 0.296930 Sum of electronic and zero-point Energies= -1101.978349 Sum of electronic and thermal Energies= -1101.944373 Sum of electronic and thermal Enthalpies= -1101.943255 Sum of electronic and thermal Free Energies= -1102.047591	46 pentaerythritol-C SCF Done: -1102.34452046 A.U. O 0.409854 -0.733062 1.257386 C 1.841057 -0.836876 1.171014 H 2.184386 0.105886 1.651263 C 2.389791 -2.035540 1.949638 H 3.499019 -2.017651 1.962940 H 2.021319 -1.994319 2.994506 H 2.037149 -2.974426 1.482095 C 2.251075 -0.791444 -0.306576 H 1.705344 0.004629 -0.846419 H 2.142301 -1.762561 -0.817627 I 4.430236 -0.224662 -0.568610 O 0.167587 -2.656825 0.005225 C -0.415384 -1.713201 0.571774 N -1.680523 -1.339827 0.702114 C -2.721827 -2.049783 0.128198 C -4.036937 -1.519912 0.314422 C -2.620116 -3.252166 -0.643153 C -5.169333 -2.132763 -0.236939 H -4.135269 -0.600995 0.915006 C -3.762630 -3.856936 -1.189267 H -1.621845 -3.682440 -0.800453 C -5.047481 -3.312001 -0.999062 H -6.163784 -1.683633 -0.069720 H -3.645238 -4.781292 -1.782470 H -5.936721 -3.796099 -1.435497 H -0.245877 0.669915 2.077073 C -1.743960 2.502883 0.447612 C -1.837648 1.722612 1.787668 H -2.498733 2.299985 2.480509 H -2.305464 0.732668 1.579733 C -3.149567 2.584229 -0.188471 H -3.853015 3.103201 0.502398 H -3.543223 1.550791 -0.349674 C -1.201027 3.922372 0.730631 H -0.210708 3.833600 1.225305 H -1.885599 4.435224 1.454761 O -0.579900 1.543627 2.412645 O -3.153272 3.327961 -1.423622 H -2.406698 2.912073 -1.937738 O -1.032832 4.721800 -0.455685 H -1.902255 4.611472 -0.925454 C -0.791165 1.747127 -0.511818 H 0.200287 1.642956 -0.015725 H -1.178474 0.721179 -0.683756 O -0.658677 2.391050 -1.799000 H -0.426918 3.327710 -1.569133

TS-CD	
Zero-point correction= 0.365951 (Hartree/Particle) Thermal correction to Energy= 0.398901 Thermal correction to Enthalpy= 0.400019 Thermal correction to Gibbs Free Energy= 0.298095 Sum of electronic and zero-point Energies= -1101.982524	46 pentaerythritol-CDdelmesoALL SCF Done: -1102.34847599 A.U. O -0.514327 0.242404 1.031541 C -1.962719 0.291771 1.074368 H -2.256601 -0.775399 1.064339

Sum of electronic and thermal Energies= -1101.949575 Sum of electronic and thermal Enthalpies= -1101.948457 Sum of electronic and thermal Free Energies= -1102.050381	C -2.427728 0.964500 2.365131 H -3.532042 0.903390 2.445089 H -1.969588 0.464207 3.240839 H -2.123419 2.031497 2.363263 C -2.503775 0.981589 -0.170499 H -2.203342 0.618251 -1.160899 H -3.036772 1.935138 -0.110715 I -4.892629 -0.230643 -0.395756 O -0.772504 2.160071 -0.119767 C 0.041177 1.370354 0.463848 N 1.352101 1.442499 0.620418 C 2.138392 2.458469 0.074997 C 3.483928 2.533457 0.540539 C 1.731159 3.402009 -0.913233 C 4.377103 3.489059 0.038591 H 3.791996 1.817203 1.318885 C 2.638286 4.351535 -1.410045 H 0.694413 3.376904 -1.274159 C 3.965739 4.408463 -0.946079 H 5.410526 3.517632 0.424048 H 2.295765 5.066090 -2.178313 H 4.667669 5.160338 -1.342296 H 2.183580 0.232478 1.425769 C 2.859870 -2.223139 0.077047 C 3.562126 -1.021402 0.772449 H 4.534981 -1.393059 1.182067 H 3.823446 -0.270789 -0.019772 C 3.847176 -2.865993 -0.924335 H 4.757000 -3.217871 -0.385930 H 4.183957 -2.091279 -1.659913 C 2.452723 -3.254589 1.155651 H 1.779906 -2.759112 1.885146 H 3.367351 -3.574113 1.718732 O 2.834394 -0.451684 1.825298 O 3.296905 -4.006353 -1.604297 H 2.403387 -3.677908 -1.908453 O 1.762191 -4.396601 0.618089 H 2.344432 -4.688968 -0.130387 C 1.602554 -1.725582 -0.675723 H 0.900198 -1.250434 0.041550 H 1.890921 -0.949130 -1.417249 O 0.936690 -2.778657 -1.413780 H 0.754020 -3.464940 -0.722394

D	
Zero-point correction= 0.369669 (Hartree/Particle) Thermal correction to Energy= 0.403232 Thermal correction to Enthalpy= 0.404350 Thermal correction to Gibbs Free Energy= 0.298764 Sum of electronic and zero-point Energies= -1102.034245 Sum of electronic and thermal Energies= -1102.000682 Sum of electronic and thermal Enthalpies= -1101.999563 Sum of electronic and thermal Free Energies= -1102.105149	46 pentaerythritol-D SCF Done: -1102.40391380 A.U. O 0.461955 -0.403765 0.077375 C -0.863551 -1.036190 0.211897 H -1.129711 -1.450326 -0.785218 C -0.814187 -2.137454 1.248227 H -1.830844 -2.580248 1.317105 H -0.098999 -2.929956 0.949130 H -0.509296 -1.733695 2.236131 C -1.785186 0.144936 0.543243 H -2.752096 0.024938 0.011041 H -1.999913 0.224793 1.633460 I -4.539352 -2.176141 -0.328032 O 1.295740 1.669258 -0.319647 C 0.333115 0.955571 -0.078920 N -0.996995 1.300660 0.094321 C -1.536933 2.606056 0.049143 C -2.917446 2.781963 0.321042 C -0.746800 3.743633 -0.258307 C -3.486149 4.064627 0.288515 H -3.558450 1.917073 0.543034 C -1.336131 5.016260 -0.284933 H 0.321360 3.613246 -0.469355 C -2.704459 5.192623 -0.011795

	H -4.562283 4.173645 0.498291 H -0.704954 5.887355 -0.525991 H -3.156406 6.196844 -0.036622 C 4.511200 -0.409363 0.352624 C 3.511421 -0.126677 1.505364 H 4.094130 0.014300 2.446766 H 2.988790 0.834695 1.288541 C 5.467588 0.797869 0.212189 H 6.016327 0.961556 1.167737 H 4.869347 1.721750 0.013264 C 5.315593 -1.687713 0.692464 H 4.606409 -2.529084 0.837874 H 5.847353 -1.535428 1.666678 O 2.594736 -1.183664 1.725415 H 1.833523 -1.023141 1.121696 O 6.459640 0.603470 -0.809967 H 5.921552 0.311503 -1.597755 O 6.244275 -2.067091 -0.337045 H 6.744200 -1.227737 -0.516151 C 3.730093 -0.605263 -0.973065 H 3.012253 -1.449738 -0.853329 H 3.127859 0.301632 -1.189662 O 4.598969 -0.832173 -2.102135 H 5.172926 -1.586682 -1.809318

D0 (without iodide)	
Zero-point correction= 0.369574 (Hartree/Particle) Thermal correction to Energy= 0.400174 Thermal correction to Enthalpy= 0.401293 Thermal correction to Gibbs Free Energy= 0.309054 Sum of electronic and zero-point Energies= -1090.449207 Sum of electronic and thermal Energies= -1090.418607 Sum of electronic and thermal Enthalpies= -1090.417489 Sum of electronic and thermal Free Energies= -1090.509727	45 pentaerythritol-DminusI SCF Done: -1090.81878127 A.U. O 2.738744 1.819914 0.626786 C 2.390123 2.024121 -0.765748 H 1.400294 2.534227 -0.762794 C 3.445119 2.870308 -1.451173 H 3.171476 3.031520 -2.514230 H 3.529527 3.859878 -0.960523 H 4.434103 2.369733 -1.409677 C 2.226850 0.592689 -1.312757 H 1.382537 0.531216 -2.028340 H 3.147622 0.220581 -1.819780 O 2.211697 0.287665 2.208917 C 2.294141 0.594115 1.032419 N 1.960784 -0.164214 -0.091862 C 1.481507 -1.495114 -0.097314 C 1.206678 -2.125397 -1.336486 C 1.229472 -2.208759 1.102753 C 0.660944 -3.418653 -1.371682 H 1.406425 -1.609729 -2.285772 C 0.683674 -3.499438 1.046015 H 1.465555 -1.741007 2.065948 C 0.386292 -4.113828 -0.183540 H 0.447806 -3.881933 -2.347882 H 0.489750 -4.033653 1.989769 H -0.046989 -5.125152 -0.214617 C -2.059608 0.639429 0.470568 C -1.005564 0.770289 1.580892 H -1.528330 0.808594 2.569979 H -0.368491 -0.144538 1.588511 C -2.815148 -0.700400 0.681467 H -3.278665 -0.717850 1.693053 H -2.082098 -1.544992 0.639738 C -3.049275 1.831251 0.550845 H -2.485560 2.781910 0.449499 H -3.527663 1.839225 1.562519 O -0.221304 1.943071 1.367225 H 0.500401 1.932911 2.026680 O -3.874729 -0.893864 -0.262484 H -3.433926 -0.773475 -1.144505 O -4.041531 1.806429 -0.483841 H -4.439240 0.899794 -0.408644 C -1.365351 0.617854 -0.916656

	H -0.777921 1.557490 -1.043030 H -0.655755 -0.235007 -0.951451 O -2.283058 0.434964 -2.003640 H -2.974026 1.133515 -1.852750

TS-CC	
Zero-point correction= 0.467809 (Hartree/Particle) Thermal correction to Energy= 0.512666 Thermal correction to Enthalpy= 0.513785 Thermal correction to Gibbs Free Energy= 0.383913 Sum of electronic and zero-point Energies= -1501.353192 Sum of electronic and thermal Energies= -1501.308334 Sum of electronic and thermal Enthalpies= -1501.307216 Sum of electronic and thermal Free Energies= -1501.437087	60 pentaerythritol-C--C SCF Done: -1501.82100055 A.U. C -1.733670 0.455419 0.638945 O -0.498463 0.335068 0.826031 O -2.530511 -0.718377 0.578256 C -1.892309 -1.979605 0.824828 H -0.995234 -1.818440 1.462105 C -2.920415 -2.864240 1.523771 H -2.498120 -3.862858 1.753735 H -3.241908 -2.381825 2.468198 H -3.816402 -2.995031 0.881420 C -1.441872 -2.465679 -0.554134 H -0.688079 -1.785668 -0.999088 H -2.300396 -2.634664 -1.232737 I -0.360888 -4.445486 -0.495961 N -2.404612 1.588656 0.541366 C -3.749884 1.739109 0.232393 C -4.442323 0.977610 -0.754091 C -4.470764 2.785146 0.876567 C -5.783593 1.246066 -1.062470 H -3.905451 0.169172 -1.269900 C -5.811277 3.046579 0.559063 H -3.935560 3.388315 1.624558 C -6.485028 2.279128 -0.410465 H -6.291129 0.638196 -1.831415 H -6.340301 3.863311 1.079640 H -7.539514 2.484453 -0.657536 C -1.085407 3.387009 0.339993 O -1.572681 4.112808 1.151480 N -0.377280 3.003930 -0.611806 C 0.973656 3.236639 -0.840082 C 1.542450 2.807473 -2.065308 C 1.822669 3.844861 0.123863 C 2.911982 2.979969 -2.311675 H 0.889074 2.305857 -2.793955 C 3.192726 4.002874 -0.130191 H 1.395330 4.161514 1.088183 C 3.751046 3.571969 -1.347848 H 3.338871 2.622222 -3.262911 H 3.834547 4.451822 0.645242 H 4.832179 3.661245 -1.530905 C 3.187290 -0.509145 0.400502 C 1.969124 -1.295233 -0.149756 H 2.344165 -2.177697 -0.719339 H 1.383981 -1.700314 0.713217 C 4.050326 -1.451501 1.268671 H 4.408069 -2.312852 0.659378 H 3.422682 -1.874556 2.094109 C 4.011595 0.007372 -0.803301 H 3.363712 0.661278 -1.419505 H 4.306766 -0.868271 -1.437477 O 1.152263 -0.532464 -1.013363 H 0.515682 -0.036838 -0.412052 O 5.216001 -0.798764 1.800491 H 4.855666 0.065242 2.149650 O 5.167629 0.772505 -0.427281 H 5.605388 0.216038 0.267418 C 2.684733 0.674658 1.263584 H 2.009316 1.319742 0.663592 H 2.083939 0.293220 2.116408 O 3.764644 1.455377 1.823249 H 4.285637 1.741955 1.030944

CC	
Zero-point correction= 0.470678 (Hartree/Particle) Thermal correction to Energy= 0.514877 Thermal correction to Enthalpy= 0.515995 Thermal correction to Gibbs Free Energy= 0.388808 Sum of electronic and zero-point Energies= -1501.376551 Sum of electronic and thermal Energies= -1501.332352 Sum of electronic and thermal Enthalpies= -1501.331234 Sum of electronic and thermal Free Energies= -1501.458421	60 pentaerythritol-CC SCF Done: -1501.84722873 A.U. C 0.496221 1.385212 -1.523294 O 0.255743 0.371737 -2.170170 O 1.794498 1.836700 -1.270147 C 2.828649 0.838214 -1.267476 H 2.479474 -0.043984 -1.847132 C 4.069086 1.452410 -1.904428 H 4.915363 0.736998 -1.885539 H 3.854717 1.726487 -2.956369 H 4.365975 2.371489 -1.357032 C 2.975922 0.473627 0.211915 H 2.002304 0.177282 0.648446 H 3.424466 1.297095 0.800562 I 4.312697 -1.292075 0.544913 N -0.412387 2.248256 -1.001559 C -0.093560 3.245873 -0.032292 C 0.404941 2.877537 1.235582 C -0.365202 4.596420 -0.323229 C 0.675767 3.871499 2.187887 H 0.535974 1.806507 1.455488 C -0.104674 5.584561 0.642312 H -0.791393 4.840291 -1.307770 C 0.427012 5.227086 1.894378 H 1.066679 3.584232 3.177896 H -0.316922 6.641869 0.413259 H 0.635957 6.003433 2.648633 C -1.894183 1.927412 -1.102254 O -2.547181 2.560449 -1.936800 N -2.203199 1.050938 -0.141000 C -3.519681 0.675363 0.126715 C -3.734912 -0.057644 1.330525 C -4.654145 0.937451 -0.696064 C -5.006564 -0.523837 1.686849 H -2.859980 -0.237577 1.975207 C -5.924393 0.467913 -0.325232 H -4.505660 1.514319 -1.618383 C -6.117826 -0.267749 0.859349 H -5.131529 -1.095881 2.621712 H -6.785175 0.678558 -0.983545 H -7.119303 -0.637501 1.134151 C -0.796449 -2.708747 0.052011 C 0.212381 -1.566720 0.341897 H 1.027619 -1.996017 0.972403 H 0.674362 -1.288423 -0.636410 C 0.013992 -3.915010 -0.488822 H 0.757174 -4.244468 0.272691 H 0.593293 -3.593415 -1.390889 C -1.523179 -3.111109 1.355909 H -2.084248 -2.238880 1.744392 H -0.757761 -3.382836 2.127797 O -0.285781 -0.442862 1.033200 H -0.997393 0.093730 0.503353 O -0.809707 -5.053604 -0.793166 H -1.559782 -4.652821 -1.320678 O -2.466825 -4.180634 1.172392 H -1.954045 -4.859976 0.661029 C -1.817148 -2.257032 -1.023629 H -2.390499 -1.381541 -0.657872 H -1.279872 -1.927740 -1.937820 O -2.721351 -3.319534 -1.412363 H -3.131167 -3.600045 -0.555250

TS-BC (with epichlorohydrin as a substrate)	
Zero-point correction= 0.326940 (Hartree/Particle) Thermal correction to Energy= 0.360898 Thermal correction to Enthalpy= 0.362016 Thermal correction to Gibbs Free Energy= 0.256342	43 Clpentaerythritol-BC SCF Done: -1522.54594790 A.U. O 0.848825 0.084474 0.361832 C 2.137073 0.023615 0.641810

Sum of electronic and zero-point Energies= -1522.219008 Sum of electronic and thermal Energies= -1522.185050 Sum of electronic and thermal Enthalpies= -1522.183932 Sum of electronic and thermal Free Energies= -1522.289606	H 2.485270 0.788388 1.378917 Cl 2.611341 -1.627363 1.604945 C 2.968943 0.030238 -0.646383 H 2.647165 0.882583 -1.274975 H 2.880436 -0.919982 -1.201068 I 5.179340 0.380484 -0.369314 O 0.643601 -1.764502 -1.488840 C -0.021338 -1.535041 -0.522584 N -0.958490 -1.719067 0.293025 C -2.233484 -2.191472 0.008662 C -3.068354 -2.571581 1.092286 C -2.779156 -2.222277 -1.304505 C -4.398003 -2.957488 0.870729 H -2.644228 -2.537195 2.107377 C -4.113604 -2.600327 -1.512448 H -2.143402 -1.927261 -2.154302 C -4.935704 -2.968949 -0.430655 H -5.029337 -3.240141 1.729483 H -4.520095 -2.599433 -2.537471 H -5.985875 -3.254878 -0.599861 H -0.053881 1.089457 1.286415 C -2.782417 1.745383 0.524954 C -1.951866 1.152272 1.701465 H -2.512665 1.361804 2.647687 H -1.909796 0.044802 1.583165 C -4.180117 1.088146 0.492876 H -4.708683 1.265061 1.457388 H -4.076308 -0.016699 0.370718 C -2.911902 3.270272 0.749013 H -1.893627 3.708689 0.804762 H -3.401763 3.450553 1.740324 O -0.664086 1.707876 1.799612 O -5.020272 1.634179 -0.547001 H -4.439156 1.584604 -1.354791 O -3.632836 3.947759 -0.298504 H -4.448396 3.388286 -0.407972 C -2.051812 1.465746 -0.811492 H -1.009644 1.853068 -0.748276 H -1.982176 0.372050 -0.971031 O -2.748568 2.005142 -1.956769 H -2.925111 2.948607 -1.703120

TS-CD (with epichlorohydrin as a substrate)	
Zero-point correction= 0.329669 (Hartree/Particle) Thermal correction to Energy= 0.362120 Thermal correction to Enthalpy= 0.363238 Thermal correction to Gibbs Free Energy= 0.261182 Sum of electronic and zero-point Energies= -1522.230608 Sum of electronic and thermal Energies= -1522.198158 Sum of electronic and thermal Enthalpies= -1522.197039 Sum of electronic and thermal Free Energies= -1522.299096	43 Clpentaerythritol-CD SCF Done: -1522.56027740 A.U. O -0.497569 0.169972 0.874426 C -1.897721 0.194064 0.900166 H -2.232736 -0.852108 1.000627 Cl -2.492055 1.056515 2.420664 C -2.456660 0.886208 -0.330086 H -2.196404 0.482988 -1.316190 H -3.072591 1.785497 -0.254723 I -4.832660 -0.497433 -0.584840 O -0.813233 2.033646 -0.351268 C 0.033897 1.322776 0.286868 N 1.320927 1.469761 0.489415 C 2.068539 2.527542 -0.044045 C 3.381726 2.697155 0.479362 C 1.641264 3.422383 -1.065748 C 4.228457 3.706418 0.001992 H 3.705210 2.011816 1.278744 C 2.501881 4.426503 -1.537866 H 0.627007 3.321061 -1.474063 C 3.798569 4.581082 -1.014274 H 5.238790 3.812058 0.431797 H 2.146717 5.104854 -2.332204 H 4.464000 5.375066 -1.390475 H 2.240645 0.317281 1.350739 C 3.118785 -2.129435 0.063243

	C 3.686804 -0.801904 0.637646 H 4.735975 -0.998298 0.972623 H 3.757247 -0.059908 -0.199377 C 4.065207 -2.648140 -1.043731 H 5.081856 -2.822179 -0.622341 H 4.172104 -1.865076 -1.837464 C 3.027345 -3.164229 1.209682 H 2.385626 -2.748539 2.013341 H 4.047684 -3.312918 1.647930 O 2.960986 -0.295366 1.728056 O 3.629159 -3.892865 -1.613667 H 2.663844 -3.725998 -1.808798 O 2.463651 -4.422070 0.797742 H 2.990042 -4.659166 -0.009228 C 1.712752 -1.872028 -0.529561 H 1.042416 -1.471276 0.260802 H 1.775924 -1.097057 -1.324455 O 1.137276 -3.049437 -1.139748 H 1.168817 -3.724642 -0.414191

TS-CC (with epichlorohydrin as a substrate)	
Zero-point correction= 0.430937 (Hartree/Particle) Thermal correction to Energy= 0.475437 Thermal correction to Enthalpy= 0.476555 Thermal correction to Gibbs Free Energy= 0.346011 Sum of electronic and zero-point Energies= -1921.603119 Sum of electronic and thermal Energies= -1921.558619 Sum of electronic and thermal Enthalpies= -1921.557501 Sum of electronic and thermal Free Energies= -1921.688045	57 Clpentaerythritol-C--C SCF Done: -1922.03405588 A.U. C -1.528740 -0.799164 -0.617930 O -0.349680 -0.560001 -0.956423 O -2.365360 0.319576 -0.244750 C -1.913811 1.590825 -0.583990 H -0.998220 1.533342 -1.207898 Cl -3.190235 2.418409 -1.621920 C -1.668513 2.321404 0.726849 H -0.875106 1.769544 1.273620 H -2.598841 2.428348 1.314898 I -0.832926 4.381090 0.504693 N -2.112744 -1.974913 -0.545983 C -3.400049 -2.280423 -0.109402 C -4.051635 -1.653294 0.988910 C -4.069536 -3.358903 -0.750767 C -5.321368 -2.079727 1.405698 H -3.546776 -0.826238 1.505943 C -5.336842 -3.779372 -0.322938 H -3.554037 -3.858189 -1.584350 C -5.978257 -3.141918 0.756098 H -5.804910 -1.573866 2.258745 H -5.832370 -4.617212 -0.842062 H -6.976241 -3.470421 1.089245 C -0.672953 -3.538205 -0.493878 O -1.051804 -4.305154 -1.330300 N 0.028227 -3.140008 0.467386 C 1.402026 -3.258058 0.625850 C 1.978742 -2.859077 1.859407 C 2.268658 -3.700775 -0.411003 C 3.368021 -2.894692 2.041691 H 1.307442 -2.487897 2.647971 C 3.657860 -3.724632 -0.219111 H 1.834125 -3.996264 -1.378756 C 4.221753 -3.320643 1.005629 H 3.797943 -2.559773 2.999788 H 4.309032 -4.042445 -1.049564 H 5.313020 -3.306632 1.145431 C 3.176061 0.865769 -0.235006 C 1.831791 1.482255 0.226316 H 2.046815 2.377606 0.854566 H 1.282408 1.859468 -0.673051 C 3.993734 1.949287 -0.977440 H 4.181895 2.814514 -0.301357 H 3.396833 2.335976 -1.842726 C 3.949231 0.386671 1.019442 H 3.335261 -0.369127 1.547846 H 4.078184 1.258122 1.712559

	O 1.035726 0.602511 0.993645 H 0.552293 0.019339 0.336487 O 5.274901 1.471582 -1.417575 H 5.057829 0.591976 -1.839450 O 5.215762 -0.217158 0.720611 H 5.642959 0.422596 0.094940 C 2.901275 -0.319036 -1.195403 H 2.268530 -1.083522 -0.696311 H 2.329983 0.038736 -2.078603 O 4.114413 -0.920558 -1.698480 H 4.586283 -1.220403 -0.881752

Table S7. The xyz coordinates for all the DFT optimized structures (absolute energies in a.u.) using epichlorohydrin as the substrate.

HBD = Ascorbic acid

TS-BC (2a)	
Zero-point correction= 0.324362 (Hartree/Particle) Thermal correction to Energy= 0.361302 Thermal correction to Enthalpy= 0.362420 Thermal correction to Gibbs Free Energy= 0.251514 Sum of electronic and zero-point Energies= -1747.554248 Sum of electronic and thermal Energies= -1747.517308 Sum of electronic and thermal Enthalpies= -1747.516190 Sum of electronic and thermal Free Energies= -1747.627096	45 EpiYso-BC SCF Done: -1747.87861017 A.U. O 1.332842 -0.695973 1.440654 O 0.431852 -3.144956 -0.343929 H -0.197528 -2.357123 -0.223073 C 2.026456 -1.682972 0.860295 O 3.022074 -4.484390 -0.972804 C 1.649485 -2.738705 0.064741 O 3.984879 -2.792944 0.220195 C 2.877631 -3.468973 -0.322726 O 3.625983 -0.360448 -1.256363 H 2.665669 -0.564670 -1.346327 O 5.809935 1.073844 -0.641260 H 5.247829 0.980268 -1.440330 C 3.530732 -1.601936 0.869929 H 3.940641 -1.569953 1.908015 C 3.990773 -0.331564 0.121173 H 3.496650 0.526190 0.645214 C 5.499523 -0.091448 0.116472 H 5.864154 0.065154 1.154752 H 5.996092 -1.006312 -0.293244 H 0.353492 -0.753678 1.128642 O -0.861419 -0.909054 0.145166 C -2.185493 -0.693818 0.526200 H -2.636459 -1.632661 0.939616 C -2.330089 0.411936 1.582836 H -3.392877 0.658702 1.773255 H -1.775306 1.310278 1.249776 C -2.903463 -0.323246 -0.779789 H -2.730901 -1.103790 -1.542578 H -2.589833 0.670035 -1.154383 I -5.168011 -0.196795 -0.631993 O 0.798029 -0.261166 -1.695158 C 0.230334 0.504769 -0.974150 N -0.104523 1.606977 -0.484690 C 0.766188 2.706587 -0.378802 C 0.252656 3.941276 0.082711 C 2.152472 2.606679 -0.663250 C 1.109069 5.039109 0.266885 H -0.823347 4.015300 0.304328 C 3.004275 3.698679 -0.448765 H 2.570927 1.660207 -1.037250 C 2.489380 4.925214 0.013280 H 0.692541 5.993595 0.629386 H 4.083640 3.561874 -0.627304 H 3.159321 5.783270 0.183240 Cl -1.611850 -0.109658 3.167206

TS-CD (2a)	
Zero-point correction= 0.325699 (Hartree/Particle) Thermal correction to Energy= 0.362689 Thermal correction to Enthalpy= 0.363808 Thermal correction to Gibbs Free Energy= 0.248844 Sum of electronic and zero-point Energies= -1747.561410 Sum of electronic and thermal Energies= -1747.524420 Sum of electronic and thermal Enthalpies= -1747.523301 Sum of electronic and thermal Free Energies= -1747.638265	45 EpiYso-CD SCF Done: -1747.88710908 A.U. O 2.472079 -1.232308 -0.041984 O 2.752536 1.956260 0.229999 H 1.921187 1.520381 0.582730 C 3.404873 -0.361388 -0.436950 O 5.311901 2.492381 -1.110815 C 3.546807 1.002553 -0.304348 O 5.437811 0.239751 -1.444282 C 4.815682 1.395929 -0.960045 O 5.804533 -1.092719 1.083574 H 5.058875 -0.495835 1.304727 O 7.475252 -3.084084 0.289729 H 7.435354 -2.532638 1.098529 C 4.659709 -0.906203 -1.076943 H 4.420646 -1.495884 -1.993552 C 5.445300 -1.804563 -0.097996 H 4.778623 -2.670428 0.146867 C 6.761112 -2.328153 -0.677235 H 6.552886 -2.992369 -1.544540 H 7.343166 -1.448693 -1.048526 H 1.694888 -0.717890 0.382842 O 0.706361 0.412808 0.859606 C -0.545003 0.276467 0.699342 O -0.966458 -1.018009 0.528569 C -3.111427 -0.115848 -0.309086 H -2.651634 0.206434 -1.252477 H -3.759201 0.612005 0.189232 C -2.397176 -1.206726 0.488556 H -2.508486 -2.186594 -0.014886 I -5.066515 -1.352342 -1.365733 C -2.998236 -1.292293 1.893590 H -4.089470 -1.465429 1.809304 H -2.805997 -0.348890 2.440969 N -1.518037 1.168746 0.701378 C -1.377015 2.545617 0.585780 C -0.300170 3.183977 -0.089686 C -2.411566 3.364618 1.114570 C -0.260665 4.581221 -0.205613 H 0.516785 2.582464 -0.510371 C -2.368709 4.759727 0.982929 H -3.249466 2.872588 1.634056 C -1.290336 5.381062 0.324563 H 0.594672 5.047784 -0.721085 H -3.185708 5.370129 1.402506 H -1.253066 6.477789 0.225568 Cl -2.297277 -2.652392 2.858739

TS-CD+AcidAscorbic (2a)	
Zero-point correction= 0.475688 (Hartree/Particle) Thermal correction to Energy= 0.529208 Thermal correction to Enthalpy= 0.530327 Thermal correction to Gibbs Free Energy= 0.380181 Sum of electronic and zero-point Energies= -2431.777341 Sum of electronic and thermal Energies= -2431.723820 Sum of electronic and thermal Enthalpies= -2431.722702 Sum of electronic and thermal Free Energies= -2431.872848	65 EpiYso-CD+Acid SCF Done: -2432.25302861 A.U. O 2.337205 0.377796 -0.353485 O 1.503074 3.454627 -0.260551 H 0.785311 2.768542 -0.199930 C 3.066926 1.514191 -0.286529 O 4.090194 4.837070 -0.063225 C 2.701422 2.832031 -0.246941 O 5.031898 2.759469 -0.130134 C 3.938760 3.636410 -0.136892 O 4.642638 1.358823 2.268676 H 4.935001 2.285386 2.142597 O 7.016142 -0.294938 -0.040839 H 6.641841 -1.211301 0.028015 C 4.560902 1.397370 -0.177933 H 5.020661 0.883268 -1.053210 C 5.044844 0.672125 1.097447 H 4.545735 -0.321407 1.115870 C 6.573576 0.450332 1.070633

	H 7.062697 1.449570 1.021519 H 6.853575 -0.003981 2.055074 H 1.345528 0.565938 -0.286126 O -0.093410 1.273694 -0.251337 C -1.302166 0.999690 -0.036581 O -1.573922 -0.352963 0.223567 C -3.944374 0.252685 -0.087011 H -3.914571 0.299561 -1.182206 H -4.555146 0.986600 0.442689 C -2.952210 -0.639664 0.644615 H -3.079261 -1.701262 0.358849 I -6.043450 -1.353840 -0.097929 C -3.095092 -0.472696 2.153984 H -4.131030 -0.739225 2.441658 H -2.880617 0.575387 2.442997 N -2.385024 1.737748 -0.000037 C -2.488622 3.080089 -0.374915 C -1.610554 3.710123 -1.295958 C -3.559436 3.836059 0.166809 C -1.795152 5.057974 -1.637568 H -0.769683 3.146933 -1.722782 C -3.742671 5.178689 -0.192875 H -4.240648 3.351277 0.883459 C -2.859496 5.800222 -1.095074 H -1.088877 5.532822 -2.337057 H -4.580963 5.747210 0.241432 H -2.997371 6.857778 -1.370142 O 0.741900 -1.718258 1.124685 O -0.894415 -2.360494 -1.555034 H -1.118970 -1.544097 -1.049224 C 0.910668 -2.622408 0.139223 O 0.655459 -4.564482 -2.746486 C 0.226953 -2.896375 -1.011451 O 2.028591 -4.370282 -0.935108 C 0.925407 -4.001907 -1.708657 O 3.440110 -1.909919 -1.196257 H 2.969292 -1.050283 -1.033215 O 5.793201 -2.696752 -0.494655 H 5.335973 -2.162354 -1.193451 C 2.151199 -3.474712 0.175511 H 2.211054 -4.068275 1.118904 C 3.434393 -2.623599 0.028935 H 3.451184 -1.917883 0.895306 C 4.717352 -3.476276 0.021045 H 4.973465 -3.813855 1.047267 H 4.544219 -4.376318 -0.614634 H -0.112398 -1.234919 1.003696 Cl -1.963125 -1.548534 3.059747

TS-CC (2a)	
Zero-point correction= 0.428963 (Hartree/Particle) Thermal correction to Energy= 0.476362 Thermal correction to Enthalpy= 0.477481 Thermal correction to Gibbs Free Energy= 0.340640 Sum of electronic and zero-point Energies= -2146.938609 Sum of electronic and thermal Energies= -2146.891210 Sum of electronic and thermal Enthalpies= -2146.890091 Sum of electronic and thermal Free Energies= -2147.026932	59 EpiYso-C--C SCF Done: -2147.36757189 A.U. O -2.639428 1.339444 -1.588295 O -1.339046 -1.602775 -1.608970 H -0.667323 -0.858679 -1.636478 C -3.152327 0.109714 -1.741800 O -3.662239 -3.342688 -1.866153 C -2.602612 -1.145469 -1.737229 O -4.902135 -1.431739 -2.006583 C -3.701243 -2.128211 -1.863677 O -4.868146 -0.396847 0.629400 H -3.903457 -0.264727 0.794781 O -7.328923 0.634528 0.831627 H -6.678412 0.205767 1.431976 C -4.653197 -0.037919 -1.791236 H -5.107320 0.549631 -2.624868 C -5.288978 0.412843 -0.451926 H -4.995529 1.483734 -0.303149 C -6.818337 0.310806 -0.451290

	H -7.249632 1.018669 -1.193810 H -7.088588 -0.727555 -0.769891 H -1.778668 1.318981 -1.016117 C 0.585136 1.091639 -0.679617 O 0.616207 0.234705 -1.571665 O 1.721252 1.779326 -0.326113 C 2.962878 1.227255 -0.803037 H 2.841266 0.868580 -1.846662 C 3.997839 2.340402 -0.725992 H 5.006742 1.938155 -0.938855 H 3.987272 2.801827 0.282067 C 3.261656 0.046314 0.128615 H 2.416899 -0.668212 0.118457 H 3.463044 0.376033 1.165820 I 5.048735 -1.131445 -0.494063 N -0.539196 1.391905 0.032043 C -0.608511 2.443379 0.991076 C 0.335065 2.601123 2.034616 C -1.744257 3.283151 0.960761 C 0.160358 3.605843 2.997498 H 1.189620 1.913459 2.084827 C -1.913242 4.285153 1.930688 H -2.491799 3.127489 0.168016 C -0.959422 4.457833 2.948909 H 0.903228 3.718123 3.804600 H -2.803950 4.933189 1.890955 H -1.092654 5.244321 3.709283 C -0.997263 -0.226078 1.005544 O -2.176857 -0.162587 1.259920 N 0.125379 -0.797578 1.169200 C 0.264072 -2.140720 1.547706 C 1.413674 -2.508495 2.290540 C -0.653787 -3.151048 1.159278 C 1.629299 -3.845660 2.657758 H 2.128609 -1.720282 2.575262 C -0.423231 -4.484629 1.527433 H -1.511611 -2.886869 0.523815 C 0.710645 -4.843238 2.282151 H 2.527911 -4.110507 3.239515 H -1.140725 -5.257137 1.205781 H 0.883220 -5.894392 2.564409 Cl 3.663812 3.650698 -1.928179

TS-CC+AcidAscorbic (2a)	
Zero-point correction= 0.575611 (Hartree/Particle) Thermal correction to Energy= 0.640949 Thermal correction to Enthalpy= 0.642068 Thermal correction to Gibbs Free Energy= 0.465220 Sum of electronic and zero-point Energies= -2831.152397 Sum of electronic and thermal Energies= -2831.087059 Sum of electronic and thermal Enthalpies= -2831.085940 Sum of electronic and thermal Free Energies= -2831.262787	79 EpiYso-C--C+Acid SCF Done: -2831.72800767 A.U. O -3.625480 1.745454 0.045077 O -2.255581 -0.231695 -2.079851 H -1.568866 0.419444 -1.707444 C -4.088113 1.085571 -1.023808 O -4.518105 -1.112516 -3.703234 C -3.515854 0.231696 -1.930419 O -5.785858 0.317516 -2.453269 C -4.582966 -0.294183 -2.808122 O -5.951431 -0.831212 0.179216 H -4.989731 -0.859810 0.369754 O -8.490139 -0.158478 0.821793 H -7.910261 -0.924710 1.020965 C -5.576297 1.111878 -1.279040 H -5.952646 2.145798 -1.465789 C -6.340192 0.510964 -0.076343 H -6.122105 1.172432 0.800574 C -7.854734 0.451623 -0.290183 H -8.262328 1.480201 -0.403179 H -8.041015 -0.098370 -1.246095 H -2.719778 1.376402 0.360568 C -0.412121 1.478862 0.123589 O -0.454459 1.384260 -1.118089 O 0.500239 2.319974 0.723213

	C 1.409985 3.035442 -0.133474 H 0.944787 3.183467 -1.130318 C 1.690122 4.372170 0.540638 H 2.486576 4.916583 -0.002480 H 2.002584 4.212600 1.592480 C 2.638337 2.132703 -0.255240 H 2.331823 1.154049 -0.664853 H 3.146650 1.993779 0.718675 I 4.198544 2.889985 -1.653125 N -1.267889 0.854568 0.961956 C -1.107164 0.788220 2.357679 C 0.148713 0.604622 2.995923 C -2.279478 0.765051 3.155741 C 0.219210 0.403975 4.385206 H 1.068228 0.634608 2.394549 C -2.196773 0.565913 4.541172 H -3.251557 0.898125 2.657293 C -0.949048 0.381749 5.166746 H 1.203207 0.243648 4.853727 H -3.121859 0.550509 5.140280 H -0.888135 0.217168 6.253983 C -1.923699 -1.234071 0.491674 O -3.083355 -1.176902 0.735356 N -0.799760 -1.767383 0.290323 C -0.626378 -2.989329 -0.433665 C -1.269514 -3.210096 -1.670700 C 0.278731 -3.941754 0.085302 C -0.999808 -4.393025 -2.378623 H -1.938372 -2.436042 -2.079676 C 0.540739 -5.116802 -0.642148 H 0.735772 -3.764112 1.069978 C -0.093896 -5.345470 -1.876563 H -1.500581 -4.560037 -3.345665 H 1.252420 -5.852035 -0.234417 H 0.117902 -6.264304 -2.445950 O 1.569755 -0.701984 0.094771 O 1.217408 -2.292326 2.845808 H 0.494538 -1.653455 2.650827 C 2.443137 -1.292876 0.919722 O 3.963003 -3.145509 3.457361 C 2.306434 -1.977274 2.094501 O 4.562568 -2.068324 1.537099 C 3.637657 -2.488585 2.492504 O 3.412967 -3.467122 -0.739654 H 2.435731 -3.394231 -0.767236 O 5.477096 -3.159803 -2.486625 H 4.812706 -3.865499 -2.333147 C 3.881558 -1.383387 0.478018 H 4.346084 -0.378094 0.338539 C 3.990995 -2.169502 -0.850216 H 3.471778 -1.560988 -1.630484 C 5.439605 -2.405065 -1.288660 H 5.939098 -1.429534 -1.473850 H 5.974162 -2.908333 -0.444894 H 0.601972 -1.019928 0.254411 Cl 0.216926 5.420375 0.560560

HBD = *meso*-erythritol

TS-BC (2a)	
Zero-point correction= 0.326081 (Hartree/Particle) Thermal correction to Energy= 0.359846 Thermal correction to Enthalpy= 0.360965 Thermal correction to Gibbs Free Energy= 0.257890 Sum of electronic and zero-point Energies= -1522.217864 Sum of electronic and thermal Energies= -1522.184099 Sum of electronic and thermal Enthalpies= -1522.182981 Sum of electronic and thermal Free Energies= -1522.286055	43 EpiMeso-BC SCF Done: -1522.54394514 A.U. O 0.339405 0.572617 0.080273 C 1.691516 0.691565 -0.203888 H 1.868268 0.808793 -1.307288 C 2.389048 1.875781 0.496695 H 3.492119 1.771185 0.477473 H 2.027095 1.947744 1.539302 C 2.306192 -0.647428 0.241333

	H 1.759987 -1.495370 -0.208605 H 2.357114 -0.749200 1.341467 I 4.465870 -1.019042 -0.436201 O 0.608988 0.472219 2.737282 C -0.116235 -0.161827 2.022738 N -1.019362 -1.018491 1.906256 C -1.701228 -1.724970 0.938182 C -2.867095 -2.421967 1.355501 C -1.330781 -1.787621 -0.434039 C -3.622584 -3.170750 0.442990 H -3.166946 -2.336686 2.409882 C -2.096282 -2.536592 -1.338649 H -0.484467 -1.159260 -0.752487 C -3.246719 -3.236070 -0.916103 H -4.527383 -3.696613 0.789642 H -1.798565 -2.560594 -2.399914 H -3.837535 -3.829049 -1.632732 C -2.268576 2.303331 0.965248 H -1.906682 1.967414 1.966864 H -2.943646 3.174330 1.134326 C -3.051472 1.148570 0.328730 H -2.280660 0.404388 0.015850 C -3.799821 1.572199 -0.956386 H -4.709679 2.142055 -0.619131 C -4.253442 0.330335 -1.749248 H -4.855757 0.658724 -2.628837 H -3.329760 -0.155006 -2.137072 O -1.208936 2.717114 0.114124 H -0.538443 1.946017 0.077157 O -3.002201 2.347189 -1.833852 H -2.194685 2.612640 -1.304888 O -3.943166 0.602685 1.291634 H -4.527655 0.005881 0.766118 O -5.022037 -0.589597 -0.950978 H -4.519778 -1.433108 -0.918799 Cl 2.011173 3.454661 -0.323525

TS-CD (2a)	
Zero-point correction= 0.327635 (Hartree/Particle) Thermal correction to Energy= 0.361016 Thermal correction to Enthalpy= 0.362135 Thermal correction to Gibbs Free Energy= 0.257079 Sum of electronic and zero-point Energies= -1522.228009 Sum of electronic and thermal Energies= -1522.194627 Sum of electronic and thermal Enthalpies= -1522.193509 Sum of electronic and thermal Free Energies= -1522.298565	43 EpiMeso-CD SCF Done: -1522.55564380 A.U. O 0.183481 -0.103963 0.157060 C -1.125455 -0.508279 -0.274036 H -1.812351 0.173863 0.261650 C -1.296168 -0.348613 -1.787619 H -2.329085 -0.639668 -2.064056 H -0.568679 -0.998016 -2.314586 C -1.382059 -1.958235 0.115503 H -1.268217 -2.252351 1.165788 H -1.539755 -2.744803 -0.627649 I -4.083297 -1.906233 0.381603 O 0.634545 -2.278492 -0.215643 C 1.111273 -1.116207 0.025782 N 2.353863 -0.707197 0.178628 C 3.476705 -1.531210 0.124581 C 4.731518 -0.887130 0.327614 C 3.483063 -2.935044 -0.118346 C 5.931385 -1.608415 0.291975 H 4.721636 0.198689 0.515764 C 4.694254 -3.645195 -0.150432 H 2.525452 -3.448322 -0.279162 C 5.926561 -2.996972 0.052168 H 6.885638 -1.078862 0.453231 H 4.671781 -4.732136 -0.340153 H 6.870797 -3.564899 0.022697 C 2.149024 2.549300 -0.364627 H 2.977746 2.977197 -0.982151 H 1.556682 1.874244 -1.024283 C 1.231786 3.707119 0.060675 H 1.812604 4.366823 0.765099

	C 0.012990 3.188744 0.865707 H -0.556458 2.501916 0.187018 C -0.930692 4.317974 1.288018 H -1.694729 3.888742 1.979168 H -0.340056 5.075258 1.860318 O 2.648307 1.854453 0.774142 H 2.549716 0.848288 0.562416 O 0.418220 2.557407 2.064189 H 1.282419 2.115737 1.824783 O 0.855040 4.406938 -1.119311 H -0.045869 4.763353 -0.946137 O -1.544195 4.893162 0.118351 H -1.964658 5.731055 0.381612 Cl -1.026189 1.348328 -2.344049

TS-CC (2a)	
Zero-point correction= 0.429621 (Hartree/Particle) Thermal correction to Energy= 0.474750 Thermal correction to Enthalpy= 0.475868 Thermal correction to Gibbs Free Energy= 0.341856 Sum of electronic and zero-point Energies= -1921.585344 Sum of electronic and thermal Energies= -1921.540215 Sum of electronic and thermal Enthalpies= -1921.539096 Sum of electronic and thermal Free Energies= -1921.673108	57 EpiMeso-C--C SCF Done: -1922.01496435 A.U. C -1.919644 0.154657 -1.489440 O -0.836655 0.299657 -2.095388 O -2.404433 1.237362 -0.705308 C -1.422161 2.183805 -0.295913 H -0.703614 2.382323 -1.120725 C -2.146300 3.462083 0.103995 H -1.445393 4.165065 0.594339 H -2.981918 3.224400 0.792915 C -0.692648 1.523589 0.883470 H -0.282743 0.545375 0.568225 H -1.348409 1.405227 1.767512 I 1.098739 2.652414 1.591436 N -2.687790 -0.923169 -1.504744 C -3.818110 -1.098463 -0.701649 C -3.829315 -0.872787 0.703395 C -4.979744 -1.664233 -1.288073 C -4.961398 -1.178917 1.471914 H -2.923103 -0.468730 1.174988 C -6.112153 -1.963663 -0.514920 H -4.957384 -1.864677 -2.370498 C -6.115191 -1.720241 0.871369 H -4.941559 -0.998850 2.560426 H -7.002949 -2.397716 -1.000184 H -7.003251 -1.957622 1.479832 C -1.410209 -2.635351 -0.953612 O -1.872765 -3.528478 -1.592107 N -0.669659 -2.042191 -0.128570 C 0.195060 -2.689601 0.767588 C 1.175826 -1.909867 1.430152 C 0.122740 -4.078528 1.051246 C 2.053371 -2.504282 2.348282 H 1.265622 -0.846070 1.165154 C 1.002457 -4.660050 1.977065 H -0.629075 -4.694006 0.532230 C 1.972614 -3.880242 2.634603 H 2.816472 -1.879201 2.840725 H 0.930239 -5.740930 2.184878 H 2.662932 -4.342946 3.358344 C 2.212958 -0.968288 -1.663841 H 1.732274 -1.951134 -1.448877 H 2.254023 -0.855220 -2.775497 C 3.650117 -1.010166 -1.133884 H 3.592652 -1.105635 -0.015818 C 4.423175 0.299248 -1.437860 H 4.535607 0.347590 -2.557289 C 5.830339 0.288862 -0.827184 H 6.285818 1.295774 -0.984792 H 5.722425 0.134177 0.273275 O 1.519527 0.106322 -1.046311 H 0.601842 0.182560 -1.469554 O 3.794576 1.445884 -0.905835

	H 2.817697 1.242453 -0.906479 O 4.277326 -2.137266 -1.731309 H 5.244180 -1.965780 -1.672067 O 6.627647 -0.746844 -1.434659 H 7.375811 -0.931700 -0.839437 Cl -2.857747 4.316257 -1.328081

HBD = pentaerythritol

TS-BC (2a)	
Zero-point correction= 0.354167 (Hartree/Particle) Thermal correction to Energy= 0.389855 Thermal correction to Enthalpy= 0.390974 Thermal correction to Gibbs Free Energy= 0.278960 Sum of electronic and zero-point Energies= -1561.467130 Sum of electronic and thermal Energies= -1561.431442 Sum of electronic and thermal Enthalpies= -1561.430323 Sum of electronic and thermal Free Energies= -1561.542338	46 EpiPenta-BC SCF Done: -1561.82129709 A.U. O 0.707936 -0.674900 0.623850 C 2.082330 -0.655237 0.744072 H 2.415001 -0.295127 1.755936 C 2.772871 -2.006224 0.492257 H 3.867187 -1.932350 0.645409 H 2.562038 -2.373560 -0.529484 C 2.445551 0.381024 -0.317420 H 2.030739 1.372348 -0.064571 H 2.150713 0.053655 -1.331613 I 4.739500 0.884663 -0.553671 O 0.553097 -2.038214 -1.710960 C -0.294588 -1.952163 -0.876855 N -1.337334 -2.164006 -0.242170 C -2.685909 -2.035555 -0.517813 C -3.626245 -2.461626 0.455276 C -3.172004 -1.448843 -1.718922 C -5.001607 -2.299881 0.234627 H -3.243908 -2.902752 1.387964 C -4.549198 -1.282659 -1.922143 H -2.450770 -1.104733 -2.476800 C -5.475623 -1.705325 -0.950236 H -5.714711 -2.628222 1.008603 H -4.902673 -0.803021 -2.849242 H -6.555455 -1.559787 -1.109347 H 0.065727 0.301747 1.629554 C -2.343872 1.718412 0.872432 C -1.794014 0.737650 1.951876 H -2.411313 0.875869 2.877573 H -1.982812 -0.305617 1.594656 C -3.838661 1.425008 0.623454 H -4.415959 1.576899 1.564050 H -3.971901 0.359309 0.325502 C -2.165979 3.166103 1.381763 H -1.090360 3.339922 1.592799 H -2.715882 3.282237 2.350924 O -0.443307 0.946441 2.249956 O -4.419250 2.300163 -0.367036 H -3.767855 2.250761 -1.120044 O -2.602364 4.160215 0.432843 H -3.500723 3.833730 0.158398 C -1.538588 1.520131 -0.433620 H -0.456240 1.664314 -0.221947 H -1.650908 0.476604 -0.783261 O -1.985712 2.373869 -1.511044 H -1.985644 3.279197 -1.103947 Cl 2.148445 -3.273292 1.640310

TS-CD (2a)	
Zero-point correction= 0.459263 (Hartree/Particle) Thermal correction to Energy= 0.505341 Thermal correction to Enthalpy= 0.506460 Thermal correction to Gibbs Free Energy= 0.373037 Sum of electronic and zero-point Energies= -1960.863322 Sum of electronic and thermal Energies= -1960.817243 Sum of electronic and thermal Enthalpies= -1960.816125 Sum of electronic and thermal Free Energies= -1960.949547	60 EpiPenta-C--C SCF Done: -1961.32258461 A.U. C 1.362295 -0.960053 0.406303 O 0.342539 -0.331443 0.782087 O 2.492597 -0.201778 -0.017963 C 2.441690 1.205976 0.185621 H 1.779921 1.448709 1.045408 C 3.869782 1.671129 0.450254 H 3.927999 2.775824 0.484829 H 4.548227 1.283651 -0.336205 C 1.844105 1.789448 -1.097247 H 0.816759 1.404835 -1.261034 H 2.490759 1.619549 -1.979781 I 1.530930 4.021415 -1.006657 N 1.485110 -2.265826 0.304887

	C 2.643535 -2.985856 0.064896 C 3.940781 -2.623333 0.537548 C 2.526939 -4.219925 -0.637379 C 5.047886 -3.450981 0.301989 H 4.065031 -1.679848 1.087887 C 3.641214 -5.038548 -0.867574 H 1.530388 -4.510948 -1.004896 C 4.916533 -4.663931 -0.402256 H 6.036707 -3.141170 0.682349 H 3.511496 -5.984912 -1.420105 H 5.792673 -5.308493 -0.580993 C -0.614323 -3.230975 0.402380 O -0.460841 -3.925785 1.353661 N -1.084071 -2.695587 -0.620878 C -2.428935 -2.529087 -0.955056 C -2.743645 -2.065763 -2.255320 C -3.490998 -2.765058 -0.040902 C -4.078789 -1.857246 -2.632084 H -1.912954 -1.849482 -2.942718 C -4.820801 -2.543140 -0.426261 H -3.256656 -3.091417 0.984549 C -5.127386 -2.094005 -1.723749 H -4.302103 -1.482933 -3.644710 H -5.629609 -2.705324 0.304215 H -6.171846 -1.898263 -2.010996 C -2.985628 1.344232 0.766662 C -1.718748 1.792441 -0.006611 H -1.955306 2.726189 -0.568660 H -0.919491 2.052708 0.730757 C -3.451154 2.494824 1.687992 H -3.693840 3.397285 1.081117 H -2.614931 2.779117 2.376345 C -4.091979 1.006912 -0.264010 H -3.738478 0.191281 -0.924359 H -4.265041 1.904613 -0.911417 O -1.262906 0.829669 -0.936098 H -0.711068 0.190204 -0.392548 O -4.632480 2.160387 2.435738 H -4.440301 1.240830 2.776264 O -5.325058 0.574389 0.337335 H -5.498674 1.251143 1.041690 C -2.653501 0.100395 1.630470 H -2.221969 -0.694683 0.988444 H -1.873635 0.352470 2.379694 O -3.801354 -0.392095 2.356536 H -4.496789 -0.501316 1.656298 Cl 4.486055 1.050222 2.039940

TS-CC (2a)	
Zero-point correction= 0.357489 (Hartree/Particle) Thermal correction to Energy= 0.391730 Thermal correction to Enthalpy= 0.392848 Thermal correction to Gibbs Free Energy= 0.286262 Sum of electronic and zero-point Energies= -1561.489513 Sum of electronic and thermal Energies= -1561.455272 Sum of electronic and thermal Enthalpies= -1561.454154 Sum of electronic and thermal Free Energies= -1561.560740	46 EpiPenta-CD SCF Done: -1561.84700199 A.U. O -0.433365 0.276983 0.811055 C -1.868524 0.328209 0.720879 H -2.186408 -0.729409 0.787502 C -2.472488 1.128020 1.877860 H -3.576444 1.128444 1.780684 H -2.092060 2.168896 1.852412 C -2.299595 0.936949 -0.606996 H -1.927271 0.494288 -1.538725 H -2.848327 1.881311 -0.666110 I -4.683639 -0.304272 -0.927934 O -0.606747 2.115636 -0.475345 C 0.170160 1.365098 0.209243 N 1.464727 1.444156 0.440255 C 2.290818 2.425072 -0.114432 C 3.608303 2.513740 0.421438 C 1.947732 3.316330 -1.172188 C 4.537057 3.435796 -0.078865 H 3.866553 1.834123 1.249157

	C 2.890021 4.232418 -1.666549 H 0.933145 3.278556 -1.590452 C 4.189510 4.304573 -1.131516 H 5.547799 3.477455 0.361241 H 2.598131 4.907226 -2.489523 H 4.919687 5.029702 -1.526381 H 2.265837 0.241615 1.326733 C 2.973610 -2.234577 0.040393 C 3.658655 -1.017085 0.724773 H 4.623683 -1.375962 1.162281 H 3.932973 -0.280650 -0.076003 C 3.976325 -2.883974 -0.941246 H 4.882970 -3.221044 -0.388291 H 4.315102 -2.117319 -1.684344 C 2.561558 -3.253030 1.129671 H 1.877973 -2.752224 1.845403 H 3.472314 -3.558997 1.706286 O 2.907671 -0.428710 1.752145 O 3.441757 -4.037873 -1.610267 H 2.549916 -3.720702 -1.929952 O 1.883763 -4.406348 0.600711 H 2.476878 -4.707518 -0.135325 C 1.720782 -1.756784 -0.732162 H 1.008631 -1.277473 -0.027645 H 2.010925 -0.987986 -1.481156 O 1.068767 -2.823172 -1.462015 H 0.884128 -3.502095 -0.763627 Cl -2.056157 0.422965 3.488967

S10. Supporting references

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