Developing Non-Radioactive, Radical Methods to Screen for Radiolytic Stability

Supplemental Information

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Experimental Methods

General. Butyryl chloride (Thermo Scientific), bis(2-ethylhexyl)amine (Thermo Scientific), isobutyryl chloride (Alfa Aesar), *N,N*-diisopropylethylamine (Chem-Impex International), *tert*-butylhydrazone hydrochloride (TCI America), and bibenzyl (TCI America) were of reagent quality and used as received. GC-MS grade toluene, acetone, and diethyl ether solvents were purchased from Fisher Chemical. Silica gel 40 – 63 μm (230 – 400 mesh) was purchased from Silicycle and used as received.

Instrumentation. Gamma radiolysis was performed in an MDS Nordion GammaCell 220 Excel self-contained ^{60}Co gamma irradiator at Idaho National Laboratory (INL). Initial gas chromatography-mass spectrometry (GC-MS) studies were conducted at INL on a Thermo Scientific Trace GC Ultra coupled with an ISQ series mass spectrometer. All irradiated samples were then shipped to Clemson University for in-depth analysis and further GC-MS studies using a Shimadzu GC-2010 Plus coupled with a QP2010 SE mass spectrometer.

GC-MS studies at INL and Clemson were conducted using a Resteck SH-Rxi-5MS 30 m × 0.25 mm × 0.25 μm df column with the following method parameters: injector 280 °C; split injection; oven conditions of 40 to 60 °C (5 °C/min), 60 to 260 °C (20 °C/min), and hold at 260 °C for 5 min; ion source 200 °C; and interface 250 °C. The MS program was gated to remove the very large toluene and parent monoamide peaks so that minor degradation products could be observed: 0 min to 2.8 min filament on, 2.8 to 4.5 min filament off, and 4.5 – 19 min filament on. The filament was also turned off from 13.15 – 13.45 and 12.80 – 13.10 min for DEHBA and DEH*i*BA respectively. All GC-FID was conducted on the Thermo Scientific instrument at INL using a TR-35ms 30 m × 0.32 mmID × 0.25 μm df column and the same oven conditions as described for the GC-MS analyses.

^{1}H, ^{13}C{^{1}H}, and NMR spectra were recorded using a Bruker Avance Neo 300 MHz or 500 MHz spectrometer. Chemical shifts δ (in ppm) for ^{1}H and ^{13}C NMR are referenced to tetramethylsilane relative to solvent as an internal standard. Coupling constants (*J*) are expressed in Hertz (Hz). Elemental analyses were performed at Atlantic Microlab, Inc. (Norcross, GA). UV-vis studies were performed using a Thermo Scientific BioMate 160 UV-visible spectrophotometer. All syntheses and purifications were performed at ambient conditions unless otherwise specified.

Tert-*butyl hydrazone synthesis (**1**)*. **1** was synthesized by combining sodium hydroxide, *tert*-butyl hydrazine hydrochloride, acetone, water, and acetic acid as reported,[1] with the exception of scaling up the reaction using 10.22 g, 82 mmol of *tert*-butyl hydrazine hydrochloride and 2.5 equivalents of acetone (15 mL, 203 mmol) and stirring for 48 h instead of 2 h. The reaction mixture was washed with ether (3 × 80 mL) and combined. These combined ether layers were then washed with deionized water (1 × 100 mL), dried over $MgSO_4$, and filtered. The solvent was removed under vacuum to yield a clear, colorless oil. The longer reaction time and the addition of a water wash of the combined ether layers yielded **1** that was 95% pure by ^{1}H NMR measurements, preventing vacuum distillation from being needed as reported.[1] **Note: 1** decomposed ~27% in two months stored at -20 °C. Yield: 39%. ^{1}H NMR spectroscopy ($CDCl_3$, 500 MHz): δ_H 1.17 (9H, s), 1.70 (3H, s), 1.91 (3H, s), 4.19 (1H, bs). ^{13}C NMR ($CDCl_3$, 75 MHz) δ_C 15.35, 25.58, 28.71, 53.13, 144.23.

General amide synthesis. A 500 mL round-bottomed flask was charged with a stir bar and flame dried before use. After cooling, the secondary amine (26 - 250 mmol, 1 equiv) was added, followed by dichloromethane (100 mL; dried over sodium sulfate for at least 24 h). The clear,

colorless/light yellow solution was stirred in an ice bath under a nitrogen atmosphere. After cooling, *N*,*N*-diisopropylethylamine (29 – 276 mmol, 1.1 equiv) was added, and the reaction mixture was stirred cold for 10 min. The flask was then vented with needle through a rubber septum, and the appropriate acyl chloride (29 – 276 mmol, 1.1 equiv) was added dropwise to the reaction while stirring on ice over 10 min. **Note:** this reaction is exothermic and releases HCl gas, so the acyl chloride should be added slowly and carefully.

After acyl chloride addition, the vent needle was removed, and the reaction was allowed to stir for 24 – 48 h and warm slowly to room temperature. During this time, the reaction mixture varied between light to dark yellow, and in some cases, red. The reaction then was poured into a separatory funnel, the organic layer was separated, and then it was washed successively with 75 mL of the following: 1.0 M KOH, 1.0 M HCl, saturated $NaHCO_3$, and deionized water. After wash steps were complete, the organic layer was separated, dried over anhydrous magnesium sulfate, filtered, and evaporated under reduced pressure to yield the products as yellow oils. The crude monoamides were purified using flash column chromatography using 100% dichloromethane as the eluent (R_f = 0.4 DEHBA, R_f = 0.68 DEH*i*BA).

DEHBA: Yield 82%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ_H 0.85 – 0.91 (12H, m), 0.95 (3H, t, *J* = 7.4 Hz), 1.18 – 1.36 (16H, m), 1.58 (1H, m), 1.67 (2H, sext, *J* = 7.5 Hz), 2.29 (2H, t, *J* = 7.5 Hz), 3.14 (2H, d, *J* = 7.6 Hz), 3.27 (2H, m). ^{13}C NMR ($CDCl_3$, 125 MHz) δ_C 10.84, 11.05, 14.19, 14.20, 14.23, 19.19, 23.19, 23.25, 23.96, 24.05, 28.90, 28.97, 30.68, 30.75, 35.63, 37.15, 38.70, 48.85, 51.57, 173.58. Anal. Calcd for $C_{20}H_{41}NO$: C, 77.10; H, 13.27; N, 4.50. Found: C, 77.28; H, 13.32; N, 4.57.

DEH*i*BA: Yield 84%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ_H 0.85 – 0.91 (12H, m), 1.11 (6H, d, *J* = 6.5 Hz), 1.18 – 1.34 (16H, m), 1.55 (1H, sept, *J* = 6.0 Hz), 1.68 (1H, sept, *J* = 6.0 Hz), 2.80 (1H, sept, *J* = 6.5 Hz), 3.16 (2H, d, *J* = 6.5 Hz), 3.25 (m, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ_C 10.84, 11.06, 14.19, 14.22, 19.78, 23.19, 23.24, 23.90, 24.03, 28.90, 28.96, 30.42, 30.64, 30.72, 37.26, 39.13, 49.19, 51.55, 177.87. Anal. Calcd for $C_{20}H_{41}NO$: C, 77.10; H, 13.27; N, 4.50. Found: C, 77.14; H, 13.27; N, 4.60.

*2-(*tert-*Butylazo)-2-hydroperoxypropane (azoperoxide) synthesis (**2**).* A 25 mL graduated cylinder was charged with **1** (615 mg, 4.796 mmol) dissolved in toluene (10 mL) and capped with a septum secured with parafilm to prevent evaporation and monitor gas bubbling. A long needle was attached to tubing connected to an oxygen tank. This long needle was then put through the septum (two exit needles were also inserted into the septum to allow for gas to escape; see picture) and the oxygen tank was turned on to vigorously bubble oxygen into the solution for 1-2 h. Azoperoxide formation of was followed via UV-Vis spectroscopy. To measure azoperoxide concentration, an aliquot of the solution in the graduated cylinder (0.1 mL) was added to 1.9 mL toluene (2 mL total volume) and placed in a 3 mL quartz cuvette with a path length of 1 cm. Note: toluene evaporated during oxygen bubbling, so prior to removing an aliquot of the reaction mixture, toluene was added to the reaction mixture to ensure that it remained at its starting volume of 10 mL.

Picture of experimental setup for azoperoxide synthesis.

The UV-Vis absorbance was measured at 368 nm, the absorbance maximum for **2**. Aliquots were checked in this manner starting after 1 h of oxygen bubbling, and oxygen bubbling was discontinued when the

absorbance at 382 nm leveled off, indicating maximum azoperoxide formation. The last absorbance measurement of azoperoxide **2** was used to calculate final azoperoxide concentration using a reported extinction coefficient of 17 $M^{-1}cm^{-1}$ in benzene,[1] correcting for the dilution when preparing the UV-Vis sample. Azoperoxide generation using this method was successful in benzene and toluene but not in *n*-dodecane, acetonitrile, or dioxane.

Gamma radiolysis of monoamides. A stock solution of each monoamide (100 mM) was prepared in toluene and partitioned in 5.0 mL aliquots into 20 mL screw-cap scintillation vials. Irradiation was performed using a cobalt-60 irradiator at the Idaho National Laboratory. Samples were irradiated to approximately 50, 250, 500, 650, and 1000 kGy at a dose rate of 2-3 $kGy \cdot h^{-1}$, measured using Fricke dosimetry and correcting for cobalt-60 decay.[2] The absorbed doses were also corrected by multiplying by toluene density (0.87 g/mL).[2] All irradiations were performed in triplicate, except for ~50 and ~500 kGy which were performed in duplicate.

Azoperoxide assay. A 1.0 M monoamide stock solution was prepared volumetrically by weighing 1.56 g (5.0 mmol) of the corresponding monoamide into a 5.00 mL volumetric flask and filling to the line with toluene. In a 20 mL scintillation vial, varying volumes of a freshly synthesized ~480 mM azoperoxide stock solution in toluene (yielding 20, 40, 80, 120, 250, or 400 mM final concentrations) were added to a toluene solution containing 0.2 mL of the 1.0 M monoamide stock solution. Additional toluene was then added to the monoamide/azoperoxide solution to reach a total volume of 2.0 mL for each sample (100 mM final amide concentration). Azoperoxide-only (20, 40, 80, 120, 250, or 400 mM), amide-only (100 mM), and toluene-only samples were also prepared as controls. Samples were capped and heated at 75 °C for 2 h in a water bath to generate the radical species. All assays were performed in triplicate.

GC-MS/GC-FID analysis. To analyze the GC-MS and GC-FID data, all the peaks in each TIC were integrated using the automatic integration function in the analysis software, Shimadzu LabSolutions version 4.54. The automatic integration was checked, and smaller intensity peaks were manually integrated, if necessary. Degradation products were identified as any peak not observed in the control TICs, and mass spectra were collected for all degradation products. The chemical identities of the degradation products were determined from their parent *m*/*z* peaks in the mass spectra, without distinguishing between isomers of the same mass. The percentage of each product was determined by dividing its TIC peak area by the total of the peak areas in the TIC. Several parent peaks that eluted close together had the same *m*/*z* values, so these were identified as isomers, based on the small energy differences for isomers found in DFT calculations, and their peak areas were combined. Generally, the vast majority of peaks that were identified as isomers with the same parent *m/z* values eluted within 1 – 2 minutes from one another. In a very few cases, there were degradation product isomers identified with larger differences between the retention times (retention times are provided in Table S1). All identified degradation products were with ±1 *m/z* of theoretical values, consistent with instrument error. In the few cases where parent *m*/*z* peaks were within ±1 *m/z* of each other for two (or more) TIC peaks, they were treated as the same degradation product. All radiolytic and radical assay degradation products with normalized peak area percentages ≥ 1% are listed in Table S1.

The radiolytic and radical assay samples were analyzed in triplicate by comparing the TICs for each set of conditions. To obtain the percent relative standard deviation for all TICs of each dose, TIC intensities were averaged at each retention time for the triplicate measurements, and standard deviations were calculated for each point. These standard deviations were used to calculate a relative standard deviation for each set of triplicate TICs, ranging from 2.5 ± 2.7% to

4.6 ± 3.3% for the radical assay and from 3.4 ± 3.0% to 5.0 ± 7.0% for gamma radiolysis across the entire TIC (Table S2).

Radical and gamma radiolytic correlation using bibenzyl. In both the radiolysis and the radical assay samples, bibenzyl was formed from the coupling of two tolyl radicals (retention time ~10.6 min), and its formation was linear with respect to dose. Therefore, bibenzyl formation was used as an internal standard to correlate these two methods. A GC-MS calibration curve was determined using commercial bibenzyl (0.1 to 3 mM), and then radiolysis and radical assay samples for the middle and high doses were diluted so that the bibenzyl concentration was in the middle of the linear region of the calibration curve (~0.5 mM; the lowest-dose radiation and azoperoxide samples did not require dilution). The TIC bibenzyl peak in each sample was integrated, and the exact bibenzyl concentration was calculated from the calibration curve. Graphs of bibenzyl concentration vs. radiation dose or vs. azoperoxide concentration were used to correlate radiation dose with azoperoxide concentration (Figure 5).

Density functional theory (DFT) calculations. Quantum chemical calculations were performed using the Gaussian 16 software package.[3] Geometry optimization calculations were performed using the B3LYP theory with a 6-311g+(d,p) basis set specified in Cartesian format. The initial geometry was drawn using Avogadro software (version 1.2.0).[4] Conformer searches were conducted in Avogadro, employing random and weighted rotor searches with 1000 conformers. The weighted rotor search provided generally lower energy values compared to the random rotor search. A systematic rotor search was not used because it required 10-24 h to complete for each molecule, compared to 5 to 10 min for other methods, and the energy differences from the resulting calculations were negligible.

MMFF94 force fields are used to predict molecular conformations and energy minima but lack specific parameterization for radicals, since they are not closed-shell molecules.[5,6] To avoid this issue, radical energies were determined using a single-point energy calculation from the initial monoamide geometry, systematically removing one hydrogen atom at a time from different sites without adjusting atomic positions. This mimics hydrogen abstraction by a radical species, a major pathway for monoamide decomposition.[7] The energy difference between each radical and the ground state was calculated to determine the relative energies of radical formation.

For DEHBA and DEH*i*BA, radical species near the amide functional group have lower energies than radical species farther from the functional group (Tables S3-S4). The *C*-terminal and *N*-terminal radicals closest to the amide in DEHBA and DEH*i*BA have very little difference in energy (less than 5 kJ/mol). For DEHBA, the lowest-energy radicals are the *cis* radical of the *N*-terminal C2 carbon (see atom numbering scheme in Figure S26) and the *cis* radical of the *N*-terminal C1 carbon. For DEH*i*BA, the lowest energy radicals are the *cis* radical of the *N*-terminal C1 carbon and the *trans* radical of the *N*-terminal C2 carbon. Most of the *N*-terminal radicals have lower formation energies (radical - ground state energies) for DEHBA than DEH*i*BA, whereas *C*-terminal radicals have lower formation energies for DEH*i*BA compared to DEHBA. The energy differences between most DEHBA and DEH*i*BA radicals are less than 8 kJ/mol, differences that are low enough that radicals may form at multiple locations during radiolytic or radical treatment. This result is consistent with the formation of multiple isomers of monoamide degradation products, suggesting that after irradiation or azoperoxide treatment, degradation products with the same *m*/*z* values by GC/MS that elute close together in the TICs are isomers of the same products.

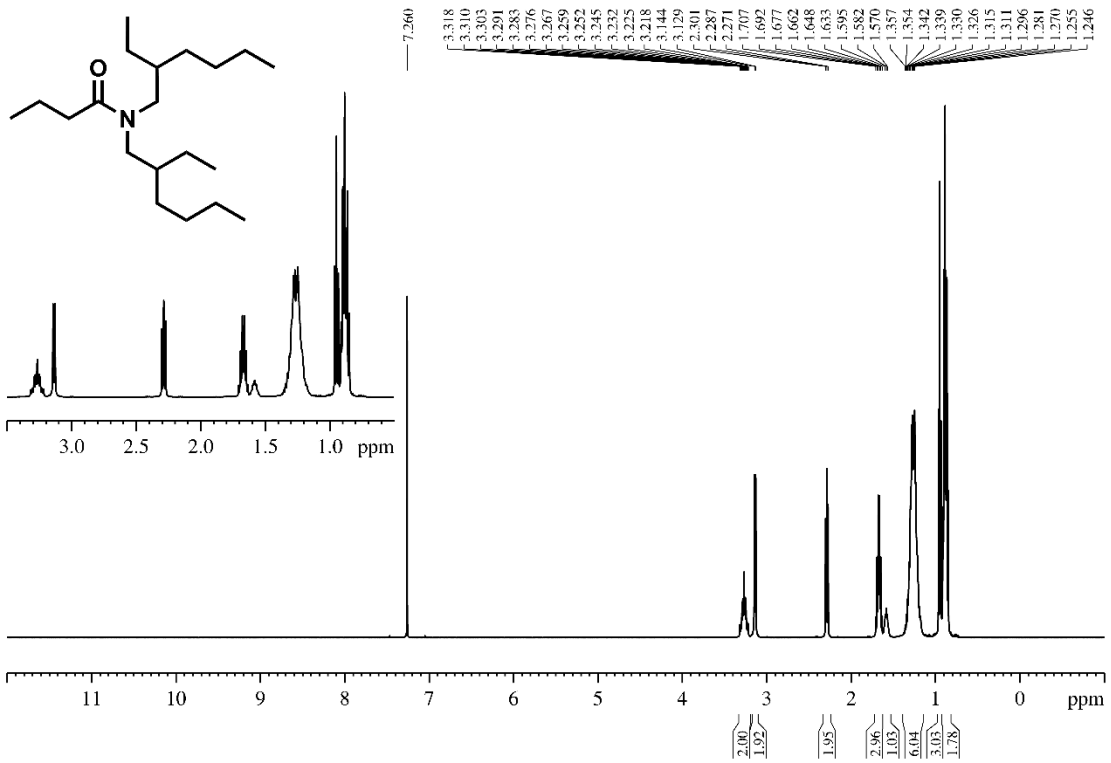


Figure S1. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of DEHBA.

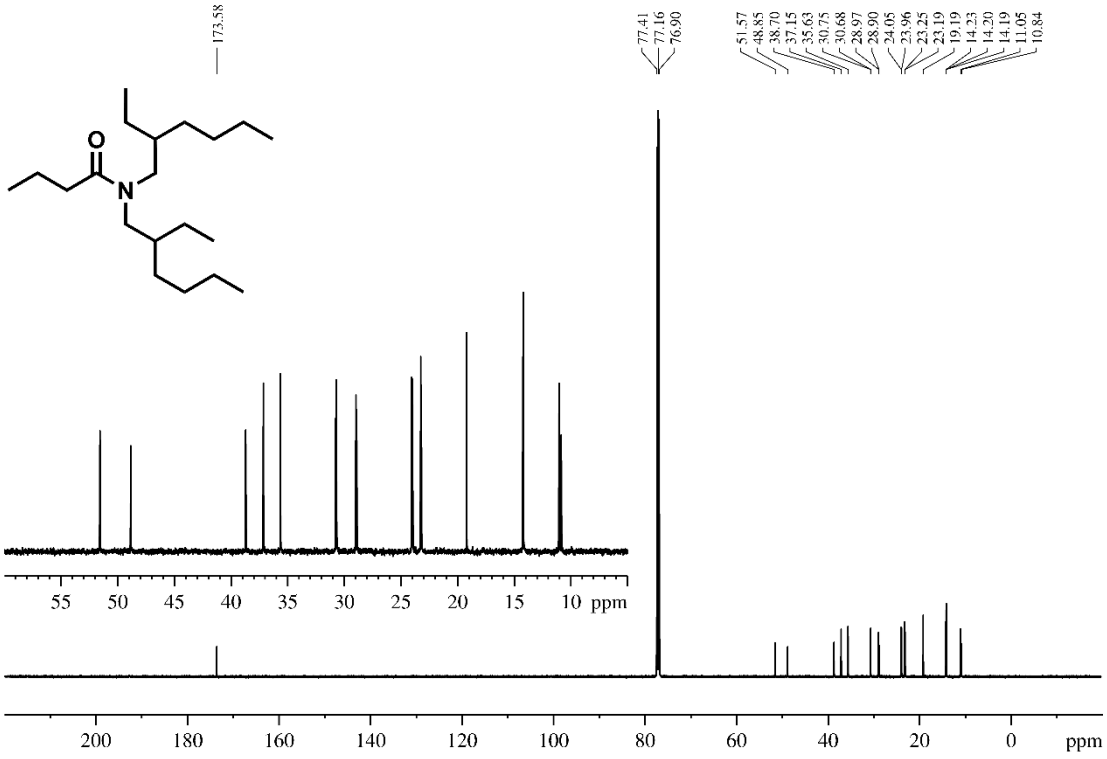


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125 MHz) of DEHBA.

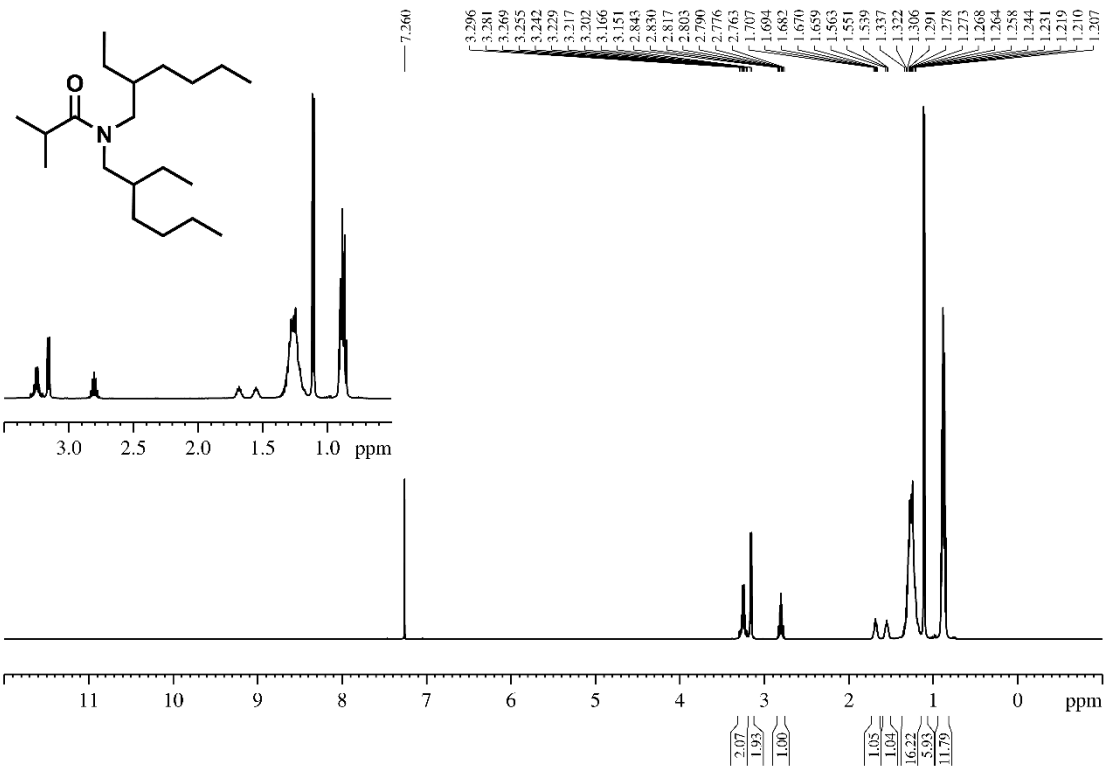


Figure S3. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of DEH*i*BA.

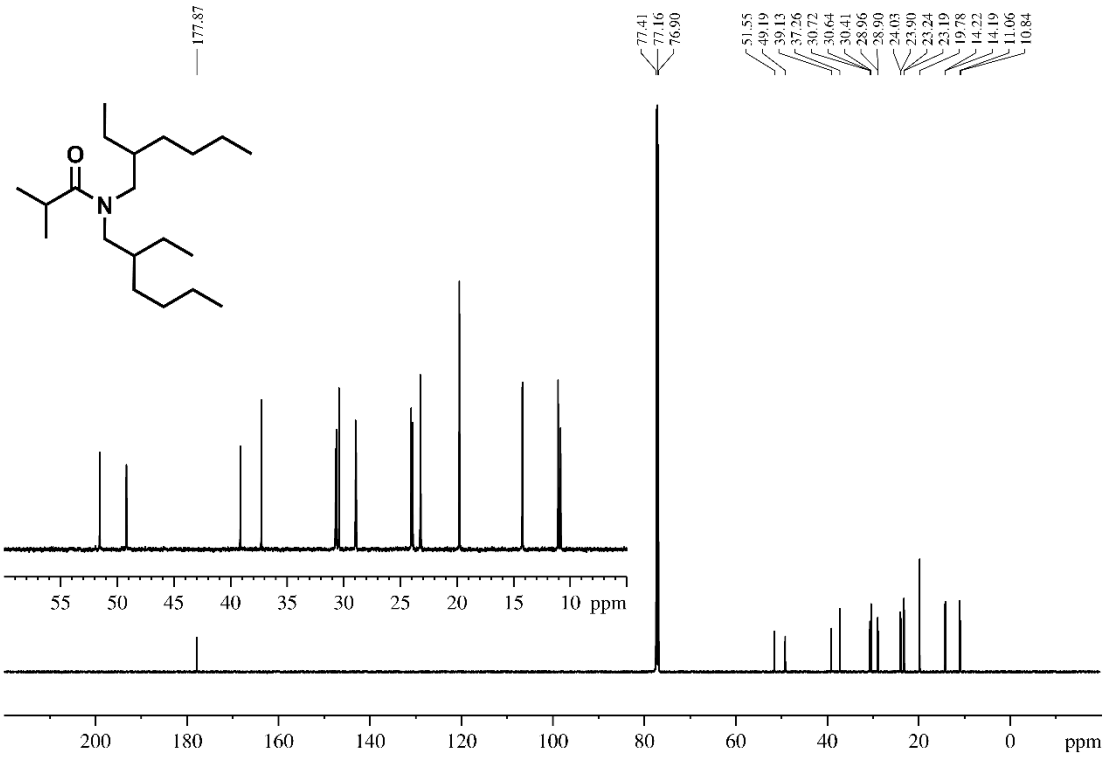


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125 MHz) of DEH*i*BA.

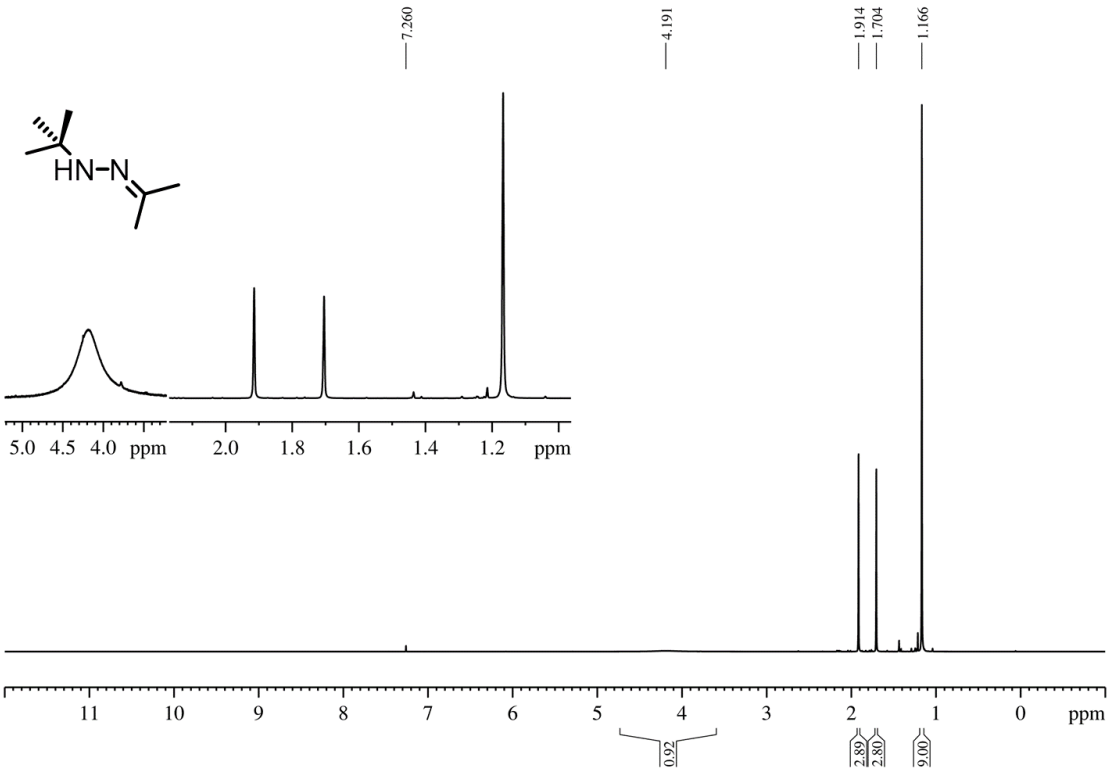


Figure S5. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of *tert*-butyl hydrazone (**1**).

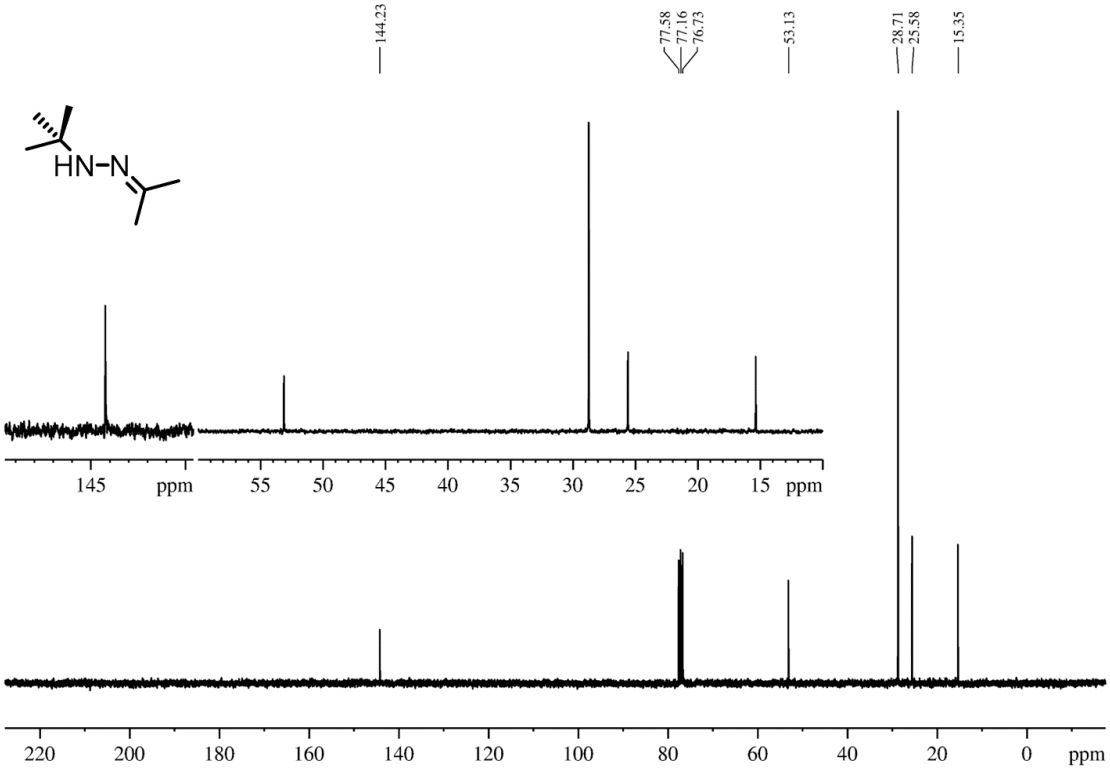


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 75 MHz) of *tert*-butyl hydrazone (**1**).

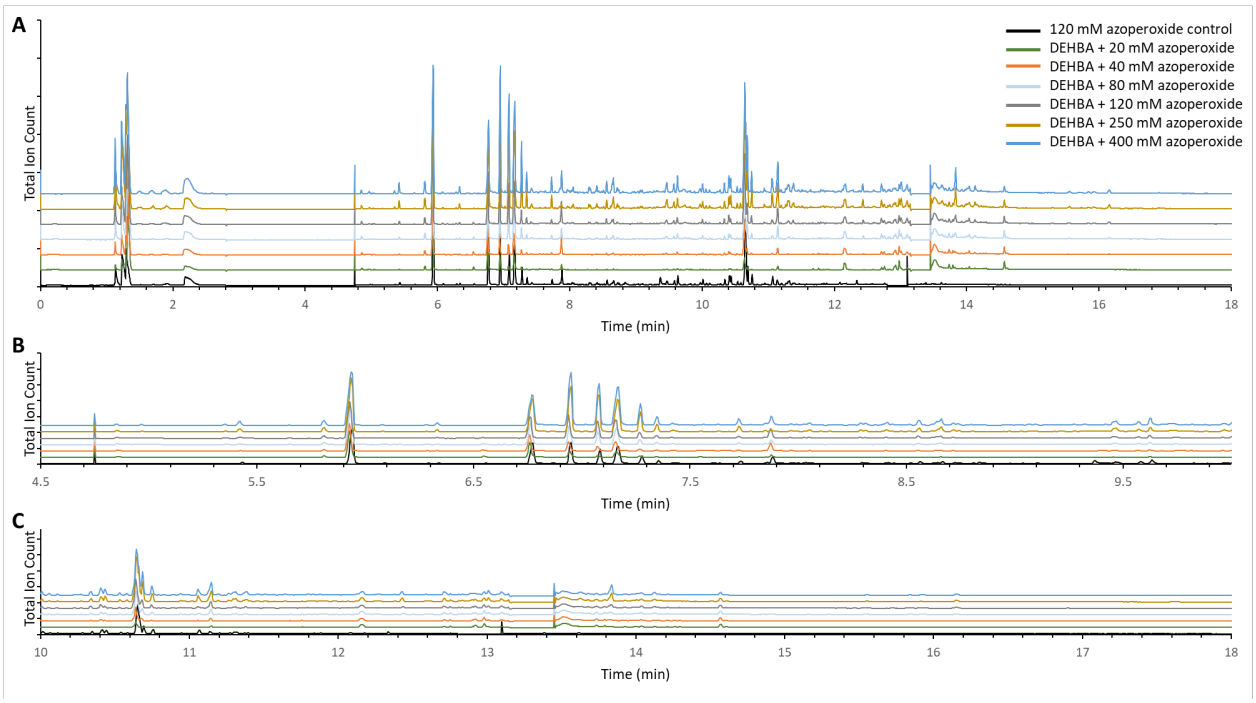


Figure S7. A) Full TICs for DEHBA treated with azoperoxide at the indicated concentrations and B and C) insets of the TICs in A.

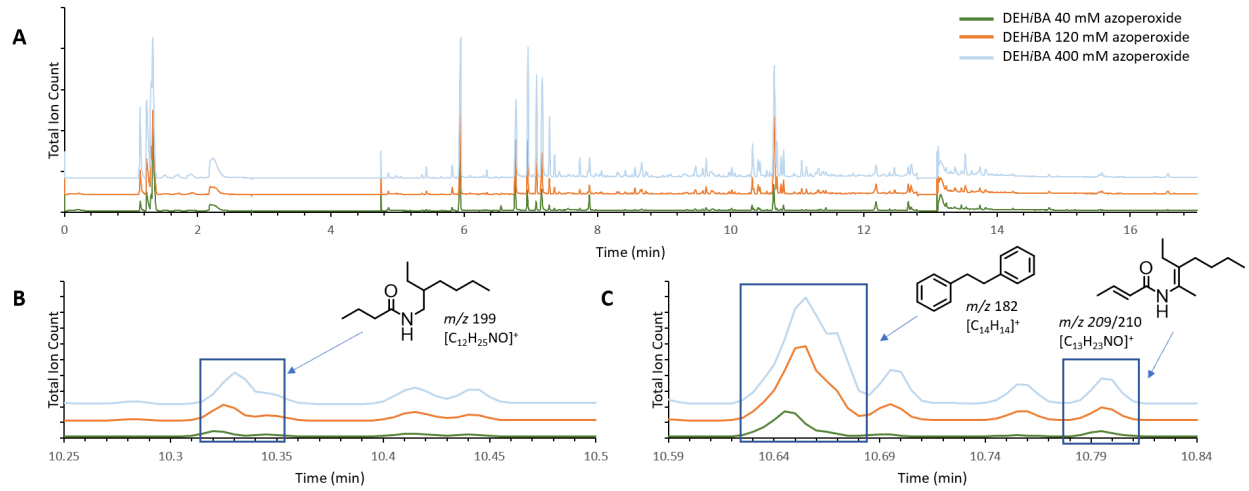


Figure S8. A) Full TICs for DEH*i*BA treated with azoperoxide at the indicated concentrations and B and C) insets of the TICs in A.

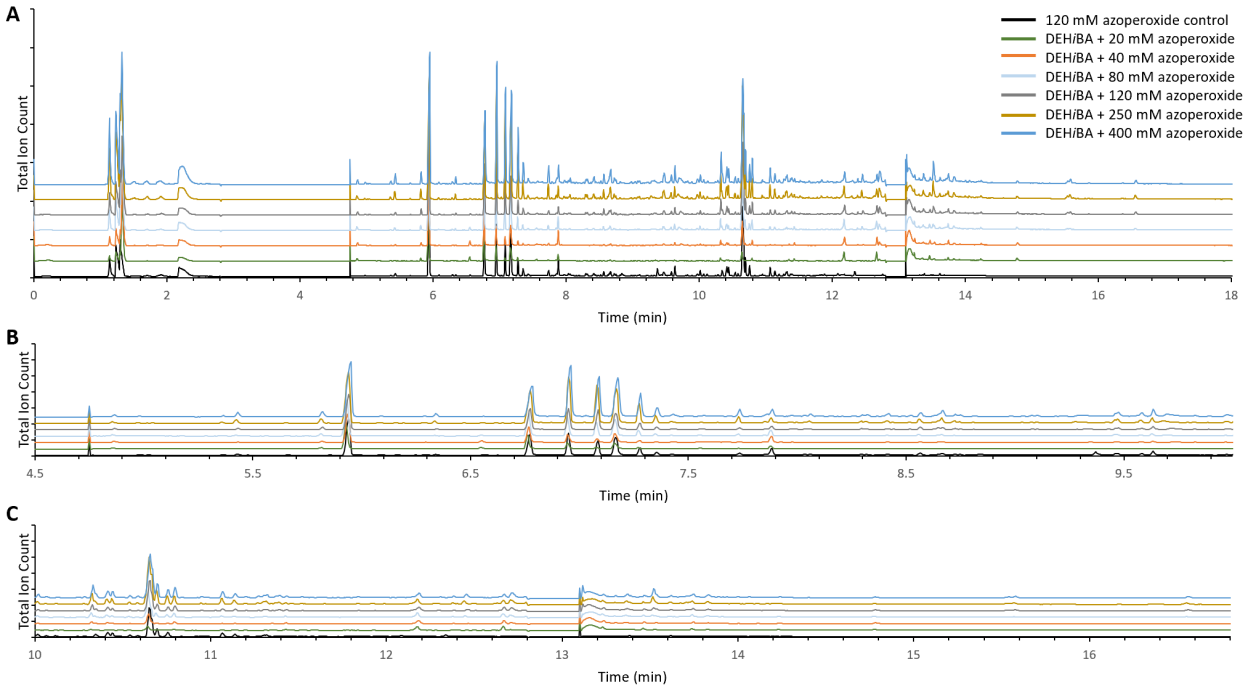


Figure S9. A) Full TICs for DEH*i*BA treated with azoperoxide at the indicated concentrations and B and C) insets of the TICs in A.

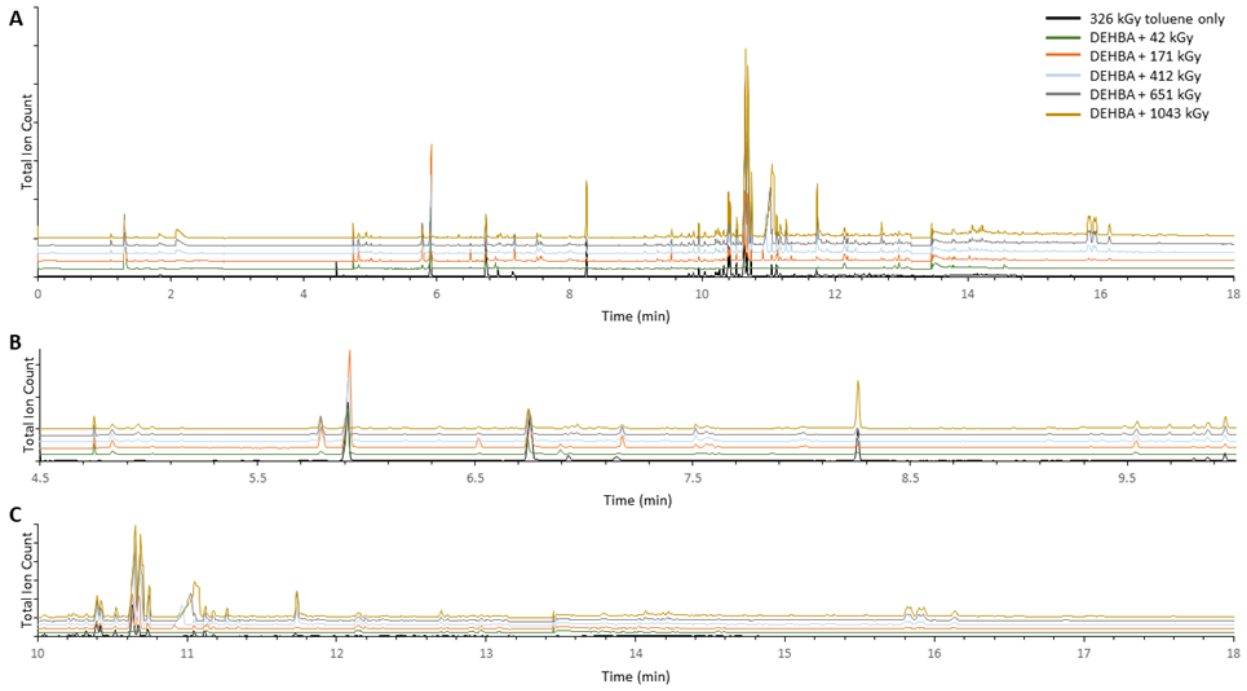


Figure S10. A) Full TICs for DEHBA irradiated at the indicated doses and B and C) insets of the TICs in A.

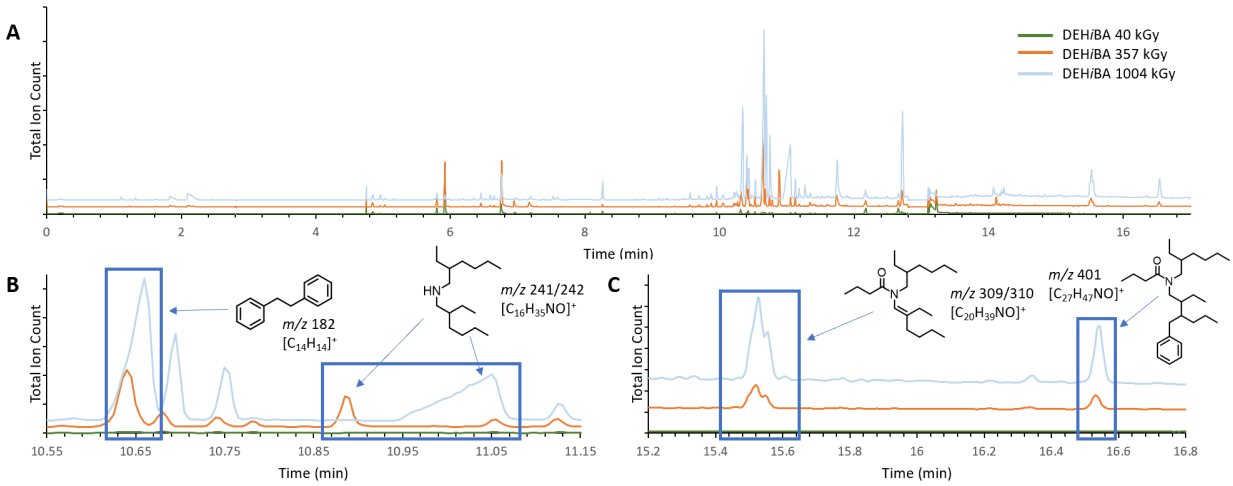


Figure S11. A) Full TICs for DEH*i*BA irradiated at the indicated doses and B and C) insets of the TICs in A.

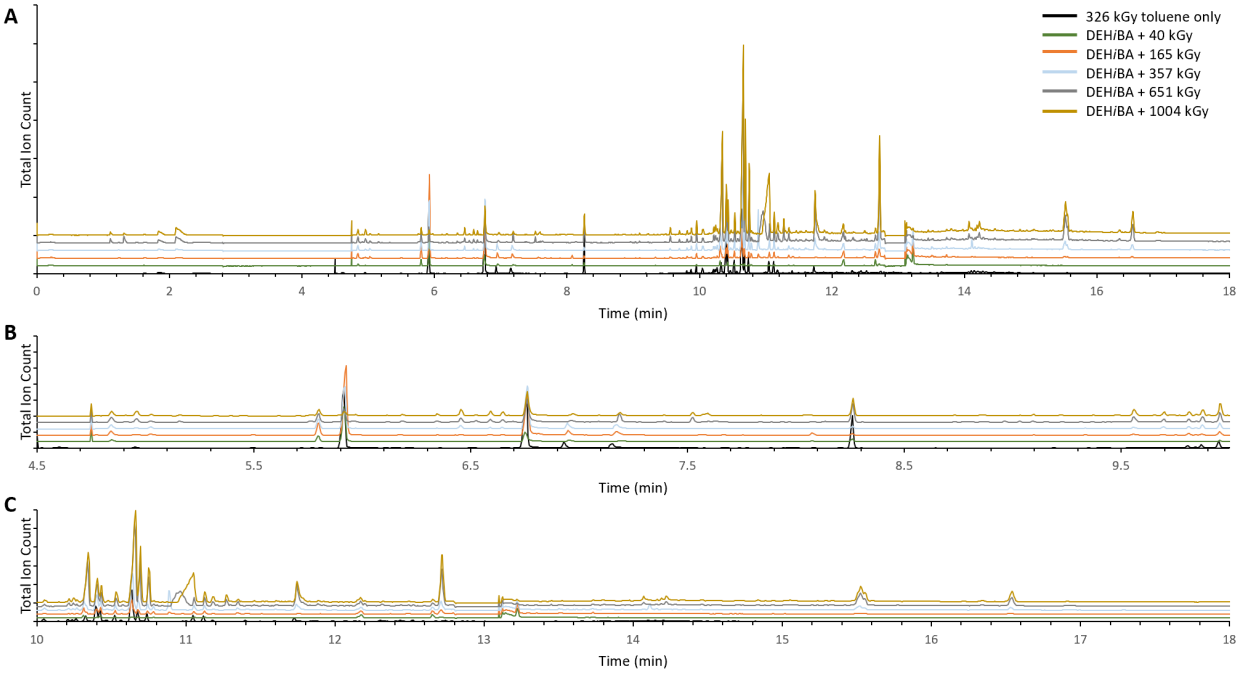


Figure S12. A) Full TICs for DEH*i*BA irradiated at the indicated doses and B and C) insets of the TICs in A.

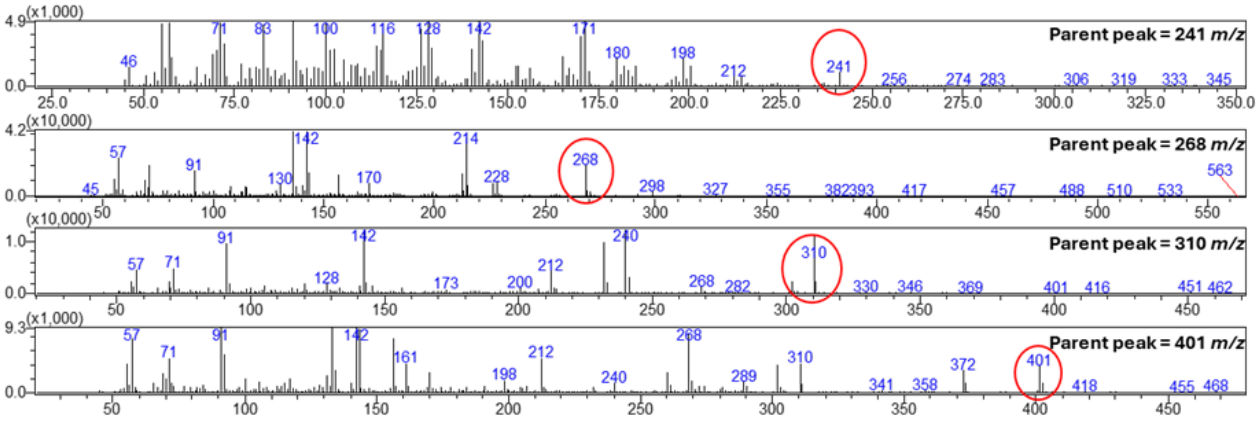


Figure S13. Selected mass spectra for DEHBA and DEH*i*BA degradation products formed in the radical assay. Similar mass spectra were observed for DEHBA and DEH*i*BA degradation products formed during gamma radiolysis.

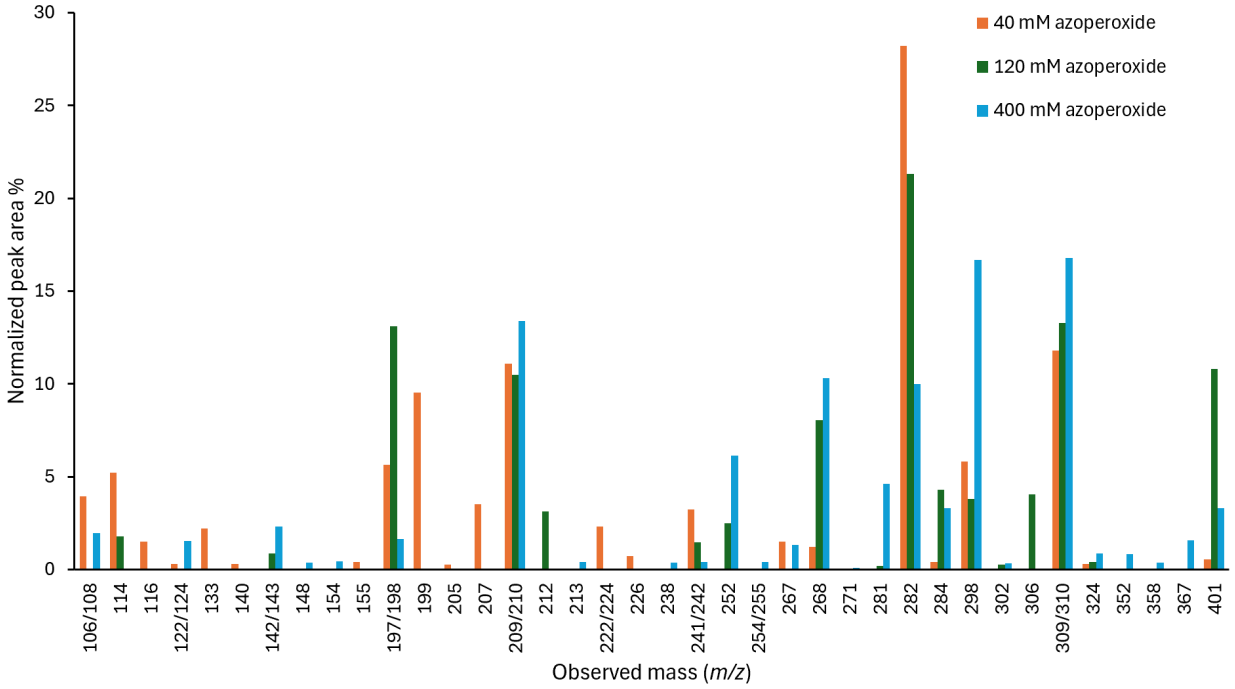


Figure S14. Normalized peak area percentages for all DEHBA degradation products upon treatment with 40 (orange), 120 (green), or 400 mM (blue) azoperoxide.

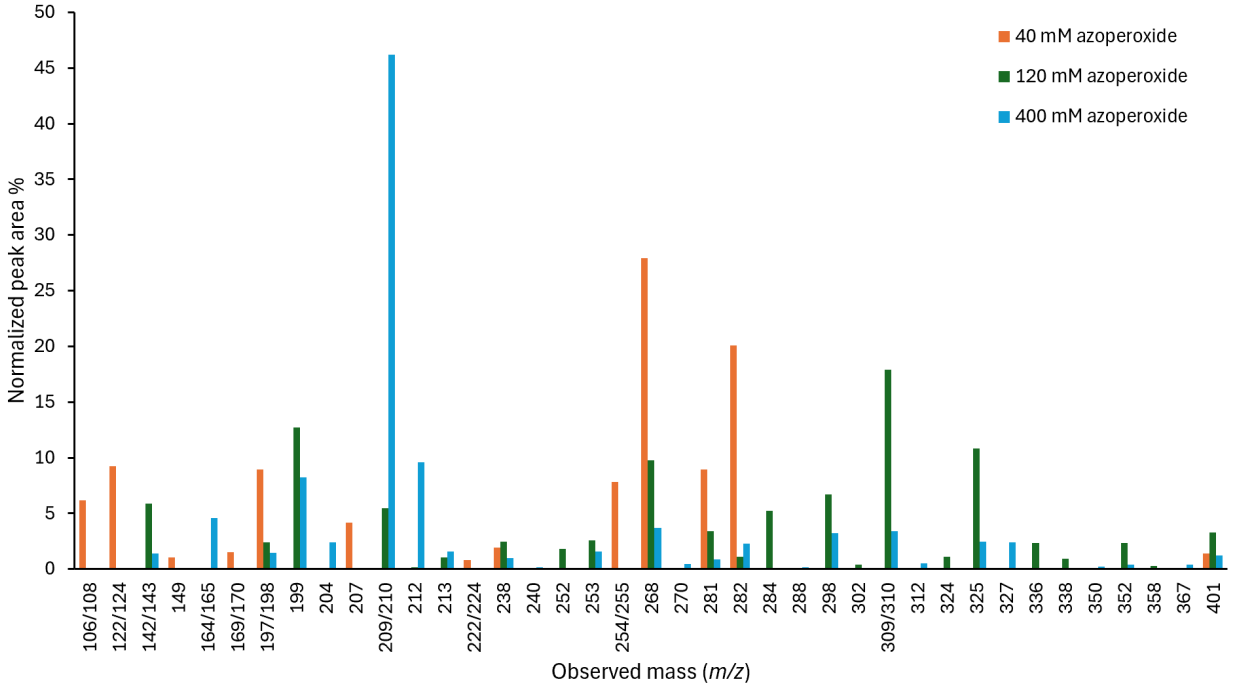


Figure S15. Normalized peak area percentages for all DEH*i*BA degradation products upon treatment with 40 (orange), 120 mM (green), or 400 mM (blue) azoperoxide.

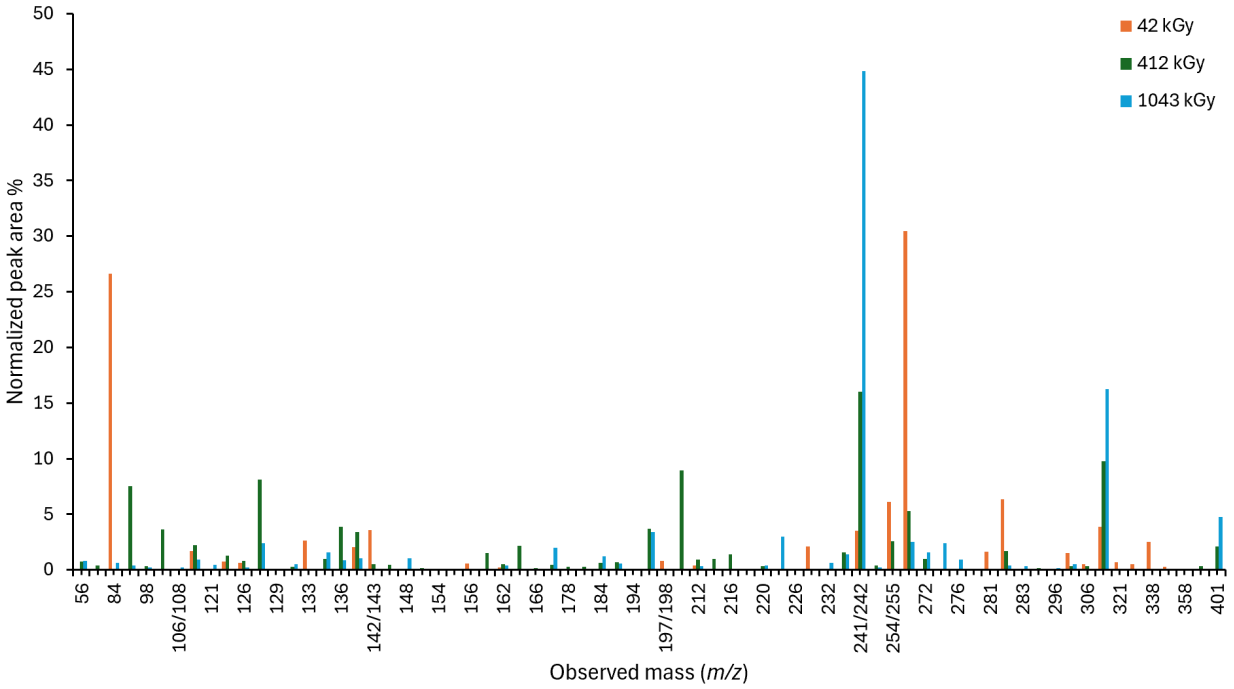


Figure S16. Normalized peak area percentages for all DEHBA degradation products upon treatment with 42 (orange), 412 (green), or 1043 kGy (blue) gamma radiation.

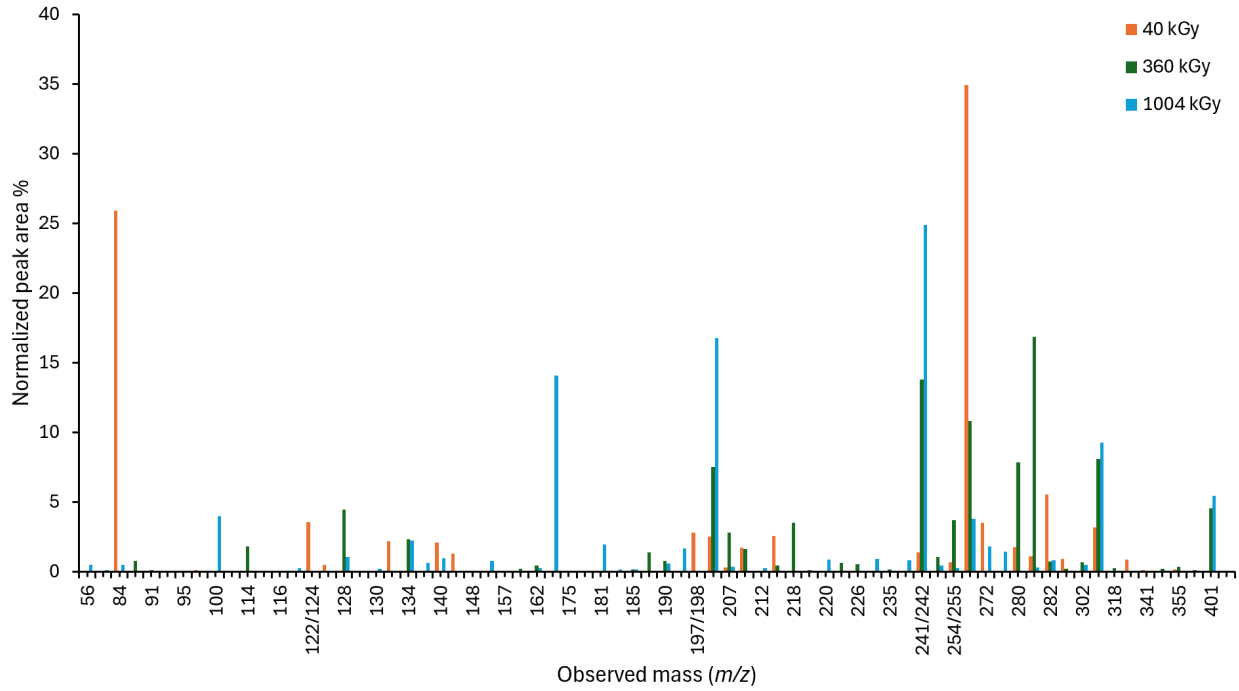


Figure S17. Normalized peak area percentages for all DEH*i*BA degradation products upon treatment with 40 (orange), 360 (green), or 1004 kGy (blue) gamma radiation.

Context for radiolytic and radical assay comparisons. The goal of this work is not to obtain exact correlations between gamma radiolytic and non-radiolytically generated radical degradation. Gamma radiolysis is *the* gold standard, but gamma irradiators are expensive, difficult to maintain (by replacing their radioactive sources), and are increasingly only available in national laboratories due to security concerns about radiological terrorism. A synthetic laboratory can produce dozens of compounds to be tested for various applications (antioxidants for astronaut food, radical scavengers to lengthen the lifetime of electronics components in spacecraft, radioprotectants to modulate side effects from Gamma Knife® cancer treatments, etc.), but testing dozens of compounds via gamma radiolysis would be slow and expensive. Therefore, there is a great need for a rapid, inexpensive protocol that can qualitatively or semi-quantitatively predict gamma irradiation results for use as a prescreen to narrow the pipeline.

Additionally, as we demonstrated using the bibenzyl internal standard, the damage that is done during the radical assay at its highest does is not as high as was achieved using gamma radiolysis. For example, in Figure 3C, 120 mM azoperoxide correlates to ~2.8 mM bibenzyl formation and 412 kGy correlates to ~5.2 mM bibenzyl formation. The graphs in Figure 3 and S18 show results for only the most formed monoamide degradation products; the following Table S1 contains additional information for all 58 compounds.

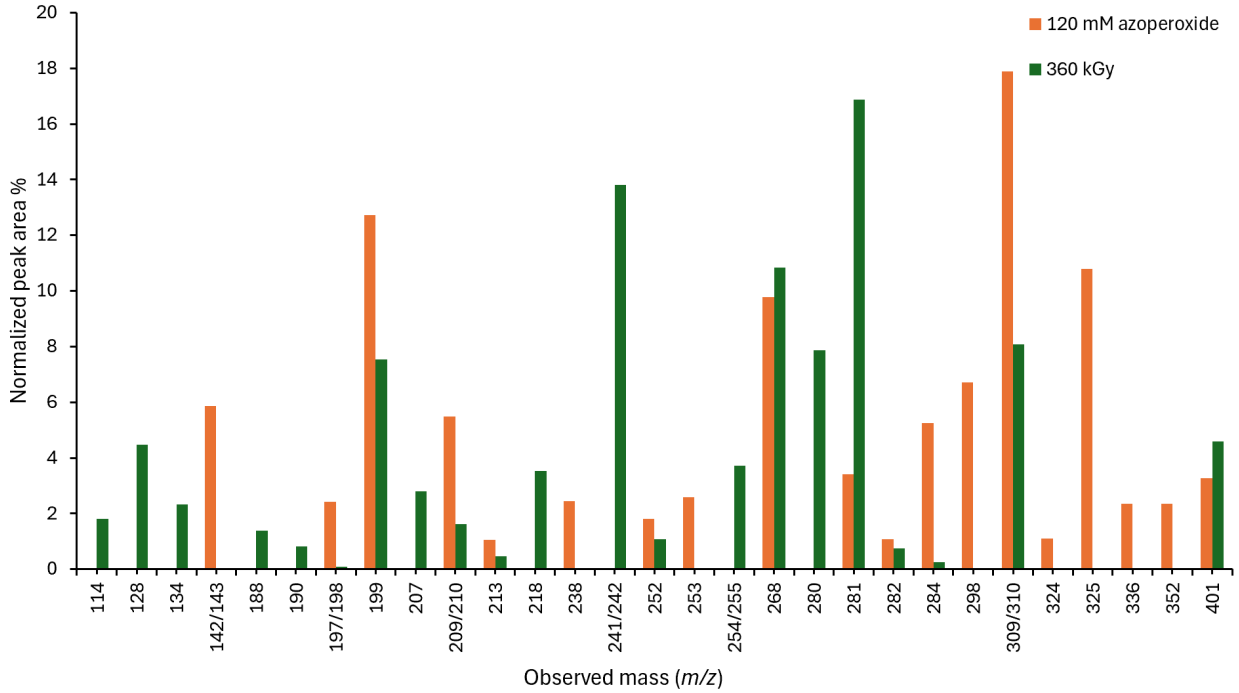
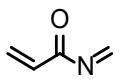
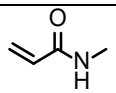
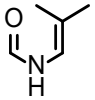
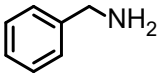
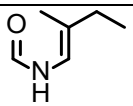
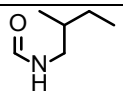
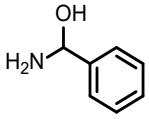
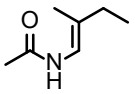
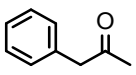
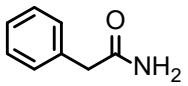
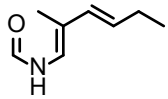
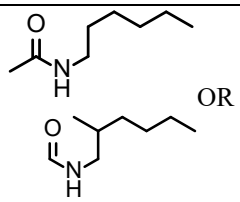
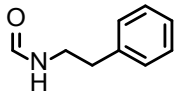
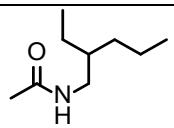
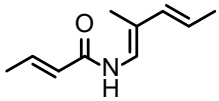
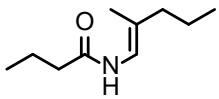
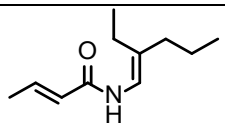
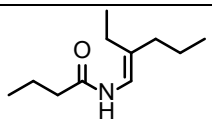
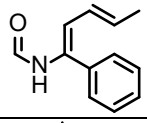
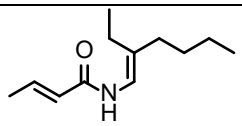
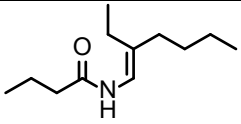
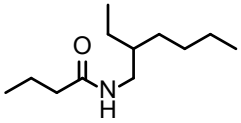
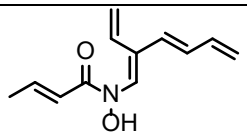
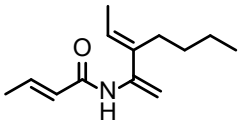
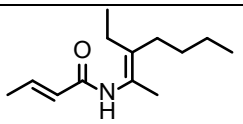
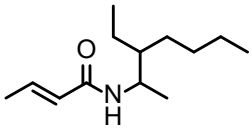
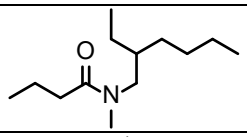
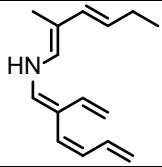
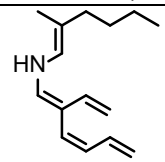
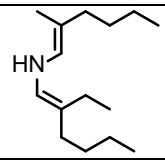


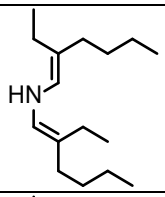
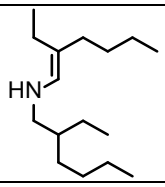
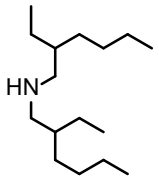
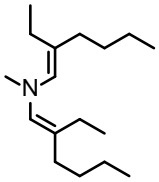
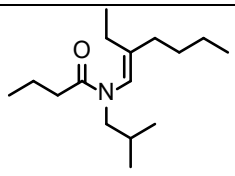
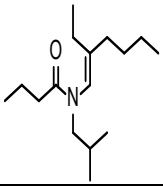
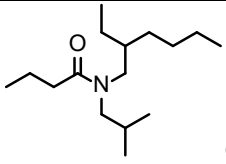
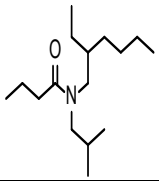
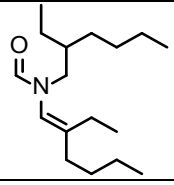
Figure S18. Graph comparing DEH*i*BA degradation products formed from treatment with 120 mM azoperoxide (orange) or 360 kGy gamma radiolysis (green) that have ≥ 1% normalized peak area percentages in either method.

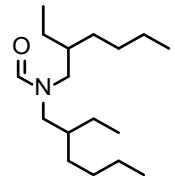
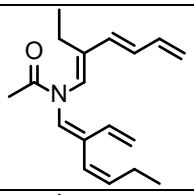
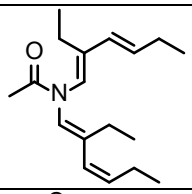
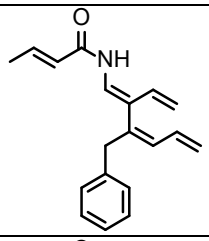
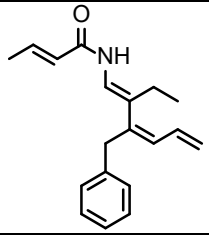
Table S1. Percentages of DEHBA and DEH*i*BA degradation products with ≥ 1% normalized peak areas formed during gamma radiolysis or azoperoxide treatment at low (L), medium (M), and high (H) doses with corresponding possible structure (NA = not observed). *Reported degradation product for both DEHBA and DEH*i*BA.[8-10] #Reported degradation product for DEH*i*BA only.[8] ##Reported as an unidentified degradation product for DEH*i*BA.[8] ‡Reported as unidentified degradation product for DEHBA.[10] Reported DEH*i*BA degradation products were formed under the following indicated conditions: c = contacted; o = organic only; b = both (for DEHBA, the reported degradation products were only done under contacted conditions)[8-10]; a = % product was determined by adding peaks with *m/z* values within ± 1 mass unit.

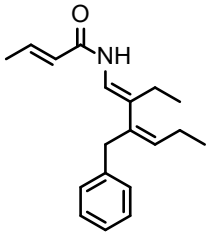
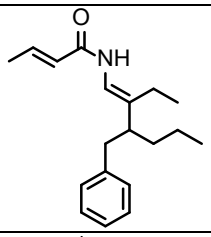
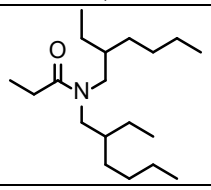
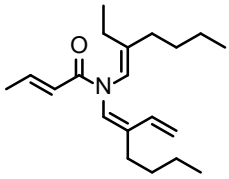
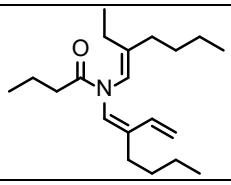
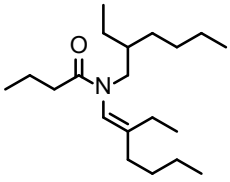
Entry #	Observed *m/z* value and empirical formula	Possible degradation product	% Product observed for DEHBA (radical assay/ radiolysis)	% Product observed for DEH*i*BA (radical assay/ radiolysis)	Retention times for DEHBA (radical assay/ radiolysis)	Retention times for DEH*i*BA (radical assay/ radiolysis)
1	84 $[C_4H_5NO]^+$		L: 0/26.6 M: 0/0 H: 0/0.649	L: 0/25.9 M: 0/0 H: 0/0.488	L: NA/1.316 M: NA H: NA/1.309	L: NA/1.315 M: NA H: NA/1.313, 1.494
2	86 $[C_4H_7NO]^+$		L: 0/0 M: 0/7.55 H: 0/0.374	L: 0/0 M: 0/0 H: 0/0	L: NA M: NA/1.307 H: NA/1.476	NA
3	100 $[C_5H_9NO]^+$		L: 0/0 M: 0/3.67 H: 0/0	L: 0/0 M: 0/0 H: 0/4.02	L: NA M: NA/2.094 H: NA	L: NA M: NA H: NA/2.101
4	106/108 $[C_7H_9N]^+$		L: 3.94/ 0 M: 0/0 H: 1.98/0.221	L: 6.20/0 M: 0/0 H: 0/0	L: 6.820/NA M: NA/NA H: 4.515/5.960	L: 6.827/NA M: NA H: NA
5	114 $[C_6H_{11}NO]^+$		L: 5.21/ 1.70 M: 1.79/2.21 H: 0/0.925	L: 0/0 M: 0/1.81 H: 0/0	L: 4.865/4.858 M: 4.854/4.831 H: NA/4.834	L: NA M: NA/4.842 H: NA
6	116 $[C_6H_{13}NO]^+$		L: 1.51/0 M: 0/0 H: 0/0	L: 0/0 M: 0/0.076 H: 0/0	L: 7.558/NA M: NA H: NA	L: NA M: NA/7.583 H: NA
7	122/124 $[C_7H_9NO]^+$		L: 0.316/0 M: 0/1.29 H: 1.53/0	L: 9.25/3.58 M: 0/0 H: 0/0.04	L: 8.084/7.959 M: NA/8.024, 8.073 H: 9.704/NA	L: 9.737/7.868, 7.954 M: NA H: NA/8.044
8	128 $[C_7H_{15}NO]^+$		L: 0/0 M: 0/8.12 H: 0/2.38	L: 0/0 M: 0/4.47 H: 0/1.09	L: NA M: NA/5.316, 5.752, 5.794, 5.862, 5.95, 6.338 H: NA/5.751, 5.791, 6.016, 6.337	L: NA M: NA/5.798, 9.556 H: NA/5.755, 5.799
9	133	Unidentified	L: 2.22/2.64 M: 0/0 H: 0/0	L: 0/2.20 M: 0/0 H: 0/0	L: 8.571/6.910 M: NA H: NA	L: NA/6.907 M: NA H: NA
10	134 $[C_9H_{10}O]^+$		L: 0/0 M: 0/0.980 H: 0/1.57	L: 0/0 M: 0/2.32 H: 0/2.26	L: NA M: NA/6.6, 6.896, 6.919, 6.939, 6.972, 7.07 H: NA/6.590, 6.916, 6.948,	L: NA M: NA/6.455, 6.590, 6.646 H: NA/6.456, 6.592, 6.649, 6.971

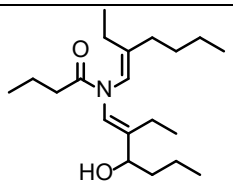
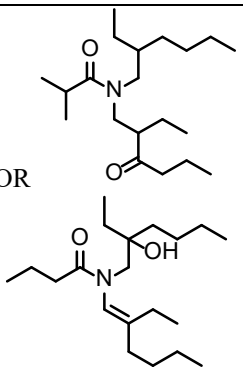
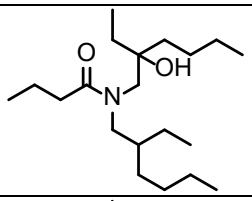
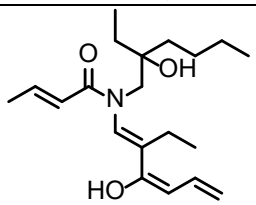
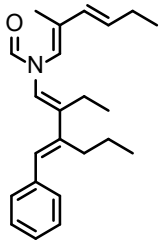
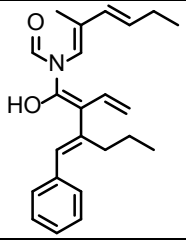
					6.971, 7.069, 8.072	
11	136 $[C_8H_9NO]^+$		L: 0/0 M: 0/3.86 H: 0/0.870	L: 0/0 M: 0/0 H: 0/0.659	L: NA M: NA/7.179 H: NA/7.178	L: NA M: NA H: NA/6.526, 7.189
12	140 $[C_8H_{13}NO]^+$		L: 0.314/2.03 M: 0/3.38 H: 0/1.06	L: 0/2.10 M: 0/0 H: 0/0.993	L: 10.579/7.534, 7.578, 7.603 M: NA/7.516, 7.566, 7.62, 8.64 H: NA/7.517, 7.591, 12.194	L: NA/7.530, 7.575, 7.600, 7.631 M: NA H: NA/7.369, 7.524, 7.594, 12.199
13	142/143[a] $[C_8H_{17}NO]^+$		L: 0/3.59 M: 0.882/0.511 H: 2.34/0	L: 0/1.30 M: 5.85/0 H: 1.41/0.038	L: NA/5.175, 7.424, 7.871 M: 6.820/5.014 H: 4.549, 4.874, 6.716/NA	L: NA/7.390, 7.421, 10.906 M: 9.720/NA H: 5.836/8.065
14	149 $[C_9H_{11}NO]^+$		L: 0/0 M: 0/0 H: 0/0	L: 1.04/0 M: 0/0 H: 0/0	NA	L: 9.586/NA M: NA H: NA
15	157 $[C_9H_{19}NO]^+$		L: 0/0 M: 0/1.52 H: 0/0	L: 0/0 M: 0/0 H: 0/0.036	L: NA M: NA/9.540 H: NA	L: NA M: NA H: NA/7.839
16	164/165[a] $[C_{10}H_{15}NO]^+$		L: 0/0 M: 0/2.14 H: 0/0	L: 0/0 M: 0/0 H: 4.58/0	L: NA M: NA/8.744, 12.192, 12.312 H: NA	L: NA M: NA H: 9.576/NA
17	169/170[a] $[C_{10}H_{19}NO]^+$		L: 0/0 M: 0/0.441 H: 0/1.98	L: 1.51/0 M: 0/0 H: 0/14.1	L: NA M: NA/9.332 H: NA/12.701	L: 10.846/NA M: NA H: NA/9.225, 12.717
18	181 $[C_{11}H_{19}NO]^+$		L: 0/0 M: 0/0 H: 0/0	L: 0/0 M: 0/0 H: 0/1.98	NA	L: NA M: NA H: NA/14.220
19	184 $[C_{11}H_{21}NO]^+$		L: 0/0 M: 0/0.615 H: 0/1.23	L: 0/0 M: 0/0 H: 0/0.180	L: NA M: NA/9.606, 12.742 H: NA/9.545	L: NA M: NA H: NA/10.780
20	188 $[C_{12}H_{13}NO]^+$		L: 0/0 M: 0/0 H: 0/0	L: 0/0 M: 0/1.38 H: 0/0	NA	L: NA M: NA/11.350 H: NA
21	196 $[C_{12}H_{21}NO]^+$		L: 0/0 M: 0/3.70 H: 0/3.40	L: 0/0 M: 0/0 H: 0/1.67	L: NA M: NA/11.176, 11.264, 11.450 H: NA/11.121	L: NA M: NA H: NA/11.208, 11.350, 11.459
22[#,b]	197/198[a] $[C_{12}H_{23}NO]^+$		L: 5.64/ 0.805 M: 13.1/8.94 H: 1.65/0	L: 8.97/2.80 M: 2.41/0.093 H: 1.43/0.044	L: 11.679, 11.759, 12.445/11.629	L: 12.471/11.339, 11.417

					M: 11.755, 12.435, 12.600/10.874, 11.731, 12.245 H: 12.290/NA	M: 12.509/11.820 H: 11.933/8.973
23*,[b]	199 $[C_{12}H_{25}NO]^+$		L: 9.53/0 M: 0/0 H: 0/0	L: 0/2.55 M: 12.7/7.55 H: 8.25/16.8	L: 10.679/NA M: NA H: NA	L: NA/10.310 M: 10.326, 12.462/10.320 H: 10.344/10.340
24	204 $[C_{12}H15NO_2]^+$		L: 0/0 M: 0/0 H: 0/0	L: 0/0 M: 0/0 H: 2.40/0	NA	L: NA M: NA H: 9.736/NA
25	207 $[C_{13}H_{21}NO]^+$		L: 3.51/0 M: 0/0 H: 0/0	L: 4.16/0.311 M: 0/2.81 H: 0/0.343	L: 8.032, 9.077, 9.142, 9.279, 10.225, 11.295, 11.644/NA M: NA H: NA	L: 5.668, 8.579, 11.815/5.175 M: NA/2.099, 7.936 H: NA/5.027, 5.159
26	209/210 $[C_{13}H_{23}NO]^+$		L: 11.1/0 M: 10.5/0 H: 13.4/0	L: 0/1.71 M: 5.49/ 1.61 H: 46.2/0	L: 11.146/NA M: 11.143/NA H: 11.165/NA	L: NA/13.403 M: 10.796/10.780 H: 10.810/NA
27	212 $[C_{13}H_{25}NO]^+$		L: 0/0.382 M: 3.13/0.937 H: 0/0.322	L: 0/0 M: 0.156/0 H: 9.61/0.287	L: NA/5.042, 5.225 M: 9.739/11.875, 14.928, 14.979 H: NA/9.487, 11.896	L: NA M: 6.826/NA H: 6.845, 8.971/11.520
28	213 $[C_{13}H_{27}NO]^+$		L: 0/0 M: 0/0.981 H: 0.413/0	L: 0/2.57 M: 1.06/0.471 H: 1.59/0	L: NA M: NA/11.134 H: 10.906/NA	L: NA/10.786, 10.830 M: 10.500/1.231 H: 10.515/NA
29	216 $[C_{15}H_{21}N]^+$		L: 0/0 M: 0/1.41 H: 0/0	L: 0/0 M: 0/0 H: 0/0	L: NA M: NA/11.344 H: NA	NA
30	218 $[C_{15}H_{23}N]^+$		L: 0/0 M: 0/0.067 H: 0/0	L: 0/0 M: 0/3.54 H: 0/0	L: NA M: NA/11.913 H: NA	L: NA M: NA/14.110 H: NA
31	222/224 $[C_{15}H_{29}N]^+$		L: 2.31/0 M: 0/0 H: 0/3.01	L: 0.815/0 M: 0/0 H: 0/0	L: 11.798/NA M: NA/NA H: NA/11.267, 11.346, 11.453, 11.694	L: 11.3/NA M: NA/11.400 H: NA
32	229	Unidentified	L: 0/2.10 M: 0/0 H: 0/0	L: 0/0 M: 0/0 H: 0/0	L: NA/12.707 M: NA H: NA	NA

33	238 $[C_{16}H_{31}N]^+$		L: 0/0 M: 0/0 H: 0.383/0	L: 1.94/0 M: 2.44/0 H: 1.01/0	L: NA M: NA H: 12.395/NA	L: 11.784/NA M: 11.781/NA H: 12.452/NA
34*[,b]	240 $[C_{16}H_{33}N]^+$		L: 0/0 M: 0/1.60 H: 0/1.42	L: 0/0 M: 0/0 H: 0.180/0.826	L: NA M: NA/12.699, 15.198 H: NA/13.781	L: NA M: NA H: 12.521/13.800, 15.023
35*[,b]	241/242[a] $[C_{16}H_{35}N]^+$		L: 3.23/3.50 M: 1.46/16.0 H: 0.423/ 44.8	L: 0/1.39 M: 0/13.8 H: 0/24.9	L: 12.815, 12.838/10.880, 11.674, 12.531 M: 11.675/10.966 H: 5.059/11.052	L: NA/12.532 M: NA/10.890 H: NA/11.050
36	252 $[C_{17}H_{33}N]^+$		L: 0/0 M: 2.51/0.413 H: 6.13/ 0.203	L: 0/0 M: 1.80/1.07 H: 0.090/ 0.455	L: NA M: 12.630/12.028, 12.105, 12.496 H: 12.438, 12.892/12.498	L: NA M: 12.415/11.886, 12.471, 12.489 H: 12.504/11.886, 11.924
37[#,c] (top)	253 $[C_{17}H_{35}N]^+$	 OR 	L: 0/0 M: 0/0 H: 0/0	L: 0/0 M: 2.58/0 H: 1.57/0	NA	L: NA M: 11.432/NA H: 11.446/NA
38*[,o] (top)	254/255 $[C_{16}H_{33}NO]^+$	 OR 	L: 0/6.128 M: 0/2.58 H: 0.403/0	L: 7.824/ 0.699 M: 0/3.71 H: 0/0.271	L: NA/12.148 M: NA/12.147 H: 12.602/NA	L: 12.506/12.115 M: NA/12.170 H: NA/12.490
39	267 $[C_{17}H_{33}NO]^+$		L: 1.51/0 M: 0/0 H: 1.34/0	L: 0/0 M: 0/0 H: 0/0	L: 12.123/NA M: NA H: 12.142/NA	NA

40	268 $[C_{17}H_{35}NO]^+$		L: 1.21/ 30.5 M: 8.07/5.29 H: 10.3/ 2.50	L: 27.9/34.9 M: 9.77/ 10.9 H: 3.72/ 3.81	L: 14.010/0.210, 7.393, 12.919, 12.978, 13.511, 13.786 M: 5.039, 6.987, 7.548, 13.629/0.094, 0.232, 4.899, 4.95, 12.844, 12.91, 12.966, 13.776, 13.968, 14.214 H: 13.649/0.089, 0.220, 4.900, 5.016, 12.894, 12.969	L: 13.537, 13.621/ 4.858, 4.927, 9.536, 12.23, 12.661, 13.151, 13.228, 13.458, 14.226 M: 5.049, 7.564, 11.934, 12.296/0.061, 0.208, 12.654, 13.222, 13.288, 13.355, 13.433, 13.505, 13.559, 13.621, 13.801, 16.214 H: 4.925, 5.062, 6.717, 9.252, 13.404, 14.188/0.064, 0.215, 4.844, 4.910, 12.527, 13.165, 13.221, 13.452
41	272 $[C_{18}H_{25}NO]^+$		L: 0/0 M: 0/0.963 H: 0/1.57	L: 0/3.54 M: 0/0 H: 0/1.84	L: NA M: NA/14.065, 14.108, 15.323 H: NA/12.027, 12.249, 12.849, 14.067	L: NA/12.000, 12.753 M: NA H: NA/14.070, 14.738, 14.837
42	275 $[C_{18}H_{29}NO]^+$		L: 0/0 M: 0/0 H: 0/2.41	L: 0/0 M: 0/0 H: 0/1.45	L: NA M: NA H: NA/11.537, 12.105, 12.147	L: NA M: NA H: NA/12.171, 13.402
43	280 $[C_{19}H_{21}NO]^+$		L: 0/0 M: 0/0.083 H: 0/0.125	L: 0/1.76 M: 0/7.87 H: 0/0	L: NA M: NA/13.011 H: NA/13.000	L: NA/12.711 M: NA/12.710 H: NA
44	281 $[C_{19}H_{23}NO]^+$		L: 0/1.65 M: 0.201/0.056 H: 4.63/0	L: 8.92/1.14 M: 3.40/16.9 H: 0.868/ 0.319	L: NA/5.812 M: 6.690/6.109 H: 12.732/NA	L: 12.385/5.811 M: 12.385/5.917, 5.97, 6.345 H: 12.302, 12.371/5.970, 6.115

45	282 $[C_{19}H_{25}NO]^+$		L: 28.2/6.35 M: 21.3/1.67 H: 10.0/ 0.417	L: 20.1/5.56 M: 1.08/0.748 H: 2.28/ 0.830	L: 13.605, 13.681, 13.820, 14.040, 14.211/13.098, 14.035 M: 13.096, 13.680, 13.820, 14.036/13.084, 13.804, 14.025 H: 13.116, 13.697/13.086, 14.027	L: 13.700, 13.915/13.292, 13.525, 13.735 M: 13.914/13.730 H: 13.386/13.354, 13.525, 13.733
46[##,c]	284 $[C_{19}H_{27}NO]^+$		L: 0.418/0 M: 4.32/0 H: 3.32/0	L: 0/0.948 M: 5.25/0.244 H: 0/0	L: 14.131/NA M: 14.123/NA H: 14.145/NA	L: NA/13.903 M: 13.831/13.830 H: NA
47[##,b]	298 $[C_{19}H_{39}NO]^+$		L: 5.82/0 M: 3.82/0 H: 16.7/0	L: 0/0 M: 6.70/0 H: 3.23/0	L: 13.837/NA M: 13.834/NA H: 13.857, 14.056/NA	L: NA M: 13.521/NA H: 13.535/NA
48	302 $[C_{20}H_{31}NO]^+$		L: 0/1.53 M: 0.270/0.339 H: 0.343/0.528	L: 0/0 M: 0.369/0.699 H: 0/0.510	L: NA/14.167 M: 15.294/17.010 H: 15.326/15.042, 15.283	L: NA M: 15.628/14.876, 14.936, 15.772 H: NA/14.887, 14.940, 15.051, 15.091, 15.238
49	306 $[C_{20}H_{35}NO]^+$		L: 0/0.538 M: 4.07/0.349 H: 0/0	L: 0/0 M: 0/0 H: 0/0	L: NA/14.291 M: 14.004/14.279 H: NA	NA
50*[,b]	309/310[a] $[C_{20}H_{39}NO]^+$		L: 11.8/3.87 M: 13.3/9.78 H: 16.8/ 16.2	L: 0/0.177 M: 17.9/8.09 H: 3.40/9.30	L: 13.011, 13.990/13.733,14.566 M: 13.008, 13.927, 14.210, 15.833, 15.850, 15.937/13.056, 13.722, 13.890, 14.553, 14.875, 15.616, 15.699, 15.829, 15.891, 16.231, 16.421, 16.546, 18.491 H: 13.029, 13.085, 13.945, 14.024, 15.881, 15.948/13.100,	L: NA/13.346, 13.820 M: 12.711, 13.710, 13.744, 13.970, 14.115, 15.541/15.520 H: 12.726, 13.928, 13.951, 13.985, 15.600/15.293, 15.334, 15.527

					14.883, 15.330, 15.838, 15.929	
51	324 $[C_{20}H_{37}NO_2]^+$		L: 0.314/0 M: 0.428/0 H: 0.857/0	L: 0/0 M: 1.09/0 H: 0/0	L: 14.512/NA M: 14.500/NA H: 14.241, 14.371/NA	L: NA M: 13.935/NA H: NA
52*,[b] (top)	325 $[C_{20}H_{39}NO_2]^+$	OR 	L: 0/0 M: 0/0 H: 0/0	L: 0/0 M: 10.8/0 H: 2.47/0	NA	L: NA M: 13.304, 13.371/NA H: 13.318, 13.759/NA
53*,[b]	327 $[C_{20}H_{41}NO_2]^+$		L: 0/0 M: 0/0 H: 0/0	L: 0/0 M: 0/0 H: 2.40/0	NA	L: NA M: NA H: 13.726, 13.845/NA
54	336 $[C_{20}H_{33}NO_3]^+$		L: 0/0 M: 0/0 H: 0/0	L: 0/0 M: 2.34/0 H: 0/0	NA	L: NA M: 14.063/NA H: NA
55	338 $[C_{23}H_{31}NO]^+$		L: 0/2.50 M: 0/0 H: 0/0	L: 0/0 M: 0.942/0 H: 0/0	L: NA/12.751 M: NA H: NA	L: NA M: 15.169/NA H: NA
56	352 $[C_{23}H_{29}NO_2]^+$		L: 0/0 M: 0/0 H: 0.847/0	L: 0/0 M: 2.35/0 H: 0.379/0	L: NA M: NA H: 14.342, 14.459, 14.531/NA	L: NA M: 14.002, 14.205/NA H: 13.905, 14.221/NA

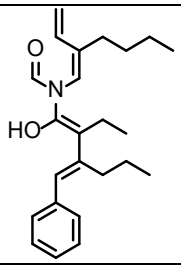
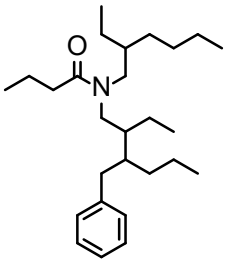
57‡	367 $[C_{24}H_{33}NO_2]^+$		L: 0/0 M: 0/0 H: 1.59/0	L: 0/0 M: 0/0 H: 0.409/0	L: NA M: NA H: 13.995/NA	L: NA M: NA H: 14.016/NA
58*,b	401 $[C_{27}H_{47}NO]^+$		L: 0.552/0 M: 10.8/2.09 H: 3.31/ 4.77	L:1.41/0 M:3.27/4.58 H: 1.23/5.48	L: 16.153/NA M: 15.551, 15.725, 15.915, 16.151, 16.901/16.130, 16.877 H: 15.586, 15.764, 16.189/15.710, 16.138, 16.884, 17.023, 17.112, 17.596	L: 16.558/NA M: 15.577, 15.858, 16.561/16.333, 16.42, 16.532, 16.906, 16.95, 17, 17.296 H: 15.562, 15.880, 16.389, 16.589/15.778, 16.217, 16.341, 16.541, 16.909

Table S2. The percent relative standard deviations for triplicate TICs of each azoperoxide or γ-radiation dose with DEHBA.

Azoperoxide (mM) or Radiolysis Dose (kGy)	**Relative Standard Deviation (RSD)**
40 mM azoperoxide	2.54 ± 2.65
120 mM azoperoxide	3.31 ± 2.89
400 mM azoperoxide	4.86 ± 3.33
42 kGy	N/A (only 2 samples)
171 kGy	3.43 ± 3.02
412 kGy	N/A (only 2 samples)
651 kGy	3.56 ± 3.56
1043 kGy	5.03 ± 6.99

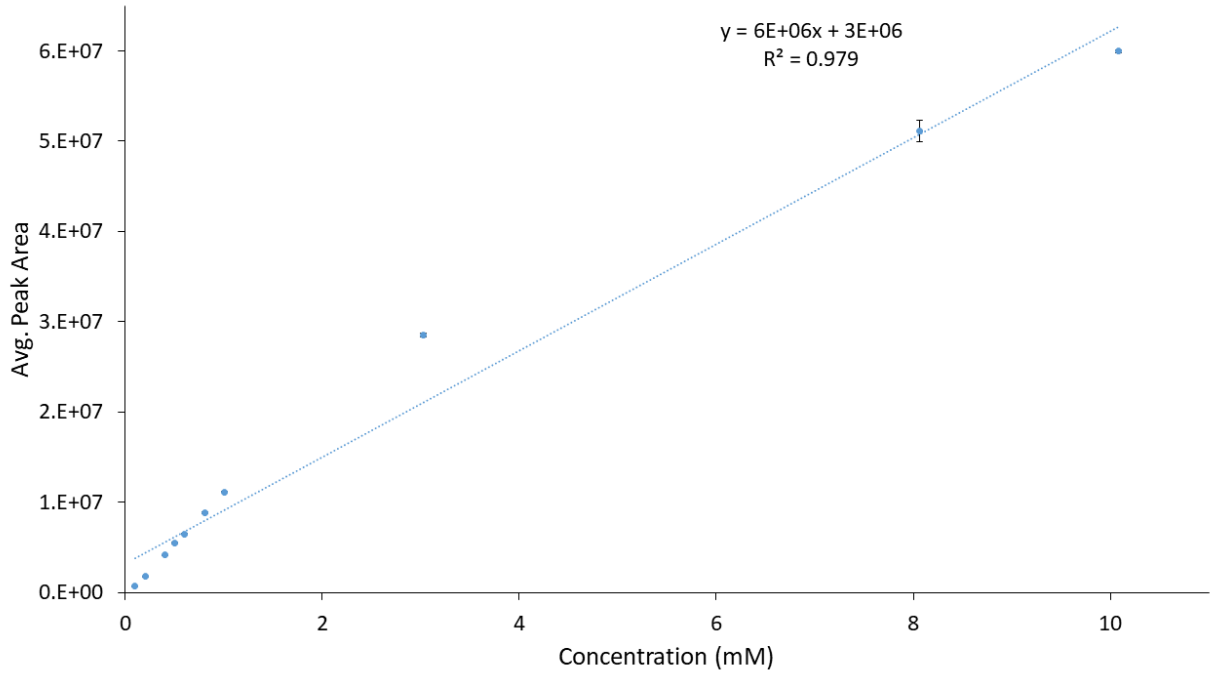


Figure S19. Calibration curve of DEHBA in toluene (0.1 to 10 mM). Instrument response was non-linear above 1 mM DEHBA.

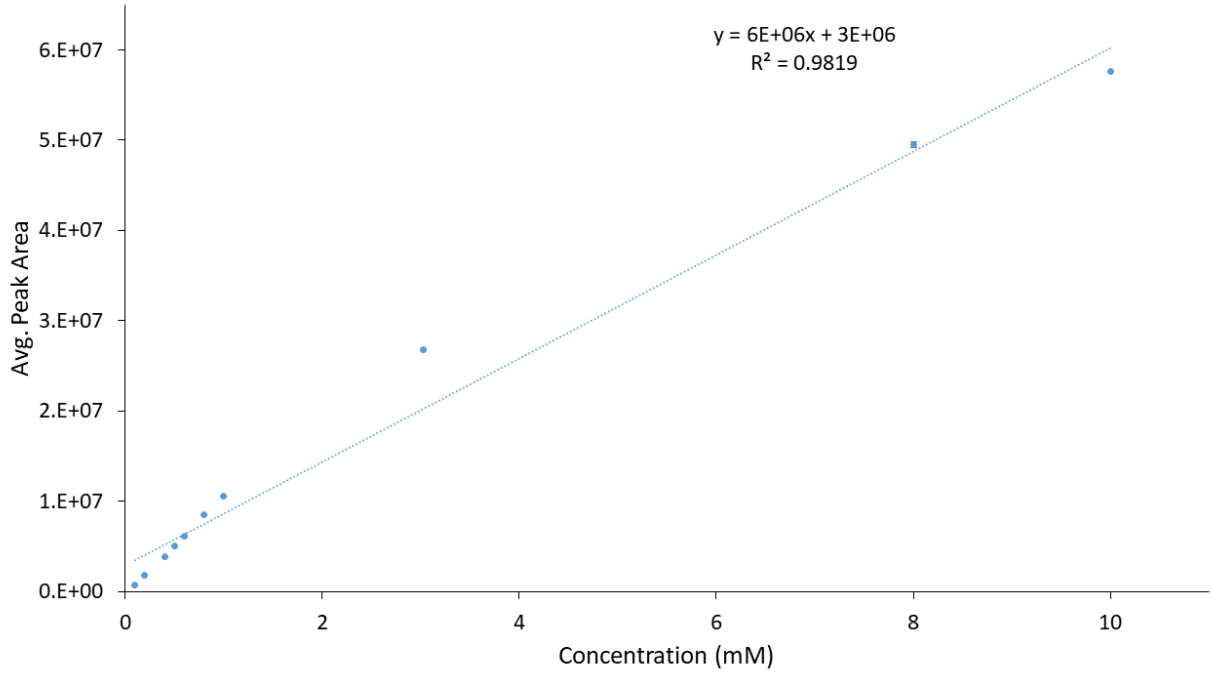


Figure S20. Calibration curve of DEH*i*BA in toluene (0.1 to 10 mM). Instrument response was non-linear above 1 mM DEH*i*BA.

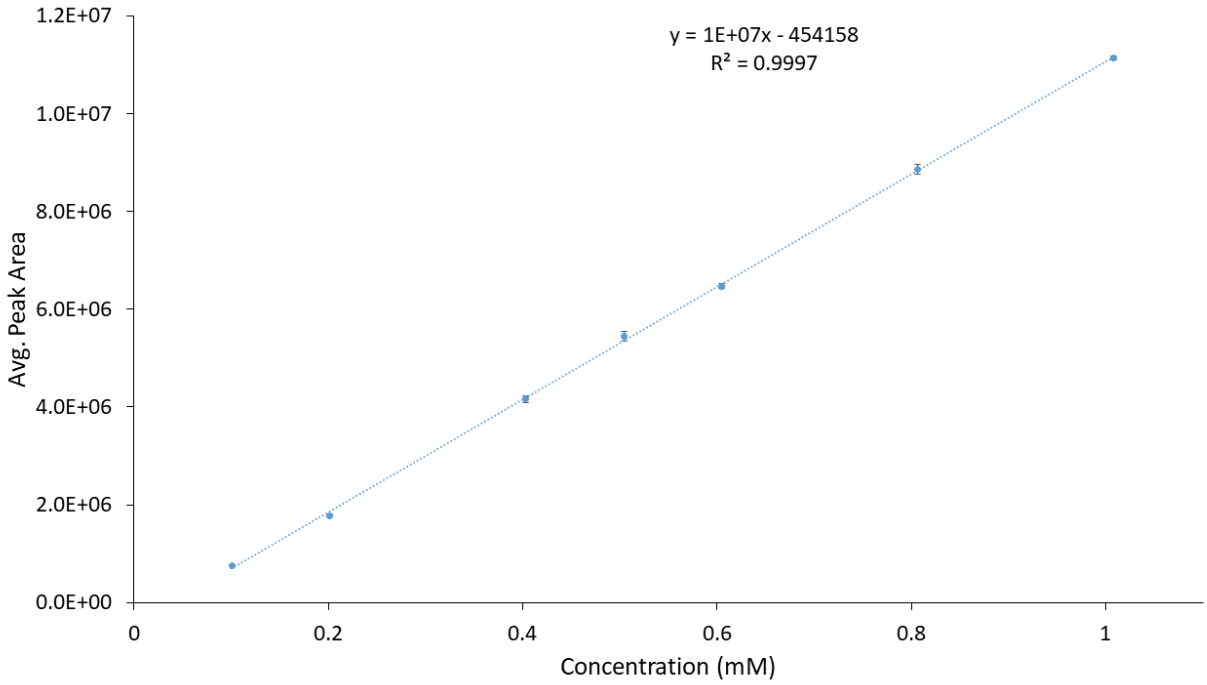


Figure S21. Linear region of the DEHBA calibration curve in toluene (0.1 to 1 mM).

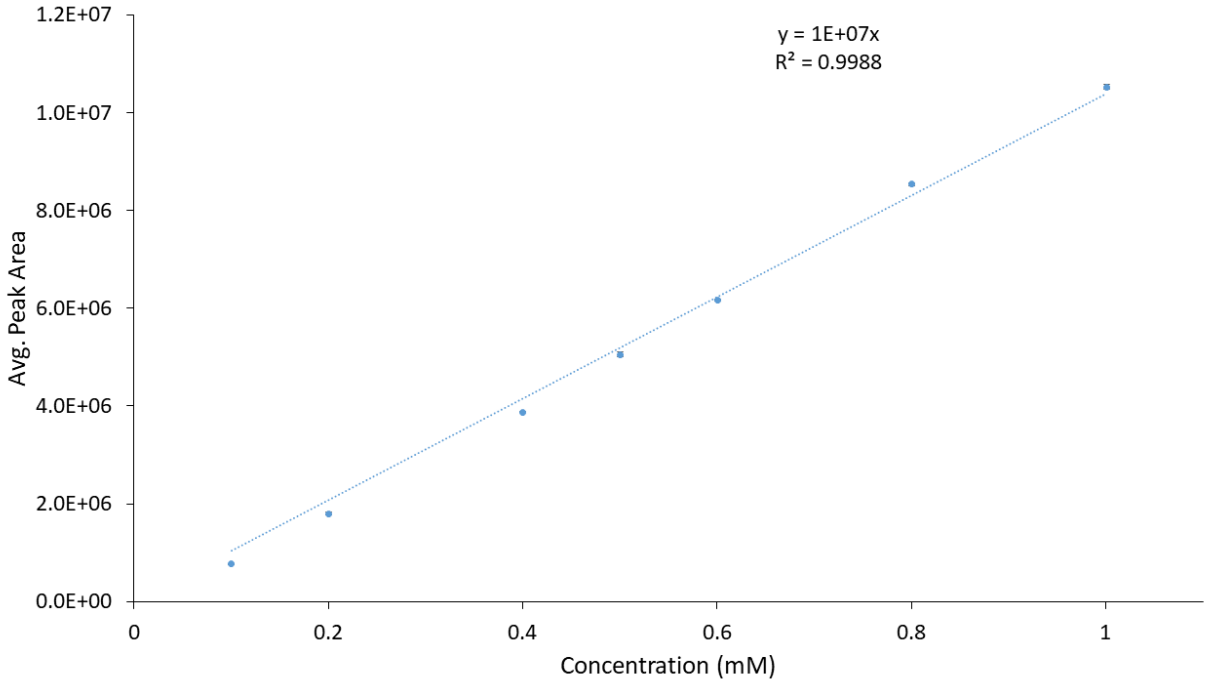


Figure S22. Linear region of the DEH*i*BA calibration curve in toluene (0.1 to 1 mM).

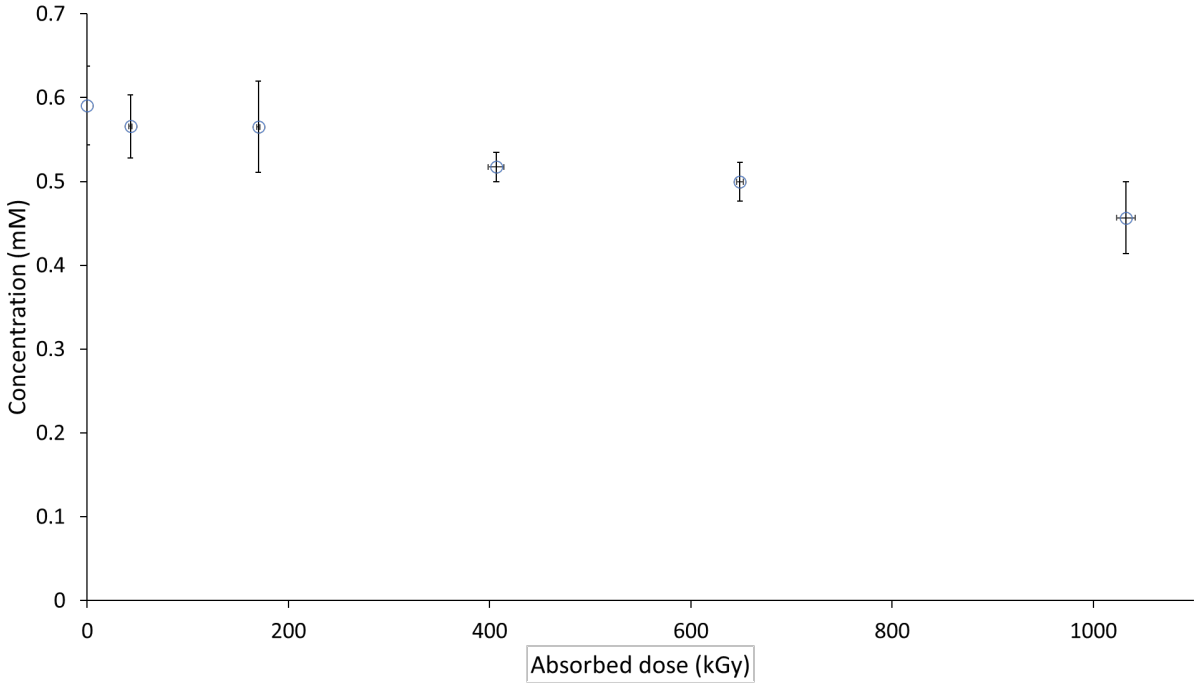


Figure S23. DEHBA concentration (mM) vs. absorbed dose (kGy) determined by GC-FID methods. The dose constants (d, kGy^{-1}) were calculated using the natural log of DEHBA concentration (mM) vs. absorbed dose (kGy).

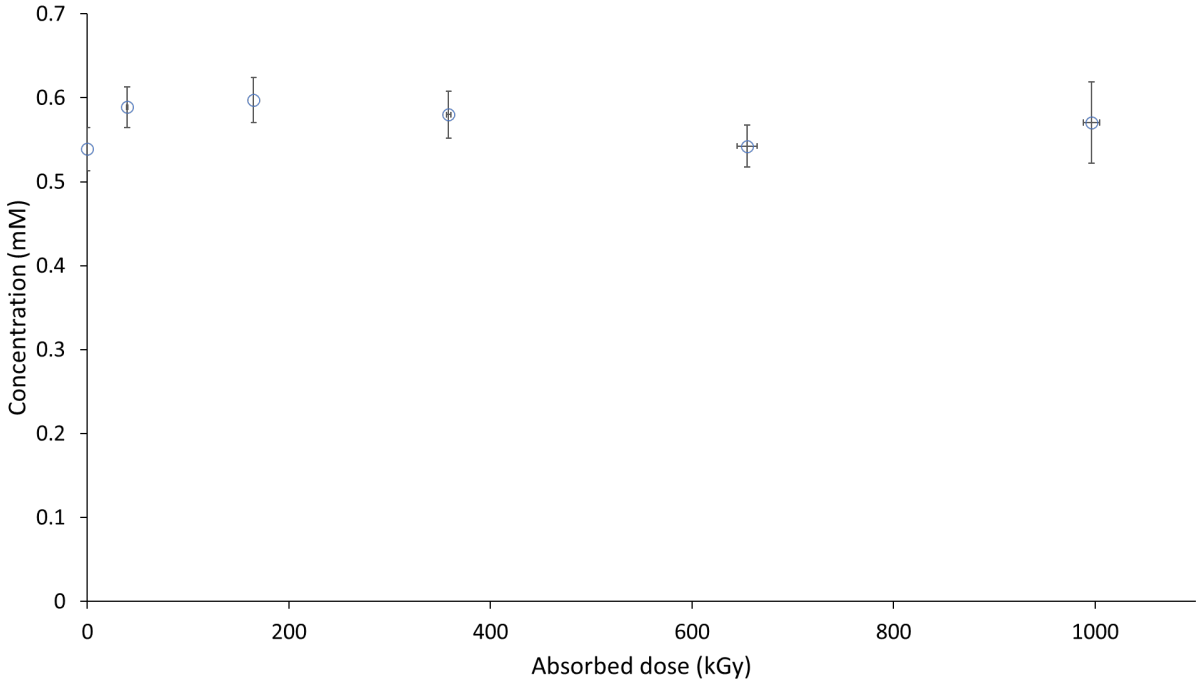


Figure S24. DEH*i*BA concentration (mM) vs. absorbed dose (kGy) determined by GC-FID methods. The dose constants (d, kGy^{-1}) were calculated using the natural log of DEH*i*BA concentration (mM) vs. absorbed dose (kGy)

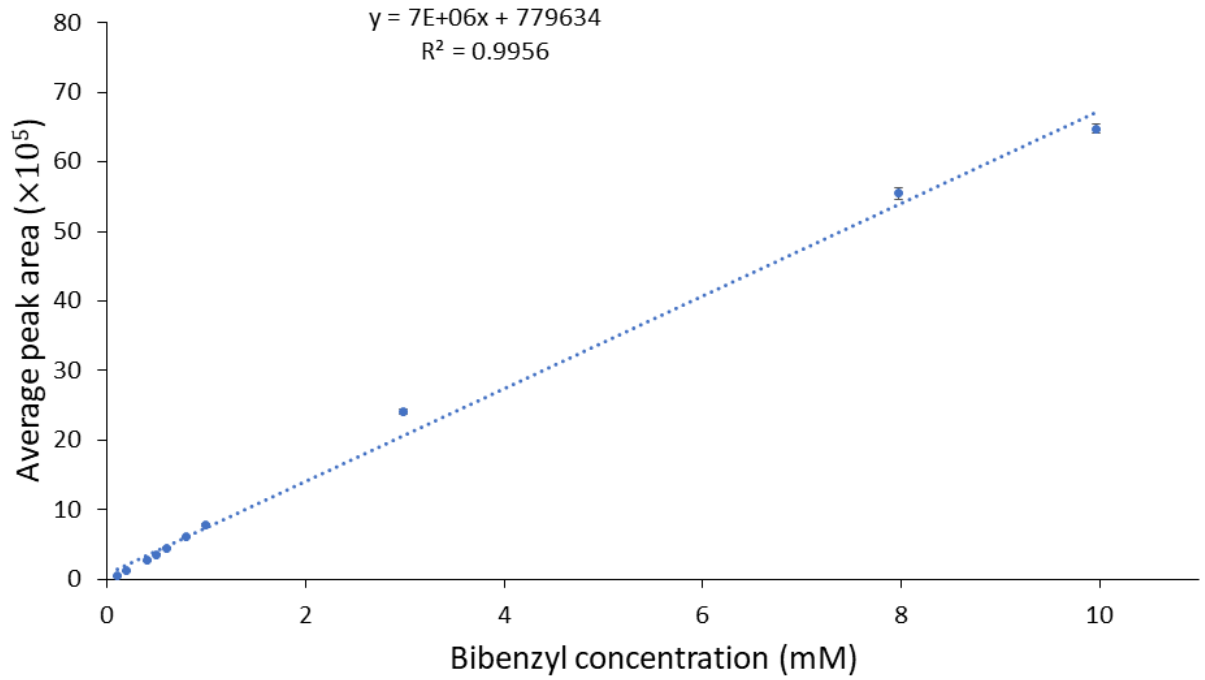


Figure S25. Calibration curve of bibenzyl in toluene (0.1 to 10 mM). Instrument response was non-linear after 3 mM dibenzyl.

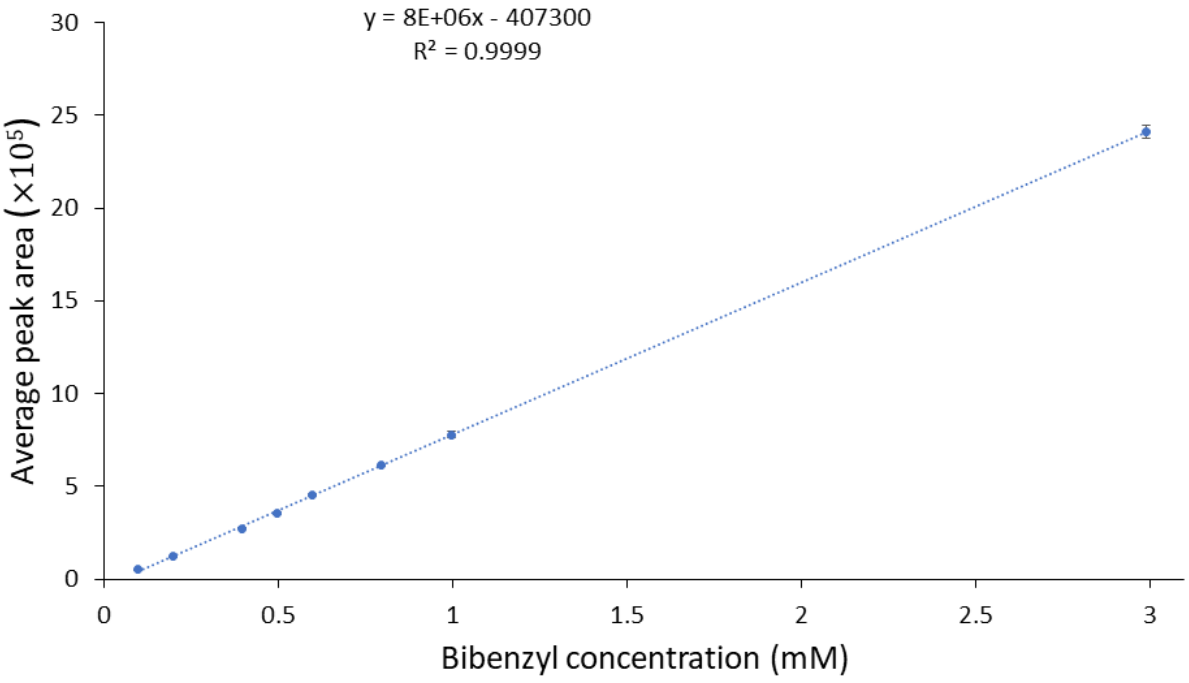


Figure S26. Linear region of the calibration curve of bibenzyl in toluene (0.1 to 3 mM).

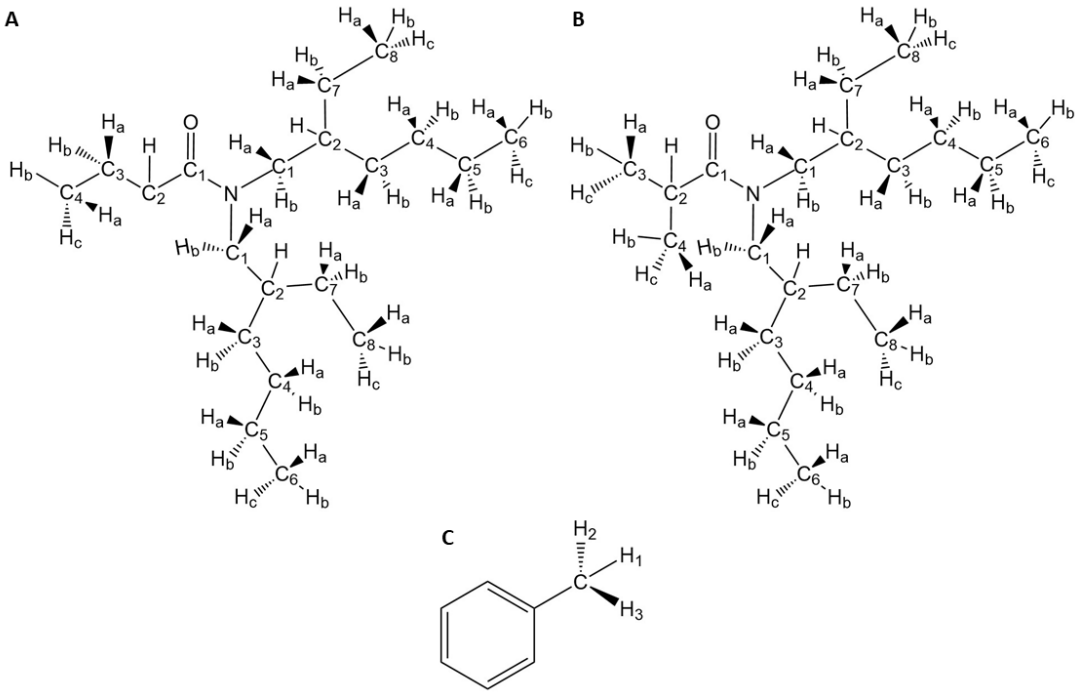
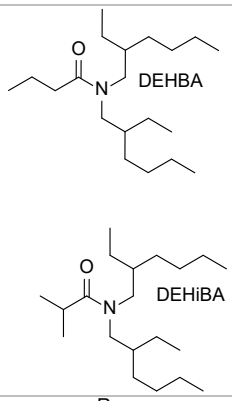
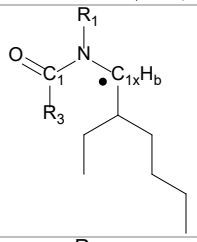
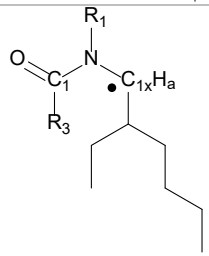
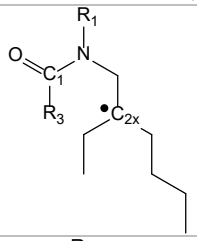
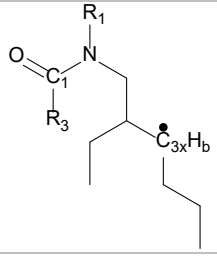
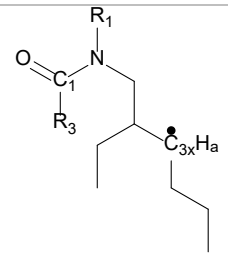
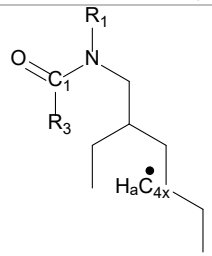
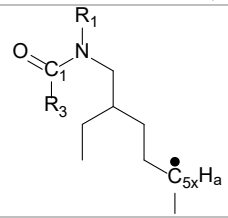
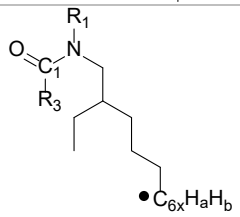
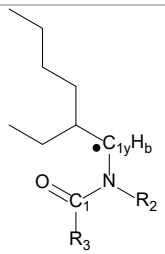
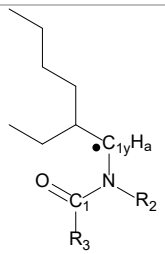
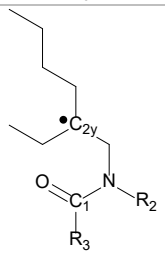


Figure S27. Monoamide and toluene structures showing labeling schemes for computations of radical energies (Tables S3-S5).

Table S3. Calculated energies of *N*-terminal radicals at different positions of the monoamide chain for DEHBA and DEH*i*BA (R_1 = *N*-terminal alkyl, *trans* branching; R_2 = *N*-terminal alkyl, *cis* branching; and R_3 = *C*-terminal alkyl branching; x = *cis* branching; y = *trans* branching.)

Structure Number	**Structure**	**Radical Position**	**Energy, kJ/mol**		**Energy difference from ground state, kJ/mol**	
			DEHBA	DEH*i*BA	DEHBA	DEH*i*BA
1.		Ground state	-2407369	-2407374	0	0
2.		*N*-terminal *cis* C1	-2405607	-2405618	1762	1756
3.		*N*-terminal *cis* C1	-2405600	-2405601	1769	1773
4.		*N*-terminal *cis* C2	-2405609	-2405612	1760	1762
5.		*N*-terminal *cis* C3	-2405593	-2405597	1776	1776

6.		*N*-terminal *cis* C3	-2405596	-2405599	1772	1775
7.		*N*-terminal *cis* C4	-2405596	-2405600	1773	1774
8.		*N*-terminal *cis* C5	-2405591	-2405596	1778	1778
9.		*N*-terminal *cis* C6	-2405578	-2405581	1791	1793
10.		*N*-terminal *trans* C1	-2405601	-2405586	1767	1788
11.		*N*-terminal *trans* C1	-2405589	-2405611	1780	1763
12.		*N*-terminal *trans* C2	-2405601	-2405614	1767	1760

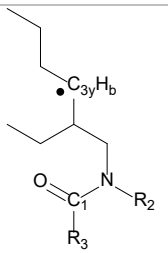
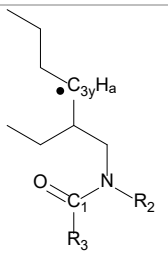
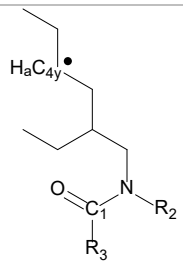
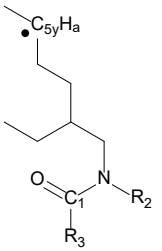
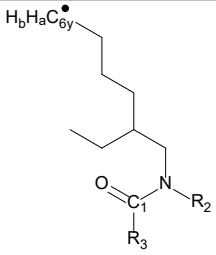
13.		*N*-terminal *trans* C3	-2405597	-2405599	1772	1775
14.		*N*-terminal *trans* C3	-2405596	-2405602	1773	1772
15.		*N*-terminal *trans* C4	-2405599	-2405599	1769	1774
16.		*N*-terminal *trans* C5	-2405592	-2405596	1777	1778
17.		*N*-terminal *trans* C6	-2405578	-2405583	1790	1791

Table S4. Calculated energies of *C*-terminal radicals at different positions of the monoamide chain for DEHBA and DEH*i*BA (R_1 = *N*-terminal alkyl, *trans* branching; R_2 = *N*-terminal alkyl, *cis* branching; and R_3 = *C*-terminal alkyl branching; x = *cis* branching; y = *trans* branching).

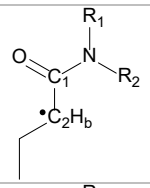
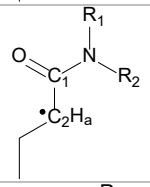
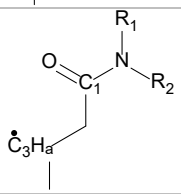
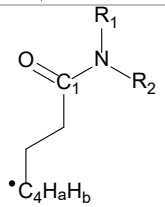
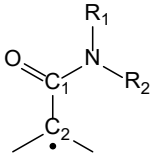
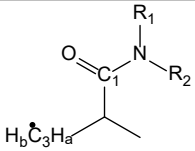
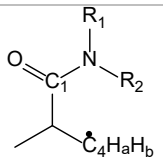
Structure Number	Structure	Radical Position	Energy, kJ/mol	Energy difference from ground state, kJ/mol
18.		*C*-terminal C2	-2405604	1764
19.		*C*-terminal C2	-2405602	1766
20.		*C*-terminal C3	-2405585	1783
21.		*C*-terminal C4	-2405577	1792
22.		*C*-terminal C2	-2405613	1761
23.		*C*-terminal C3	-2405573	1801
24.		*C*-terminal C4	-2405574	1799

Table S5. Calculated energies of toluene and its radicals.

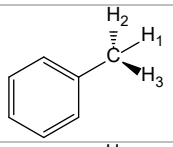
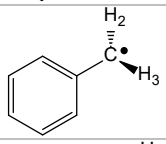
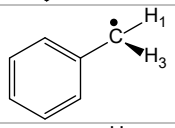
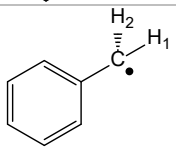
Structure Number	Structure	Radical Position	Energy, kJ/mol	Energy difference from ground state, kJ/mol
25.		Ground state	-713051	0
26.		Toluene_H1	-711288	1763
27.		Toluene_H2	-711260	1792
28.		Toluene_H3	-711260	1792

Table S6. DFT Cartesian coordinates for DEHBA, DEH*i*BA, toluene, and their radicals. Structures numbers correspond to entry numbers in Tables S3-S5.

Structure 1 DEHBA

C	-16.74645000	-7.29581000	-29.07958000
N	-16.24120000	-8.46124000	-28.50212000
O	-17.13335000	-7.27087000	-30.25033000
C	-16.80109000	-6.03588000	-28.22304000
H	-15.79834000	-5.59850000	-28.18194000
H	-17.11444000	-6.27946000	-27.20810000
C	-17.79291000	-5.01342000	-28.78734000
H	-17.40030000	-4.58740000	-29.71767000
C	-18.07850000	-3.89601000	-27.79616000
H	-18.73923000	-5.50798000	-29.03850000
H	-17.16214000	-3.36138000	-27.52836000
H	-18.52706000	-4.29260000	-26.87909000
H	-18.78133000	-3.17661000	-28.22863000
C	-15.72908000	-8.57200000	-27.13701000
C	-16.27237000	-9.68589000	-29.31095000
H	-15.95374000	-9.39046000	-30.31432000
C	-17.66291000	-10.37276000	-29.36502000
H	-15.51164000	-10.38738000	-28.94876000
C	-17.72524000	-11.38505000	-30.54216000
H	-18.43189000	-9.61085000	-29.54264000
C	-17.99572000	-11.15323000	-28.05866000
H	-18.20876000	-12.19828000	-28.32383000
C	-19.23453000	-10.67037000	-27.28309000
H	-17.12800000	-11.22084000	-27.39618000
H	-19.67520000	-11.56199000	-26.81654000
H	-20.00158000	-10.28012000	-27.96136000
C	-18.93954000	-9.69279000	-26.14219000
H	-19.54234000	-9.97207000	-25.26887000
C	-19.28448000	-8.25633000	-26.49161000
H	-17.89832000	-9.76916000	-25.81731000
H	-20.36914000	-8.11468000	-26.51882000
H	-18.88722000	-7.97430000	-27.46695000
H	-18.87685000	-7.57434000	-25.73797000
H	-16.37582000	-7.99570000	-26.47395000
C	-14.26609000	-8.12237000	-26.93826000
H	-15.82952000	-9.61507000	-26.82743000
H	-14.14530000	-7.12236000	-27.37416000
C	-13.28946000	-9.06537000	-27.67244000
C	-13.97633000	-7.98973000	-25.42045000
H	-12.97645000	-7.56505000	-25.28188000
C	-14.10512000	-9.29902000	-24.62788000
H	-14.67201000	-7.25244000	-24.99835000
H	-13.37736000	-10.03379000	-24.98945000
H	-15.09809000	-9.73359000	-24.78517000
C	-13.93307000	-9.11889000	-23.11841000
H	-13.49034000	-9.01594000	-28.74932000
H	-13.46247000	-10.10518000	-27.37111000
C	-11.81939000	-8.72955000	-27.46484000
H	-11.50800000	-8.90452000	-26.43091000
H	-11.61360000	-7.68583000	-27.72079000
H	-11.19742000	-9.36506000	-28.10377000
C	-17.44869000	-10.80928000	-31.92359000
H	-18.72865000	-11.83025000	-30.56290000
H	-17.02001000	-12.20659000	-30.36154000
H	-18.04746000	-9.91361000	-32.11026000
H	-17.69581000	-11.55191000	-32.69002000
H	-16.39105000	-10.56222000	-32.05368000
C	-12.53619000	-8.67646000	-22.71749000
H	-14.14851000	-10.07768000	-22.63107000
H	-14.66993000	-8.40068000	-22.74037000
H	-12.43599000	-8.69492000	-21.62766000
H	-12.32961000	-7.65608000	-23.05268000
H	-11.77677000	-9.34191000	-23.13978000

Structure 1 DEH*i*BA

C	-41.58679000	4.90840000	17.54866000
N	-40.40565000	4.16886000	17.43926000
O	-42.46741000	4.84248000	16.68693000
C	-41.80805000	5.73836000	18.81953000
C	-43.04898000	6.62506000	18.66204000
H	-40.94941000	6.39635000	18.97825000
C	-42.00503000	4.82763000	20.03439000
C	-39.14957000	4.54266000	18.10778000
C	-40.34167000	3.13945000	16.39363000
H	-40.90520000	3.48091000	15.51708000
C	-40.85643000	1.72930000	16.82710000
H	-39.29987000	3.04778000	16.07187000
C	-42.33895000	1.80160000	17.26276000
H	-40.25649000	1.39936000	17.68544000
C	-40.59982000	0.77384000	15.63220000
H	-41.30333000	1.02071000	14.82899000
C	-40.66297000	-0.72535000	15.94008000
H	-39.59470000	0.97506000	15.23659000
H	-41.67502000	-1.02935000	16.20096000
H	-40.02700000	-0.94777000	16.80593000
C	-40.21390000	-1.60177000	14.76485000
H	-39.16103000	-1.40725000	14.53168000
C	-41.05506000	-1.40977000	13.51077000
H	-40.28237000	-2.65212000	15.07305000
H	-40.87864000	-0.42805000	13.05982000
H	-42.12323000	-1.50164000	13.73052000
H	-40.79492000	-2.16585000	12.76245000
H	-39.38193000	4.74223000	19.15357000
C	-38.46371000	5.79467000	17.49483000
H	-38.47689000	3.67809000	18.11337000
H	-39.20904000	6.60037000	17.45222000
C	-37.98706000	5.58506000	16.03772000
C	-37.29012000	6.30426000	18.36509000
H	-36.54602000	5.50965000	18.48980000
C	-37.70263000	6.80926000	19.75240000
H	-36.79105000	7.12662000	17.83438000
H	-38.10084000	5.98279000	20.34955000
H	-38.49695000	7.55914000	19.65762000
C	-36.50788000	7.42037000	20.48951000
H	-37.67359000	6.55426000	15.62789000
H	-38.82848000	5.26515000	15.41408000
C	-36.83092000	4.60754000	15.86181000
H	-37.03830000	3.63606000	16.31719000
H	-35.90788000	5.00059000	16.29890000
H	-36.64110000	4.44314000	14.79613000
C	-42.96271000	0.53120000	17.81312000
H	-42.95478000	2.16753000	16.43235000
H	-42.42555000	2.53440000	18.06950000
H	-42.26594000	-0.02093000	18.45054000
H	-43.84214000	0.78419000	18.41731000
H	-43.32314000	-0.11542000	17.00961000
C	-36.85314000	7.75926000	21.93024000
H	-36.17833000	8.32913000	19.97199000
H	-35.66452000	6.71982000	20.48195000
H	-37.67997000	8.47454000	21.98012000
H	-35.98788000	8.20059000	22.43409000
H	-37.14298000	6.85943000	22.48334000
H	-43.95665000	6.02176000	18.53225000
H	-42.95572000	7.27581000	17.78848000
H	-43.19217000	7.25603000	19.54480000
H	-42.87147000	4.17091000	19.89708000
H	-42.17046000	5.42109000	20.93936000
H	-41.14308000	4.18079000	20.21577000

Structure 2

DEHBA_Ncis_C1H1_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100

H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 2

DEH*i*BA_Ncis_C1H1_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 3

DEHBA_Ncis_C1H2_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300

H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 3

DEH*i*BA_Ncis_C1H2_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 4

DEHBA_Ncis_C2_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700

C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 4

DEH*i*BA_Ncis_C2_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 5

DEHBA_Ncis_C3H1_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800

C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 5

DEH*i*BA_Ncis_C3H1_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 6

DEHBA_Ncis_C3H2_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100

H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 6

DEH*i*BA_Ncis_C3H2_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 7

DEHBA_Ncis_C4H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700

H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 7

DEH*i*BA_Ncis_C4H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 8

DEHBA_Ncis_C5H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100

H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 8

DEH*i*BA_Ncis_C5H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 9

DEHBA_Ncis_C6H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700

C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.49026600	-1.98043800	0.41356400

Structure 9

DEH*i*BA_Ncis_C6H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 10

DEHBA_Ntrans_C1H1_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500

H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 10

DEH*i*BA_Ntrans_C1H1_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 11

DEHBA_Ntrans_C1H2_radical

C	-0.73583700	1.61820700	-0.52402800

N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 11

DEH*i*BA_Ntrans_C1H2_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100

H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 12

DEHBA_Ntrans_C2_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 12

DEH*i*BA_Ntrans_C2_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100

H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 13

DEHBA_Ntrans_C3H1_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 13

DEH*i*BA_Ntrans_C3H1_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200

H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 14

DEHBA_Ntrans_C3H2_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 14

DEH*i*BA_Ntrans_C3H2_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800

H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 15

DEHBA_Ntrans_C4H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 15

DEH*i*BA_Ntrans_C4H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200

H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 16

DEHBA_Ntrans_C5H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 16

DEH*i*BA_Ntrans_C5H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200

C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 17

DEHBA_Ntrans_C6H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 17

DEH*i*BA_Ntrans_C6H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200

H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 18

DEHBA_C_C1H1_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 19

DEHBA_C_C1H2_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100

H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 20

DEHBA_C_C2H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	1.26092000	5.19373700	0.60073100
H	0.09731600	4.98041100	1.91254900
H	-0.21299200	6.16409000	0.64049700
C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 21

DEHBA_C_C3H_radical

C	-0.73583700	1.61820700	-0.52402800
N	-0.27068800	0.32792800	-0.44596000
O	-1.73426000	1.89354300	-1.18133900
C	0.00447800	2.69682300	0.27040600
H	1.07450600	2.66739700	0.04314000
H	-0.07919500	2.45388300	1.33798700
C	-0.54109500	4.10348600	0.01663500
H	-0.46170600	4.33136700	-1.05013600
C	0.19204800	5.16789800	0.83775700
H	-1.60972000	4.12009800	0.24355400
H	1.26092000	5.19373700	0.60073100
H	-0.21299200	6.16409000	0.64049700

C	0.96878400	-0.04869100	0.24450900
C	-1.05608000	-0.71113400	-1.13514000
H	-1.28738300	-0.34574100	-2.13623100
C	-2.36705000	-1.11367300	-0.42335400
H	-0.41685400	-1.59132400	-1.23986000
C	-3.17385600	-2.07578600	-1.31943100
H	-2.94565300	-0.19504600	-0.29574700
C	-2.07483500	-1.72591200	0.96103600
H	-1.53429400	-2.67197500	0.81327000
C	-3.26803600	-1.99755100	1.89794300
H	-1.38575700	-1.06251100	1.49614800
H	-2.86442900	-2.52155400	2.77171700
H	-3.96882100	-2.70258300	1.43602700
C	-4.04298200	-0.75664200	2.39182800
H	-4.41889300	-0.96242400	3.40022000
C	-5.23368900	-0.33271100	1.52213600
H	-3.34791900	0.08520700	2.49965300
H	-5.95824900	-1.14851800	1.43142100
H	-4.93140400	-0.04388300	0.51348200
H	-5.75414300	0.52184300	1.96444600
H	1.04843200	0.52101300	1.17397100
C	2.27546400	0.13519100	-0.56590300
H	0.86385400	-1.09420200	0.53970900
H	2.29409600	1.17744400	-0.90947800
C	2.31046600	-0.74453000	-1.83052400
C	3.50713600	-0.03723000	0.35464400
H	4.39441100	0.29377600	-0.19234000
C	3.74995300	-1.44875200	0.91243600
H	3.40440900	0.65896700	1.19769600
H	3.91231300	-2.15363400	0.08820100
H	2.85429300	-1.79756200	1.43805700
C	4.94053900	-1.53874000	1.88236900
H	1.40739500	-0.54195900	-2.41358200
H	2.26006500	-1.80315500	-1.54883300
C	3.52957800	-0.51274300	-2.73030800
H	4.46436900	-0.80248600	-2.24347000
H	3.61556700	0.54122700	-3.01405300
H	3.44690800	-1.09552300	-3.65171000
C	-3.77086000	-1.44394500	-2.58344500
H	-3.99192700	-2.50181400	-0.73129400
H	-2.53439800	-2.92552200	-1.59662800
H	-4.41485200	-0.59648300	-2.33171500
H	-4.37618600	-2.17297800	-3.12992100
H	-3.00461300	-1.07655300	-3.27009500
C	6.30902100	-1.28504500	1.23980300
H	4.94324700	-2.53594300	2.33642100
H	4.78723400	-0.83140400	2.70692000
H	7.11382200	-1.42062000	1.96757300
H	6.39598800	-0.26958500	0.84435700
H	6.49026600	-1.98043800	0.41356400

Structure 22

DEH*i*BA_C_C1_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 23

DEH*i*BA_C_C21H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500

C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	1.18515500	4.23449000	0.67960100
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 24

DEH*i*BA_C_C22H_radical

C	0.49597200	2.02591200	-0.75819800
N	0.09767200	0.72712900	-0.53994800
O	-0.26178800	2.85875500	-1.24596200
C	1.91065300	2.45908300	-0.34531200
C	2.58349500	3.19685300	-1.51244100
H	2.52458600	1.59635200	-0.08776500
C	1.80658100	3.36313600	0.89731600
C	0.95709900	-0.32328900	0.02519500
C	-1.28656200	0.36037900	-0.87360900
H	-1.66929300	1.13337200	-1.54004300
C	-2.23868700	0.20013700	0.33470200
H	-1.26620600	-0.58093200	-1.42945600
C	-2.33504400	1.50080600	1.15278300
H	-1.82239400	-0.57727500	0.99172100
C	-3.61480900	-0.30215500	-0.17891500
H	-4.30971200	0.54324000	-0.21735500
C	-4.22299600	-1.45388100	0.63637600
H	-3.51296800	-0.64585100	-1.21647000
H	-4.35957200	-1.14382700	1.67885300
H	-3.50068100	-2.27944600	0.65978000
C	-5.55683600	-1.98587900	0.08881500
H	-5.42106100	-2.28953000	-0.95686300
C	-6.72559700	-0.99828400	0.18529100
H	-5.81896600	-2.89817300	0.63663200
H	-6.55296900	-0.09910400	-0.41197100
H	-6.88899300	-0.68275300	1.22102000
H	-7.65381000	-1.45340400	-0.17146800
H	1.49439900	0.07222800	0.88884700
C	1.96073800	-0.97450800	-0.95644100
H	0.29399200	-1.09464600	0.42378900
H	2.56420400	-0.16599400	-1.38658200
C	1.28103000	-1.68029600	-2.15072700
C	2.92357900	-1.91643000	-0.20101500
H	2.34990800	-2.59197800	0.44649400
C	4.00376100	-1.21450000	0.63397200
H	3.42259700	-2.56072300	-0.93527400
H	3.54381000	-0.57453700	1.39659200
H	4.58303800	-0.54617200	-0.01618100
C	4.96044800	-2.19238000	1.32729600
H	2.06490100	-1.93851300	-2.87216700
H	0.63342500	-0.96203000	-2.66349100
C	0.48430300	-2.94961100	-1.82163800
H	-0.32338600	-2.76178500	-1.10835800
H	1.12129400	-3.73086400	-1.39878100
H	0.02661100	-3.35716800	-2.72709900
C	-3.15852600	1.39556900	2.44052100
H	-2.74804900	2.28857300	0.51282500
H	-1.32332600	1.82812200	1.41064900
H	-2.76800700	0.61548600	3.10269200
H	-3.13229500	2.33967200	2.99199900
H	-4.20849000	1.16593700	2.24041200
C	6.04806800	-1.49488500	2.14928200
H	5.42887000	-2.83404300	0.57113800
H	4.38353500	-2.86119900	1.97757400
H	6.66416100	-0.84483300	1.52002100
H	6.71269700	-2.21924000	2.62800900
H	5.61171000	-0.87372700	2.93794300
H	1.98130500	4.05533300	-1.81442600
H	2.70108100	2.54589600	-2.38359700
H	3.57571400	3.54865300	-1.21575000
H	2.79931100	3.71073600	1.19688000
H	1.36444800	2.83505000	1.74745100

Structure 25

toluene111023

C	1.21251000	-0.22245000	0.07073000
C	0.98967000	-1.60049000	0.06353000
C	-0.31087000	-2.09712000	-0.00052000
C	-1.38911000	-1.21630000	-0.06137000
C	-1.16754000	0.16195000	-0.05424000
C	0.13480000	0.67059000	0.02488000
C	0.37545000	2.15069000	-0.00365000
H	2.23316000	0.15066000	0.11339000
H	1.83165000	-2.28630000	0.10491000
H	-0.48377000	-3.16986000	-0.00735000
H	-2.40342000	-1.60231000	-0.11743000
H	-2.01821000	0.83727000	-0.10984000
H	0.48728000	2.49177000	-1.03742000
H	1.28099000	2.40991000	0.55493000
H	-0.45701000	2.69082000	0.45947000

Structure 26

toluene_H1

C	-0.19419000	-1.20051900	-0.00872800
C	1.19960200	-1.20355100	0.00198200
C	1.90261900	-0.00003200	0.00840800
C	1.19967500	1.20351100	0.00198100
C	-0.19413600	1.20055200	-0.00872600
C	-0.91275300	0.00004500	-0.01130000
C	-2.42351500	0.00001500	0.00941400
H	-0.73161400	-2.14362200	-0.01778700
H	1.73600400	-2.14611900	0.00163000
H	2.98673700	-0.00006200	0.01374800
H	1.73612300	2.14605200	0.00162600
H	-0.73151100	2.14367900	-0.01778200
H	-2.82894000	-0.88282400	-0.49054700
H	-2.82891400	0.88515300	-0.48646000

Structure 27

toluene_H2

C	-0.19419000	-1.20051900	-0.00872800
C	1.19960200	-1.20355100	0.00198200
C	1.90261900	-0.00003200	0.00840800
C	1.19967500	1.20351100	0.00198100
C	-0.19413600	1.20055200	-0.00872600
C	-0.91275300	0.00004500	-0.01130000
C	-2.42351500	0.00001500	0.00941400
H	-0.73161400	-2.14362200	-0.01778700
H	1.73600400	-2.14611900	0.00163000
H	2.98673700	-0.00006200	0.01374800
H	1.73612300	2.14605200	0.00162600
H	-0.73151100	2.14367900	-0.01778200
H	-2.80170400	-0.00238200	1.03738800

Structure 28

toluene_H3

C	-0.19419000	-1.20051900	-0.00872800
C	1.19960200	-1.20355100	0.00198200
C	1.90261900	-0.00003200	0.00840800
C	1.19967500	1.20351100	0.00198100
C	-0.19413600	1.20055200	-0.00872600
C	-0.91275300	0.00004500	-0.01130000
C	-2.42351500	0.00001500	0.00941400
H	-0.73161400	-2.14362200	-0.01778700
H	1.73600400	-2.14611900	0.00163000
H	2.98673700	-0.00006200	0.01374800
H	1.73612300	2.14605200	0.00162600
H	-0.73151100	2.14367900	-0.01778200
H	-2.80170400	-0.00238200	1.03738800
H	-2.82894000	-0.88282400	-0.49054700

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