Electronic Supplementary Information

for the article entitled

Isotopically Coded *N*-Methoxy Amide Reagents for GC-MS Profiling of Carbonyl Compounds via Mass Spectral Tag Generation

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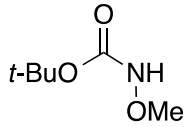
I. General Synthesis Procedures

A. Reagents and Methods

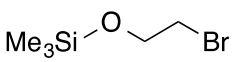
Methoxyamine hydrochloride (98%), sodium hydroxide (≥98%), 2-bromoethanol (95%), imidazole (>99%), chlorotrimethylsilane (99%), triphenyl phosphine (99%), diisopropyl azodicarboxylate (98%), trifluoroacetic acid (99%), *N,N'*-diisopropylcarbodiimide (99%), 4-dimethylaminopyridine (DMAP) (≥98%), and all solvents were purchased from Sigma-Aldrich and used without further purification. Sodium hydride (60% dispersion in mineral oil) was purchased from Acros Organics. Di-*tert*-butyl dicarbonate (99%) was purchased from Oakwood Chemical. *N*-Hydroxyphthalimide (98%), *N,N'*-diisopropylcarbodiimide (99%), and hydrazine monohydrate (99%) were purchased from Alfa Aesar. 3,3,3-$^{2}H_3$-Propionic acid was purchased from Cambridge Isotope Laboratories, Inc. 3-$^{13}C_1$-3,3,3-$^{2}H_3$-Propionic acidand 2,3-$^{13}C_2$-3,3,3-$^{2}H_3$-propionic acid were synthesized using the published procedures.[1,2] The progress of reactions was monitored by thin-layer chromatography (TLC, silica gel 60 Å F-254 plates). The plates were visualized first with UV illumination followed by staining either with phosphomolybdic acid, ninhydrin, or *p*-anisaldehyde solution. Column chromatography was performed using silica gel (230-400 mesh). NMR spectra were obtained using a Varian/Agilent 400-MR NMR spectrometer equipped with a 5 mm *z*-axis gradient AutoX probe operating at the nominal ^{1}H frequency of 399.66 MHz and ^{13}C frequency of 100.49 MHz. All spectra are reported in parts per million (ppm) relative to the residual solvent peak in ^{1}H NMR and the deuterated solvent peak in ^{13}C NMR.

B. MAP Synthesis



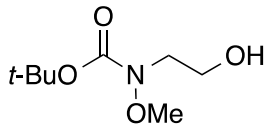
7

***tert*-Butyl *N*-methoxycarbamate (7).** To a solution of methoxyamine hydrochloride (1.50 g, 179.60 mmol) and sodium hydroxide (7.18 g, 179.60 mmol) in a solution of dioxane/water (2:1, 210 mL) at 0 °C was added di-*tert*-butyl dicarbonate (43.1 g, 197.55 mmol). The solution was stirred for 5 minutes at 0 °C and then at room temperature overnight. Dioxane was removed via rotary evaporation and the aqueous layer was extracted with ethyl acetate (3 x 20 mL). The combined organic layer was washed with brine (20 mL), dried over sodium sulfate and concentrated by rotary evaporation. The crude liquid was purified via column chromatography (SiO_2, hexane:ethyl acetate, 1:1 v/v, R_f = 0.70) to afford amide **7** (25.4 g, 96% yield) as a clear liquid, having spectral characteristics in agreement with published data;[3] IR ν (cm^{-1}) 1714, 3276; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.71 (s, 3H), 1.49 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 81.2, 64.0, 28.1; FT-ICR-MS (ESI^+, *m/z*) calcd for $C_7H_{15}NO_3$, $[M + Na]^+$ 170.0788, found 170.0789.



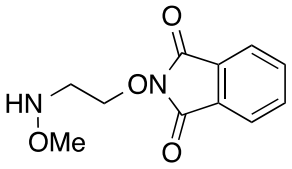
(2-Bromoethoxy)trimethylsilane. To a solution of 2-bromoethanol (10.0 g, 80.0 mmol), imidazole (13.62 g, 200.05 mmol), and DMAP (cat.) in dry CH_2Cl_2 (150 mL) at 0 °C was added chlorotrimethylsilane (10.43 g, 96.03 mmol). The solution was allowed to come to room temperature and stirred overnight. The reaction solution was washed with

water (2 x 50 mL) and brine (1 x 50 mL), dried over sodium sulfate, and purified by short path distillation (20 mbar, collect bp 149.5 °C) with the aid of an acetone-dry ice bath to cool the collection vessel. The product was isolated (14.3 g, 90% yield) as a clear liquid; IR ν (cm^{-1}) 1093, 1255; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (t, J = 8.0 Hz, 2H), 3.34 (t, J = 8.0 Hz, 2H), 0.08 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 62.7, 35.2, 28.2.



8

***tert*-Butyl *N*-(2-hydroxyethyl)-*N*-methoxycarbamate (8).** To a slurry of sodium hydride (2.46 g of 60% in mineral oil, 61.43 mmol) in dry DMF (80 mL) at 0 ˚C was added carbamate **7** (8.59 g, 58.5 mmol). The suspension was stirred until hydrogen evolution ceased whereupon (2-bromoethoxy)trimethylsilane (12.7 g, 64.4 mmol) was added dropwise. The reaction mixture was allowed to warm to room temperature and stirred overnight. The reaction mixture then was diluted with water (80 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic extract was washed successively with 1M citric acid solution (80 mL) and brine (50 mL), and then dried over sodium sulfate. The solvents were removed by rotary evaporation, and the crude liquid was purified by column chromatography (SiO_2, hexane:ethyl acetate, 7:3 v/v, R_f = 0.43) to afford carbamate **8** (5.13 g, 50% yield) as a clear liquid; IR ν (cm^{-1}) 1053, 1699, 3428; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.81 (t, J = 4.0 Hz, 2H), 3.71 (s, 3H), 3.64 (t, J = 4.0 Hz, 2H), 1.51 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 82.1, 62.6, 60.9, 52.0, 28.5; FT-ICR-MS (ESI$^+$, *m/z*) calcd for $C_8H_{17}NO_4$, $[M + H]^+$ 192.1230, found 192.1232.

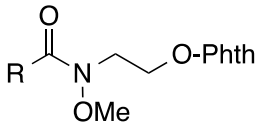


9

2-(2-(Methoxyamino)ethoxy)isoindoline-1,3-dione (9). To a mixture of carbamate **8** (0.813 g, 4.65 mmol), *N*-hydroxyphthalimide (0.985 g, 6.04 mmol) and triphenylphosphine (1.58 g, 6.04 mmol) in dry THF (20 mL) at 0 °C was added diisopropyl azodicarboxylate (1.2 mL, 6.04 mmol). The reaction solution was stirred at room temperature overnight whereupon the solvent was removed via rotary evaporation. The residue was diluted with ethyl acetate (20 mL) and the resultant solution was washed successively with sodium bicarbonate (3 x 20 mL) and brine (20 mL). The organic layer was dried over sodium sulfate and then concentrated by rotary evaporation. The crude product was purified via column chromatography (SiO_2, CH_2Cl_2:ethyl acetate, 9:1 v/v, R_f = 0.65) to afford intermediate *tert*-butyl *N*-(2-((1,3-dioxoisoindolin-2-yl)oxy)ethyl)-*N*-(methoxy)carbamate (1.4 g, 90% yield) as a clear oil; IR ν (cm^{-1}) 1702, 1730; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (m, 2H), 7.76 (m, 2H), 4.39 (t, J = 4.0 Hz, 2H), 3.86 (t, J = 4.0 Hz, 2H), 3.81 (s, 3H), 1.50 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 156.5, 134.7, 129.1, 123.8, 82.1, 63.2, 48.3, 28.4; FT-ICR-MS (ESI^+, *m/z*) calcd for $C_{16}H_{20}N_2O_6$, $[M + Na]^+$ 359.1214, found 359.1213.

To a stirred solution of the *N*-methoxycarbamate intermediate (5.56 g, 16.5 mmol) in CH_2Cl_2 (57 mL) at 0 ˚C was added trifluoroacetic acid (3.8 mL, 49.5 mmol). After stirring 1 h, the reaction mixture was concentrated by rotary evaporation and then diluted by addition of ethyl acetate (20 mL). The resultant solution was washed with sodium bicarbonate (3 x 20 mL) and brine (20 mL), dried over sodium sulfate, and concentrated

via rotary evaporation. The crude product was purified via column chromatography (SiO_2, hexane:ethyl acetate, 1:1 v/v, R_f = 0.53) to afford amine **9** (2.57 g, 66% yield) as a white solid, mp 65.6-65.9 °C; IR ν (cm^{-1}) 1711, 3265; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 (m, 2H), 7.76 (m, 2H), 4.39 (t, J = 8.0 Hz, 2H), 3.61 (s, 3H), 3.25 (t, J = 4.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 134.6, 128.8, 123.6, 74.8, 61.6, 49.6; FT-ICR-MS (ESI^+, *m/z*) calcd for $C_{11}H_{12}N_2O_4$, $[M + H]^+$ 237.0870, found 237.0872.

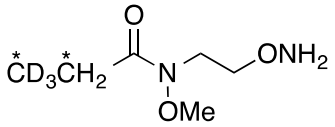


10a: R = CD_3CH_2
10b: R = $^{13}CD_3CH_2$
10c: R = $^{13}CD_3{}^{13}CH_2$

***N*-(2-((1,3-Dioxoisoindolin-2-yl)oxy)ethyl)-*N*-methoxy-3,3,3-$^2H_3$-propionamide (10a).** To a solution of amine **9** (0.405 g, 1.72 mmol) and DMAP (cat.) in CH_2Cl_2 (6 mL) at 0 ˚C was added *N,N'*-diisopropylcarbodiimide (0.7 mL, 4.44 mmol). After 5 minutes of stirring, 3,3,3-$^2H_3$-propionic acid (0.116 mL, 1.56 mmol) was added and the reaction mixture was allowed to warm to room temperature and stirred overnight. The reaction mixture was filtered through a fritted glass funnel and then concentrated by rotary evaporation. The crude residue was purified by column chromatography (SiO_2, hexane:ethyl acetate, 3:7 v/v, R_f = 0.65) to afford amide **10a** (0.399 g, 91% yield) as a colorless oil; IR ν (cm^{-1}) 1728; ^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (m, 2H), 7.75 (m, 2H), 4.39 (t, J = 4 Hz, 2H), 4.02 (t, J = 4 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.3, 163.5, 134.7, 129.3, 123.8, 75.4, 62.7, 45.6, 25.4, 14.4,; FT-ICR-MS (ESI^+, *m/z*) calcd for $C_{14}H_{13}D_3N_2O_5$, $[M + H]^+$ 296.1320, found 296.13226.

***N*-(2-((1,3-Dioxoisoindolin-2-yl)oxy)ethyl)-*N*-methoxy-3-$^{13}C_1$-3,3,3-$^{2}H_3$-propionamide (10b).** Using the procedure outlined above for the synthesis of amide **10a**, amine **9** (0.330 g, 1.40 mmol) was reacted with *N,N'*-diisopropylcarbodiimide (0.3 mL, 1.91 mmol), 3-$^{13}C_1$-3,3,3-$^{2}H_3$-propionic acid (0.1 mL, 1.27 mmol) and DMAP (cat.) to afford amide **10b** (0.265 g, 79% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (m, 2H), 7.75 (m, 2H), 4.39 (t, *J* = 4 Hz, 2H), 4.00 (t, *J* = 4 Hz, 2H), 3.80 (s, 3H), 2.50 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5, 134.8, 129.1, 123.8, 75.3, 62.6, 45.4, 25.2, 8.6-7.4 (m); FT-ICR-MS (ESI^+, *m/z*) calcd for $C_{13}{}^{13}CH_{13}D_3N_2O_5$, $[M + H]^+$ 297.1354, found 297.1356.

***N*-(2-((1,3-Dioxoisoindolin-2-yl)oxy)ethyl)-*N*-methoxy-2,3-$^{13}C_2$-3,3,3-$^{2}H_3$-propionamide (10c).** Using the procedure outlined above for the synthesis of amide **10a**, amine **9** (0.359 g, 1.52 mmol) was reacted with *N,N'*-diisopropylcarbodiimide (0.7 mL, 4.34 mmol), 2,3-$^{13}C_2$-3,3,3-$^{2}H_3$-propionic acid (0.115 mL, 1.45 mmol) and DMAP (cat.) to afford amide **10c** (0.062 g, 14% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (m, 2H), 7.75 (m, 2H), 4.38 (t, *J* = 4 Hz, 2H), 4.01 (t, *J* = 4 Hz, 2H), 3.80 (s, 3H), 2.50 (dd, *J* = 4, 128 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 134.5, 128.8, 123.6, 75.0, 62.4, 45.2, 25.3-24.8 (m), 8.5-7.0 (m); FT-ICR-MS (ESI^+, *m/z*) calcd for $C_{12}{}^{13}C_2H_{11}D_3N_2O_5$, $[M + H]^+$ 298.1384, found 298.1389.



MAP-32
MAP-33
MAP-34

***N*-(2-(Aminooxy)ethyl)-*N*-methoxy-3,3,3-$^{2}H_3$-propionamide (MAP-32).** To a solution of **10a** (0.399 g, 1.35 mmol) in CH_2Cl_2 (5 mL) at 0 ˚C was added hydrazine monohydrate (0.069 mL, 1.42 mmol) dropwise. The reaction mixture was stirred at 0 ˚C for 10 minutes before warming to room temperature and then stirring 45 minutes. The reaction was filtered through a fritted glass funnel, and the filtrate was concentrated by rotary evaporation. The crude product was purified by column chromatography (SiO_2, CH_2Cl_2:MeOH, 9:1 v/v, R_f = 0.41) to afford **MAP-32** (0.118 g, 53% yield) as a clear liquid; IR ν (cm^{-1}) 1728, 2942, 2983; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.66 (br. S, 2H) 4.04 (t, *J* = 4 Hz, 2H), 3.56 (s, 3H), 3.15 (t, *J* = 4 Hz, 2H), 2.11 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 70.9, 61.6, 50.0, 25.2, 14.0; FT-ICR-MS (ESI^+, *m/z*) calcd for $C_6H_{11}D_3N_2O_3$, $[M + H]^+$ 166.1265, found 166.1268.

***N*-(2-(Aminooxy)ethyl)-*N*-methoxy-3-$^{13}C_1$-3,3,3-$^{2}H_3$-propionamide (MAP-33).** Using the procedure outlined above for the synthesis of **MAP-32**, amide **10b** (0.265 g, 1.00 mmol) was reacted with hydrazine monohydrate (0.058 mL, 1.05 mmol) to afford **MAP-33** (0.034 g, 20% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.03 (t, *J* = 4 Hz, 2H), 3.55 (s, 3H), 3.14 (t, *J* = 4 Hz, 2H), 2.48 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 80.0, 61.6, 50.0, 25.0, 8.9-7.3 (m); FT-ICR-MS (ESI^+, *m/z*) calcd for $C_5{}^{13}CH_{11}D_3N_2O_3$, $[M + H]^+$ 167.1299, found 167.1301.

***N*-(2-(Aminooxy)ethyl)-*N*-methoxy-2,3-$^{13}C_2$-3,3,3-$^{2}H_3$-propionamide (MAP-34).** Using the procedure outlined above for the synthesis of **MAP-32**, amide **10c** (0.062 g, 0.21 mmol) was reacted with hydrazine monohydrate (0.011 mL, 0.22 mmol) to afford **MAP-33** (0.018 g, 51% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.79 (br. s, 2H), 4.03 (t, *J* = 4.0 Hz, 2H), 3.55 (s, 3H), 3.14 (t, *J* = 4.0 Hz, 2H), 2.12 (d, *J* = 128, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 73.1, 61.6, 49.8, 26.5-25.1 (m), 7.54-9.27 (m); FT-ICR-MS (ESI^+, *m/z*) calcd for $C_4{}^{13}C_2H_9D_3N_2O_3$, $[M + H]^+$ 168.1330, found 168.1335.

II. GC-MS Analyses

A. General Procedure

All GC-MS analyses were performed using an Agilent Technologies GC-MS instrument (Agilent Technologies, Palo Alto, CA); GC consisting of an Agilent 7820A gas chromatograph, and an Agilent 5975 MSD. The GC was fitted with an HP-5MS column 30 m long with an internal diameter of 250 μm and a stationary-phase film thickness of 0.25 μm. The carrier was high-purity helium at a flow rate of 1.0 mL/min. Sample size was 1 μL with a 10:1 split ratio. The injector temperature was 275 °C; the column temperature was programmed to start at 60 °C and increase at 20 °C/min, to a maximum of 315 °C, giving a 12.5 minute run, although the run was usually stopped at about 10 minutes. A 120 second solvent delay was allowed. The transfer line temperature was 250 °C. The MS ion source was held at 230 °C and the MS Quad at 150 °C. The electron ionization energy was 70 eV. Mass spectra were collected from 25 to 400 m/z.

B. Sample Preparation for Study of GC Retention Time and MST Generation

Representative sample mixtures were prepared and derivatized by treatment with an excess (~2 equiv) of reagent, either MAP-32 or MAP-33, to afford the derivatized mixtures A1-32, A2-32, B1-33 and B2-33. Aliquots (0.5 mL) of the A1 and B1 derivatized mixtures, and the A2 and B2 mixtures, were combined, respectively, and then directly injected into the GC-MS instrument for analysis. The two sample mixtures were analyzed by GC-MS a total of three times.

Sample Mixture A1-32. To generate sample mixture A1-32, solutions of benzaldehyde (50 μL of a 0.01 M solution), hexanal (50 μL of a 0.01 M solution), and 2-propoxyacetaldehyde (50 μL of a 0.01 M solution) were added to acetonitrile (5 mL). To this mixture at room temperature was added MAP-32 (250 μL of a 0.015 M solution). After the solution was heated at 60 °C for 16 hours, the solution was allowed to cool to room temperature and the acetonitrile was removed via rotary evaporation. The mixture then was reconstituted by dissolving in acetonitrile (2 mL) to generate mixture A1-32.

Sample Mixture B1-33. To generate sample mixture B1-33, solutions of benzaldehyde (50 μL of a 0.01 M solution), hexanal (50 μL of a 0.01 M solution), and 2-propoxyacetaldehyde (50 μL of a 0.01 M solution) were added to acetonitrile (5 mL). To this mixture at room temperature was added MAP-33 (200 μL of a 0.019 M solution). After the solution was heated at 60 °C for 16 hours, the solution was allowed to cool to room temperature and the acetonitrile was removed via rotary evaporation. The mixture then was reconstituted by dissolving in acetonitrile (2 mL) to generate mixture B1-33.

Sample Mixture A2-32. To generate sample mixture A2-32, solutions of benzaldehyde

(50 μL of a 0.01 M solution), hexanal (150 μL of a 0.01 M solution), and 2-propoxyacetaldehyde (50 μL of a 0.01 M solution) were added to acetonitrile (5 mL). To this mixture at room temperature was added MAP-32 (500 μL of a 0.015 M solution). After the solution was heated at 60 °C for 16 hours, the solution was allowed to cool to room temperature and the acetonitrile was removed via rotary evaporation. The mixture then was reconstituted by dissolving in acetonitrile (2 mL) to generate mixture A2-32.

Sample Mixture B2-33. To generate sample mixture B2-33, solutions of benzaldehyde (50 μL of a 0.01 M solution), hexanal (50 μL of a 0.01 M solution), and 2-propoxyacetaldehyde (150 μL of a 0.01 M solution) were added to acetonitrile (5 mL). To this mixture at room temperature was added MAP-33 (400 μL of a 0.019 M solution). After the solution was heated at 60 °C for 16 hours, the solution was allowed to cool to room temperature and the acetonitrile was removed via rotary evaporation. The mixture then was reconstituted by dissolving in acetonitrile (2 mL) to generate mixture B2-33.

C. GC-MS Study of Pooled Sample Mixtures A1-B1 and A2-B2

Tables 1 and 2 summarize the MST ion counts measured for each injection of the multiplexed sample mixtures.

Table 1. Summary of measured ion counts for MSTs generated on analysis of multiplexed A1–B1 (*E*-isomer comparison).

Carbonyl Substrate	MST (*m/z*)	Actual Substrate Ratio (source)	Measured ion counts (*E*-isomer) over three injections	Total ion counts	Ratio
Benzaldehyde	32	1 (fr. A1)	398, 722, 608	1,728	0.94
	33	1 (fr. B1)	604, 628, 599	1,831	
Hexanal	32	1 (fr. A1)	6982, 6584, 7283	20,849	0.94
	33	1 (fr. B1)	6528, 6926, 6076	19,530	
n-Propoxy-acetaldehyde	32	1 (fr. A1)	6819, 7009, 7409	21,237	0.88
	33	1 (fr. B1)	8115, 7668, 8433	24,216	

Carbonyl Substrate	MST (*m/z*)	Actual Substrate Ratio (source)	Measured ion counts (*E*-isomer) over three injections	Total ion counts	Ratio
Benzaldehyde	32	1 (fr. A2)	6549, 6435, 6617	19,601	0.92
	33	1 (fr. B2)	6510, 7172, 7566	21,248	
Hexanal	32	3 (fr. A2)	55800, 66744, 60656	183,200	0.34
	33	1 (fr. B2)	18360, 23064, 20904	62,328	
n-Propoxy-acetaldehyde	32	1 (fr. A2)	11742, 14967, 13662	40,371	0.42

	33	3 (fr. B2)	27259, 35464, 32664	95,387	

Table 2. Summary of measured ion counts for MSTs generated on analysis of multiplexed A2–B2 (*E*-isomer comparison).

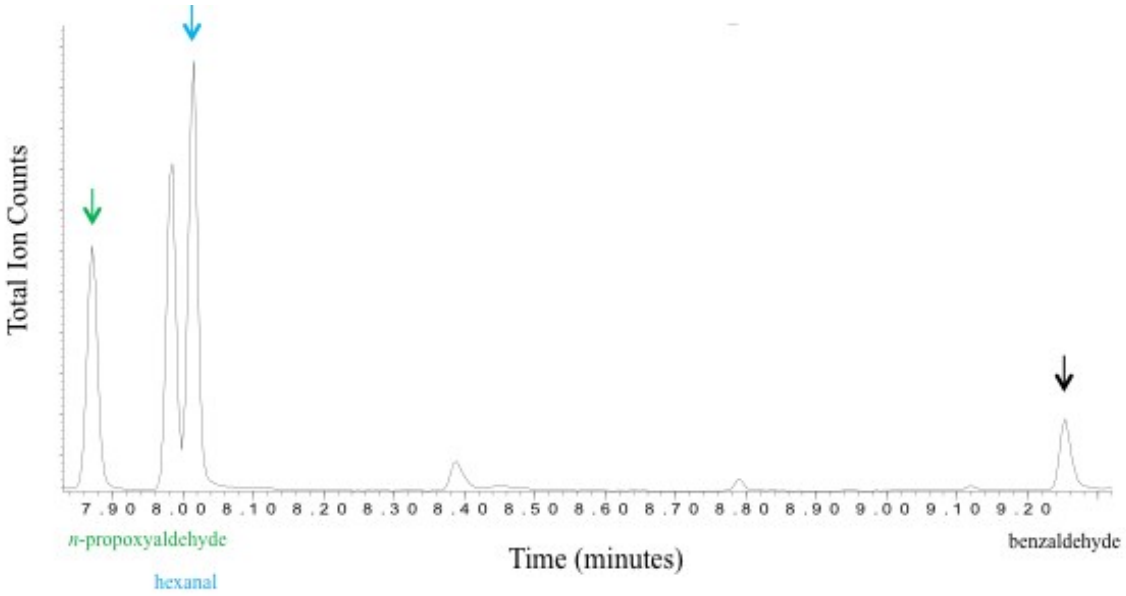
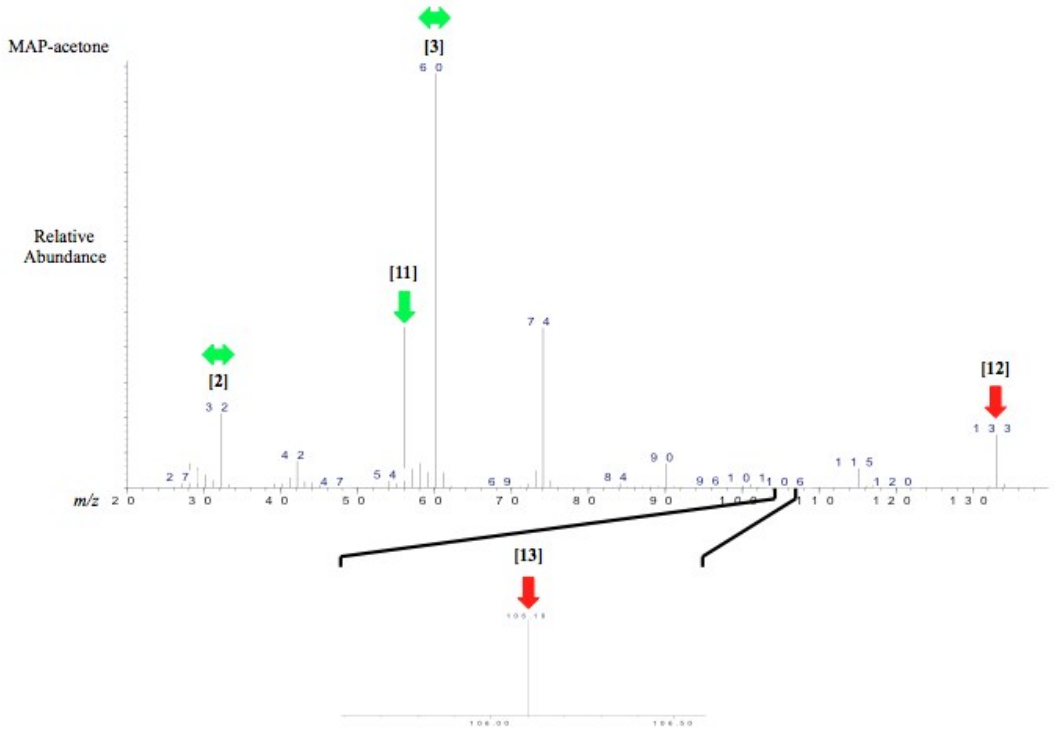


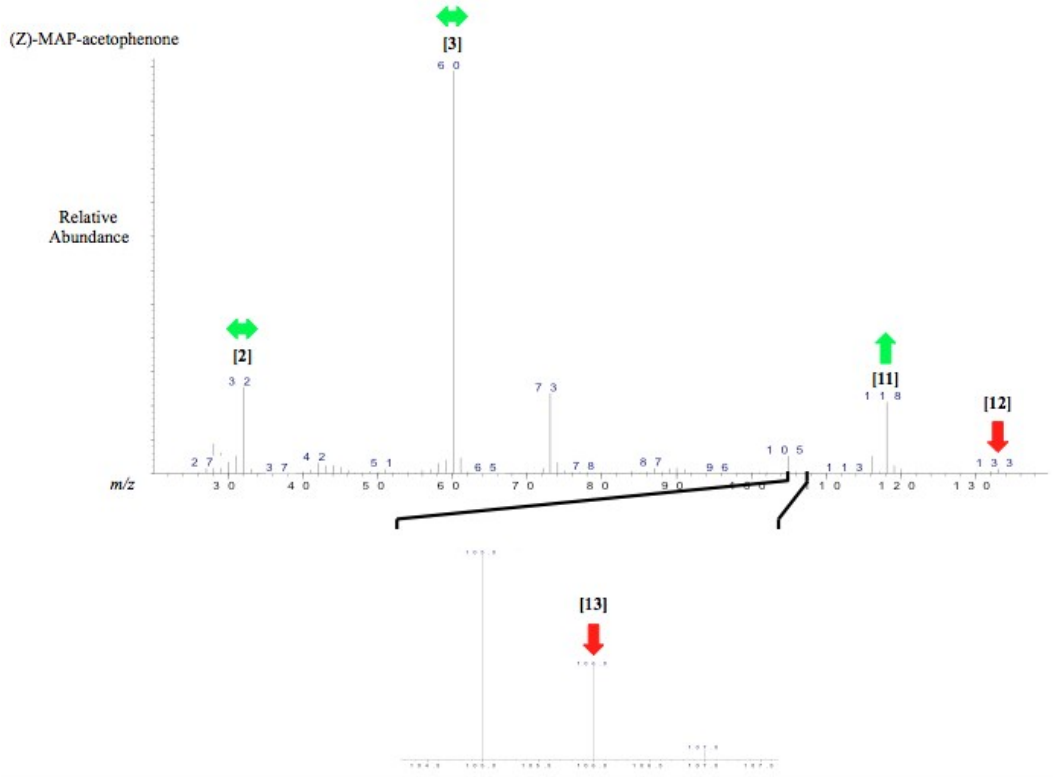
Figure S1. GC trace obtained on injection of pooled sample mixture A2-B2 showing the retention times of MAP32- and MAP33-carbonyl adducts. The *E*-isomer adducts are indicated by colored arrows. The *Z*-isomer adducts of *n*-propoxyacetaldehyde and benzaldehyde are present in trace amounts, so all calculations were preformed using the *E*-isomers.

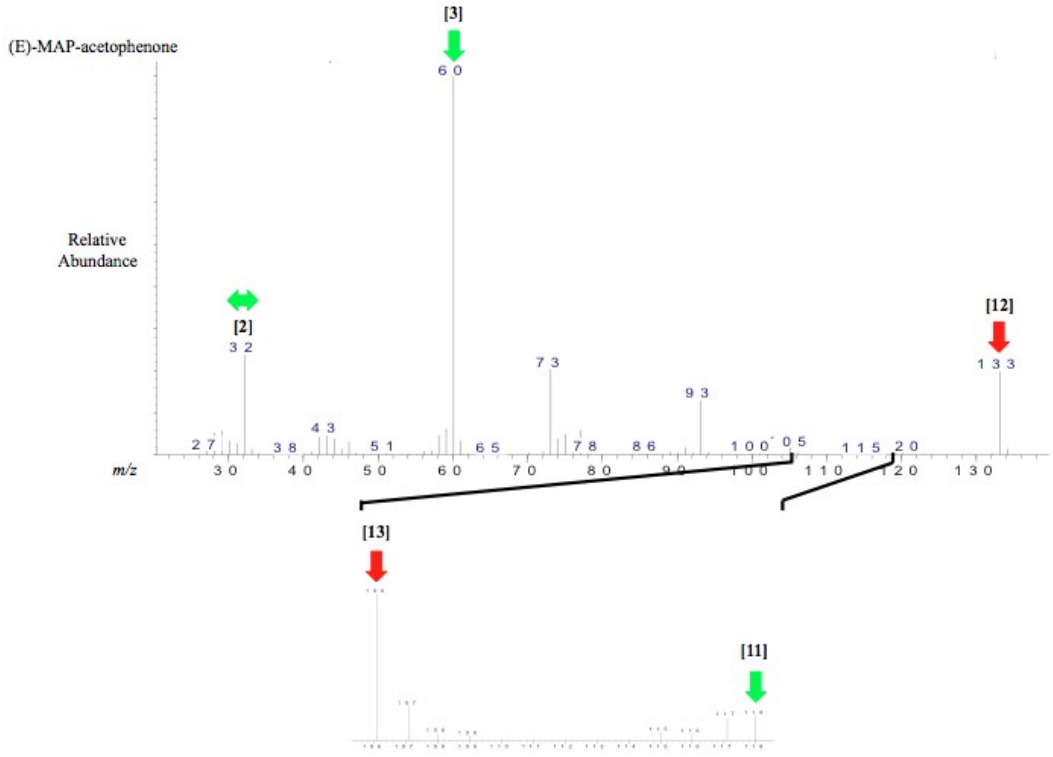
III. Comparisons of EI-Induced Fragmentations of MAP- and AEP-Adducts

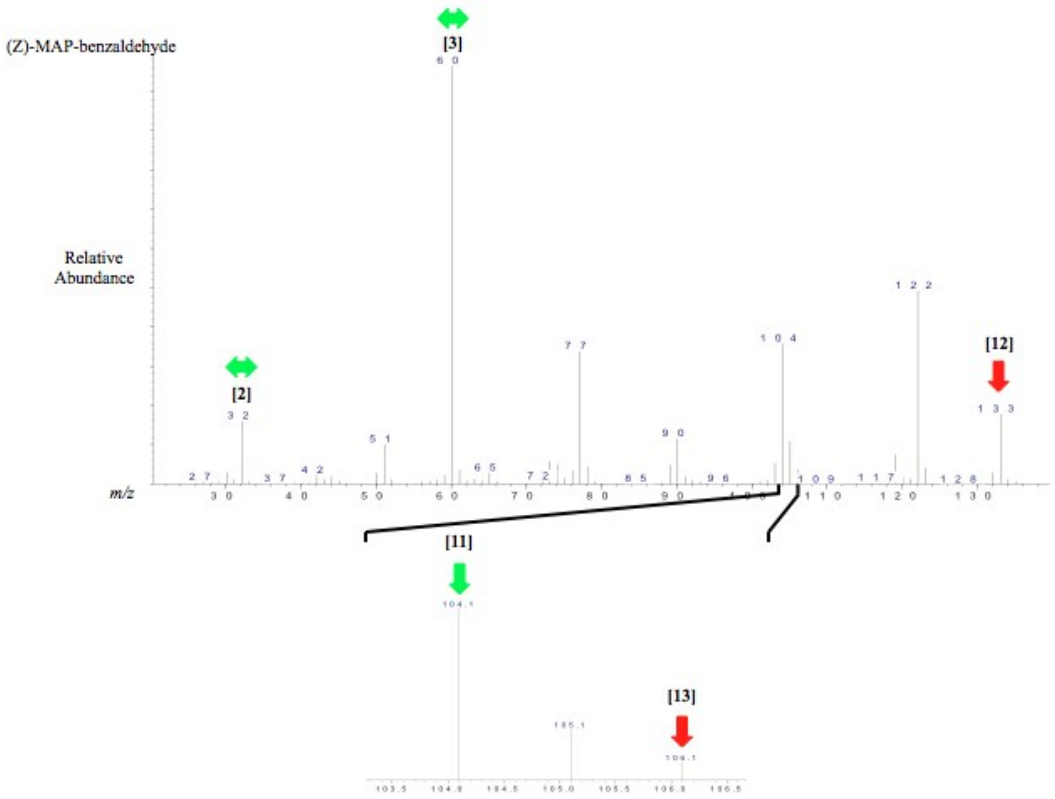
Shown below are the MS spectra obtained for the MAP-carbonyl adducts. To correlate signals of specific fragment ions derived from the MAP adducts to the corresponding ions derived from the AEP adducts, arrows are added to reflect relative changes: (1) an increase (up arrow) in signal intensity or decrease (down arrow) in signal intensity relative to the corresponding AEP-derived fragment ion; (2) ion resulting from

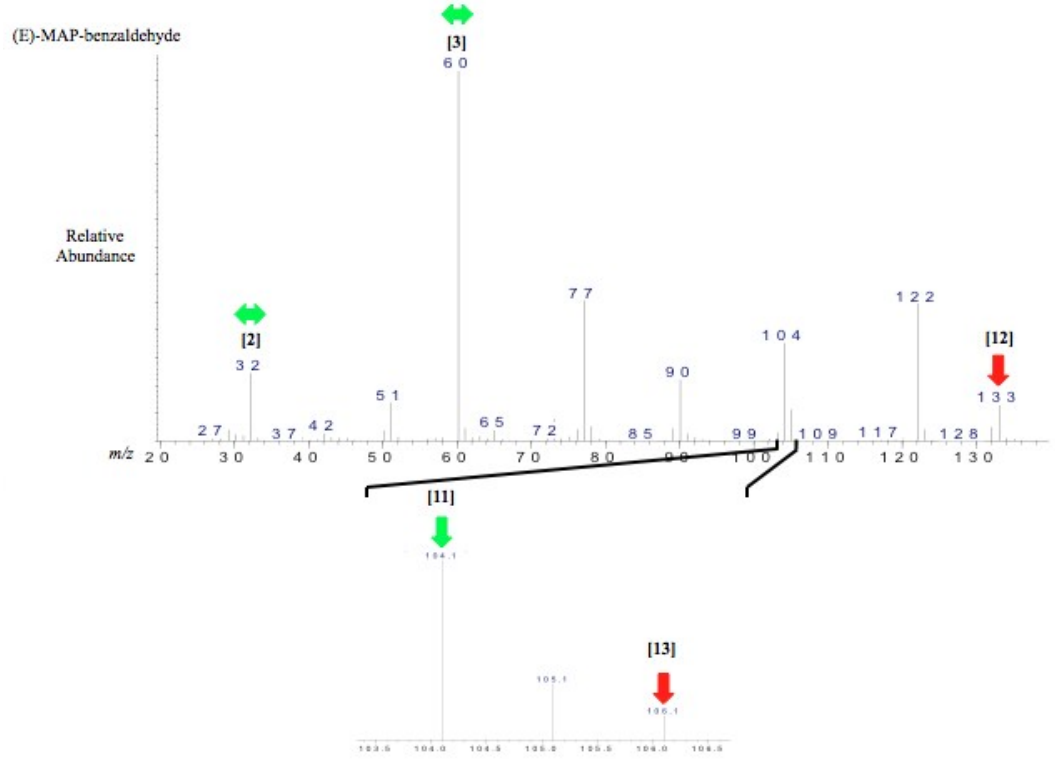
an informative (green) or uninformative (red) fragmentation. The fragment ion labels correspond to those identified in Scheme 5.

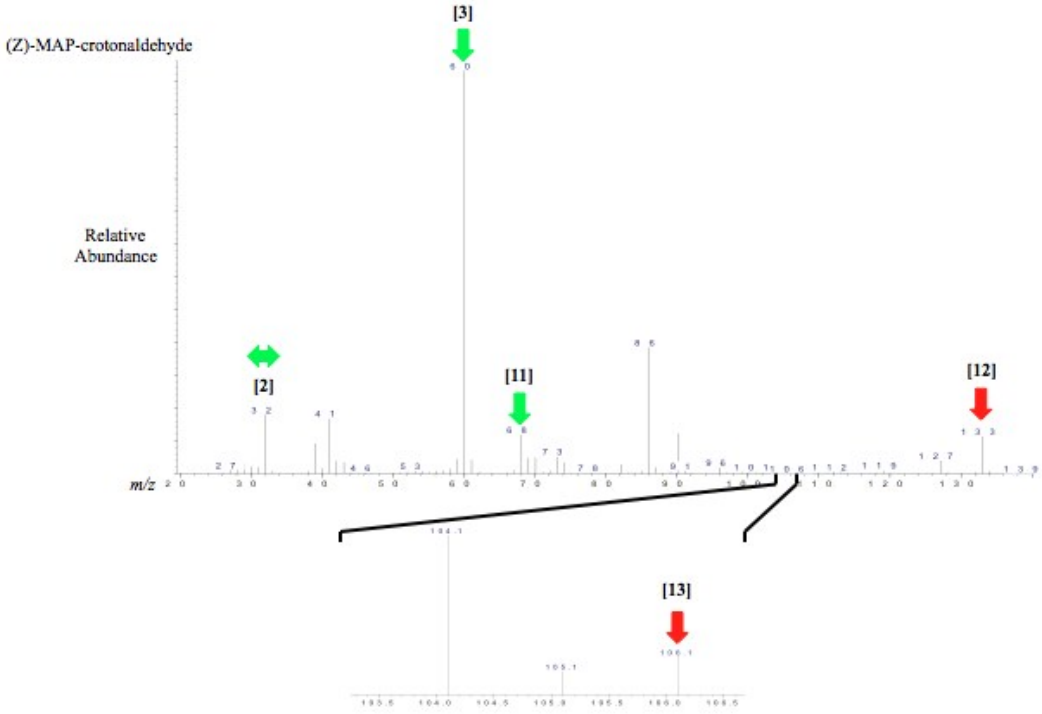


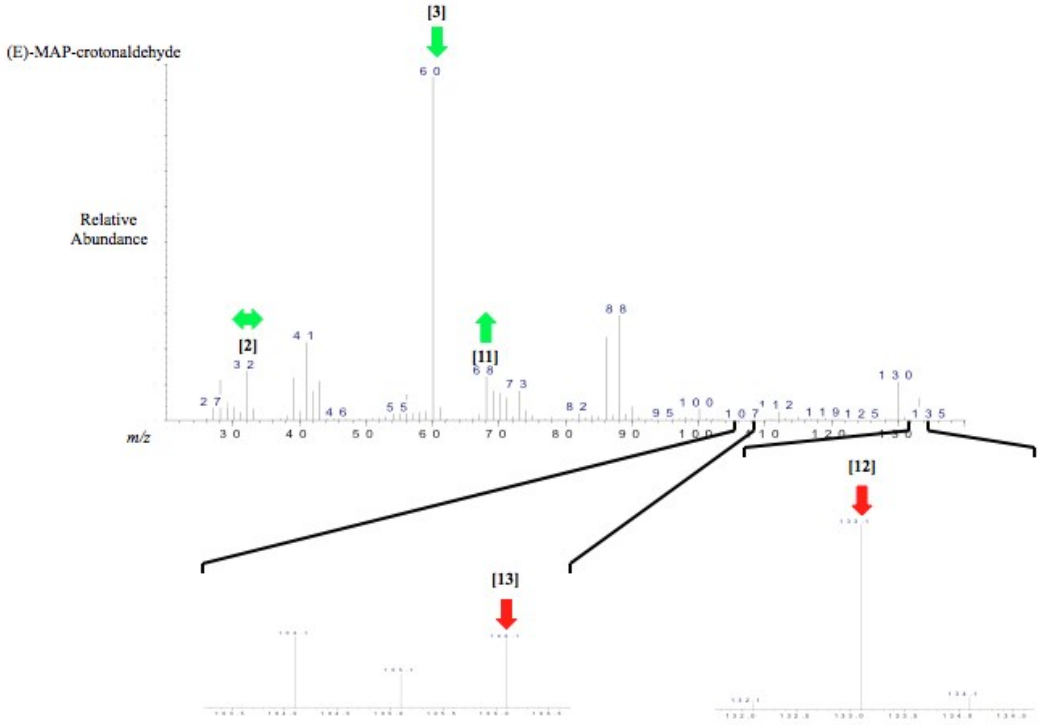

(Z)-MAP-acetophenone
[3]
Relative Abundance
[2]
[11]
[12]
[13]
m/z

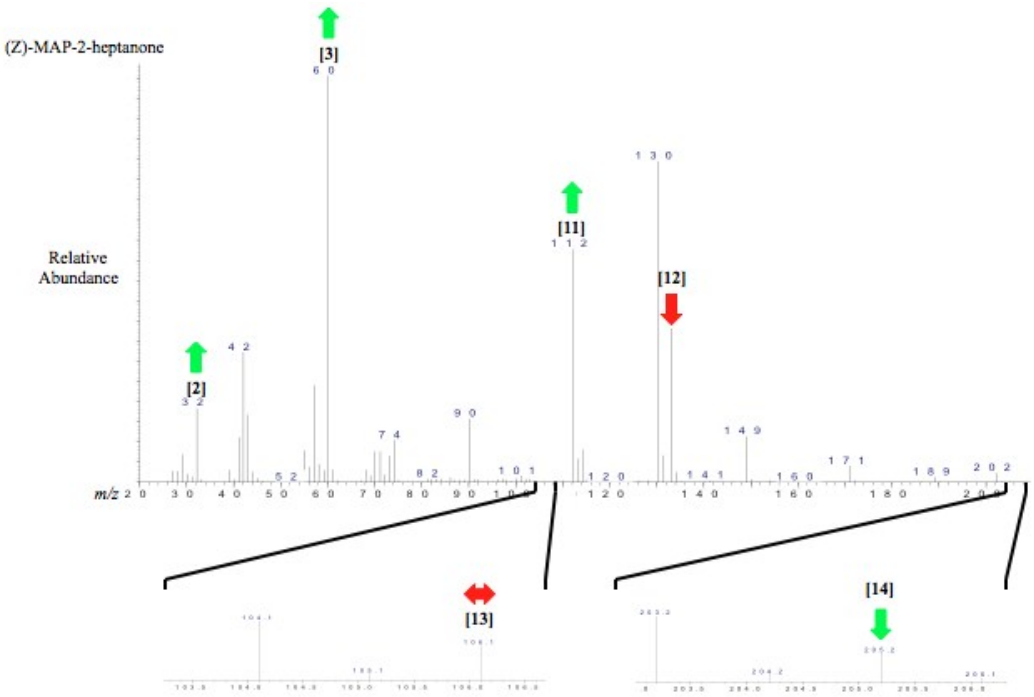

(E)-MAP-acetophenone
[3]
Relative Abundance
[2]
[12]
[13]
[11]
m/z

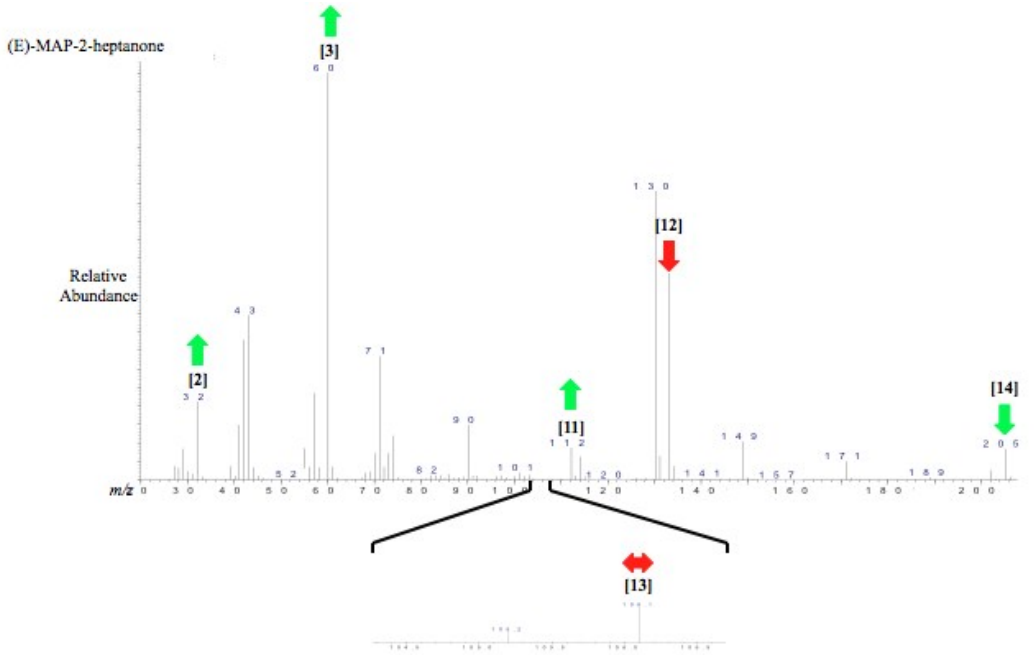

(Z)-MAP-benzaldehyde
Relative Abundance
m/z
[2]
[3]
[11]
[12]
[13]

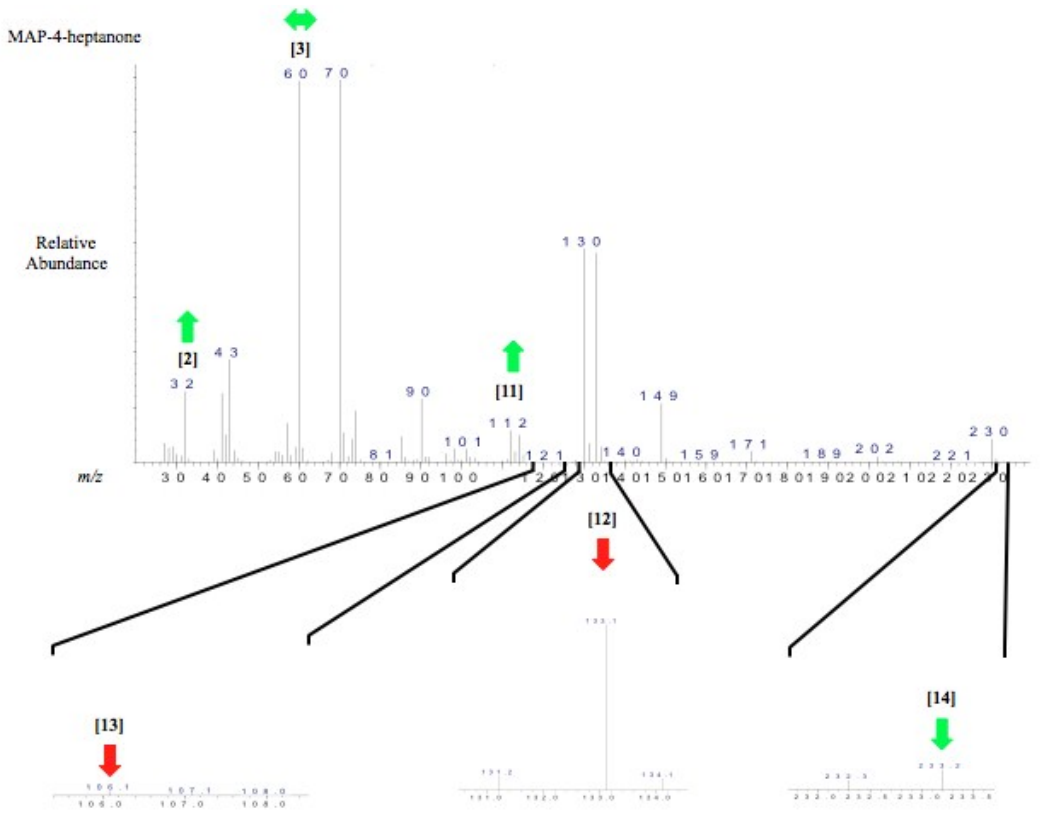

(E)-MAP-benzaldehyde
Relative Abundance
m/z
[2]
[3]
[11]
[12]
[13]

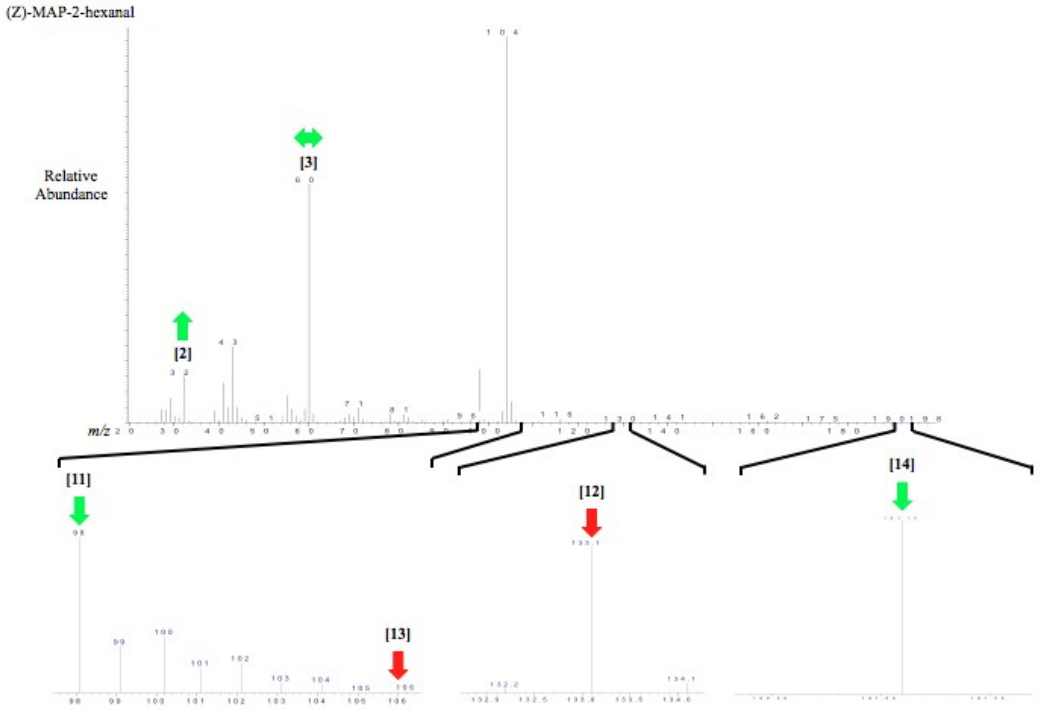

(Z)-MAP-crotonaldehyde
Relative Abundance
m/z
[2]
[3]
[11]
[12]
[13]


(E)-MAP-crotonaldehyde
Relative Abundance
m/z
[2]
[3]
[11]
[12]
[13]

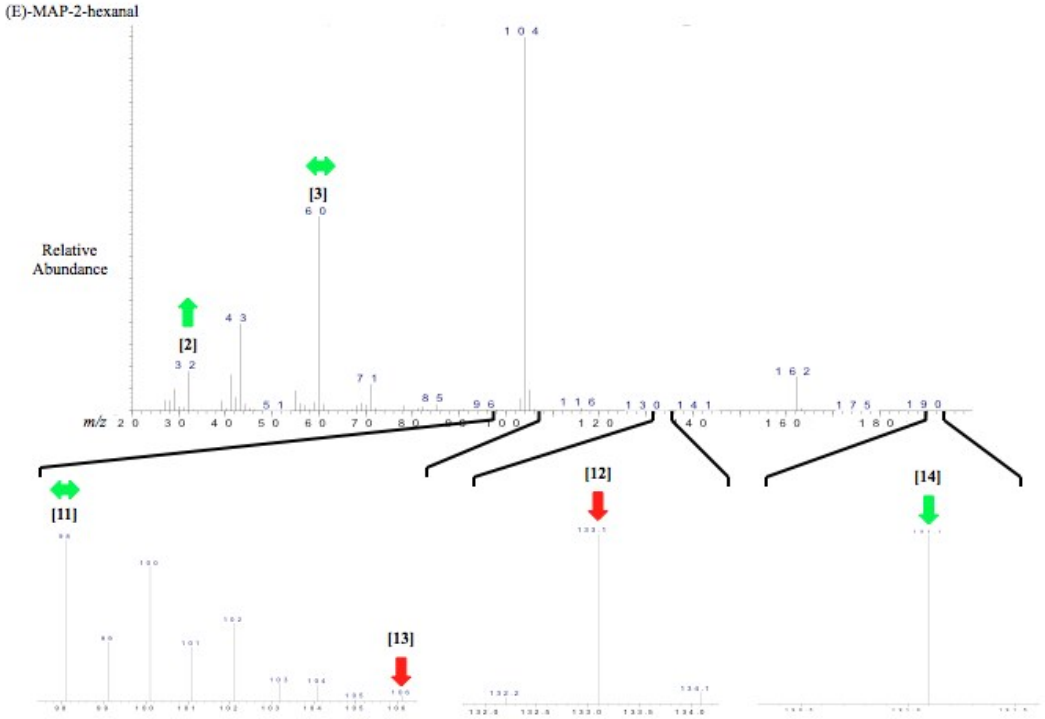

(Z)-MAP-2-heptanone
Relative Abundance
m/z
[2]
[3]
[11]
[12]
[13]
[14]


(E)-MAP-2-heptanone
Relative Abundance
m/z
[2]
[3]
[11]
[12]
[13]
[14]

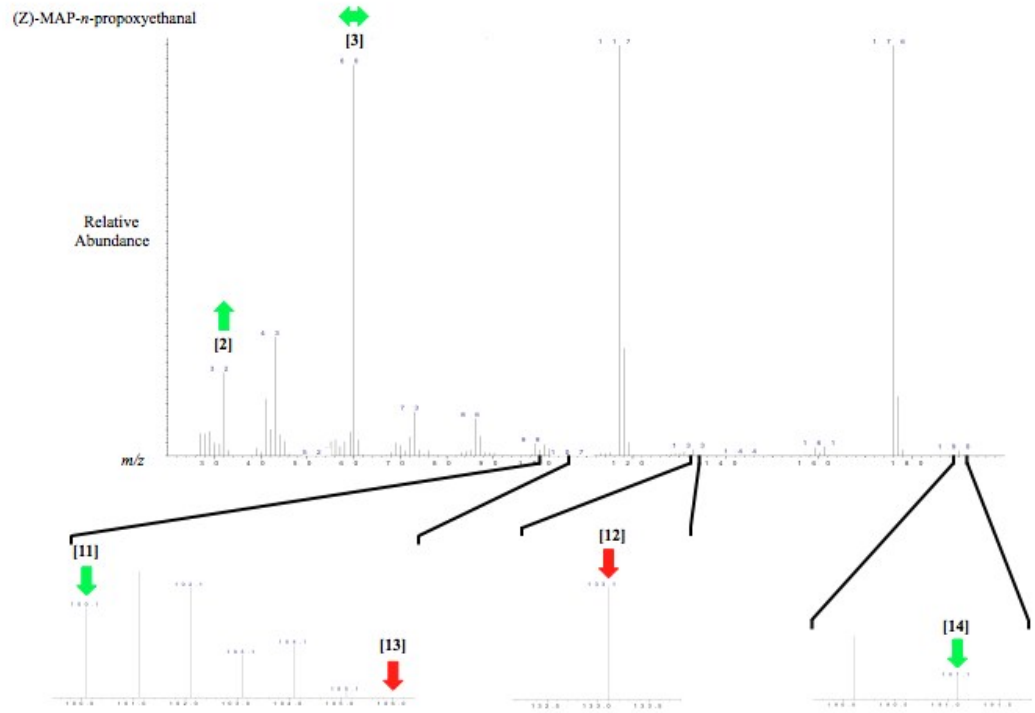

MAP-4-heptanone
[3]
Relative Abundance
[2]
[11]
[12]
[13]
[14]
m/z

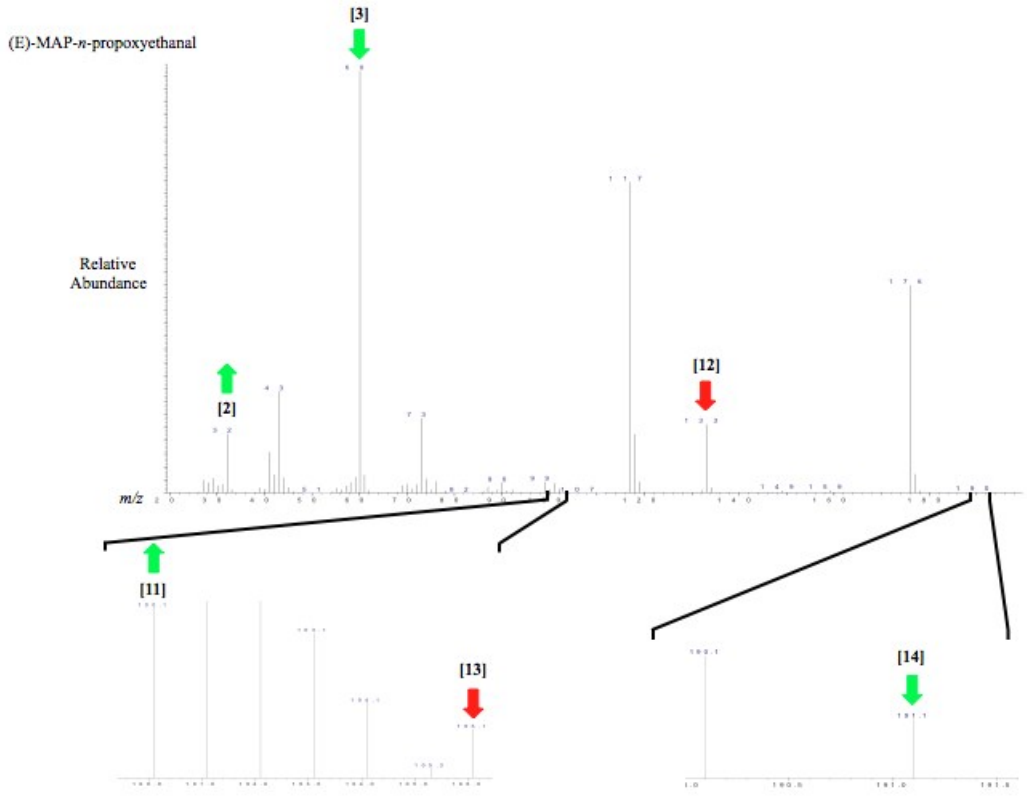

(Z)-MAP-2-hexanal
[3]
Relative Abundance
[2]
[11]
[12]
[13]
[14]
m/z

(E)-MAP-2-hexanal

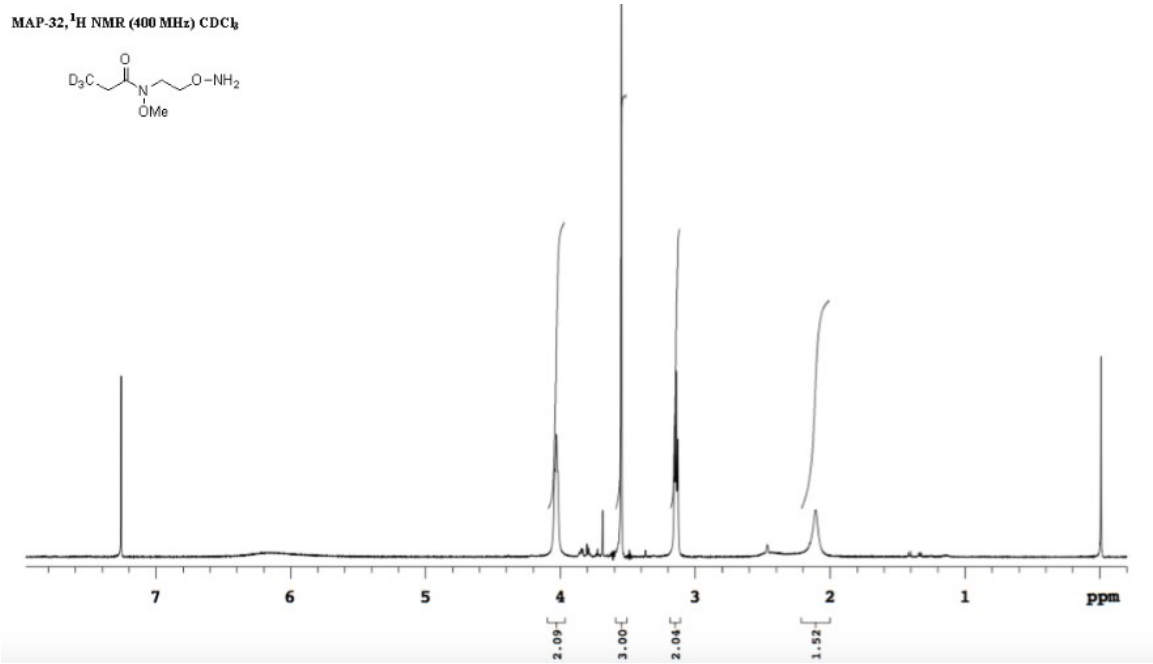


(Z)-MAP-*n*-propoxyethanal

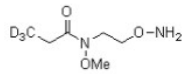




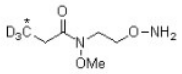
IV. ^{1}H and ^{13}C NMR Spectra of MAP Reagent Panel



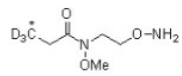
MAP-32, ^{13}C NMR (125 MHz) $CDCl_3$



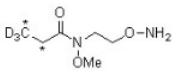
MAP-33, ^{1}H NMR (500 MHz) $CDCl_3$

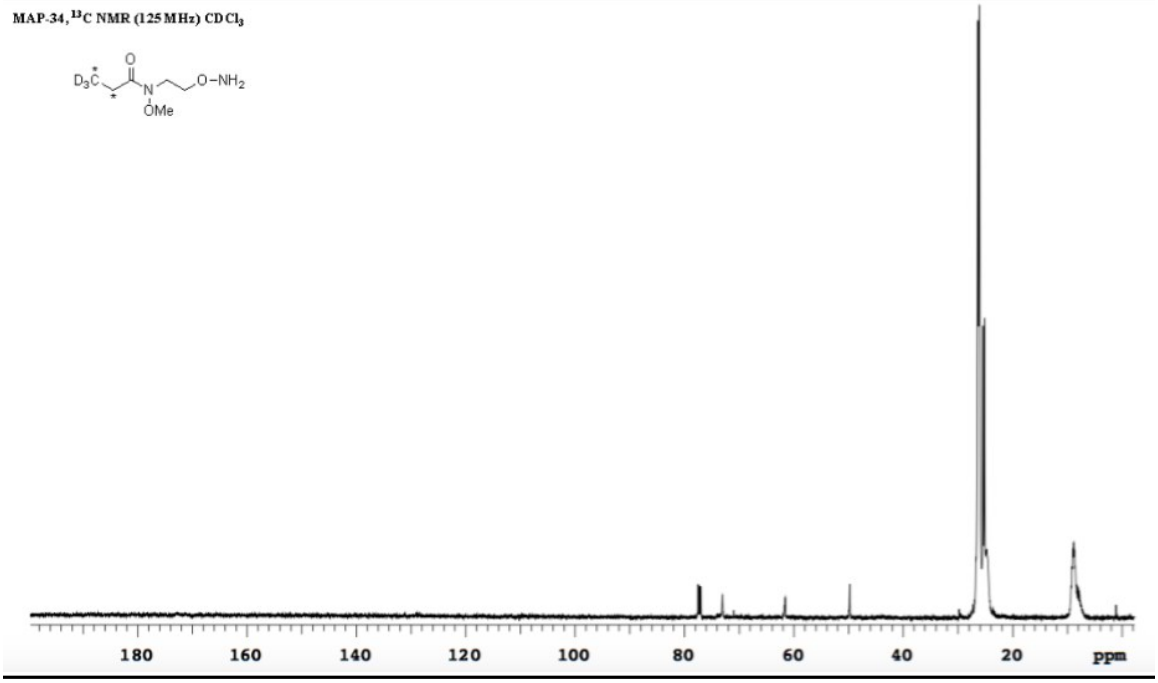


MAP-33, ^{13}C NMR (125 MHz) $CDCl_3$



MAP-34, ^{1}H NMR (500 MHz) $CDCl_3$





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