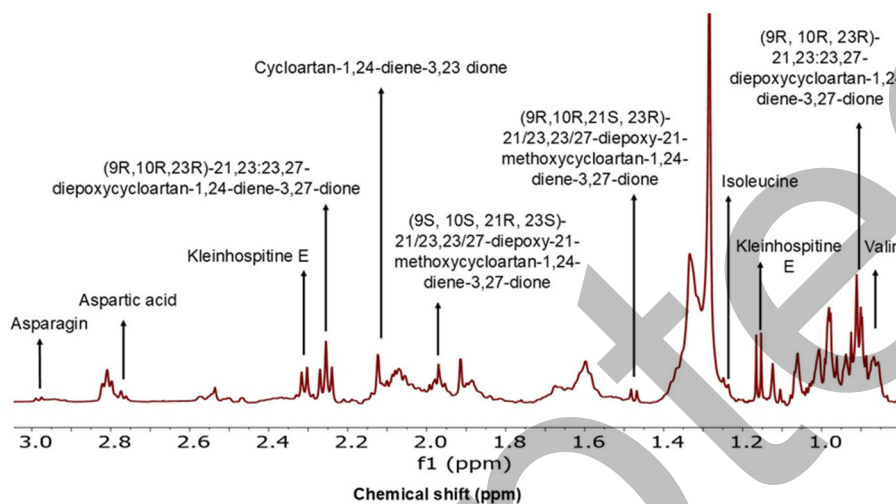
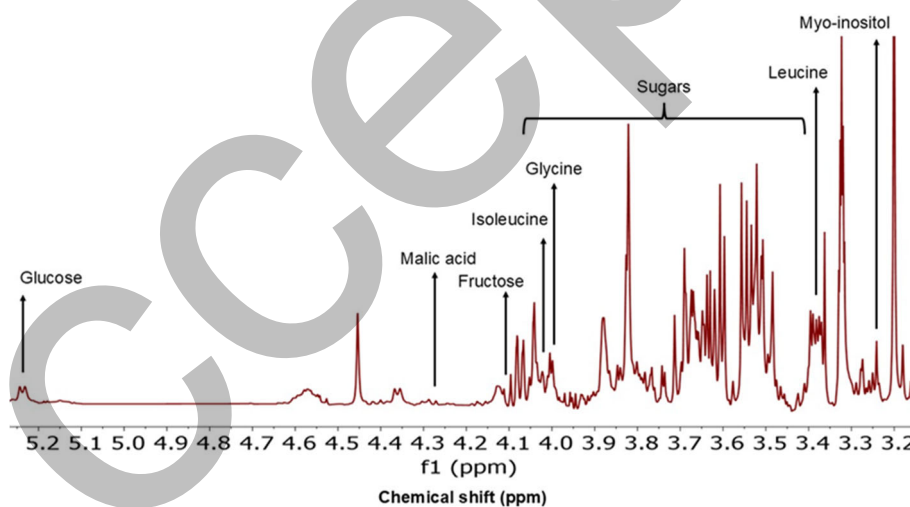


### Supplementary Data

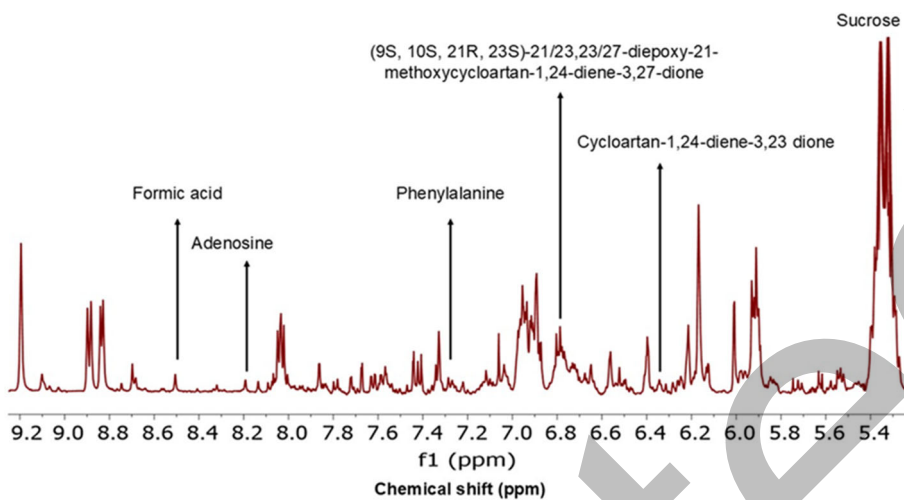
This supplementary data is a part of a paper entitled “Evaluation of *Kleinhovia hospita* Metabolite Profiles Exposed to Diverse Gamma-Irradiation Doses by  $^1\text{H}$ -NMR Combined with Chemometric Modeling”.



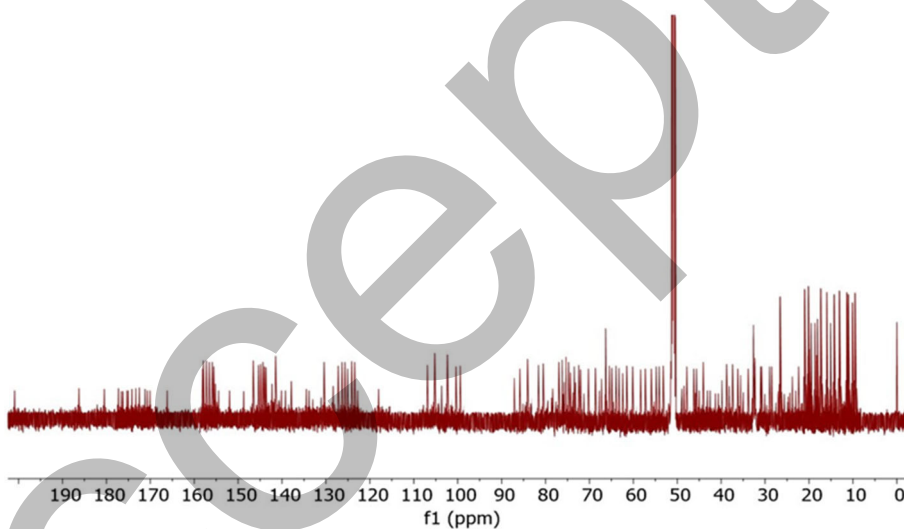
**Fig S1.** Magnification of the  $^1\text{H}$ -NMR spectrum of the group that was not treated to gamma irradiation in the 0.8–3.0 ppm region



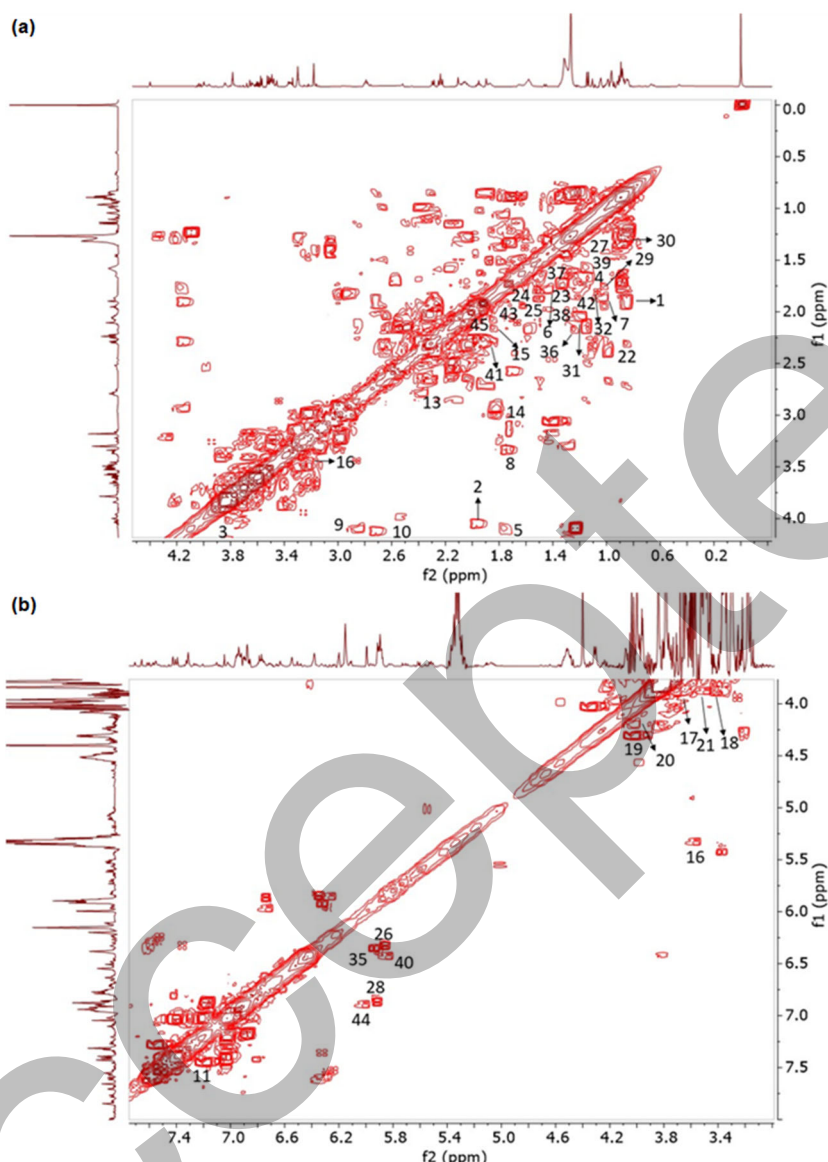
**Fig S2.** Magnification of the  $^1\text{H}$ -NMR spectrum of the group that was not exposed to gamma irradiation in the 3.2–5.3 ppm region



**Fig S3.** Magnification of the <sup>1</sup>H-NMR spectrum of the group that was not exposed to gamma irradiation in the 5.3–9.2 ppm region

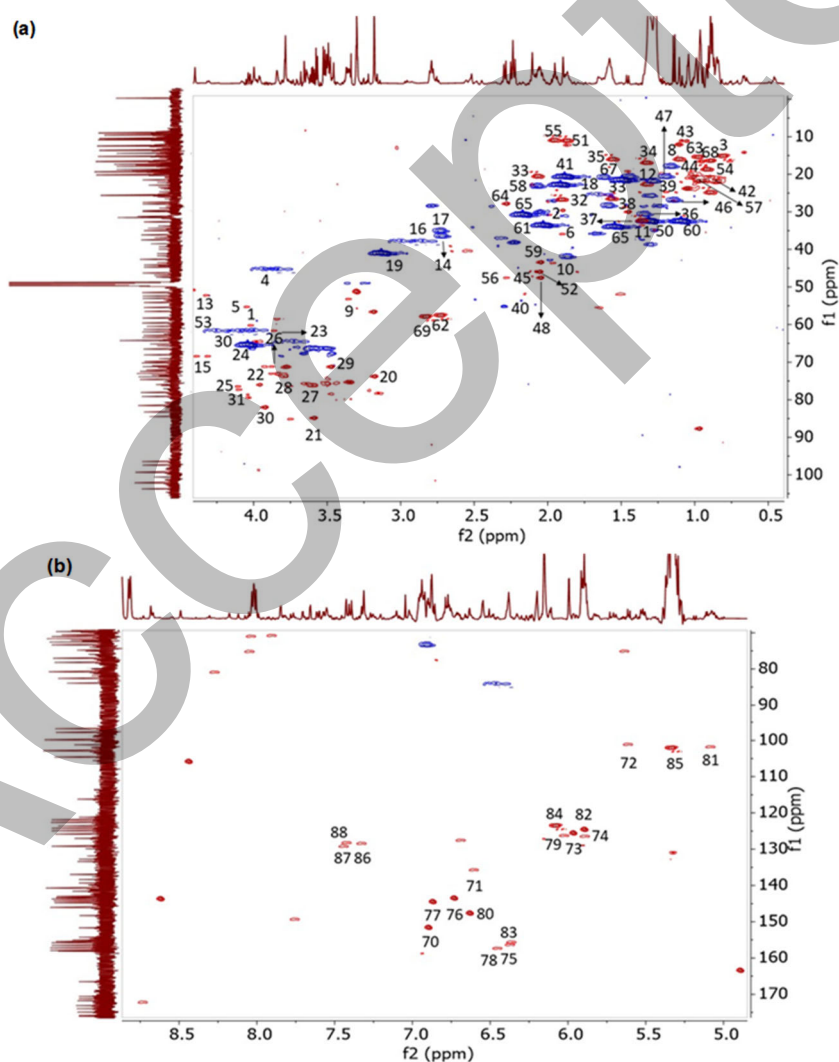


**Fig S4.** The <sup>13</sup>C-NMR spectrum of the group that was not exposed to gamma irradiation



**Fig S5.** The signal correlation of identified metabolites in the COSY spectrum of the group untreated sample. (a) Magnification COSY spectrum in the 0.2–4.2 ppm region, (b) Magnification COSY spectrum in the 3.4–7.5 ppm region. **1.** CH<sub>3</sub>/H<sub>3</sub> of valine, **2.** H<sub>2</sub>/H<sub>3</sub> of valine, **3.** H<sub>2</sub>/H<sub>2</sub> of glycine, **4.** H<sub>4</sub>/H<sub>3</sub> of isoleucine, **5.** H<sub>3</sub>/H<sub>2</sub> of isoleucine, **6.** CH<sub>3</sub>/H<sub>4</sub> of leucine, **7.** H<sub>3</sub>/H<sub>4</sub> of leucine, **8.** H<sub>3</sub>/H<sub>2</sub> of leucine, **9.** H<sub>3</sub>/H<sub>2</sub> of asparagine, **10.** H<sub>3</sub>/H<sub>2</sub> of aspartic acid, **11.** H<sub>6</sub>/H<sub>5</sub> of phenylalanine, **12.** H<sub>5</sub>/H<sub>4</sub> of phenylalanine, **13.** H<sub>2</sub>/H<sub>1</sub> of malic acid, **14.** H<sub>4</sub>/H<sub>3</sub> of GABA, **15.** H<sub>3</sub>/H<sub>2</sub> of GABA, **16.** H<sub>1</sub>/H<sub>2</sub> of sucrose, **17.** H<sub>2</sub>/H<sub>3</sub> of sucrose, **18.** H<sub>4</sub>/H<sub>5</sub> of sucrose, **19.** H<sub>3</sub>'/H<sub>4</sub>' of sucrose, **20.** H<sub>2</sub>/H<sub>3</sub> of sucrose, **21.** H<sub>4</sub>/H<sub>3</sub> of glucose, **22.** H<sub>28</sub>/H<sub>5</sub> of cycloartan-1,24-diene-3,23-dione, **23.** H<sub>5</sub>/H<sub>6</sub> of cycloartan-1,24-diene-3,23-dione, **24.** H<sub>7</sub>/H<sub>8</sub> of cycloartan-1,24-diene-3,23-dione, **25.** H<sub>12</sub>/H<sub>11</sub> of cycloartan-1,24-diene-3,23-dione, **26.** H<sub>1</sub>/H<sub>2</sub> of cycloartan-1,24-diene-3,23-dione, **27.** H<sub>15</sub>/H<sub>16</sub> of cycloartan-1,24-diene-3,23-dione, **28.** H<sub>1</sub>/H<sub>2</sub> of (9*S*,10*S*,21*R*,23*S*)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **29.** H<sub>11</sub>/H<sub>12</sub> of (9*S*,10*S*,21*R*,23*S*)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **30.** H<sub>6</sub>/H<sub>7</sub> of (9*S*,10*S*,21*R*,23*S*)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **31.** H<sub>7</sub>/H<sub>8</sub> of (9*S*,10*S*,21*R*,23*S*)-21/23,23/27-

diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **32**. H12/H11 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **33**. H15/H16 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **34**. H5/H6 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **35**. H1/H2 of (9R,10R,23R)-21,23;23,27-diepoxycycloartan-1,24-diene-3,27-dione, **36**. H5/H6 of (9R,10R,23R)-21,23;23,27-diepoxycycloartan-1,24-diene-3,27-dione, **37**. H6/H7 of (9R,10R,23R)-21,23;23,27-diepoxycycloartan-1,24-diene-3,27-dione, **38**. H7/H8 of (9R,10R,23R)-21,23;23,27-diepoxycycloartan-1,24-diene-3,27-dione, **39**. H11/H12 of (9R,10R,23R)-21,23;23,27-diepoxycycloartan-1,24-diene-3,27-dione, **40**. H1/H2 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **41**. H5/H6 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **42**. H6/H7 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **43**. H11/H12 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **44**. H1/H2 of Kleinhospitine E, **45**. H8/H11 of Kleinhospitine E



**Fig S6.** The signal correlation of detected metabolites in the HSQC spectrum of the untreated sample group. (a) Magnification of the HSQC spectra in the 0.5–4.5 ppm range. (b) Magnification of the HSQC spectra in the range of 5.0–

9.0 ppm. **1.** C2/H2 of valine, **2.** C3/H3 of valine, **3.** C4/H4 of valine, **4.** C2/H2 of glycine, **5.** C2/H2 of isoleucine, **6.** C3/H3 of isoleucine, **7.** C4/H4 of isoleucine, **8.** C5/H5 of isoleucine, **9.** C2/H2 of leucine, **10.** C3/H3 of leucine, **11.** C4/H4 of leucine, **12.** C5/H5 of isoleucine, **13.** C2/H2 of aspartic acid, **14.** C3/H3 of aspartic acid, **15.** C1/H1 of malic acid, C2/H2 of malic acid, **16.** C2/H2 of malic acid, **17.** C2/H2 of GABA, **18.** C3/H3 of GABA, **19.** C4/H4 of GABA, **20.** C3/H3 of myo-inositol, **21.** C2/H2 of glucose, **22.** C4/H4 of glucose, **23.** C6/H6 of glucose, **24.** C1/H1 of fructose, **25.** C3/H3 of fructose, **26.** C5/H5 of fructose, **27.** C2/H2 of sucrose, **28.** C3/H3 of sucrose, **29.** C4/H4 of sucrose, **30.** C5/H5 of sucrose, **31.** C3'/H3' of sucrose, **32.** C26/H26 of cycloartan-1,24-diene-3,23-dione, **33.** C27/H27 of cycloartan-1,24-diene-3,23-dione, **34.** C17/H17 of cycloartan-1,24-diene-3,23-dione, **35.** C18/H18 of cycloartan-1,24-diene-3,23-dione, **36.** C16/H16 of cycloartan-1,24-diene-3,23-dione, **37.** C15/H15 of cycloartan-1,24-diene-3,23-dione, **38.** C12/H12 of cycloartan-1,24-diene-3,23-dione, **39.** C11/H11 of cycloartan-1,24-diene-3,23-dione, **40.** C8/H8 of cycloartan-1,24-diene-3,23-dione, **41.** C7/H7 of cycloartan-1,24-diene-3,23-dione, **42.** C4/H4 of cycloartan-1,24-diene-3,23-dione, **43.** C26/H26 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **44.** C28/H28 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **45.** C5/H5 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **46.** C6/H6 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **47.** C7/H7 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **48.** C8/H8 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **49.** C11/H11 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **50.** C15/H15 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **51.** C26/H26 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **52.** C23/H23 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **53.** C21/H21 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **54.** C30/H30 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **55.** C26/H26 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **56.** C5/H5 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **57.** C28/H28 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **58.** C29/H29 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **59.** C8/H8 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **60.** C15/H15 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **61.** C16/H16 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **62.** C21/H21 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **63.** C18/H18 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **64.** C26/H26 of kleinhospitine E, **65.** C16/H16 of kleinhospitine E, **66.** C15/H15 of kleinhospitine E, **67.** C11/H11 of kleinhospitine E, **68.** C18/H18 of kleinhospitine E, **69.** C21/H21 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **70.** C1/H1 of kleinhospitine E, **71.** C22/H22 of kleinhospitine E, **72.** C24/H24 of kleinhospitine E, **73.** C2/H2 of kleinhospitine E, **74.** C2/H2 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **75.** C1/H1 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **76.** C24/H24 of (9R,10R,21S,23R)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **77.** C24/H24 of (9R,10R,23R)-21,23;23,27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **78.** C1/H1 of (9R,10R,23R)-21,23;23,27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **79.** C2/H2 of (9R,10R,23R)-21,23;23,27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **80.** C24/H24 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **81.** C21/H21 of (9S,10S,21R,23S)-21/23,23/27-diepoxy-21-methoxycycloartan-1,24-diene-3,27-dione, **82.** C2/H2 of cycloartan-1,24-diene-3,23-dione, **83.** C1/H1 of cycloartan-

1,24-diene-3,23-dione, **84**. C24/H24 of cycloartan-1,24-diene-3,23-dione, **85**. C1/H1 of sucrose, **86**. C6/H6 of phenylalanine, **87**. C5/H5 of phenylalanine, **88**. C3/H3 of phenylalanine

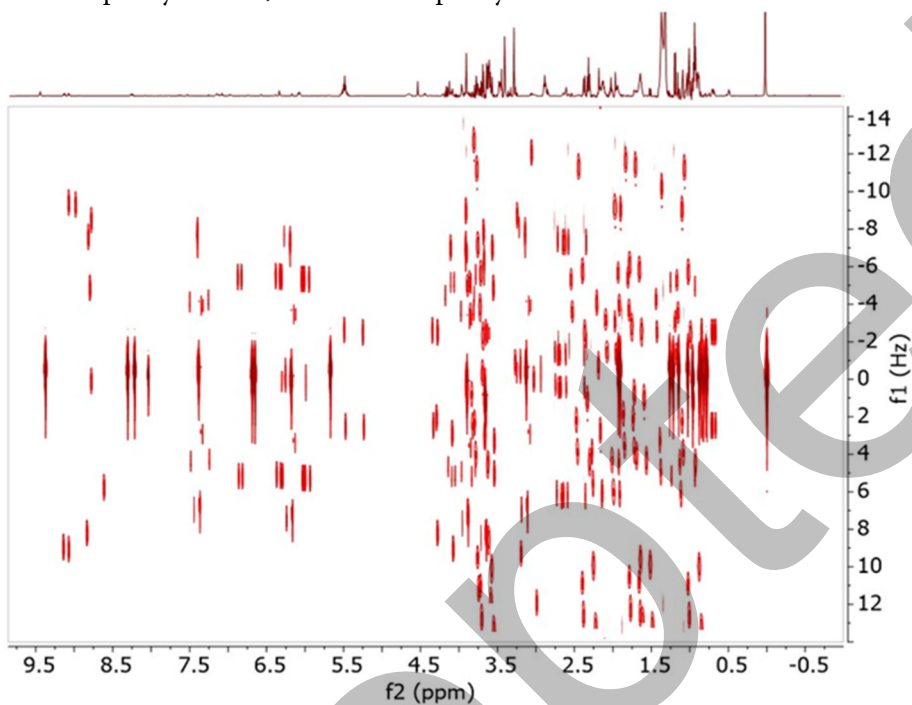
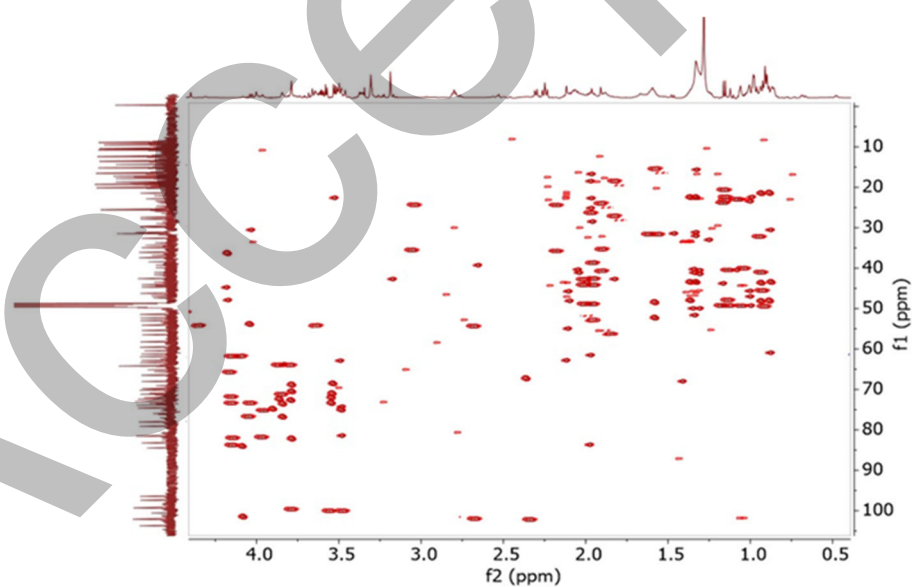


Fig S7. J-resolved spectra of the group unexposed to gamma irradiation



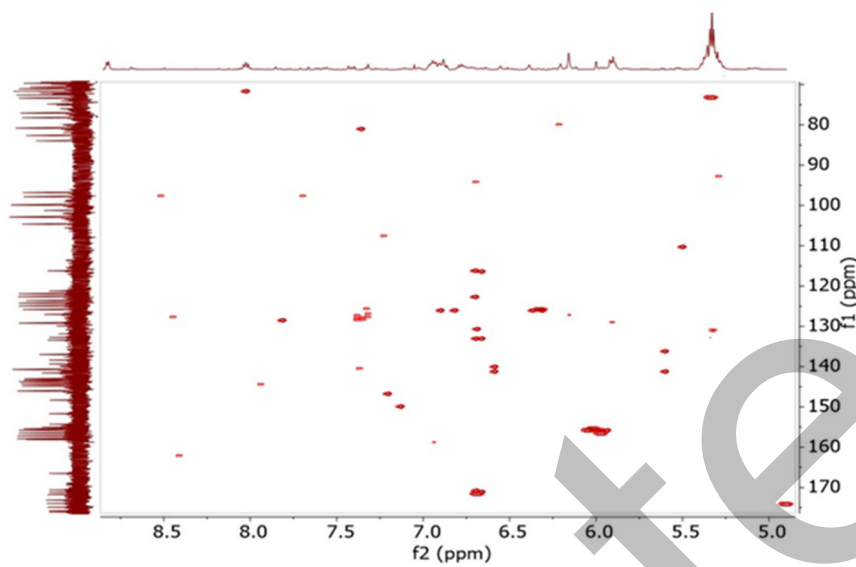


Fig S8. HMBC spectrum of the group not exposed to gamma irradiation