SUPPLEMENTARY MATERIALS

Novel phenolic constituents of *Pulmonaria officinalis* L. LC-MS/MS comparison of spring and autumn metabolite profiles

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***Correspondence**:jkrzyzanowska@iung.pulawy.pl; Tel.: +48-81-4786-881

Spis treści

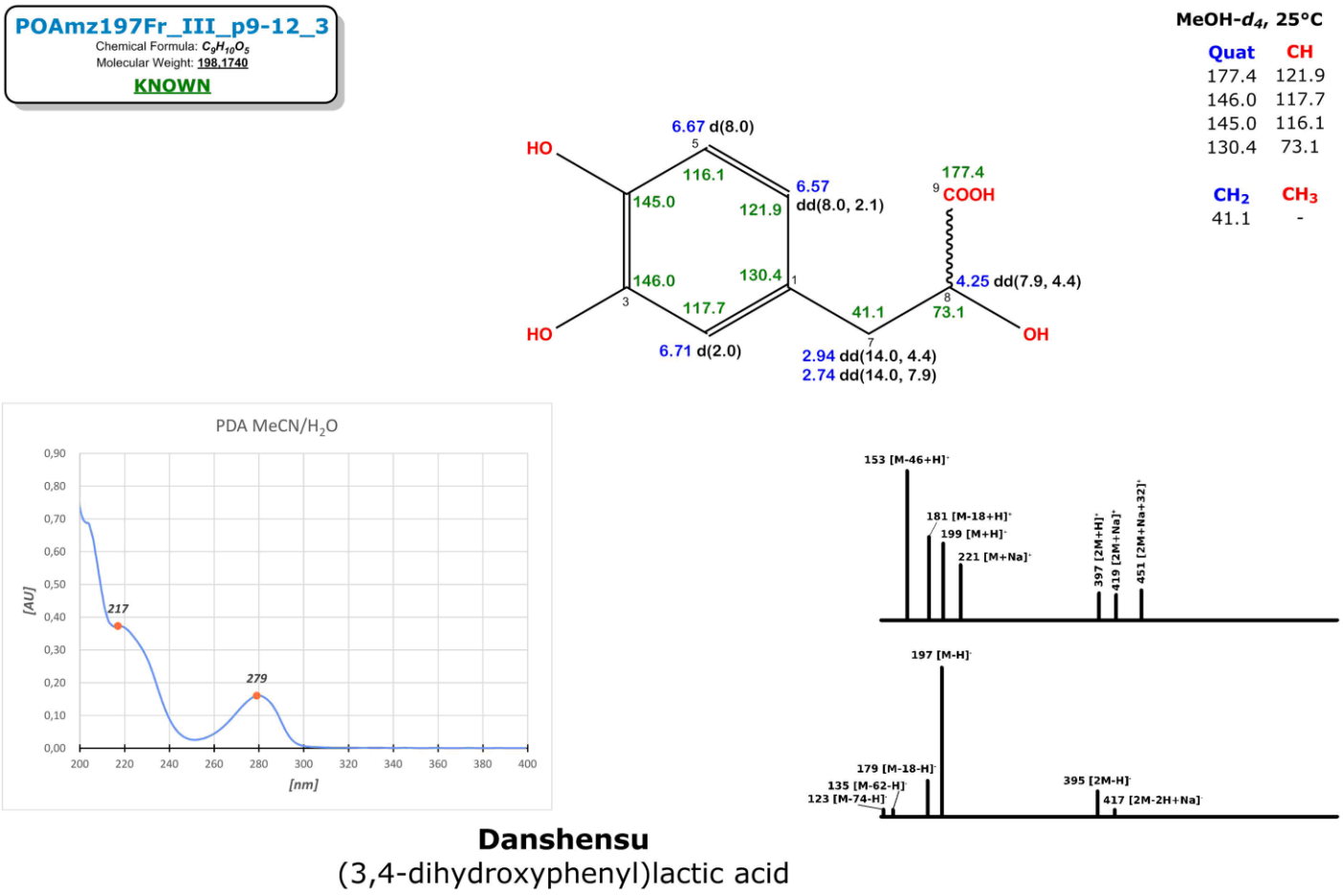
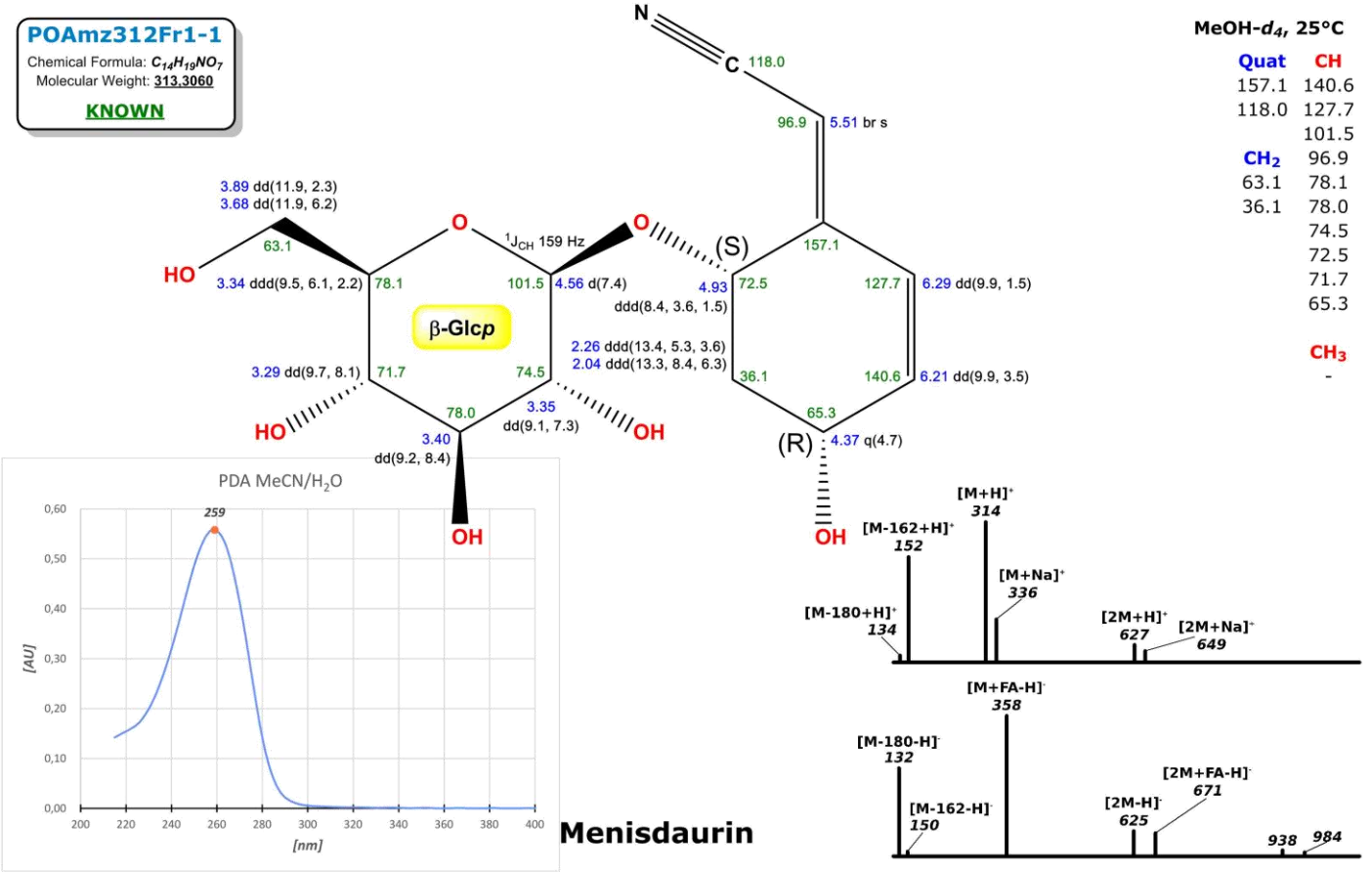


Figure 1S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 1 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O



1. Seigler, D.S., Pauli, G.F., Fröhlich, R., Wegelius, E., Nahrstedt, A., Glander, K.E., Ebinger, J.E., 2005. Cyanogenic glycosides and menisdaurin from Guazuma ulmifolia, Ostrya virginiana, Tiquilia plicata, and Tiquilia canescens. Phytochemistry 66, 1567–1580. doi:10.1016/j.phytochem.2005.02.021

Figure 2S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 2 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

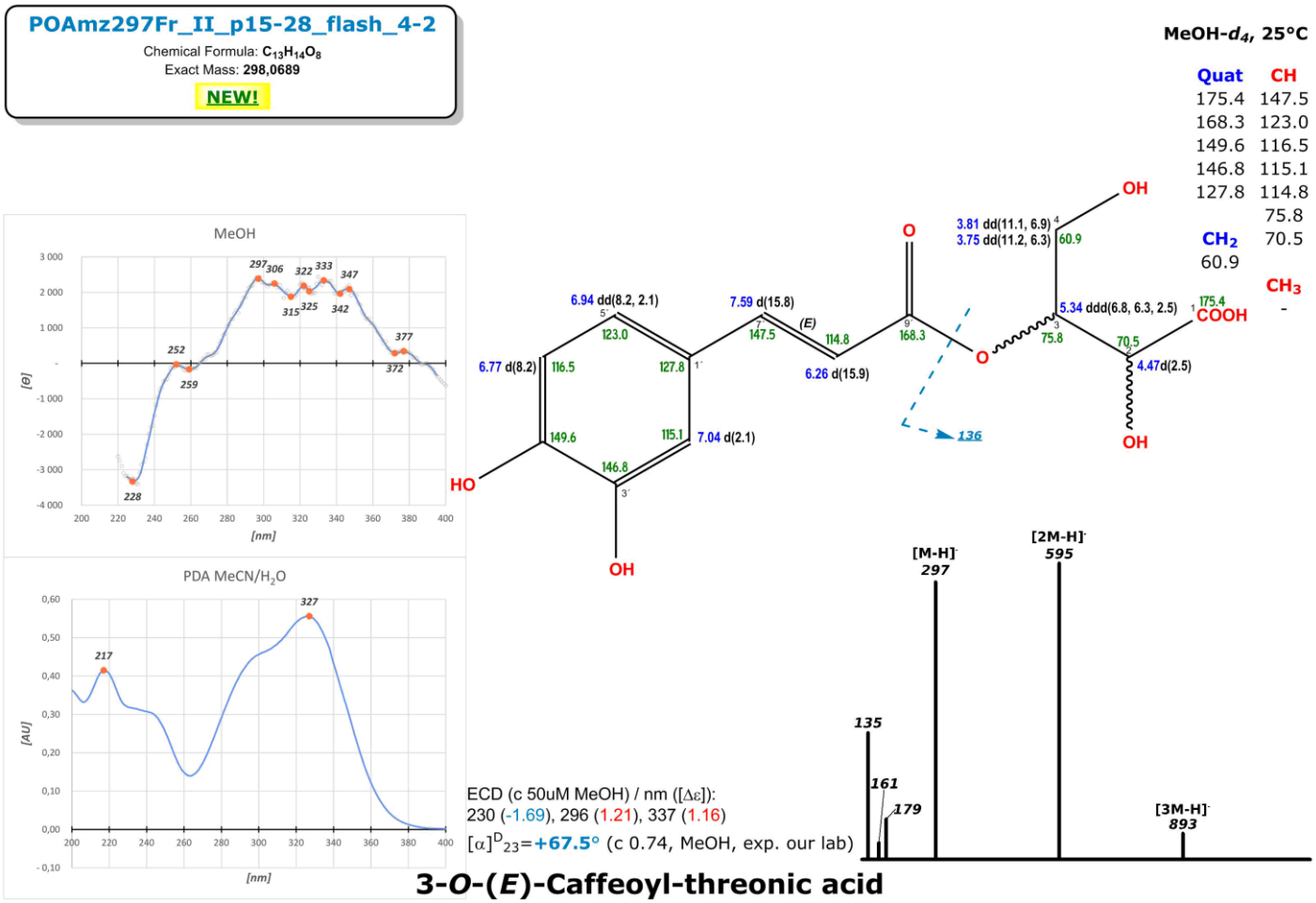


Figure 3S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 3 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O, ECD spectrum in MeOH

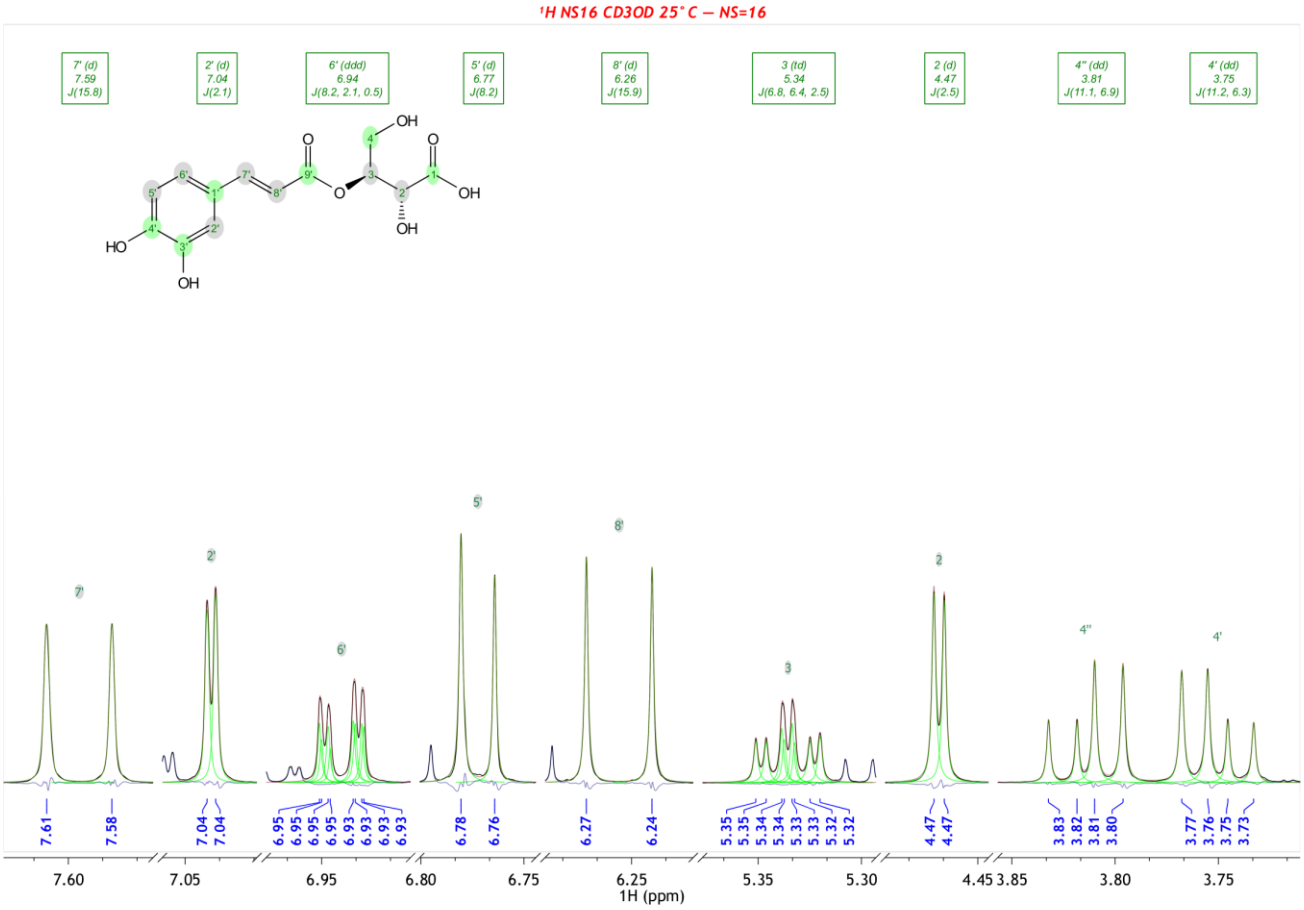


Figure 4S. ^{1}H NMR spectrum of compound 3

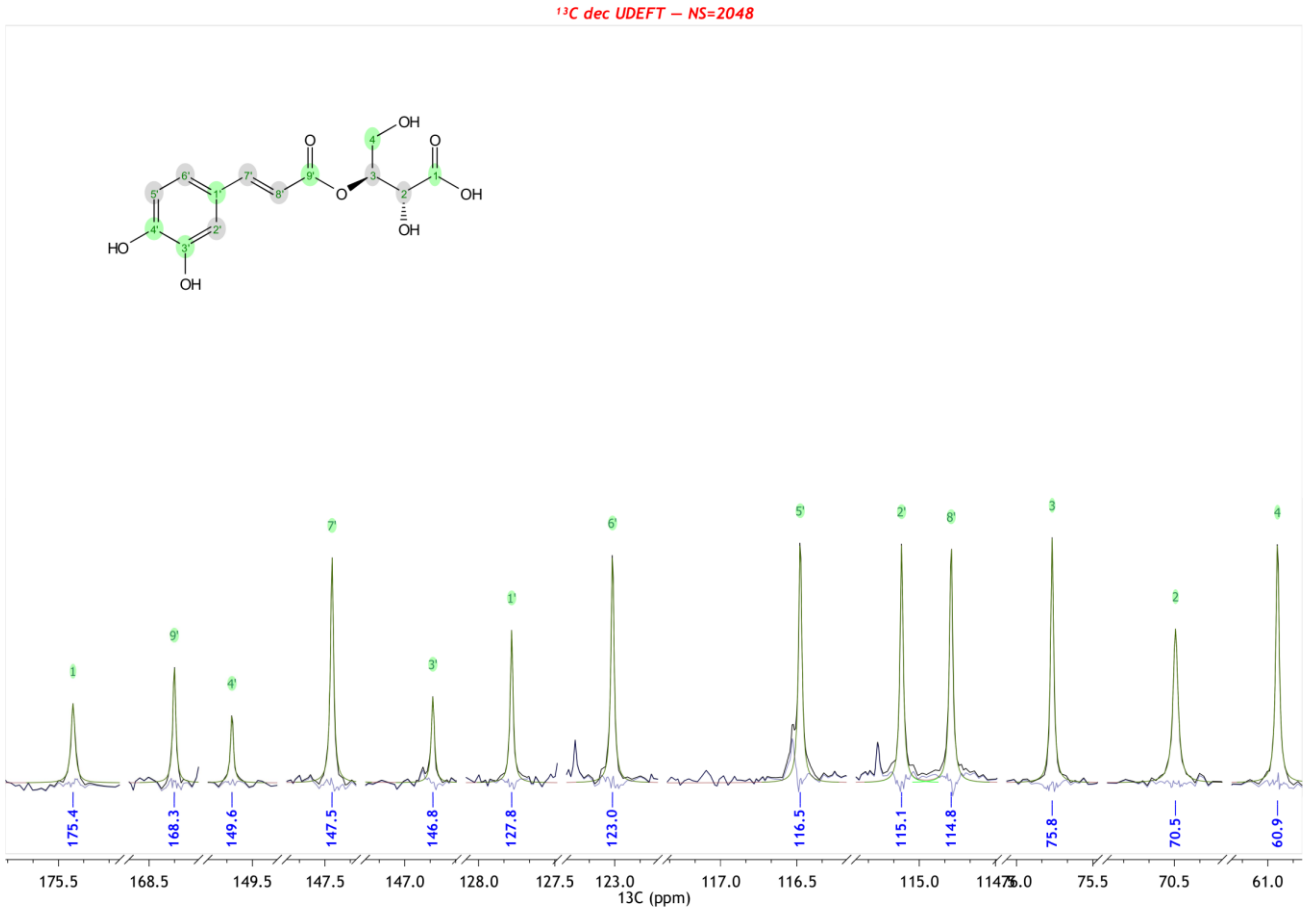


Figure 5S. ^{13}C UDEFT NMR spectrum of compound 3

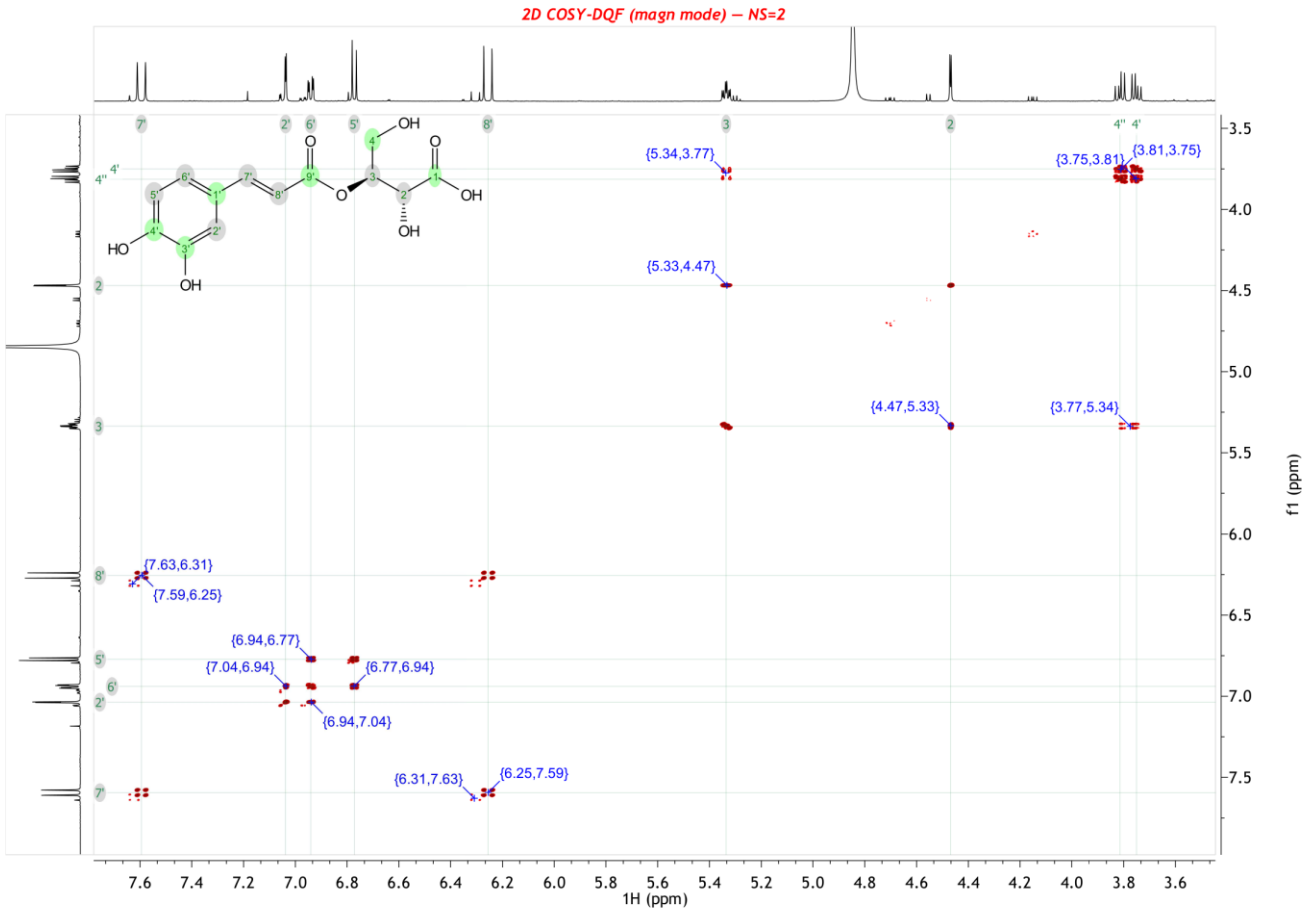


Figure 6S. ^{1}H-^{1}H COSY NMR spectrum of compound 3

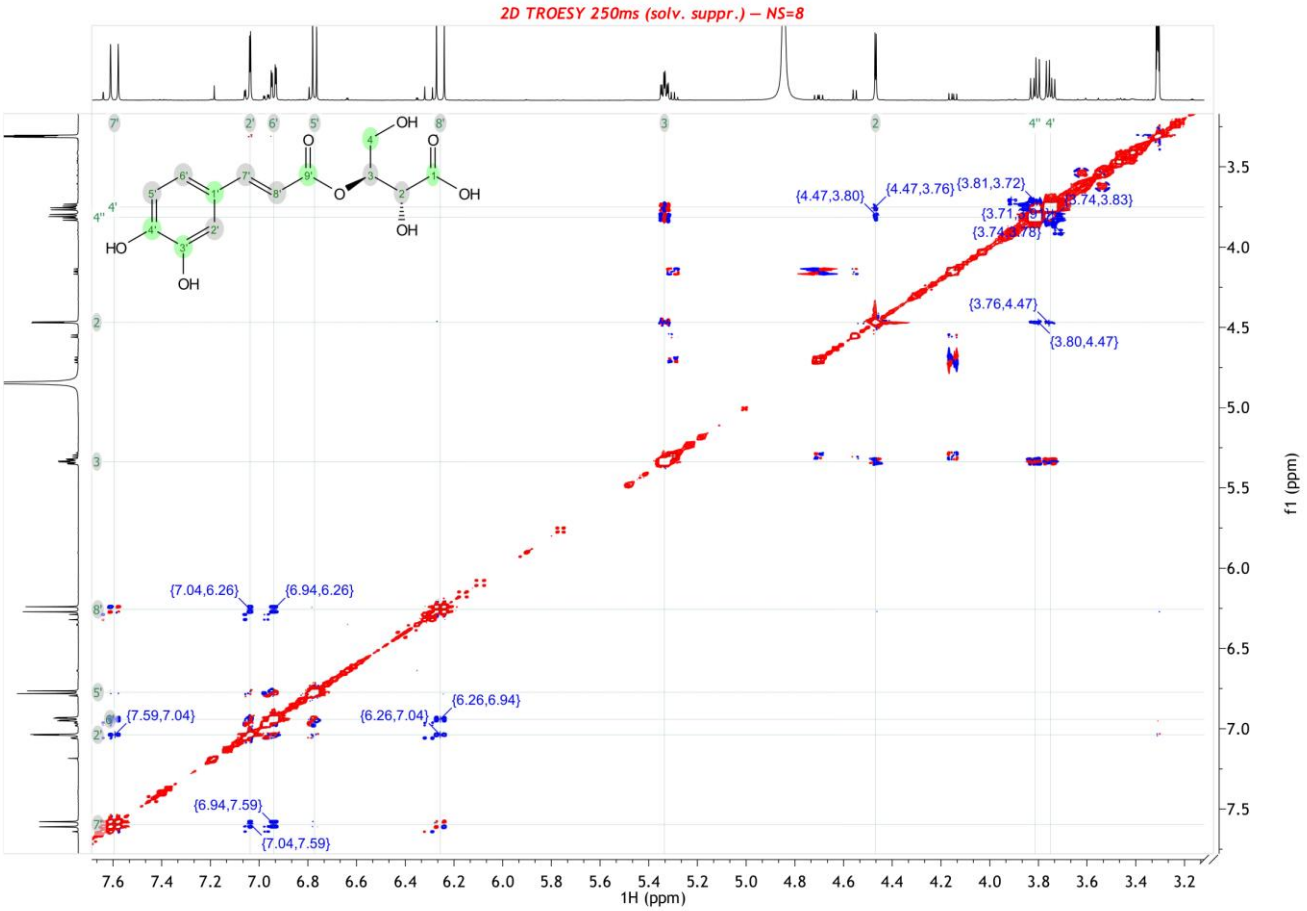


Figure 7S. ^{1}H-^{1}H TROESY (250 ms) NMR spectrum of compound 3

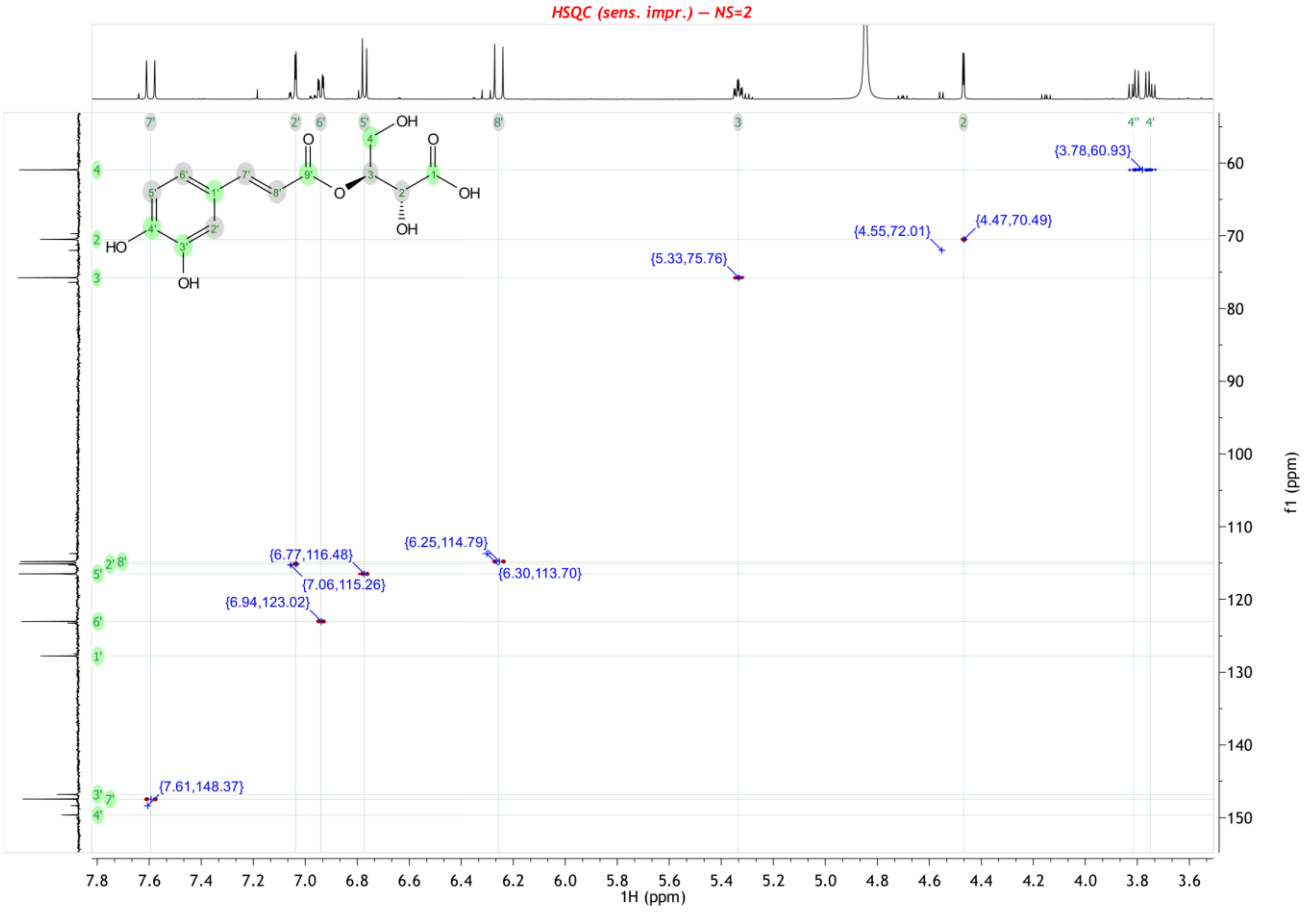


Figure 8S. ^{1}H-^{13}C HSQC NMR spectrum of compound 3

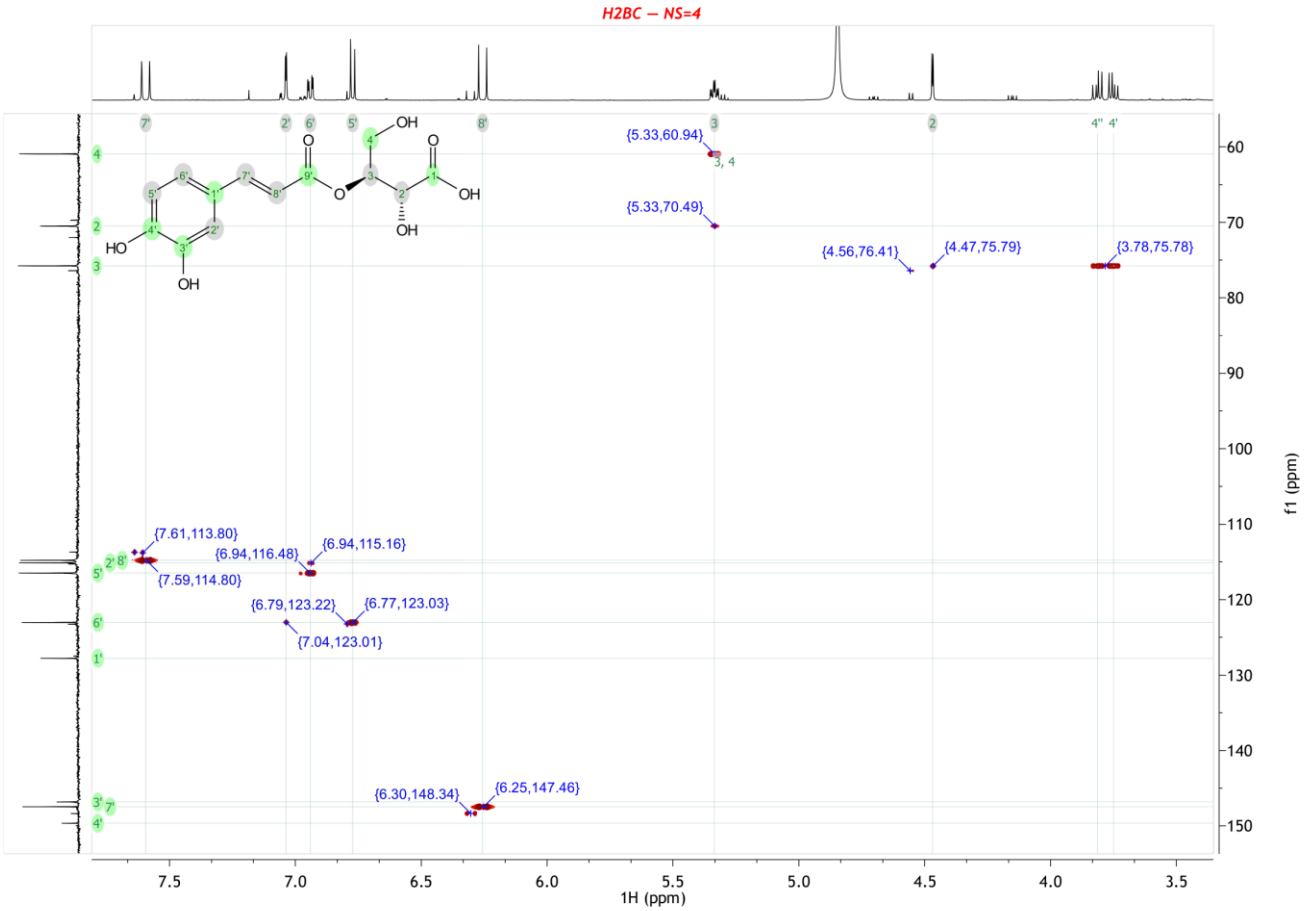


Figure 9S. ^{1}H-^{13}C H2BC NMR spectrum of compound 3

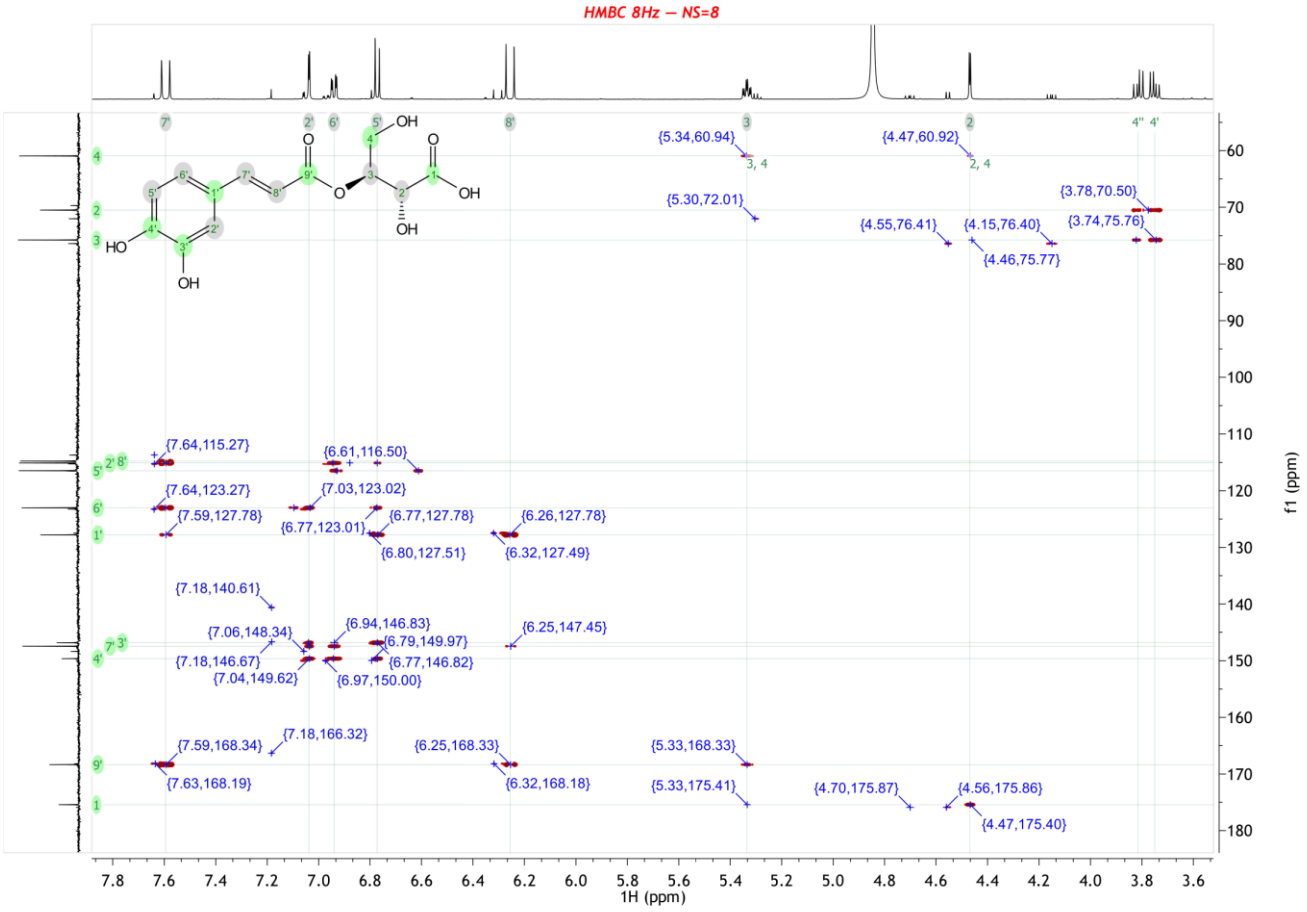
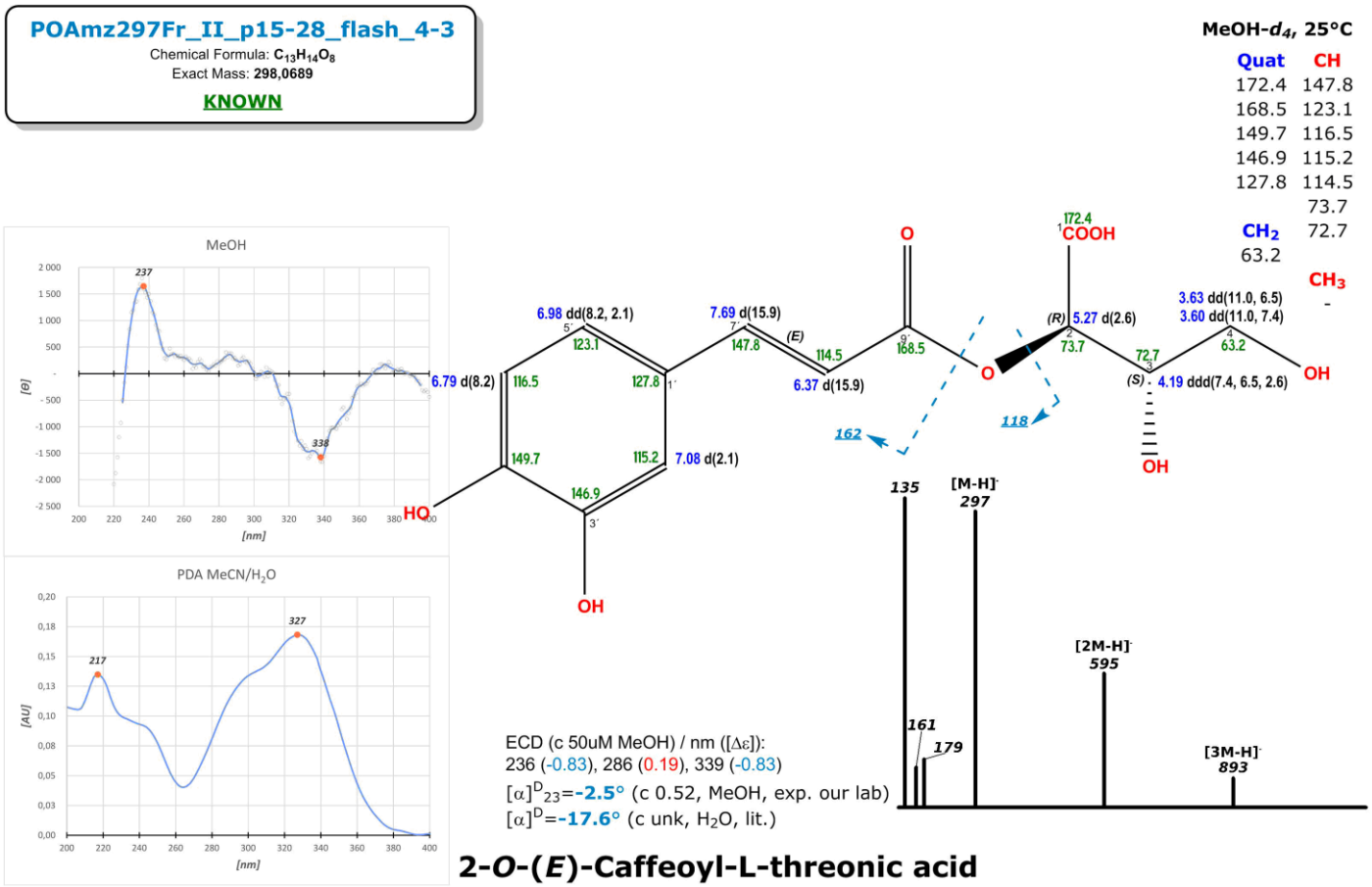
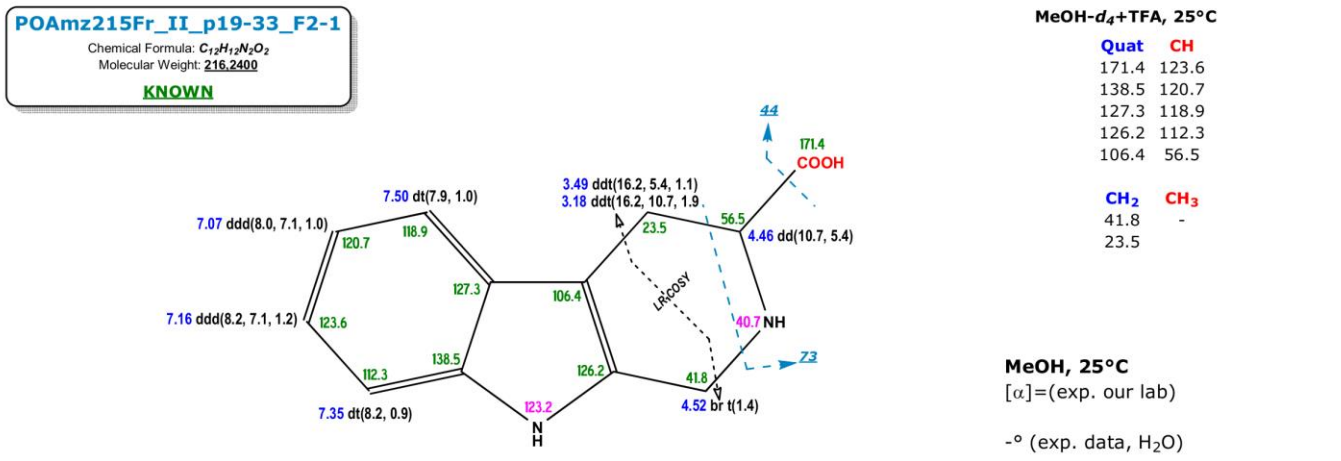


Figure 10S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 3



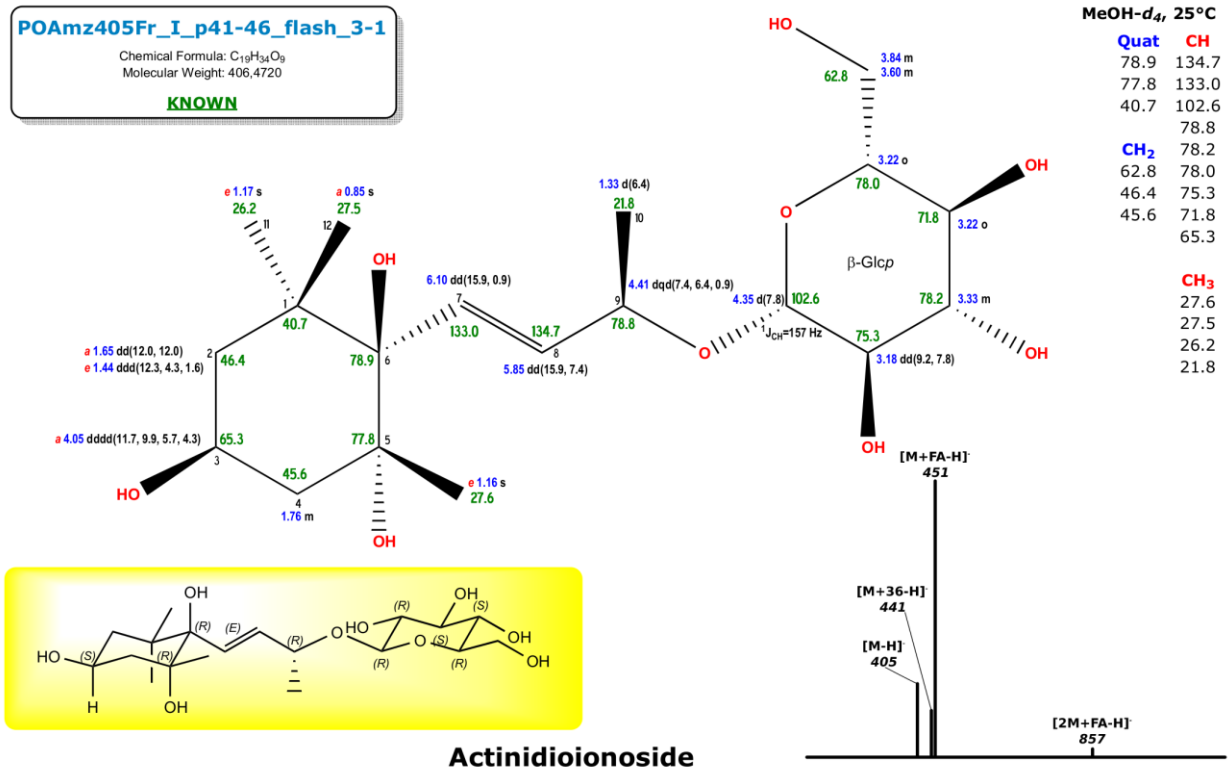
1. Kuczkowiak, U., Petereit, F., Nahrstedt, A., 2014. Hydroxycinnamic Acid Derivatives Obtained from a Commercial Crataegus Extract and from Authentic Crataegus spp. Sci. Pharm. 82, 835–846. doi:10.3797/scipharm.1404-02
2. Parveen, I., Winters, A., Threadgill, M.D., Hauck, B., Morris, P., 2008. Extraction, structural characterisation and evaluation of hydroxycinnamate esters of orchard grass (Dactylis glomerata) as substrates for polyphenol oxidase. Phytochemistry 69, 2799–2806. doi:10.1016/j.phytochem.2008.08.019

Figure 11S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 4 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O, ECD spectrum in MeOH



Lycoperodine-1

Figure 12S. ^{1}H (500 MHz) ^{13}C (125 MHz) and ^{15}N (50 MHz) NMR data of compound 5 in CD_3OD, 25°C



1. Murai, F., Tagawa, M., 1989. Relationship between ionone glycosides and terpenoids in Actinidia polygama, in: Abstract Papers of the 33rd Symposium on the Chemistry of Terpenes, Essential Oils, and Aromatics (TEAC), Sendai. pp. 68–70.
2. Otsuka, H., Hirata, E., Shinzato, T., Takeda, Y., 2003. Stereochemistry of megastigmane glucosides from Glochidion zeylanicum and Alangium premnifolium. Phytochemistry 62, 763–768. doi:10.1016/S0031-9422(02)00614-3

Figure 13S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 7 in CD_3OD, 25°C

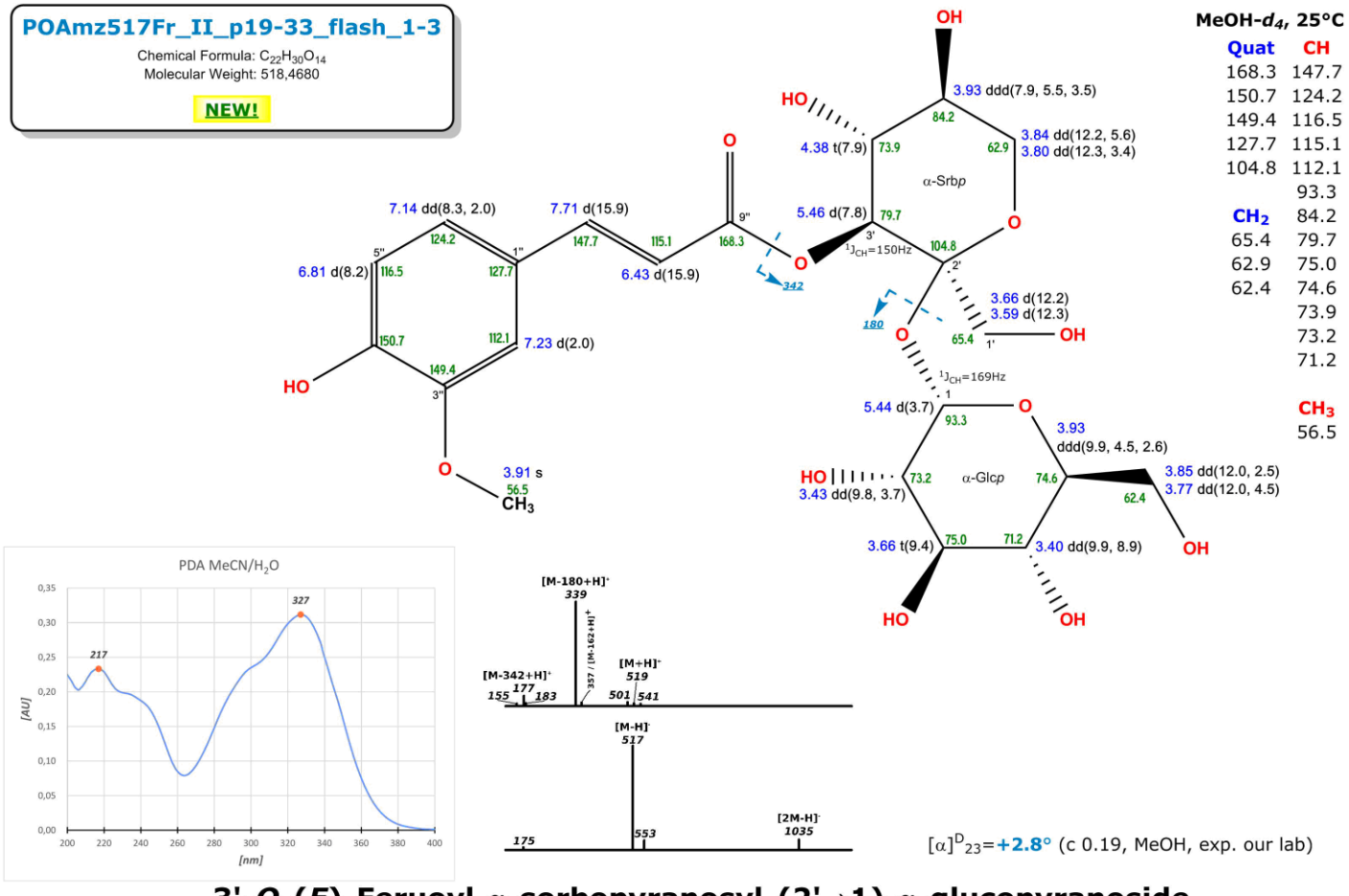


Figure 14S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 10 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$

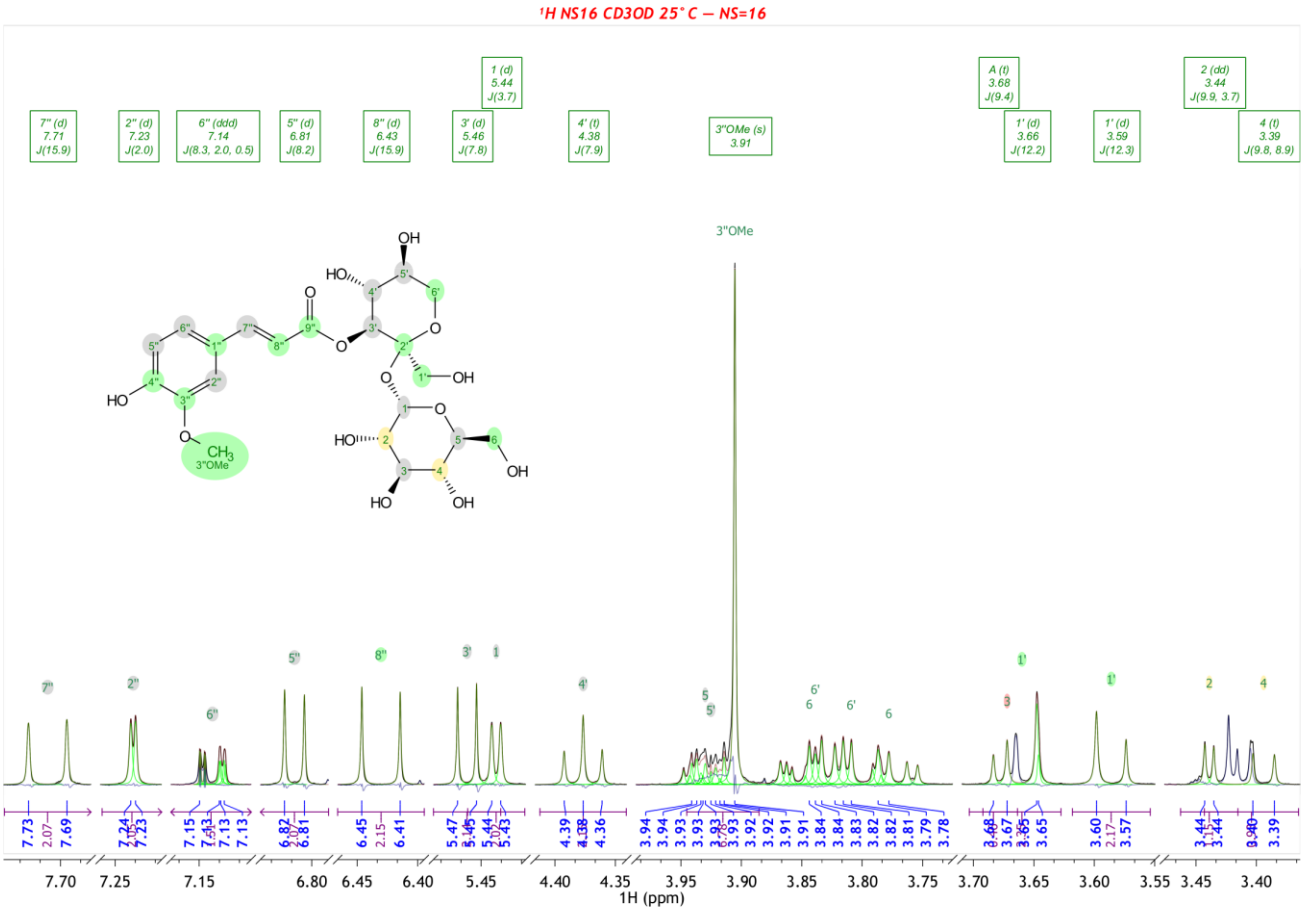


Figure 15S. ^{1}H NMR spectrum of compound 10

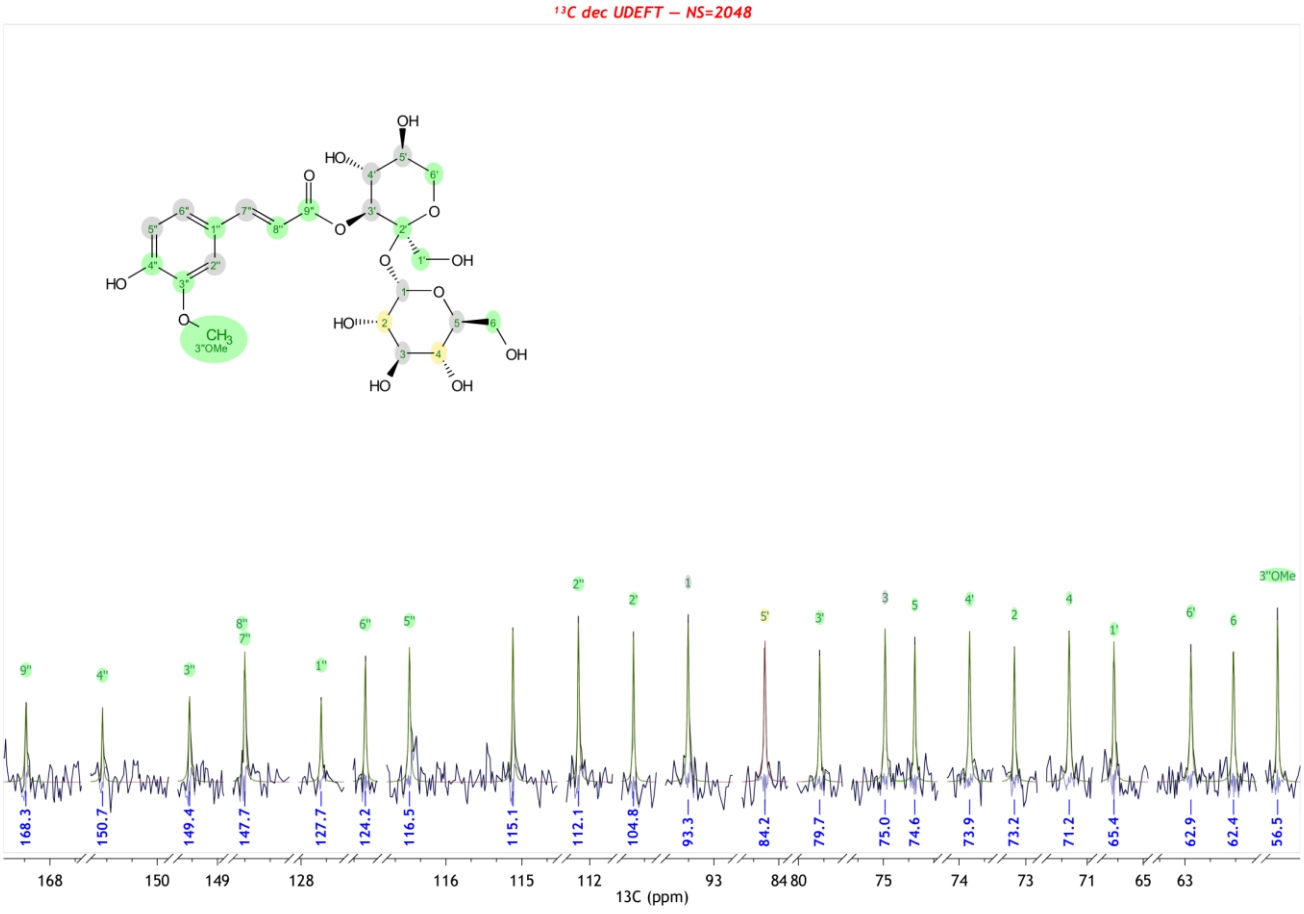


Figure 16S. ^{13}C DEPTQ NMR spectrum of compound 10

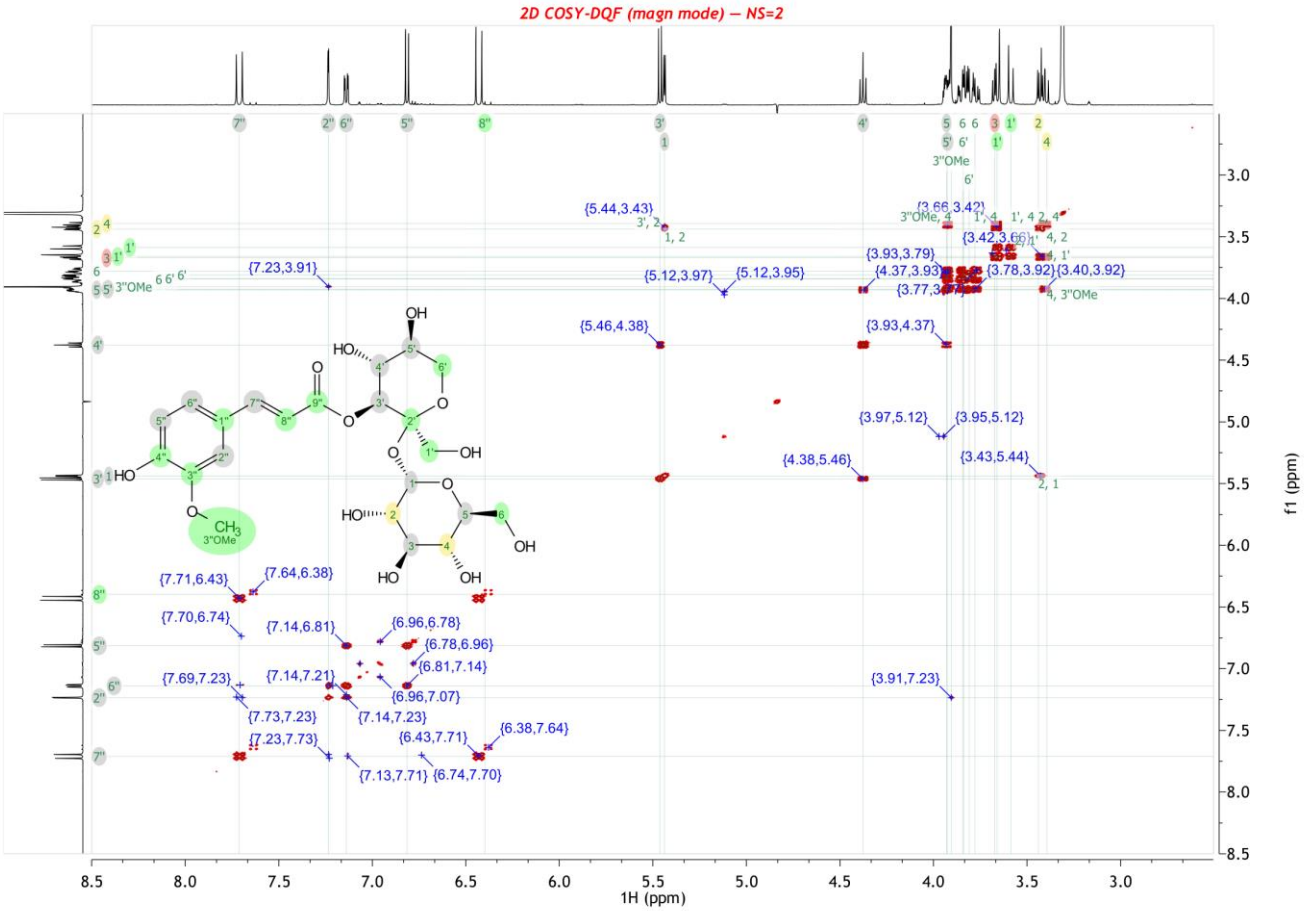


Figure 17S. ^{1}H-^{1}H COSY NMR spectrum of compound 10

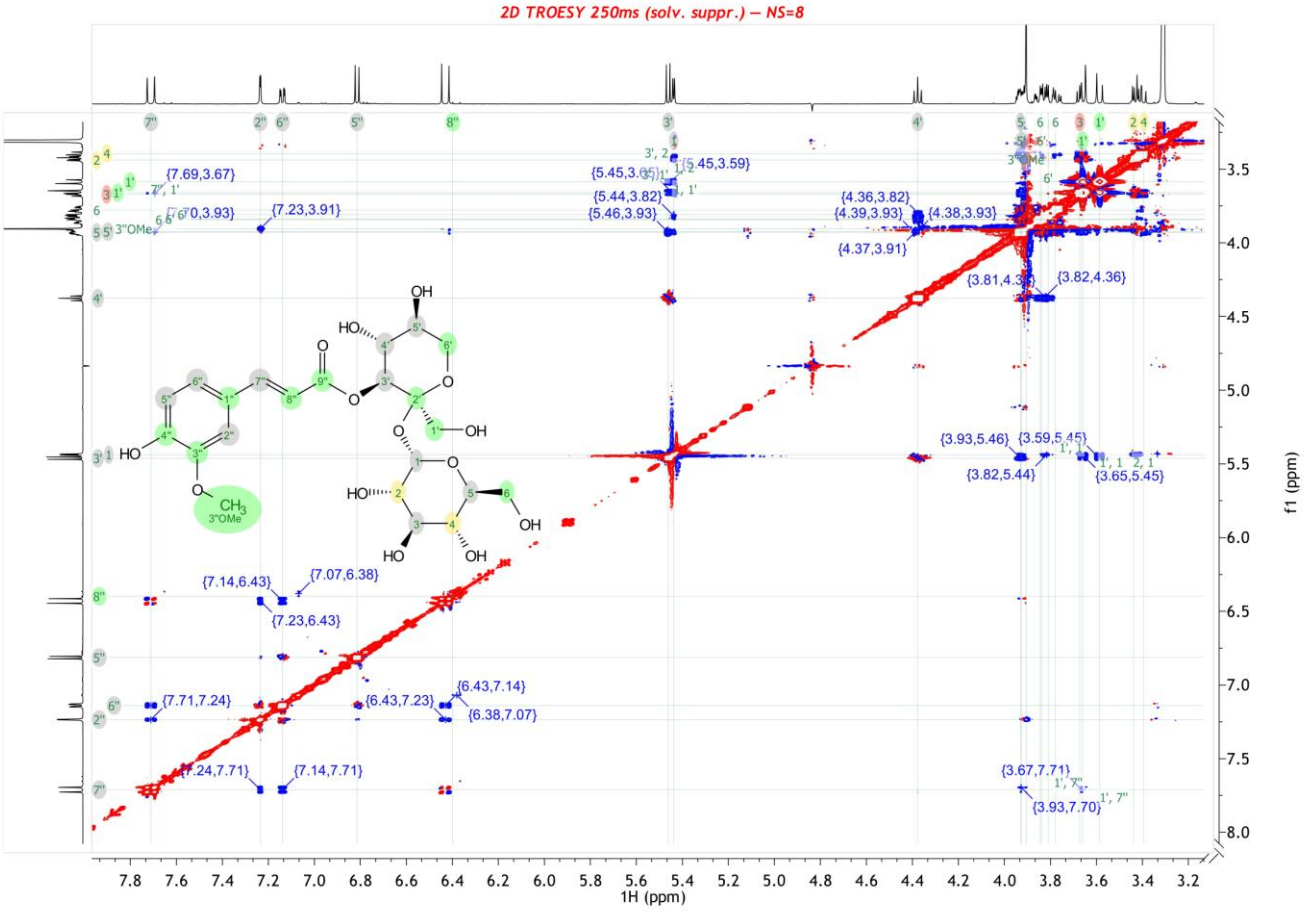


Figure 18S. ^{1}H-^{1}H TROESY (250 ms) NMR spectrum of compound 10

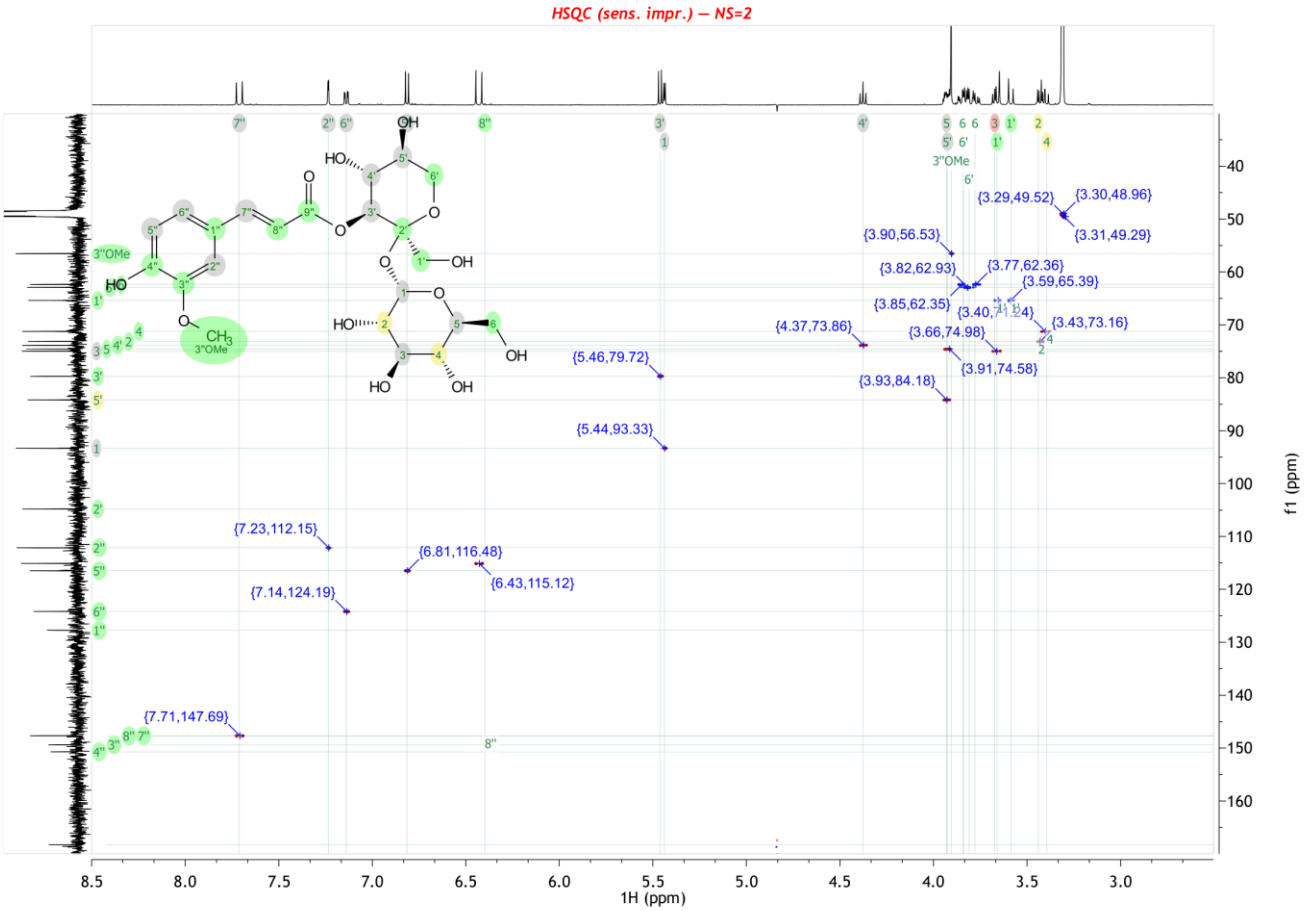


Figure 19S. ^{1}H-^{13}C HSQC NMR spectrum of compound 10

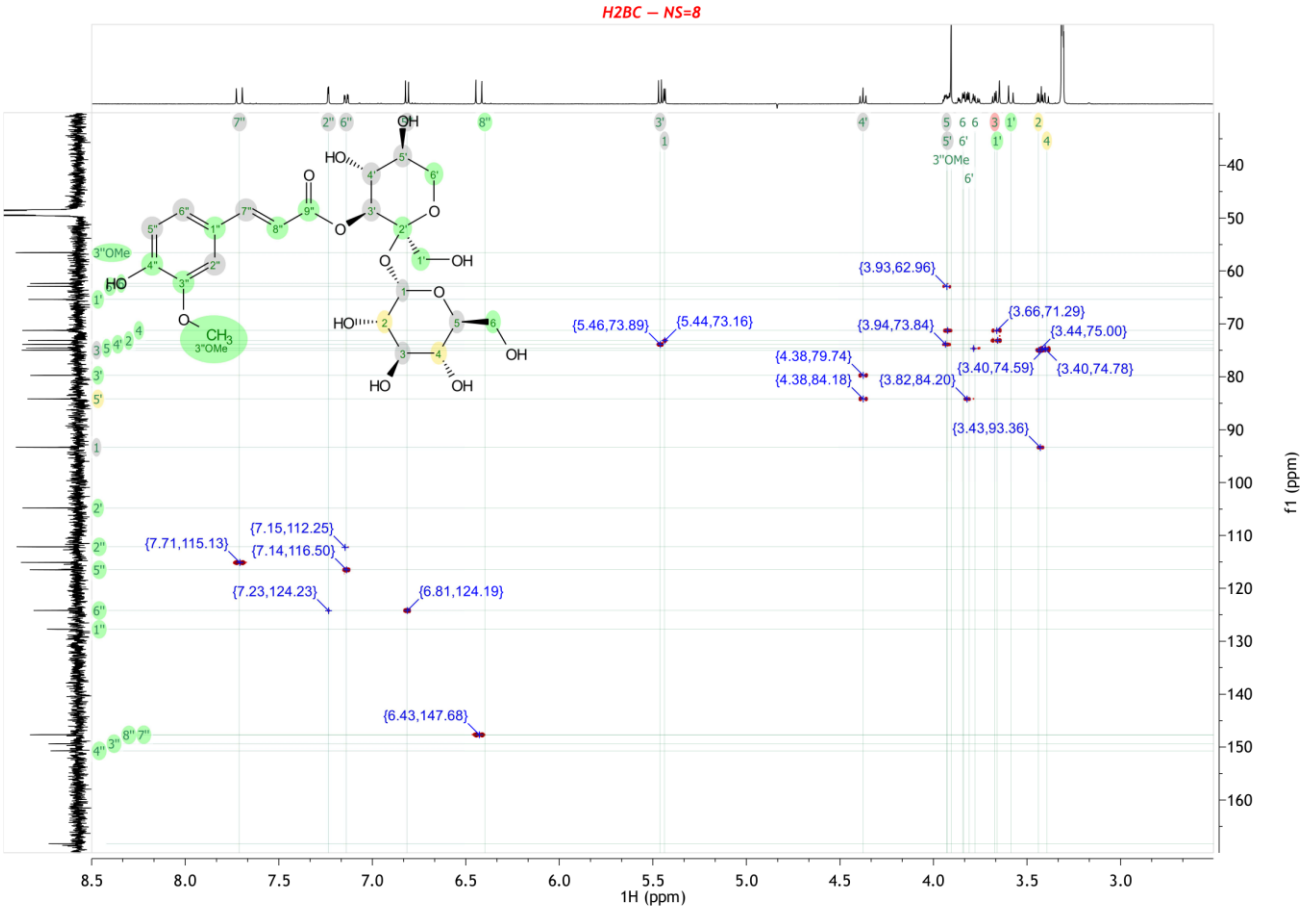


Figure 20S. ^{1}H-^{13}C H2BC NMR spectrum of compound 10

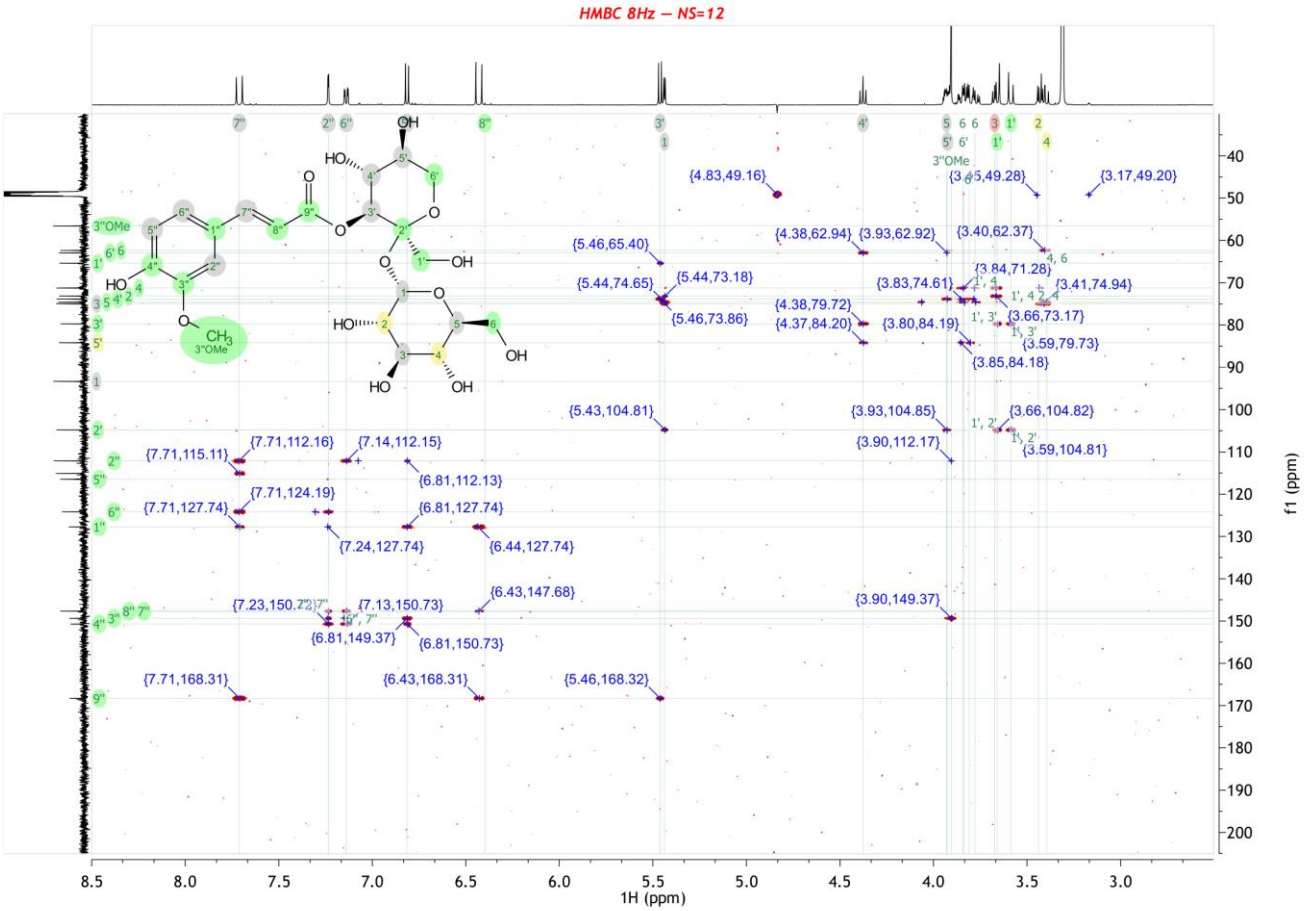
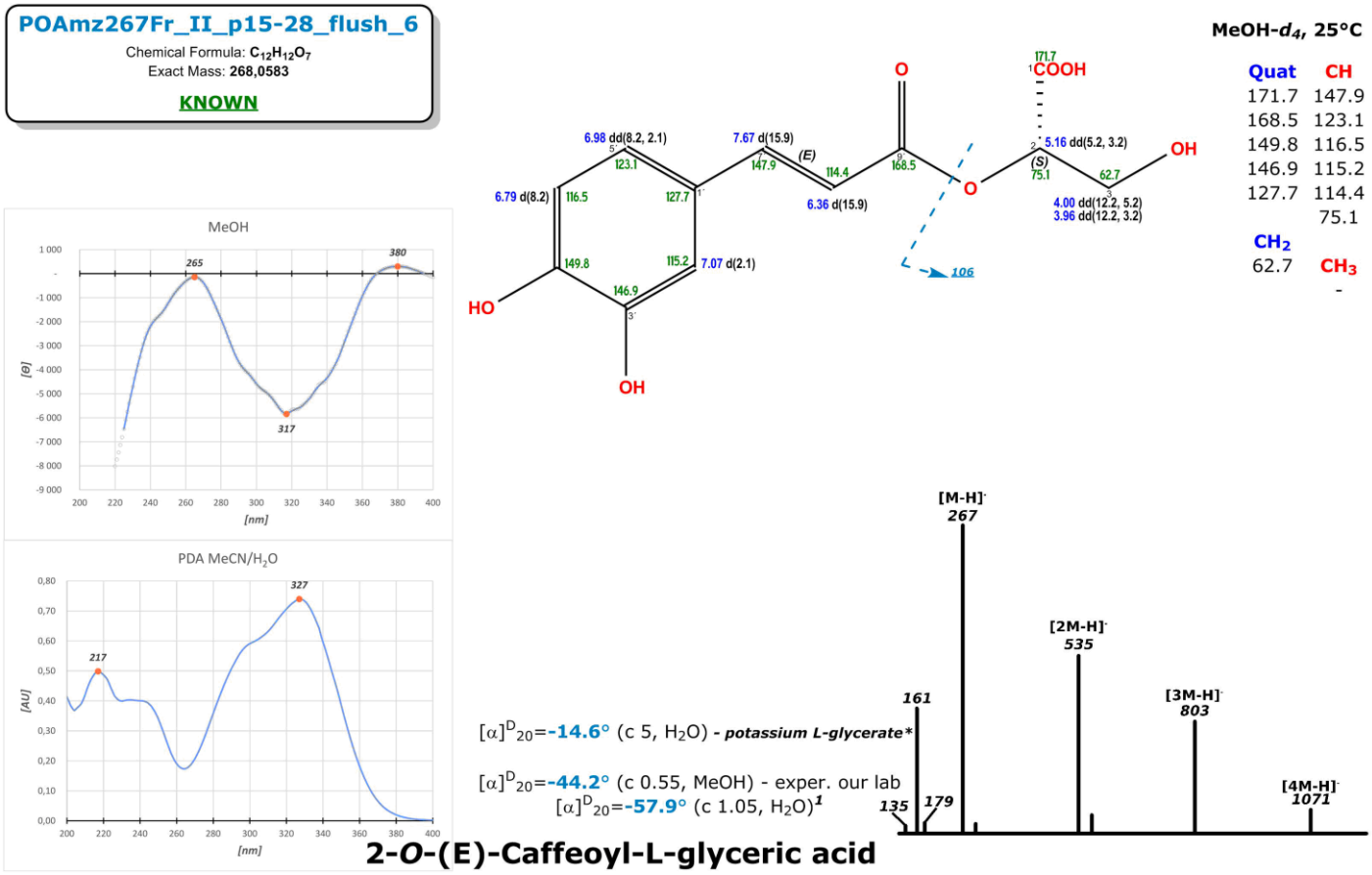
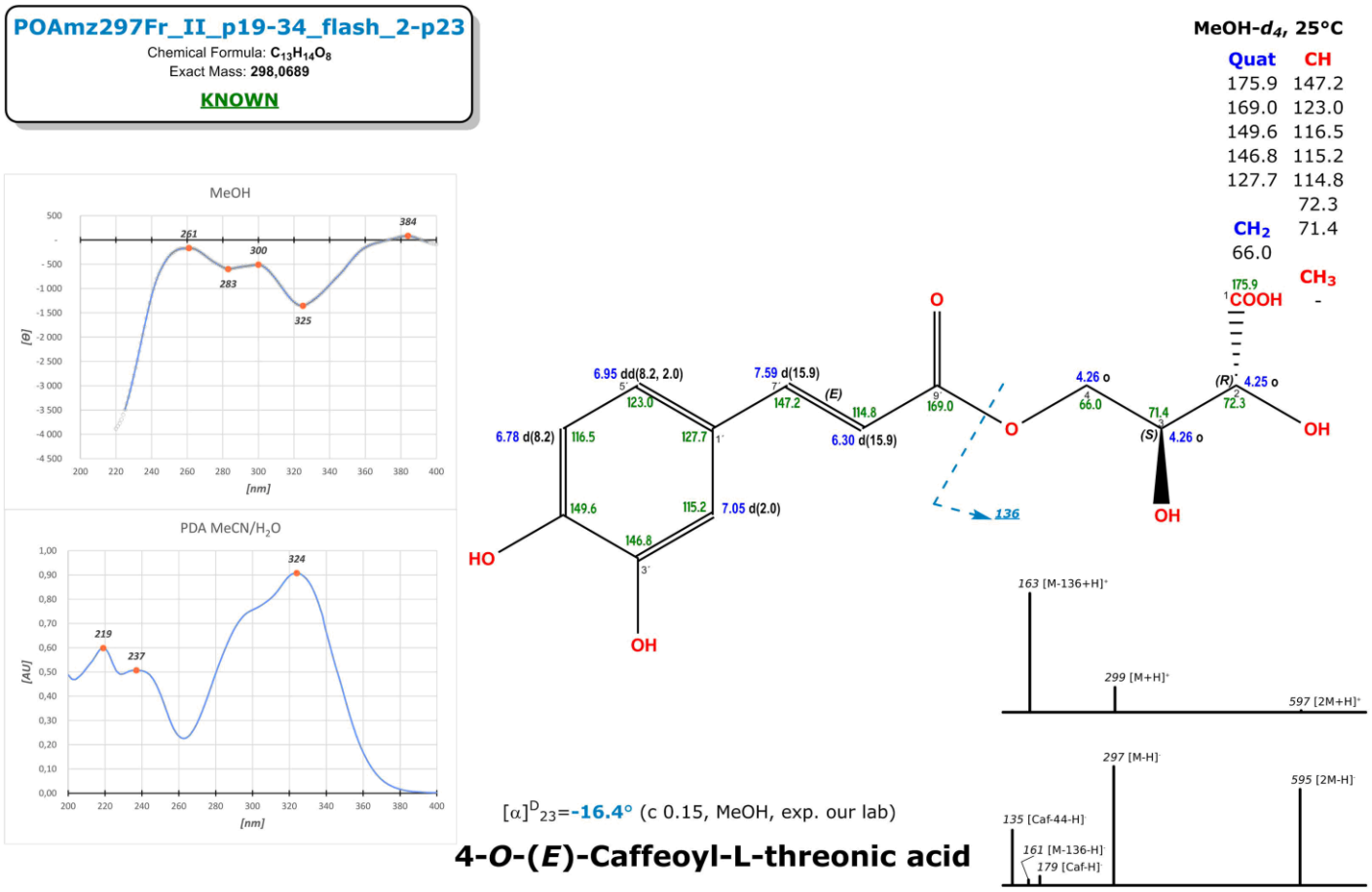


Figure 21S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 10



1. Hahn, R., Nahrstedt, A., 1993. Hydroxycinnamic acid derivatives, caffeoylmalic and new caffeoylaldonic acid esters, from Chelidonium majus. Planta Med. 59, 71–75. doi:10.1055/s-2006-959608
* http://www.drugfuture.com/chemdata/glyceric-acid.html

Figure 22S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 11 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH



Hahn, R., Nahrstedt, A., 1993. Hydroxycinnamic acid derivatives, caffeoylmalic and new caffeoylaldonic acid esters, from Chelidonium majus. Planta Med. 59, 71–75. doi:10.1055/s-2006-959608

Figure 23S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 12 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

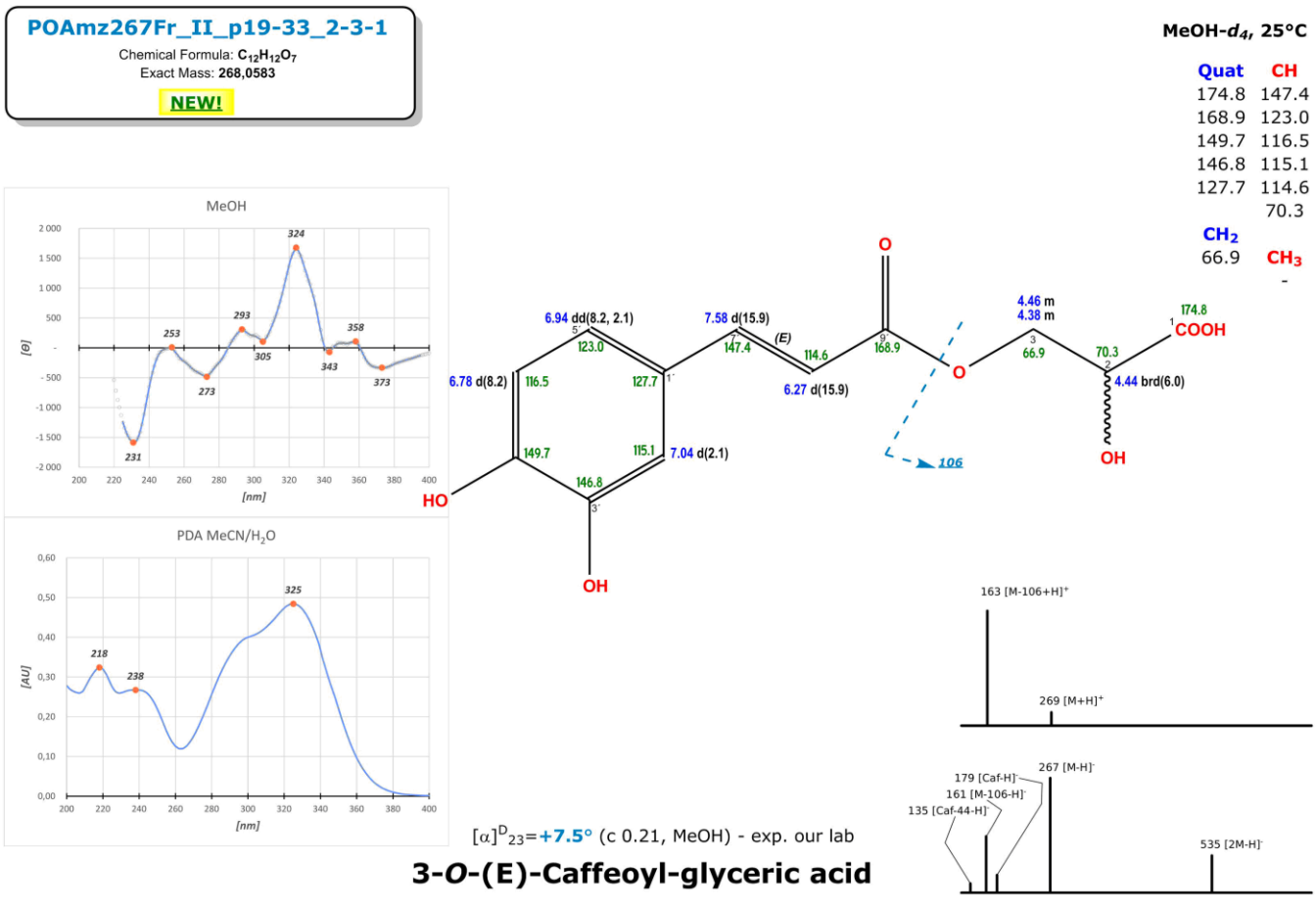


Figure 24S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 14 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

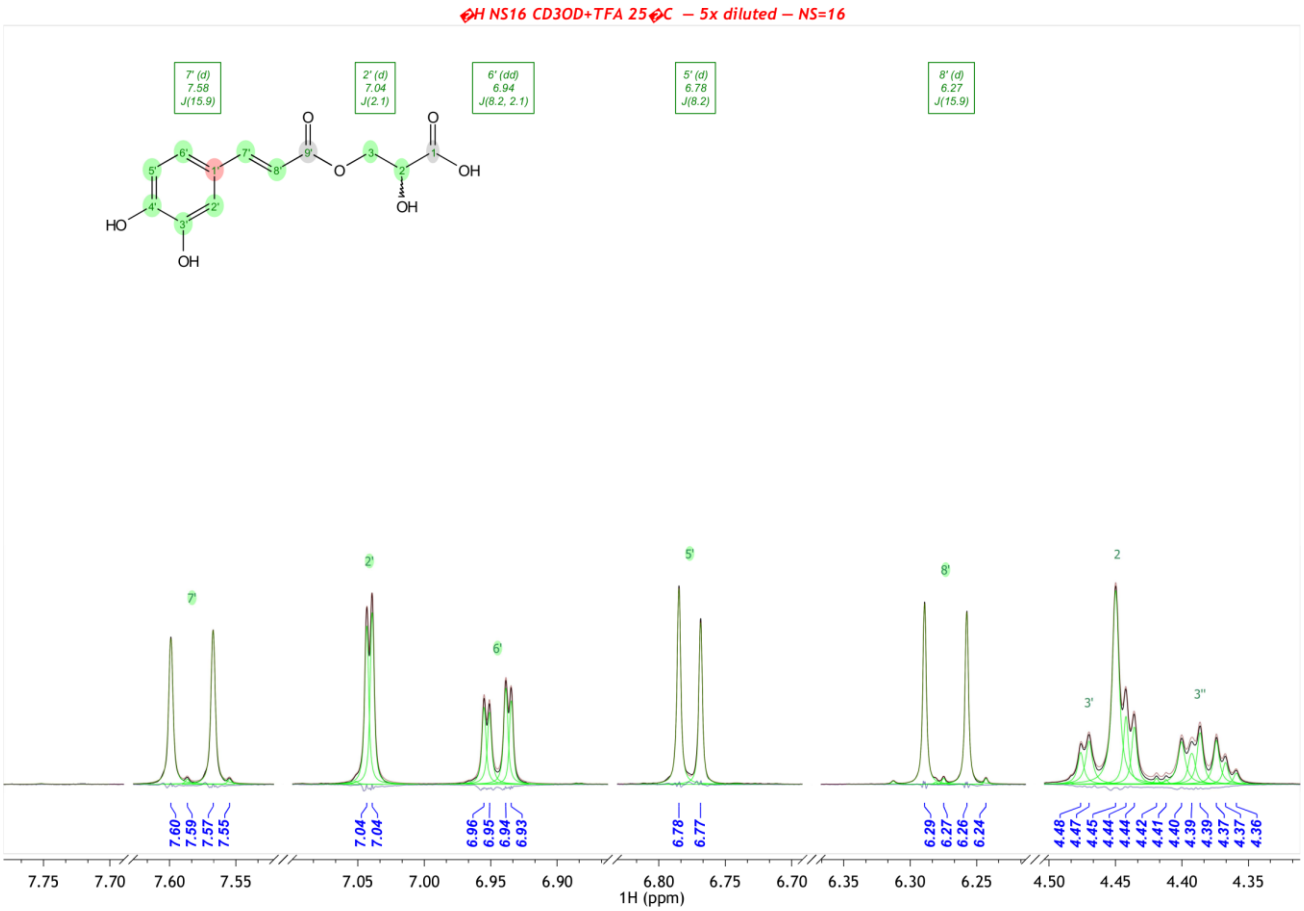


Figure 25S. ^{1}H NMR spectrum of compound 14

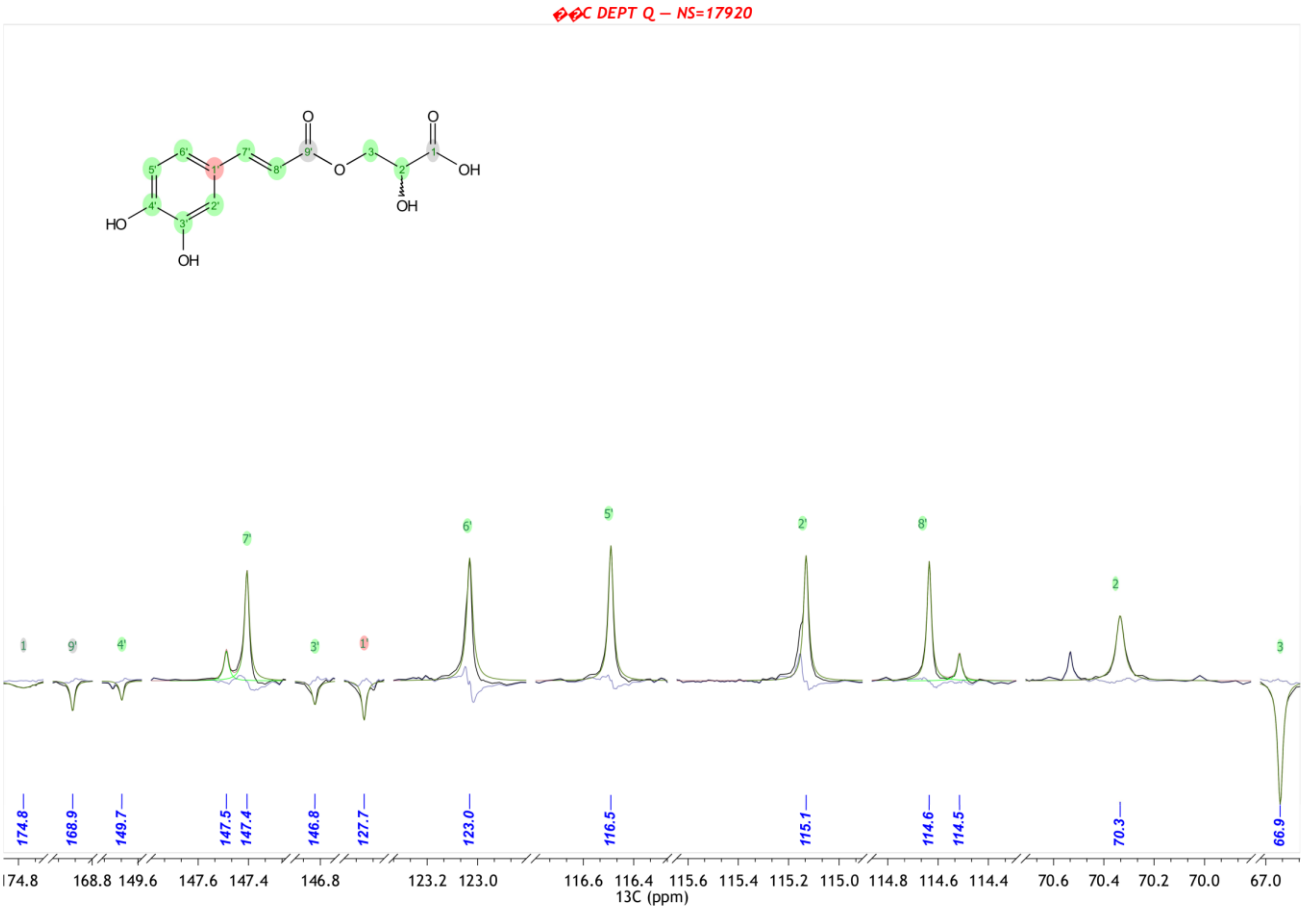


Figure 26S. ^{13}C DEPTQ NMR spectrum of compound 14

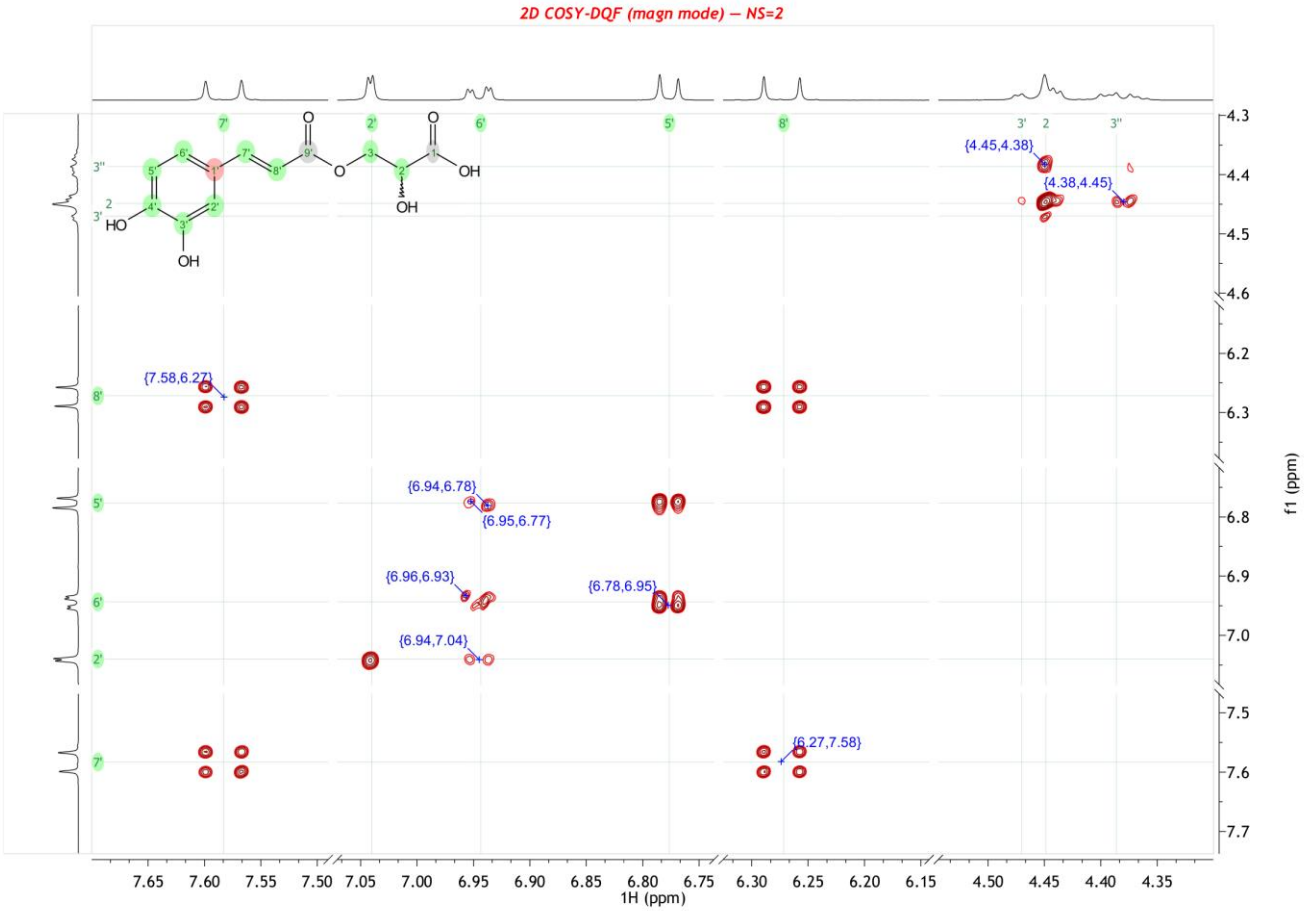


Figure 27S. ^{1}H-^{1}H COSY NMR spectrum of compound 14

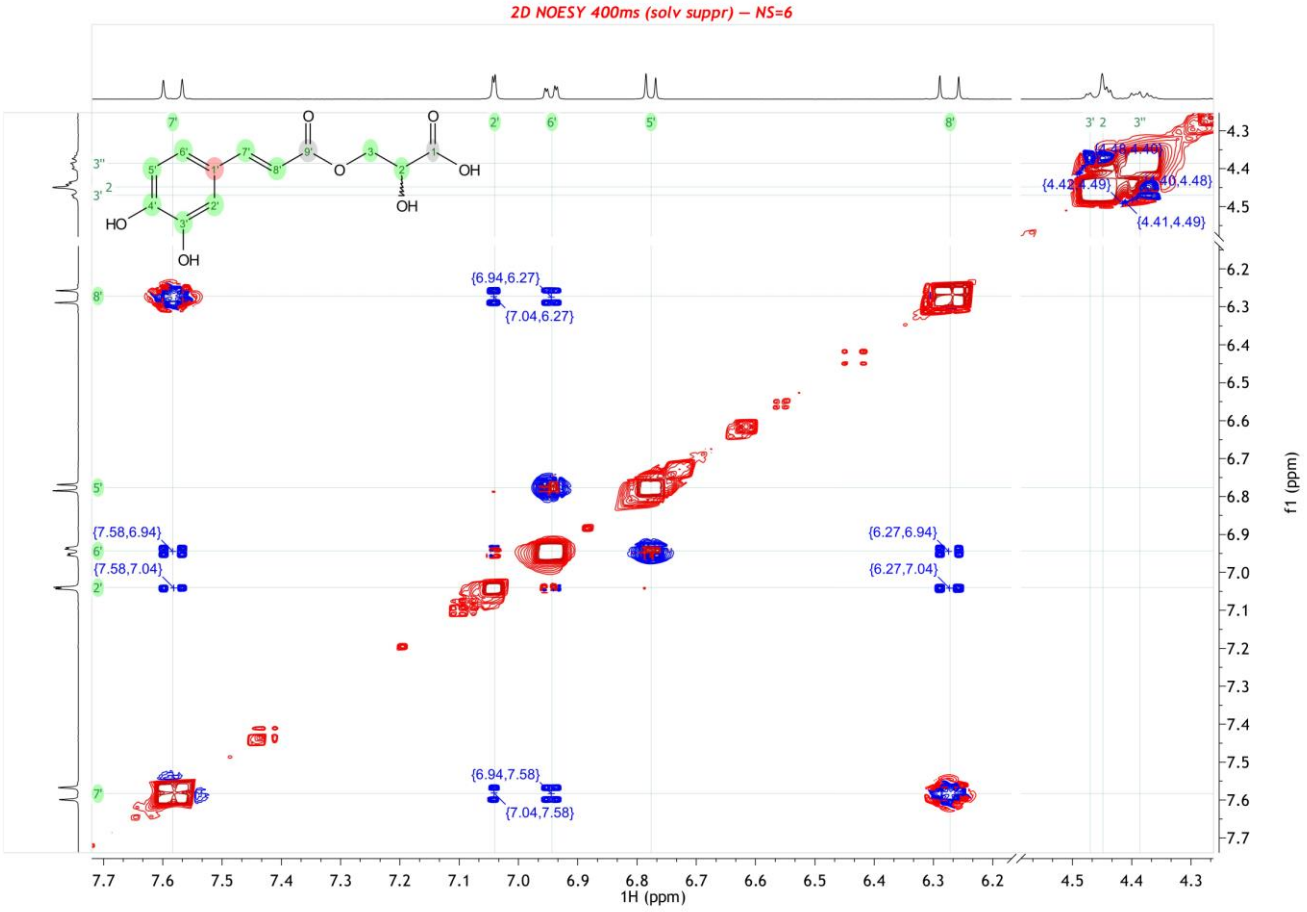


Figure 28S. ^{1}H-^{1}H NOESY (400 ms) NMR spectrum of compound 14

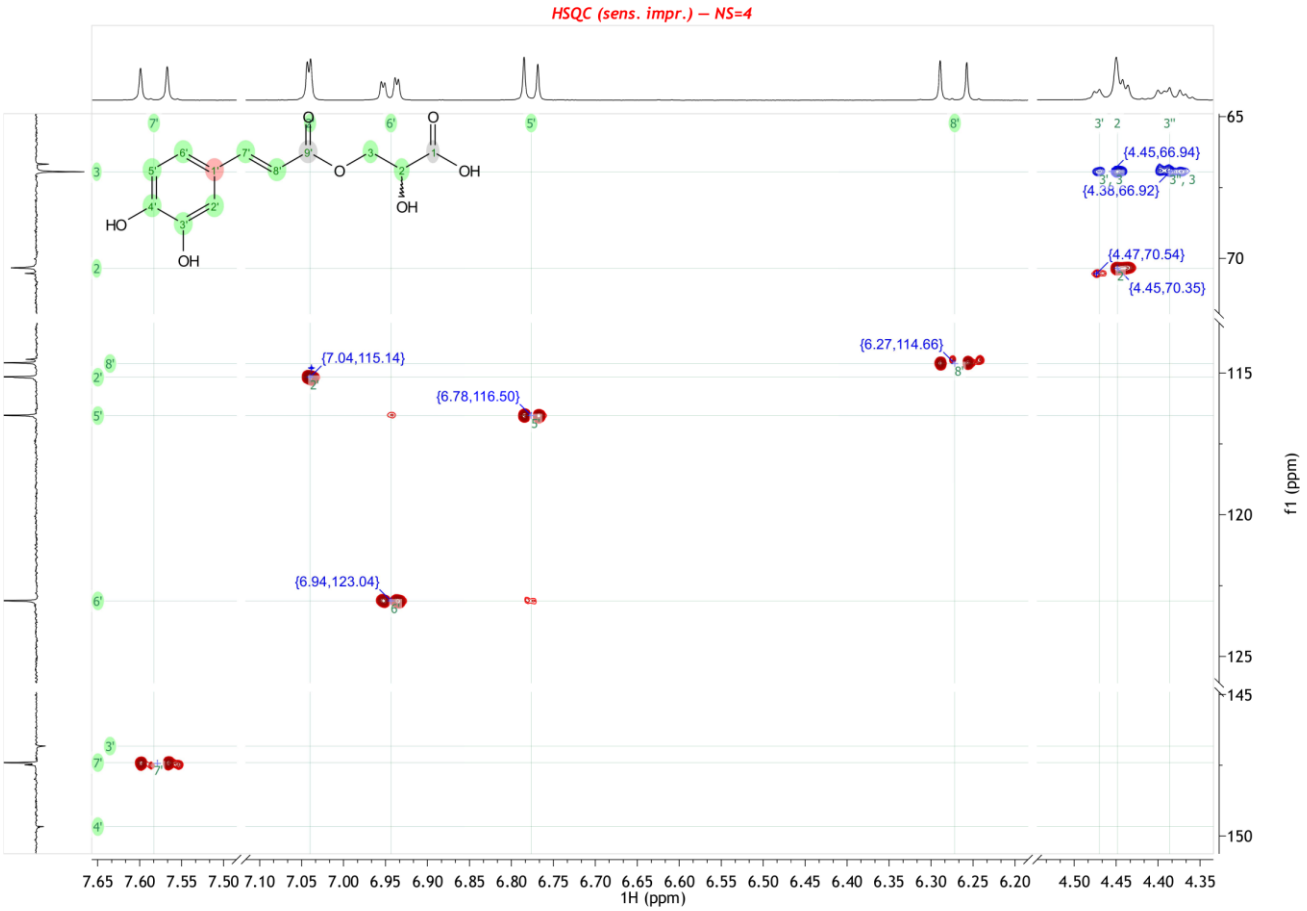


Figure 29S. ^{1}H-^{13}C HSQC NMR spectrum of compound 14

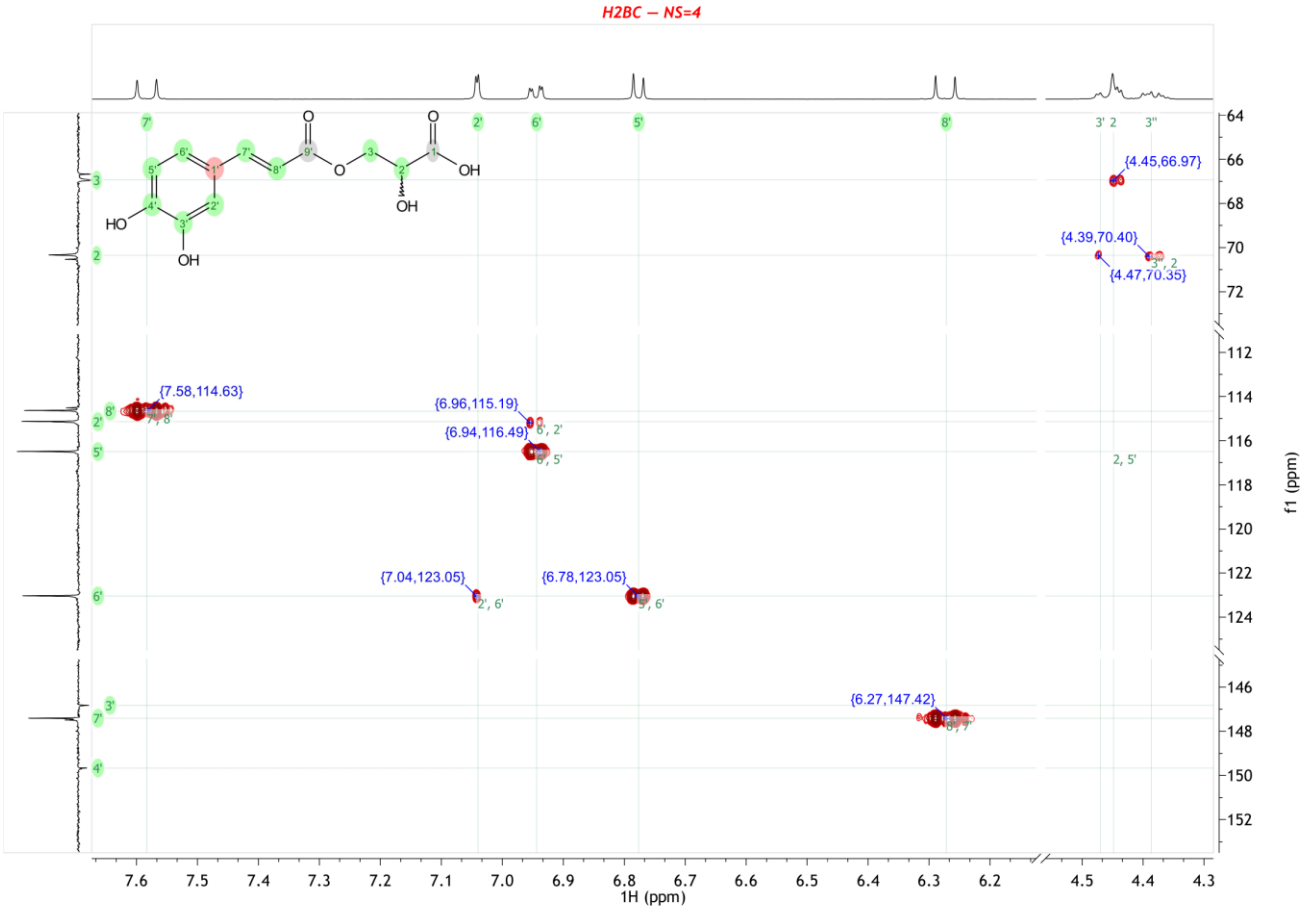


Figure 30S. ^{1}H-^{13}C H2BC NMR spectrum of compound 14

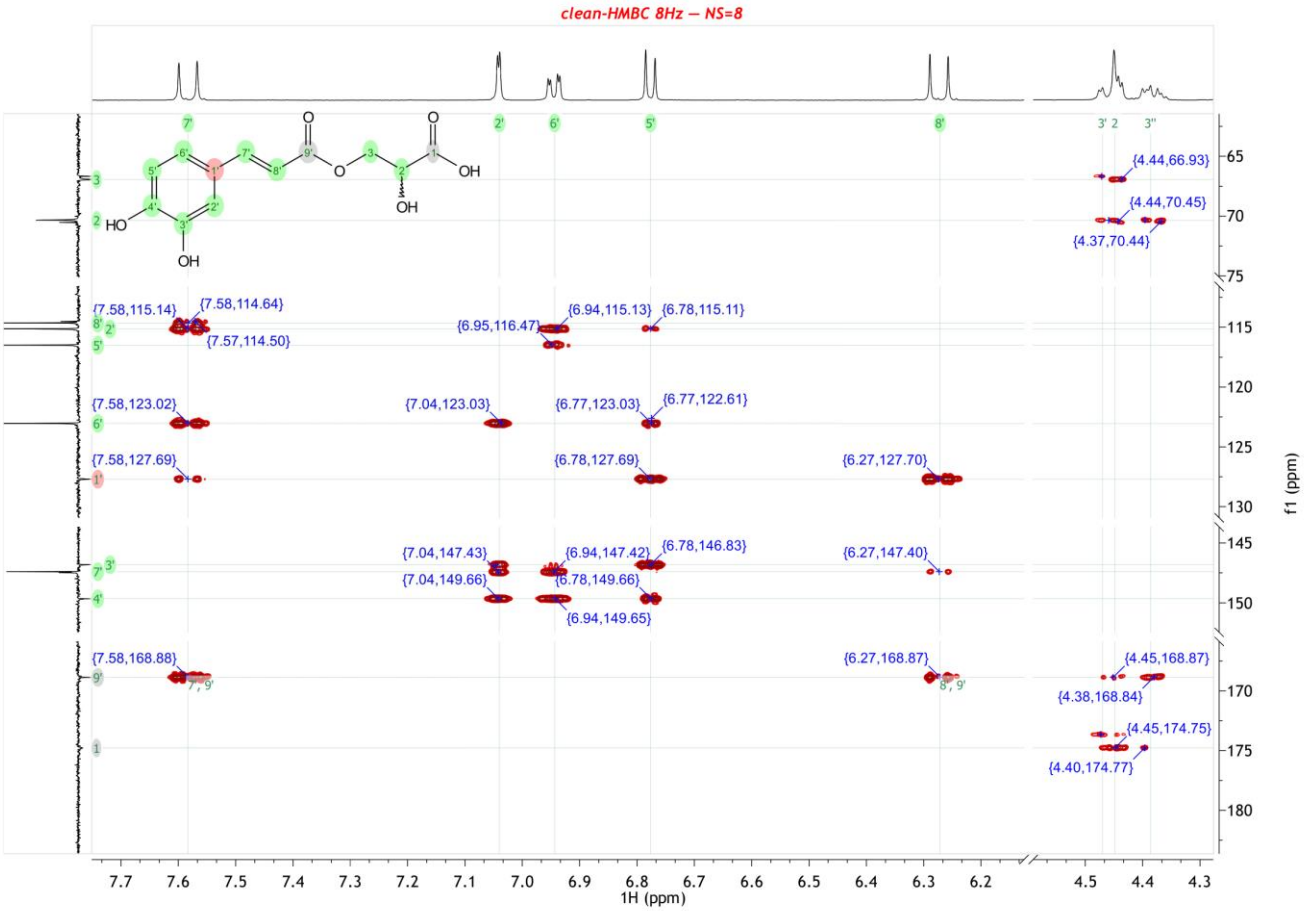


Figure 31S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 14

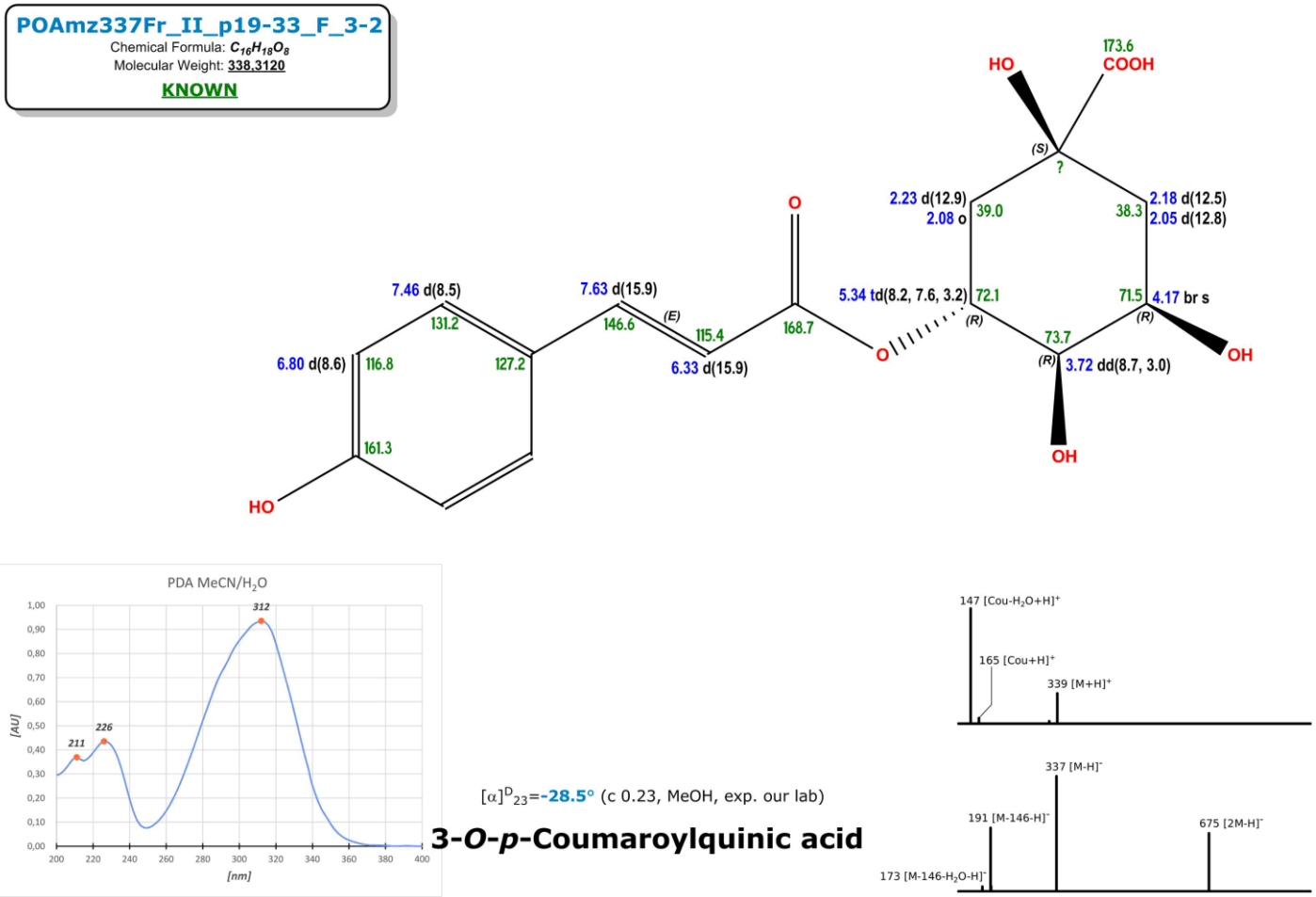
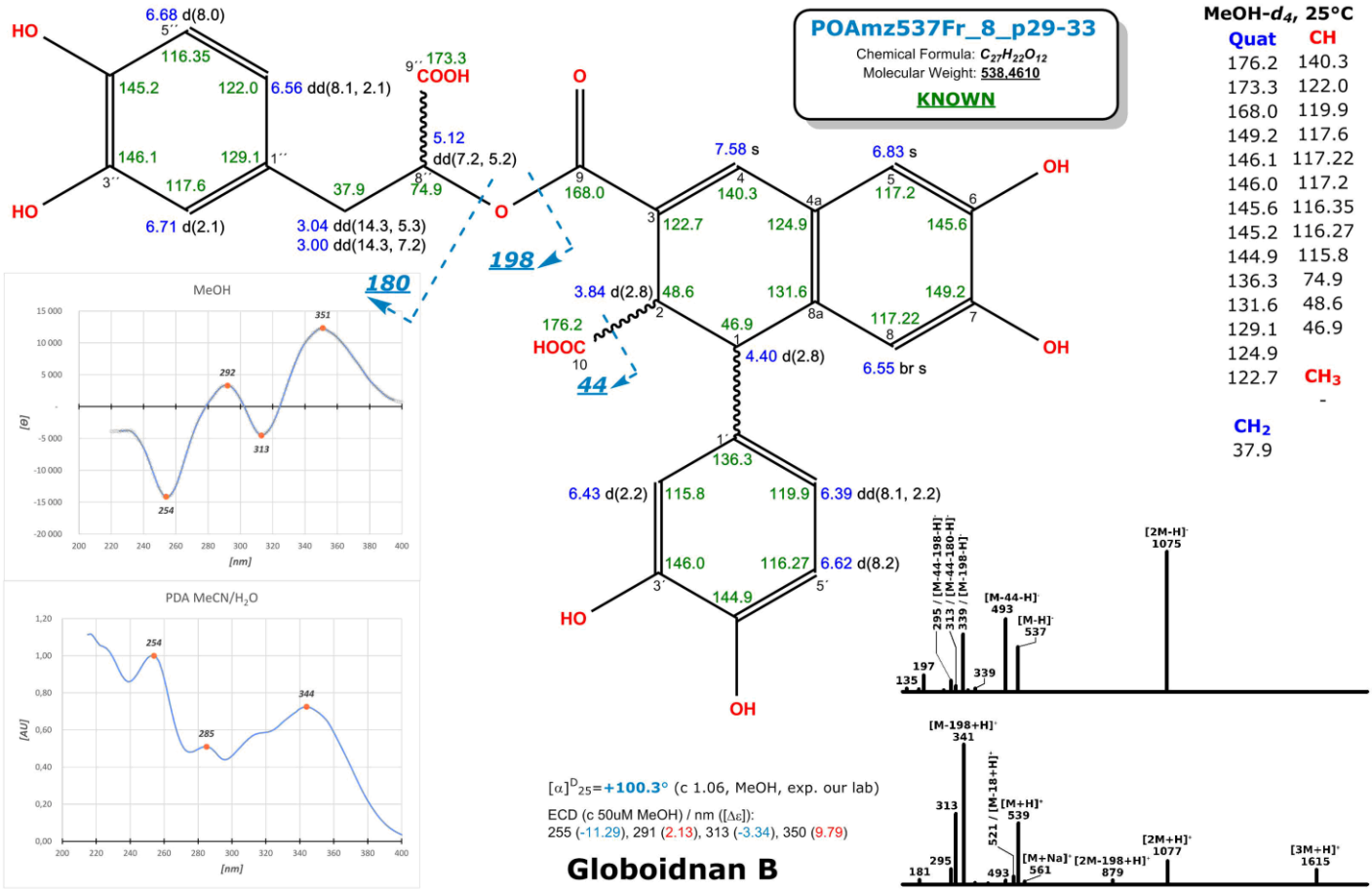


Figure 32S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 15 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O



1. Basli, A., Delaunay, J.-C., Pedrot, E., Bernillon, S., Madani, K., Monti, J.-P., Mérillon, J.M., Chibane, M., Richard, T., 2014. New Cyclolignans from Origanum glandulosum Active Against ß-amyloid Aggregation. Rec. Nat. Prod. 8, 208–216.
2. Assoumatine, T., Datta, P.K., Hooper, T.S., Yvon, B.L., Charlton, J.L., 2004. A Short Asymmetric Synthesis of (+)-Lyoniresinol Dimethyl Ether. J. Org. Chem. 69, 4140–4144. doi:10.1021/jo0497454

Figure 33S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 18 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$; ECD spectrum in MeOH

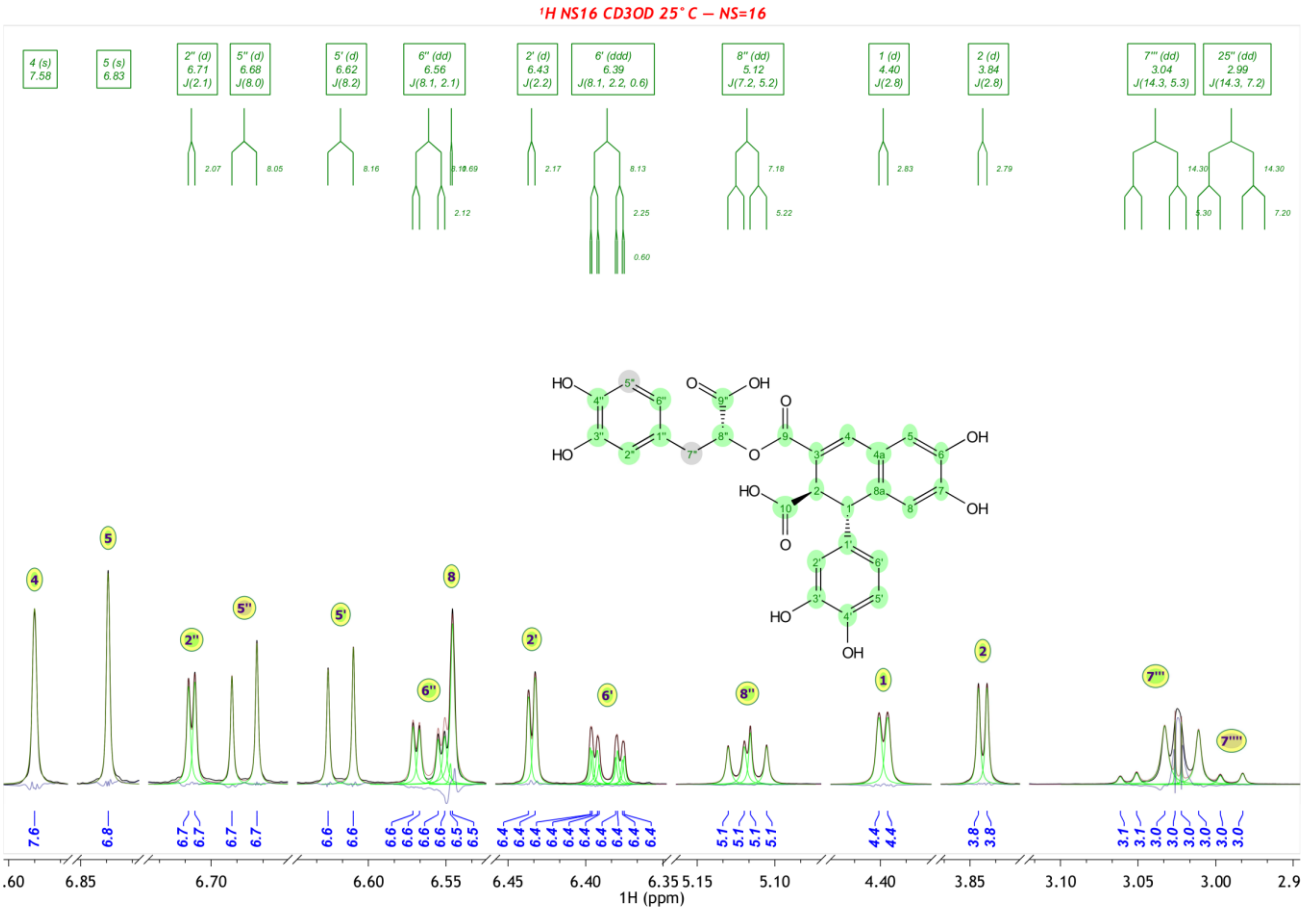


Figure 34S. ^{1}H NMR spectrum of compound 18

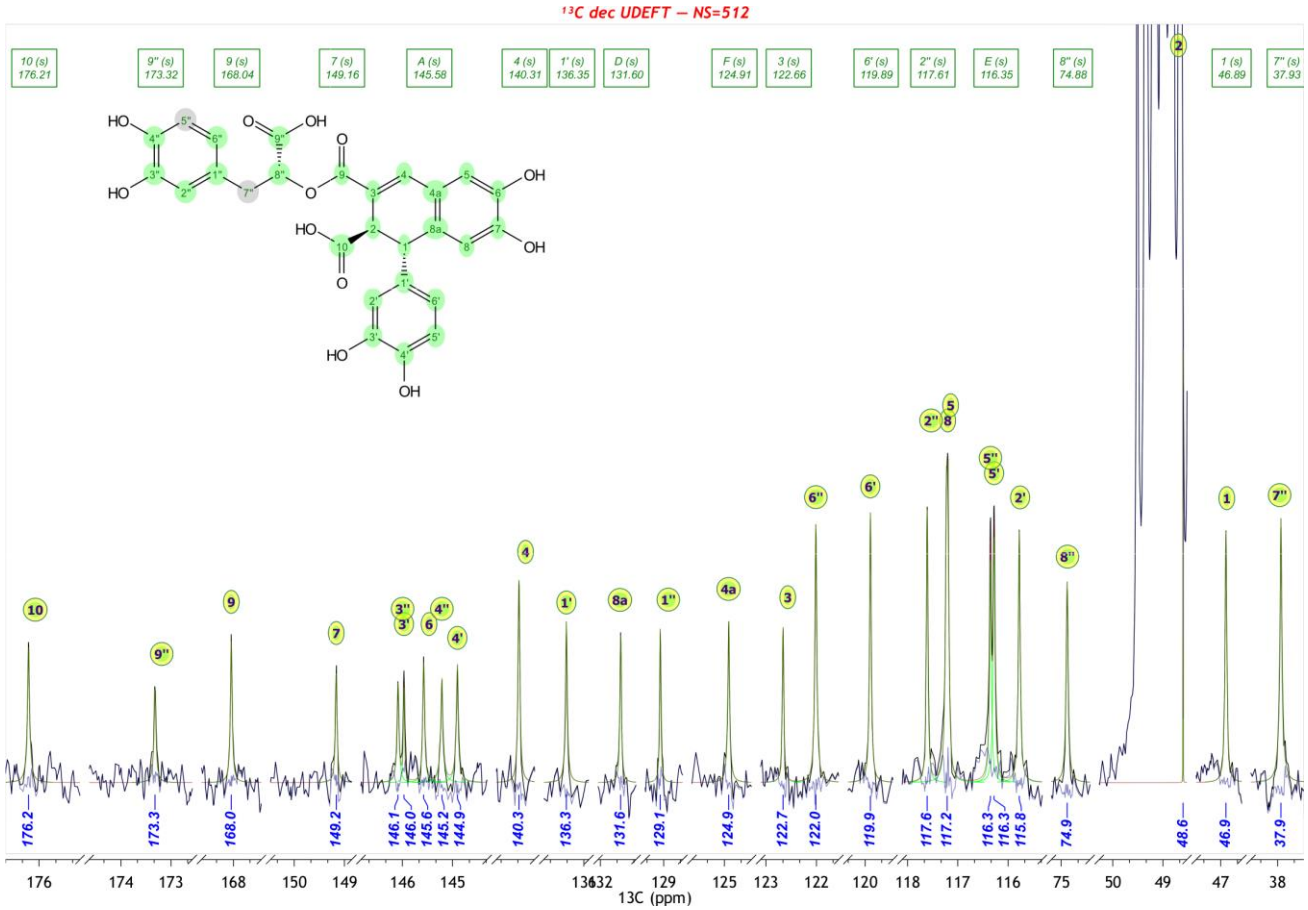


Figure 35S. ^{13}C DEPTQ NMR spectrum of compound 18

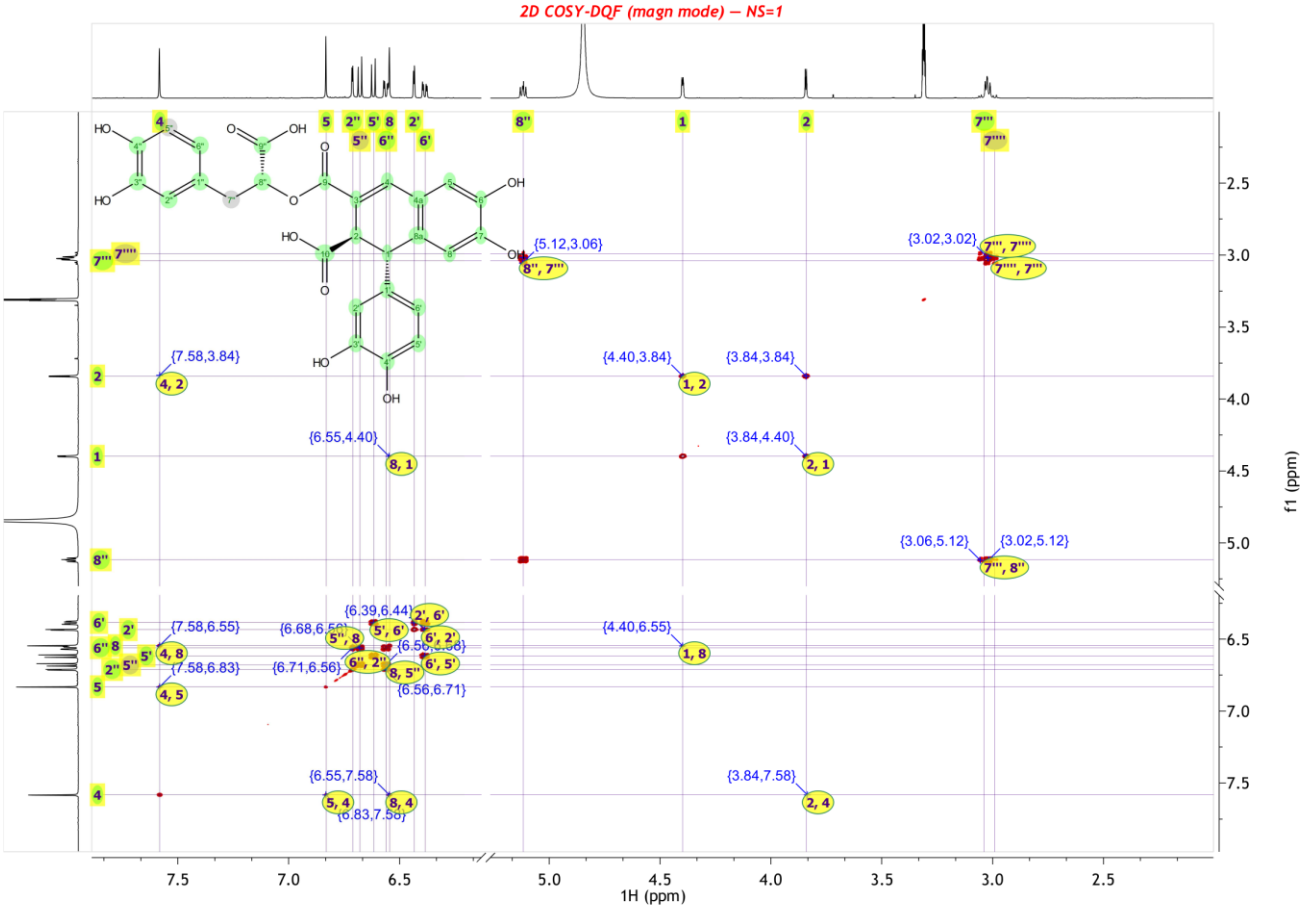


Figure 36S. ^{1}H-^{1}H COSY NMR spectrum of compound 18

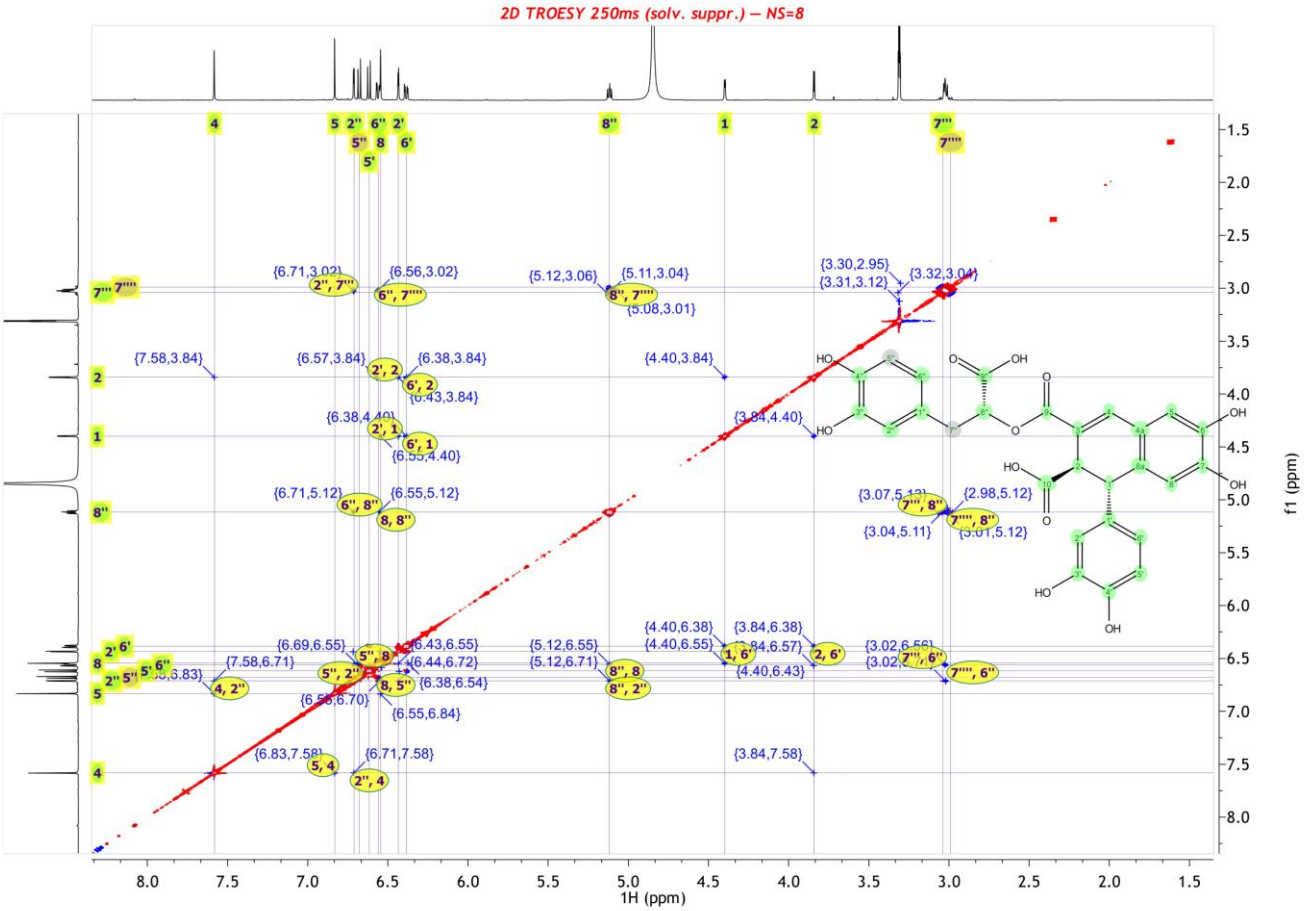


Figure 37S. ^{1}H-^{1}H TROESY (250 ms) NMR spectrum of compound 18

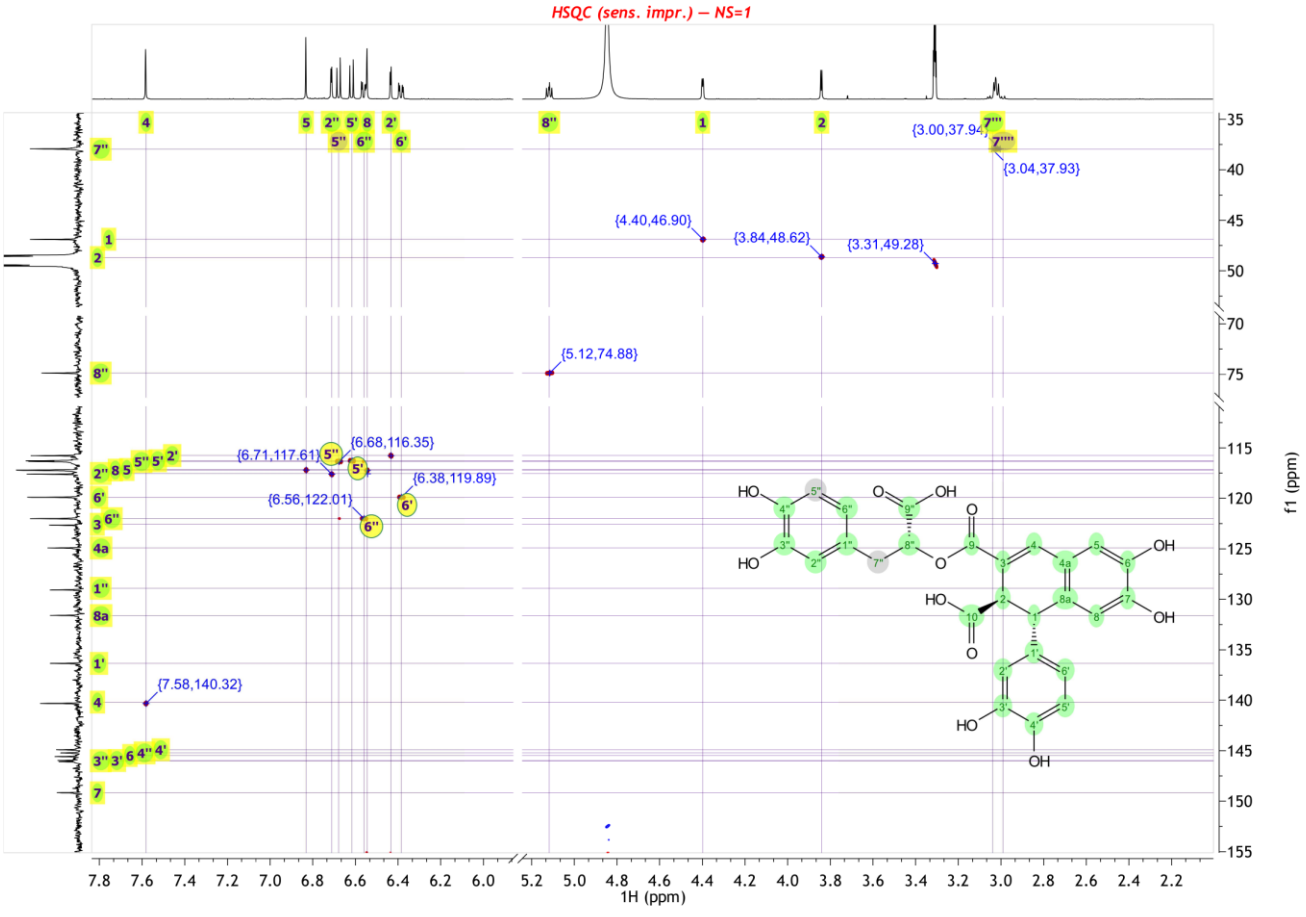


Figure 38S. ^{1}H-^{13}C HSQC NMR spectrum of compound 18

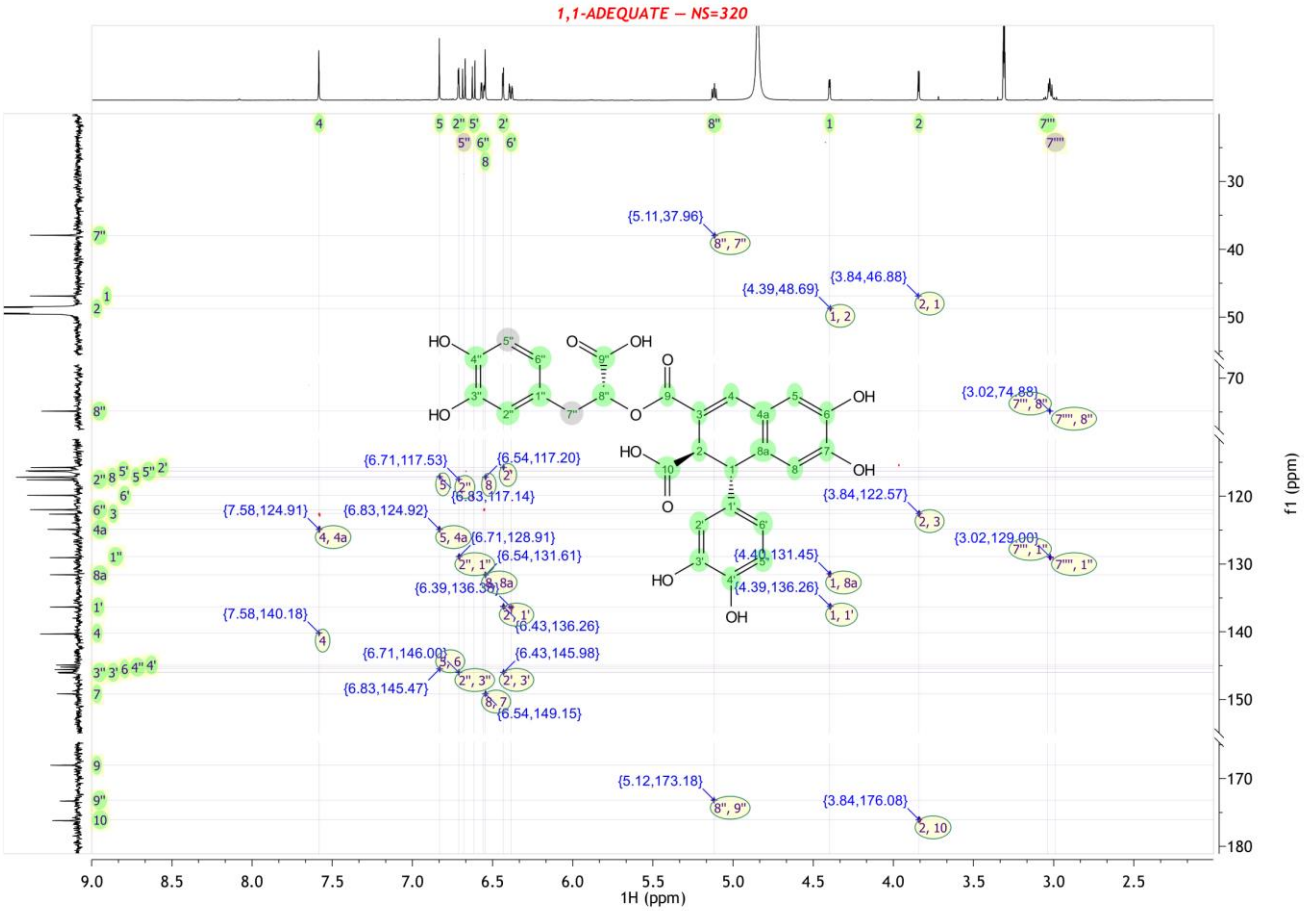


Figure 39S. ^{1}H-^{13}C 1,1-ADEQUATE NMR spectrum of compound 18

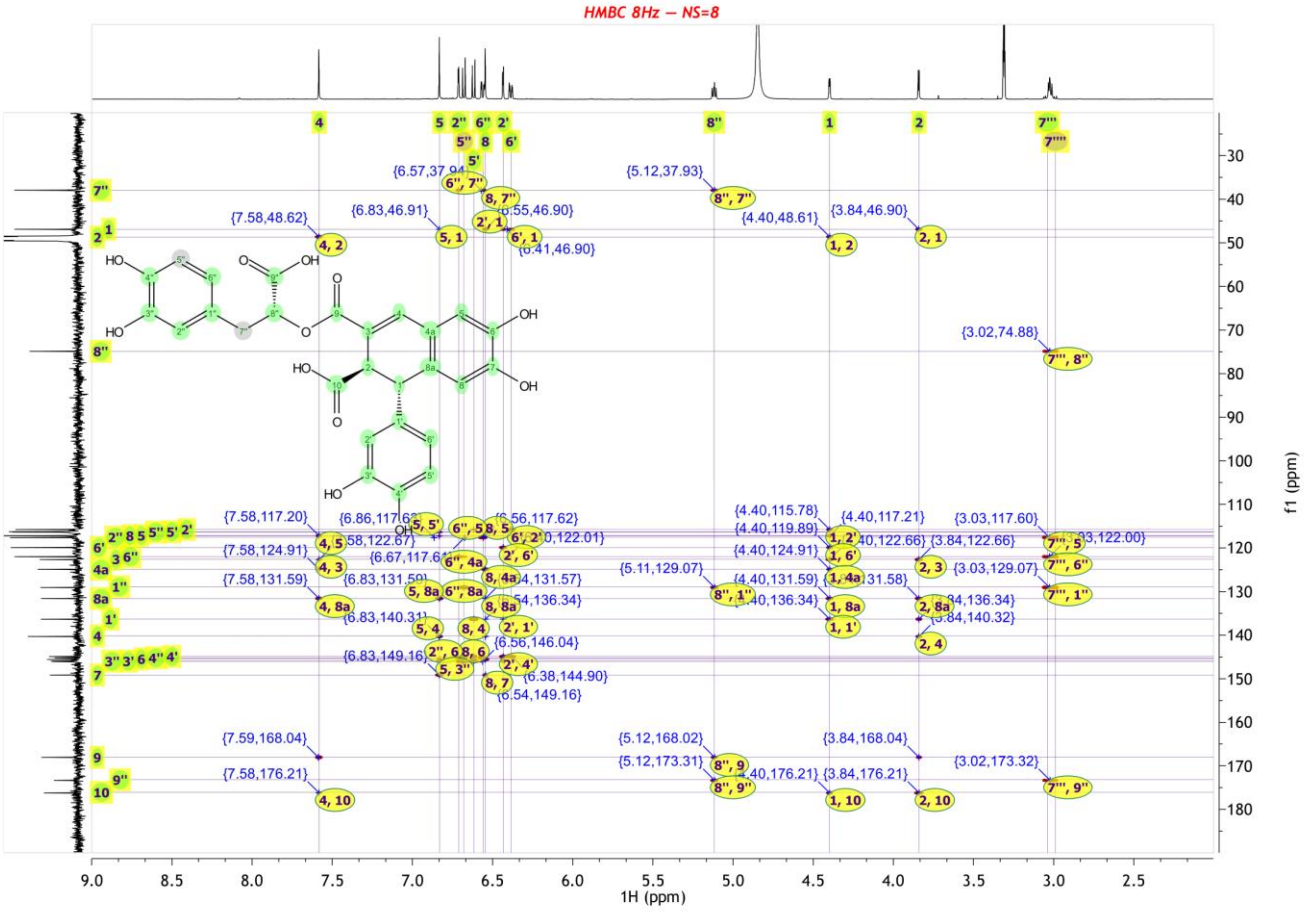


Figure 40S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 18

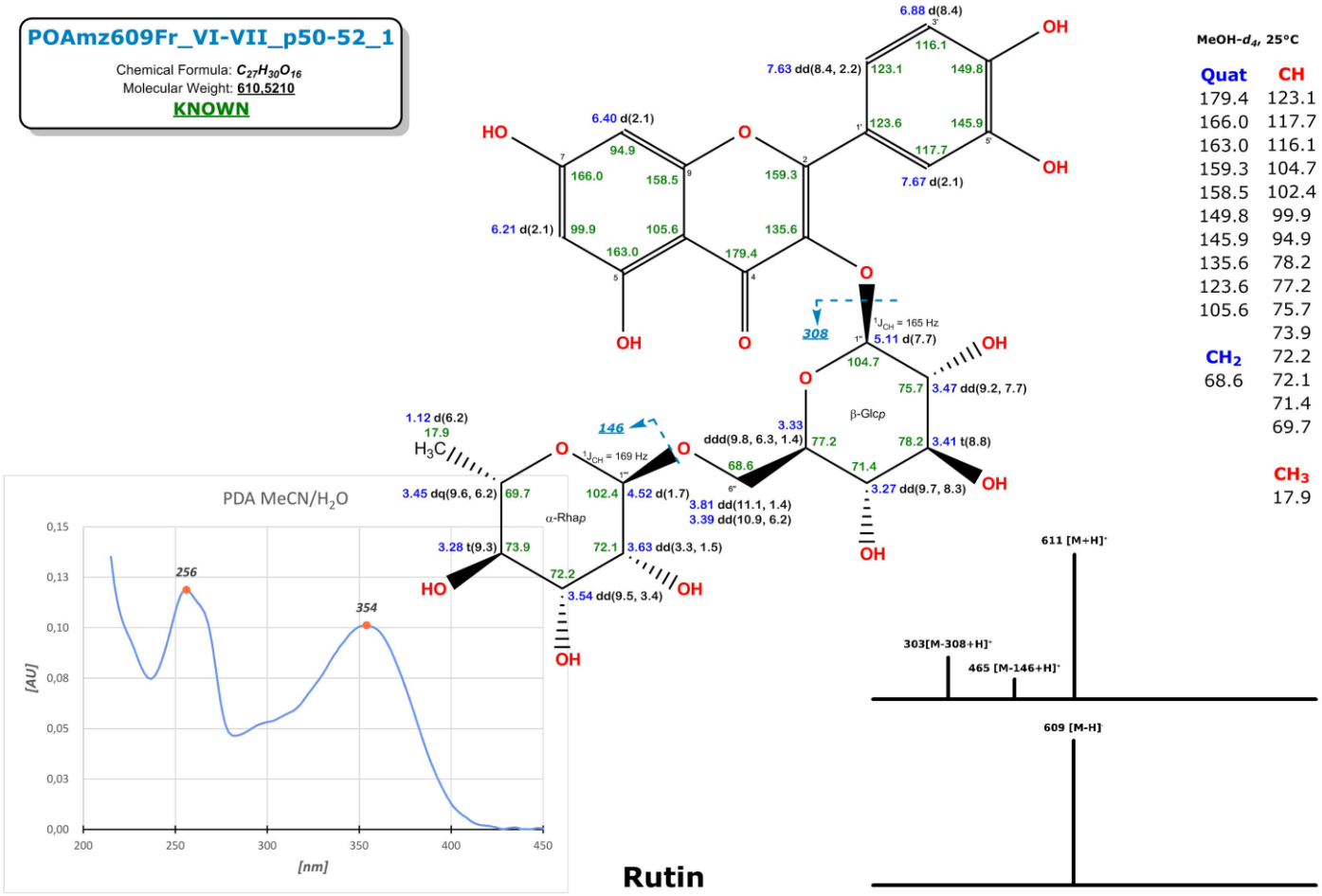


Figure 41S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 19 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$

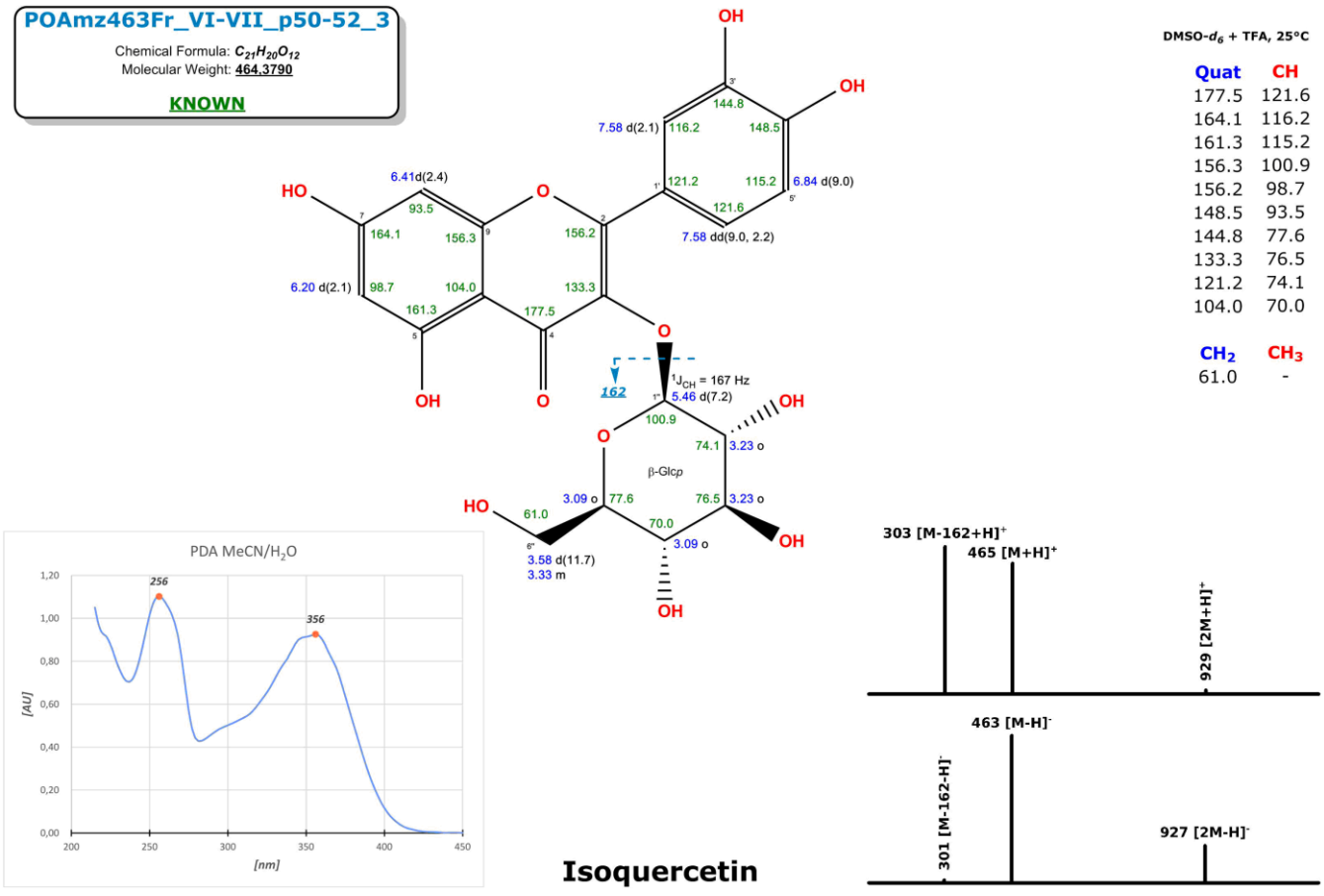


Figure 42S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 21 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$

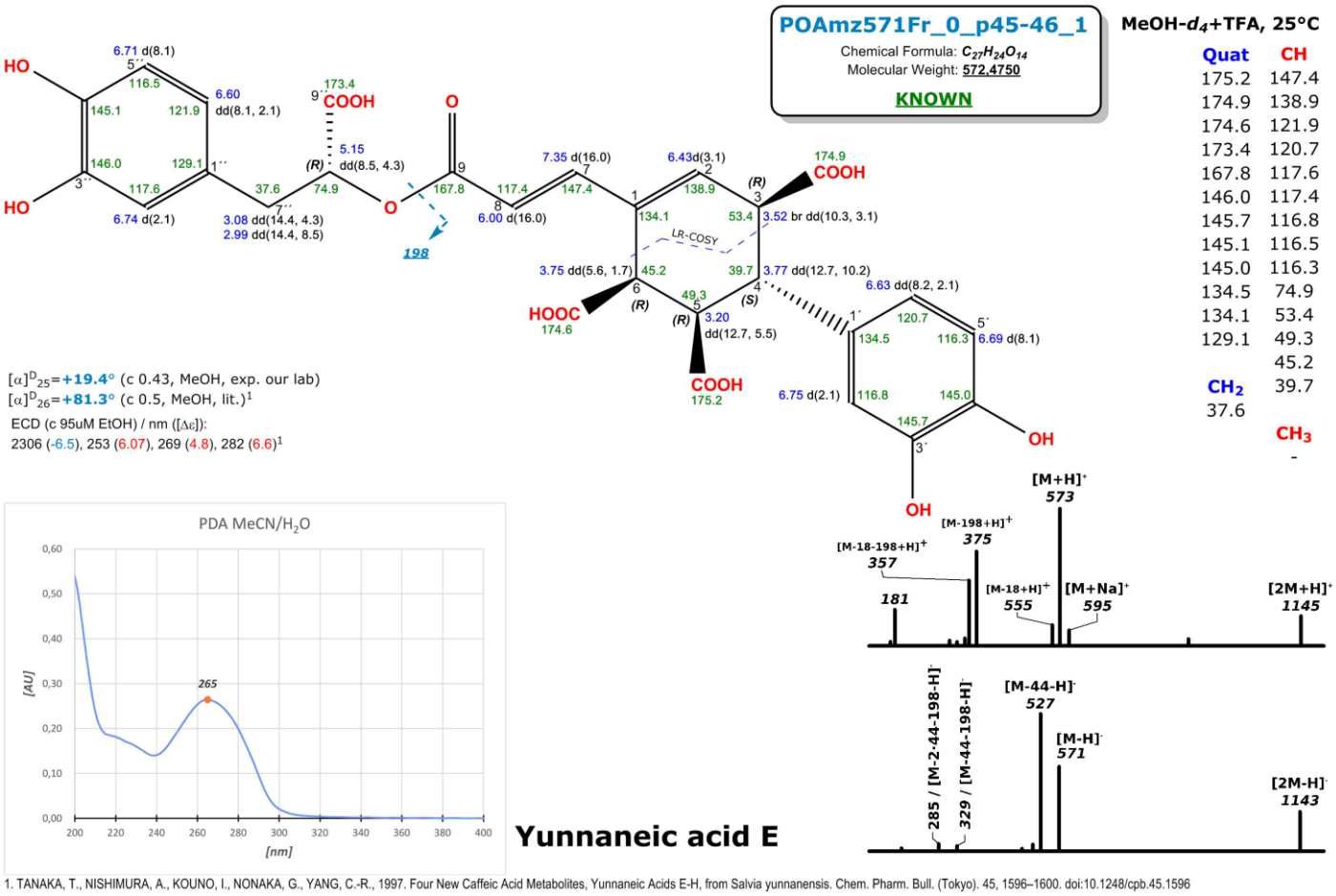


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Figure 43S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 22 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

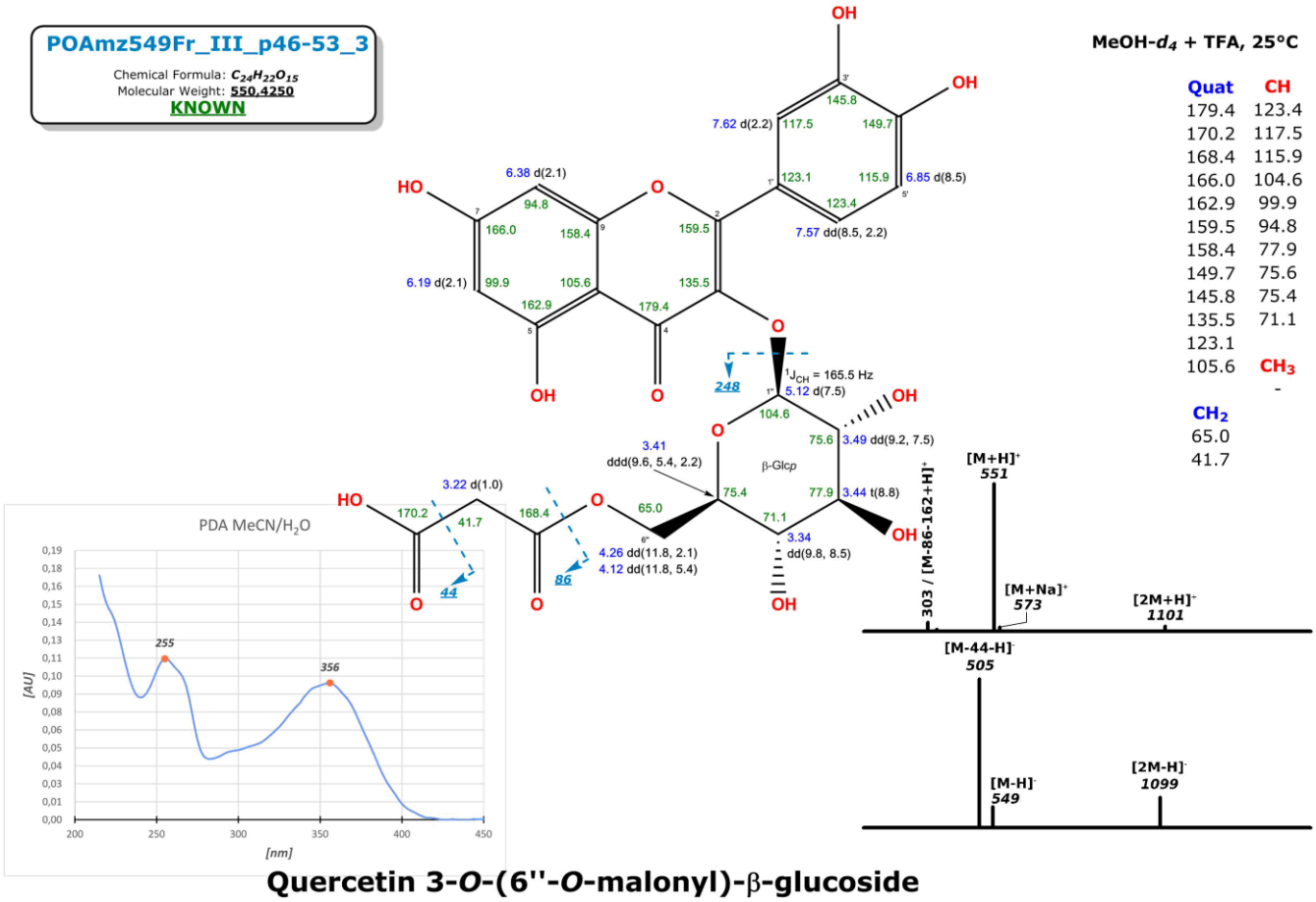

Figure 44S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 23 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

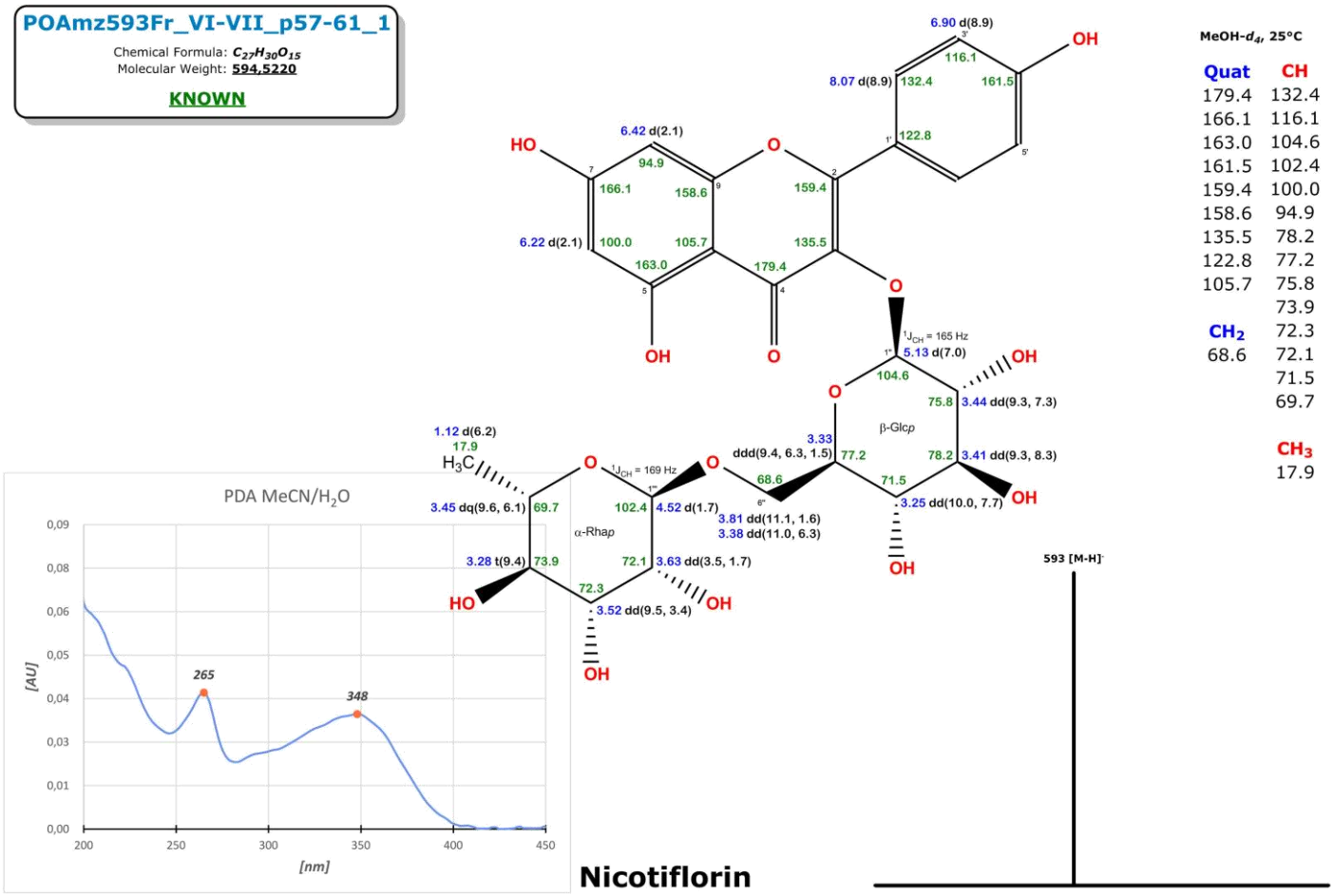

Figure 45S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 24 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$

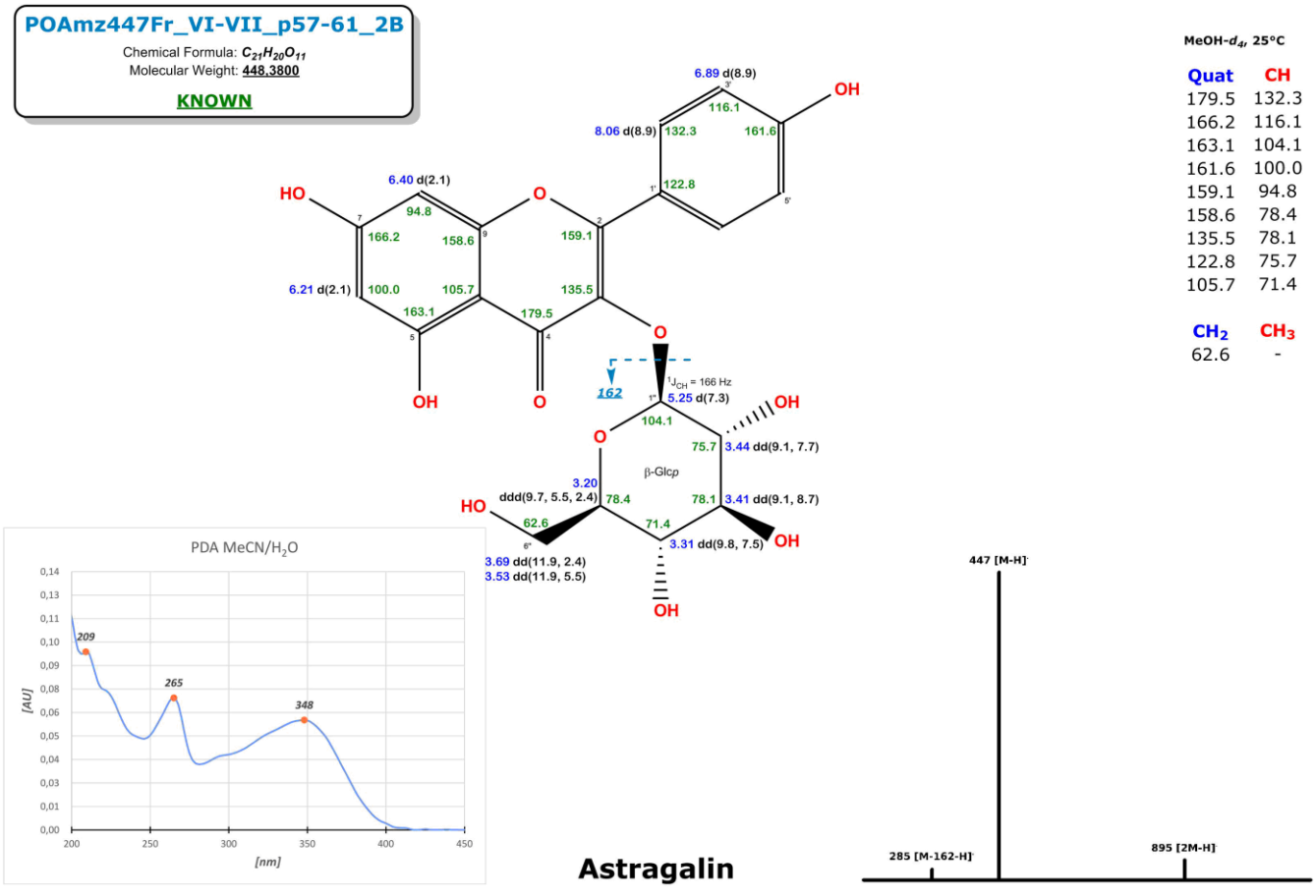

Figure 46S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 25 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$

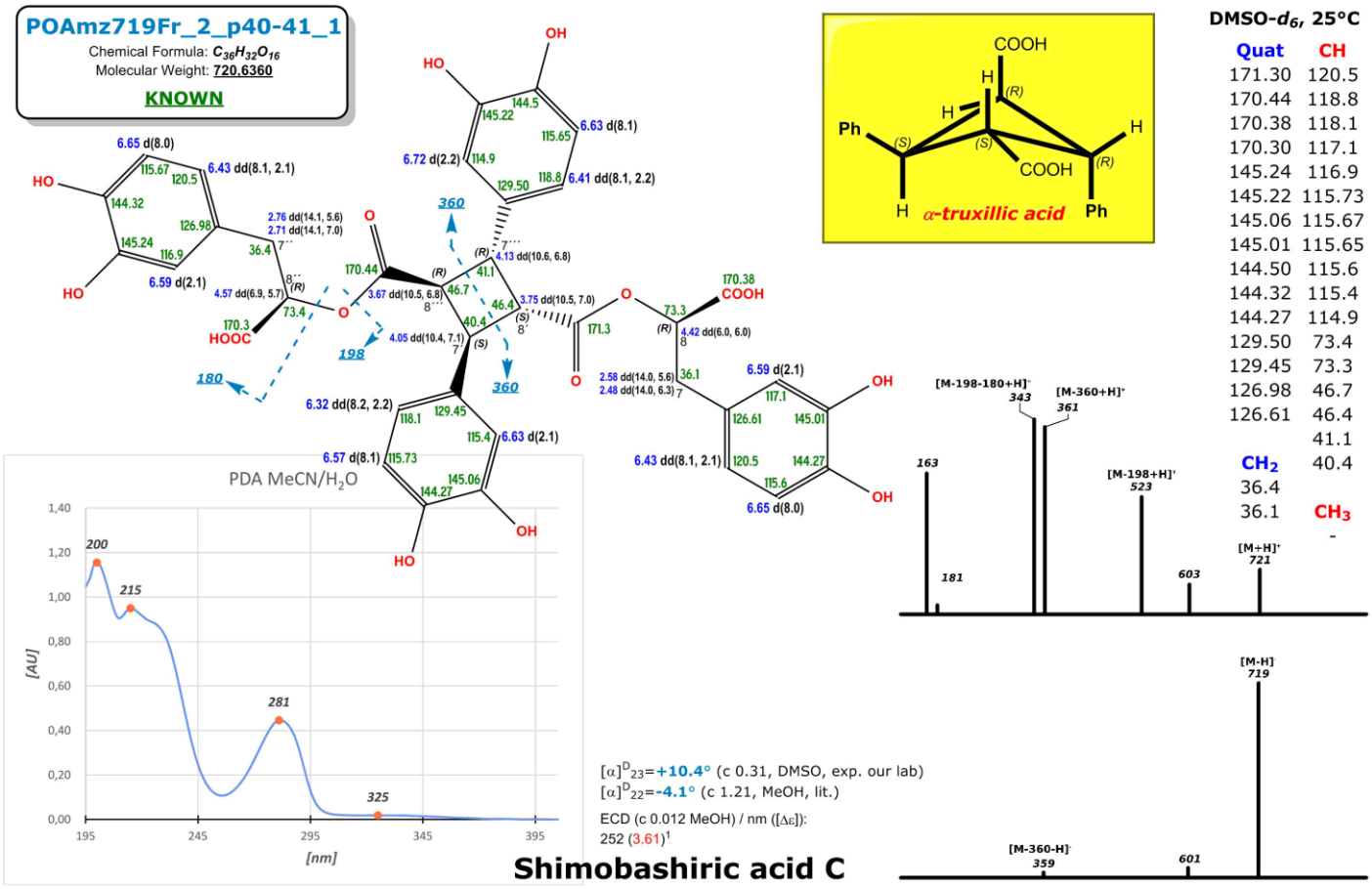

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Figure 47S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 26 in DMSO-d_6, 25°C; on-line PDA UV spectrum in MeCN/H_2O

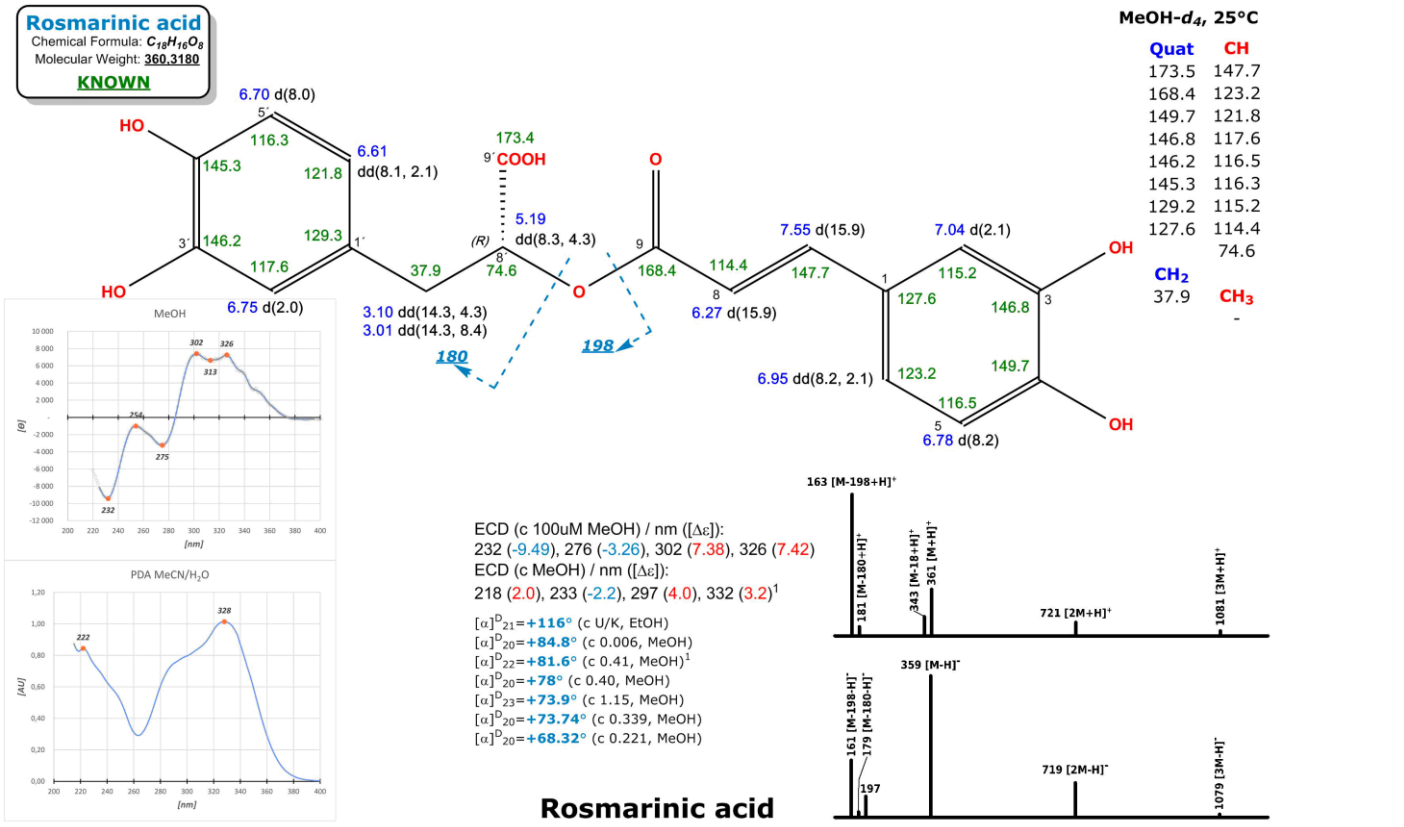

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Figure 48S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 27 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

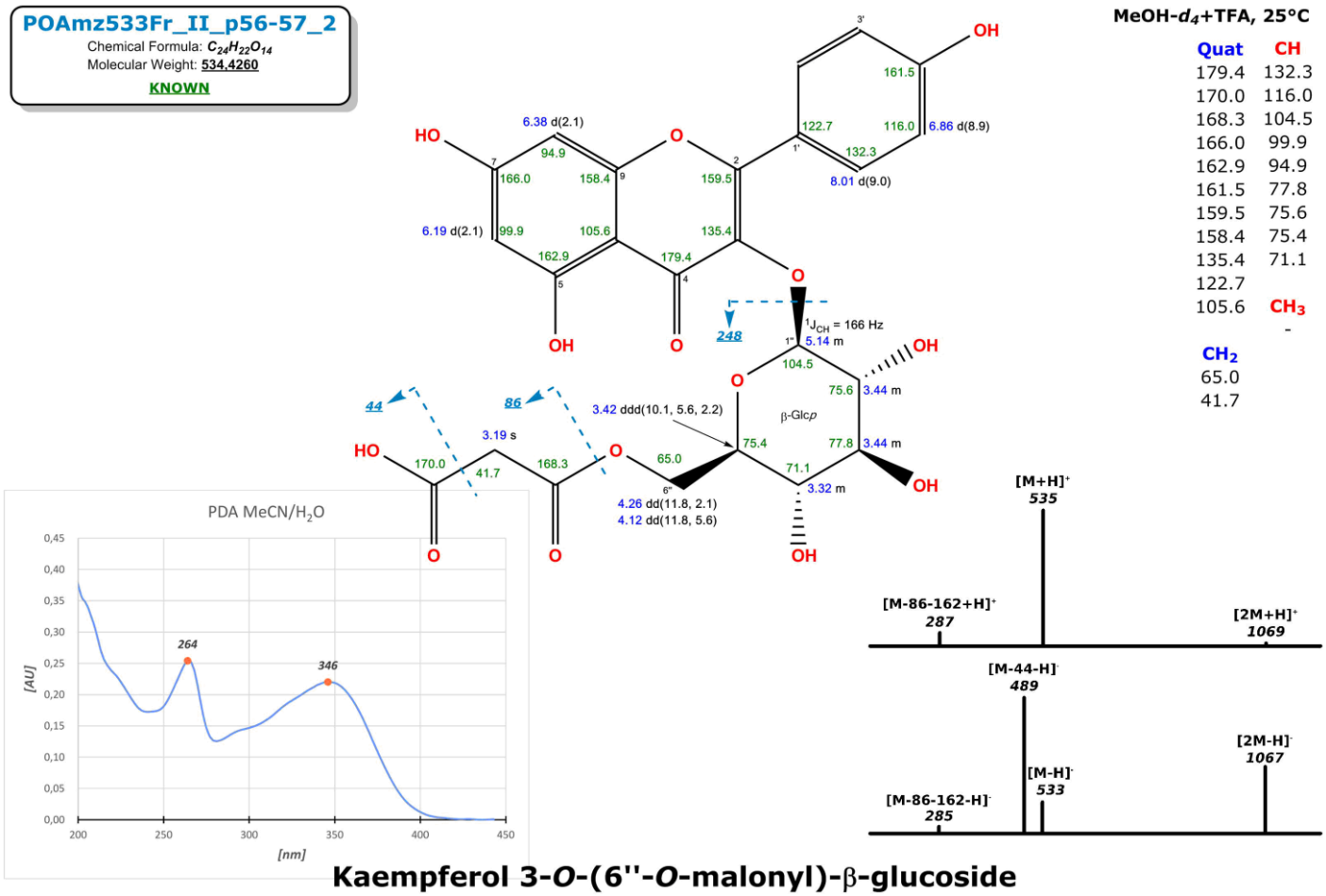

Figure 49S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 28 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$

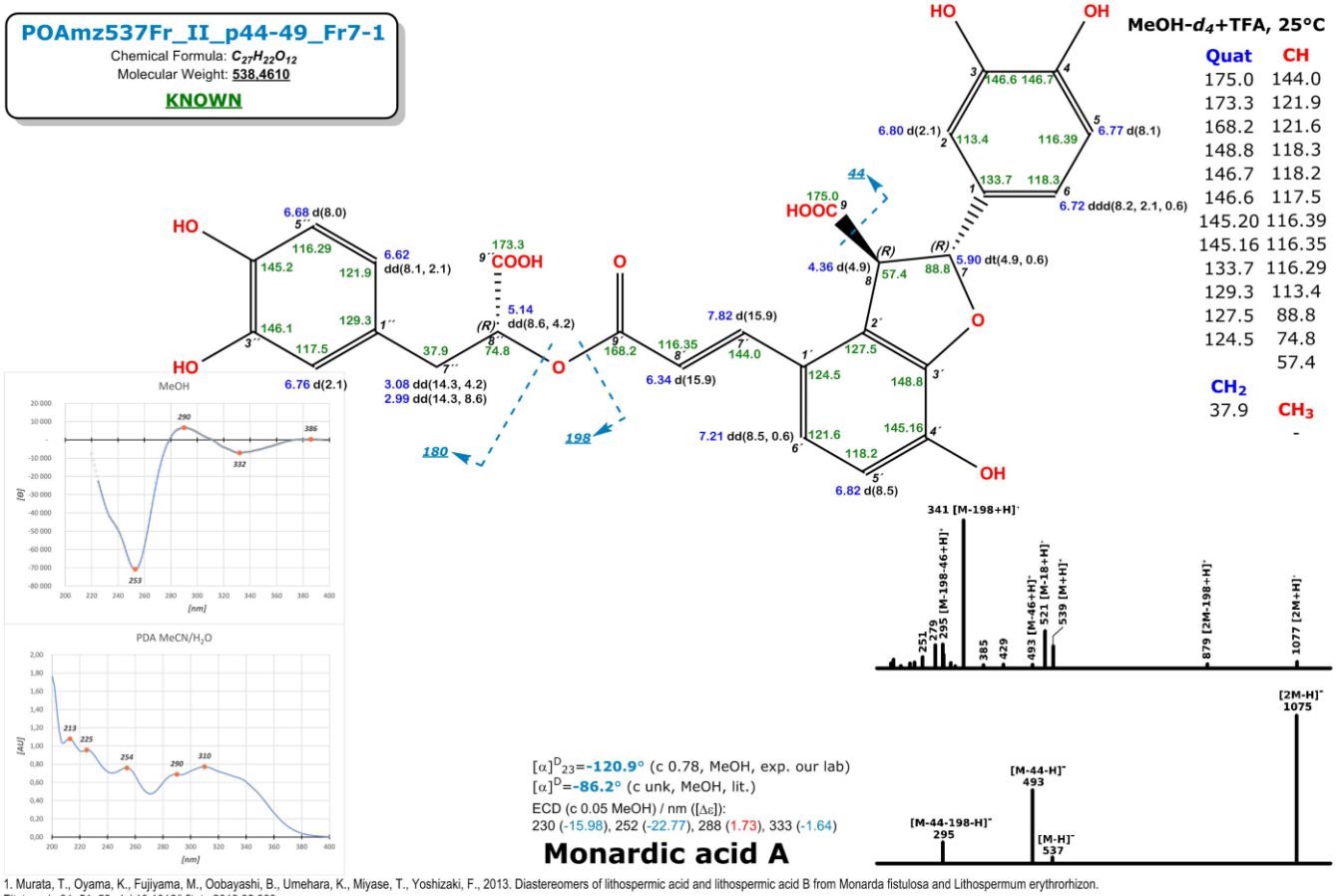

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Figure 50S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 29 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$; ECD spectrum in MeOH

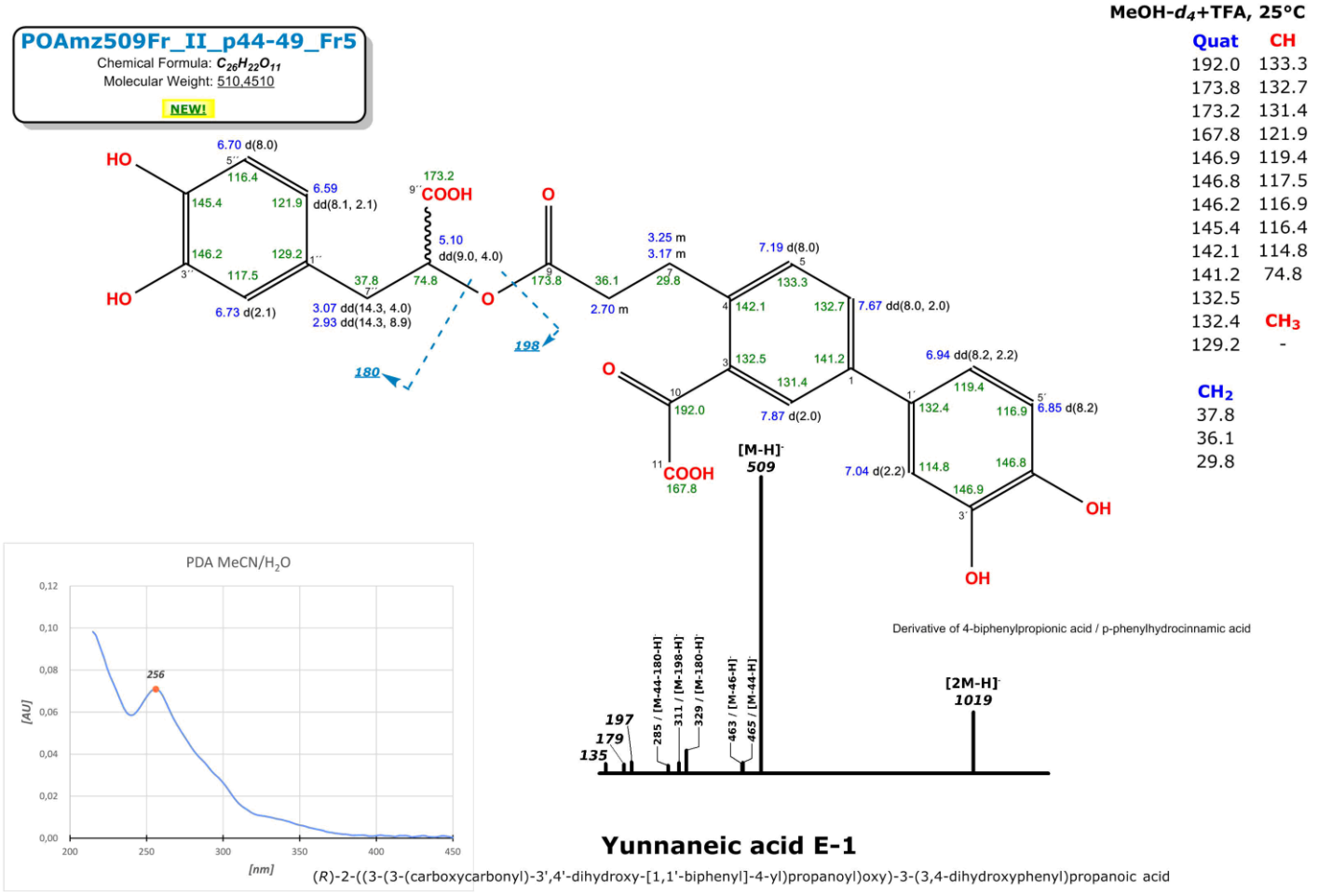

Figure 51S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 30 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

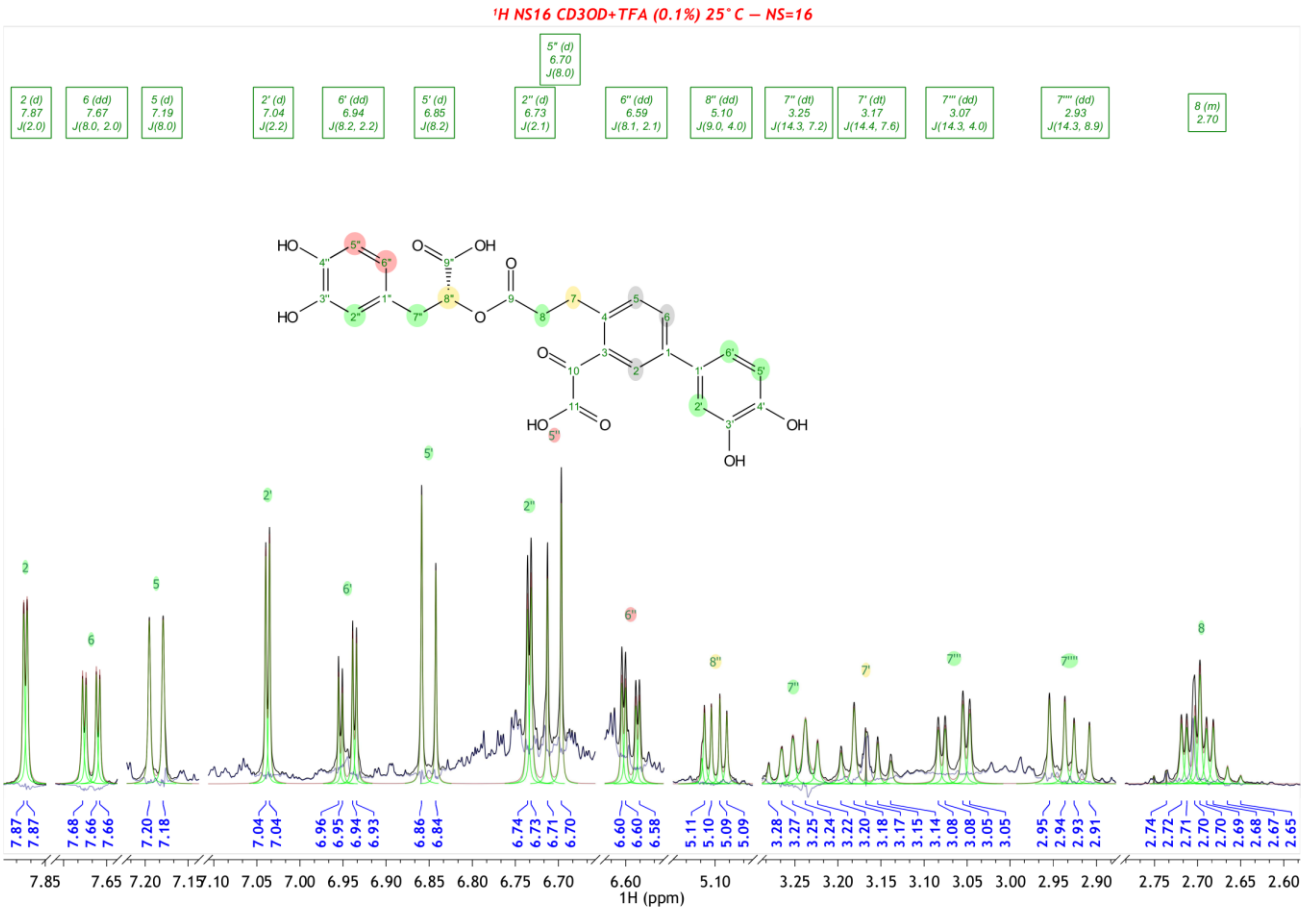

Figure 52S. ^{1}H NMR spectrum of compound 30

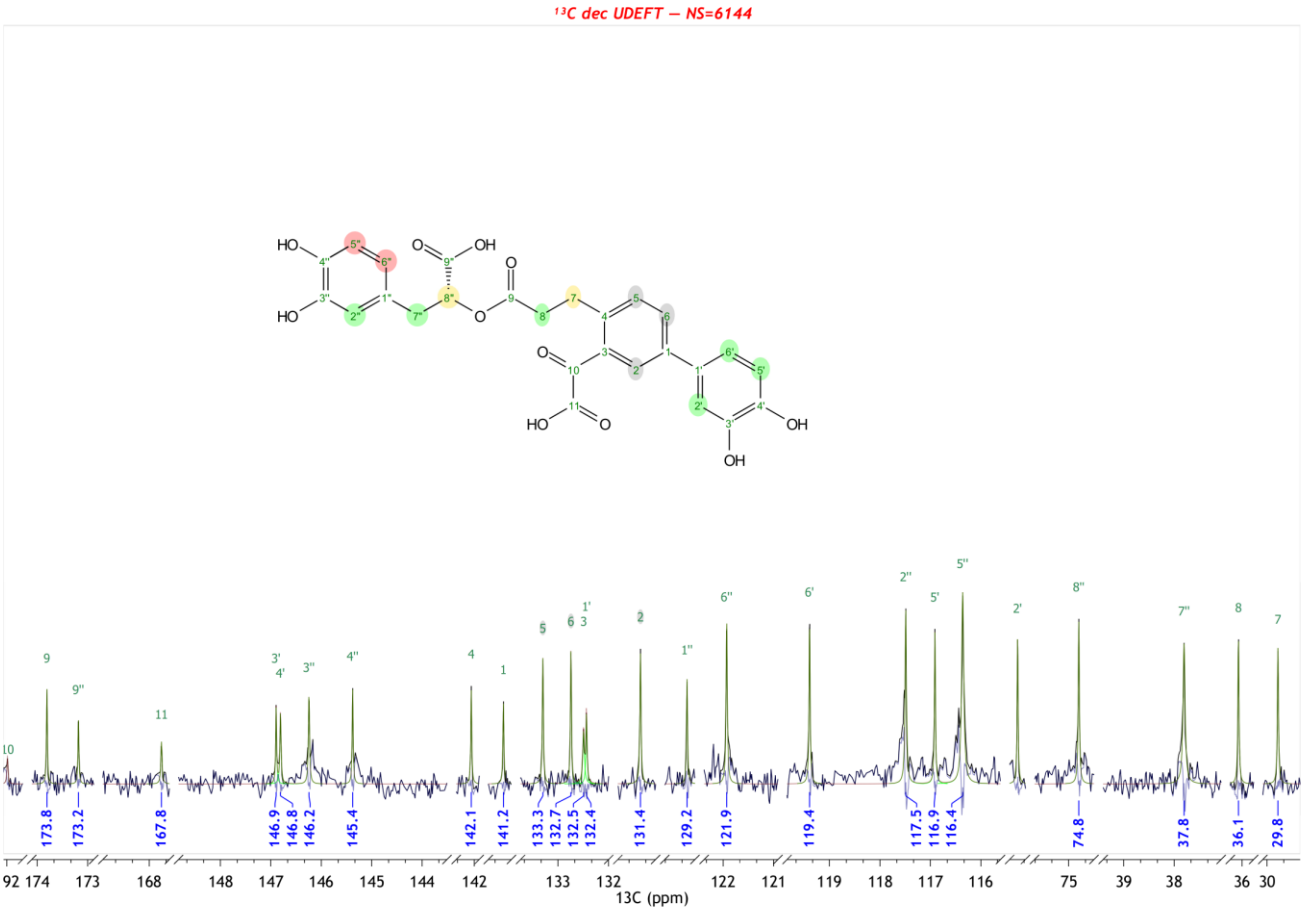

Figure 53S. ^{13}C DEPTQ NMR spectrum of compound 30

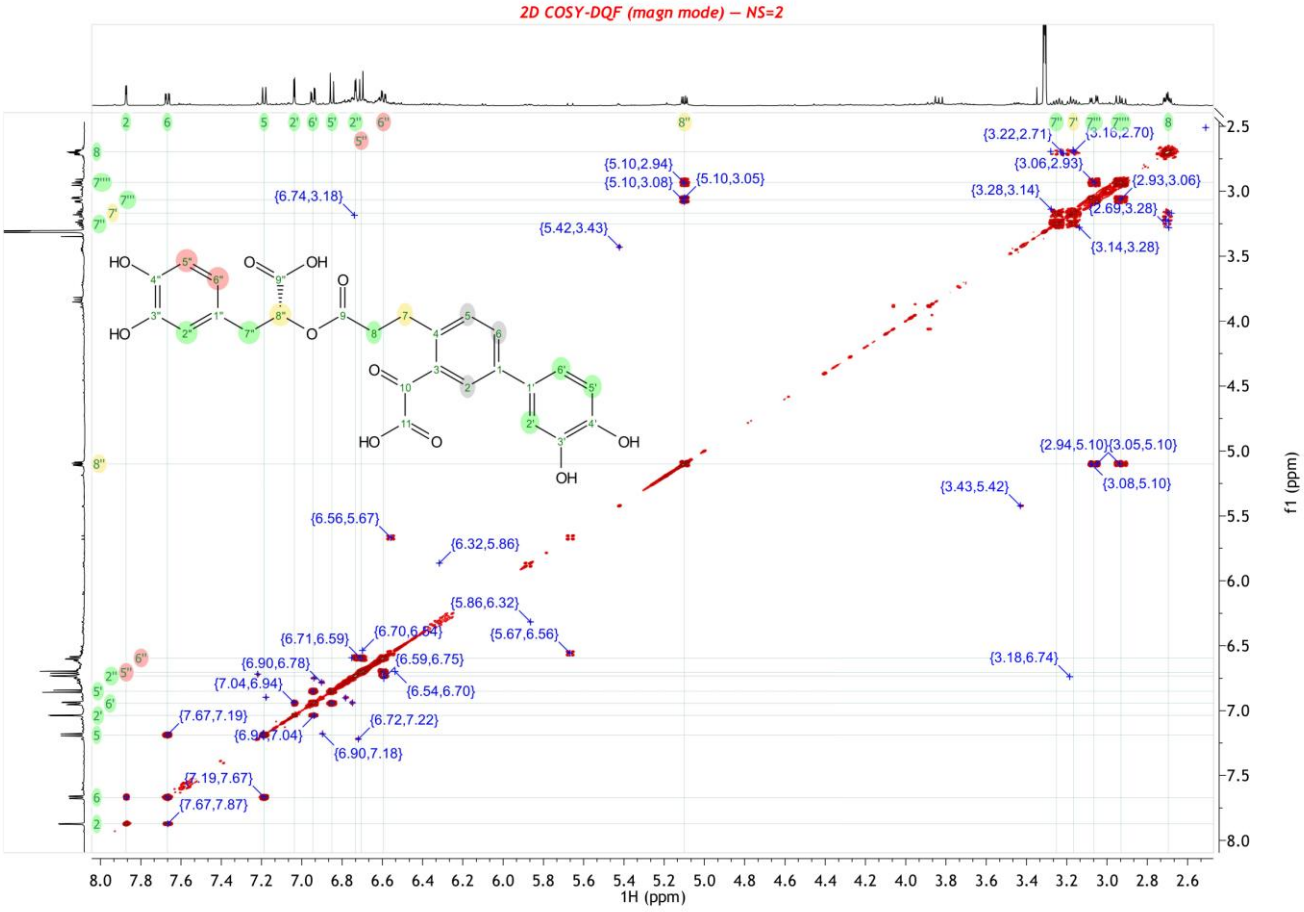

Figure 54S. ^{1}H-^{1}H COSY NMR spectrum of compound 30

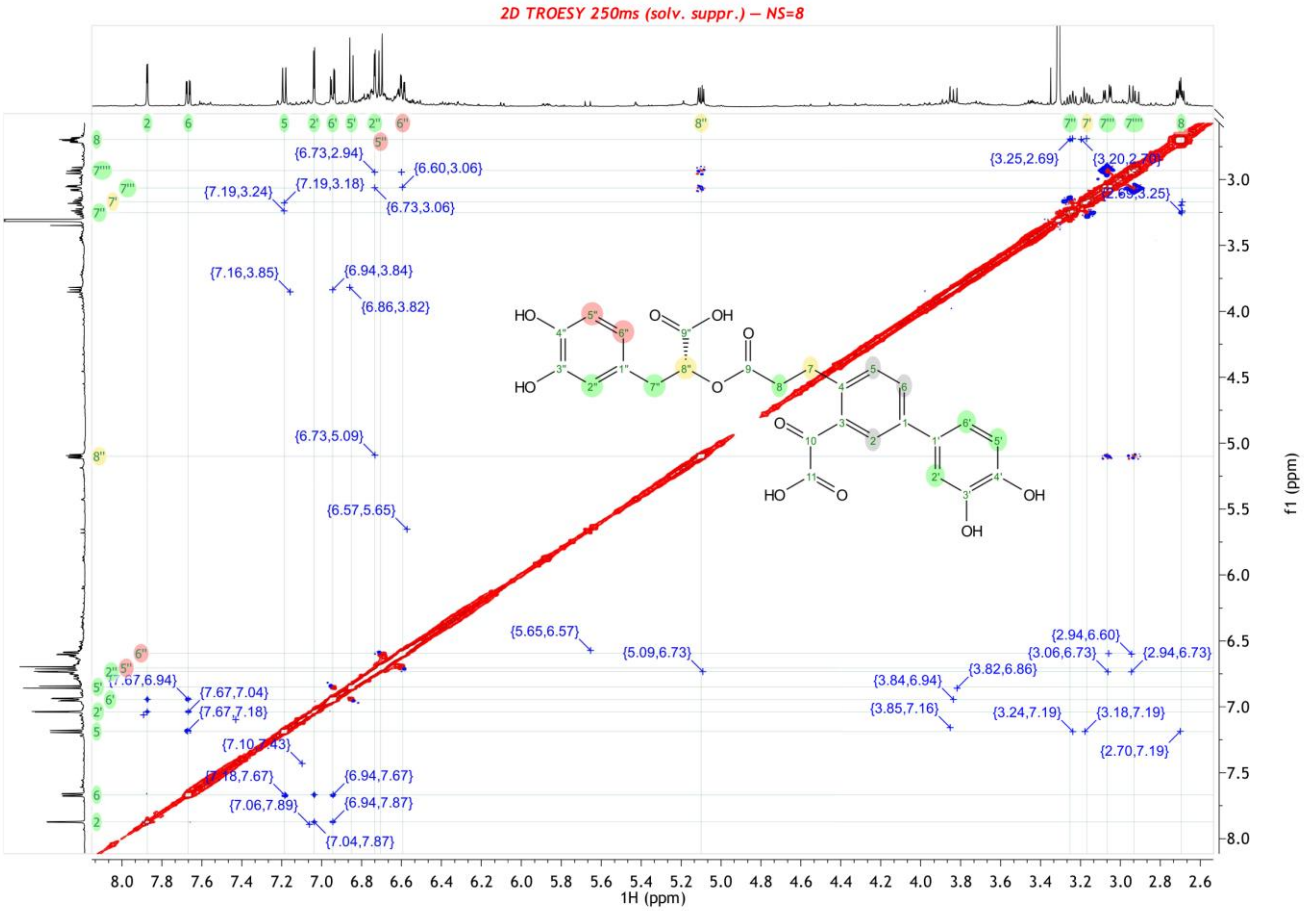

Figure 55S. ^{1}H-^{1}H TROESY (250 ms) NMR spectrum of compound 30

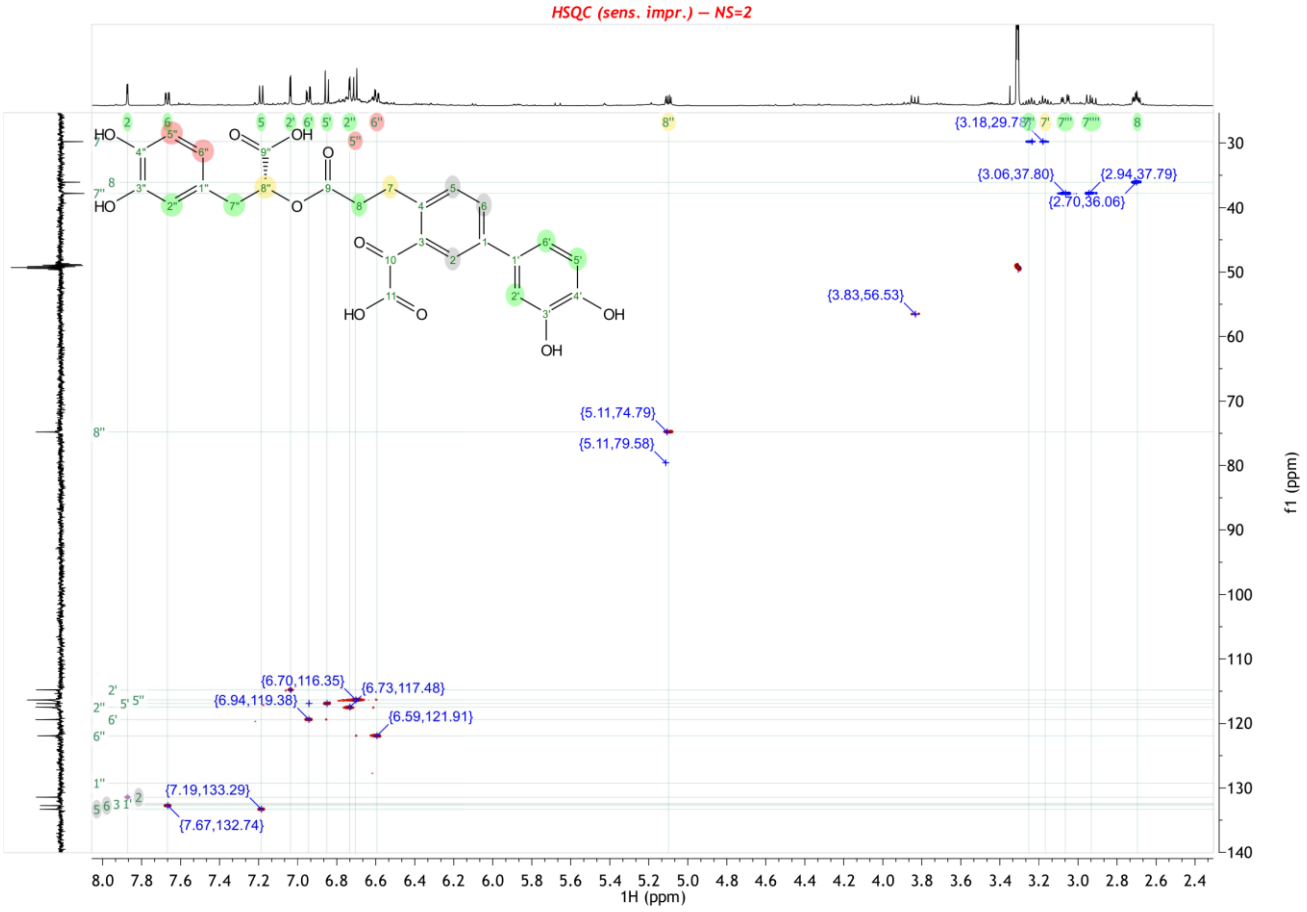

Figure 56S. ^{1}H-^{13}C HSQC NMR spectrum of compound 30

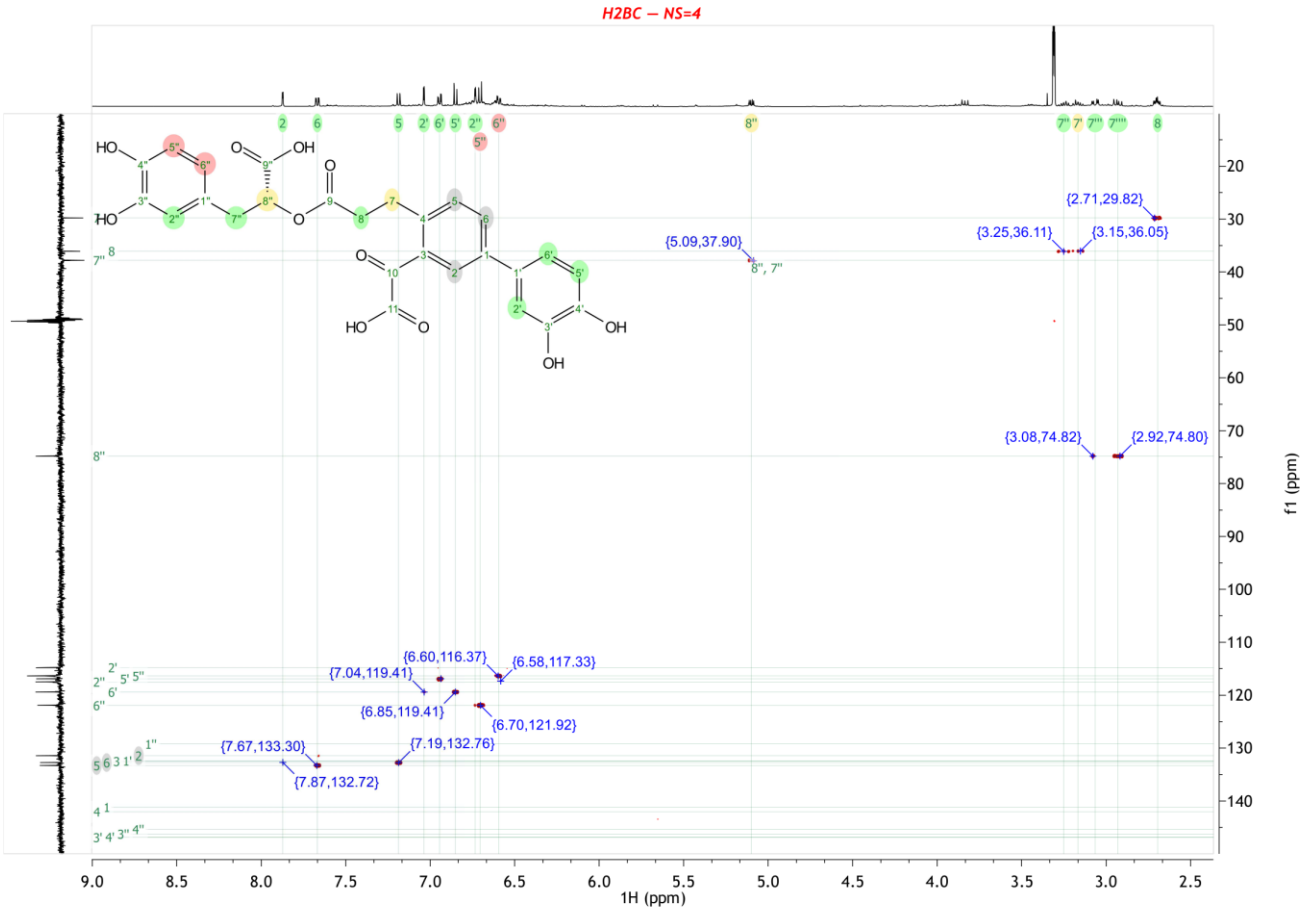

Figure 57S. ^{1}H-^{13}C H2BC NMR spectrum of compound 30

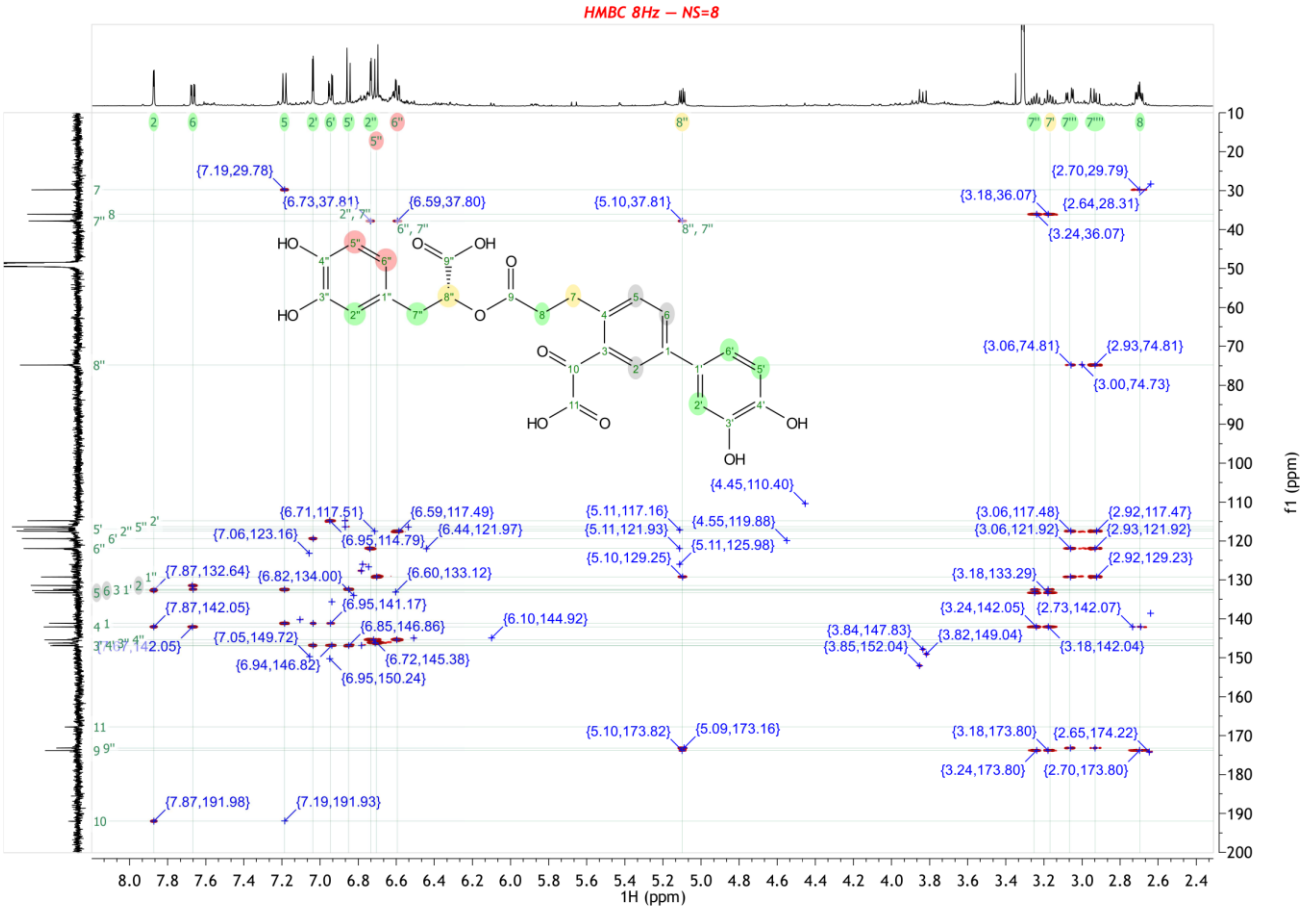

Figure 58S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 30

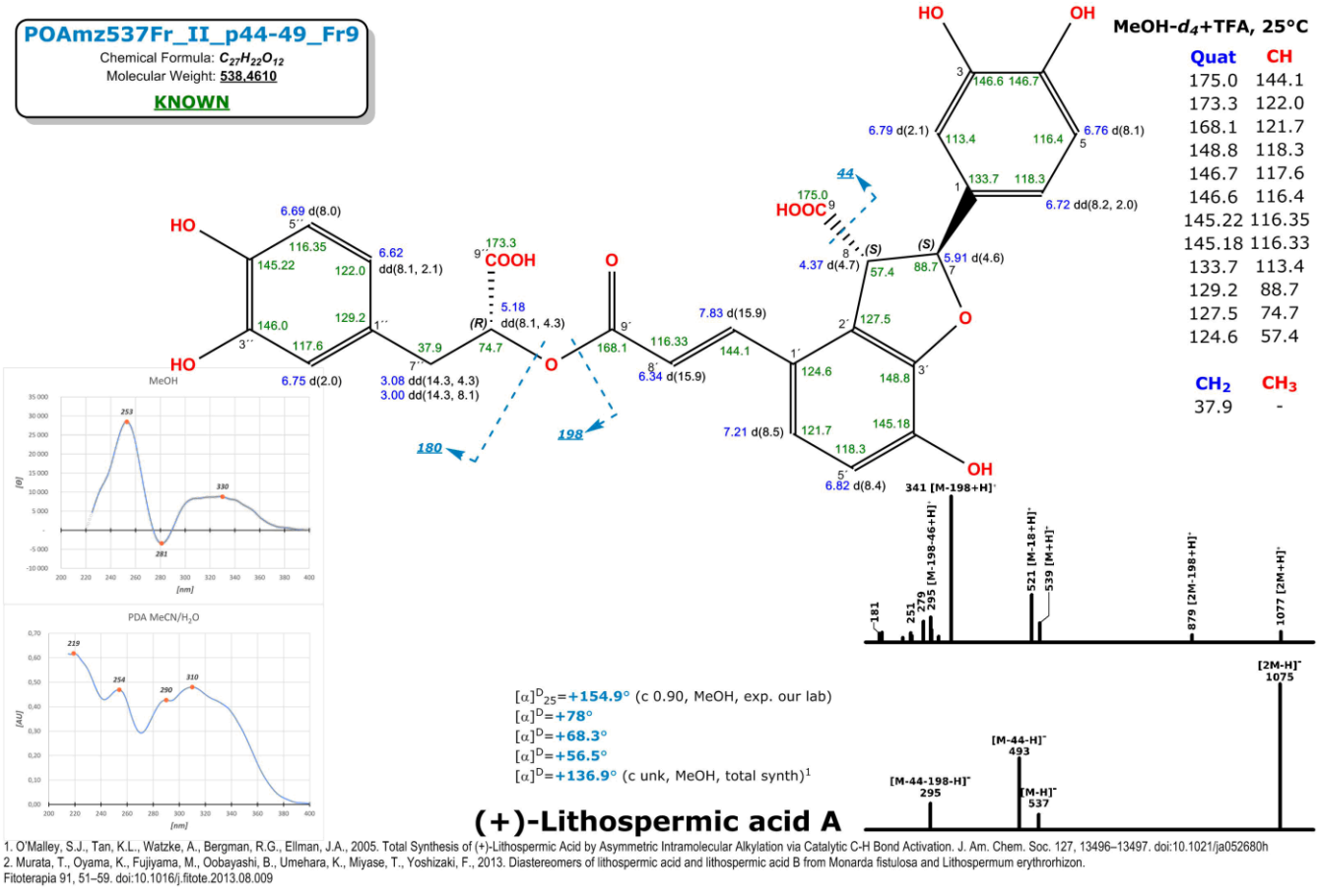

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Figure 59S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 31 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

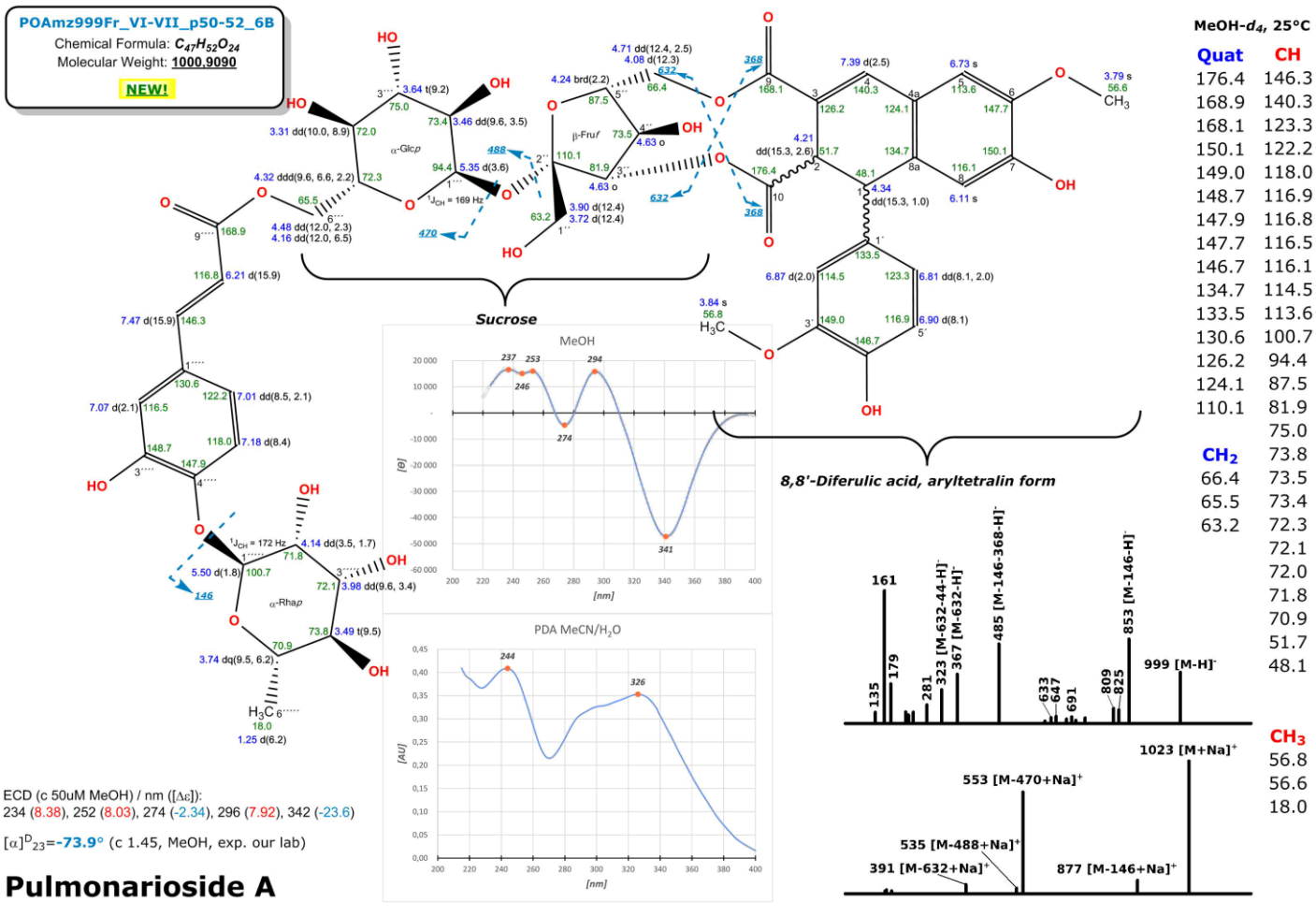

Figure 60S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 32 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

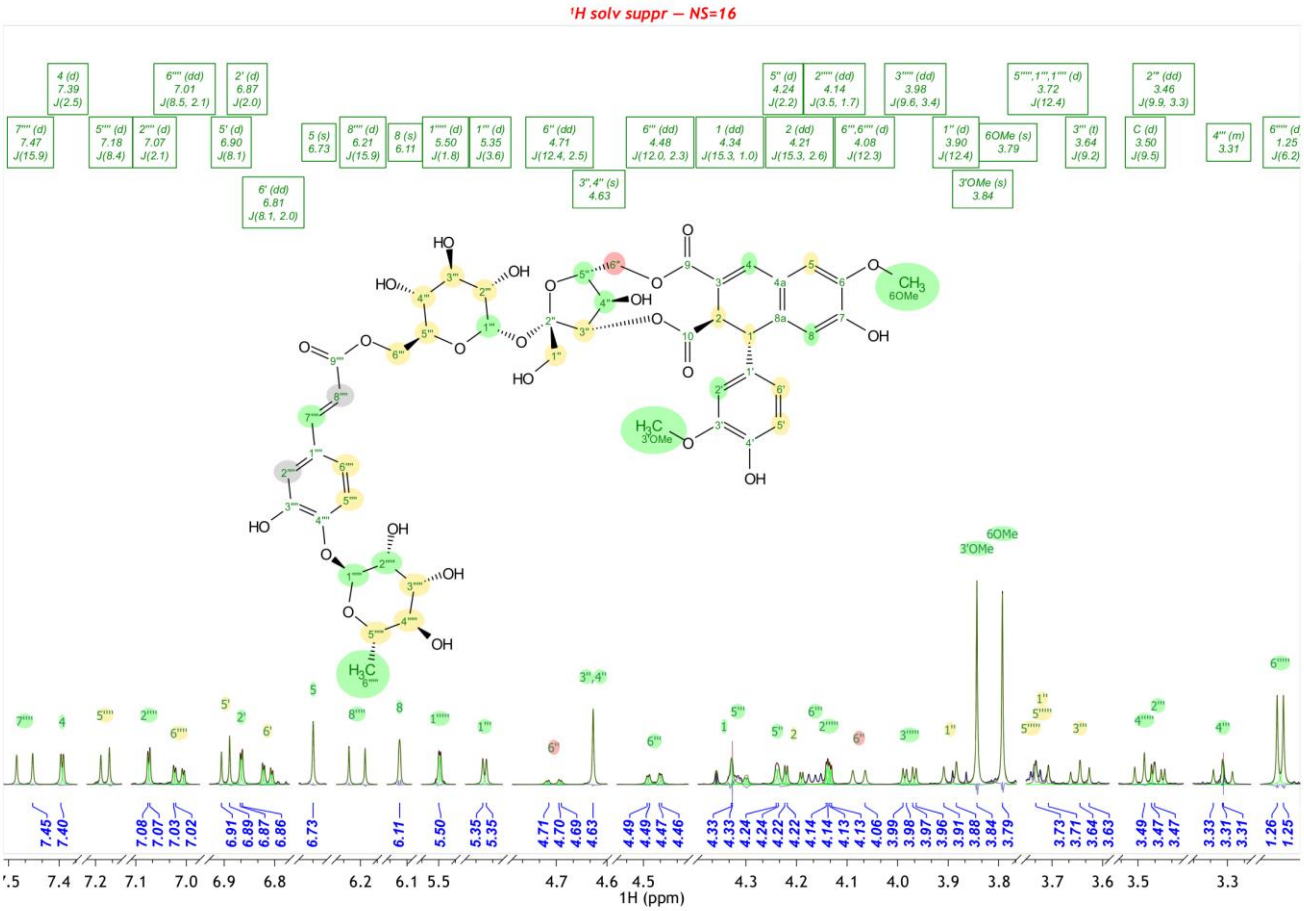

Figure 61S. ^{1}H NMR spectrum of compound 32

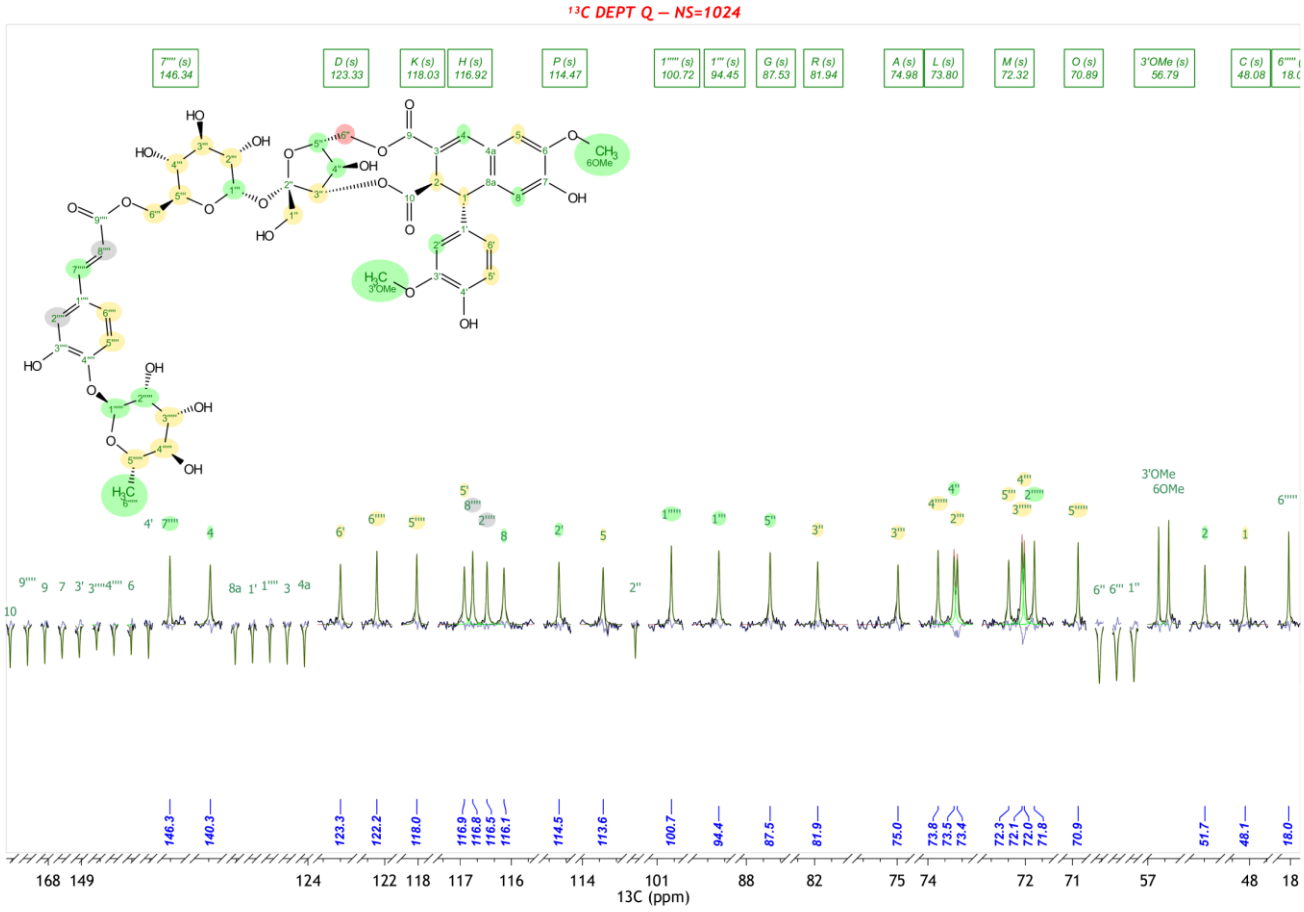

Figure 62S. ^{13}C DEPTQ NMR spectrum of compound 32

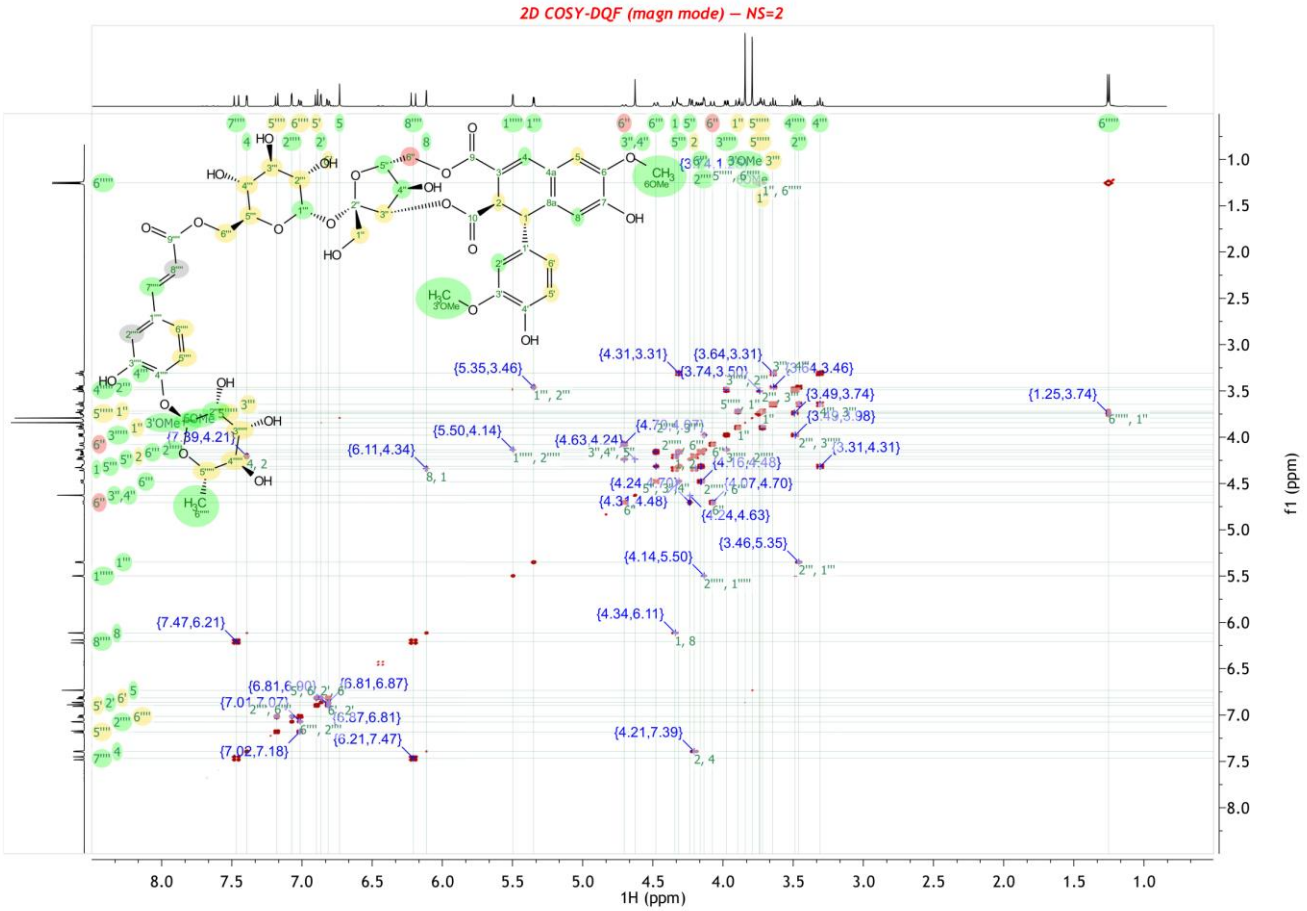

Figure 63S. ^{1}H-^{1}H COSY NMR spectrum of compound 32

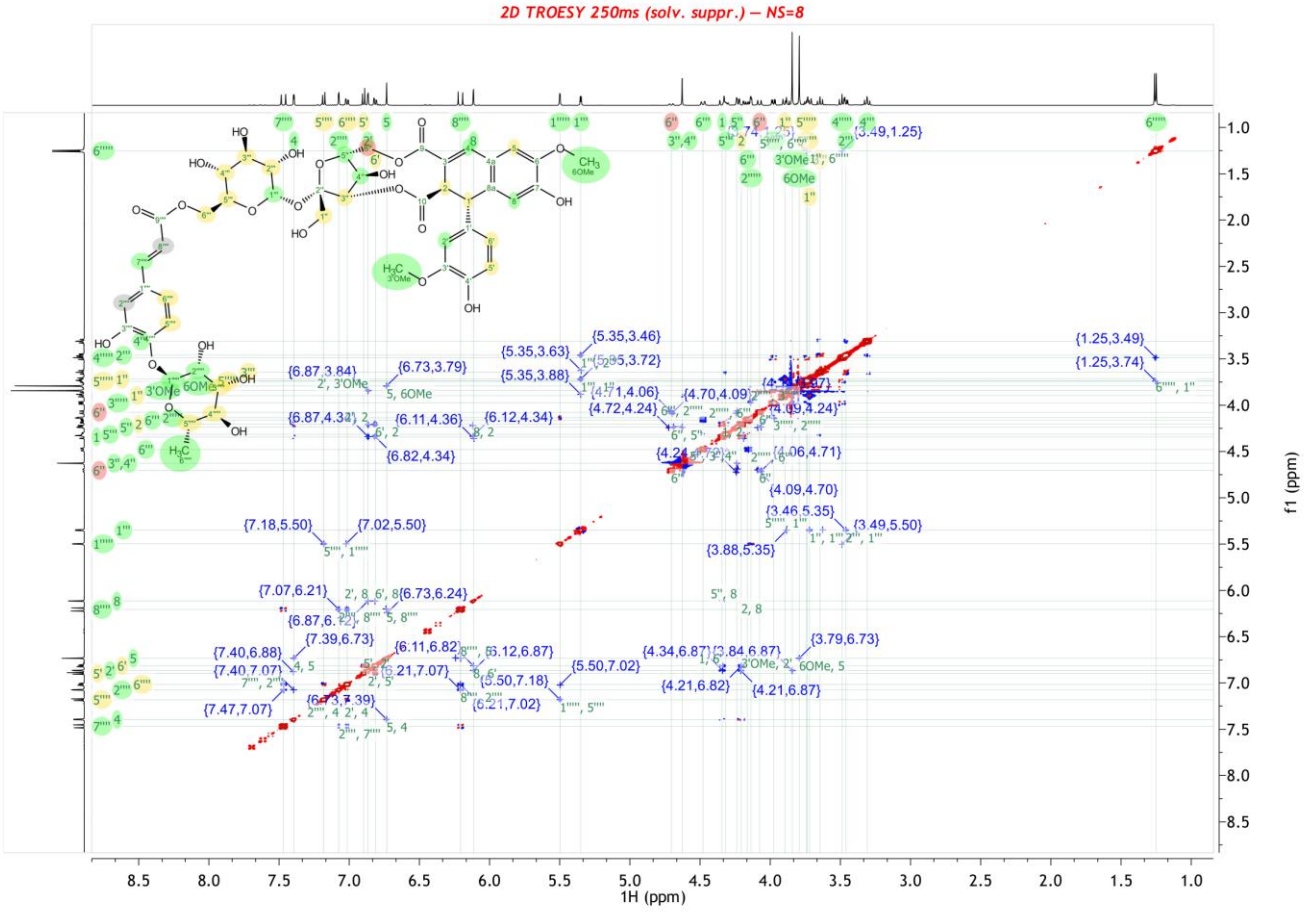

Figure 64S. ^{1}H-^{1}H TROESY (250 ms) NMR spectrum of compound 32

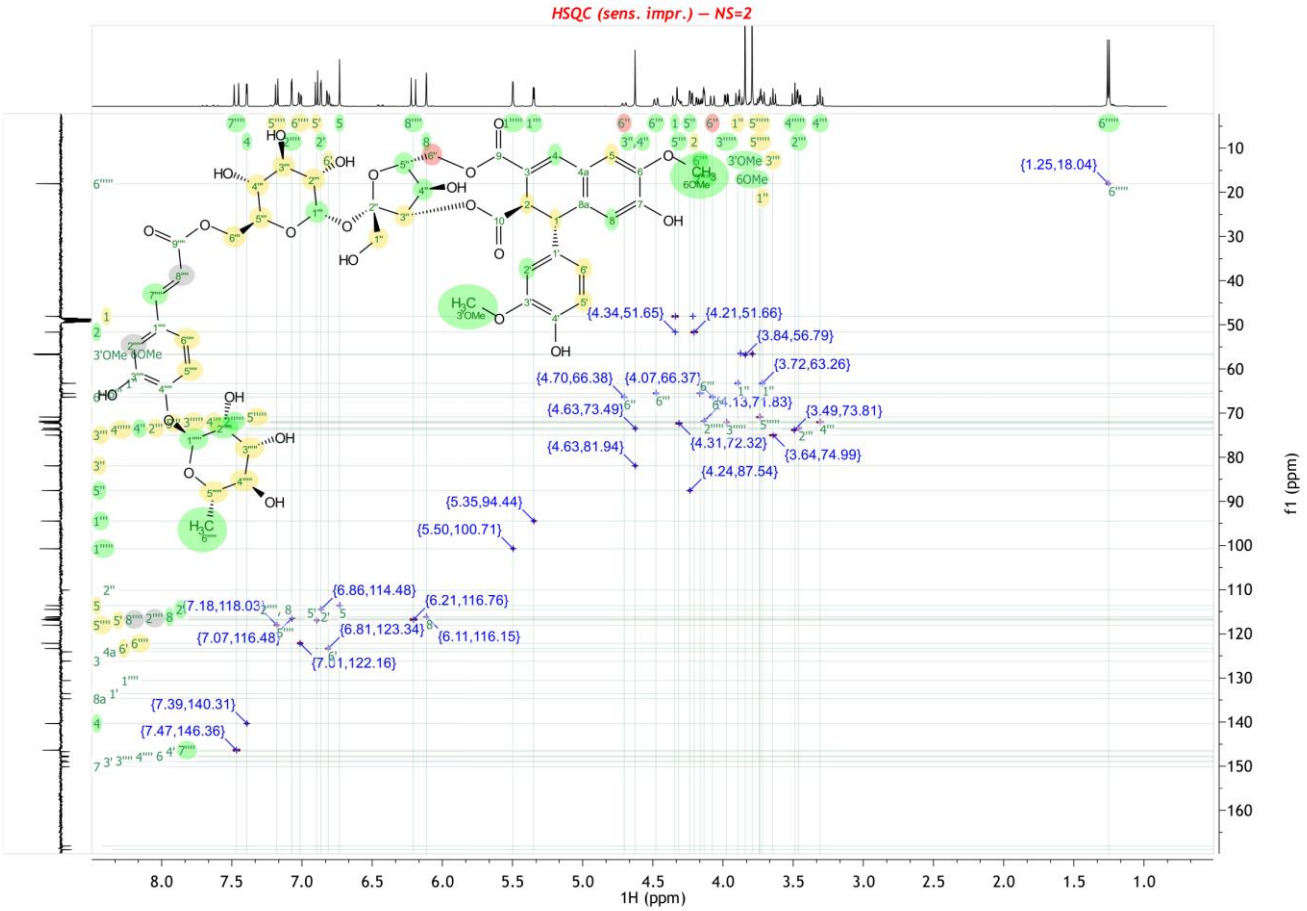

Figure 65S. ^{1}H-^{13}C HSQC NMR spectrum of compound 32

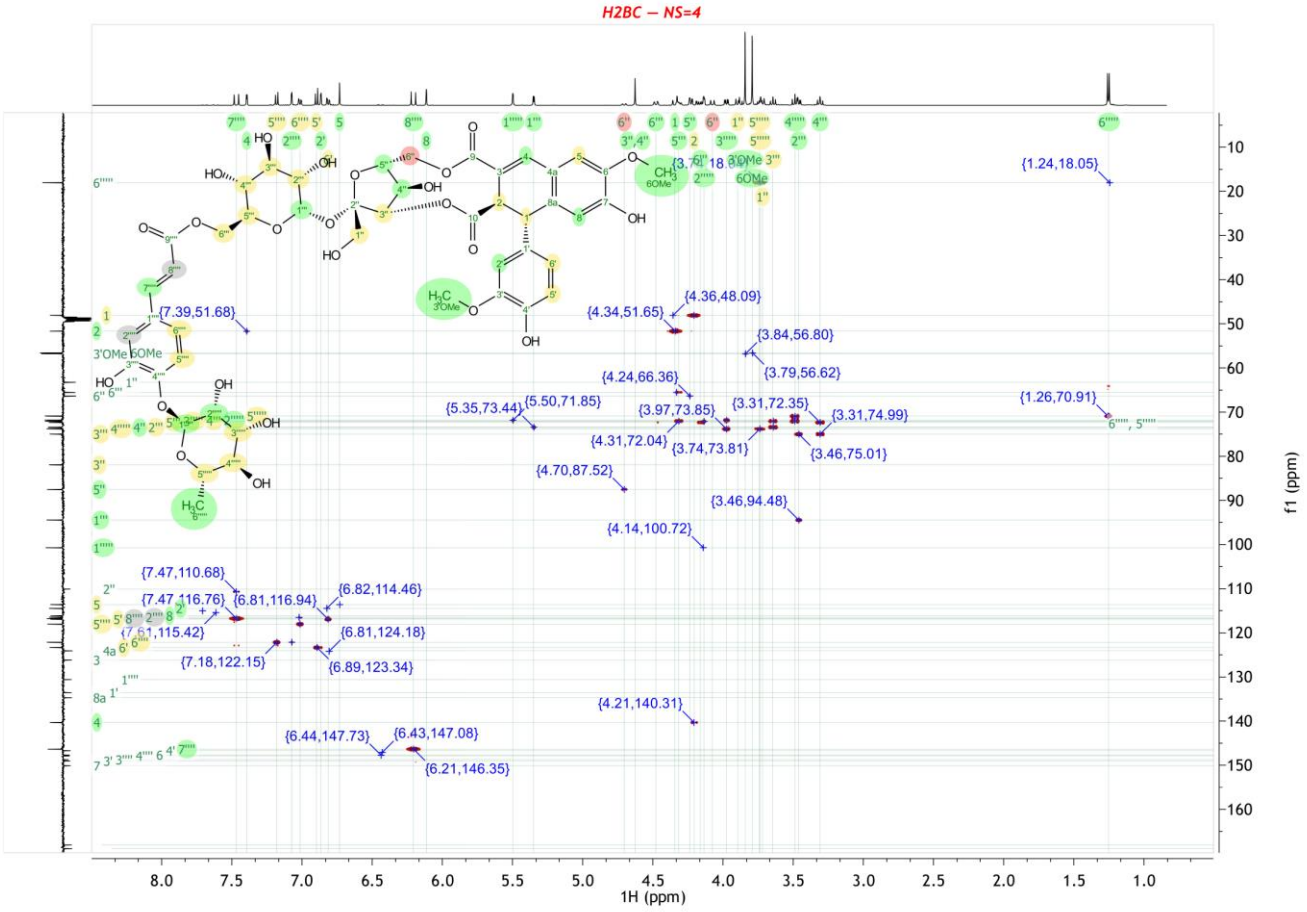

Figure 66S. ^{1}H-^{13}C H2BC NMR spectrum of compound 32

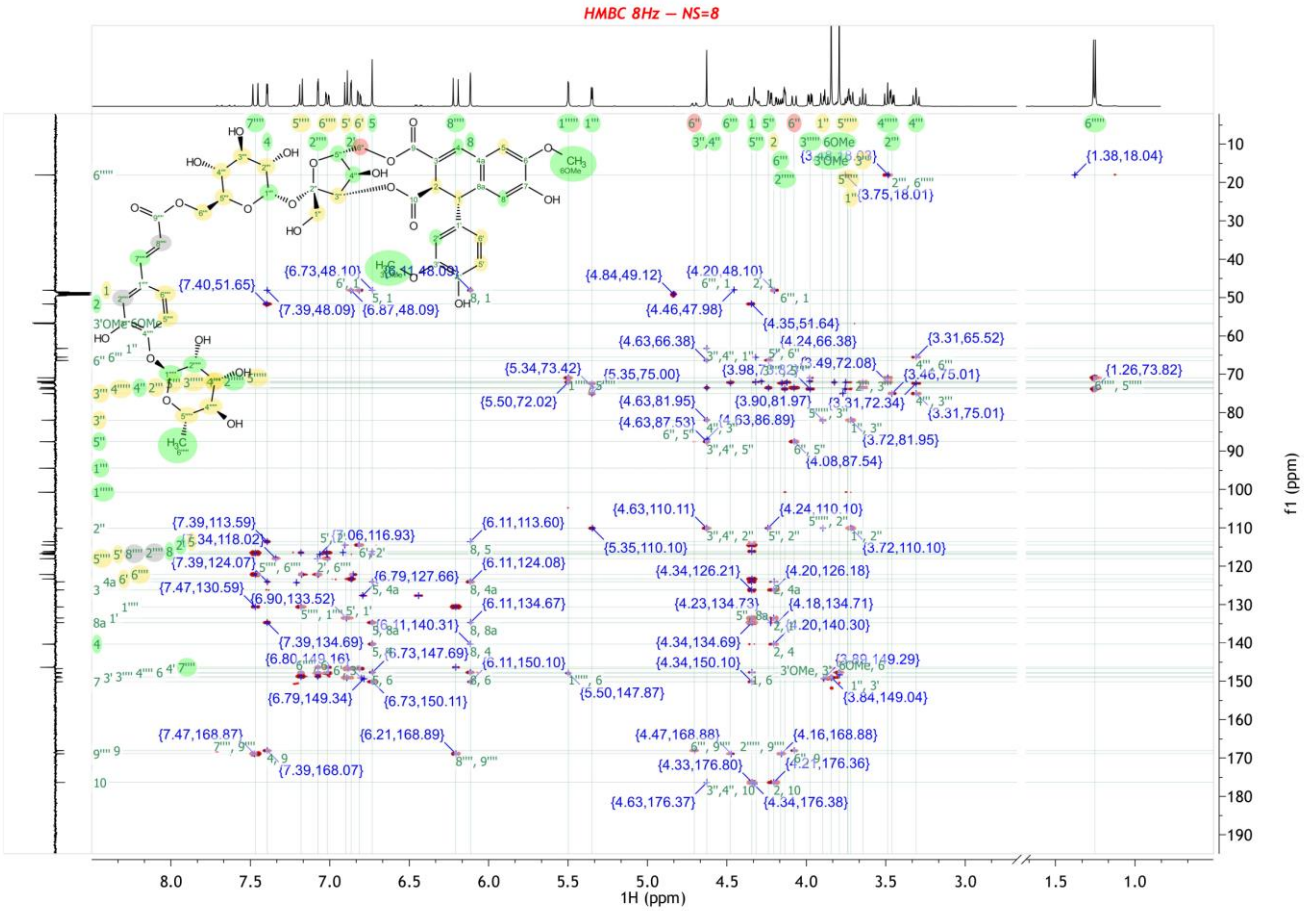

Figure 67S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 32

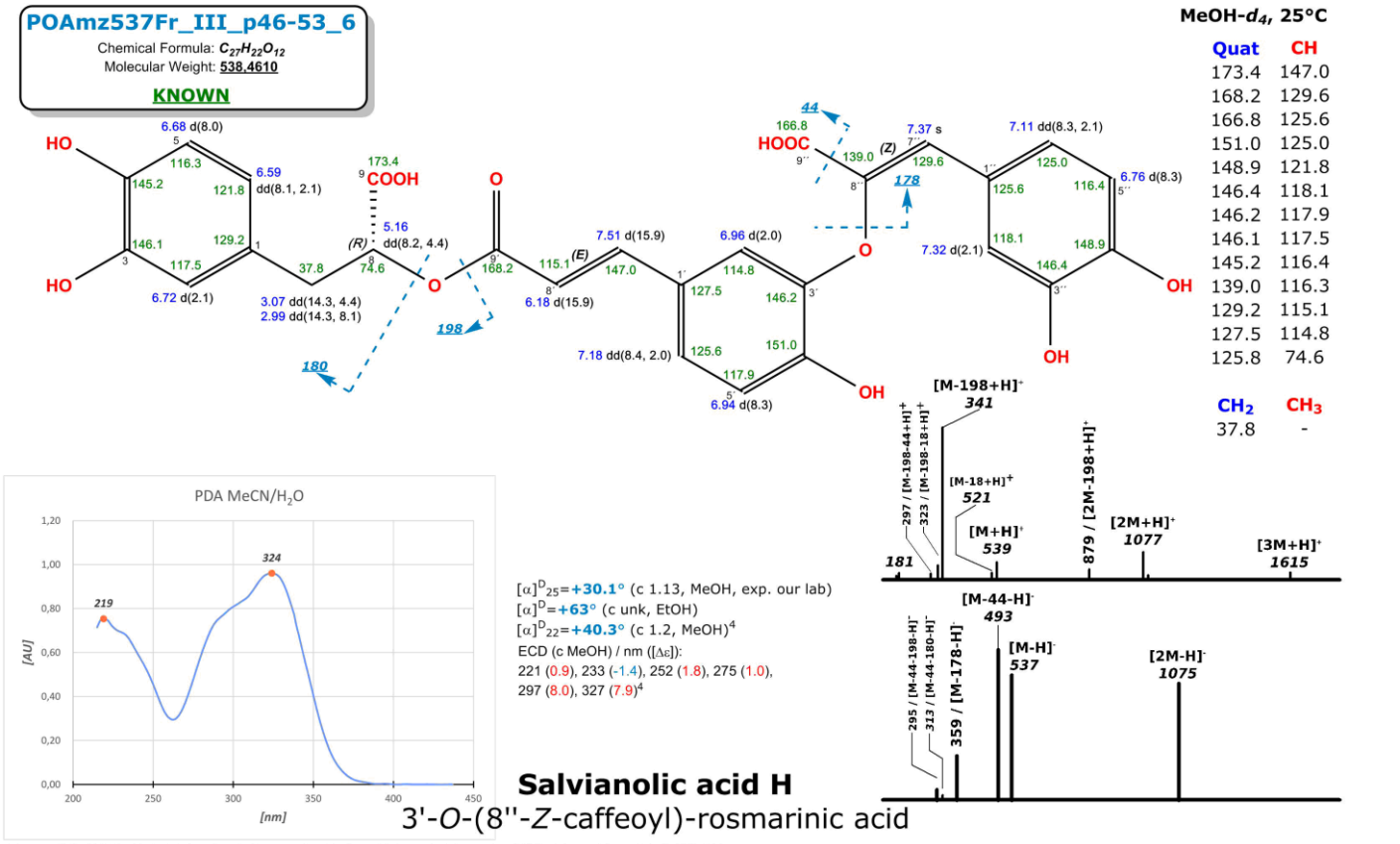

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Figure 68S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 33 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

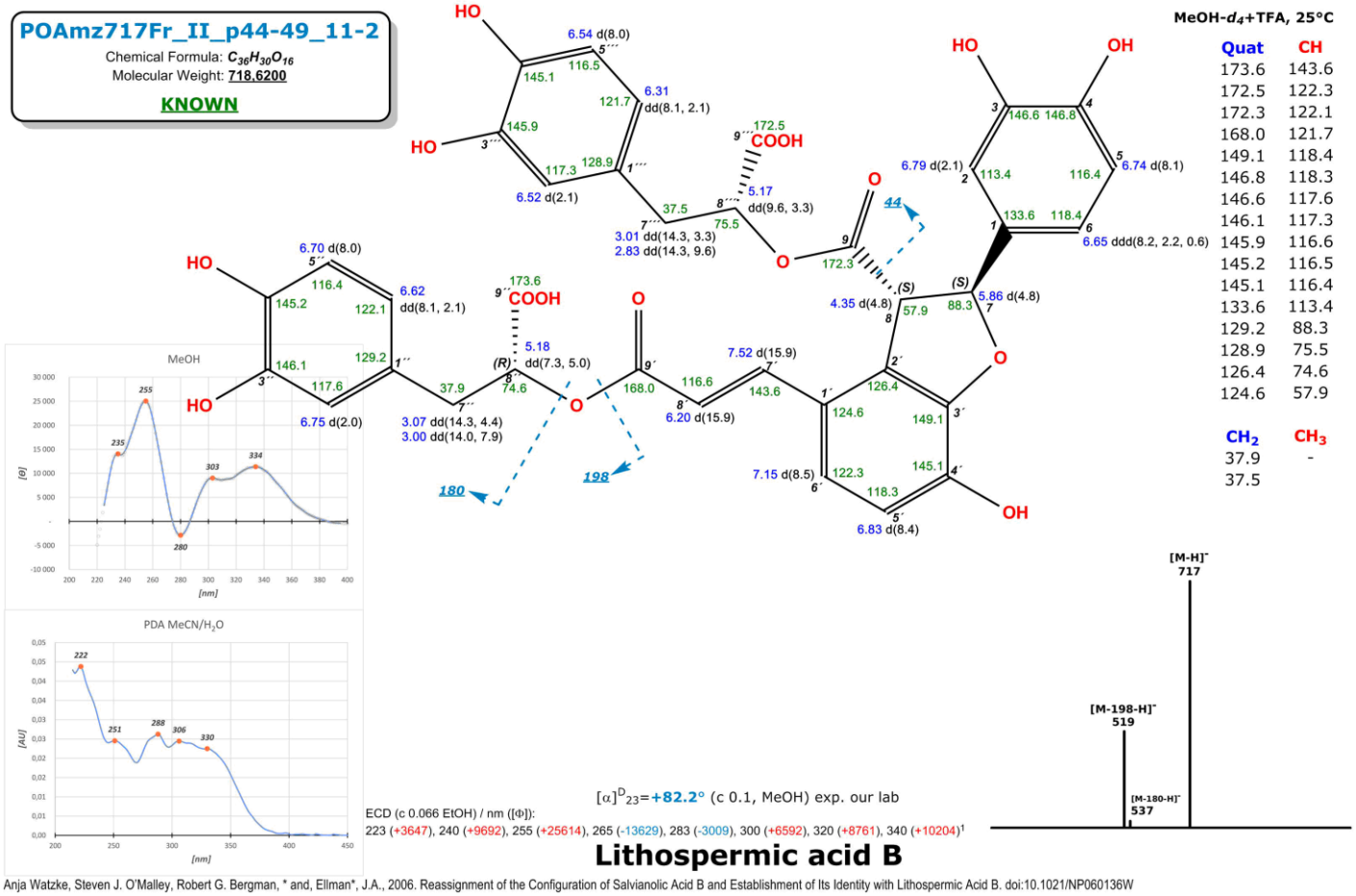


Figure 69S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 34 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

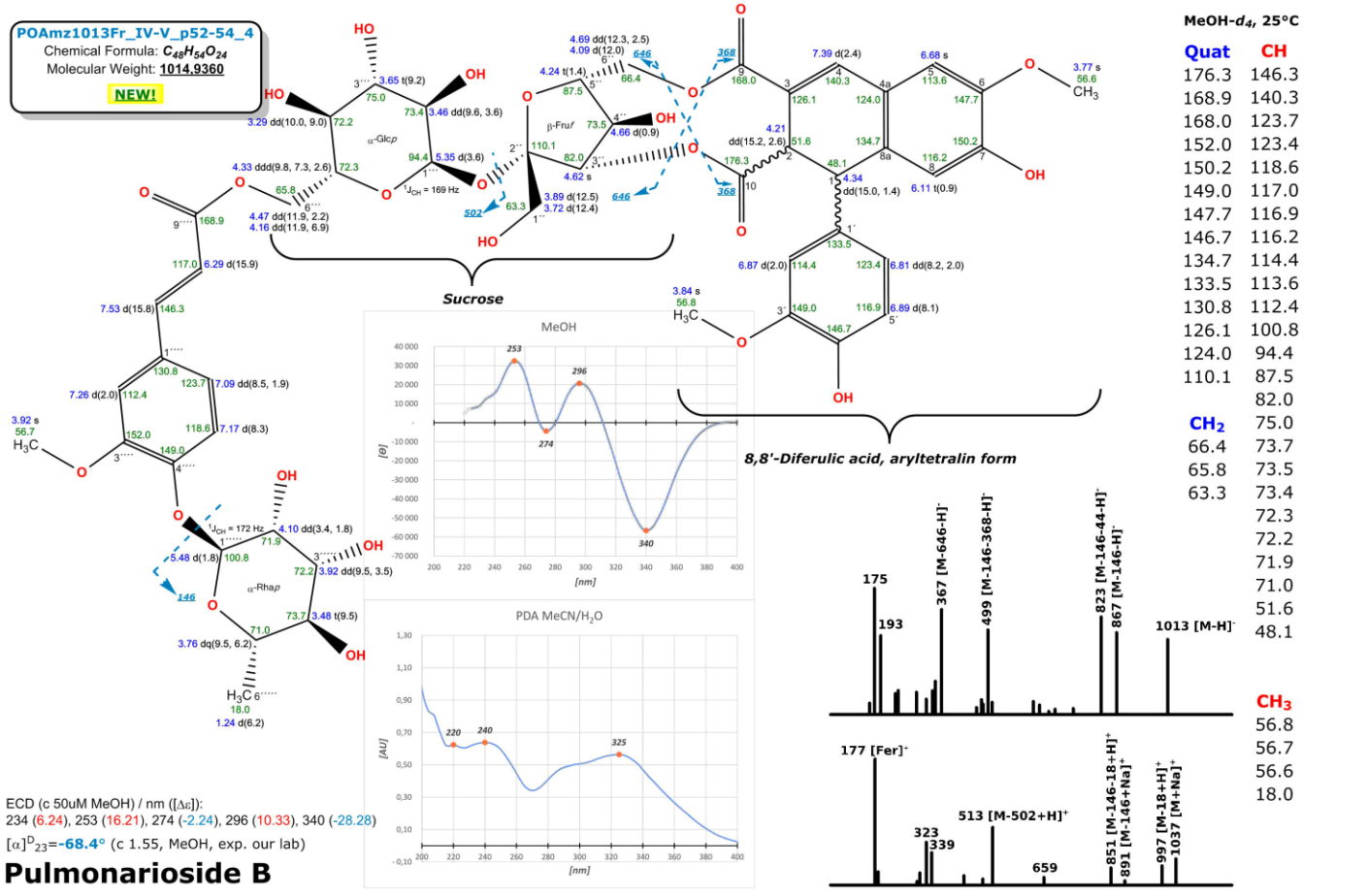


Figure 70S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 35 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

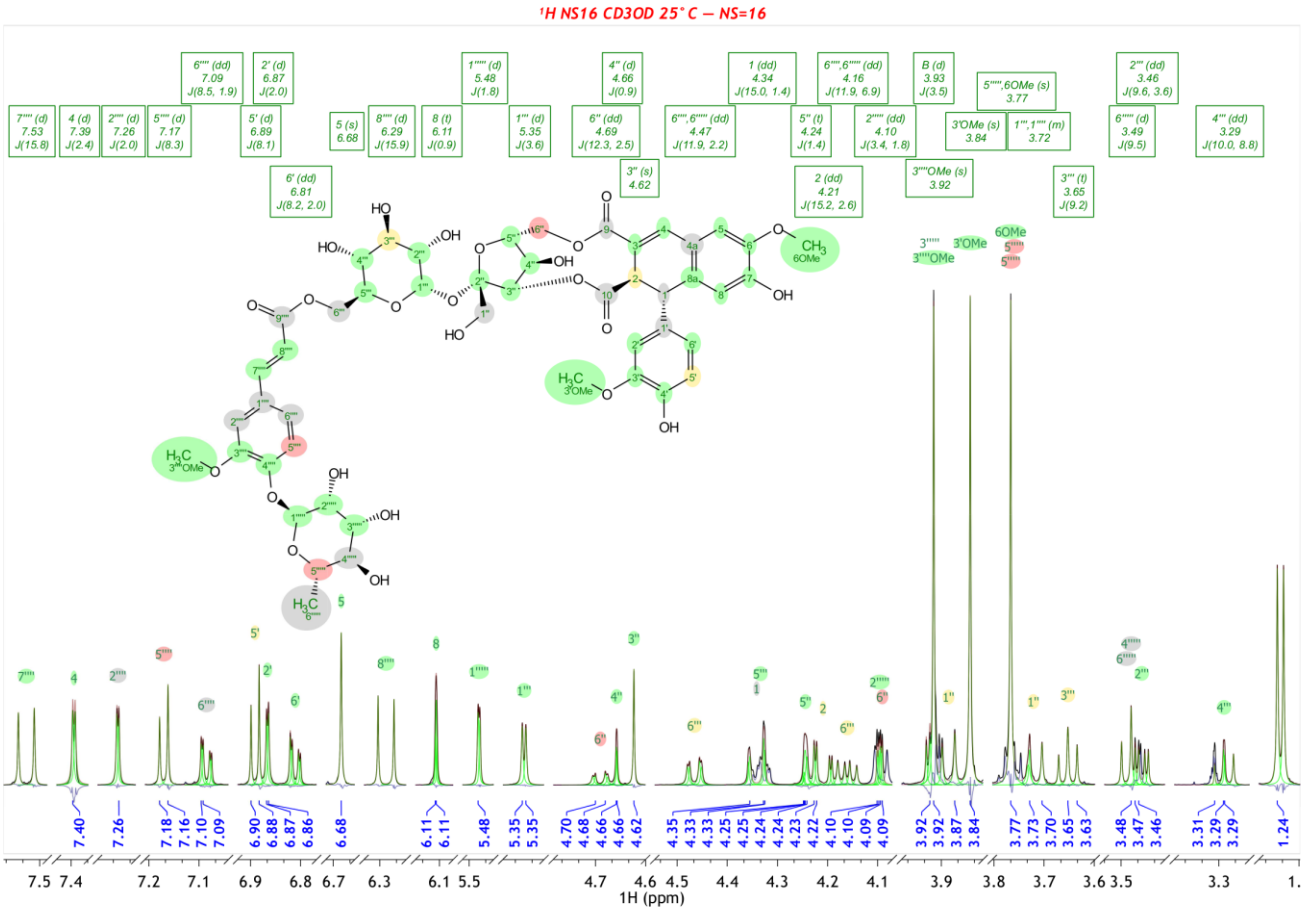


Figure 71S. ^{1}H NMR spectrum of compound 35

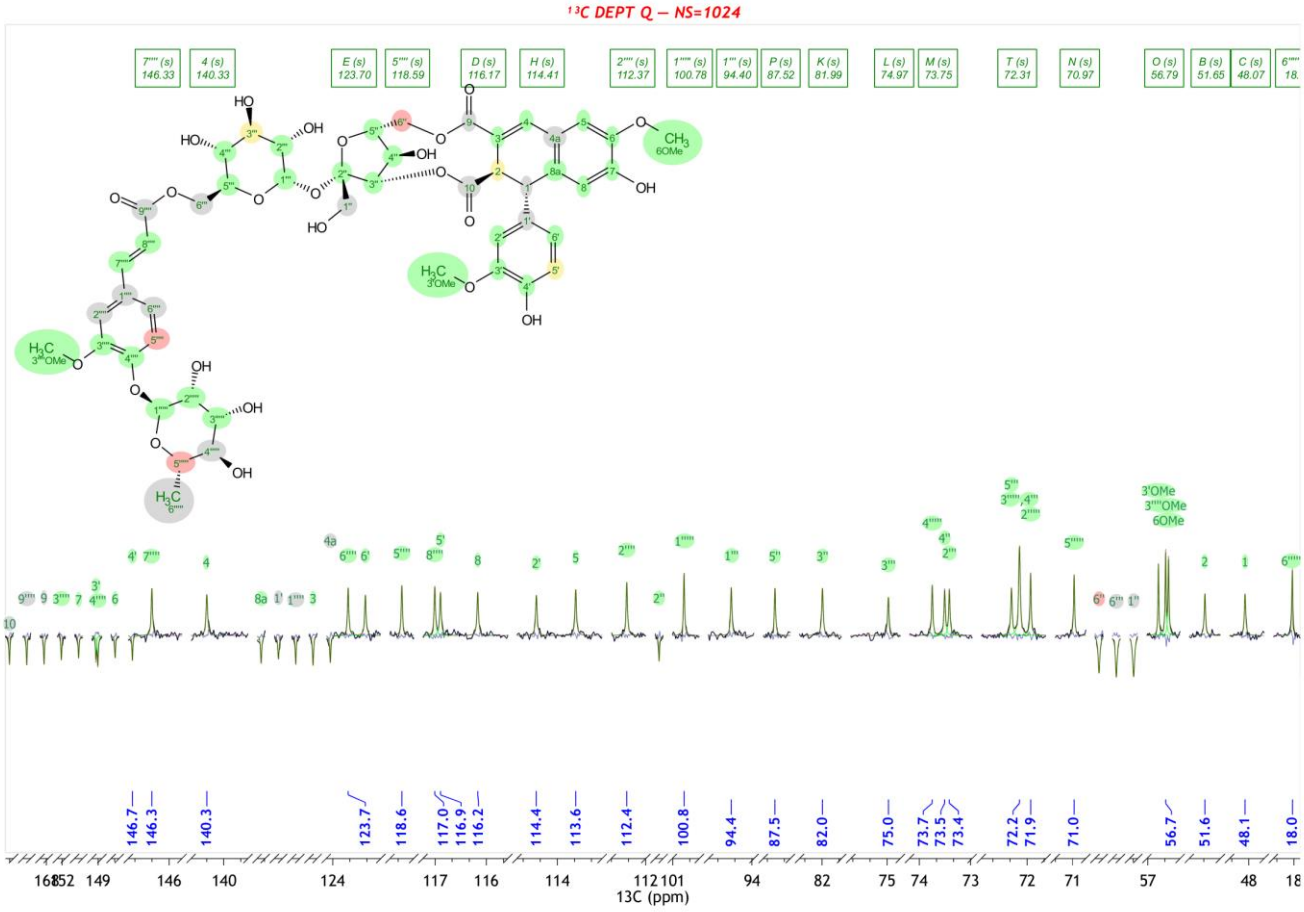


Figure 72S. ^{13}C DEPTQ NMR spectrum of compound 35

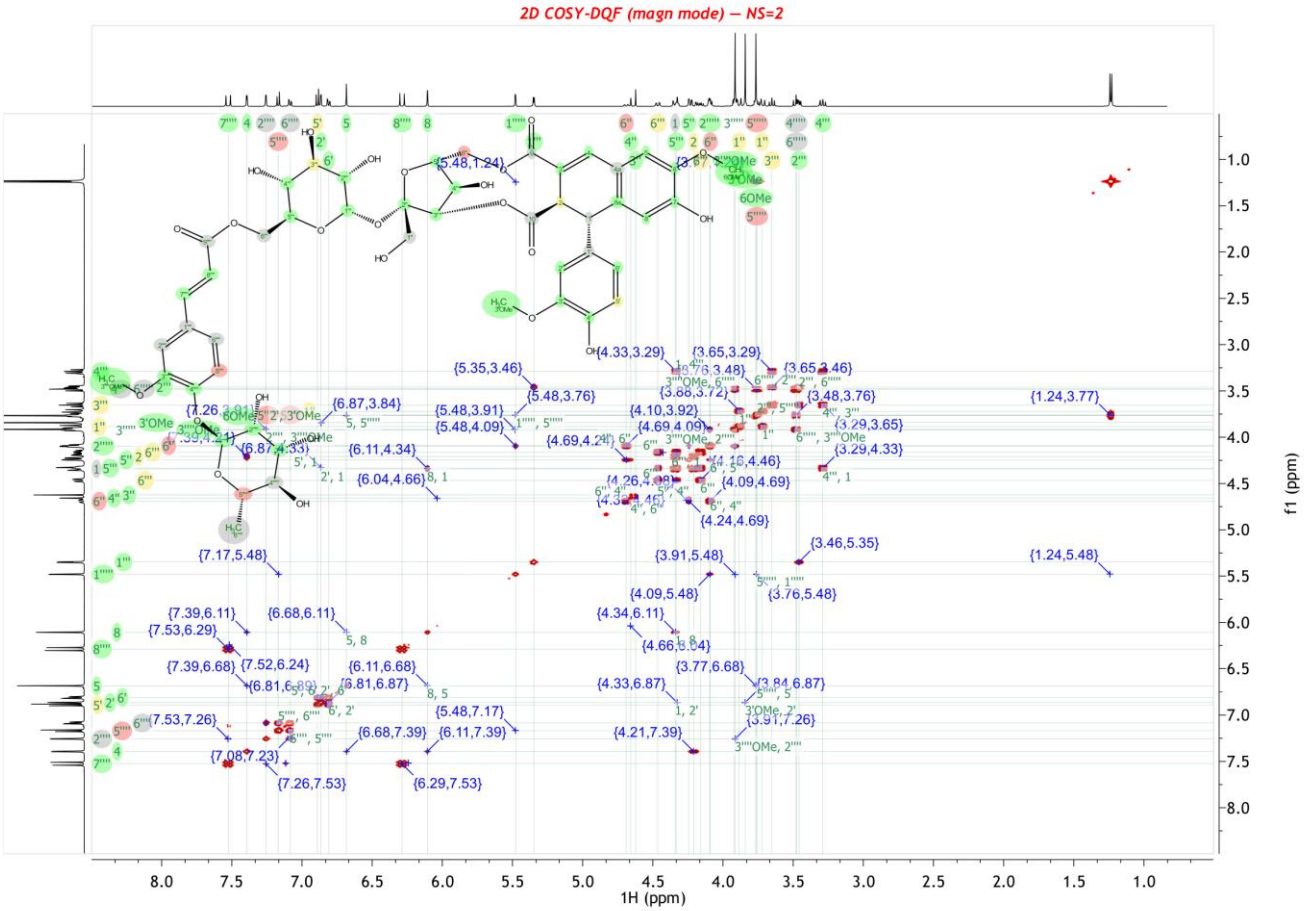


Figure 73S. ^{1}H-^{1}H COSY NMR spectrum of compound 35

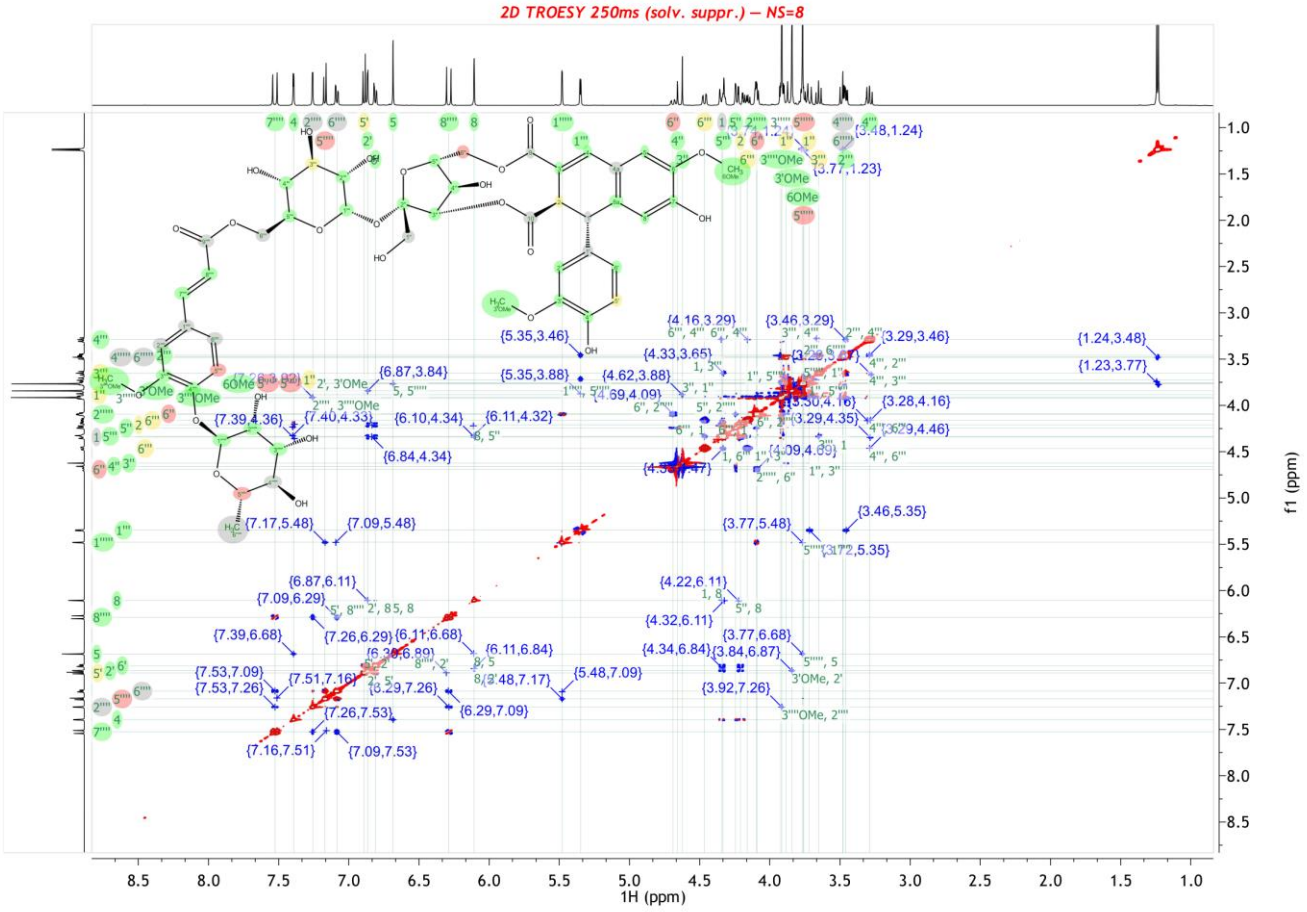


Figure 74S. ^{1}H-^{1}H TROESY (250 ms) NMR spectrum of compound 35

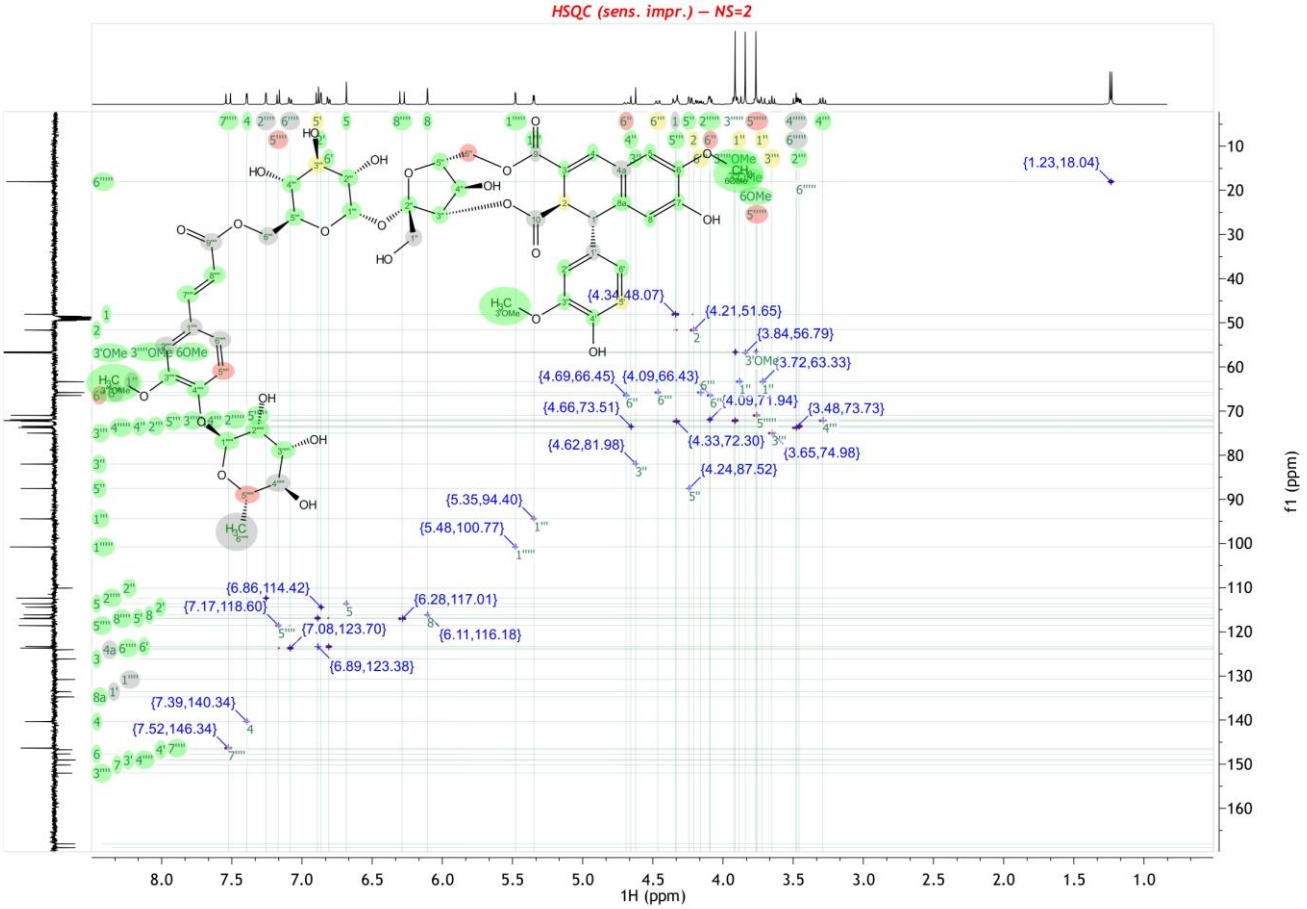


Figure 75S. ^{1}H-^{13}C HSQC NMR spectrum of compound 35

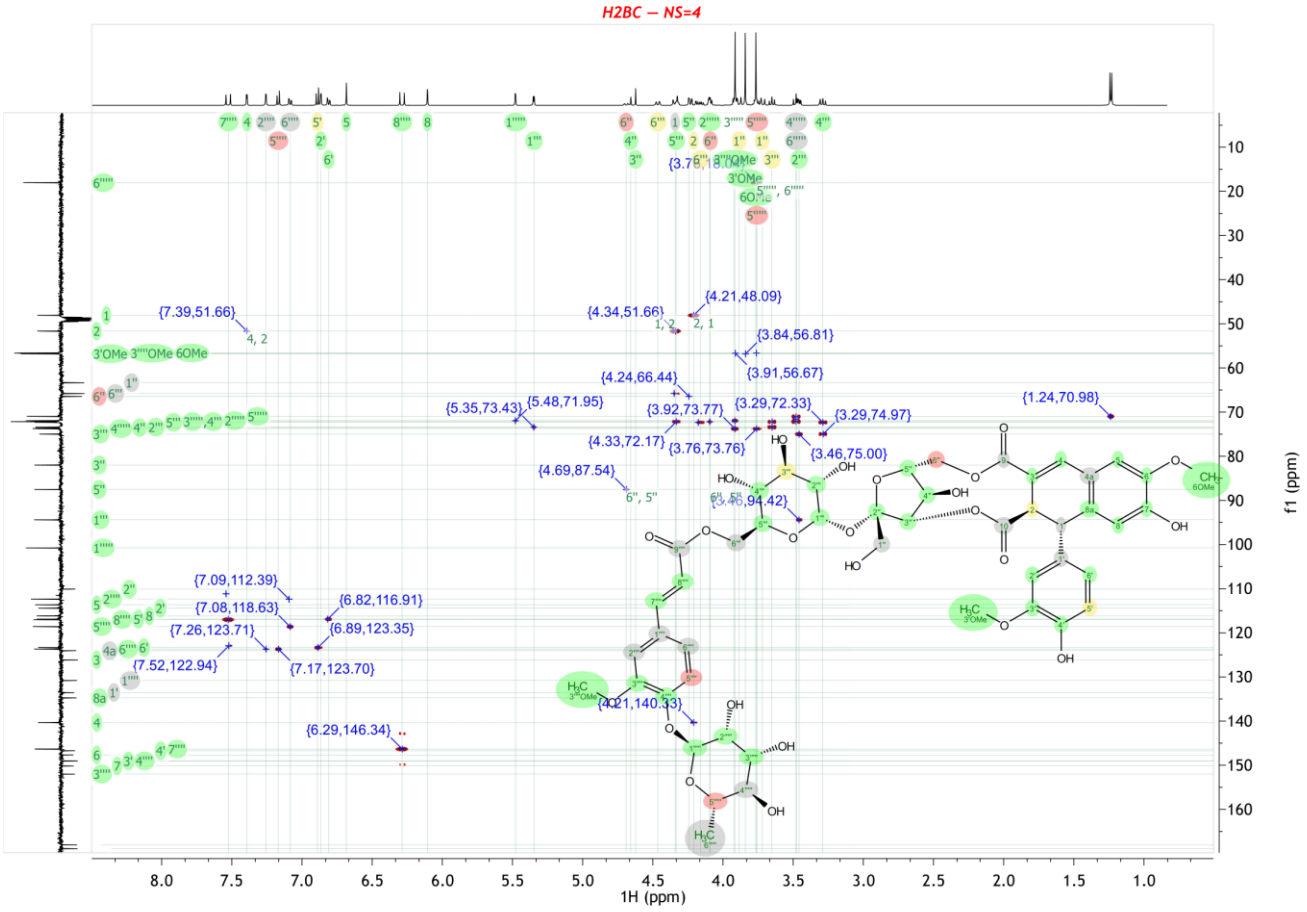


Figure 76S. ^{1}H-^{13}C H2BC NMR spectrum of compound 35

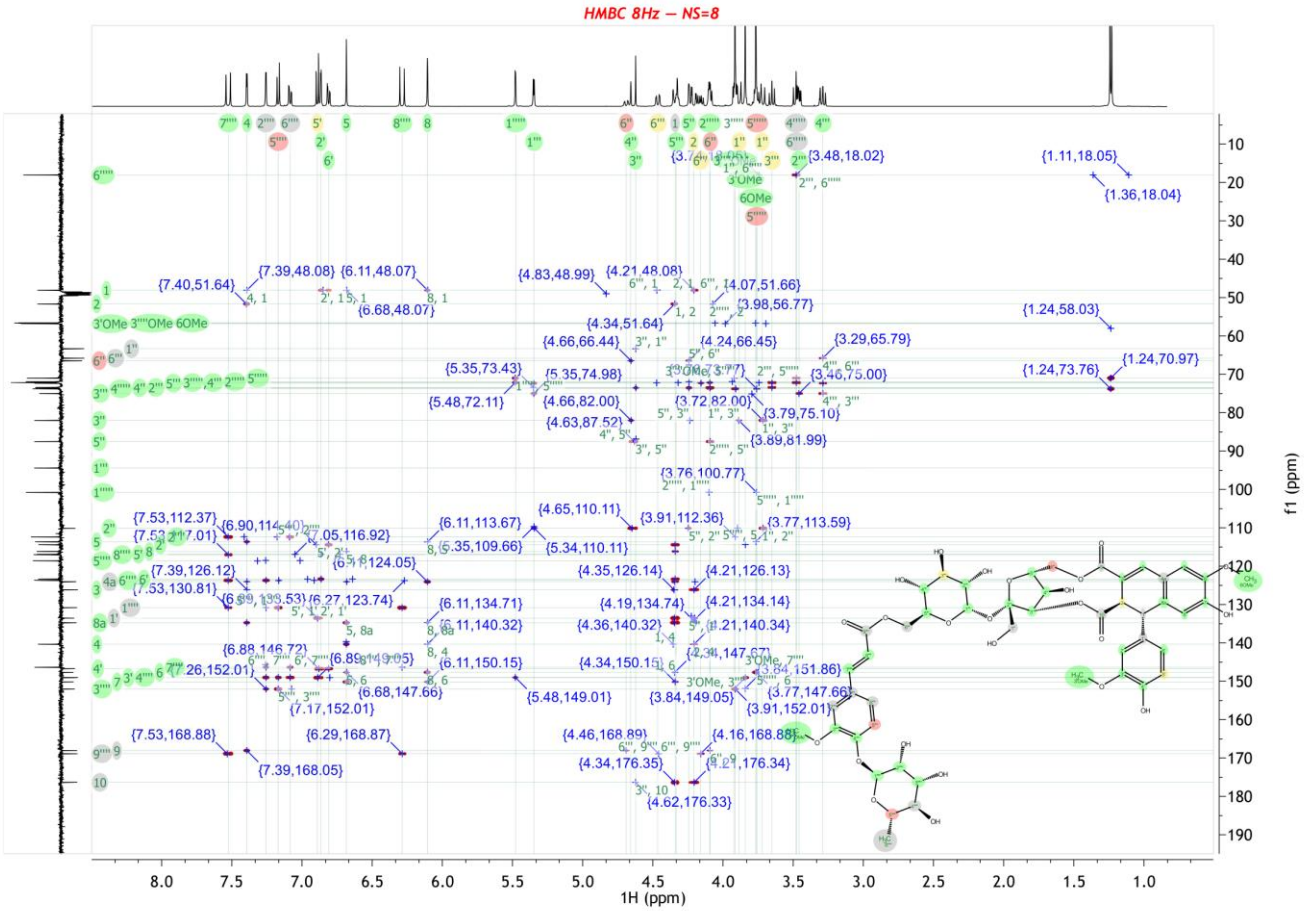
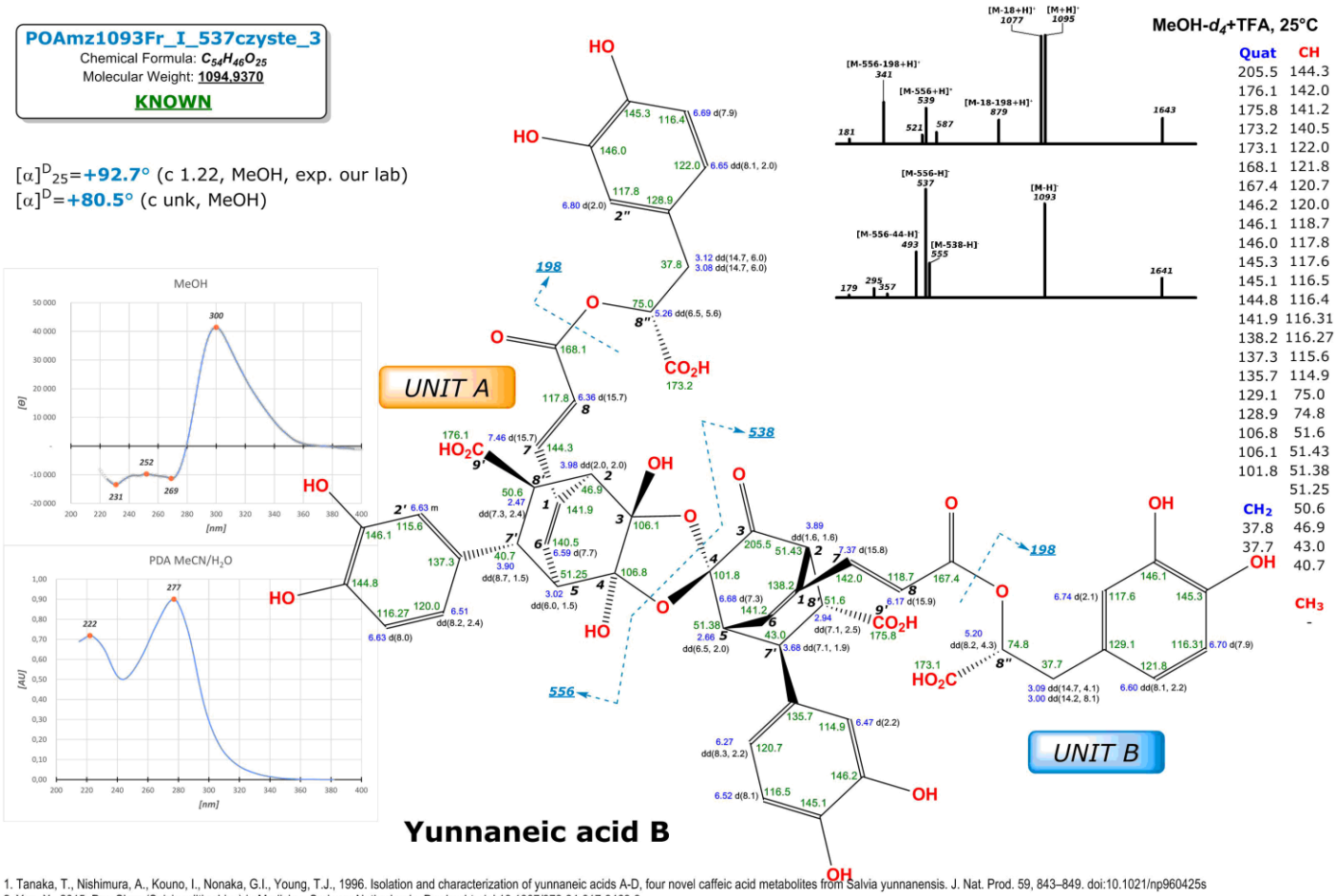


Figure 77S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 35



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2. Yan, X., 2015. Dan Shen (Salvia miltiorrhiza) in Medicine. Springer Netherlands, Dordrecht. doi:10.1007/978-94-017-9463-3

Figure 78S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 36 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

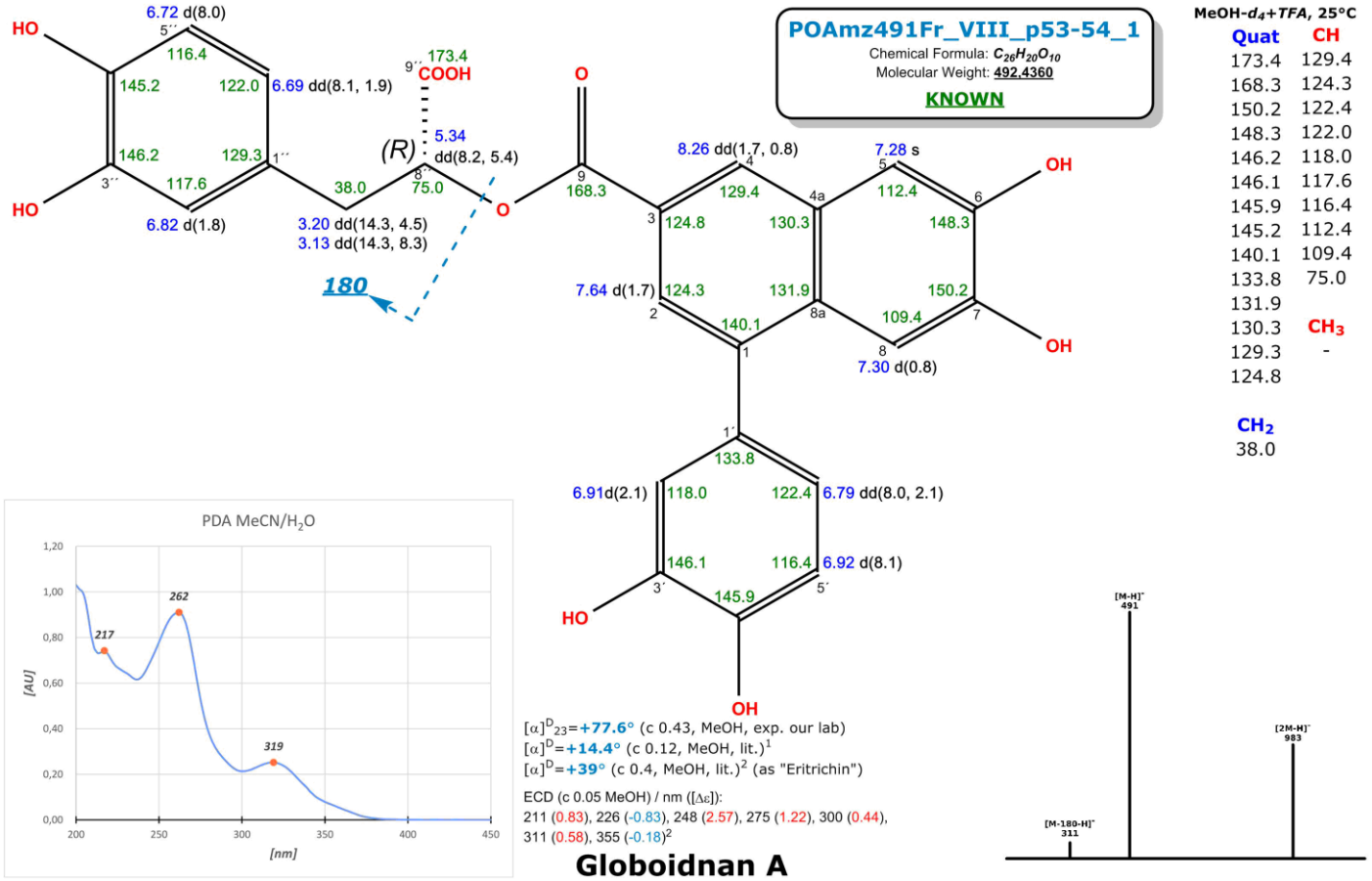

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Figure 79S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 37 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

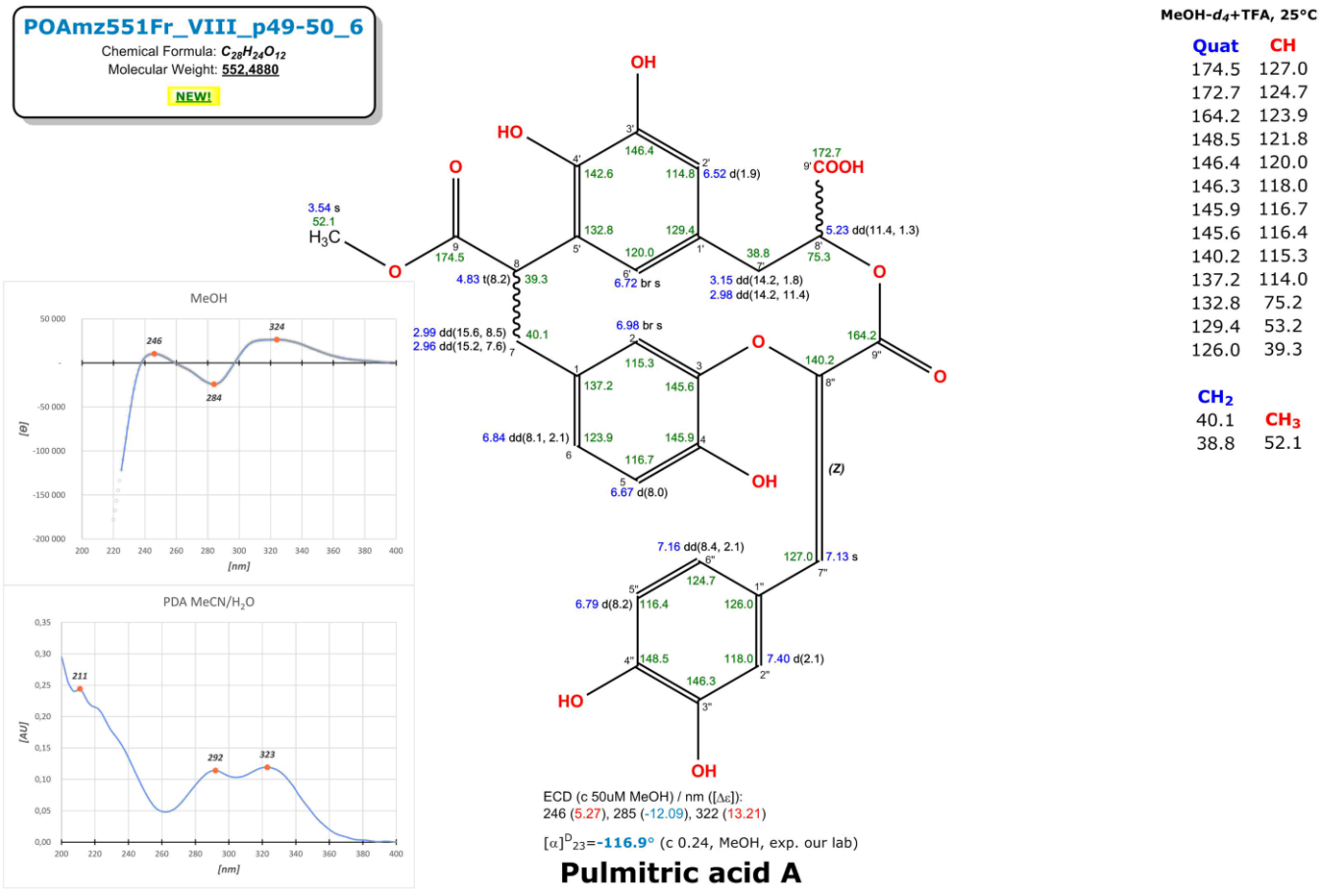


Figure 80S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 38 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O

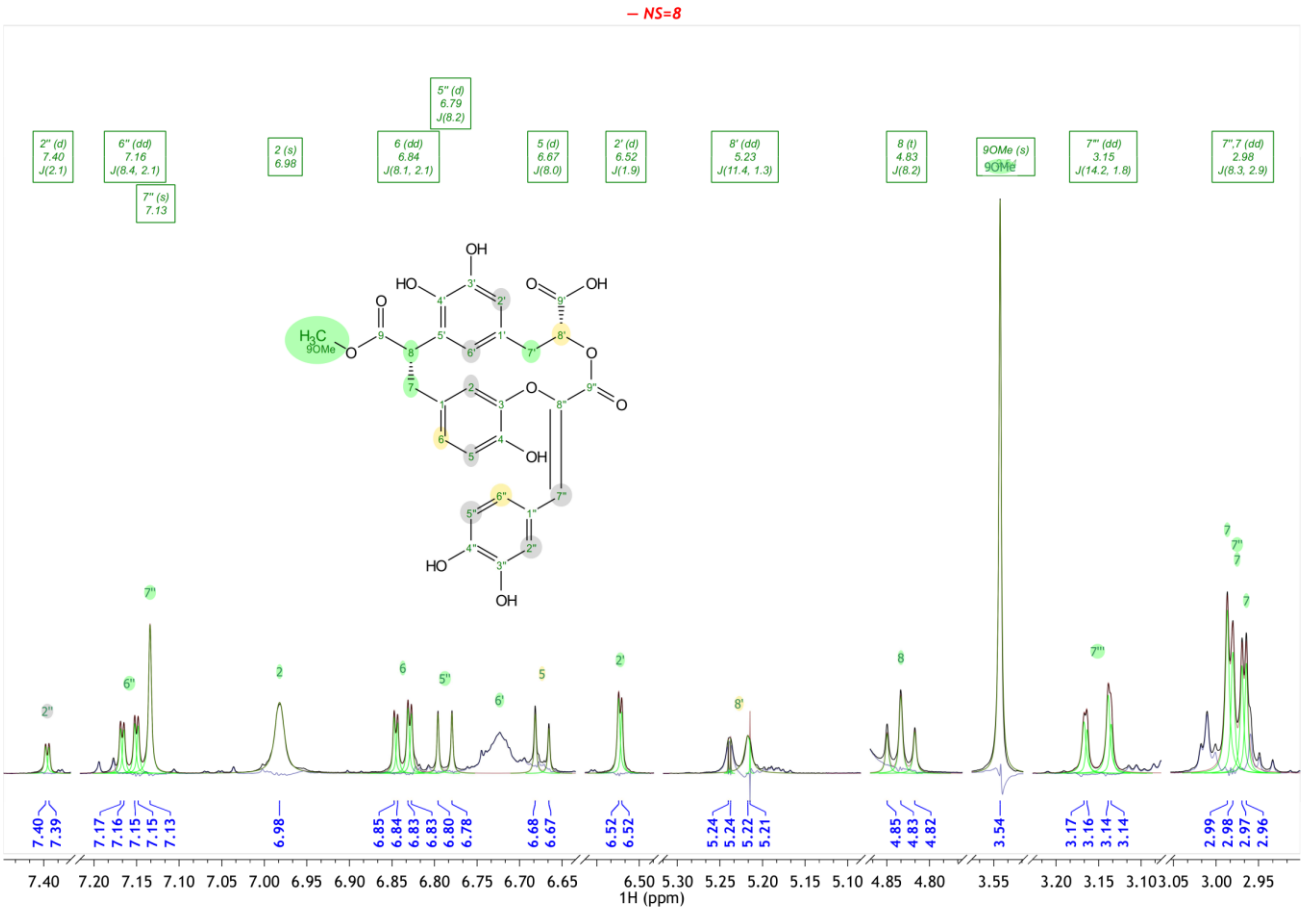


Figure 81S. ^{1}H NMR spectrum of compound 38

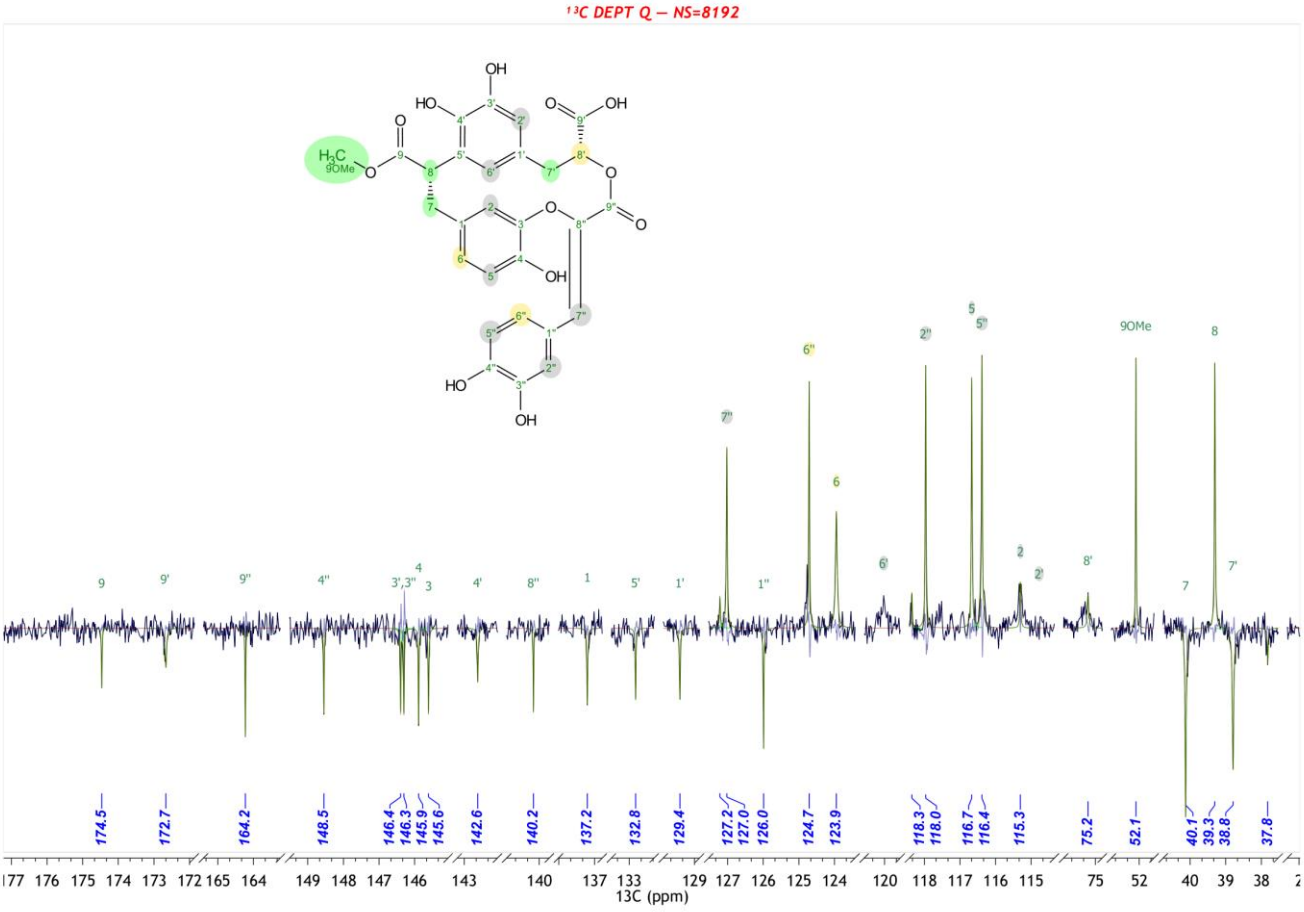


Figure 82S. ^{13}C DEPTQ NMR spectrum of compound 38

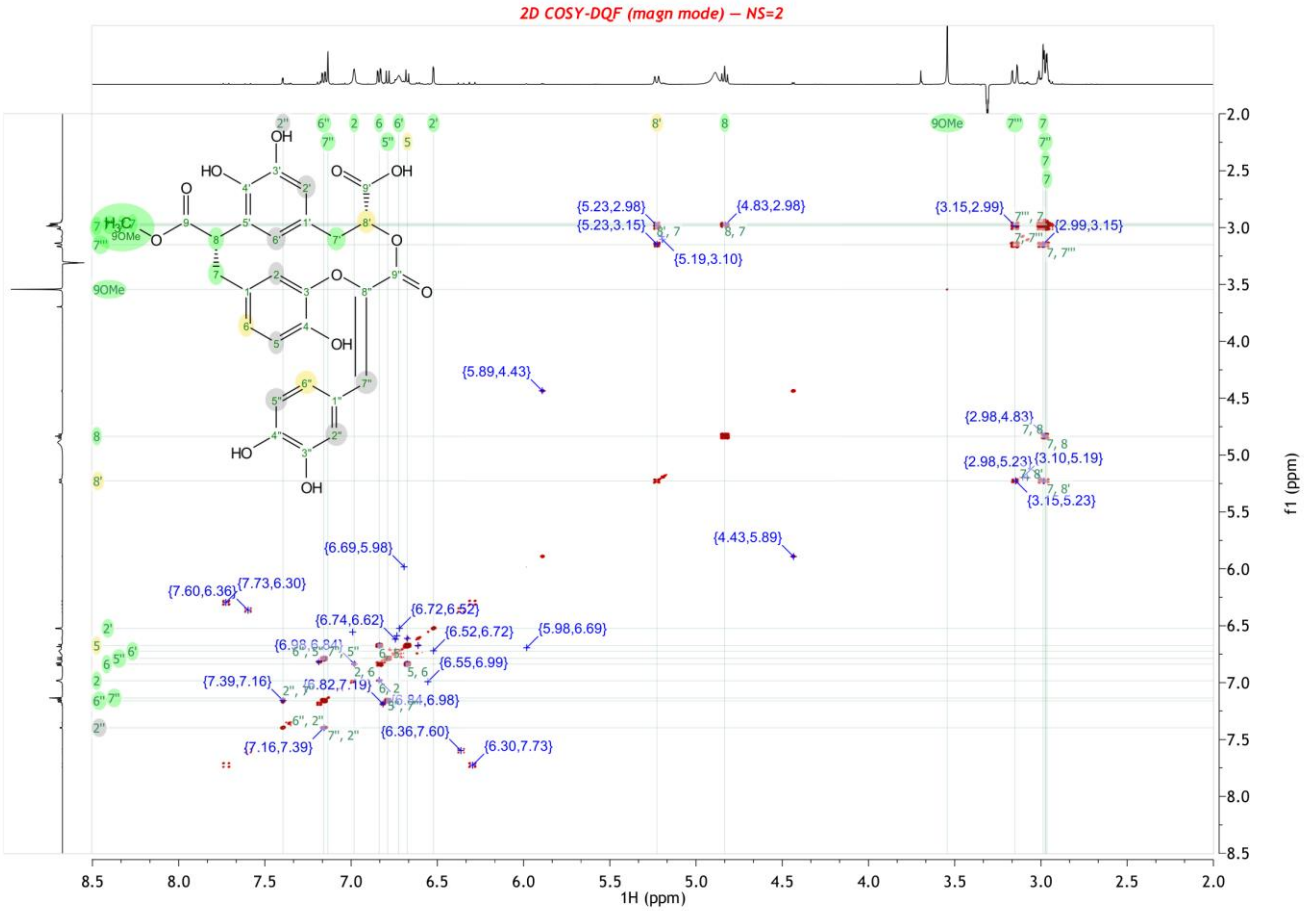


Figure 83S. ^{1}H-^{1}H COSY NMR spectrum of compound 38

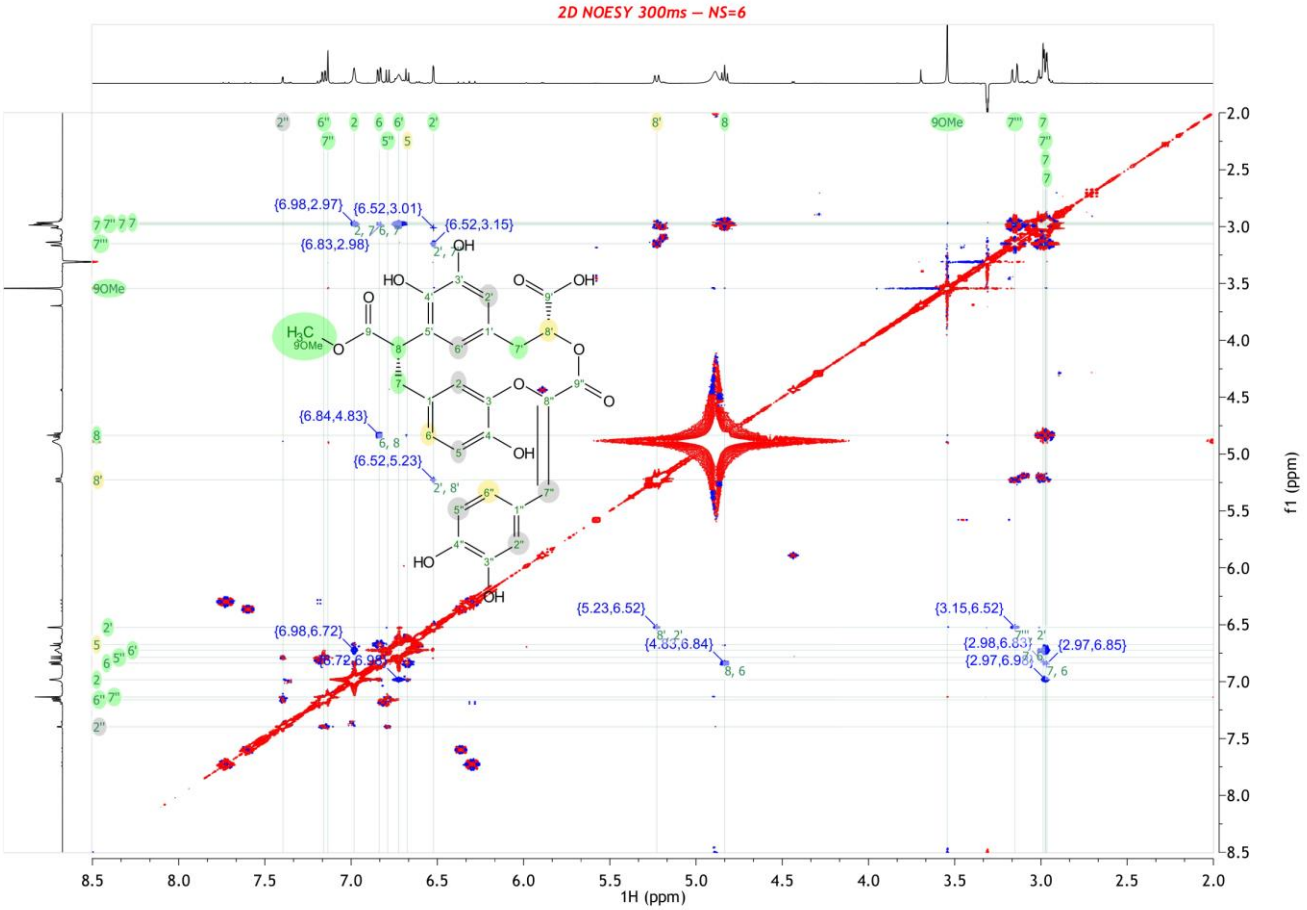


Figure 84S. ^{1}H-^{1}H NOESY (300 ms) NMR spectrum of compound 38

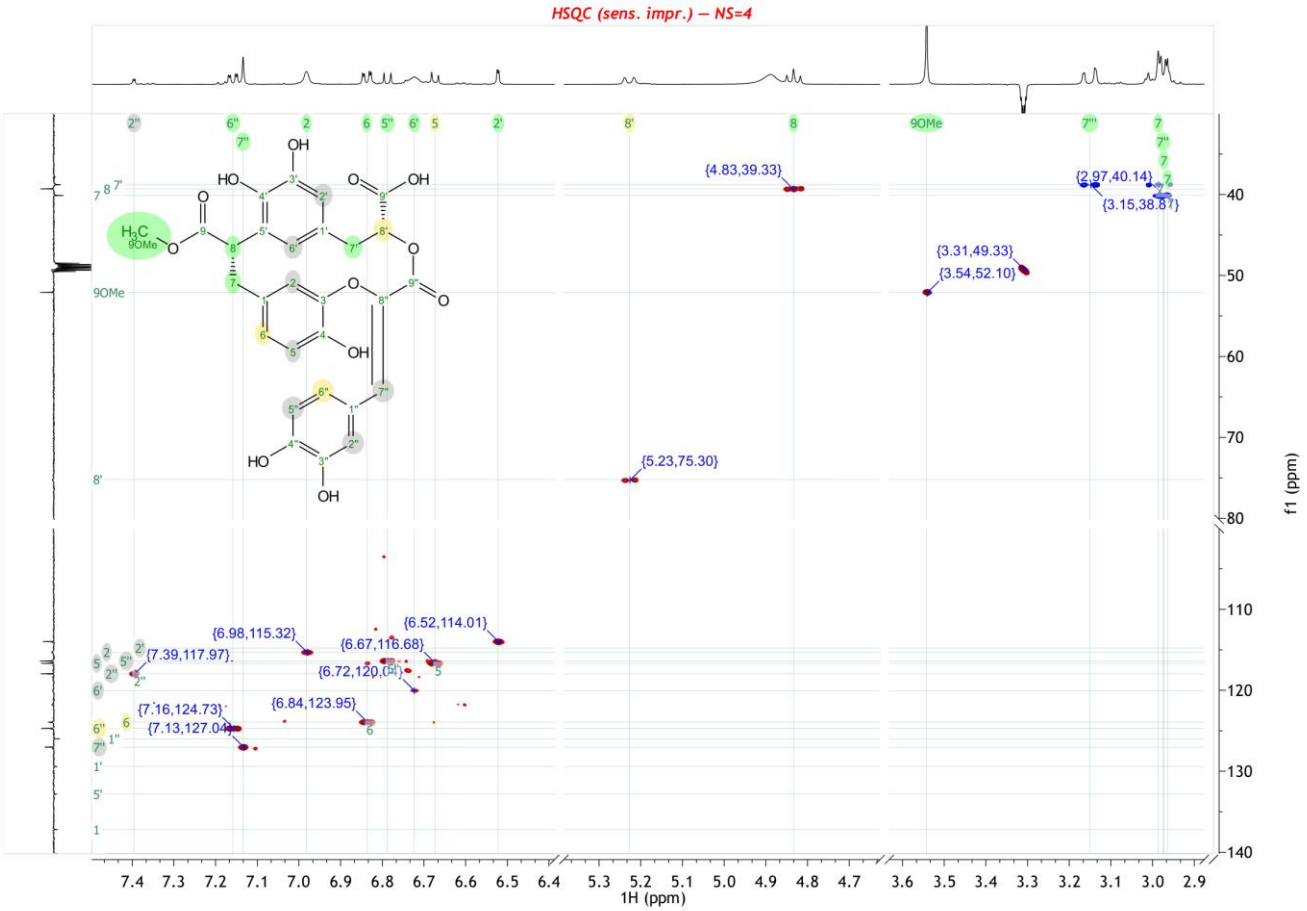


Figure 85S. ^{1}H-^{13}C HSQC NMR spectrum of compound 38

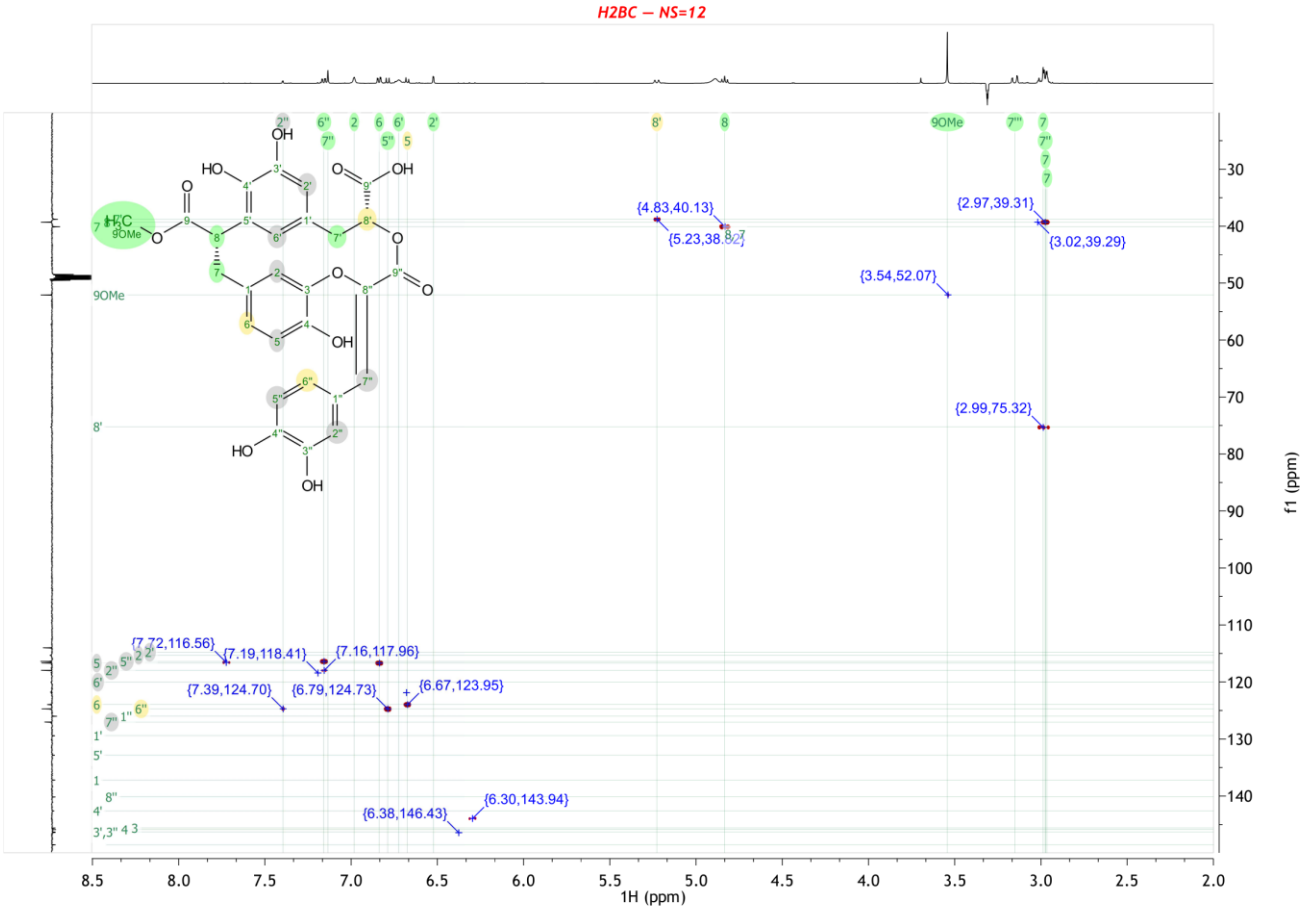


Figure 86S. ^{1}H-^{13}C H2BC NMR spectrum of compound 38

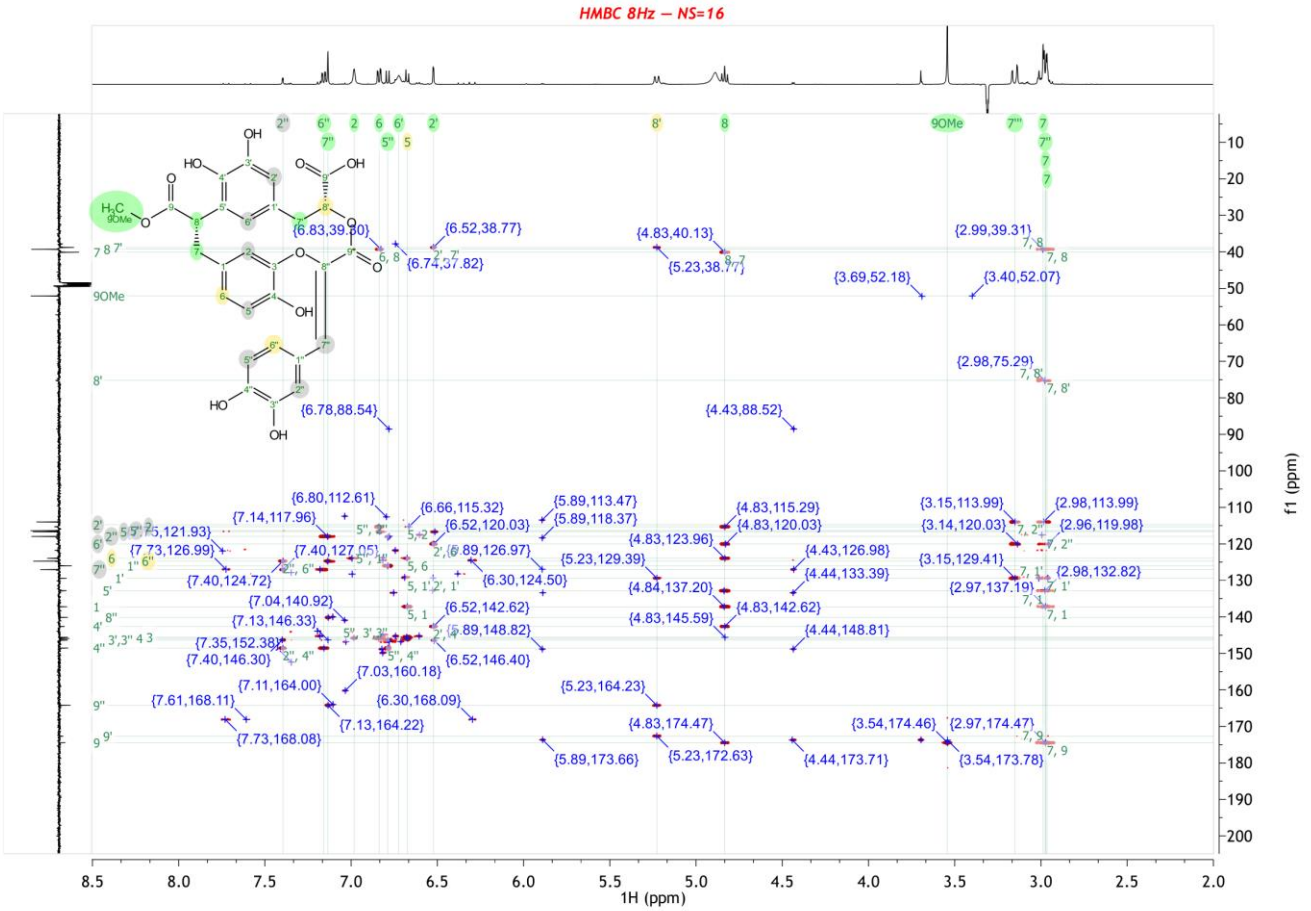
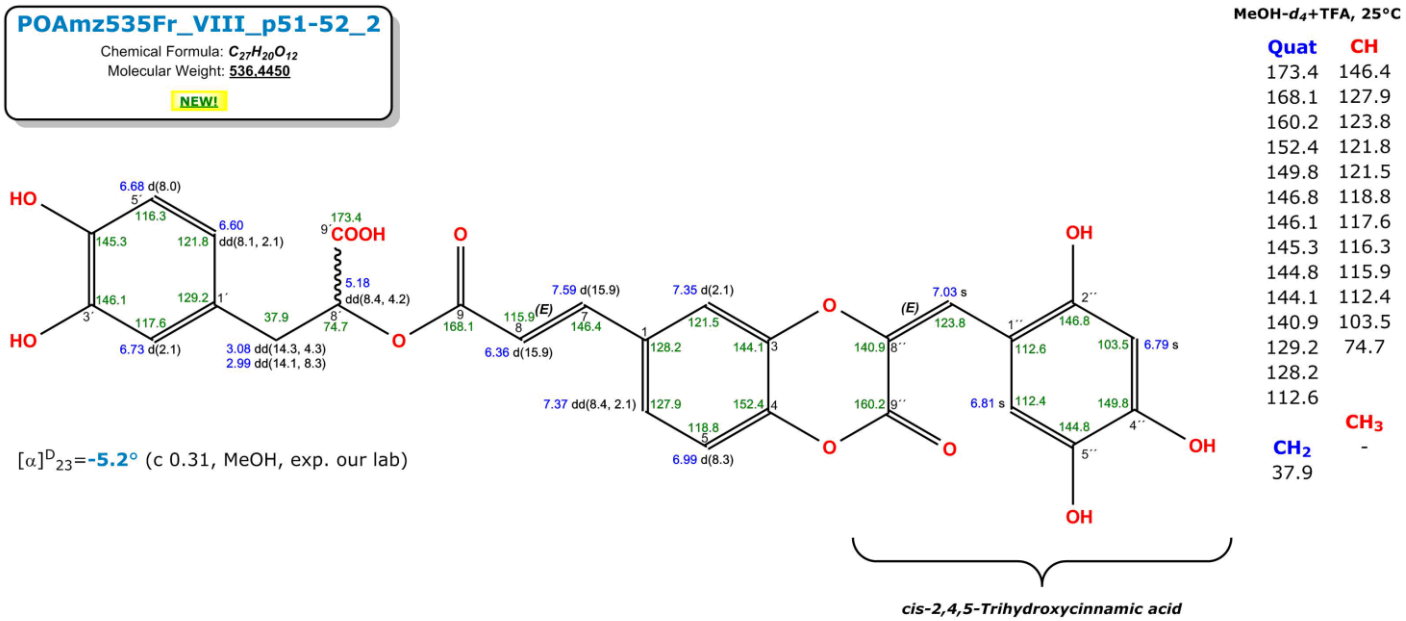


Figure 87S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 38



Pulmitric acid B

1. Murata, T., Watahiki, M., Tanaka, Y., Miyase, T., Yoshizaki, F., 2010. Hyaluronidase Inhibitors from Takuran, Lycopus lucidus. Chem. Pharm. Bull. (Tokyo). 58, 394–397. doi:10.1248/cpb.58.394

Figure 88S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 39 in CD_3OD, 25°C

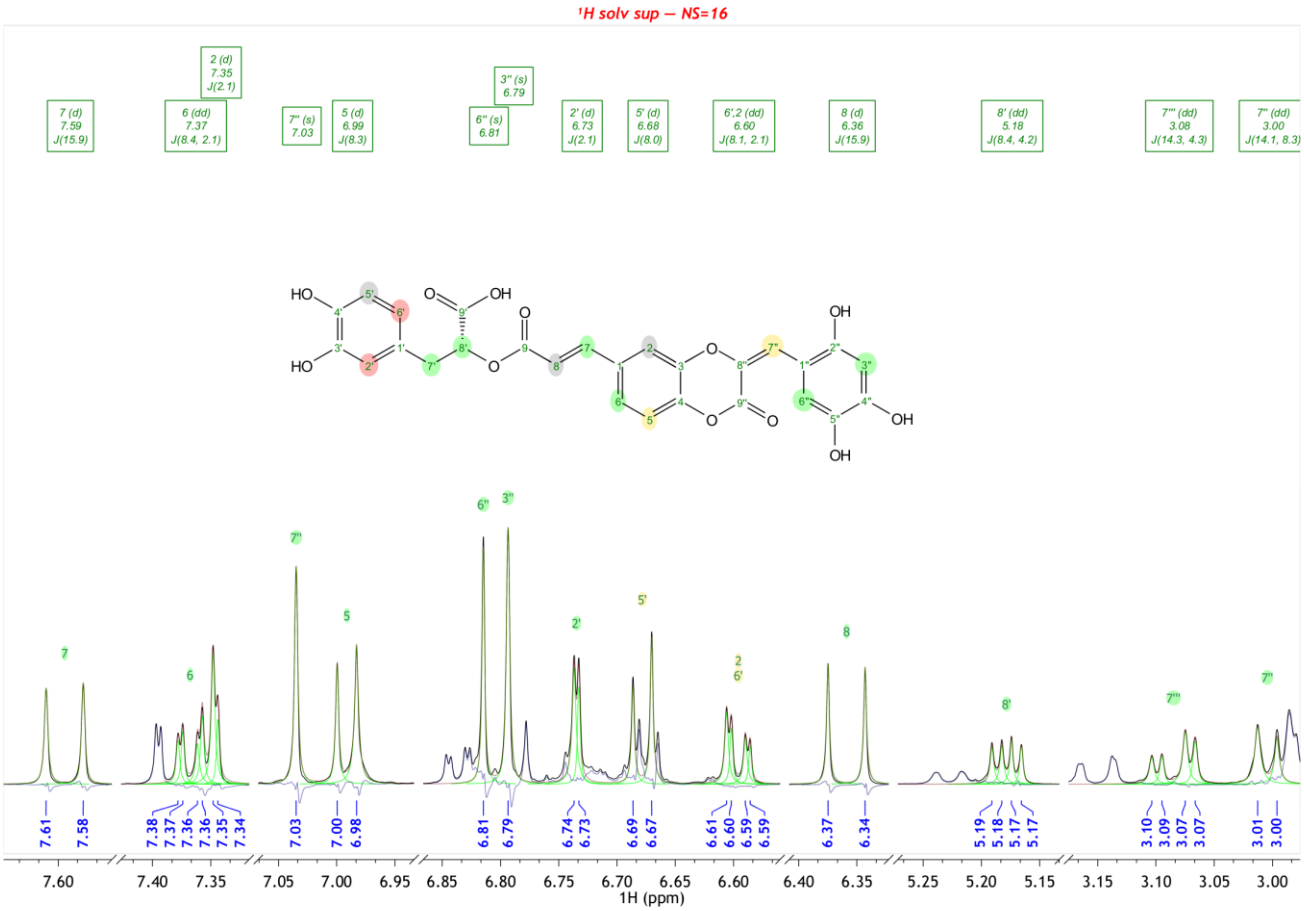


Figure 89S. ^{1}H NMR spectrum of compound 39

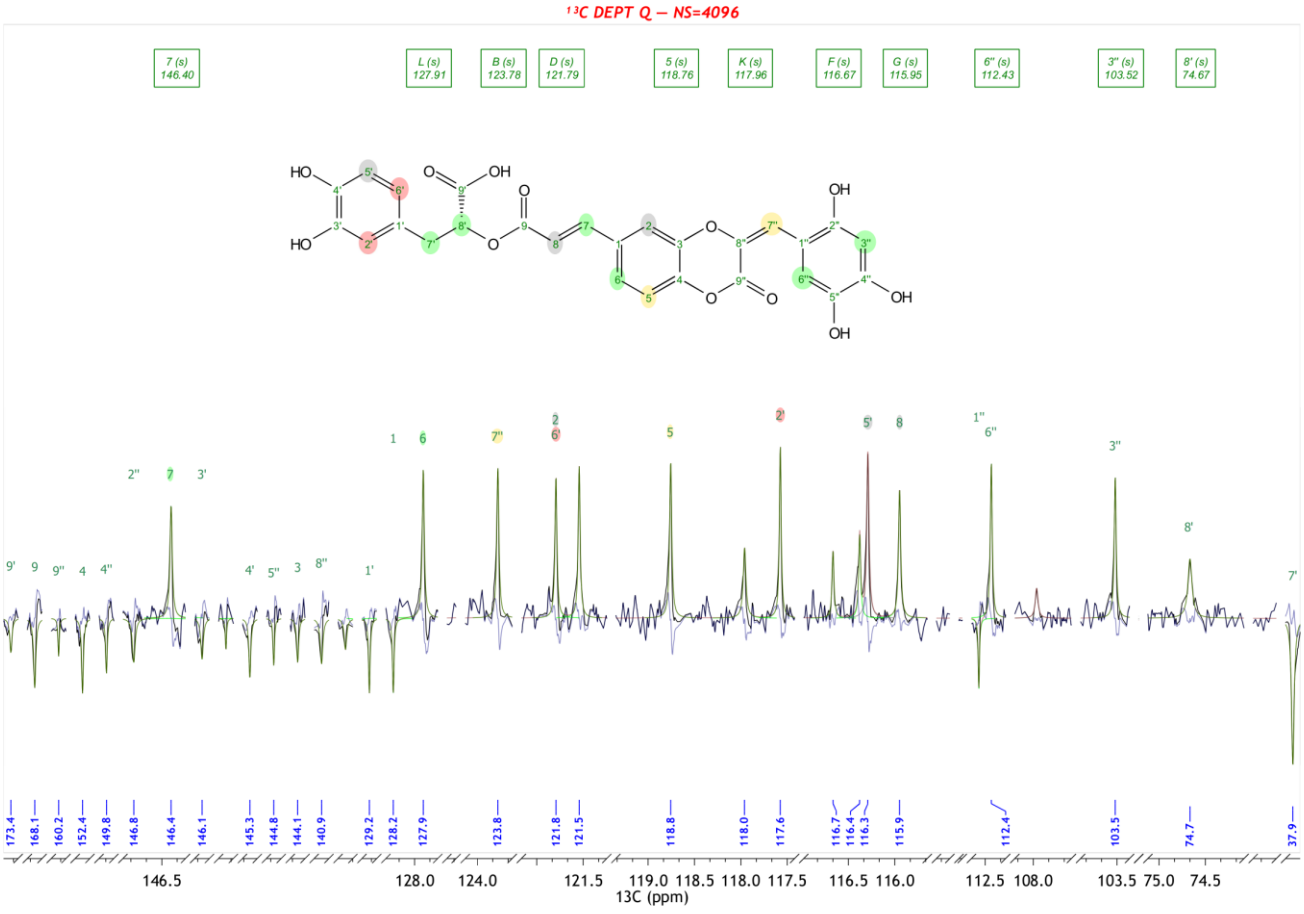


Figure 90S. ^{13}C DEPTQ NMR spectrum of compound 39

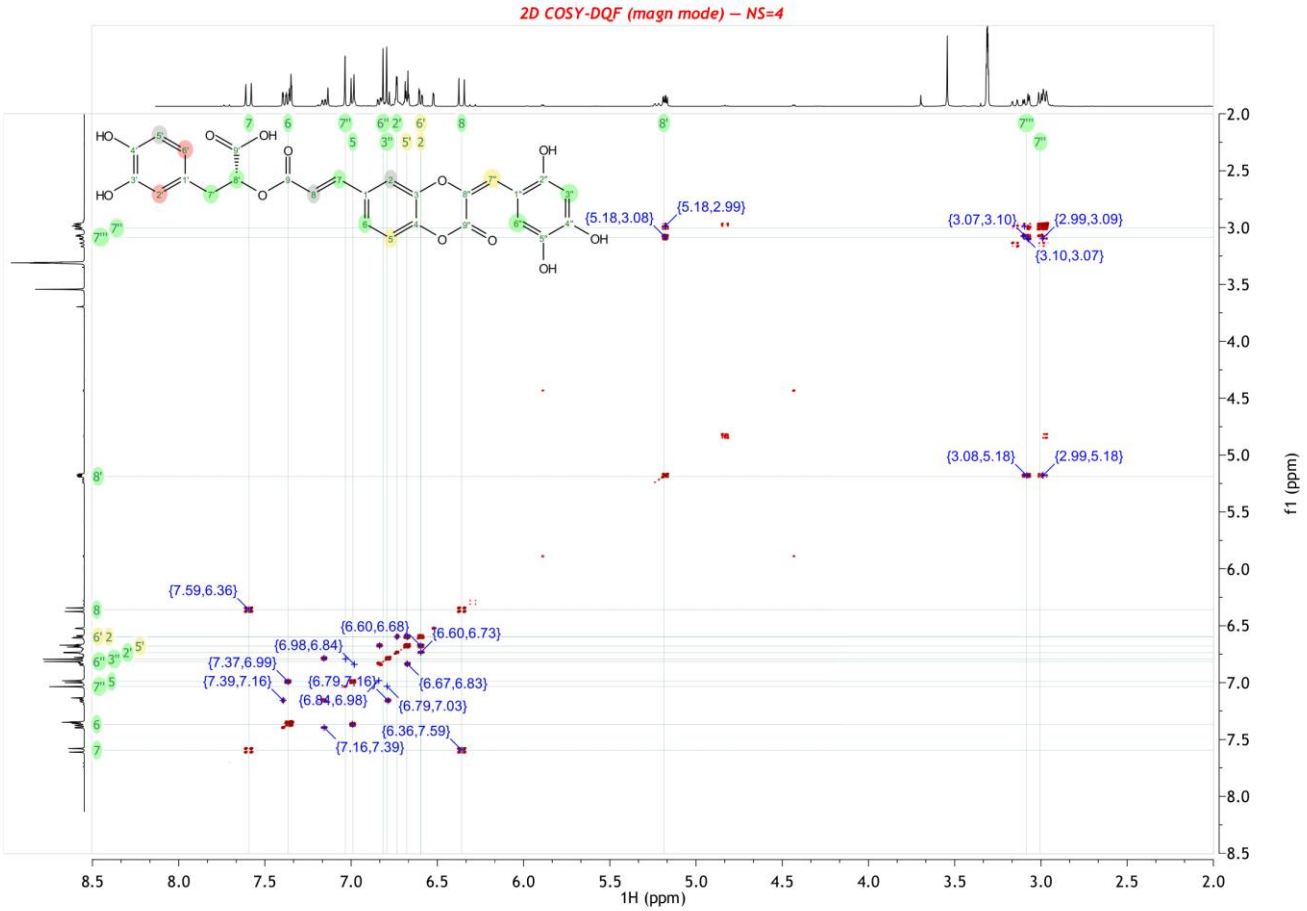


Figure 91S. ^{1}H-^{1}H COSY NMR spectrum of compound 39

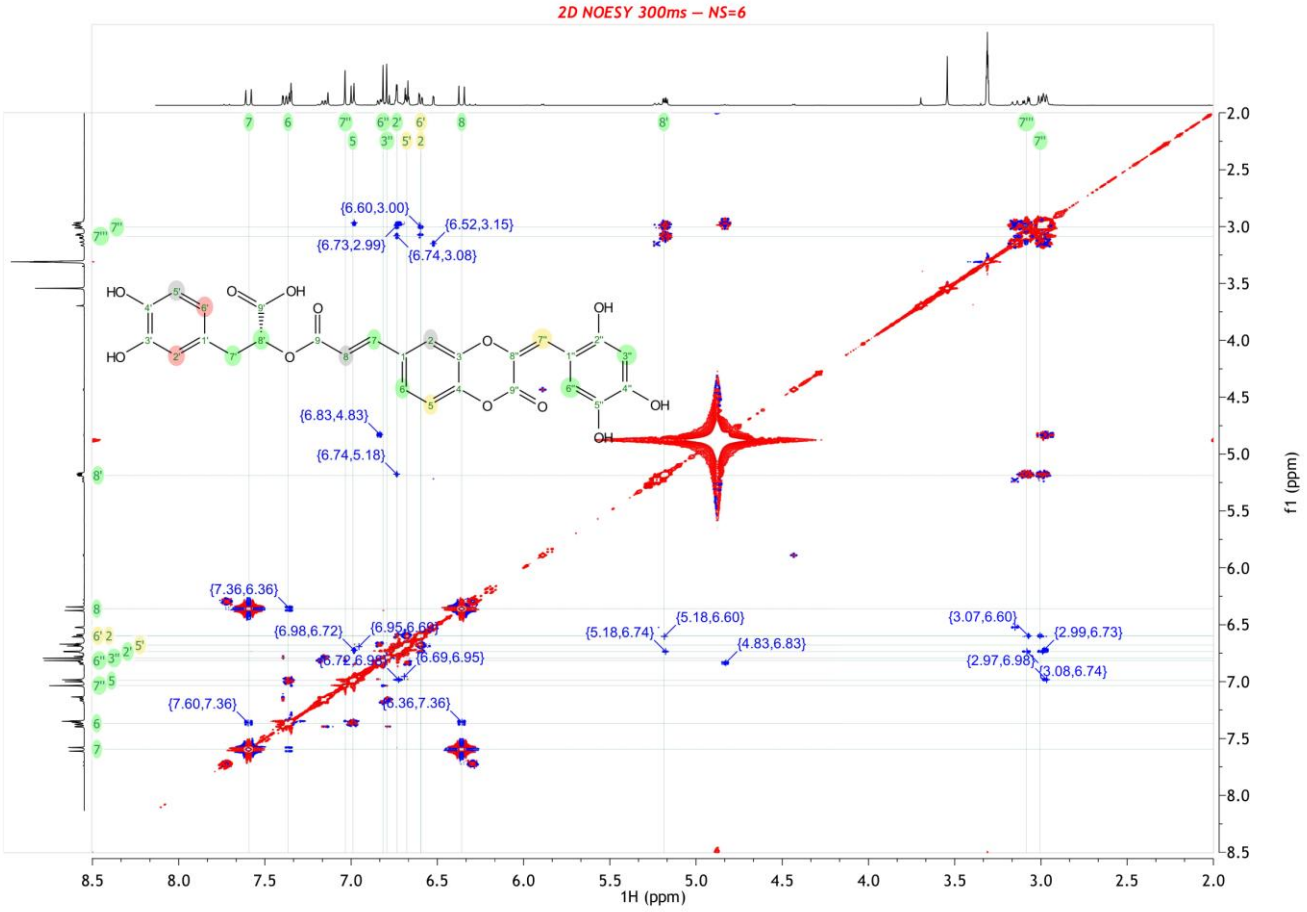


Figure 92S. ^{1}H-^{1}H NOESY (300 ms) NMR spectrum of compound 39

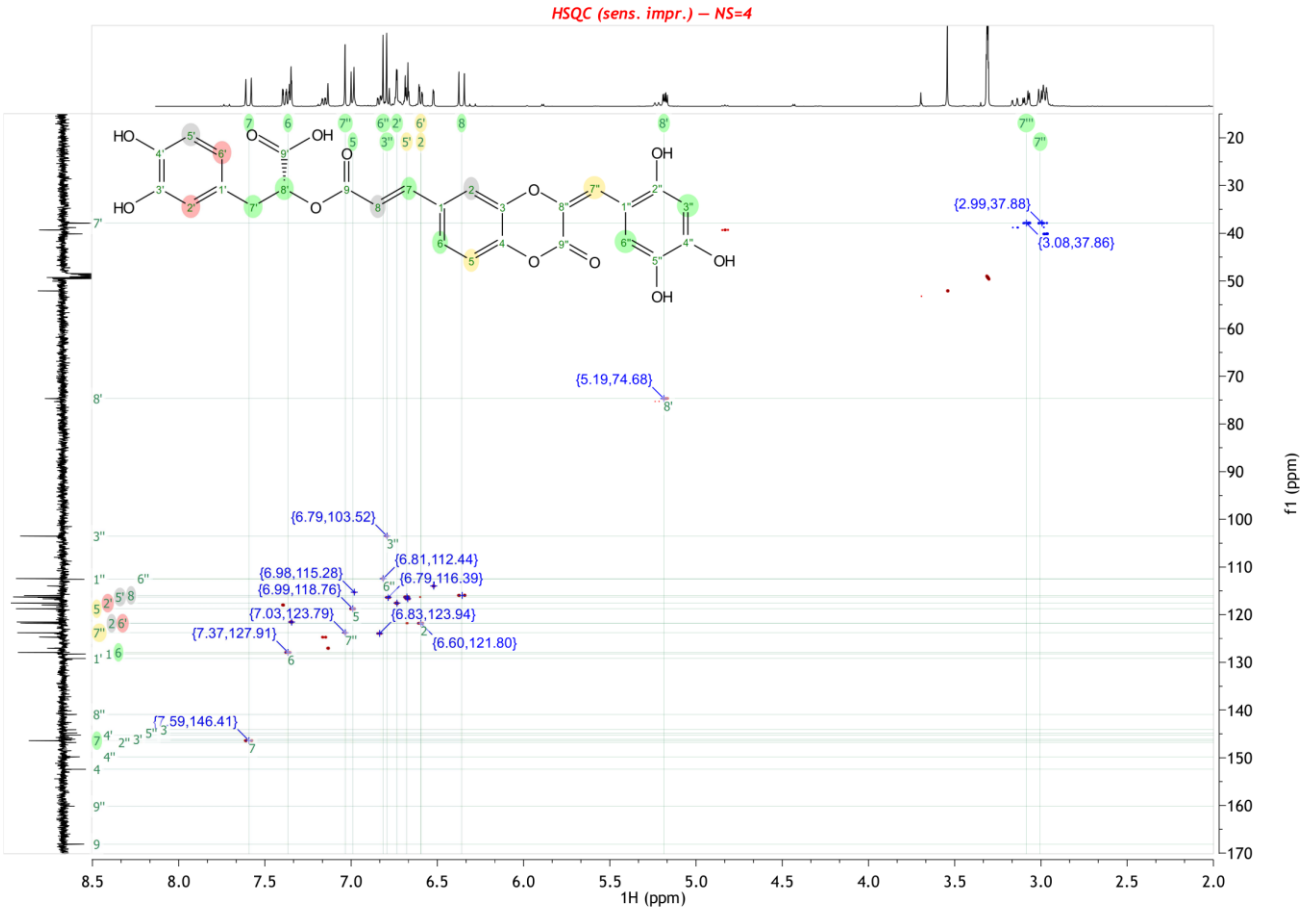


Figure 93S. ^{1}H-^{13}C HSQC NMR spectrum of compound 39

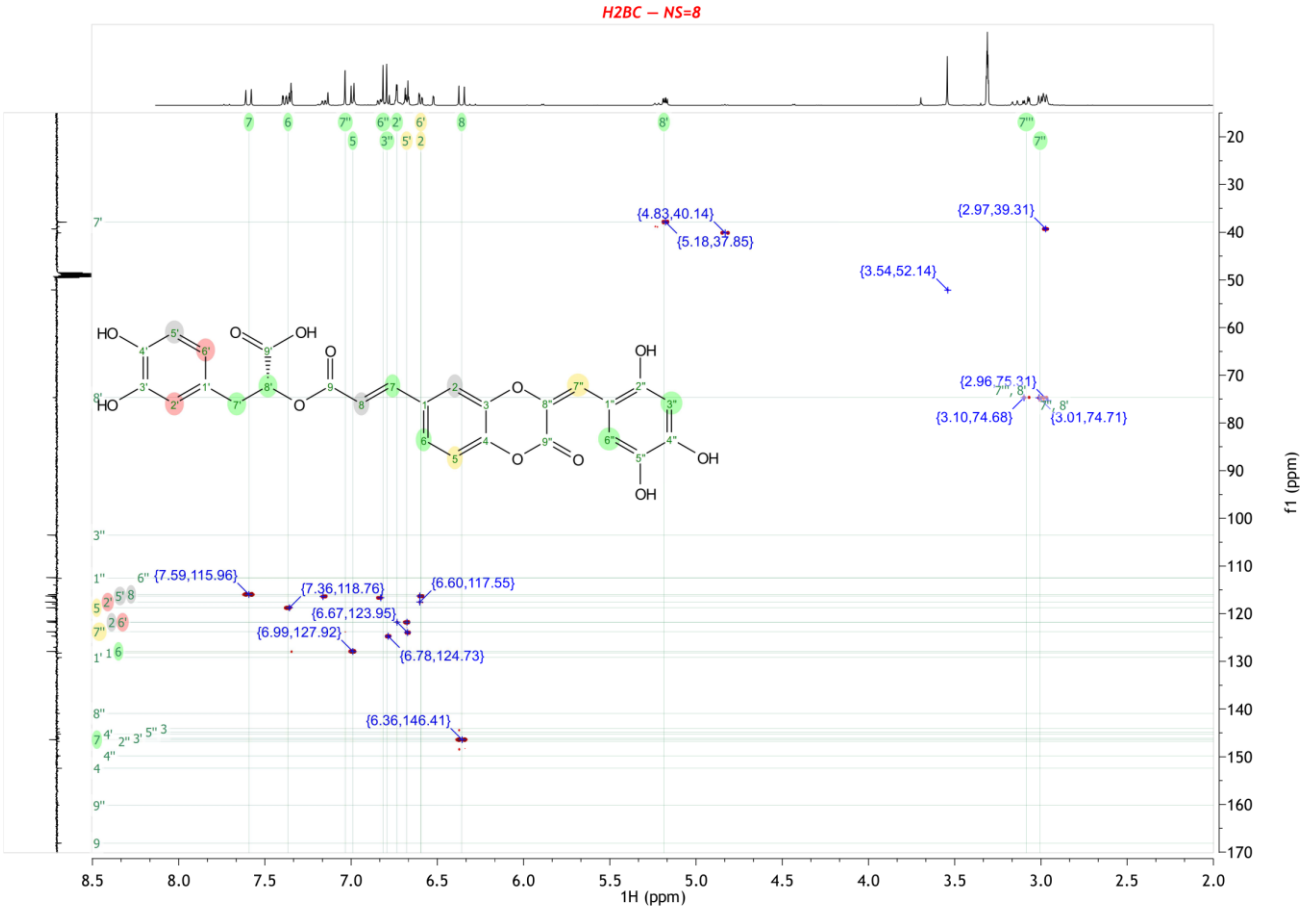


Figure 94S. ^{1}H-^{13}C H2BC NMR spectrum of compound 39

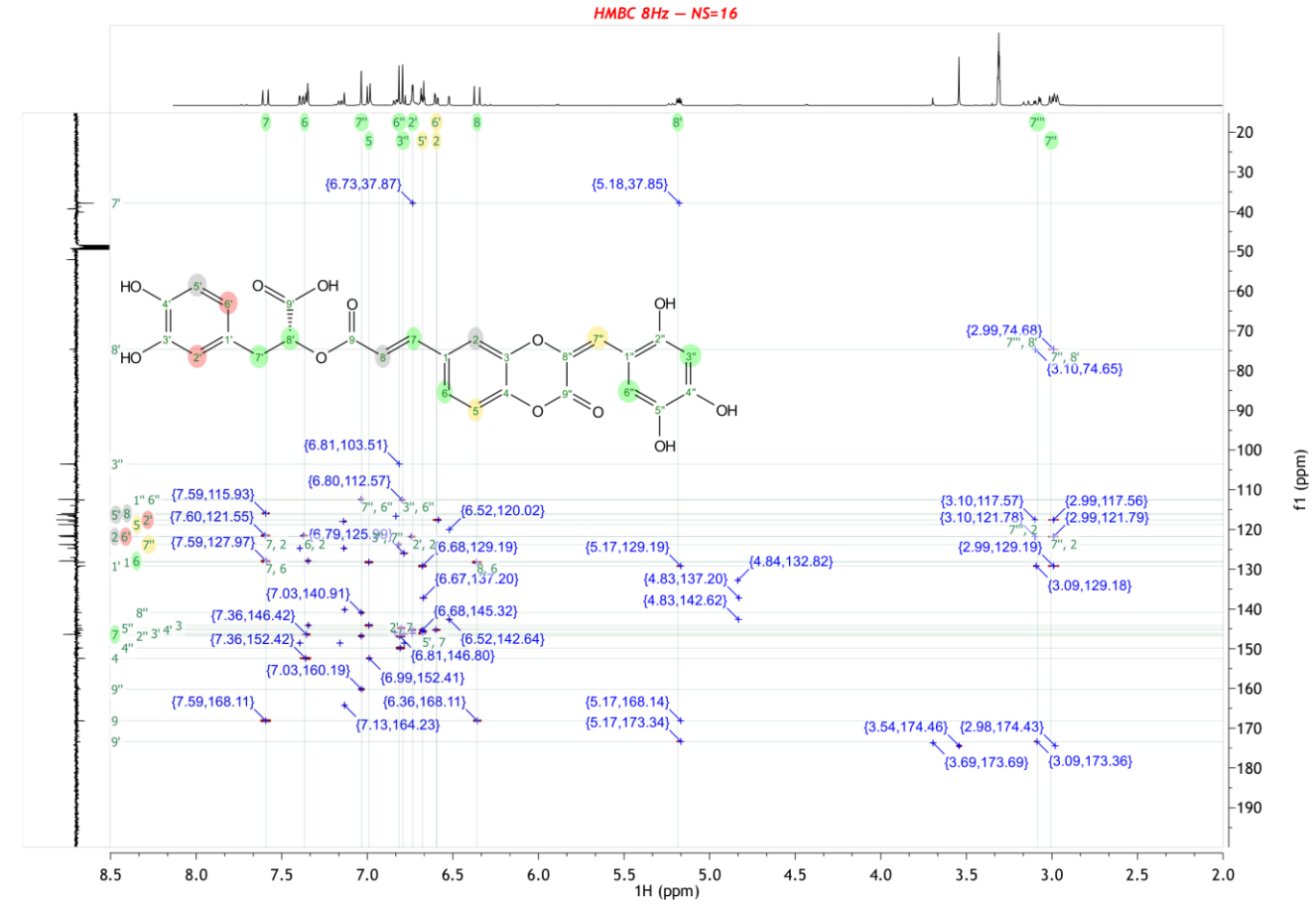
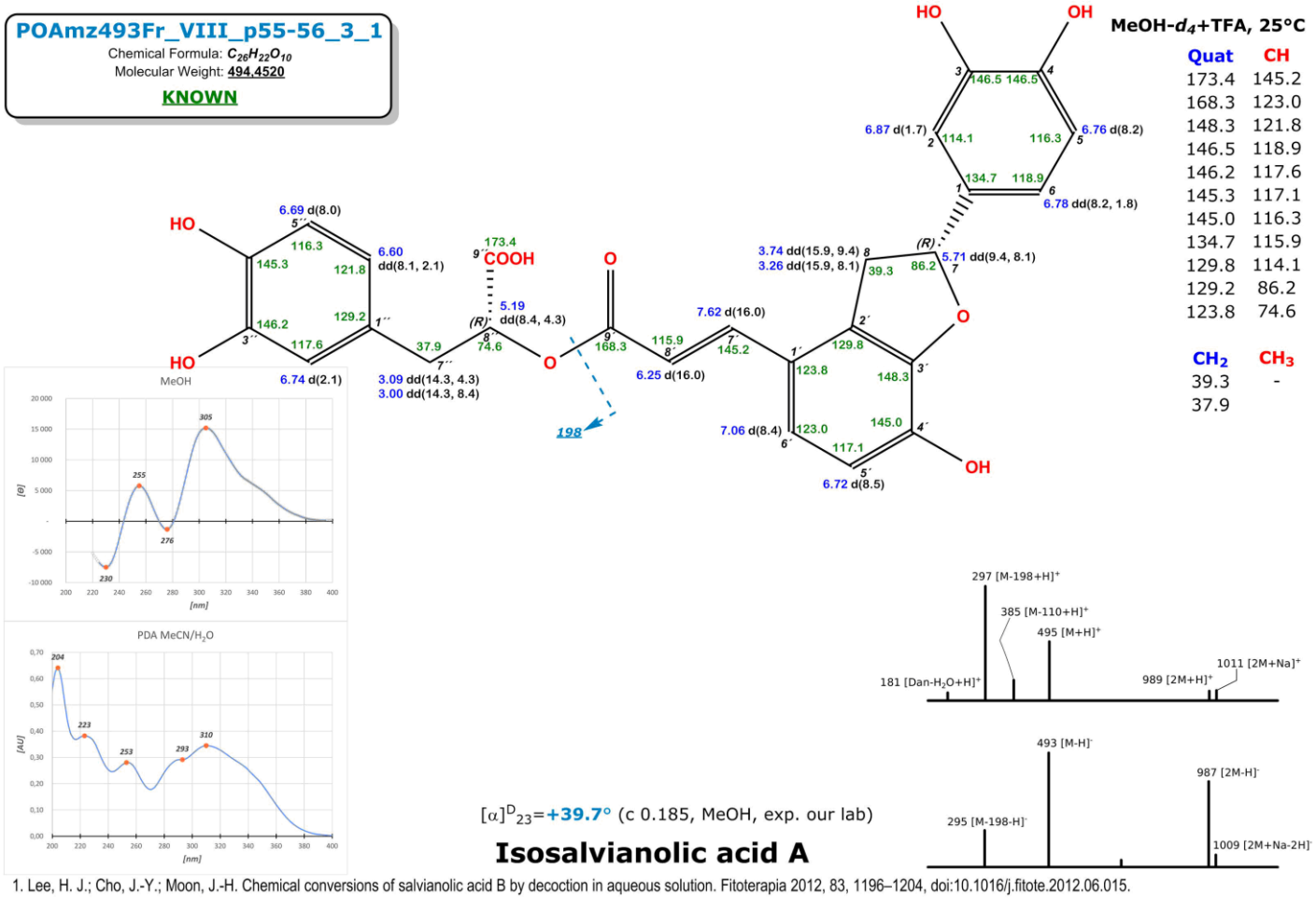


Figure 95S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 39



1. Lee, H. J.; Cho, J.-Y.; Moon, J.-H. Chemical conversions of salvianolic acid B by decoction in aqueous solution. Fitoterapia 2012, 83, 1196–1204, doi:10.1016/j.fitote.2012.06.015.

Figure 96S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 40 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

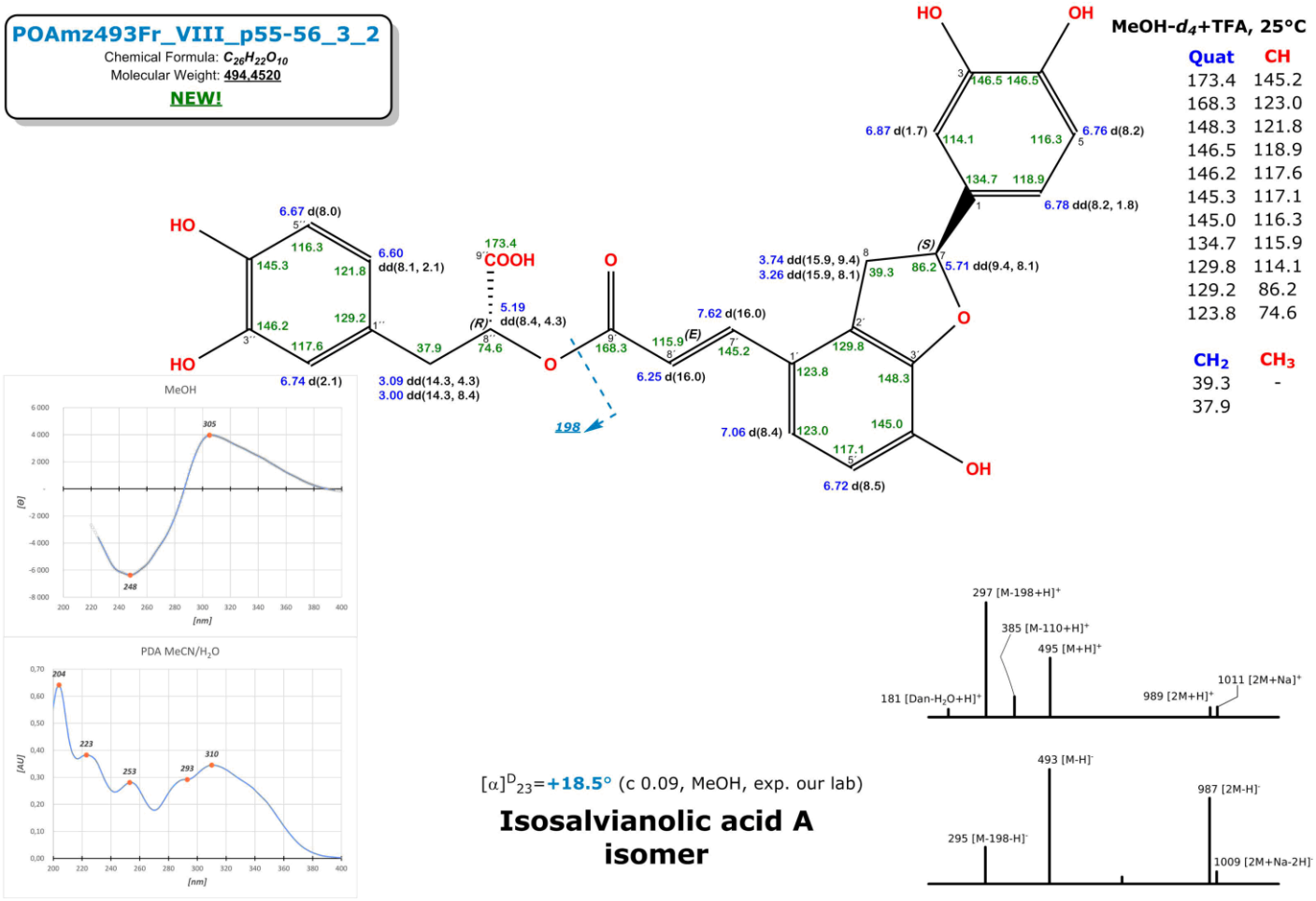


Figure 97S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 41 in CD_3OD, 25°C; on-line PDA UV spectrum in MeCN/H_2O; ECD spectrum in MeOH

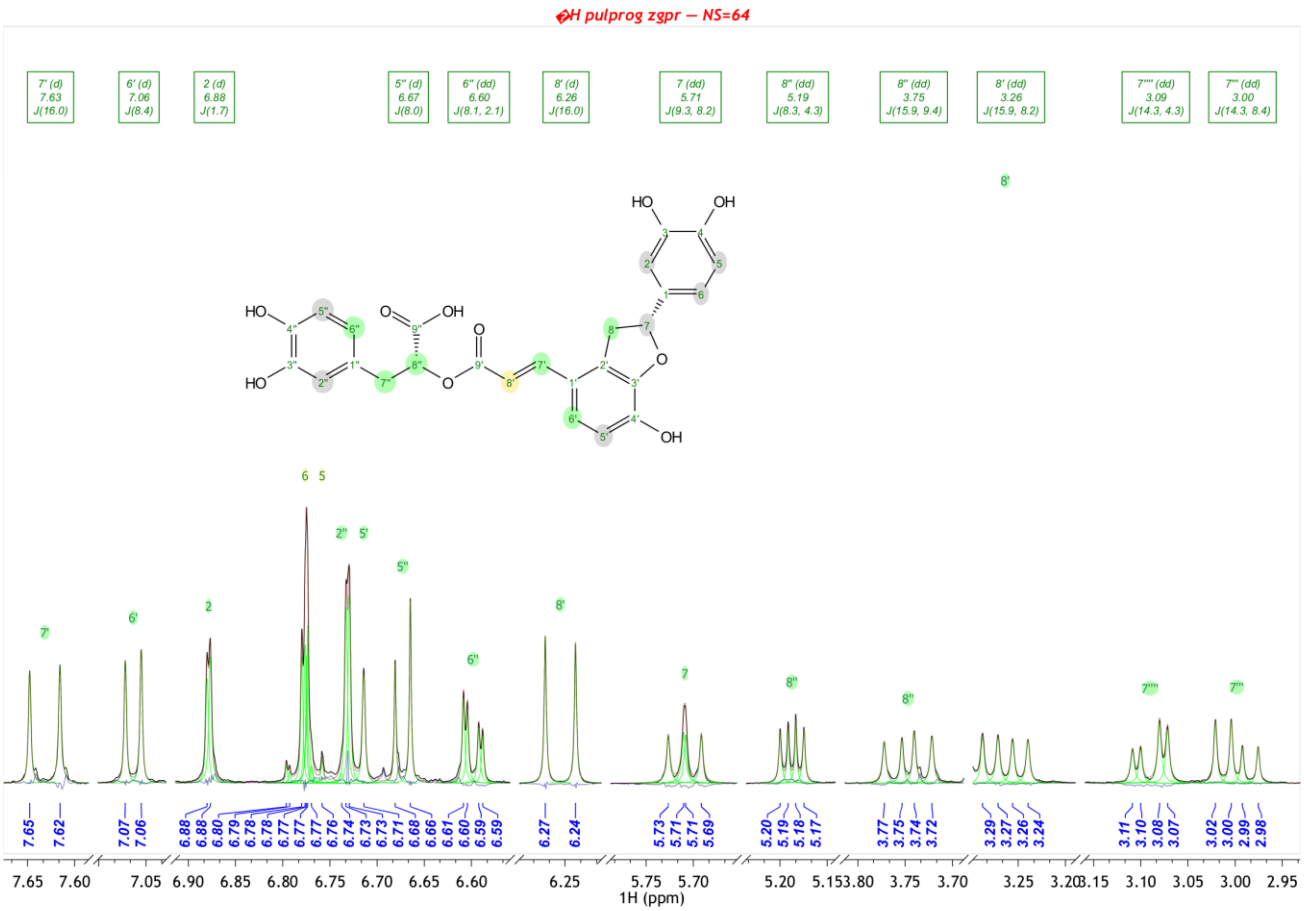


Figure 98S. ^{1}H NMR spectrum of compound 41

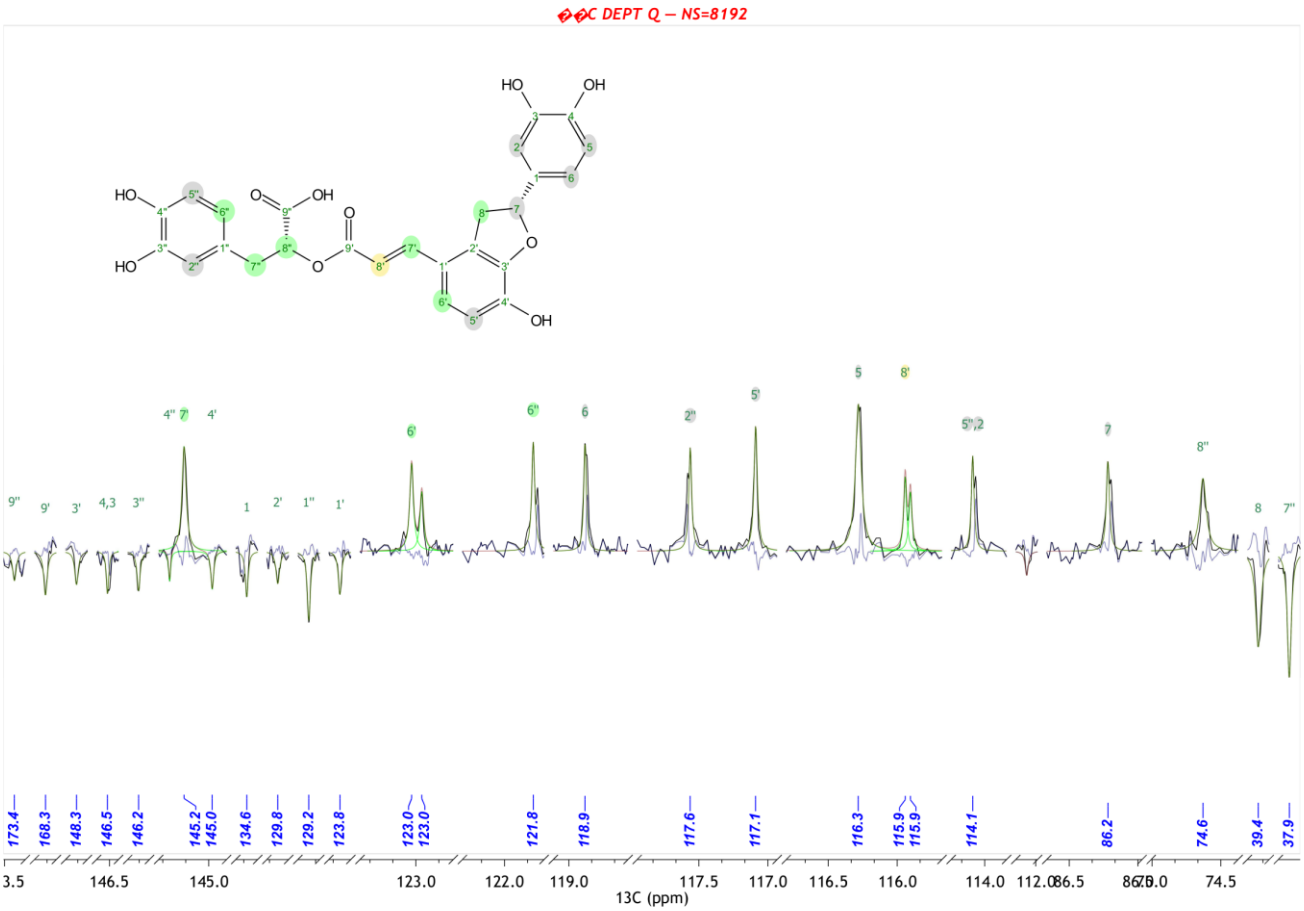


Figure 99S. ^{13}C DEPTQ NMR spectrum of compound 41

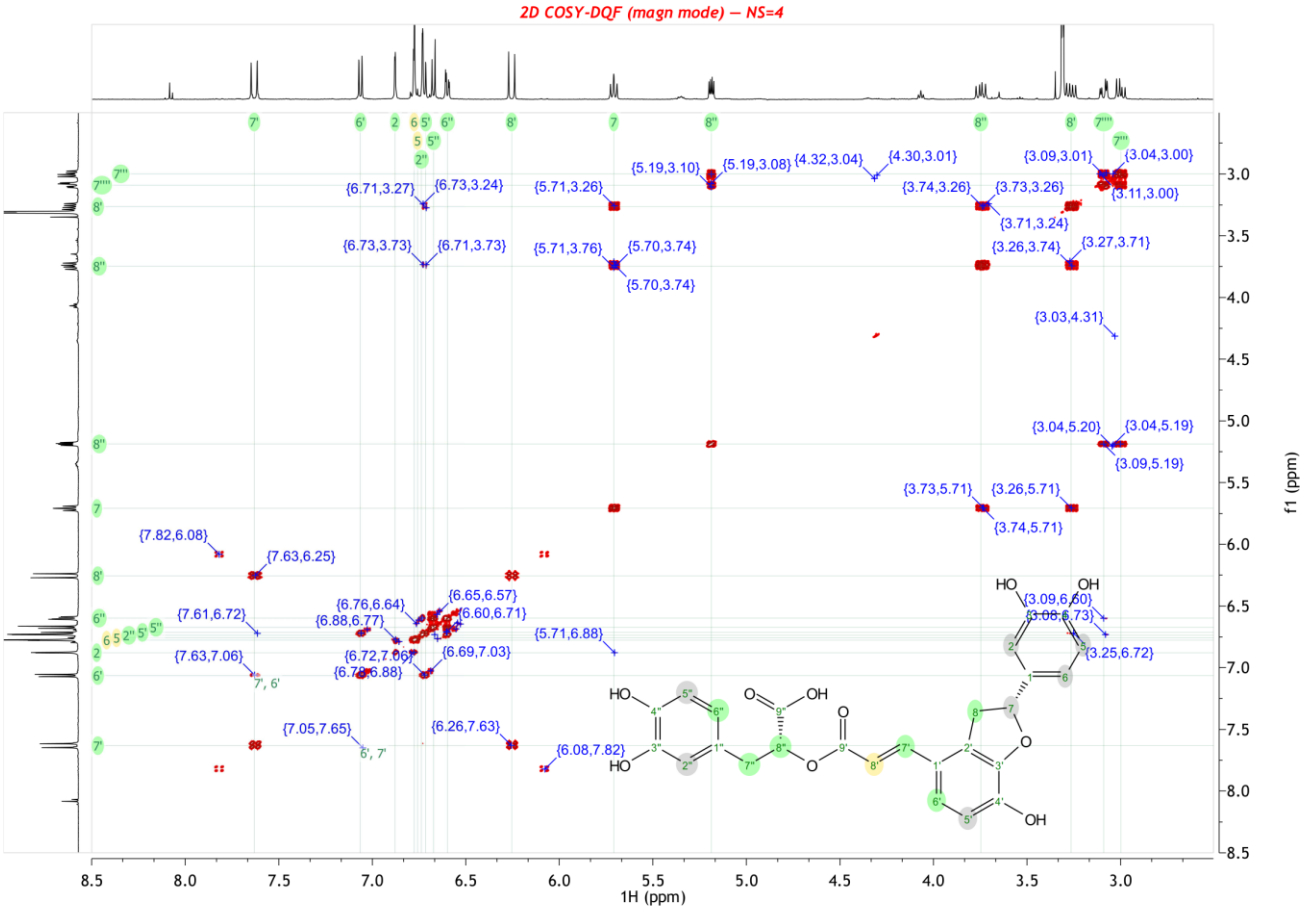


Figure 100S. ^{1}H-^{1}H COSY NMR spectrum of compound 41

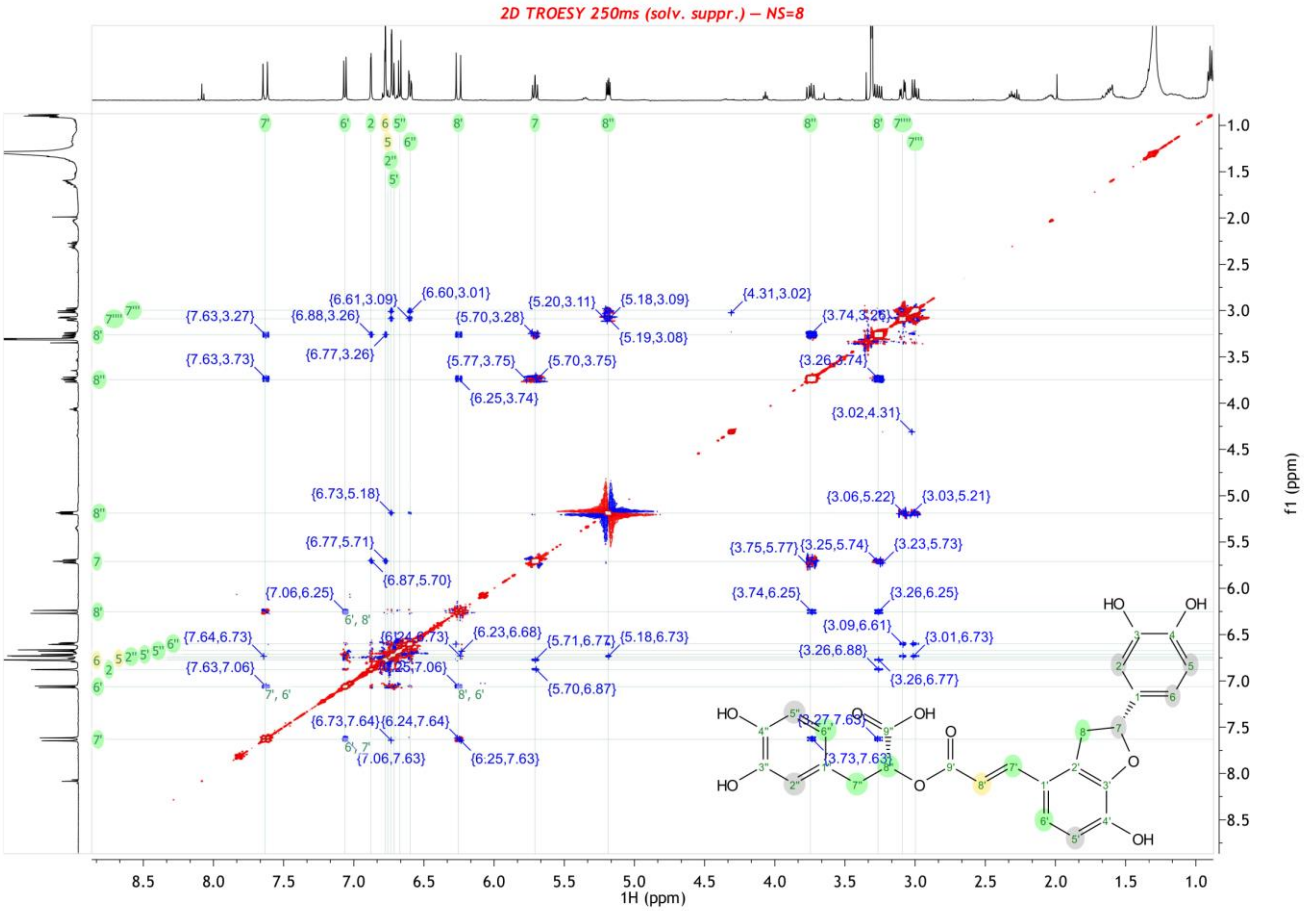


Figure 101S. ^{1}H-^{1}H TROESY (250 ms) NMR spectrum of compound 41

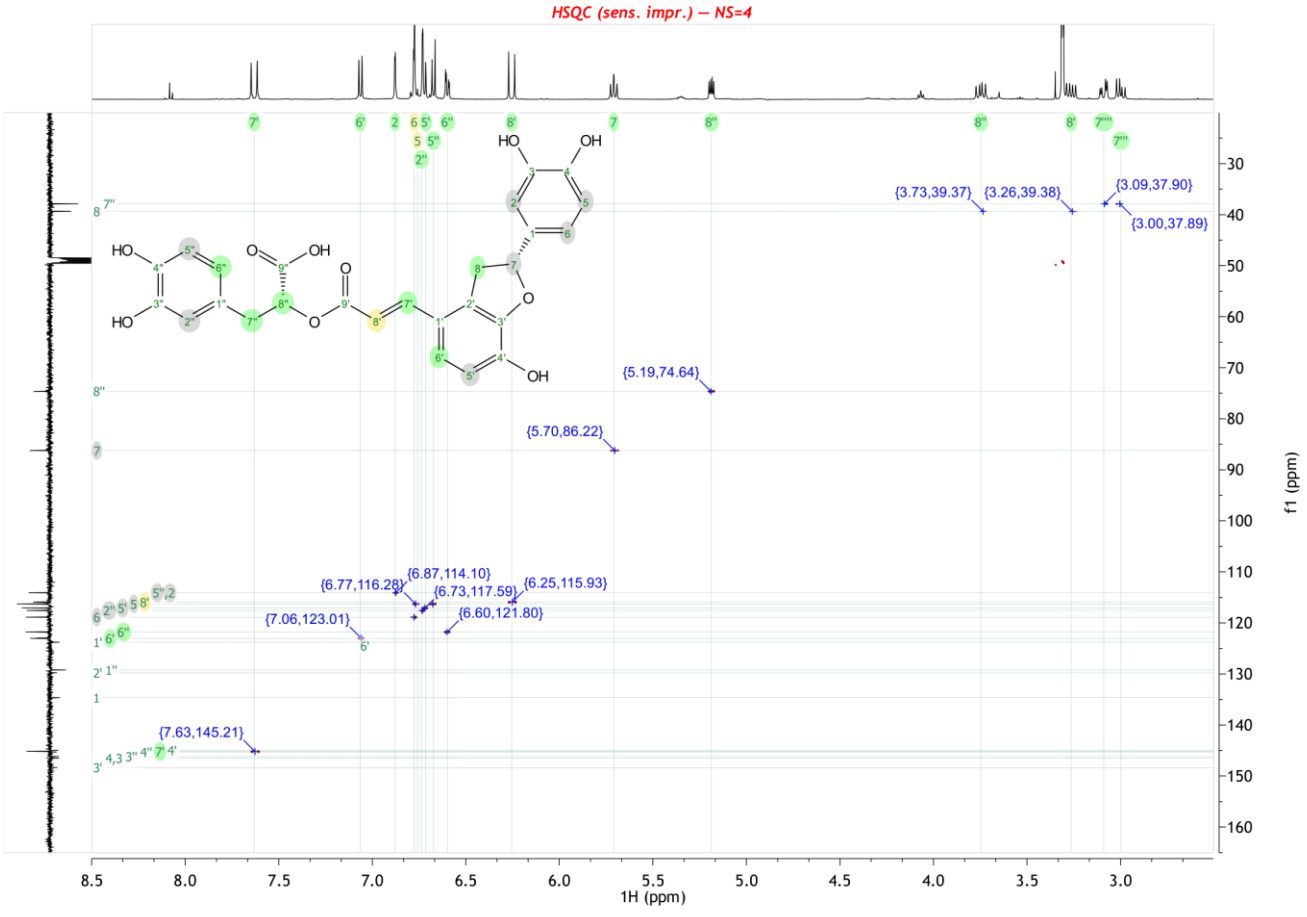


Figure 102S. ^{1}H-^{13}C HSQC NMR spectrum of compound 41

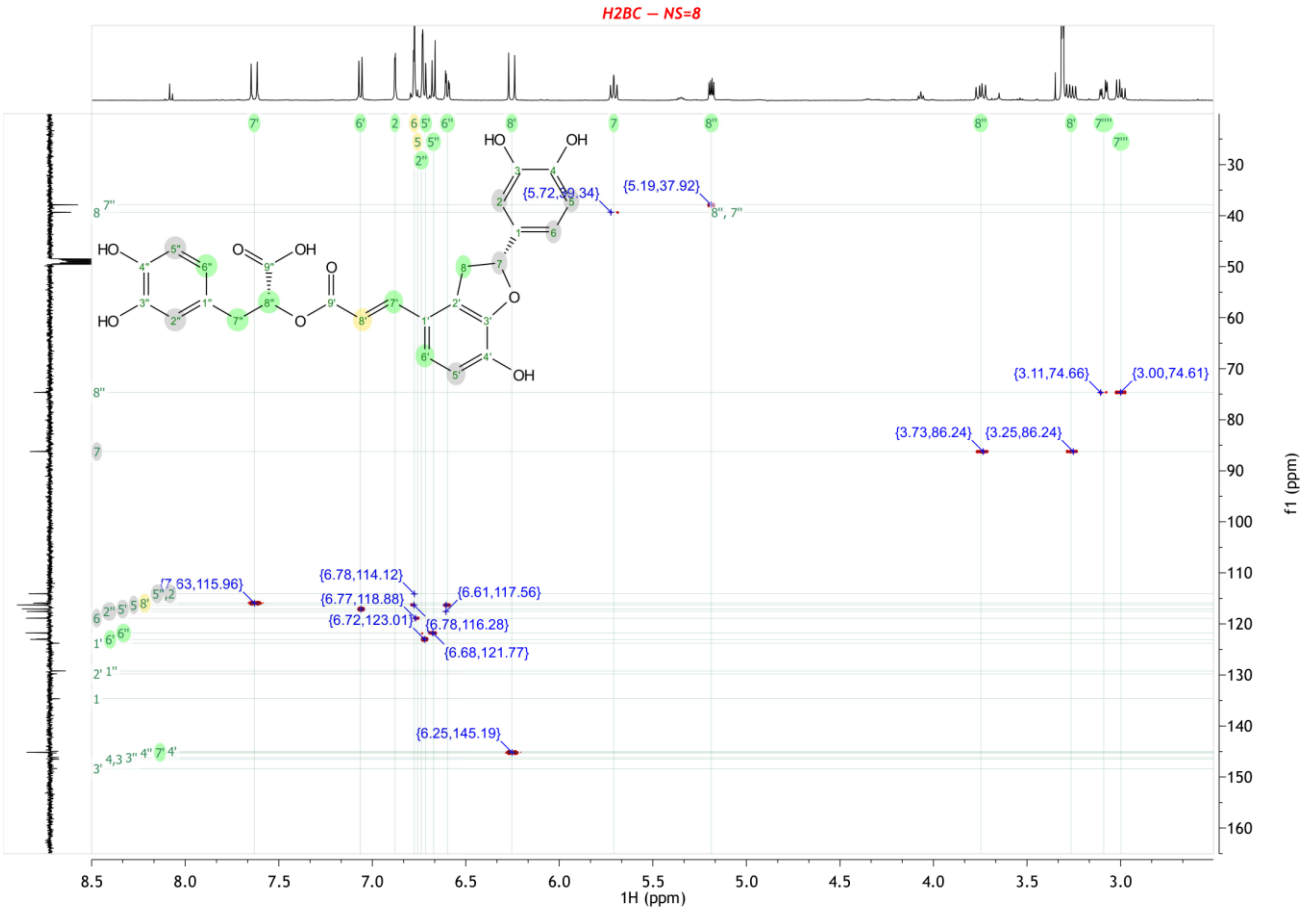


Figure 103S. ^{1}H-^{13}C H2BC NMR spectrum of compound 41

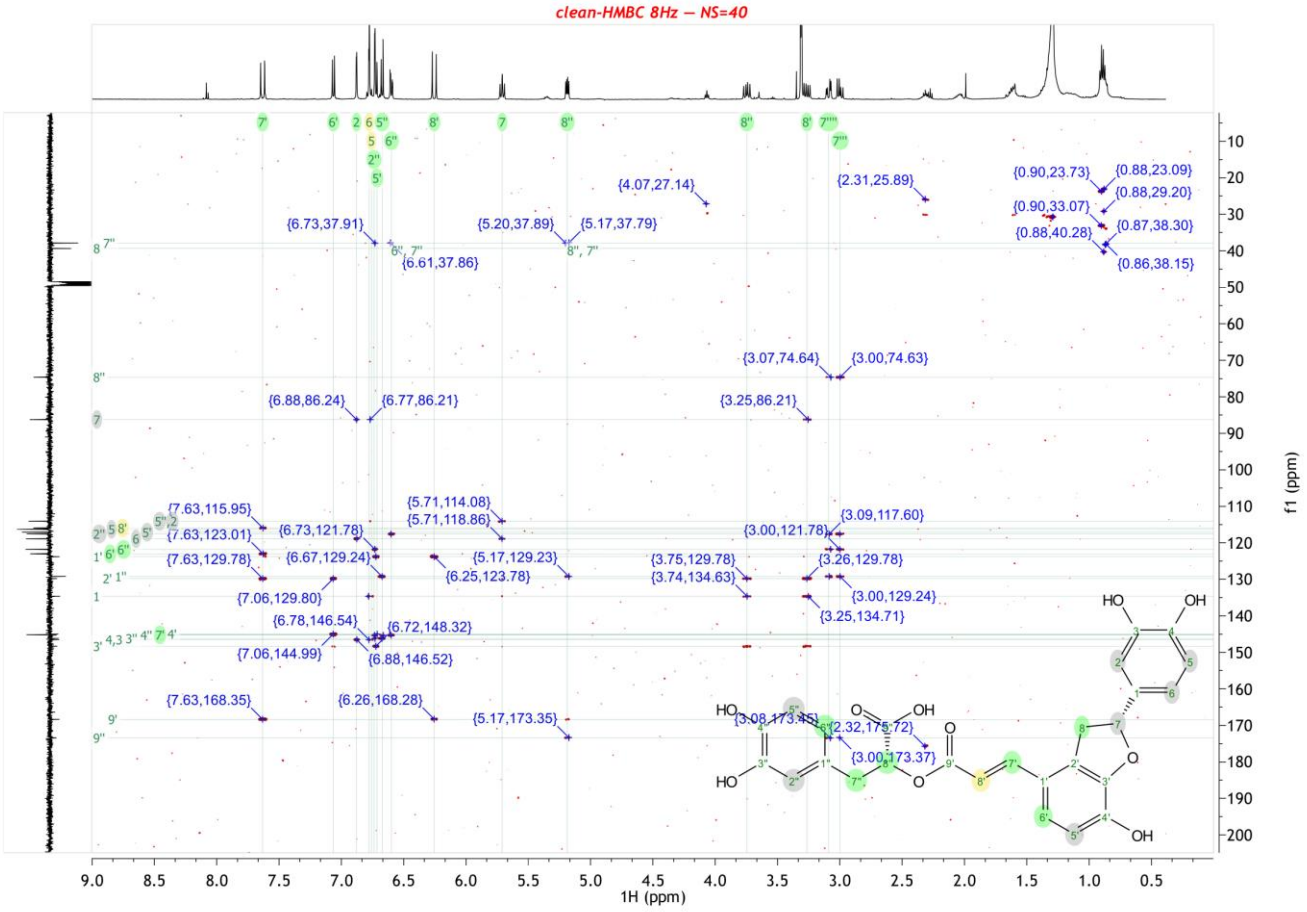


Figure 104S. ^{1}H-^{13}C HMBC (8 Hz) NMR spectrum of compound 41

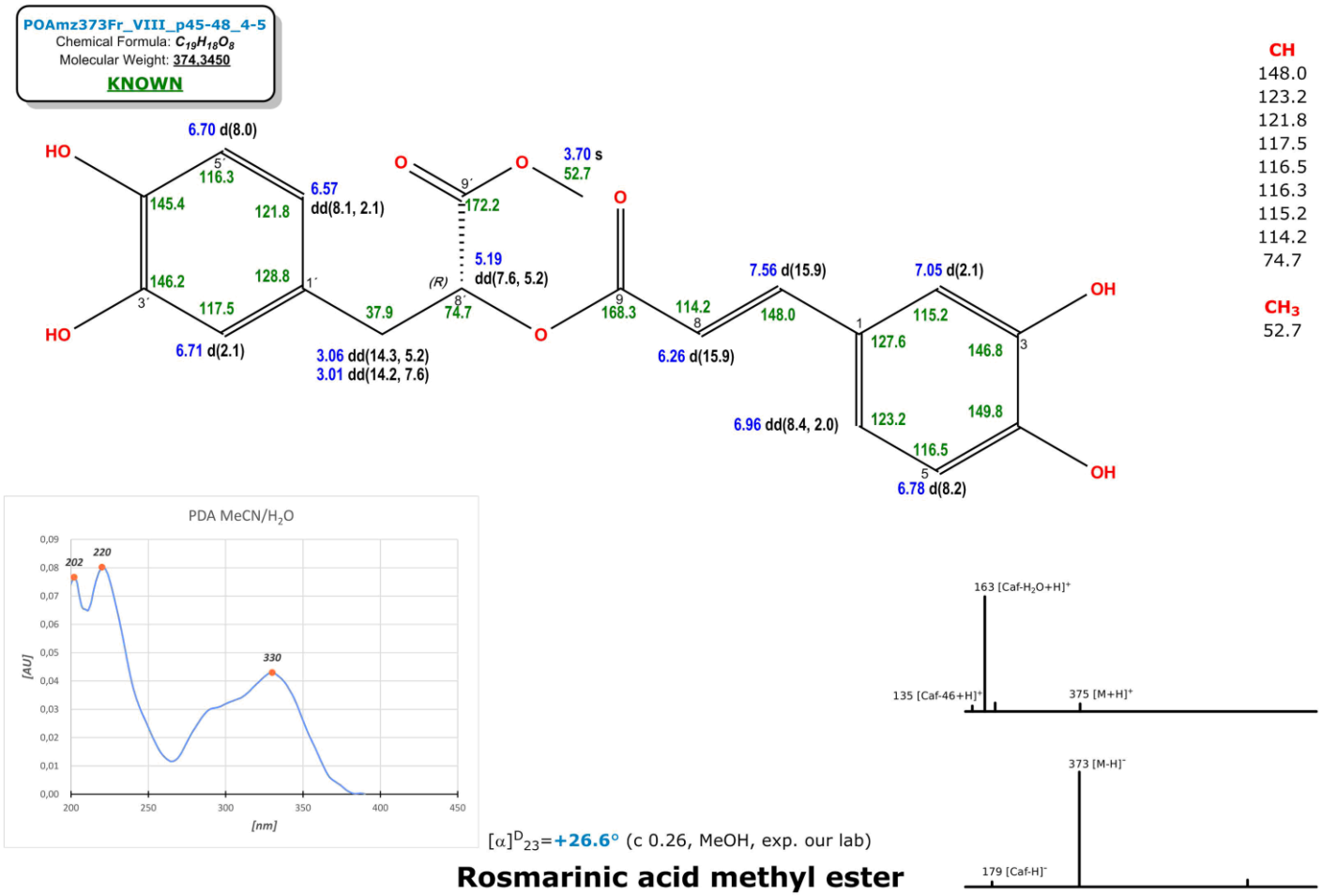
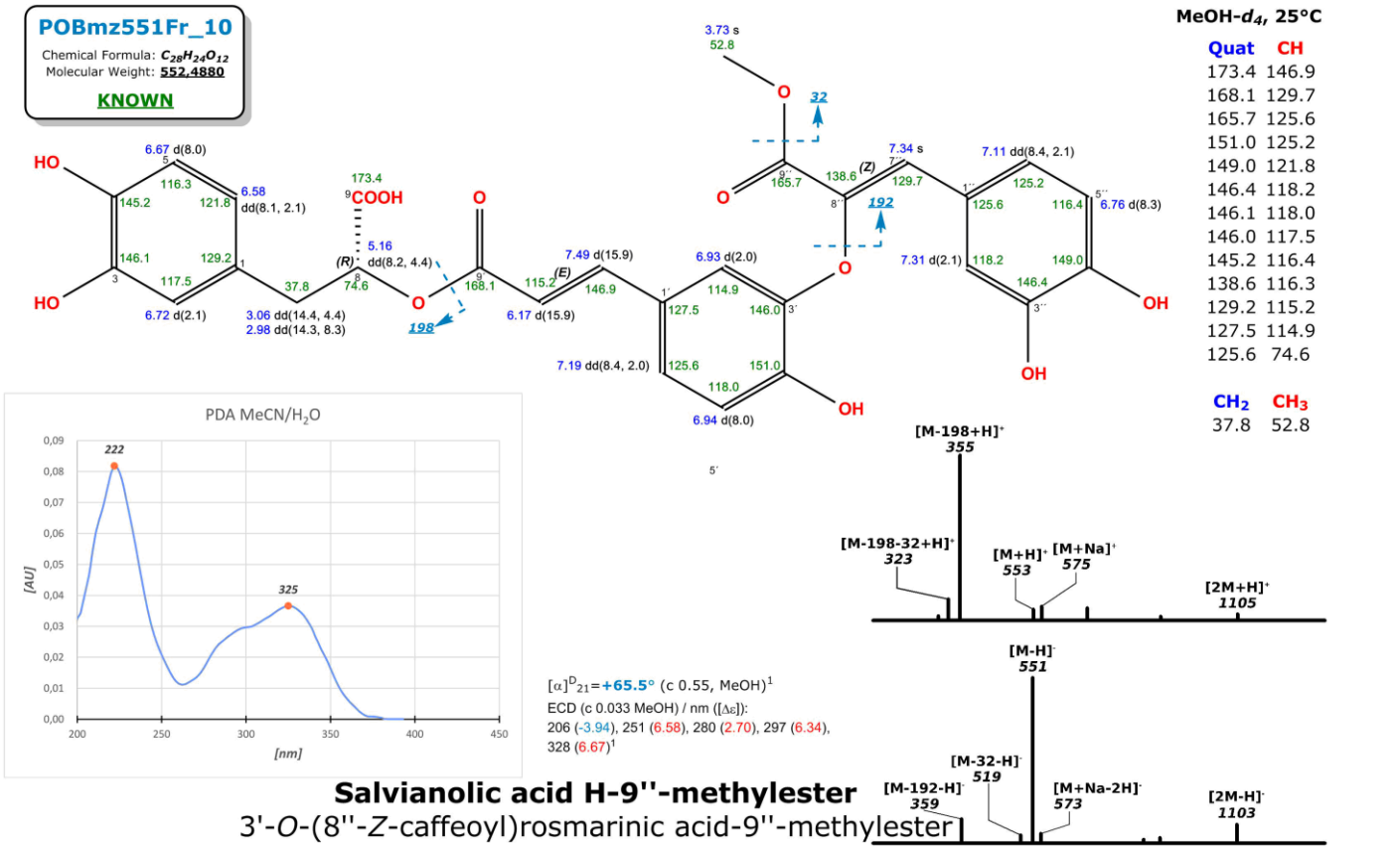


Figure 105S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 43 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$



1.Murata, T., Watahiki, M., Tanaka, Y., Miyase, T., Yoshizaki, F., 2010. Hyaluronidase Inhibitors from Takuran, Lycopus lucidus. Chem. Pharm. Bull. (Tokyo). 58, 394–397. doi:10.1248/cpb.58.394

Figure 106S. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR data of compound 44 in CD_3OD, 25°C; on-line PDA UV spectrum in $MeCN/H_2O$

Table S1.

No.	Compound name	Regression equation	R^2	Calibration range [μg/mL]	LOD [μg/mL]	LOQ [μg/mL]
1	Danshensu	$y=-0.0002x^2+0.0194x+0.0045$	0.9977	0.2-35	0.1	0.4
2	Menisdaurin	$y=-0.0004x^2+0.0374x+0.0067$	0.9987	0.2-35	0.1	0.4
3	3-*O*-(*E*)-caffeoyl-L-threonic acid	$y=-0.0024x^2+0.0577x+0.0053$	0.9995	0.2-12	0.1	0.3
4	2-*O*-(*E*)-caffeoyl-L-threonic acid	$y=-0.0004x^2+0.0400x+0.0074$	0.9989	0.2-35	0.1	0.4
5	Lycoperodine-1	$y=-0.0006x^2+0.0387x+0.0114$	0.9971	0.2-35	0.1	0.4
6	Chlorogenic acid	$y=-0.0109x^2+0.2568x+0.0126$	0.9998	0.2-12	0.1	0.3
7	Actinidioionoside	$y=-0.0013x^2+0.0762x+0.0342$	0.9937	0.2-12	0.1	0.3
8	Caffeic acid	$y=-0.0003x^2+0.0447x+0.0229$	0.9982	0.2-60	0.1	0.3
9	Cryptochlorogenic acid	Calibrated using compound **6** curve.				
10	3'-*O*-(*E*)-Feruoyl-*α*-sorbopyranosyl-(2'→1)-*α*-glucopyranoside	$y=-0.004x^2+0.0902x+0.0113$	0.9988	0.2-12	0.1	0.4
11	2-*O*-(*E*)-caffeoyl-D-glyceric acid	$y=-0.0004x^2+0.0477x+0.021$	0.9979	0.3-60	0.2	0.6
12	4-*O*-(*E*)-caffeoyl-L-threonic acid	$y=-0.005x^2+0.1131x+0.0107$	0.9992	0.2-12	0.1	0.3
13	Neochlorogenic acid	$y=-0.0109x^2+0.2568x+0.0126$	0.9998	0.2-12	0.1	0.3
14	3-*O*-(*E*)-caffeoyl-D-glyceric acid	$y=-0.0006x^2+0.0717x+0.0267$	0.9986	0.2-60	0.1	0.3
15	3-*O*-p-coumaroyl-quinic acid	$y=-0.0015x^2+0.0967x+0.0358$	0.9959	0.2-35	0.1	0.4
16	4-*O*-p-coumaroyl-quinic acid	Calibrated using compound **15** curve.				
17	5-*O*-p-coumaroyl-quinic acid	Calibrated using compound **15** curve.				
18	Globoidnan B	$y=-0.0003x^2+0.0489x+0.0157$	0.9989	0.4-60	0.3	0.9
19	Rutin	$y=-0.0012x^2+0.0739x+0.0261$	0.9948	0.2-35	0.1	0.3
20	Nicotiflorin isomer	Calibrated using compound **24** curve.				
21	Quercetin 3-O-β-glucoside	$y=-0.0064x^2+0.1414x+0.0189$	0.9984	0.2-12	0.1	0.3
22	Yunnaneic acid E	$y=-0.0001x^2+0.0077x-0.001$	0.9984	0.5-60	0.4	1.2
23	Quercetin 3-*O*-(6''-*O*-malonyl)-*β*-glucoside	$y=-0.0004x^2+0.0265x+0.009$	0.9944	0.2-35	0.1	0.3
24	Nicotiflorin	$y=-0.0018x^2+0.1125x+0.0327$	0.9966	0.2-35	0.1	0.4
25	Astragalin	$y=-0.002x^2+0.1069x+0.0483$	0.9933	0.2-35	0.1	0.3
26	Shimobashiric acid C	$y=-0.0001x^2+0.0509x+0.0116$	0.9993	0.3-60	0.2	0.9
27	Rosmarinic acid	$y=-0.0001x^2+0.0509x+0.0116$	0.9993	0.2-12	0.1	0.3
28	Kaempferol 3-*O*-(6''-*O*-malonyl)-*β*-glucoside	$y=-0.0004x^2+0.0284x+0.0073$	0.9968	0.2-35	0.1	0.3
29	Monardic acid A	$y=-0.0001x^2+0.0017x+0.0032$	0.9858	0.5-60	0.5	1.5
30	Yunnaneic acid E-1	Not measured				
31	Lithospermic acid A	$y=-0.0001x^2+0.0095x+0.0059$	0.9997	0.2-60	0.3	0.9
32	Pulmonarioside A	$y=-0.0003x^2+0.0331x+0.0145$	0.9975	0.2-60	0.2	0.6
33	Salvianolic acid H	$y=-0.0005x^2+0.0683x+0.0135$	0.9991	0.2-60	0.1	0.3
34	Lithospermic acid B	Not measured				
35	Pulmonarioside B	$y=-0.0002x^2+0.0291x+0.0105$	0.9982	0.2-60	0.1	0.3
36	Yunnaneic acid B	$y=-0.0001x^2+0.0024x-0.0017$	0.9988	0.2-60	0.1	0.3
37	Globoidnan A	$y=-0.0072x^2+0.1572x+0.0108$	0.9995	0.2-12	0.1	0.3
38	Pulmitric acid A	$y=-0.0128x^2+0.2597x+0.0201$	0.9994	0.2-12	0.1	0.3
39	Pulmitric acid B	$y=-0.0026x^2+0.2597x+0.0201$	0.9954	0.2-35	0.1	0.3
40	Isosalvianolic acid A	$y=-0.0117x^2+0.2729x+0.0298$	0.9986	0.2-12	0.1	0.3
41	Isosalvianolic acid A-1	Calibrated using compound **40** curve.				
42	Isosalvianolic acid A isomer	Calibrated using compound **40** curve.				
43	Rosmarinic acid methyl ester	$y=-0.0154x^2+0.3333x+0.0683$	0.9973	0.2-12	0.1	0.3
44	Salvianolic acid H-9''-methylester	$y=-0.001x^2+0.0691x+0.0125$	0.9984	0.2-35	0.1	0.3
45	Lycopic acid C	Not measured				

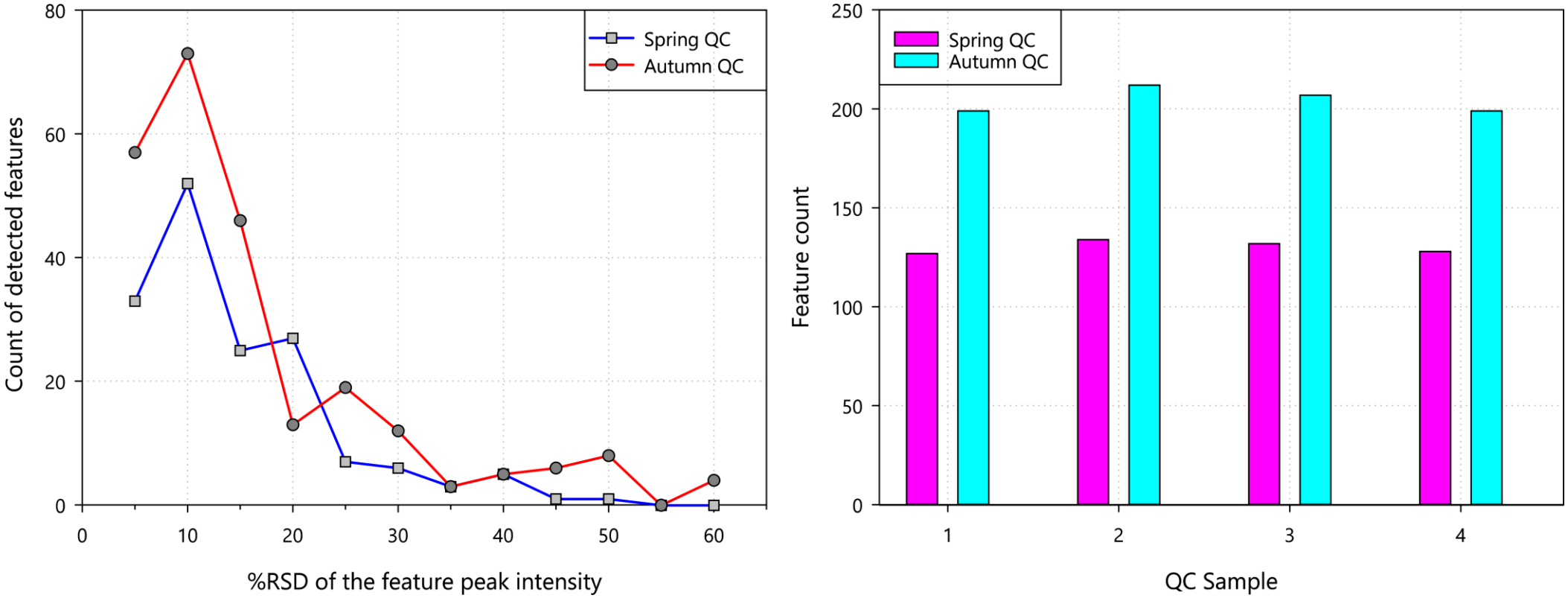


Figure 107S. Frequency distribution of the relative standard deviation for the peak intensities and peak numbers in QC samples