Supplementary Information

Isolation and identification of novel selective antitumor constituents, sidrin and sidroside, from *Zizyphus spina-christi*.

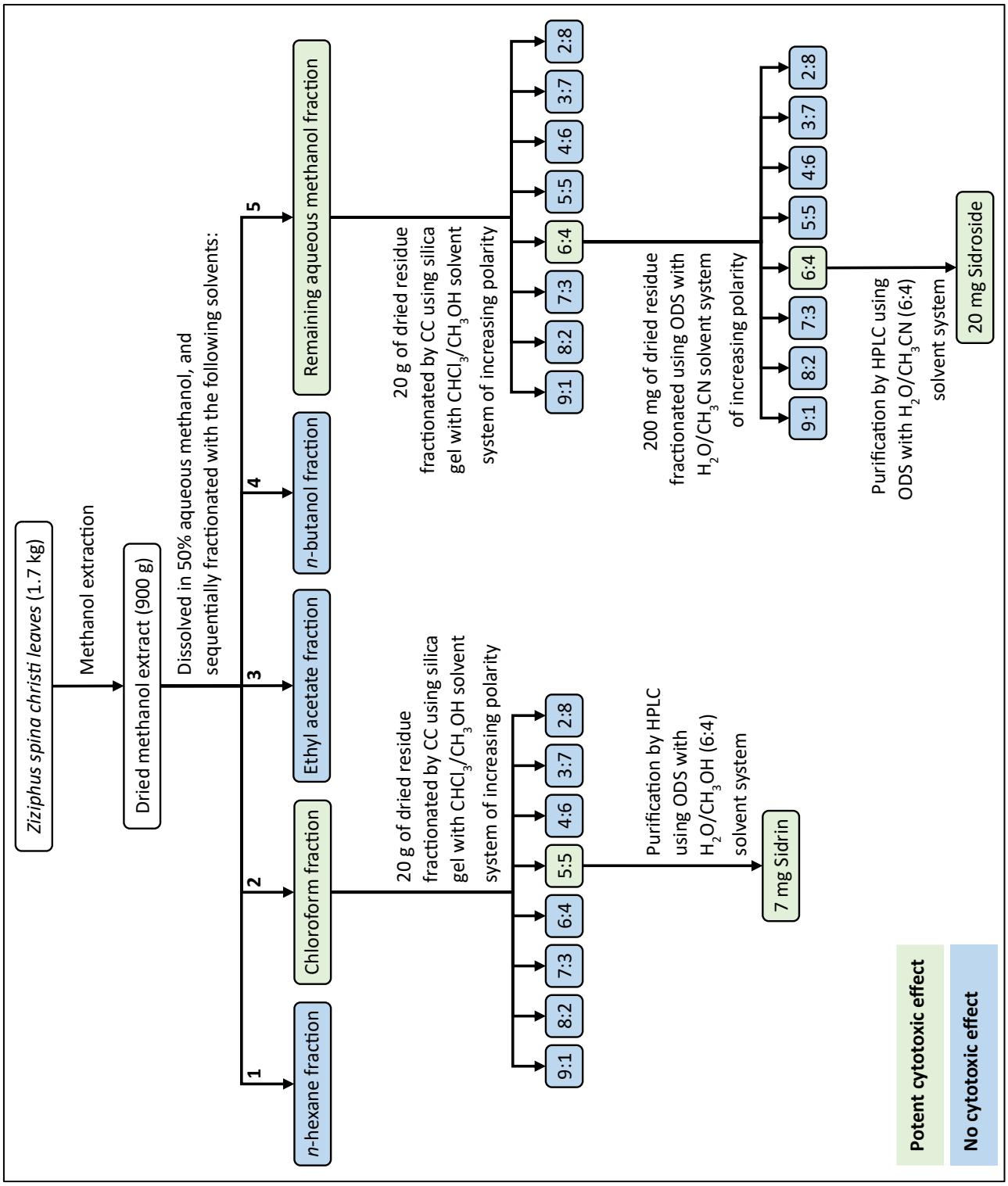


Figure 1s. Extraction and isolation scheme of sidrin and sidroside. ***CC***, column chromatography; ***HPLC***, High-performance liquid chromatography; ***ODS***, octadecylsilane.

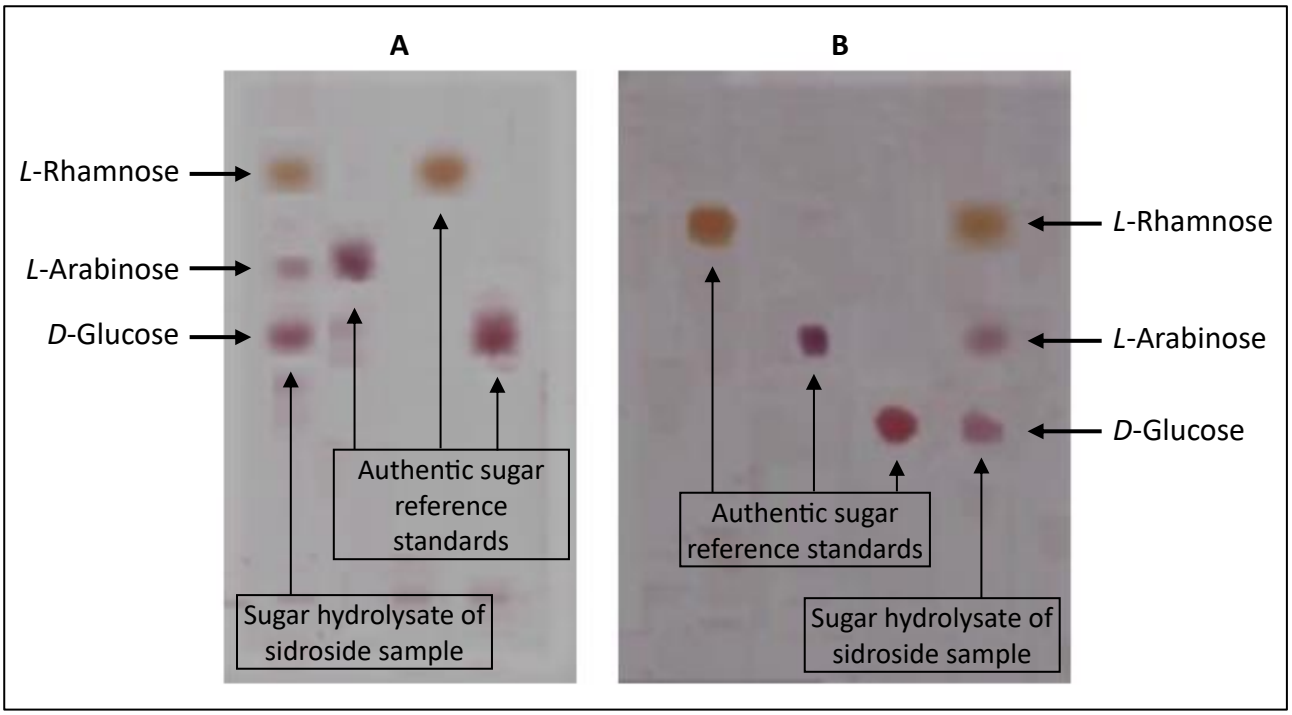


Figure 2s. Thin-layer chromatograms of sugar hydrolysate of sidroside with standard sugars. ***A.*** Using $CHCl_3$:CH_3OH:H_2O (65:40:20); ***B.*** Using CH_3CN:H_2O (17:3). Retention factors for *L*-arabinose, *L*-Rhamnose, and *D*-glucose are 0.50, 0.60, and 0.41, respectively.

Sample: T205-2-2-4-1 Matrix: Glycerol
Instrument: SX102A
Inlet: Reservoir Ionization mode: FAB-

Scan: 23 R.T.: 6.2
Base: m/z 455; 69.9%FS TIC: 26088379 #Intensities: 7249
No.220

Selected Isotopes : $H_{0-47}C_{0-31}O_{0-4}$ Error Limit : 100 mmu

Measured Mass	% Base	Formula	Calculated Mass	Error
483.34784	1.6%	$C_{31}H_{47}O_4$	483.34744	0.4

Figure 3s. Negative high resolution FAB-MS spectrum of sidrin.

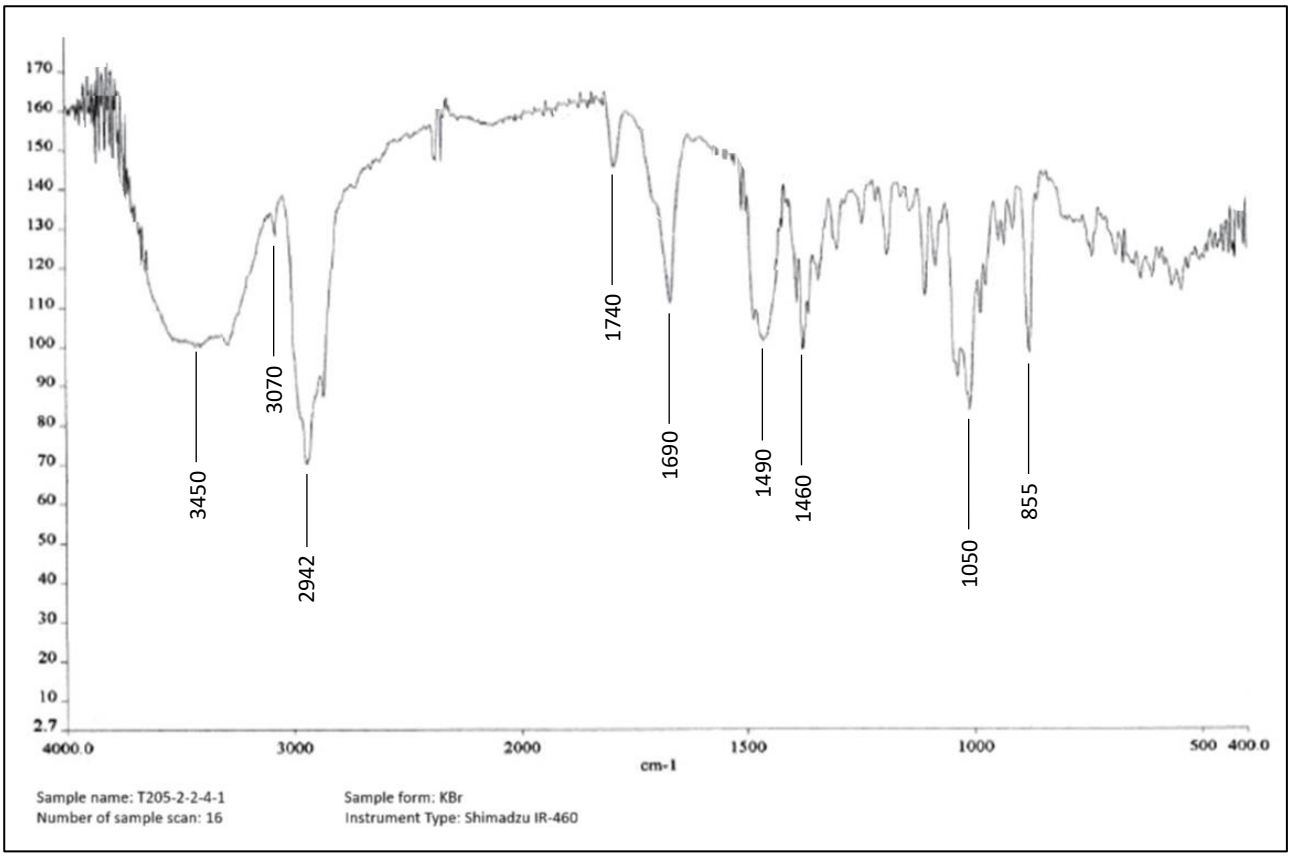


Figure 4s. Infrared spectrum of sidrin.

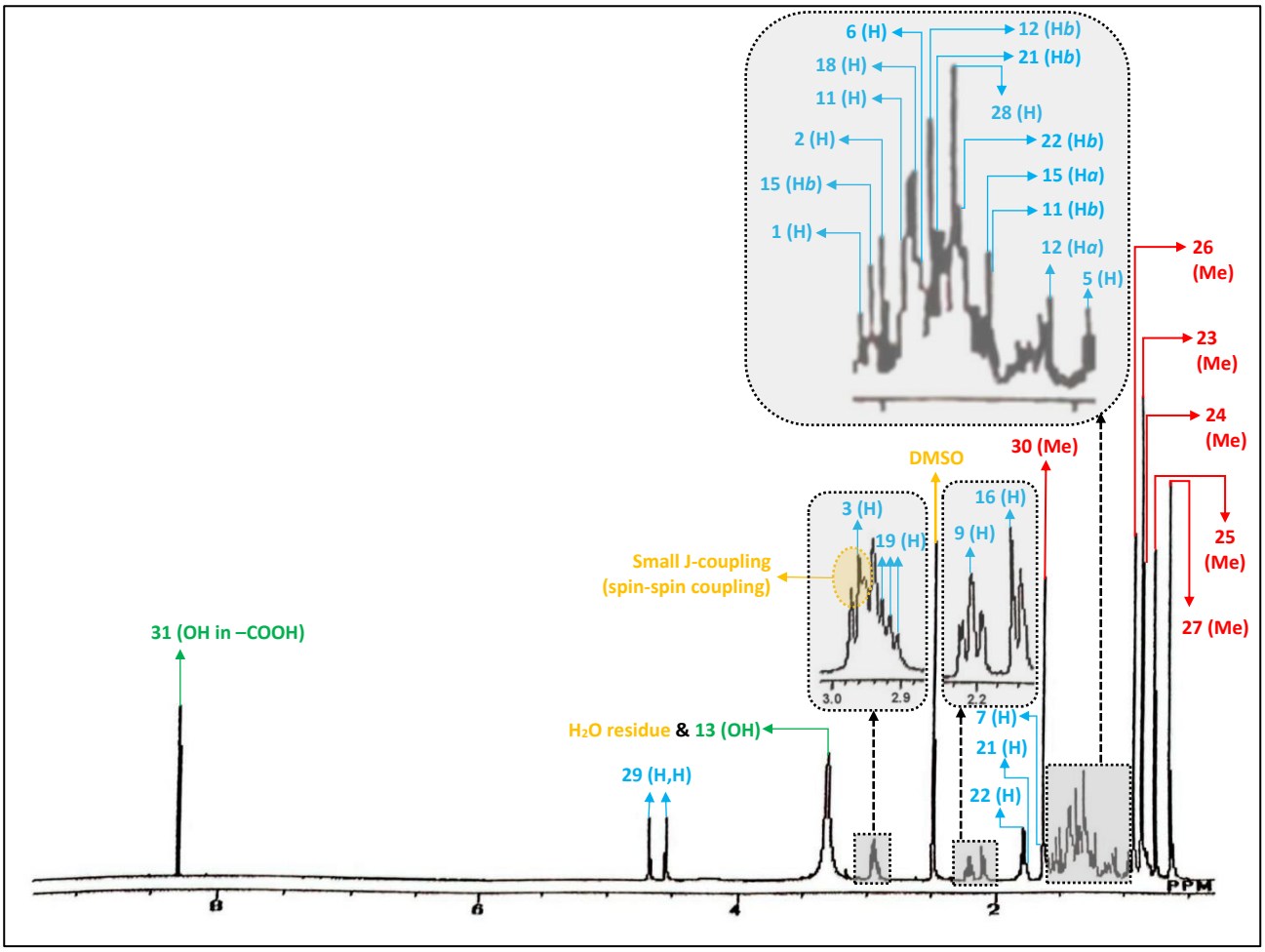


Figure 5s. ^{1}H-NMR (500 MHz, DMSO-d_6) spectrum of sidrin (13-β-hydroxy-lup-20(30)-ene-2,3-β-epoxy-28- carboxylate). ***a***, alpha; ***b***, beta; ***DMSO***, dimethyl sulfoxide; ***H,*** hydrogen proton bonded to the related carbon atom; ***Me***, methyl group bonded to the related carbon atom; ***n***, carbon atom numbers; ***OH***, hydroxyl group bonded to the related carbon atom.

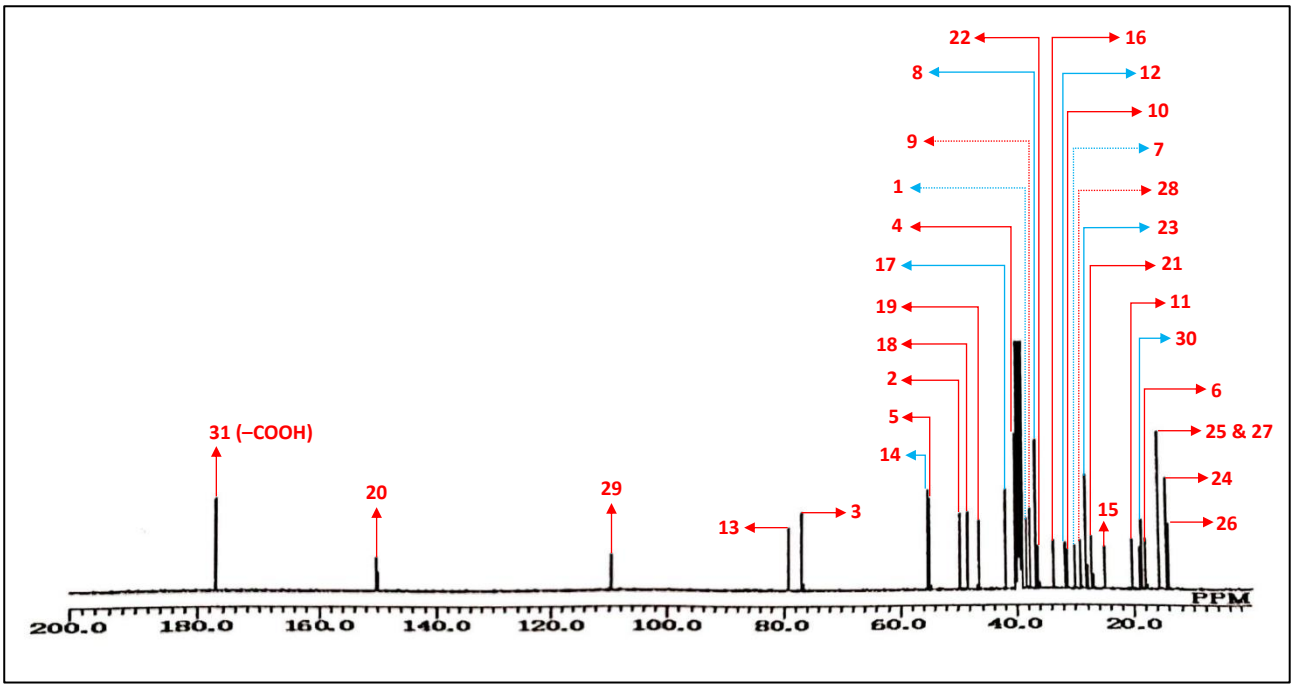


Figure 6s. ^{13}C-NMR (125 MHz, DMSO-d_6) spectrum of sidrin showing the number of each carbon atom.

Note: Arrow colors and styles have no specific indication other than tracking facilitation.

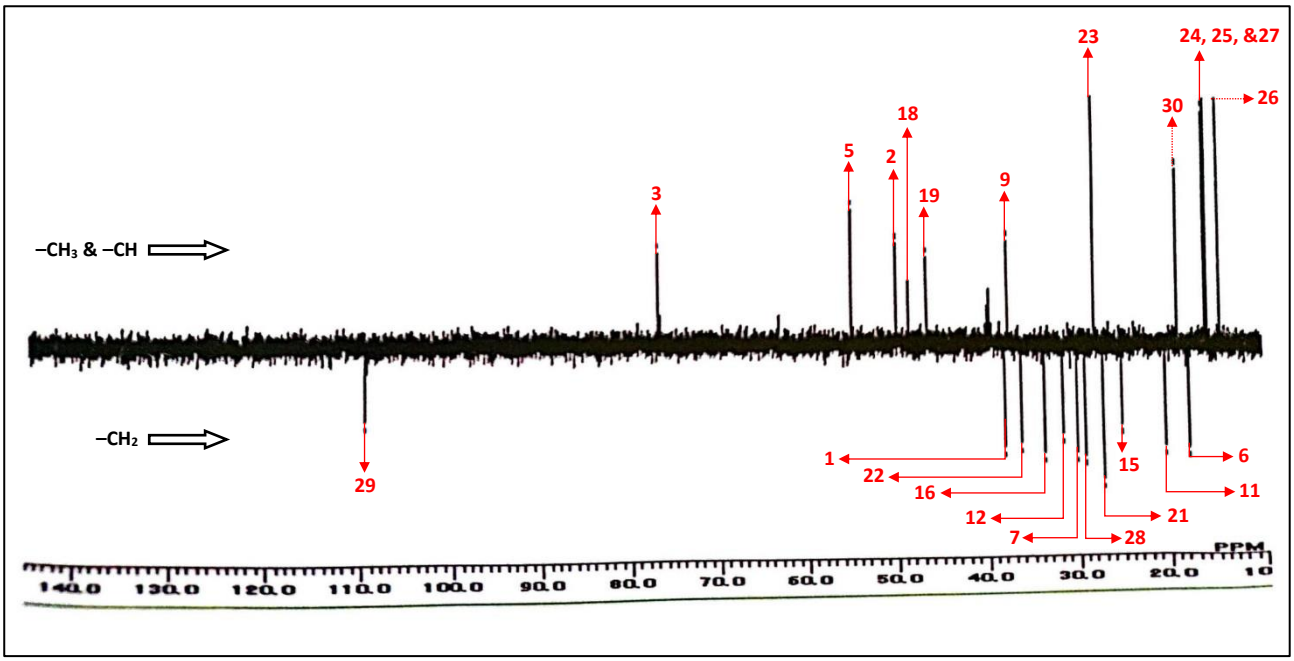


Figure 7s. DEPT 135 (125 MHz, DMSO-d_6) spectrum of sidrin showing the related numbers of all protonated carbon atoms.

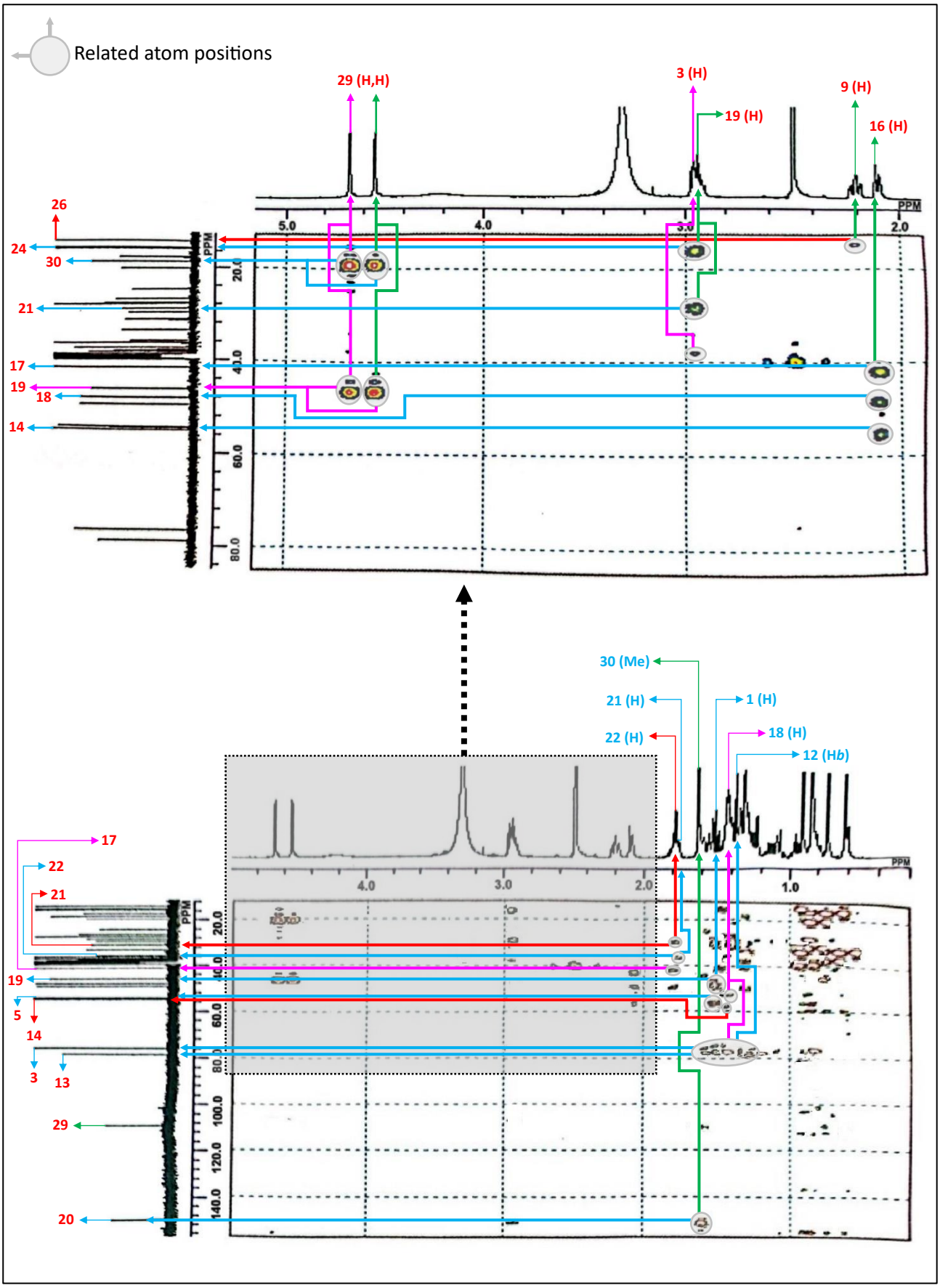


Figure 8s. HMBC spectrum of sidrin. ***H***, hydrogen proton bonded to the related carbon atom; ***n***, the number of the related carbon atom.

Note: Arrow colors and styles have no specific indication other than tracking facilitation.

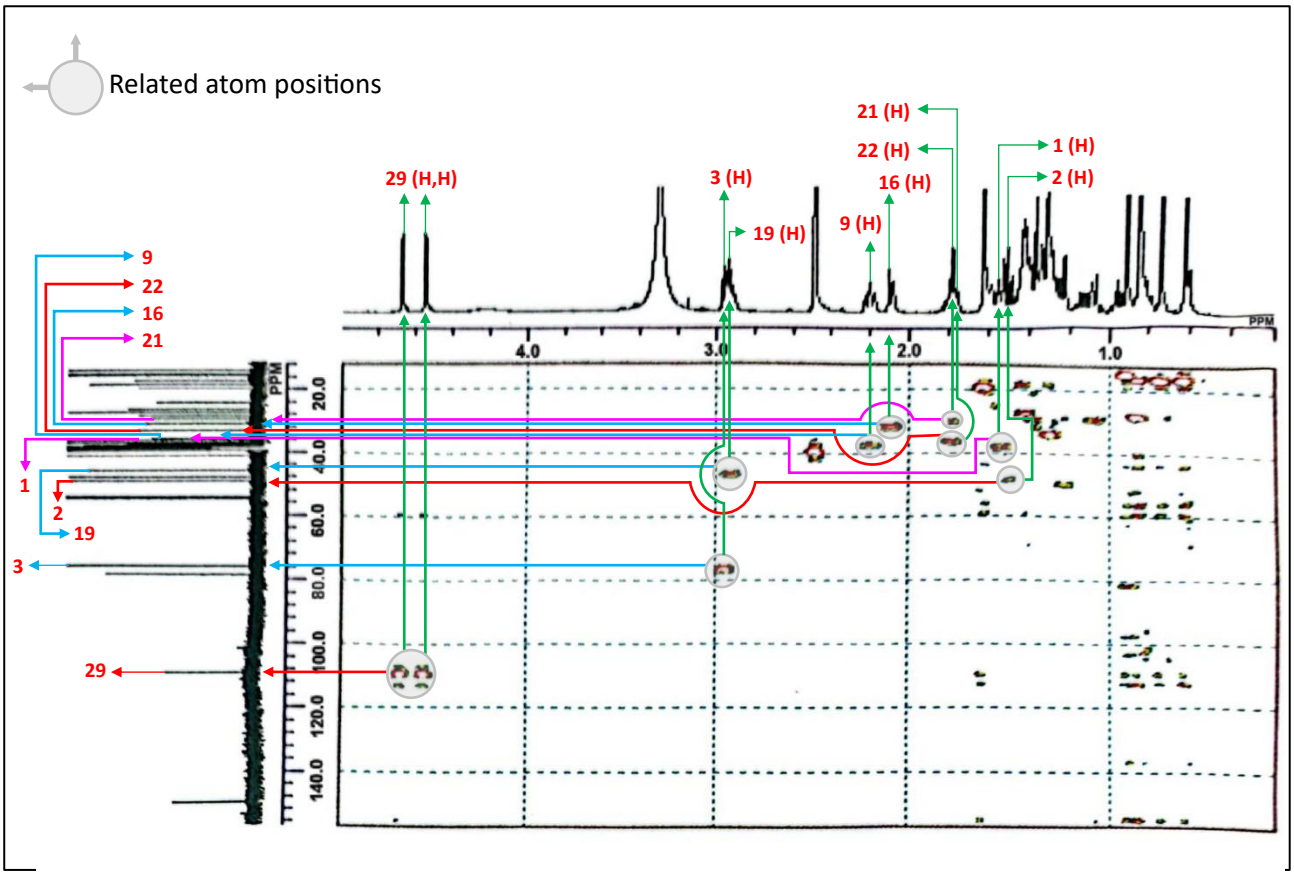


Figure 9s. HMQC spectrum of Sidrin. ***H***, hydrogen proton bonded to the related carbon atom; ***n***, the number of the related carbon atom.

Note: Arrow colors and styles have no specific indication other than tracking facilitation.

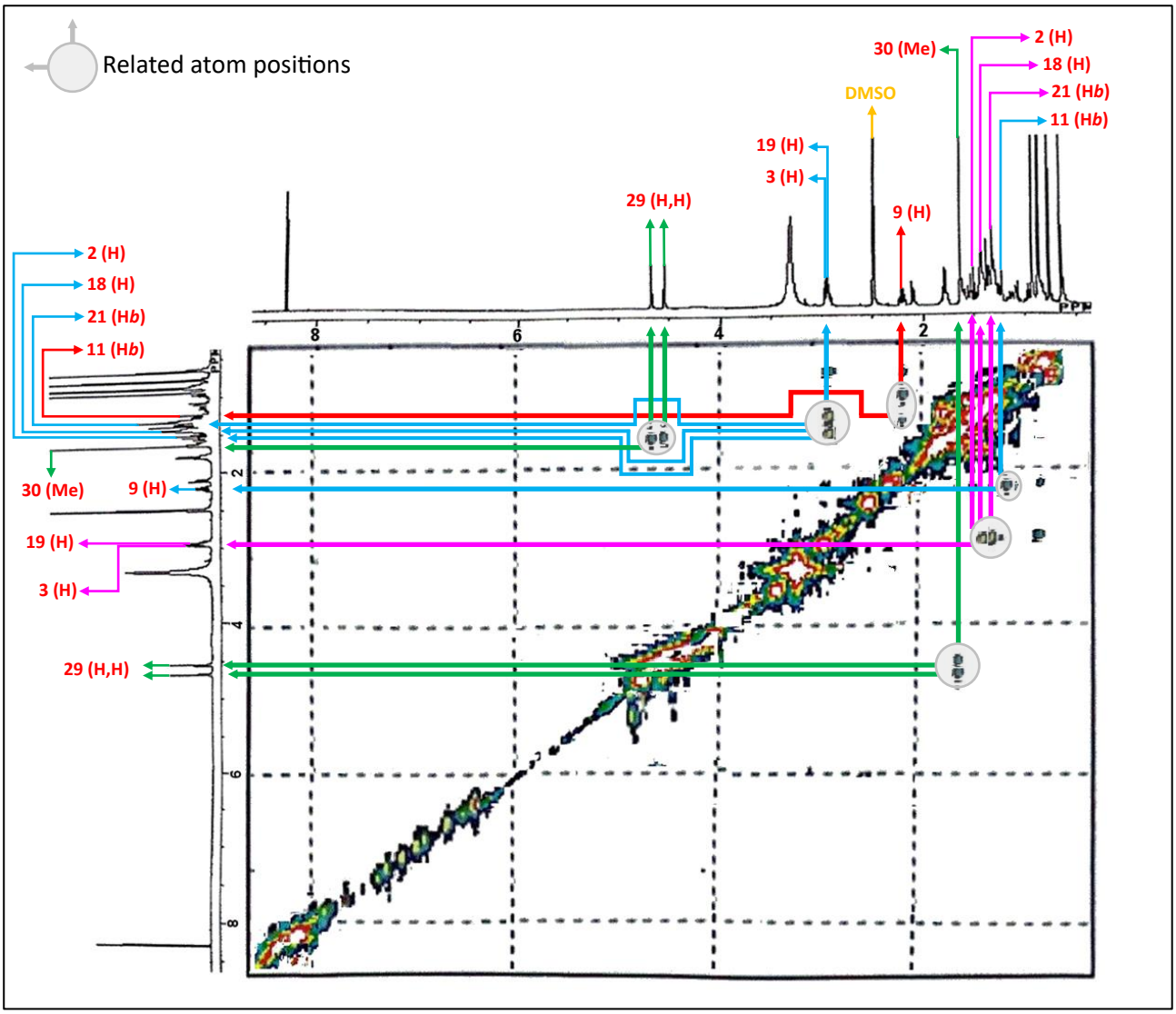


Figure 10s. ^{1}H-^{1}H COSY spectrum of sidrin. ***b***, beta; ***DMSO***, dimethyl sulfoxide; ***H***, hydrogen proton bonded to the related carbon atom; ***Me***, methyl group bonded to the related carbon atom; ***n***, the number of the related carbon atom.

Note: Arrow colors and styles have no specific indication other than tracking facilitation.

Sample: T205-2-8-20-7-8 Matrix: Glycerol
Instrument: SX102A
Inlet: Reservoir

Ionization mode: FAB+

Scan: 116

R.T.: 14.5

Base: m/z 941; .2%FS TIC: 316185

#Intensities: 148

No.465

Selected Isotopes : $H_{0-77}C_{0-47}O_{0-17}$

Error Limit : 100 mmu

Measured Mass	*% Base*	*Formula*	*Calculated Mass*	*Error*
913.51574	36.3%	$C_{47}H_{77}O_{17}$	913.51603	-0.3

Figure 11s. Positive high resolution FAB-MS spectrum of sidroside.

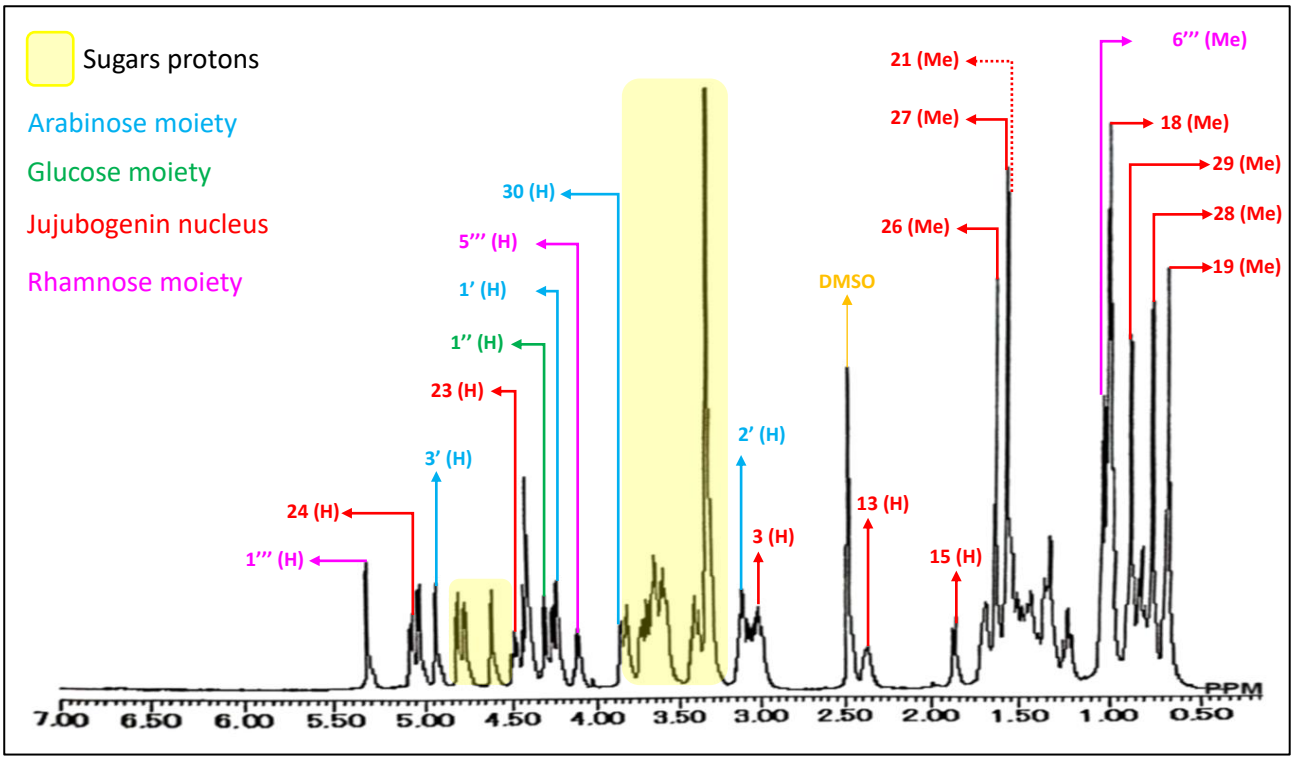


Figure 12s. ^{1}H-NMR (500 MHz, DMSO-d_6) spectrum of sidroside (3-*O*-β-D-glucopyranosyl-(1-3)-α-L-arabinopyranosyl-jujubogenin-20-*O*-α-L-rhamnopyranoside). ***DMSO***, dimethyl sulfoxide; ***H***, hydrogen proton bonded to the related carbon atom; ***Me***, methyl group bonded to the related carbon atom; ***n***, the number of the related carbon atom in the jujubogenin nucleus; ***n'***, the number of the carbon atom in arabinose moiety; ***n''***, the number of the carbon atom in glucose moiety; ***n'''***, the number of the carbon atom in rhamnose moiety.

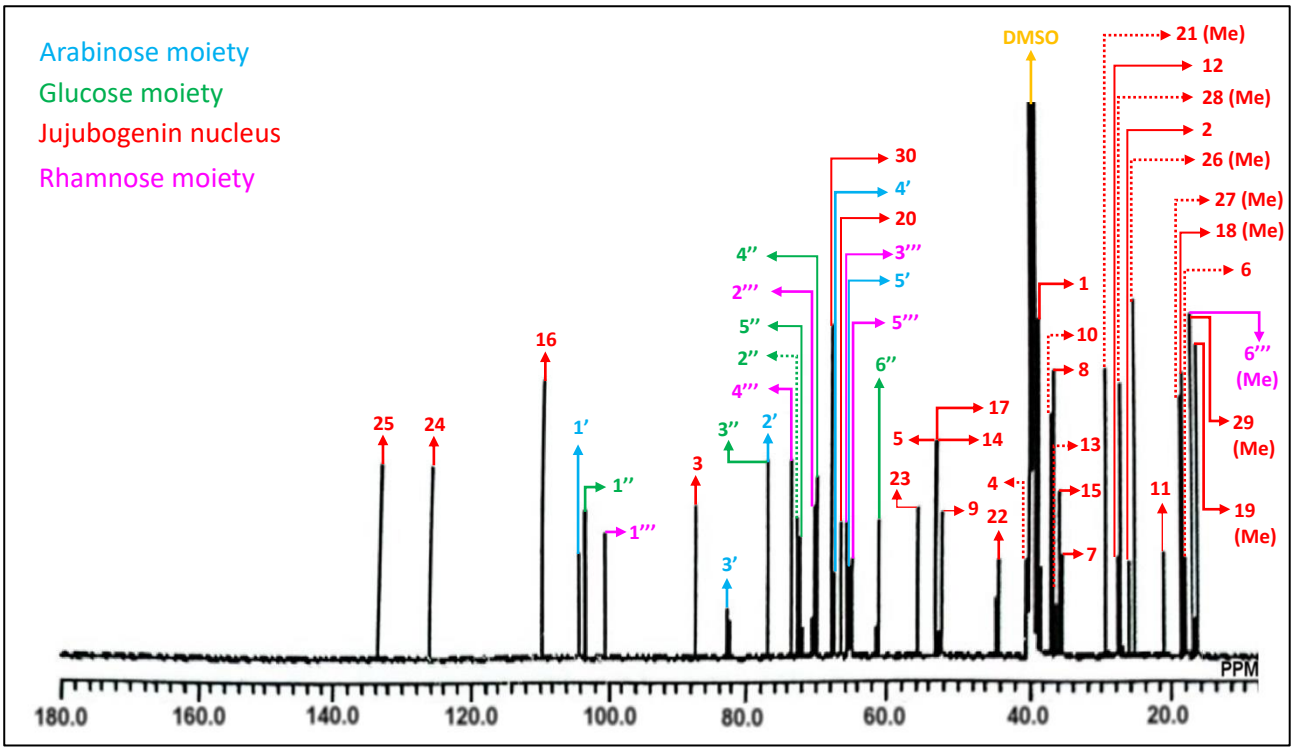


Figure 13s. ^{13}C-NMR (125 MHz, DMSO-d_6) spectrum of sidroside. ***DMSO***, dimethyl sulfoxide; ***Me***, methyl group bonded to the related carbon atom; ***n***, the number of the carbon atom in the jujubogenin nucleus; ***n'***, the number of the carbon atom in arabinose moiety; ***n''***, the number of the carbon atom in glucose moiety; ***n'''***, the number of the carbon atom in rhamnose moiety.

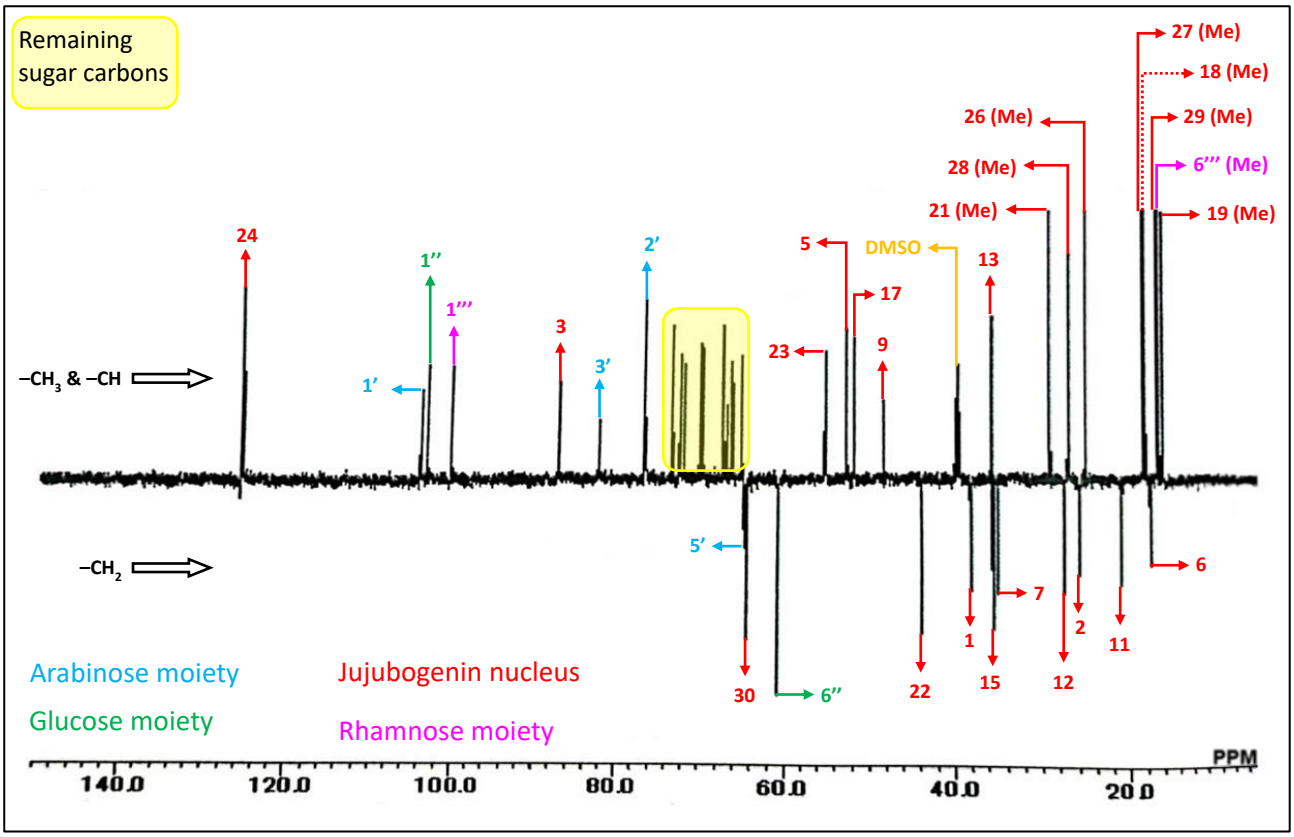


Figure 14s. DEPT 135 (125 MHz, DMSO-d_6) spectrum of sidroside. ***DMSO***, dimethyl sulfoxide; ***Me***, methyl group bonded to the related carbon atom; ***n***, the number of the carbon atom in the jujubogenin nucleus; ***n'***, the number of the carbon atom in arabinose moiety; ***n''***, the number of the carbon atom in glucose moiety; ***n'''***, the number of the carbon atom in rhamnose moiety.

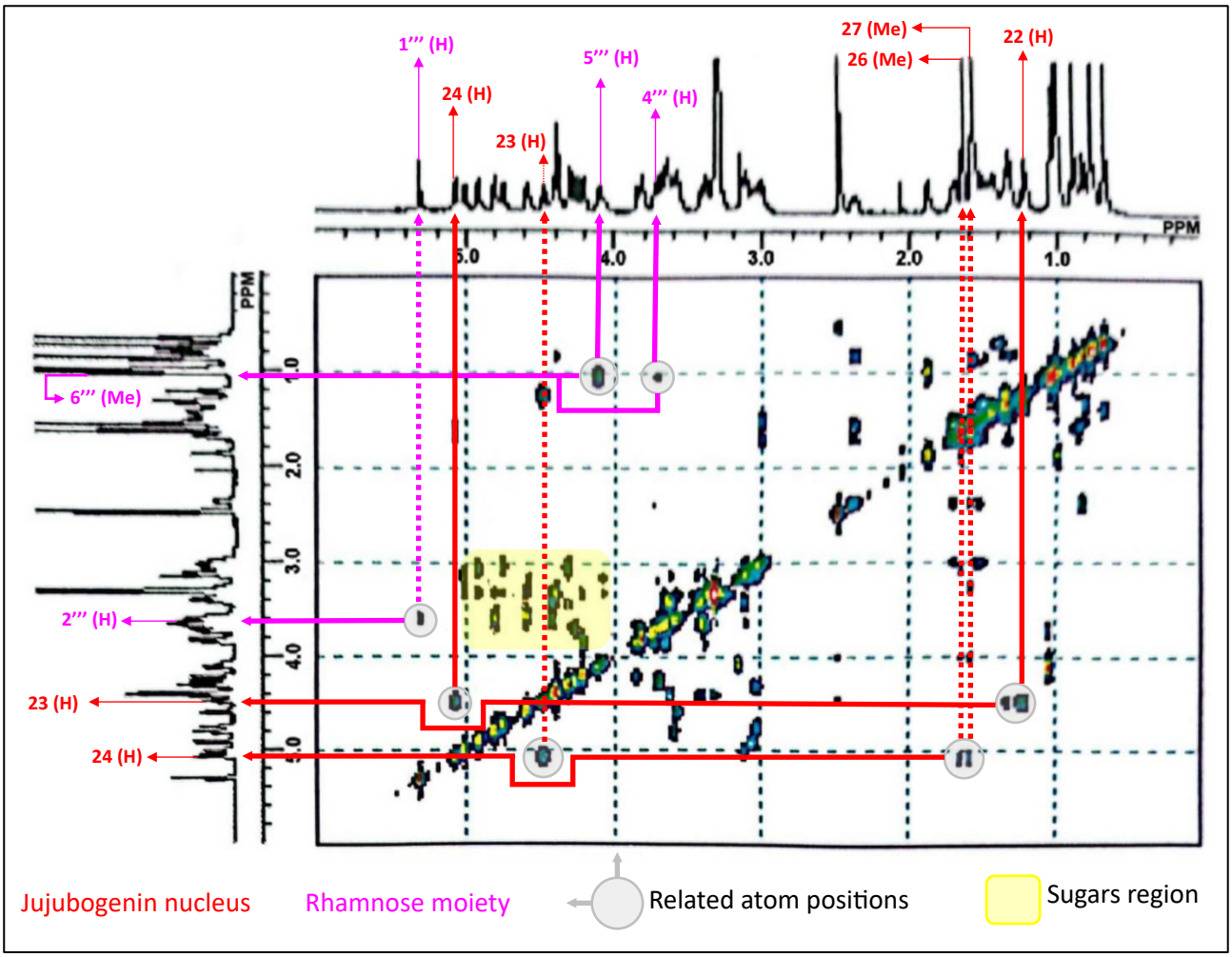


Figure 15s. ^{1}H-^{1}H COSY spectrum of sidroside. ***H***, hydrogen proton bonded to the related carbon atom; ***Me***, methyl group bonded to the related carbon atom; ***n***, the number of the carbon atom in the jujubogenin nucleus; ***n'''***, the number of carbon atom in rhamnose moiety.

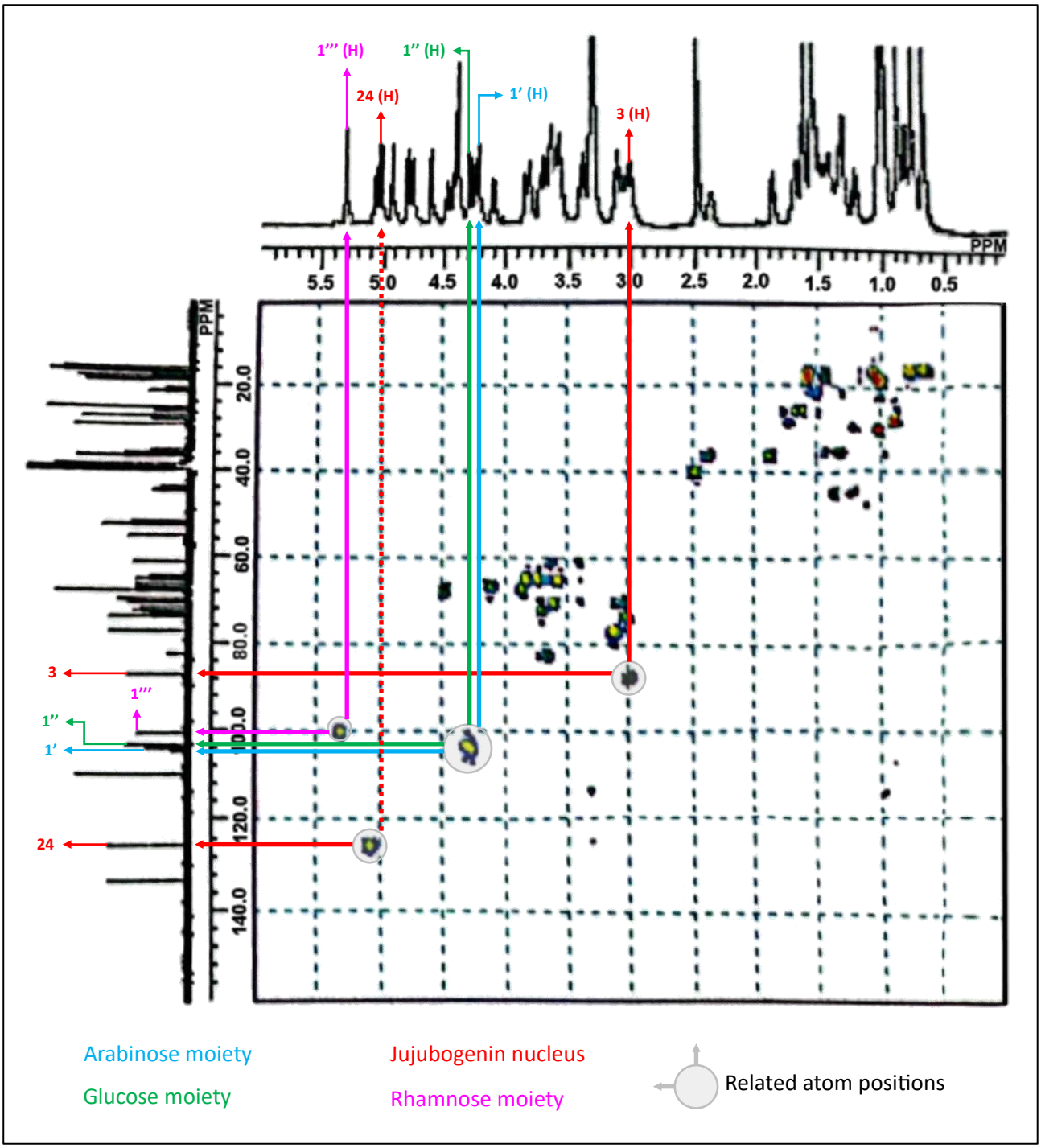


Figure 16s. HMQC spectrum of sidroside. ***H***, hydrogen proton bonded to the related carbon atom; ***n***, the number of the carbon atom in the jujubogenin nucleus; ***n'***, the number of the carbon atom in arabinose moiety; ***n''***, the number of the carbon atom in glucose moiety; ***n'''***, the number of the carbon atom in rhamnose moiety.

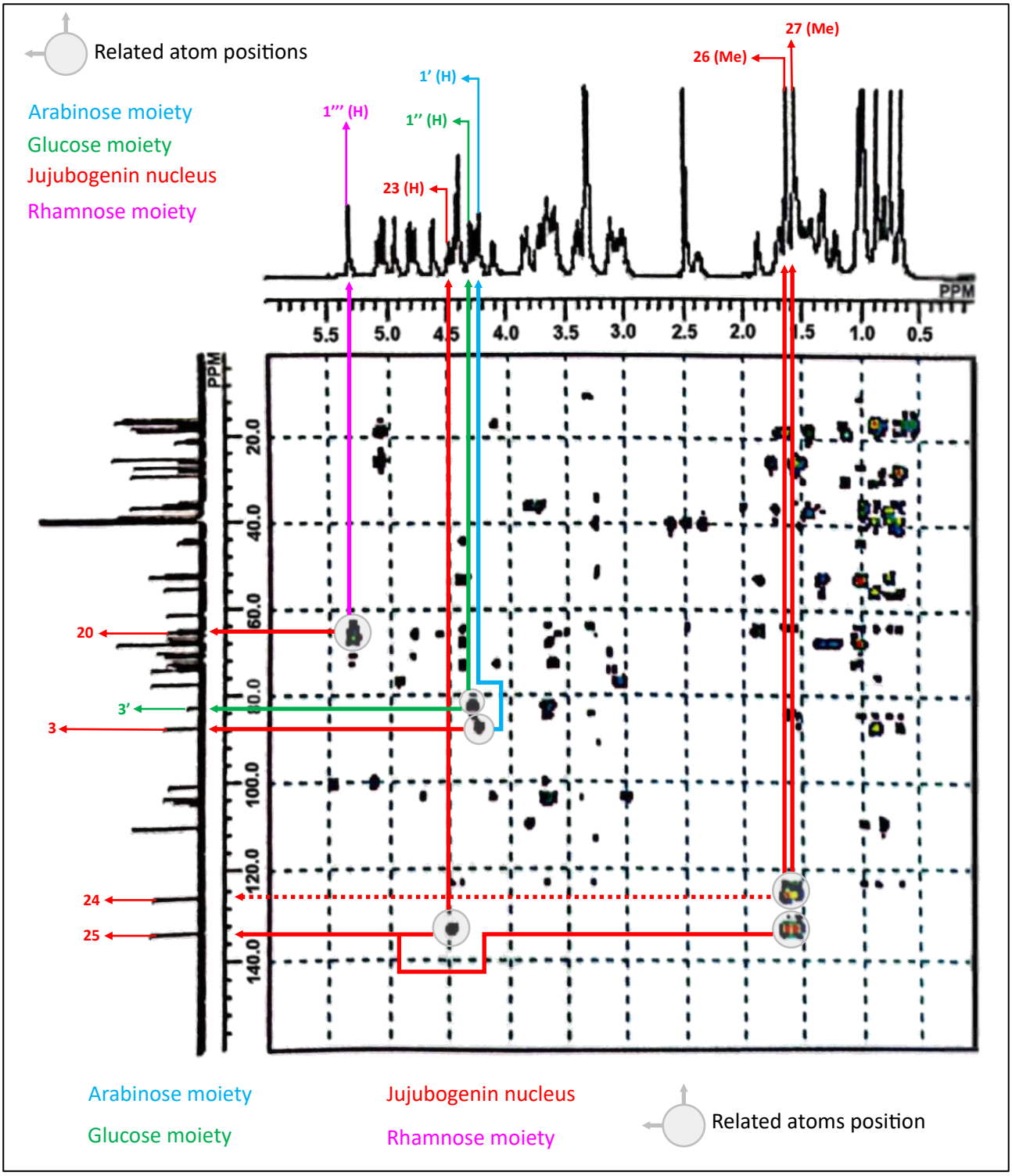


Figure 17s. HMBC spectrum of sidroside. ***H***, hydrogen proton bonded to the related carbon atom; ***Me***, methyl group bonded to the related carbon atom; ***n***, the number of the carbon atom in the jujubogenin nucleus; ***n'***, the number of the carbon atom in arabinose moiety; ***n''***, the number of the carbon atom in glucose moiety; ***n'''***, the number of the carbon atom in rhamnose moiety.

Table 1s. The cytotoxicity of sidrin against the 60 human cancer cell lines performed at the National Cancer Institute (USA).

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-750102 / 1 **Conc:** 1.00E-5 Molar

Experiment ID: 0904OS90

Panel/Cell Line	Growth Percent
Leukemia	
HL-60(TB)	72.10
K-562	71.94
MOLT-4	95.01
RPMI-8226	81.28
Non-Small Cell Lung Cancer	
A549/ATCC	74.23
EKVX	76.38
HOP-62	91.55
HOP-92	98.79
NCI-H226	89.63
NCI-H23	82.49
NCI-H322M	95.62
NCI-H460	89.48
NCI-H522	78.03
Colon Cancer	
COLO 205	112.64
HCC-2998	84.25
HCT-116	83.34
HCT-15	93.76
HT29	103.13
KM12	81.14
SW-620	107.85
CNS Cancer	
SF-268	102.35
SF-295	85.26
SF-539	93.86
SNB-19	103.20
SNB-75	100.59
U251	94.51
Melanoma	
LOX IMVI	99.82
MALME-3M	99.89
M14	86.46
MDA-MB-435	99.79
SK-MEL-2	97.89
SK-MEL-28	118.66
SK-MEL-5	84.82
UACC-257	89.88
UACC-62	80.41
Ovarian Cancer	
IGROV1	97.94
OVCAR-3	114.47
OVCAR-4	97.78
OVCAR-5	93.95
OVCAR-8	88.89
NCI/ADR-RES	91.06
SK-OV-3	90.10
Renal Cancer	
786-0	87.27
A498	125.42
ACHN	94.84
CAKI-1	80.91
RXF 393	101.42
SN12C	83.26
TK-10	108.80
UO-31	77.92
Prostate Cancer	
PC-3	80.56
DU-145	113.16
Breast Cancer	
MCF7	95.29
MDA-MB-231/ATCC	85.10
HS 578T	110.36
BT-549	66.72
T-47D	76.32
MDA-MB-468	92.46
Mean	92.31
Delta	25.59
Range	58.70

Mean Growth Percent - Growth Percent

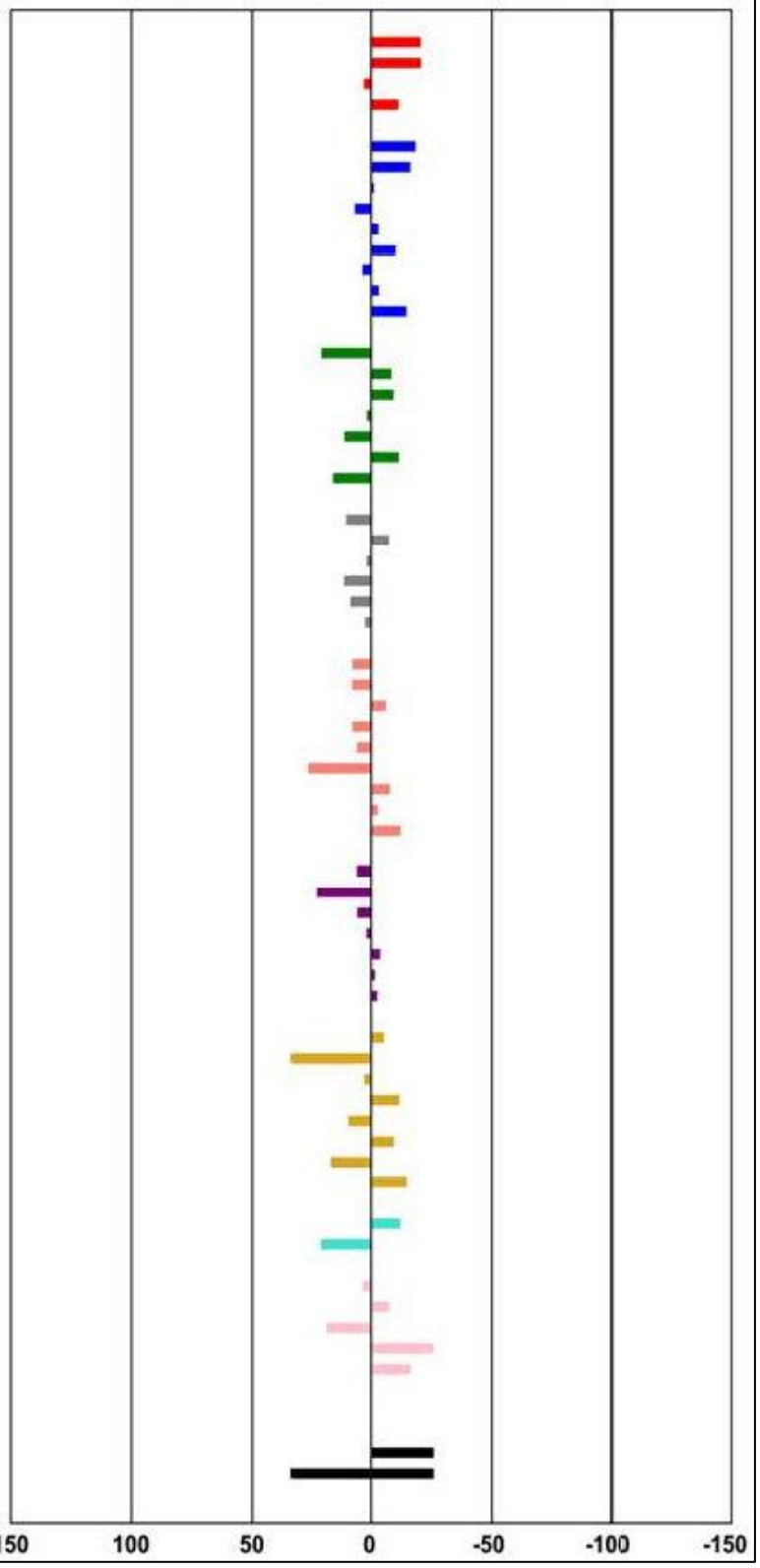


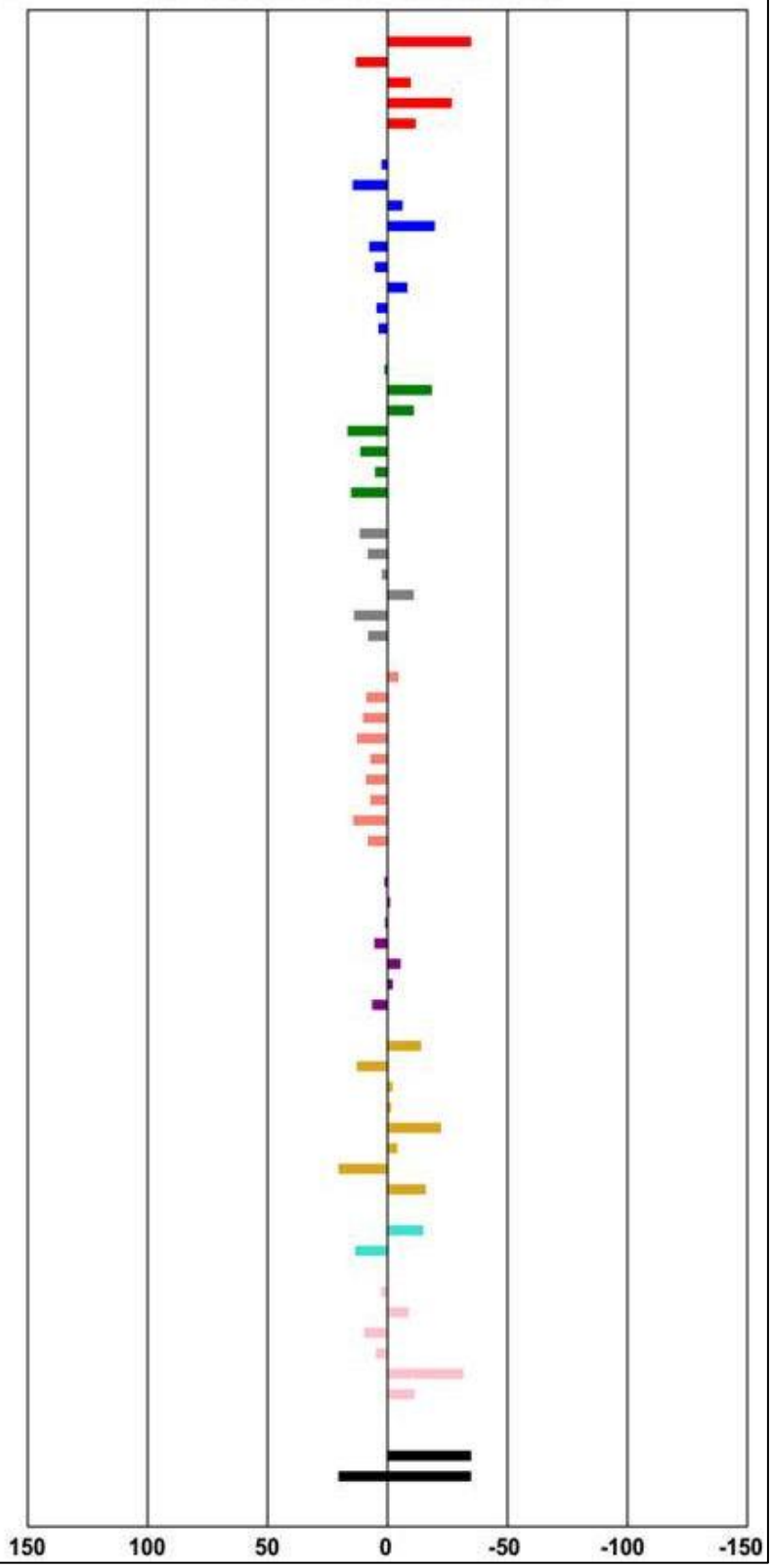
Table 2s. The cytotoxicity of sidroside against the 60 human cancer cell lines performed at the National Cancer Institute (USA).

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-750103 / 1 | **Conc:** 1.00E-5 Molar

Experiment ID: 0904OS90

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	52.60
HL-60(TB)	100.00
K-562	77.83
MOLT-4	60.67
RPMI-8226	75.75
Non-Small Cell Lung Cancer	
A549/ATCC	89.25
EKVX	101.31
HOP-62	81.21
HOP-92	67.67
NCI-H226	94.42
NCI-H23	92.10
NCI-H322M	79.14
NCI-H460	91.36
NCI-H522	90.54
Colon Cancer	
COLO 205	87.96
HCC-2998	68.94
HCT-116	76.44
HCT-15	103.49
HT29	98.16
KM12	92.02
SW-620	101.98
CNS Cancer	
SF-268	98.37
SF-295	95.06
SF-539	89.15
SNB-19	76.53
SNB-75	100.75
U251	94.94
Melanoma	
LOX IMVI	82.87
MALME-3M	95.68
M14	96.99
MDA-MB-435	99.56
SK-MEL-2	93.98
SK-MEL-28	95.86
SK-MEL-5	93.94
UACC-257	101.15
UACC-62	95.07
Ovarian Cancer	
IGROV1	87.98
OVCAR-3	86.36
OVCAR-4	87.82
OVCAR-5	92.28
OVCAR-8	82.04
NCI/ADR-RES	85.22
SK-OV-3	93.23
Renal Cancer	
786-0	73.38
A498	99.58
ACHN	85.35
CAKI-1	85.89
RXF 393	65.11
SN12C	83.43
TK-10	107.22
UO-31	71.48
Prostate Cancer	
PC-3	72.45
DU-145	100.27
Breast Cancer	
MCF7	89.46
MDA-MB-231/ATCC	78.51
HS 578T	96.54
BT-549	91.69
T-47D	55.70
MDA-MB-468	76.16
Mean	87.12
Delta	34.52
Range	54.62

Mean Growth Percent - Growth Percent