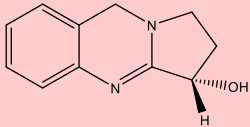
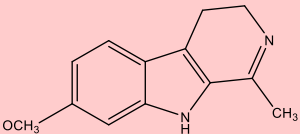
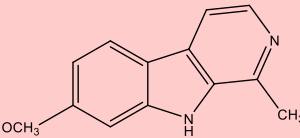
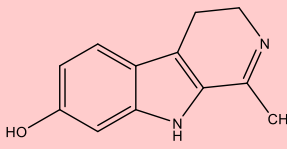
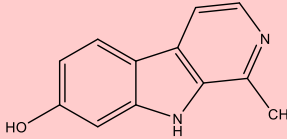
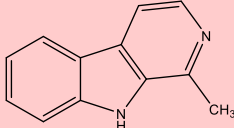
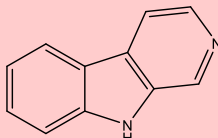
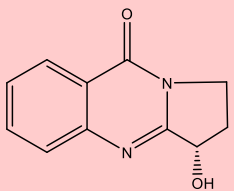
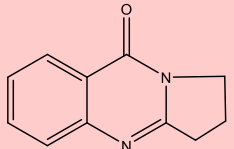


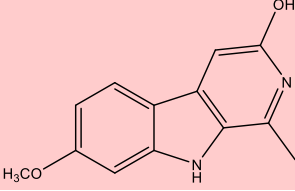

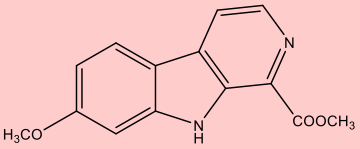
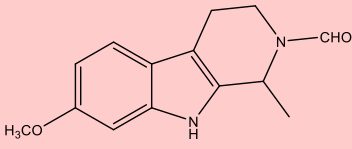
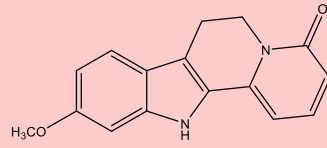
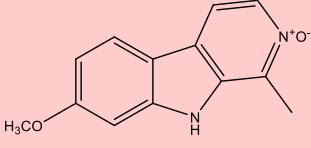
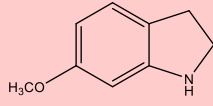
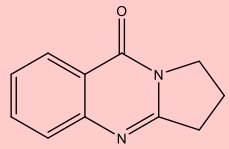
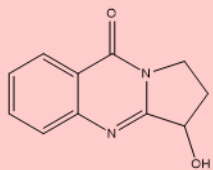
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala*

Compound name	Extracted from	Structures	References
3-Hydroxy-1,2,3,9-tetrahydro-pyrrolo-[2,1-b]quinazolin-4-ium chloride dihydrate	Leaf		Kan et al., 2009
Harmaline	Seed		Astulla et al., 2008; Tascón et al., 2016
Harmine	Aerial parts; seed		Astulla et al., 2008; Tascón et al., 2016; Zhang et al., 2022
Harmalol	Seed		Tascón et al., 2016
Harmol	Seed		Tascón et al., 2016
Harmane	Seed		Tascón et al., 2016
Horharmane	Aerial parts; seed		Tascón et al., 2016; Zhang et al., 2022
(S)-Vasicinone	Aerial parts; seed		Astulla et al., 2008; Zhang et al., 2022
Deoxyvasicinone	Aerial parts; seed		Astulla et al., 2008; Zhang et al., 2022

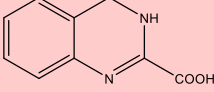
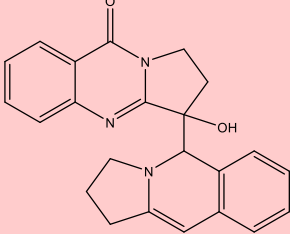
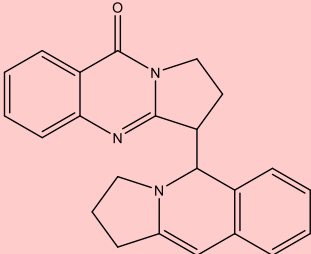
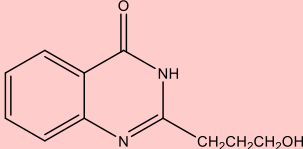
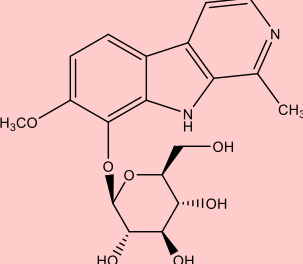
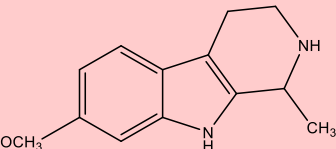
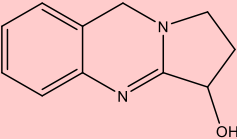
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
3-Hydroxylated harmine	Seed		Yang et al., 2015
Acetylnorharmine	Seed		Yang et al., 2015
Harmic acid methy ester	Seed		Yang et al., 2015
2-Aldehyde-tetrahydroharmine	Seed		Yang et al., 2015
Harmalanine	Seed		Yang et al., 2015
Harmine N-oxide	Seed		Yang et al., 2015
6-Methoxyindoline	Seed		Yang et al., 2015
Dexyvasicinone	Seed		Yang et al., 2015
Vasicinone	Seed		Yang et al., 2015

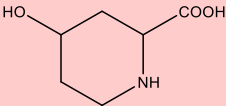
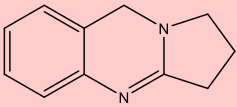
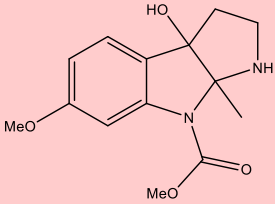
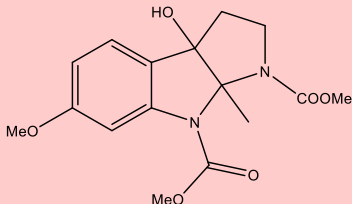
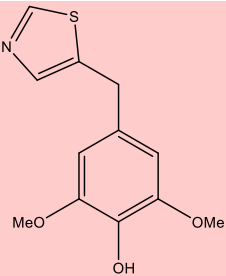
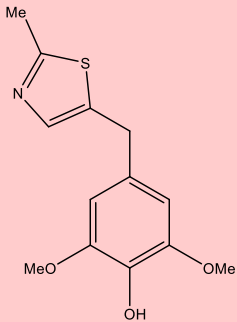
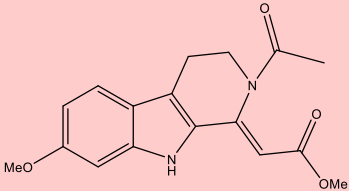
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
2-Carboxyl-3,4-dihydroquinazoline	seeds		Yang et al., 2015
Dipepine	aerial parts		Faskhutdinov et al., 2000
Dipeginol	aerial parts		Faskhutdinov et al., 2000
Pegamine	seeds		Wang et al., 2018b
Ruine	seeds		Wang et al., 2018b
Tetrahydroharmine	seeds		Wang et al., 2018b
Peganine	seeds		Wang et al., 2018b

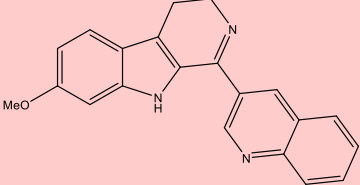
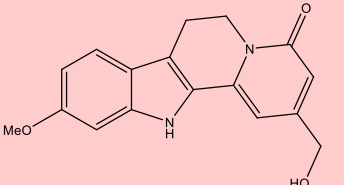
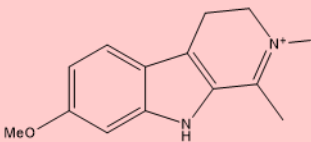
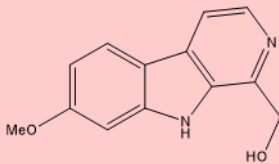
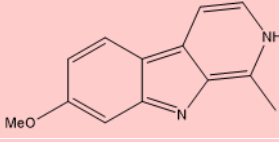
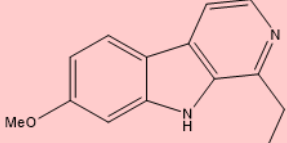
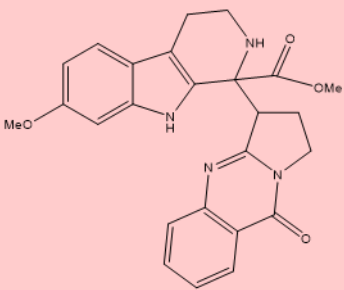
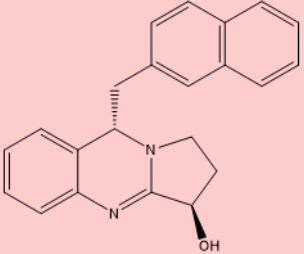
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Pegaline	Seed		Wang et al., 2018b
Dexoypeganine	Seed		Wang et al., 2018b
Pegamine A	Seed		Wang et al., 2017a
Pegamine B	Seed		Wang et al., 2017a
Peganumal A	Seed		Wang et al., 2017a
Peganumal B	Seed		Wang et al., 2017a
Pegaharmine F	Seed		Wang et al., 2017a

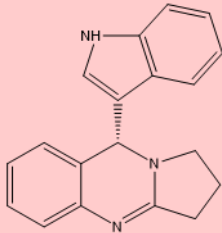
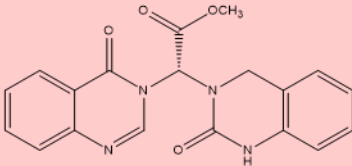
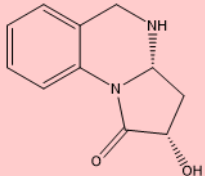
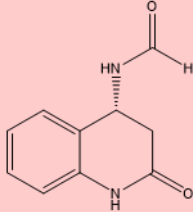
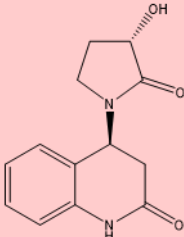
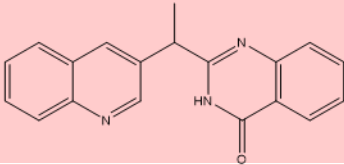
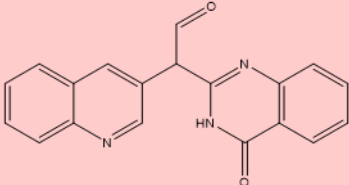
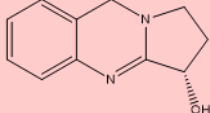
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Pegaharmine G	Seed		Wang et al., 2017a
Pegaharmine H	Seed		Wang et al., 2017a
Pegaharmine I	Seed		Wang et al., 2017a
Pegaharmine J	Seed		Wang et al., 2017a
Pegaharmine K	Seed		Wang et al., 2017a
1-Ethyl-7-methoxy-9H-pyrido [3,4-b]indole	Seed		Wang et al., 2017a
Peharmaline A	Seed		Wang et al., 2017b
Peharmaline F	Aerial parts		Zhang et al., 2022

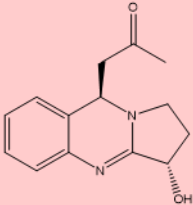
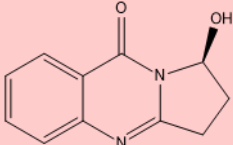
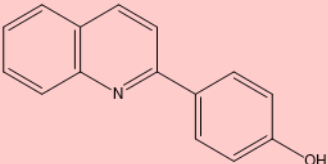
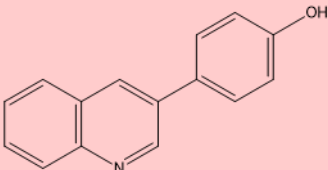
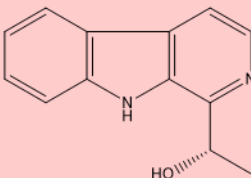
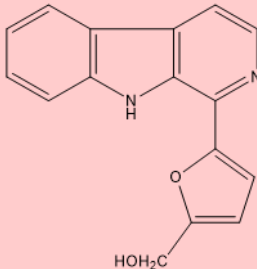
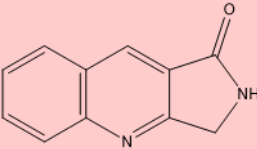
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Peharmaline I	Aerial parts		Zhang et al., 2022
Peharmaline H	Aerial parts		Zhang et al., 2022
Peharmaline G	Aerial parts		Zhang et al., 2022
Peharmaline J	Aerial parts		Zhang et al., 2022
Peharmaline K	Aerial parts		Zhang et al., 2022
2-(3-Quinolinylmethyl)-4(3H)-quinazolinone	Aerial parts		Zhang et al., 2022
luotonin F	Aerial parts		Zhang et al., 2022
(S)-Vasicine	Aerial parts		Zhang et al., 2022

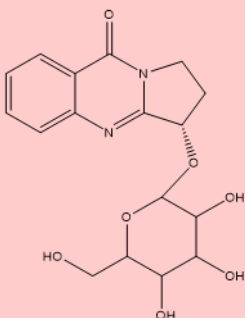
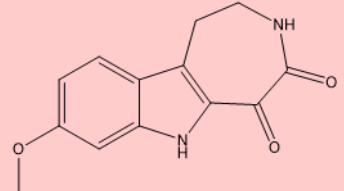
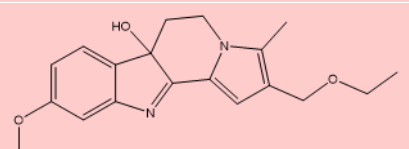
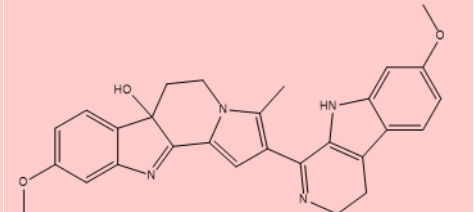
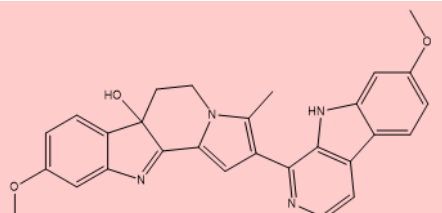
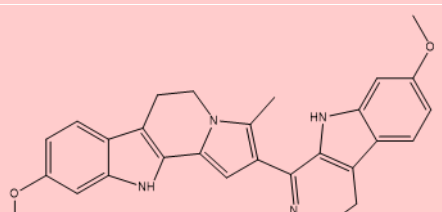
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Peganidine	Aerial parts		Zhang et al., 2022
(S)-Isovasicinone	Aerial parts		Zhang et al., 2022
2-(4-Hydroxyphenyl)quinoline	Aerial parts		Zhang et al., 2022
3-(4-Hydroxyphenyl)quinoline	Aerial parts		Zhang et al., 2022
1-(9H-Pyrido[3,4-b]indol-1-yl)ethan-1-ol	Aerial parts		Zhang et al., 2022
Perlolyrine	Aerial parts		Zhang et al., 2022
2,3-Dihydro-1H-pyrrolo[3,4-b]quinolin-1-one	Aerial parts		Zhang et al., 2022

## Supplementary Table I

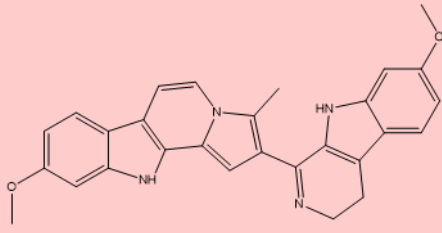
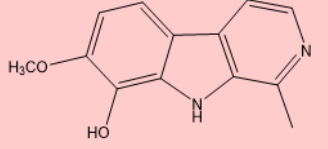
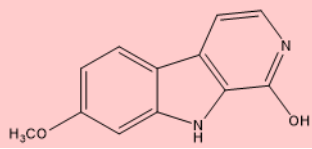
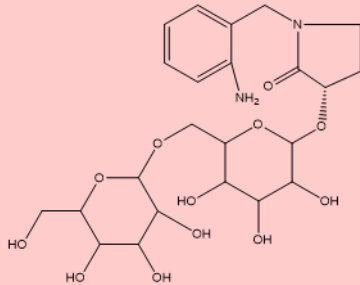
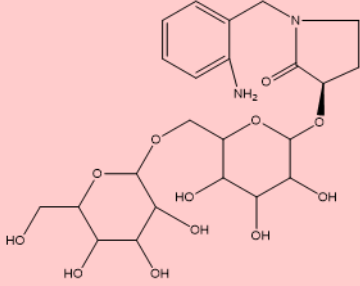
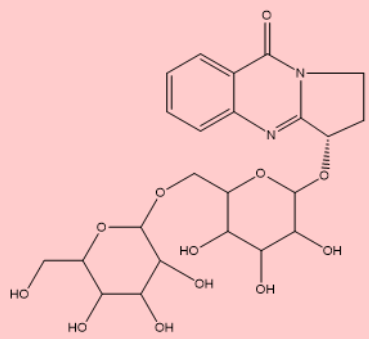
Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
( <i>R</i> )-Vasicinone-1- <i>O</i> - $\beta$ -D-glucopyranoside	Seed		Wang et al., 2015a
Pegaharines A	Seed		Wu et al., 2020
Pegaharines B	Seed		Wu et al., 2020
Pegaharines C	Seed		Wu et al., 2020
Pegaharines D	Seed		Wu et al., 2020
Pegaharines E	Seed		Wu et al., 2020



## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Pegaharines F	Seed		Wu et al., 2020
8-Hydroxyharmine	Seed		Liu et al., 2013
1-Hydroxy-7-methoxy- $\beta$ -carboline	Seed		Yang et al., 2015
(S)-1-(2-Aminobenzyl)-3-hydroxypyrrolidin-2-one $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucopyranoside	Seed		Li et al., 2018a
(R)-1-(2-Aminobenzyl)-3-hydroxypyrrolidin-2-one $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucopyranoside	Seed		Li et al., 2018a
(S)-Vasicinone $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucopyranoside	Seed		Li et al., 2018a

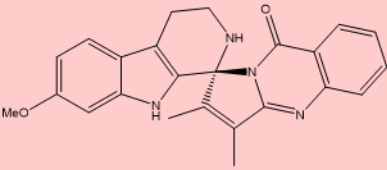
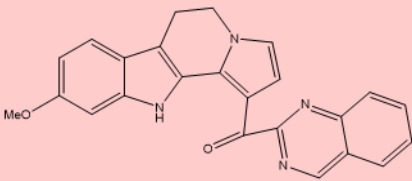
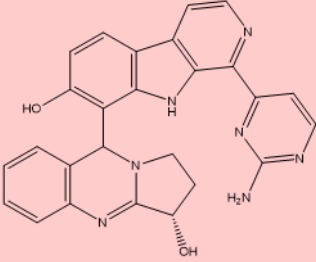
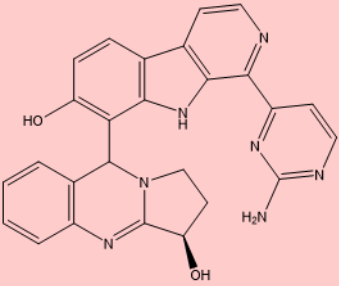
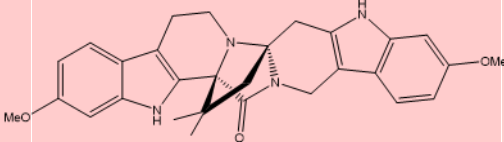
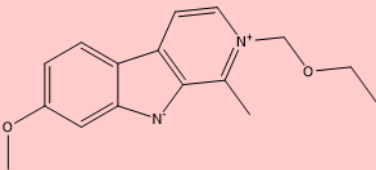
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
( <i>R</i> )-Vasicinone $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucopyranoside	Seed		Li et al., 2018a
Quinanolin-4(3 <i>H</i> )-one	Seed		Li et al., 2018a
Methyl 3-(4-oxoquinazolin-3(4 <i>H</i> )-yl)propanoate	Seed		Li et al., 2018a
Vasicinolone	Seed		Li et al., 2018a
1-(2-Aminobenzyl)-3-hydroxypyrrolidin-2-one	Seed		Li et al., 2018a
$\beta$ -D-Glucopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucopyranoside	Whole plant		Herraiz et al., 2017.

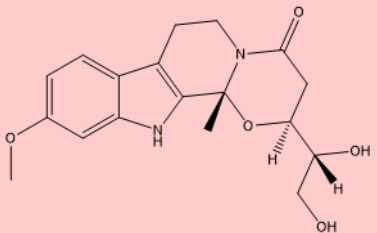
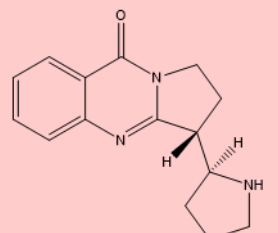
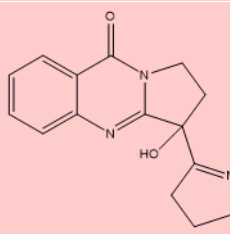
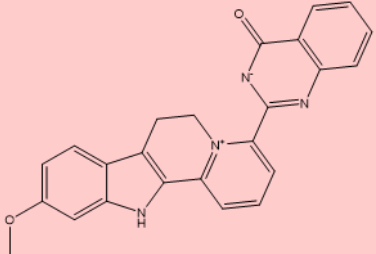
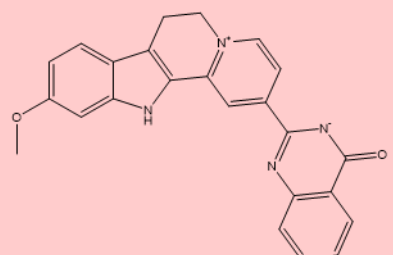
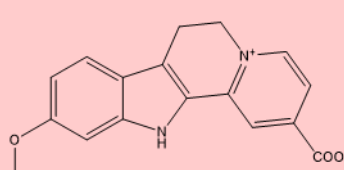
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Pegaharmalines A	Seed		Wang et al., 2014a
Pegaharmalines B	Seed		Wang et al., 2014a
Pegaharmols A	Root		Li et al., 2020b
Pegaharmols B	Root		Li et al., 2020b
Peganumine A	Seed		Wang et al., 2014b
Peganumine B	Seed		Yang et al., 2016

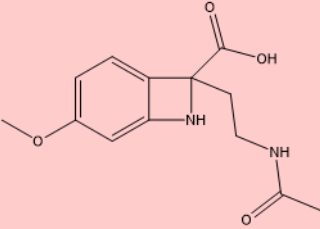
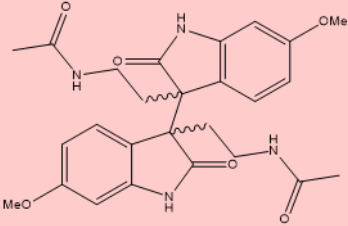
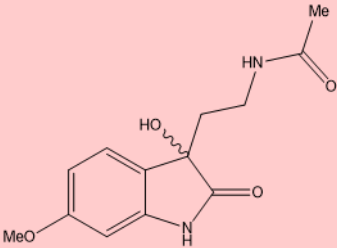
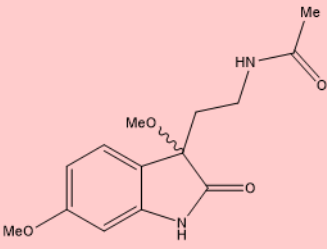
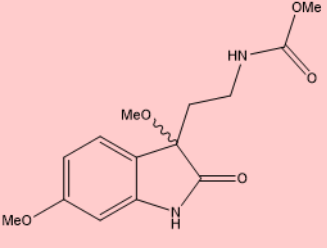
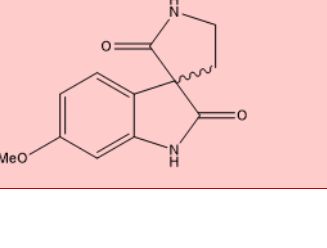
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Peganumine C	Seed		Yang et al., 2016
Peganumine D	Seed		Yang et al., 2016
Peganumine E	Seed		Yang et al., 2016
Peganumine F	Seed		Yang et al., 2016
Peganumine G	Seed		Yang et al., 2016
Peganumine H	Seed		Yang et al., 2016

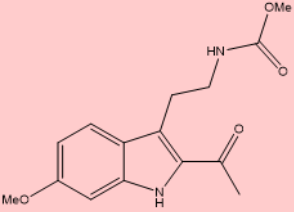
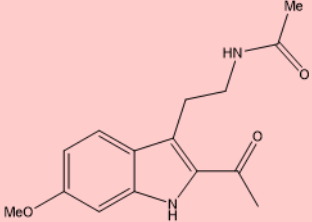
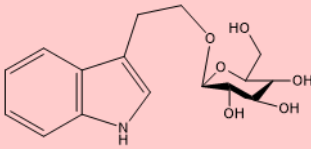
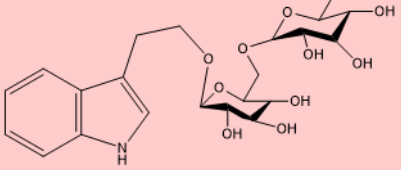
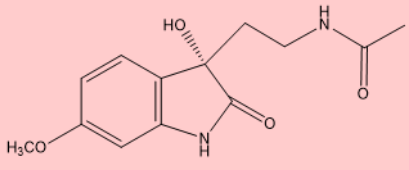
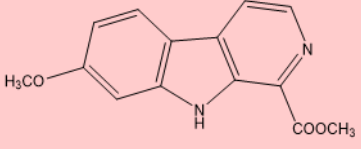
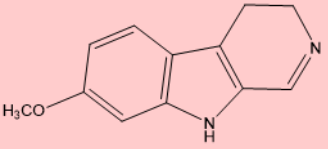
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Peganumine I	Seed		Yang et al., 2016
Peganumaline A	Seed		Wang et al., 2018a
Peganumaline B	Seed		Wang et al., 2018a
Peganumaline C	Seed		Wang et al., 2018a
Peganumaline D	Seed		Wang et al., 2018a
Peganumaline E	Seed		Wang et al., 2018a

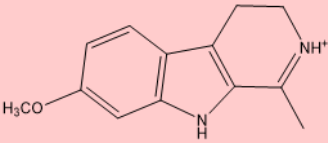
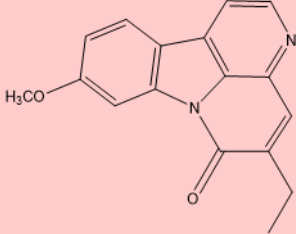
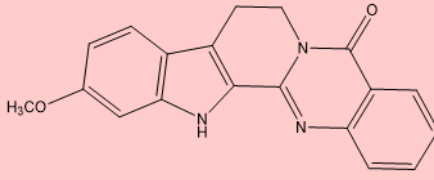
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Peganumaline F	Seed		Wang et al., 2018a
2-Acetyl-3-(2-acetamidoethyl)-7-methoxyindole	Seed		Wang et al., 2018a
2-(Indol-3-yl)ethyl-β-D-glucopyranoside	Seed		Wang et al., 2015b
2-(Indol-3-yl)ethyl-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside	Seed		Wang et al., 2015b
(S)-3-Hydroxy-3-(N-acetyl-2-aminoethyl)-6-methoxyindol-2-one	Seed		Wang et al., 2015b
Harmic acid methyl ester	Seed		Wang et al., 2015b
Harmalacidine	Seed		Wang et al., 2015b

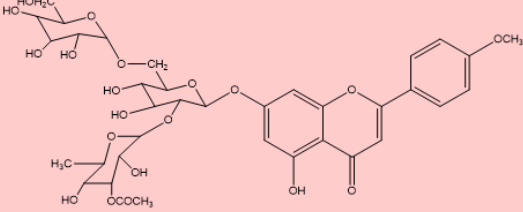
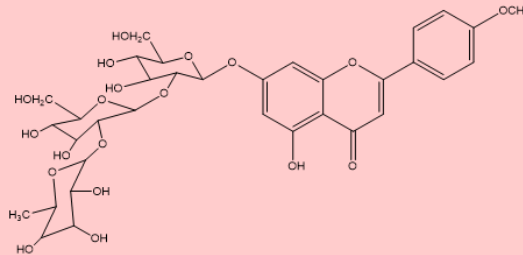
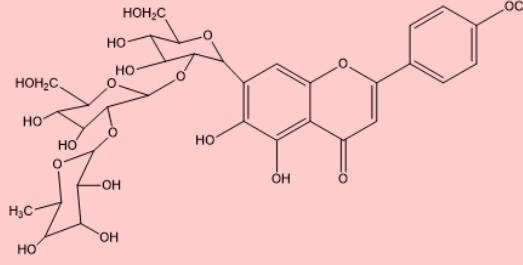
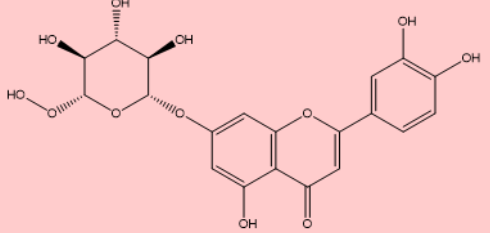
## Supplementary Table I

Alkaloids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Protonated harmaline	seeds		Wang et al., 2015b
luotonin C	seeds		Wang et al., 2015b
11-Methoxyyl-rutaecarpine	seeds		Wang et al., 2015b

## Supplementary Table I

Flavonoids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
7-O-[6''-O-Glucosyl-2''-O-(3'''-acetyl-rhamnosyl)glucoside	Aerial parts		Sharaf et al., 1997
7-O-(2'''-O-Rhamnosyl-2''-O-glucosylglucoside)	Aerial parts		Sharaf et al., 1997
2'''-O-Rhamnosyl-2''-O-glucosylcytisine	Aerial parts		Sharaf et al., 1997
Luteolin 7-glucoside	Leaf		Elansary et al., 2020



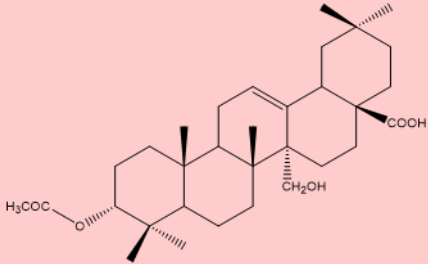
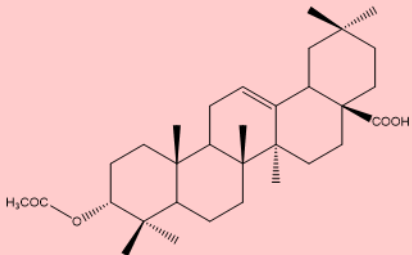
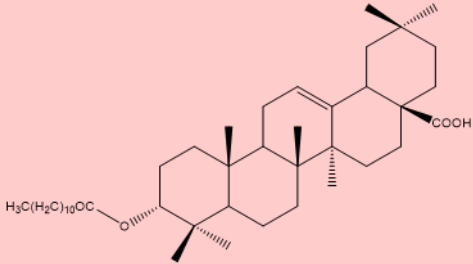
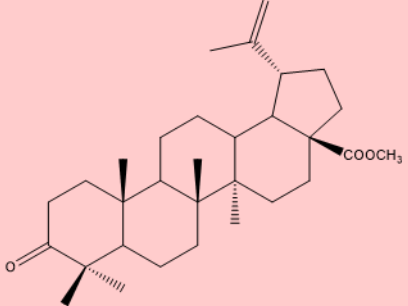
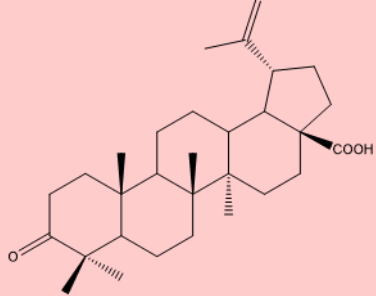
## Supplementary Table I

Triterpenoids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
3 $\alpha$ -Acetoxy-14 $\alpha$ -hydroxylup-20 (29)-en-11-oxo-28-oic acid methyl ester	Seed		Li et al., 2020a
3 $\beta$ -Acetoxy-27-(4-hydroxy-3-methoxy- <i>E</i> -cinnamoyloxy) lup- en-28-oic acid methyl ester	Seed		Li et al., 2020a
3 $\beta$ -Acetoxy-27-hydroxy-lup-20 (29)-en-28-oic acid	Seed		Li et al., 2020a
3 $\alpha$ -Acetoxy-27-hydroxy-olean-12-en-11-oxo-28-oic acid methyl ester	Seed		Li et al., 2020a
3 $\alpha$ -Hydroxy-olean-27-(4-hydroxy-3-methoxy- <i>E</i> -cinnamoyloxy)-12-en-28-oic acid methyl ester	Seed		Li et al., 2020a

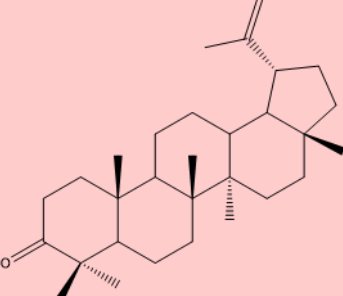
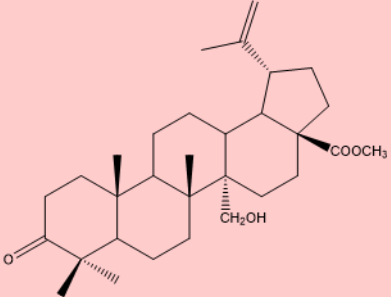
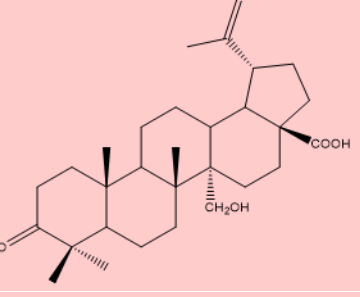
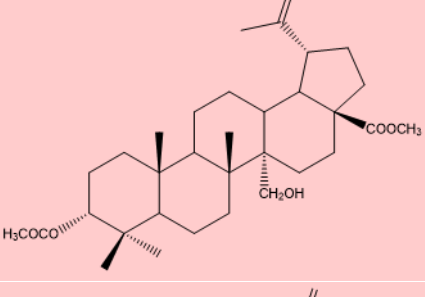
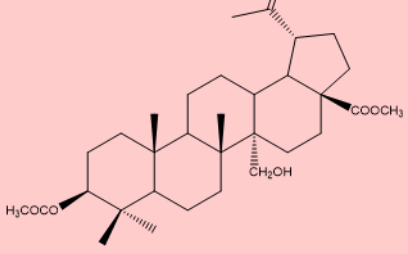
## Supplementary Table I

Triterpenoids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
3 $\alpha$ -Acetoxy-27-hydroxyolean-12-en-28-oic acid	Seed	 The structure shows a pentacyclic triterpene skeleton with a double bond at C-12. It features an acetoxy group (-O-C(=O)-CH <sub>3</sub> ) at C-3, a hydroxyl group (-OH) at C-27, and a carboxylic acid group (-COOH) at C-28. A hydroxymethyl group (-CH <sub>2</sub> OH) is attached to the C-28 ring.	Li et al., 2020a
3 $\alpha$ -Acetoxy oleanolic acid	Seed	 The structure shows a pentacyclic triterpene skeleton with a double bond at C-12. It features an acetoxy group (-O-C(=O)-CH <sub>3</sub> ) at C-3 and a carboxylic acid group (-COOH) at C-28.	Li et al., 2020a
Urs-12-ene-28-carboxy-3 $\alpha$ -tetradecanoate	Seed	 The structure shows a pentacyclic triterpene skeleton with a double bond at C-12. It features a tetradecanoate ester group (-O-C(=O)-(CH <sub>2</sub> ) <sub>13</sub> -CH <sub>3</sub> ) at C-3 and a carboxylic acid group (-COOH) at C-28.	Li et al., 2020a
Methyl-lup-20 (29)-en-3-on-28-oate	eed	 The structure shows a pentacyclic triterpene skeleton with a double bond at C-12 and a ketone group at C-20. It features a methyl ester group (-COOCH <sub>3</sub> ) at C-28 and a methyl group at C-29.	Li et al., 2020a
Betulonic acid	eed	 The structure shows a pentacyclic triterpene skeleton with a double bond at C-12 and a ketone group at C-20. It features a carboxylic acid group (-COOH) at C-28 and a methyl group at C-29.	Li et al., 2020a

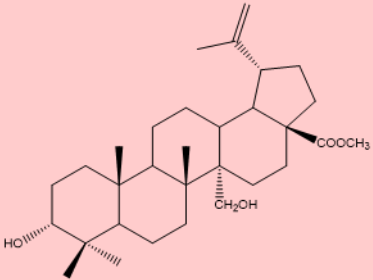
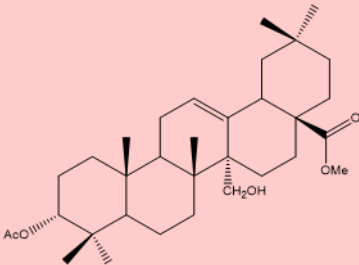
## Supplementary Table I

Triterpenoids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Lup-20 (29)-en-3-on-28-oic acid	Seed		Li et al., 2020a
3-Oxo-27-hydroxylup-20 (29)-en-28-acid methyl ester	Seed		Li et al., 2020a
3-Oxo-27-hydroxylup-20 (29)-en-28-oic acid	Seed		Li et al., 2020a
3 $\alpha$ -Acetoxy-27-hydroxylup-20 (29)-en-28-oic acid methyl ester	Seed		Li et al., 2020a
3 $\beta$ -Acetoxy-27-hydroxylup-20 (29)-en-28-oic acid methyl ester	Seed		Li et al., 2020a

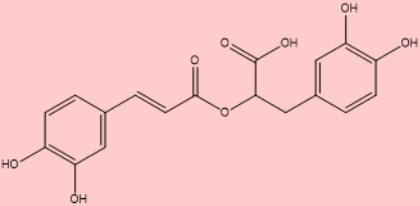
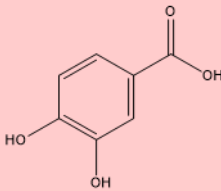
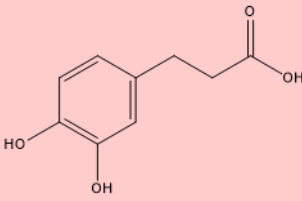
## Supplementary Table I

Triterpenoids identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
3 $\alpha$ ,27-Dihydroxylup-20 (29)-en-28-oic acid methyl ester	Seed		Li et al., 2020a
3 $\alpha$ -Acetoxy-27-hydroxyolean-12-en-28-oic acid methyl ester	Seed		Wang et al., 2016b

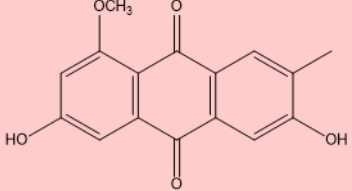
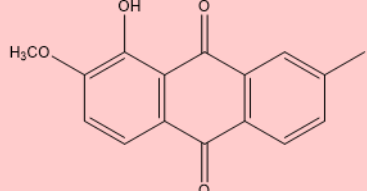
## Supplementary Table I

Phenolic acid identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Rosmarinic acid	Leaf		Elansary et al., 2020
Protocatechuic acid	Leaf		Elansary et al., 2020
Hydrocaffeic acid	Leaf		Elansary et al., 2020

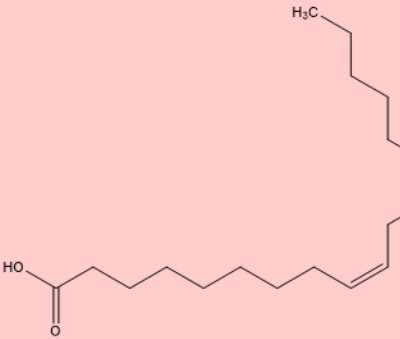
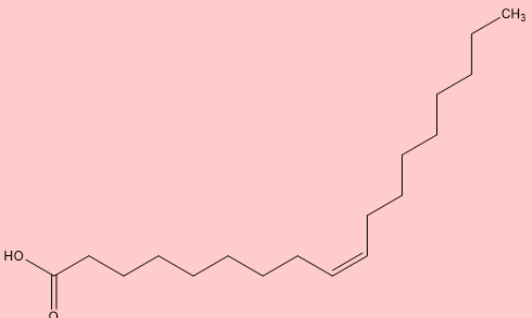
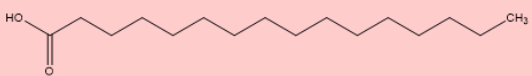
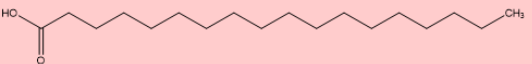
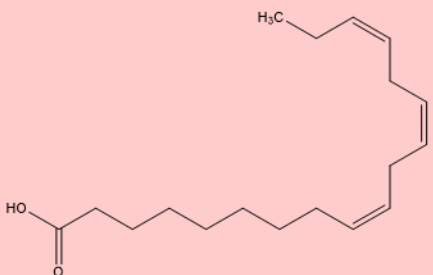
## Supplementary Table I

Anthraquinone identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
3,6-Dihydroxy-8-methoxy-2-methylanthraquinone	Seed	 <p>The structure shows an anthraquinone core with a methyl group at position 2, a methoxy group at position 8, and hydroxyl groups at positions 3 and 6.</p>	Pitret and Srivastav, 1987
8-Hydroxy-7-methoxy-2-methyl-anthraquinone	Seed	 <p>The structure shows an anthraquinone core with a methyl group at position 2, a methoxy group at position 7, and a hydroxyl group at position 8.</p>	Pitret and Srivastav, 1987

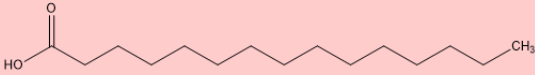

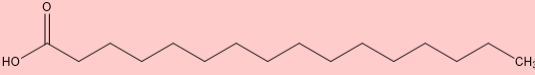
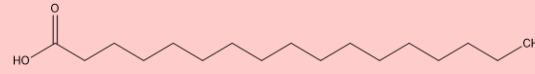
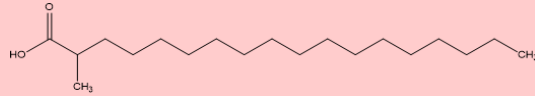
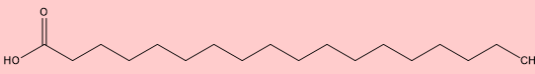
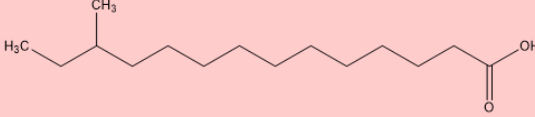
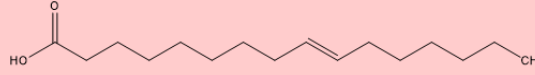
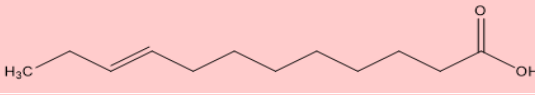
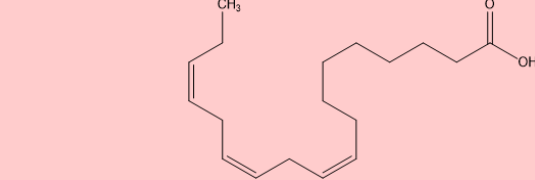

Supplementary Table I

Fatty acid identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Linoleic acid	Seed		Khadhr et al., 2016
Oleic acid	Seed		Khadhr et al., 2016
Palmitic acid	Seed		Khadhr et al., 2016
Stearic acid	Seed		Khadhr et al., 2016
Linolenic acid	Seed		Khadhr et al., 2016
Tetradecanoic acid	Whole plant		Moussa et al., 2015

## Supplementary Table I

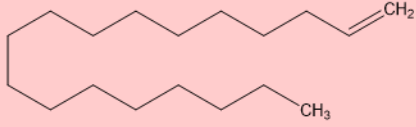
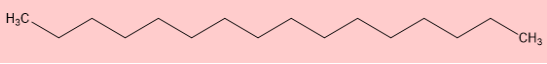
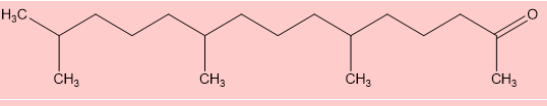
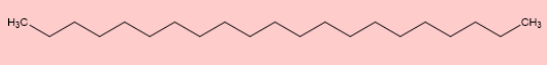
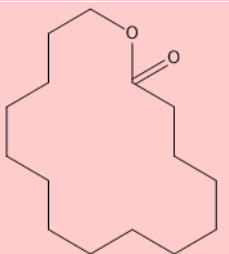

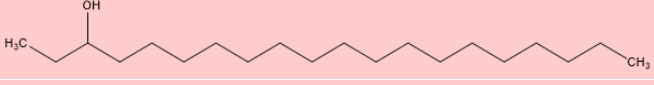
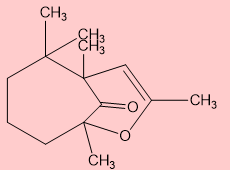
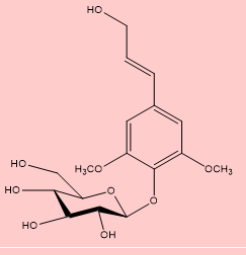
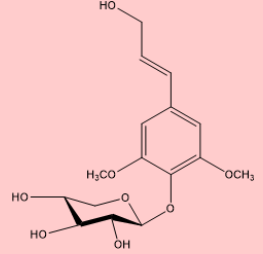
Fatty acid identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
Pentadecanoic acid	Whole plant		Moussa et al., 2015
5, 9, 13-Trimethyl-tetradecanoic acid	Whole plant		Moussa et al., 2015
Hexadecanoic acid	Whole plant		Moussa et al., 2015
Heptadecanoic acid	Whole plant		Moussa et al., 2015
2-Methyl-octadecanoic acid	Whole plant		Moussa et al., 2015
Octadecanoic acid	Whole plant		Moussa et al., 2015
12-Methyl-tetradecanoic acid	Whole plant		Moussa et al., 2015
9-Hexadecenoic acid	Whole plant		Moussa et al., 2015
9-Dodecenoic acid	Whole plant		Moussa et al., 2015
9,12,15-Octadecatrienoic acid	whole plant		Moussa et al., 2015
10,13-Octadecadienoic acid	whole plant		Moussa et al., 2015



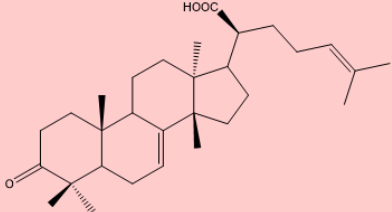
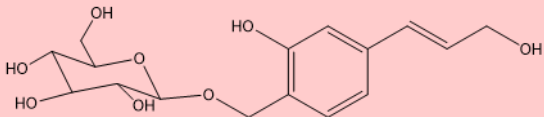
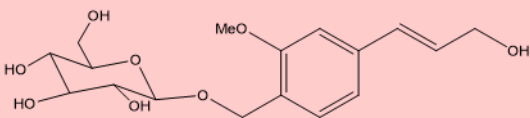
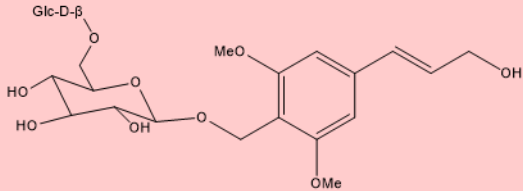
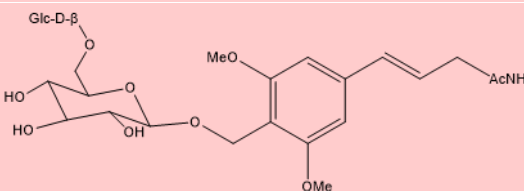
Supplementary Table I

Other compounds identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
1-Octadecene	Whole plant		Moussa et al., 2015
Hexadecane	Whole plant		Moussa et al., 2015
2-Pentadecanone, 6,10,14-trimethyl	Whole plant		Moussa et al., 2015
<i>n</i> -Heneicosane	Whole plant		Moussa et al., 2015
1-oxacyclohexadecan-2-one	Whole plant		Moussa et al., 2015
E-15-Heptadecenal	Whole plant		Moussa et al., 2015
Eicosan-3-ol	Whole plant		Moussa et al., 2015
1,2,26,8-pentamethyl-7-oxabicyclo[4.3.1]dec-8-en-1-one	Whole plant		Moussa et al., 2015
Syringin	Seed		Yang et al., 2015
1-O-β-D-xylopyranose sinapyl alcohol	Seed		Yang et al., 2015

## Supplementary Table I

Other compounds identified from different parts of *Peganum harmala* (Cont.)

Compound name	Extracted from	Structures	References
3-oxotirucalla-7,24-dien-21-oic acid	Seed		Wang et al., 2016b
( <i>E</i> )-caffeyl alcohol 4- <i>O</i> - $\beta$ -D-glucopyranoside	Seed		Wang et al., 2016b
Coniferin	Seed		Wang et al., 2016b
Syringoside	Seed		Wang et al., 2016b
<i>N</i> -acetyl-9-syringoside	Seed		Wang et al., 2016b