**Supplementary material**

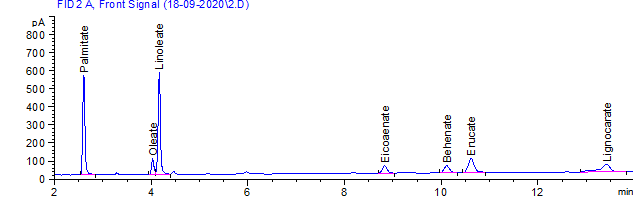
**Table S1**. Possible functional groups/ bonds originated from stretching/ bending vibrations frequencies useful in discriminating wild adlay flours.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak (s) at cm-1 animated | Origin hailing to peak (s) | possible functional group (s) reached out | wild Adlay flours | | | | | | | | | |
| PRP 2863/ 1885 cm-1 upto | YLW 2279/ 2281 cm-1 to | OWT 2279/ 2281 cm-1 to | BLK 2279/ 2281 cm-1 to | | GRY 2279/22 81 cm1 upto | | GRN 2863/1865 cm-1  upto | | BRN 2158/ 21 59; 2176 cm-1 upto |
| OOP (out of plane) region | | | | | | | | | |
| Frequencies 419 to 2863/1865 originating functional group (s) | | | | | | | | | |
| 2863/  3865 to 1865 | Shoulder peak just to right of R- C–H stretch | H-C=O nor- mally at 27 60; a known window | peak 2865 is aldehy dic H | No peak appearance (NIL)  Normally aldehydic peak originate at 2760 Cm-1 | | | | | | 2865 peak aldehydic H | | NIL |
| 2279/  2281 | -CN (2240-22 80)/ or R- CN+-O- (2280-2305); or R-N+ N (~2260) | aliphatic Nitrile/Oxid e/diazonium salt/Cyanid | Thiocyanate (2240-2260/1180-1190) accompanied with absorbance (2158/2159 | | | | | | | Absent | | associated to 2158 -2159; 2176 |
| 2225  Cm-1 | Ar-CN or R-N+N-(Diazonium salt) ~2260-2150 (-C C) | Ar– amide / or nitrile (2220-224 0) OR –C C– stretch | Absent | Absent | Absent | Absent | | ArC≡N or Nitrile is present | | absent | | Absent |
| 2176 | Ar-CN or R-N+N-(Diazonium salt) ~2260-2150 (-C C-) stretch | Ar– anide / or nitrile (2220-224 0) OR –C ≡C–stretch | absent | Absent | absent | absent | | Absent | | absent | | Thio/isothio cyanate |
| 2157 to  2159 | Single peak at 2158-59 (2140-2175) indicate thiocyanate (-SCN | | | | | | | | | |
| 2176 | Cyanide/thiocyanate /cyanate /RS-C N or -SCN- or –C=N-S stretch (2000-2200) | CN-/SCN/ OCN- iso thiocyan ates or Ar-substitut ed upper or alkyl at lower end of Isothio cyanate | Absent | Absent | Absent | Absent | | Absent | | absent | | Thio/isothio cyanate |
| 2157 to  2159 | Single peak at 2158-59 (2140-2175) indicate thiocyanate (-SCN) | | | | | | | | | |
| 2149 | Cyanide/thiocya nate/ cyanate / RS-C N or -SCN- or –C=N-S stretch (2000-2200) | CN- or SC≡N- or  OC ≡N-Thiocyan ates OR Ar- substi tuted at upper or lower R- at lower end of Iso thio- cyanate | absent | absent | -SCN (2140-2175) also C= C only ~600 OOP | Absent | | Absent | | absent | | absent |
| 2143 | Absent | absent | absent | -SCN | | -SCN | | -SCN | | absent |
| 2046/47 | present | absent | singlet | absent | | Absent | | singlet | | absent |
| 33/35-23 | Present | Present | absent | absent | | Absent | | absent | | absent |
| 2012 | present | absent | absent | absent | | Absent | | absent | | absent |
| 2005/06 | Absent | absent | singlet | singlet | | Present | | present | | singlet |
| 1993[94 | Absent | absent | absent | absent | | Present | | absent | | absent |
| 1975/76 | Absent | absent | WNB | WNB | | Present | | present | | present |
| 1961/62 | Absent | absent | as above | | | Absent | | present | | present |
| 1832 Cm-1 | acid -CO-X) or Aryl carbonate/ open chain acid anhyd (1800-1850/ 1740 to 1790 / 5-member ring anh or cyclic ketone 5-member ring/Ar- & α, ß usd ketone s/ C=O /5- member ring C=O or –CO OC- or SD 4-members ring C=O/ Lactone at 1870 -1820/ 1750-1800 | Aryl carbonate (1775-1820) | Absent | Absent | peaks 1832 & 1775 show acid anhydride or 5-member ring anhydrid | | absent | Absent | | Aryl  carbon  ate | | absent |
| 1765/  1775  cm -1 | 1,2-diketon e (s)- cis, 5- members ring (at Ʋ 1750-1800) or Aryl carbonate (1775 - 1820) | only at u 1765 or upward implicate α, α/ - di chloro and or α, α/--dibromo | Separate peaks at Ʋ 1765, 1777 >1, 2-diketon es(S) Cis, 5-member ring ahd or Ar-car bonate Separate peaks at Ʋ 1765, 1777 >> 1,2-di keton es(S) Cis, 5 members ring ahd/Ar-carbonat | | | only at Ʋ 1765 >> α, α/ -dichloro or α α/ -dibromo ketones | | | absent | | absent |
| 1753 | α, α/-di chloro or α α/- dlbromo ketones / 5-membrs ketones or lactone ring | Absent | Absent | Absent | | Absent | Absent | | alkyl car bonate or Aryl ketones | | alkyl carb onate or Aryl ketones |
| 1736/37 | C=O (735-7 50 (S) plus Ʋ 715 -730 (s) / Aryl comb bands (1500/1660-2000) several peaks due to Ar-CG C=C stretch / over tones /open chain imino (RC= N-) or amide | 6-membr Lactone or aliphatic C=O stretch (s or RCOOH /or Ketone / ester | a single band alone at Ʋ 1727 or 1720/ 1725 indicate aliphatic RC=O stretch OR Carboxylic acid (1700-1725) or triglycerides (ester) are present | | | | Singlet (S) at Ʋ 1737 indicate Ar-C =O; Separate bands at Ʋ 1720/ 1737 accompanied strong band at 1066 1134-1144 >>>> six members lactone or Aryl-C=O stretch (S) and OR α, ß-US C=O stretch, plus C-O stretch band at (Ʋ1310 -1050 (S), well known window OR Carboxylic acid (1700-1725) or triglycerides (ester) are present | | | | | |
| 1727 | Ar- C=O stretch (S) and α ß US C=O stretch | Absent | absent | absent | | Absent | Absent | absent | | absent | |
| 1719/21 | absent | Present | present | | absent | Absent | Present | | present | |
| 1690  Cm-1 | C=O (735-750 (s) and 715-730 (s) or Ar-CB (1 600-2000) several peaks due to over tones or Ar- CGD C =C stretch or open chain imino (RC =N-)/ amide | enol esters / enol ROR & enol en amines weaker than C=O (1640-1590 (s)/C=C NCG with Aryl ring (1625)/ amide (16 30-1680)/ RC =N -(16 90-1590/ dienes/ tri enes/sat ROH (1600-1725) | absent | Enol esters/ enol R-O-R or enol enamines weaker than C=O (1640-1590(s) | | | | Absent | absent | | absent | |
| 1678 | same as above | Absent | NCG C=C stretch due to 1620 -1680 or saturated ROH | NCG- C=C; amide | | NCG- C=C; amide | Non conjugated (NCG) - C=C; amide | NCG C= C stretch  due to 162 0/1680/ CJ-Ar. censure when Ʋ at 1625 | | NCG C=C. or  amide | |
| 1656 | Absent | absent | | absent | Absent | absent | |
| 1677 | Absent | Absent | present | | present | NCG C=C | present | | present | |
| 1577 | open chain azo OR aliphatic Nitro compounds or well-known NB R~ 1600; ~1580 and ~1500 due to Ar- ring stretch (NBR associated with OOP) | N=N -163 0-1575/ C=C–CAr. ring in pla ne stretch accompanied with OOP & in plane bending at 1000-1280 as well as several pe aks at 1660 -2000 due to overtone | Absent | Absent | absent | | absent | Absent | present | | absent | |
| 1574 | present | Absent | absent | | absent | Absent | absent | | absent | |
| 1560/61 | absent | Present | absent | | present | Present | present | | present | |
| 1523/25 | absent | Present | absent | | present | Present | present | | present | |
| 1491/94 | present | Absent | Absent | | present | Absent | present | | absent | |
| 1484 | present | Absent | Absent | | absent | Absent | present | | present | |
| 1441 | aliphatic symm. scissor/ bend CH | Basics skeleton o | present | absent | absent | | absent | absent | absent | | absent | |
| 1391/92 | Present | present | present | | present | present | present | | present | |
| 1348/ 1351 | Pri. /sec. OH (1350-12 60) /aliphatic Nitro cmpds/ organic P=O stretch | OH, in plane bend for simple P -Oxy/ hetro- Oxy bond | present | absent | absent | | present | present | present | | present | |
| 1291/  1284 | C=C-C-H (in-ring) plane bend | Present | Present | absent | | present | Absent | present | | present | |
| 1215/ | ArC-O stretch / C-N/-OCN+ /COCN stretch; or Cyclic ether large ring C-O stretch/ C-O-C in Acid anhydride and OR Ar-C-O sym- stretch or Pri. / Sec. ROH C-O stretch or R-substituted ether C-O stretch OR C-O and C-C- stretch of carbon and ring vibration mainly from carbohydrate | C-O-/C-O & or Sec amine C-N stretch | Absent | present | absent | | absent | Absent | absent | | present | |
| 1190/88 | Cyanate due to Ʋ 1180-1190 /2240-2260 cm-1 | Sec. /Ter. amine CN stretch (1130-1190 or 1150-1210; OR N-H bending of amide (mainly from AAs) | | | | probably Cyanassociate Ʋ 2225 | Sec./ Ter. amine C-N stretch (1130-1190 or 1150-1210; OR N-H bending of amide (mainly from AAs) | | | | |
| 1134/40 | large ring or R-sub- stituted ether CO-C | C-C stretch of carbohydrate (Anomeric Ring vibration (mainly from Carbohydrates)1. mono substituted due to Ʋ at 738 and 687cm-1; 2.- ortho at 738 and 3.- 1,3,5-tri substituted due to Ʋ at 687cm-1 and 720 and 878 cm-1 | | | | | | | | | |
| 1066/69 | Ar-OH or R-substit uted ether or ArO-gr /ArO-H or ahd or R-OH/C-O-C or Carboh |

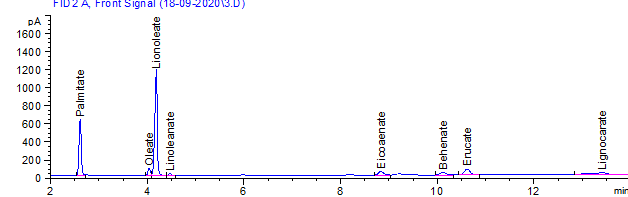
|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak animated | Origin hailing to peak (s) | Functional group (s) reached out | “OOP” (Out of plane) region 905- 632 cm-1 | | | | | | |
| 905  875/ 880 | well known OOP inter mingle with FPR =C-H OOP bend ing several peaks are present at Ʋ 631/ 632-943 / 945 witness ing mono/di/ tri/ tetra sub stituted at O-; & or m-, & or p- or ali-phatic C-Cl stretch Ʋ at 827 may also be due to (cy clic ketone) sat 5-memb er ring C=O (820 -870) associated with 1750-1800 or per oxide C-O-O-C stretch (820 -890) or anomeric region of carb. & ring vibrations (mainly from carbo- hydrate | since mono substitution Ʋ at (730-7 70 & 68 0-720)/ ortho at (735-77 0); meta (685-720, 750-810); para (800-860/ tri substituted Ʋ at 1, 2,3 (685-720, 750 -81 0); for 1,2,4 (800-810, 820-900) /1, 3, 5 (685-720, 820-90 0); for tetra substitutions due to Ʋ at 1,2,3,4 (800-840); for 1,2, 3,5 as well as for 1, 2, 4, 5 (same at 840-880) while penta substituted due to Ʋ at 8 60-900 cm-1 & last but not least hexa substituted due to Ʋ at (385 -415)/or otherwise R-C -Cl(700-800cm- | 1. ortho substituted due to Ʋ at 747.  2.-para due to Ʋ at at 878.  3.- 1,2,3 ,4- tetra & or 1, 2,3,5- & or 1,2, 4,5-tetra substituted due to Ʋ at 878.  4.- penta substituted due to Ʋ at 878 cm-1 | 1.-ortho substituted due to 745; 2.-para 846; 3.- 1,2,4-tri substituted due to Ʋ at 846 & 876  3. 1,2, 3, 4-tetra & or1,2,4,5-tetra & or 1,2,3,5-tetra substitute due to Ʋ at 846 & 8764.- penta due to Ʋ at 876 Cm-1 | 1.- para substituted 845; 2.- 1,2, 4-tri-subsituted 845 & 876; 3.-1,2,3, 4- tetra & or 1,2, 4,5-tetra & or 1,2, 4,5-tetra at 845 & 877.  4.-penta at 8777; while hexa substituted due to Ʋ at 419 cm-1 | 1.- para (Ʋ 849); 2: 1,2,4-tri-substited due to Ʋ at 849 & 905.  3. penta due to Ʋ at 905 & hexa substituted due to Ʋ at 410, and 419  Cm-1 | 1. 1,2, 3 5- & 1,2,3,4- & 1.3.4. 5-tetra substituted ted haling to Ʋ at 878 & OR otherwise penta substitution in preview of same Ʋ 878 Cm-1 | 1.ortho substituted at Ʋ 744cm-1  2: p-substituted at Ʋ 828cm-1  3. 1,2,3 5-tetra & or 1,2,4,5-tetra substitution at Ʋ 880 Cm-1  While 4. Penta substitution at Ʋ 880 Cm-1 | 1. mono substituted due to Ʋ at 738 and at 687 Cm-1  2.ortho-due to Ʋ at 738 cm-1  3. 1,3,5-tri- substituted due to Ʋ at 687 & 720 & 878 cm-1 |
| 845/ 849 |
| 827 |
| 738 | present | present | present | present |
| 663/  64 | aliphatic bromo (due to C-Br stretch & or -SH & thio substituted | ROH bend (-OH OOP)/ aliphatic Halides (RC-X) or CH-S-C-S stretch) | Present | Absent | present | present | present | present | present |
| 640/ 645 | Absent | present | absent | present | present | present | present |
| 631/ 632 | Absent | Absent | absent | present  present | present | present | present |
|  | Absent | Absent | absent | absent | absent |

Abbreviations NCG for non-conjugated; CG for conjugated; US for unsaturated, Sat for saturated. Abs means absent and pre means present while Ʋ stands for frequency number (cm-1); WNB for week narrow band; NBR for narrow band region (Ʋ 1391/1392 cm-1 – 1560/1561cm-1); OOP for out of plane (Ʋ at 650 cm-1 – 943cm-1) or FPR for fingerprint region (631/632cm-1 — 943/945cm-1; 905 cm-1); ahd for anhydride

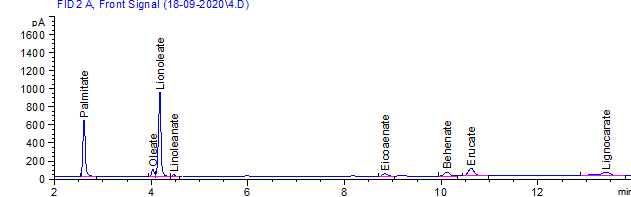
**Supplementary Figures**

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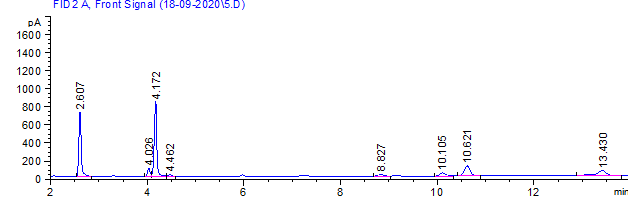
**Figure S1 GC Chromatogram of fatty acids of oil obtained from purple adlay seed**

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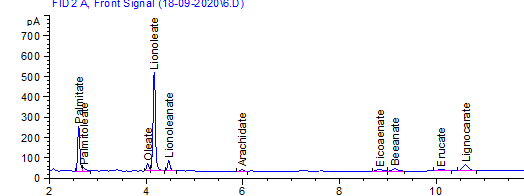
**Figure SII GC Chromatogram of fatty acids of oil obtained from black adlay seed**

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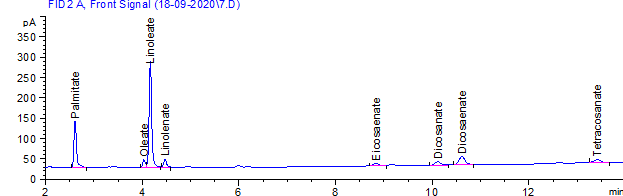
**Figure SIII GC Chromatogram of fatty acids of oil obtained from brown adlay seed**

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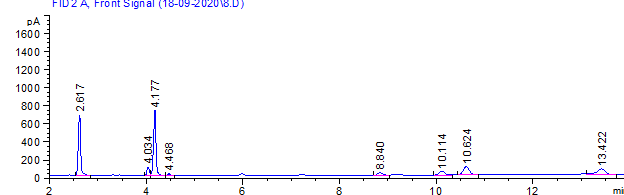
**Figure SIV GCFID Chromatogram of Green grains Triglyceride characteristics**

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**Figure SV GC Chromatogram of fatty acids of oil obtained from yellow adlay seed**

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**Figure SVI GC Chromatogram of fatty acids of oil obtained from grey adlay seed**

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**Figure SVII GC Chromatogram of fatty acids of oil obtained from Off -White adlay seed**