

## SUPPORTING INFORMATION

### Application of targeted <sup>1</sup>H NMR profiling to assess the seed vitality of soybean [*Glycine max* (L.) Merr.]

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#### Appendix A. Supplementary data

Table S1 Metabolite identification in the soybean seed

Table S2 All metabolites identified in soybean seed, showing their molecular masses, KEGG compound codes, and other corresponding information.

Fig. S1 Representative <sup>1</sup>H NMR spectra of 50% water-methanolic extracts of soybean seed.

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Table S1 Metabolite identification in the soybean seed.

No.	Compound name	No.	Compound name
1	1,3-Dimethylurate	23	Leucine
2	2-Aminoadipate	24	Lysine
3	2-Hydroxyisobutyrate	25	Malate
4	4-Aminobutyrate	26	Malonate
5	4-Hydroxyphenylacetate	27	Methionine
6	Acetate	28	N-Acetylglutamate
7	Alanine	29	Pantothenate
8	Arginine	30	Phenylacetate
9	Asparagine	31	Phenylalanine
10	Aspartate	32	Proline
11	Betaine	33	Propylene glycol
12	Carnitine	34	Pyruvate
13	Choline	35	Serine
14	Citrate	36	Succinate
15	Ethanol	37	Sucrose
16	Formate	38	Threonine
17	Fumarate	39	Tryptophan
18	Glucose	40	Tyrosine
19	Glutamate	41	Uracil
20	Glutamine	42	Valine
21	Isoleucine	43	pi-Methylhistidine
22	Lactate	44	Epicatechin

Table S2 All metabolites identified in soybean seed, showing their molecular masses, KEGG compound codes, and other corresponding information.

Compound	CAS. Registry	ChEBI. ID	Compound. ID	Formula	HMDB.Access ion. Number	KEGG.Compound. ID	PubChem. Compound	Weight
1,3-Dimethylurate	944-73-0		346	C7H8N4O3	HMDB01857		70346	196.1634
2-Hydroxyisobutyrate	594-61-6		69	C4H8O3	HMDB00729		11671	104.1045
4-Aminobutyrate	1956-12-2	CHEBI:16865	101	C4H9NO2	HMDB00112	C00334	119	103.1198
4-Hydroxyphenylacetate	156-38-7	CHEBI:18101	7	C8H8O3	HMDB00020	C00642	127	152.1473
Acetate	64-19-7	CHEBI:15366	9	C2H4O2	HMDB00042	C00033	176	60.052
Adenine	73-24-5	CHEBI:16708	272	C5H5N5	HMDB00034	C00147	190	135.1267
Adenosine	58-61-7	CHEBI:16335	276	C10H13N5O4	HMDB00050	C00212	60961	267.2413
Alanine	56-41-7	CHEBI:16977	232	C3H7NO2	HMDB00161	C00041	5950	89.0932
Arginine	74-79-3	CHEBI:16467	240	C6H14N4O2	HMDB00517	C00062	6322	174.201
Asparagine	70-47-3	CHEBI:17196	231	C4H8N2O3	HMDB00168	C00152	6267	132.1179
Aspartate	56-84-8	CHEBI:17053	234	C4H7NO4	HMDB00191	C00049	5960	133.1027
Betaine	107-43-7	CHEBI:17750	15	C5H11NO2	HMDB00043	C00719	248	117.1463
Choline	62-49-7	CHEBI:15354	302	C5H14NO	HMDB00097	C00114	305	104.1708
Citrate	77-92-9	CHEBI:30769	22	C6H8O7	HMDB00094	C00158	311	192.1235
Dimethyl sulfone	67-71-0	CHEBI:9349	3211	C2H6O2S	HMDB04983	C11142	6213	94.1328
Epicatechin	490-46-0		2	C15H14O6	HMDB01871	C09727	72276	290.2681
Ethanolamine	141-43-5	CHEBI:16000	97	C2H7NO	HMDB00149	C00189	700	61.0831
Formate	64-18-6	CHEBI:30751	32	CH2O2	HMDB00142	C00058	284	46.0254
Fumarate	110-17-8	CHEBI:18012	100	C4H4O4	HMDB00134	C00122	723	116.0722
Galactarate	526-99-8	CHEBI:30852	396	C6H10O8	HMDB00639	C00879	607	210.1388
Glucarate	87-73-0	CHEBI:16002	398	C6H10O8	HMDB00663	C00818	33037	210.1388
Glutamate	56-86-0	CHEBI:16015	229	C5H9NO4	HMDB00148	C00025	33032	147.1293
Hypoxanthine	68-94-0	CHEBI:17368	164	C5H4N4O	HMDB00157	C00262	790	136.1115

Isoleucine	73-32-5	CHEBI:17191	225	C6H13NO2	HMDB00172	C00407	6306	131.1729
Isopropanol	67-63-0	CHEBI:17824	72	C3H8O	HMDB00863	C01845	3776	60.095
Lactate	79-33-4	CHEBI:422	42	C3H6O3	HMDB00190	C00186	107689	90.0779
Leucine	61-90-5	CHEBI:15603	235	C6H13NO2	HMDB00687	C00123	6106	131.1729
Malate	6915-15-7	CHEBI:6650	94	C4H6O5	HMDB00156	C00711	525	134.0874
Malonate	141-82-2	CHEBI:30794	121	C3H4O4	HMDB00691	C00383	867	104.0615
Methionine	63-68-3	CHEBI:16643	213	C5H11NO2S	HMDB00696	C00073	6137	149.2113
myo-Inositol	87-89-8	CHEBI:17268	223	C6H12O6	HMDB00211	C00137	892	180.1559
<i>O</i> -Phosphocholine	107-73-3	CHEBI:18132	321	C5H15NO4P	HMDB00284	C00588	1014	184.1507
Propylene glycol	57-55-6	CHEBI:16997	262	C3H8O2	HMDB01881	C00583	1030	76.0944
sn-Glycero-3-phosphocholine	28319-77-9	CHEBI:16870	333	C8H21NO6P	HMDB00086	C00670	439285	258.2292
Succinate	110-15-6	CHEBI:15741	60	C4H6O4	HMDB00254	C00042	1110	118.088
Sucrose	57-50-1	CHEBI:17992	193	C12H22O11	HMDB00258	C00089	5988	342.2965
Trigonelline	535-83-1	CHEBI:18123	334	C7H7NO2	HMDB00875	C01004	5571	137.136
Trimethylamine	75-50-3	CHEBI:18139	62	C3H9N	HMDB00906	C00565	1146	59.1103
Tryptophan	73-22-3	CHEBI:16828	241	C11H12N2O2	HMDB00929	C00078	6305	204.2252
Tyrosine	60-18-4	CHEBI:17895	243	C9H11NO3	HMDB00158	C00082	6057	181.1885
Uridine	58-96-8	CHEBI:16704	162	C9H12N2O6	HMDB00296	C00299	6029	244.2014
Valine	72-18-4	CHEBI:16414	215	C5H11NO2	HMDB00883	C00183	6287	117.1463
gamma-Glutamylphenylalanine	7432-24-8		274	C14H18N2O5	HMDB00594		111299	294.3031
pi-Methylhistidine	368-16-1	□	76	C7H11N3O2	HMDB00479	C01152	64969	169.1811

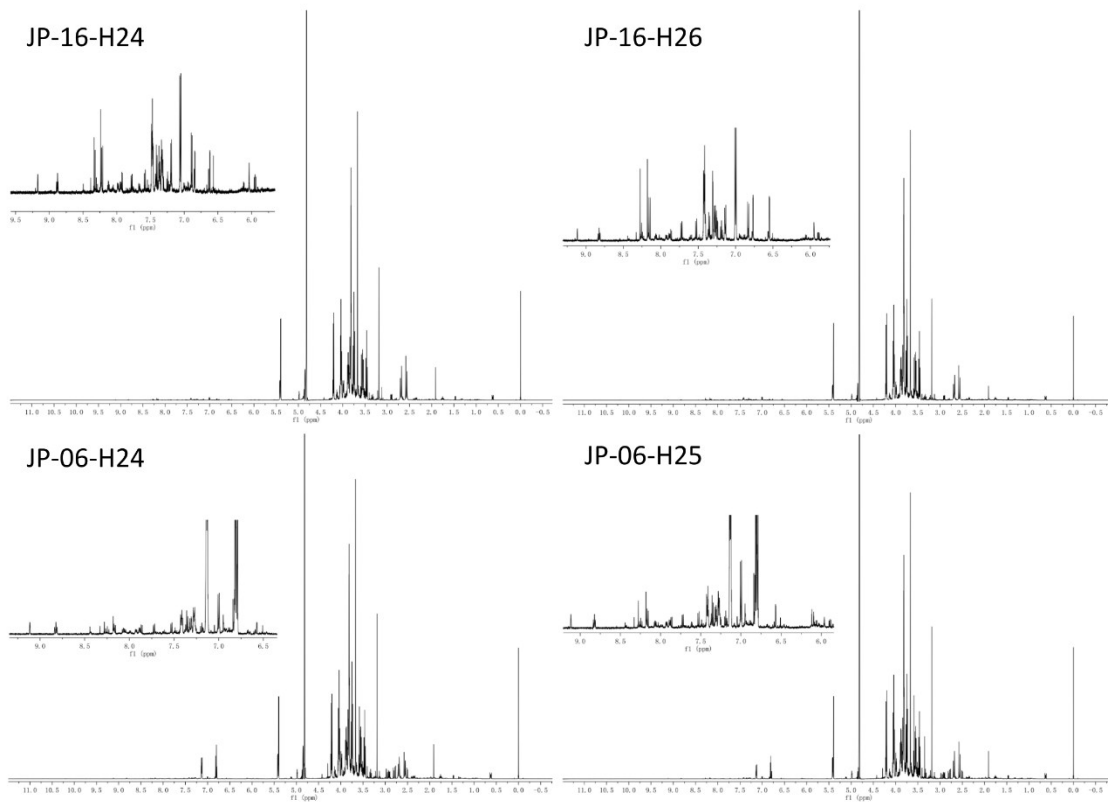


Fig. S1 Representative <sup>1</sup>H NMR spectra of 50% water-methanolic extracts of soybean seed.