

## **Supplementary materials**

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Supplementary Figure 1 Full-length blots/gels

**Supplementary Table S1. The physicochemical parameters for the active ingredients of NDSP**

Number	Name	OB (%)	DL	Mol ID	Database	Medicines
1	Mandenol	42	0.19	MOL001494	TCMSP	Ligusticum chuanxiong Hort, Panax notoginseng (Burk.) F.H. Chen
2	Myricanone	40.6	0.51	MOL002135	TCMSP	Ligusticum chuanxiong Hort
3	Perlolyrine	65.95	0.27	MOL002140	TCMSP/ETCM /Batman	Ligusticum chuanxiong Hort
4	senkyunone	47.66	0.24	MOL002151	TCMSP/ETCM	<i>Ligusticum chuanxiong</i> Hort
5	wallichilide	42.31	0.71	MOL002157	TCMSP/ETCM	<i>Ligusticum chuanxiong</i> Hort
6	sitosterol	36.91	0.75	MOL000359	TCMSP	<i>Ligusticum chuanxiong</i> Hort
7	FA	68.96	0.71	MOL000433	TCMSP/ETCM	<i>Ligusticum chuanxiong</i> Hort
8	Clionasterol	36.91	0.75	MOL001771	TCMSP/ETCM /Batman	Ligusticum chuanxiong Hort, Pueraria lobata (wild.) Ohwi, Carthamus tinctorius L, Panax notoginseng (Burk.) F.H. Chen
9	Glyceryl palmitate	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
10	Butylphthali de	NA	NA	NA	ETCM/Batman	<i>Ligusticum chuanxiong</i> Hort
11	3-[(2,6-Dide oxy-3-o-met hylhexopyra nosyl)oxy]- 14-hydroxy card-20(22) -enolide	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
12	Senkyunoli de	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
13	Spathulenol	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
14	2-Methoxy- 4-(3-Metho xy-1-Propen yl)-Phenol	NA	NA	NA	ETCM/Batman	<i>Ligusticum chuanxiong</i> Hort
15	(Z)-4,5-Dih ydro-6,7-Ci	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort

16	s-Dihydroxy-3-Butylidene Phthalide Sedanonic Acid	NA	NA	NA	ETCM/Batman	<i>Ligusticum chuanxiong</i> Hort
17	(Z)-4,5-Dihydro-6,7-Trans-Dihydroxy-3-Butylidene Phthalide	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
18	Chuanxiong zine	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
19	(Z)-6,7-Epoxy-6,7-Dihydrodigustilide	NA	NA	NA	ETCM/Batman	<i>Ligusticum chuanxiong</i> Hort
20	Z'-3,8-Dihydro-6,6',7,3'-diligustilide	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
21	(Z,Z')-Diligustilide	NA	NA	NA	ETCM/Batman	<i>Ligusticum chuanxiong</i> Hort
22	3-N-Butyl-3-Hydroxy-4,5,6,7-Tetrahydro-6,7-Dihydroxy Phthalide	NA	NA	NA	ETCM/Batman	<i>Ligusticum chuanxiong</i> Hort
23	5-Hydroxymethyl-6-Endo-(3'-Methoxy-4'-Hydroxyphenyl)-8-Oxabicyclo[3.2.1]-Oct-3-En-2-One	NA	NA	NA	ETCM	<i>Ligusticum chuanxiong</i> Hort
24	Cnidium Lactone	NA	NA	NA	ETCM/Batman	<i>Ligusticum chuanxiong</i> Hort
25	Ethyl Linoleate	46.1	0.2	MOL001495	Batman	<i>Ligusticum chuanxiong</i> Hort
26	Chrysanthe	38.72	0.58	MOL004492	Batman	<i>Ligusticum chuanxiong</i>

	maxanthin					Hort
27	L-Valine-L-Valine Anhydride	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
28	Fenchone	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
29	Epoxydihydrolinalool	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
30	Dillapiol	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
31	Methyl Phenyl Carbinol	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
32	Borneol	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
33	Sec-Butyl Isothiocyanate	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
34	Camphor	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
35	Citronellol	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
36	Z-Ligustilide	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
37	Vallesiachotamine	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
38	1-Methoxy-2-Methylanthraquinone	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
39	Vanillin Acetate	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
40	N-Butyl-2-Ethylbutylphthalate	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
41	2,3-Dihydro-5,7-Dihydroxy-2,6-Dimethyl-8-(3-Methyl-2-Butenyl)-4H-1-Benzopyran-4-One	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
42	Cocaine	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort

43	Senkyunolide K	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
44	Terpinen-4-Ol	NA	NA	NA	Batman	<i>Ligusticum chuanxiong</i> Hort
45	formononetin	69.67	0.21	MOL000392	TCMSP/Batman/ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
46	beta-sitosterol	36.91	0.75	MOL000358	TCMSP	<i>Pueraria lobata</i> (wild.) Ohwi, <i>Carthamus tinctorius</i> L, <i>Panax notoginseng</i> (Burk.) F.H. Chen
47	3'-Methoxydaidzein	48.57	0.24	MOL002959	TCMSP	<i>Pueraria lobata</i> (wild.) Ohwi
48	Daidzein-4,7-diglucoside	47.27	0.67	MOL003629	TCMSP/ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
49	Coumestrol	32.487	0.34	MOL012976	Batman/ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
50	Robinin	39.844	0.71	MOL006070	Batman/ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
51	Coumingidine	NA	NA	NA	Batman	<i>Pueraria lobata</i> (wild.) Ohwi
52	Dauricine	NA	NA	NA	Batman	<i>Pueraria lobata</i> (wild.) Ohwi
53	Tuberosin	NA	NA	NA	Batman	<i>Pueraria lobata</i> (wild.) Ohwi
54	Robustadiol A	NA	NA	NA	Batman	<i>Pueraria lobata</i> (wild.) Ohwi
55	Puerarol	NA	NA	NA	Batman/ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
56	Dalbergene	NA	NA	NA	Batman	<i>Pueraria lobata</i> (wild.) Ohwi
57	5-Methylhydantoin	NA	NA	NA	Batman	<i>Pueraria lobata</i> (wild.) Ohwi
58	3-Methoxy Pyridine	NA	NA	NA	Batman	<i>Pueraria lobata</i> (wild.) Ohwi
59	Kudzusapogenol B Methyl Ester	NA	NA	NA	ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
60	Kudzusapogenol C	NA	NA	NA	ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
61	(5S)-5-methylimidazoli	NA	NA	NA	ETCM	<i>Pueraria lobata</i> (wild.) Ohwi

	dine-2,4-dione					
62	(-)-Tuberostin	NA	NA	NA	ETCM	<i>Pueraria lobata</i> (wild.) Ohwi
63	puerarin	24.03	0.69	MOL012297	Supplement	<i>Pueraria lobata</i> (wild.) Ohwi
64	Flavoxanthin	60.41	0.56	MOL002680	TCMSP	<i>Carthamus tinctorius</i> L
65	4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	48.47	0.36	MOL002694	TCMSP	<i>Carthamus tinctorius</i> L
66	lignan	43.32	0.65	MOL002695	TCMSP	<i>Carthamus tinctorius</i> L
67	lupeol-palmitate	33.98	0.32	MOL002698	TCMSP	<i>Carthamus tinctorius</i> L
68	Phytoene	39.56	0.5	MOL002706	TCMSP	<i>Carthamus tinctorius</i> L
69	phytofluene	43.18	0.5	MOL002707	TCMSP	<i>Carthamus tinctorius</i> L
70	Pyrethrin II	48.36	0.35	MOL002710	TCMSP	<i>Carthamus tinctorius</i> L
71	6-Hydroxykaempferol	62.13	0.27	MOL002712	TCMSP	<i>Carthamus tinctorius</i> L
72	baicalein	33.52	0.21	MOL002714	TCMSP	<i>Carthamus tinctorius</i> L
73	qt_carthamone	51.03	0.2	MOL002717	TCMSP	<i>Carthamus tinctorius</i> L
74	6-Hydroxyningaringenin	33.23	0.24	MOL002719	TCMSP/ETCM /Batman	<i>Carthamus tinctorius</i> L
75	quercetagenin	45.01	0.31	MOL002721	TCMSP	<i>Carthamus tinctorius</i> L
76	7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	45.75	0.19	MOL002757	TCMSP	<i>Carthamus tinctorius</i> L
77	beta-carotene	37.18	0.58	MOL002773	TCMSP	<i>Carthamus tinctorius</i> L
78	Baicalin	40.12	0.75	MOL002776	TCMSP	<i>Carthamus tinctorius</i> L
79	kaempferol	41.88	0.24	MOL000422	TCMSP/Batma	<i>Carthamus tinctorius</i> L

80	Stigmasteryl	43.83	0.76	MOL000449	TCMSP/Batman	Carthamus tinctorius L, Panax notoginseng (Burk.) F.H. Chen
81	luteolin	36.16	0.25	MOL000006	TCMSP	Carthamus tinctorius L
82	CLR	37.87	0.68	MOL000953	TCMSP	Carthamus tinctorius L
83	quercetin	46.43	0.28	MOL000098	TCMSP/ETCM/Batman	Carthamus tinctorius L, Panax notoginseng (Burk.) F.H. Chen, Crataegus pinnatifida Bunge
84	Onjixanthone I	79.16	0.3	MOL003370	ETCM/Batman	Carthamus tinctorius L
85	Dehydrosafynol	NA	NA	NA	ETCM/Batman	Carthamus tinctorius L
86	15a,20a-Dihydroxy-a4-Pregnen-3-One	NA	NA	NA	ETCM	Carthamus tinctorius L
87	Onjixanthone II	NA	NA	NA	ETCM/Batman	Carthamus tinctorius L
88	Alpha-Onocerin	39.31	0.73	MOL005421	Batman	Carthamus tinctorius L
89	Linoleyl Acetate	42.1	0.2	MOL001645	Batman	Carthamus tinctorius L, Crataegus pinnatifida Bunge
90	Sagittariol	NA	NA	NA	Batman	Carthamus tinctorius L
91	2-Hexanol	NA	NA	NA	Batman	Carthamus tinctorius L
92	Dehydroshikimic Acid	NA	NA	NA	Batman	Carthamus tinctorius L
93	DFV	32.76	0.18	MOL001792	TCMSP	Panax notoginseng (Burk.) F.H. Chen
94	Diop	43.59	0.39	MOL002879	TCMSP/ETCM	Panax notoginseng (Burk.) F.H. Chen
95	ginsenoside rh2	36.32	0.56	MOL005344	TCMSP	Panax notoginseng (Burk.) F.H. Chen
96	ginsenoside f2	36.43	0.25	MOL007475	TCMSP	Panax notoginseng (Burk.) F.H. Chen
97	Sitogluside	20.63	0.62	MOL000357	ETCM	Panax notoginseng (Burk.) F.H. Chen
98	Dicapryl Phthalate	40.59	0.40	MOL002032	ETCM	Panax notoginseng (Burk.) F.H. Chen
99	Poriferaster	43.83	0.76	MOL001659	ETCM	Panax notoginseng

	ol					(Burk.) F.H. Chen
100	Cyclo-(Ala-Pro)	NA	NA	NA	ETCM	<i>Panax notoginseng</i> (Burk.) F.H. Chen
101	Cyclododecanone	NA	NA	NA	ETCM/Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
102	Cyclo-(Ala-Val)	NA	NA	NA	ETCM	<i>Panax notoginseng</i> (Burk.) F.H. Chen
103	Panaxydol	NA	NA	NA	ETCM	<i>Panax notoginseng</i> (Burk.) F.H. Chen
104	2,8-Dimethyl-5-Acetyl-Bicyclo[5,3,0]Decadiene-1,8	NA	NA	NA	ETCM	<i>Panax notoginseng</i> (Burk.) F.H. Chen
105	Panaxadiol	33.09	0.79	MOL005376	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
106	Cycloeucaleanol	39.73	0.79	MOL009653	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
107	(-)-Dicentrine	NA	NA	NA	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
108	(-)-2d,4d,6d,8d-Tetramethyl Undecanoic Acid	NA	NA	NA	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
109	Sandaracopimarinol	NA	NA	NA	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
110	Ethyl Pyroglutamate	NA	NA	NA	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
111	Dithiocyclopentene	NA	NA	NA	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
112	Coprine	NA	NA	NA	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
113	3,4-Dimethylbenzoic Acid	NA	NA	NA	Batman	<i>Panax notoginseng</i> (Burk.) F.H. Chen
114	Suchilactone	57.519	0.56	MOL005384	Batman	<i>Crataegus pinnatifida</i> Bunge
115	Proscillaridin A	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
116	Ethylnotopterol	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge



117	4-Methylcyclohexanone	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
118	Citronellal	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
119	3-Methylhistidin	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
120	3,7,11-Trimethyldodecan-1,7,10-Trien-3-Ol-9-One	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
121	Epicatechin	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
122	Gamma-Decanolactone	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
123	Dimethyl Camphorate	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
124	3-Methyl-1,2-Cyclopentanediol	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
125	1-Ethyl-4,8-Dimethoxy-Beta-Carboline	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
126	2-Methylcyclopentanone	NA	NA	NA	Batman	<i>Crataegus pinnatifida</i> Bunge
127	Squalene	33.55	0.42	MOL001506	ETCM	<i>Crataegus pinnatifida</i> Bunge
128	Eburicoic Acid	38.70	0.81	MOL000287	ETCM	<i>Crataegus pinnatifida</i> Bunge
129	Lanosterol	42.12	0.75	MOL001979	ETCM	<i>Crataegus pinnatifida</i> Bunge
130	Eburicol	42.37	0.77	MOL002588	ETCM	<i>Crataegus pinnatifida</i> Bunge
131	Dehydroeburicoic Acid	44.17	0.83	MOL000300	ETCM	<i>Crataegus pinnatifida</i> Bunge
132	Officinalic Acid	NA	NA	NA	ETCM	<i>Crataegus pinnatifida</i> Bunge
133	ursolic acid	16.77	0.75	MOL000511	Supplement	<i>Crataegus pinnatifida</i> Bunge
134	Hydroxysafflor Yellow	NA	NA	NA	Supplement	<i>Carthamus tinctorius</i> L

135	A Notoginsenoside R1	4.27	0.13	MOL012851	Supplement	<i>Panax notoginseng</i> (Burk.) F.H. Chen
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**Supplementary Table S2. Drug targets of NDSP**

STAT3	GRM2	ALOX12	LIMK2	PDE8B	FASN	RPA1	CA5A	EPHB4
ESR1	JAK3	AKR1B1	CDC25B	HTR2A	GPR119	OAT	ERCC5	NFKB1
ESR2	JAK2	PDE5A	GRIA1	DRD3	PPP5C	DHODH	FEN1	CFTR
BRD4	PLK1	TAS2R31	APP	HTR6	PPP1CA	FABP2	TOP1	GLO1
BRD2	HSP90AA 1	ANPEP	CTSD	MCHR1	AKR1C2	ABCC9	FCER2	ARG1
MDM2	ECE1	PPIA	ACACA	HTR1F	RARG	KCNJ11	PLAA	AHR
ADORA2 A	HCRTR2	GCGR	SLC5A2	HTR7	RARB	KCNE1	WEE1	EZR
MAPK14	HCRTR1	ALPL	S1PR3	SLC22A2	RARA	TRPV3	CCR9	NTRK1
KCNA5	PYGL	PLA2G1B	S1PR1	SLC47A1	RXRG	TOP2A	GRK6	DAPK3
P2RX7	TRPA1	FGFR1	ACACB	DRD5	NPY2R	CA3	F8	BRSK2
EPHX1	NPY5R	CDK5R1	PDE2A	HTR3B	OXTR	CA6	ADAM10	MARK3
TNKS2	GABRA2	NOX4	CA2	HTR5A	PTGIR	PSMB5	CD81	SCN10A
FADS1	SAE1	LDHA	CA4	PBK	ASAH1	PSMB2	CYP24A1	PARP10
CHRM4	NR1H3	FLT3	CDC25A	SLC18A2	MGAT2	PSMB1	ACVRL1	BCL2A1
CHRM5	NR1H2	EGLN1	NR1I3	PHLPP2	PDE6D	ICMT	GSK3A	PDE1C
CHRM2	NAAA	MMP3	NR1H4	CHEK2	ITK	UTS2R	XIAP	DAPK1
CHRM3	PDE4B	ROCK2	GPBAR1	NMT1	SLC6A15	ACPP	NR1D1	MPG
MTNR1A	CCKBR	ROCK1	SHH	PKN2	CETP	BRS3	MALT1	PIK3R1
GABRA1	CACNA1 D	PTK2B	UGT2B7	PKN1	MAP3K5	EIF2AK3	GLP1R	CAMK2B
GABRB3	HTR2B	KDM1A	POLA1	DRD4	BRD3	STK3	NUAK1	NEK6
GABRA6	HTR2C	DHFR	NPC1L1	HIF1A	GSR	STK26	SPHK2	AXL
GABRA5	LIMK1	MSR1	G6PD	DPP4	TXK	HTR4	SPHK1	AKR1C4
CYP11B1	EGFR	GSTA1	GABBR1	BIRC2	FGR	BDKRB1	KCNN3	AMY1A
IMPDH2	DUSP3	PIM2	NR3C1	CDK1	EPHA6	PARP3	S1PR2	MAPT
CYP11B2	CASP3	ADAM17	DRD2	PRCP	PTK6	MMP1	SRD5A1	INSR
MTNR1B	PTP4A3	MMP7	AKR1B10	MELK	EPHB3	RASGRP3	CCR4	APEX1
PTGS1	FNTA	ERN1	POLB	HCN4	EPHA3	PLA2G2A	PDK1	KLK1
CCR2	CYP19A1	HDAC7	KCNK2	HCN1	BTK	CTSF	HSP90B1	KLK2
ADORA2 B	KCNA3	CALM1	ALDH2	HTR1A	COQ8B	GLI2	AGTR1	PGD
GRM5	FTO	ADRA2B	TBXAS1	NQO1	EPHA1	CACNA2 D1	IKBKB	SNCA
PABPC1	GAPDH	FLT4	CTRC	ERG	FPR1	AVPR1A	KLKB1	DNMT1
HSD17B2	BCL2	PDGFRA	IDO1	CHRN3	MYLK	TRPV1	SERPINE 1	MMP14
PDE10A	ALDH1A 1	MME	CYP2A6	NOS1	HSP90AB 1	C3AR1	PLA2G5	STAT1
JUN	PARP1	LTB4R	XPO1	CDK9	STAT6	CAPN1	PLA2G10	FBP1
MAOB	TNKS	OPRD1	CTRB1	DYRK1A	CXCR2	TACR1	HNF4A	PARP14

CTSV	SOAT1	MAOA	CTSH	PDE7A	KCNMA1	RORB	COMT	PARP15
CTSL	HDAC6	QPCT	METAP1	MPI	MAP2K2	CDK8	DRD1	NR1I2
CHRM1	HDAC1	FDFT1	CTSC	TYK2	MIF	THRA	F3	H LCS
ELANE	RPS6KA2	RORC	CCR8	METAP2	NCOR1	SLC5A1	CHRNA4	PRKACA
PRKDC	HSD11B1	FYN	CEL	KAT2B	MAPKAP K2	CCR3	KCNN1	ADA
CTSB	BRAF	EPHA2	CHRNA3	GRM4	HDAC11	CACNA2 D2	KCNN2	NTRK2
ALOX5	SIGMAR1	YES1	MPO	NISCH	HDAC10	PDE4A	ADRB2	NAE1
CNR1	CSNK2A1	BLK	ADH1A	TNNI3K	CMA1	GNRHR	ADRB1	CYP1A1
MEN1	AR	SYK	ADH1C	GCK	RPS6KB1	MCL1	ADRB3	ST6GAL1
FKBP1A	SLC6A2	CSK	SERPINA 6	CDC7	MKNK1	F13A1	OPRM1	TACR2
PSEN2	CYP17A1	PIK3CG	VDR	CISD1	SLC29A1	CFD	RBBP9	SIRT1
P2RX3	CXCR3	EPHB2	SQLE	PTPRC	PLG	TEK	PDE1A	PLA2G4A
MAPK11	CACNA1 B	BMX	HMGCR	DGAT1	CTSG	GLI1	EHMT2	PI4KB
SMO	CCNE2	LYN	CYP2C19	AKT1	PDE9A	KCNJ1	EHMT1	FKBP5
TBXA2R	CCNB3	EPHA5	SLC6A4	HDAC2	GPR18	G6PC	MAP2	ERBB4
LIPE	CDK7	EPHA4	SREBF2	CA13	TDO2	PTPRF	AVPR1B	KNG1
TAAR1	BACE1	ATP1A1	FABP4	CCNE1	PGGT1B	PTPN2	MLNR	TUBB1
PLAU	CTSK	TTL	PPARA	XDH	CPB1	ADRA1B	EZH2	TRHR
TRPM8	CCNC	F2RL1	TERT	AOC3	RGS4	MMP9	MAPK7	FPR2
SLC6A9	ICAM1	PRKCA	FABP3	CNR2	CASP7	HPGDS	FGFR3	NR5A1
TRPC6	VCAM1	GLRA1	FABP5	PTGES	GABRG2	KCNJ6	IGF1R	BRD9
TRPC3	SELE	GLRA2	PPARD	FFAR1	MMP2	TTK	PDPK1	BACE2
CYP26A1	SLC6A3	ALK	FABP1	F2R	CLK3	RIPK1	MYLK2	PGK1
PTGDR2	ADORA3	MTOR	CYP51A1	GRIN2B	PKM	WNT3A	CLK1	MAP3K7
ELOVL6	GPR139	PRKCQ	JAK1	AKR1C1	PPOX	TK1	SELP	ATM
ALOX15	NQO2	ERBB2	RORA	NPY1R	KCNN4	MMP12	MAP4K4	AGPAT2
NAMPT	KCNB1	CCNT1	PTGER1	AVPR2	DYRK1B	CAPN2	CALCRL	F9
RBP4	HDAC3	PDE3A	PTGER2	AKR1C3	TNF	F11	AKT2	GRIN1
TACR3	PARP2	PDE3B	DHCR7	F2RL3	SRD5A2	NFKBIA	ATP12A	HPGD
MDM4	TLR9	SORD	PTPN6	CYP26B1	PTPN11	NEK2	DPP8	HRH2
BCHE	SIRT2	MAPK1	NOS2	NR3C2	HSPA1A	POLR1A	DPP7	ABHD6
CES1	CSF1R	NR4A2	HSD11B2	TGM1	CXCL8	CPT1A	DPP9	NOD1
EPHX2	FAAH	PIK3CA	PRKCE	INCENP	KDM6B	CPT2	MC4R	NOD2
CCR1	CSNK1E	PRKCD	IL1B	PYGM	MAPK3	CCND1	SSTR2	BMP1
IDH1	CHEK1	AMPD3	ADRA2A	GRM1	TTR	SLC2A1	SSTR4	BAD
CTSS	PGR	GYS1	ADRA2C	NLRP3	CXCR1	SLC2A3	NPBWR1	CCND3
HSD17B3	GUSB	PRKCB	ADRA1A	SOAT2	KDM4E	PTK2	GHSR	HDAC5
ALOX5A P	CELA1	CDK4	PCSK7	ABL1	GRK2	CPT1B	HCN2	HDAC4

CRHR1	PREP	ADK	C1R	CASR	KDM4A	SLC6A1	HCN3	HDAC9
RAF1	C5AR1	F2	EDNRA	PFKFB3	KDM4D	HCK	TPSAB1	NCOR2
CDK2	BMP4	RPS6KA5	PLA2G6	SCARB1	NR4A1	ACE	MC1R	ALPG
PIM1	PDE4C	F10	ADRA1D	TYMS	SORT1	PSENEEN	CAMK2D	EP300
MAPK8	TGFBR1	GSTP1	PDE4D	SLC19A1	PTGER4	LGMN	LNPEP	DBF4
KCNH2	CA1	GSTM2	HRH3	FOLR1	SLCO1B1	SLC2A2	PRKCZ	CSNK1G1
PTAFR	FAP	PPP2CA	HRH4	FOLR2	BCAT2	CSNK1D	BRPF1	RPS6KA1
MAPK10	CA7	REN	PRSS1	SLC46A1	DAO	P2RY1	BIRC3	IGFBP6
SRC	TGM2	PRF1	CHRNA4	HDAC8	MAP2K1	PHOSPH O1	AURKB	IGFBP4
MAPK9	CENPE	CBFB	THRB	FPGS	ACE2	CACNA1 C	CACNA1 H	IGFBP5
DYRK2	KDM4C	ITGAL	RAPGEF4	GART	CASP1	SSTR3	AKT3	IGFBP2
PIM3	PPARG	LRRK2	CREBBP	ATIC	MKNK2	GPR55	MBTPS1	IGFBP1
VCP	ABCG2	PIK3CD	KCNJ5	PRKCH	CTSA	CYP1A2	HTR1B	HLA-DR B1
PANK3	CES2	PIK3CB	ALDH3A 1	PRKCG	SLC22A1 2	TYR	HTR1D	SCN5A
TSPO	PTPN1	SCD	CDC25C	PAM	AKR1A1	CBR1	UGCG	NPEPPS
FLT1	SHBG	GBA	HTT	TRPV4	HCAR2	PTPRS	PAK1	RHOA
SCN9A	RXRA	CDK6	HMOX1	ACP1	CCR5	MGAM	MAP4K2	SLC6A5
LCK	PTGS2	BCL2L1	ABCC1	ABCB1	PLEC	ESRRA	BIRC8	PRLHR
MMP13	ACHE	AURKA	EGLN3	LPAR6	IDE	ESRRB	MC5R	CAMKK2
KIF11	ADORA1	MAP3K14	CHRNA7	LPAR5	ITGB1	PON1	ITGA2B	SELL
MMP8	HSD17B1	PDGFRB	HTR3A	IL2	GPR35	PLAT	CXCR4	MMP16
MAP3K8	PLA2G7	KIT	ACKR3	IKBKE	HAO2	CYP1B1	CPB2	NEU4
CA12	RET	TYRO3	BDKRB2	TBK1	FOLH1	STS	NMUR2	GABBR2
CA9	GSK3B	CYP2C9	IRAK4	OPRK1	KMO	IGFBP3	RPS6KA3	SLC22A6
MGLL	KDR	CYP3A4	HRH1	PPM1B	KDM5A	CA14	CD38	PHF8
SLC18A3	MET	GRB2	LTA4H	PPP1CC	KDM5B	CA5B	PLK4	PTGFR
KDM5C	USP13	TH	FES	PEPD	PDE11A	HGFAC	ITGB7	HSD17B1 4
KDM2A	PDE7B	NUDT1	ROS1	ENPEP	ATP4B	FURIN	ITGB5	YWHAG
GSTK1	EPAS1	BAZ2B	NTRK3	SLC15A1	QTRT1	PCSK6	MPL	PGF
HAO1	HPRT1	BAZ2A	LTK	ERAP2	PORCN	PGC	P2RY12	VEGFA
PTGES2	PER2	NOS3	IL6	KISS1R	SLC9A1	TNFRSF1 0A	PPM1A	PDE1B
PTGDR	KMT5A	ADAMTS 5	UPP1	WDR5	CHUK	LAP3	ITGA4	MAP3K12
CDC45	GLUL	CSNK2A2	EIF2AK1	GZMB	GRIK1	NTSR1	APLNR	RAP1A
TP53	SLC1A2	DYRK4	STK16	XPNPEP1	GRIK2	DNM1	CASP8	KRAS
PTGER3	RNPEP	PLA2G4B	CDK5	XPNPEP2	HSF1	PDF	PLAUR	DNAJA1
RXRβ	ADH7	PLA2G4C	GRK3	TMPRSS6	CCKAR	CSNK1A1	FKBP4	CASP6

SLC16A1	SLC5A7	PIN1	CASP9	HPN	EDNRB	ADH1B	GCG	DUSP1
DAGLA	FER	KYNU	CASP2	HLA-A	ITGAV	TPO	CYSLTR1	TDP2
PTPRCAP	TNK2	GFPT1	GRK5	ST14	TLR4	PAOX	PLCG1	TYMP
PLA2G2C	LGALS3	PIK3C3	S1PR5	HASPIN	CCND2	KCNK9	CLK2	GPR88
KDM4B	LGALS8	SLC10A2	S1PR4	DYRK3	TMIGD3	PRMT3	KCNK3	KARS
FGF1	IL6ST	OPRL1	PPP2R5A	MECP2	SLC1A1	GRIN2A	HPSE	
FGF2	LSS	AMPD2	CLK4	ATR	USP10	GRIA2	LGALS4	

**Table S3 Therapeutic targets for ischemic stroke**

APP	SOD2	FGA	CLU	ALOX5	LAMA2	HCRT	SLC6A8	HLRC1	CHRM5
IL6	LCN2	PDGFB	EGF	CD40LG	ABCB1	EDNRA	BCAP31	CRTR	CACNA2D1
TNF	IL18	CASP9	PLA2G2A	IL13	NAGLU	RELA	CCCSX	CMS15	CACNB2
KRIT1	PRNP	GRIK2	HSPA5	SLC1A3	SRC	EDNRB	RPRGL2	CLOVE	CACNA1D
F2	NFE2L2	ANGPT1	MIR210	CDH5	TF	NOD2	RPRGL1	CHDS7	CALM1
CST3	HMGB1	SLC17A5	IL17A	CTSB	ACHE	IL15	PRKCL	CEDNIK	CYP2B6
COL4A1	MB	PARP1	SMAD2	CTSD	MAPK10	CNTF	NEDMIC	CCM1	CYP2E1
NOS2	GRIN1	IL1A	APOB	ESR1	ADORA3	SOD3	NEDMLHB	CCDS2	CYP3A5
NOS3	ADAMTS13	F8	TXN	PIK3CG	MME	PRKN	MGC4067	CADASIL1	CACNA1G
ICAM1	NGF	EGR1	MBL2	BMP6	IDO1	HSPD1	MCAP	C7orf22	CACNA1H
SOD1	CD36	MAP2	ATP1A2	MAOA	CD34	TFPI	KURU	BSS	CACNA1I
MPO	NPPA	G6PD	TIMP1	CYP2C19	AQP1	PRKAA2	IDDEBF	BAP31	CACNG1
PIK3CA	TSC2	SETD2	LTA	GLUL	ITPR1	SST	GLNRS	ARMD11	CACNG2
GFAP	SLC1A2	SHH	SDHB	CD46	ACE2	MYH7	DXS1357E	AGS1	CACNG3
ACE	IGF1	SNCA	ITGAM	ANGPT2	SLC8A1	TOMM40	CVAP	AGAT	CACNG4
IL10	MAPK1	MBP	YRDC	PPARA	IL33	MAPK3	CRV	ADDL	CACNG5
TP53	MTOR	KCNJ5	SLC6A3	NEFL	SMPD1	CACNA1B	CPSQ3	AAA	CACNG6
CRP	PTGS2	REN	HP	TSPO	LPL	MYC	CCM3	AKR1C1	CACNG7
F5	PLG	FLT1	SMARCA1	TIMP2	CAMK2G	IL2RA	CCDS3	SLC22A6	CACNG8
CASP3	PIK3CA	HSPB1	HAVCR1	MAP2K1	IKBKG	STING1	CCDS1	CYP2C9	CACNA2D2
VEGFA	NTRK1	CR1	GRIN2A	MT-CO1	SLC9A1	RHOA	CASIL	RPS6KA3	CACNA2D3
MTHFR	AGTR1	CDK5	MIF	LOX	MALAT1	OLR1	CAM	NFKBIA	CACNA2D4

IL1B	SERPINA3	HSPA1A	CXCL10	COL1A1	PCNA	AOC3	BDPLT10	TNFAIP6	CACNA1F
BDNF	HSPA4	ACTA2	PECAM1	MIR155	PLA2G7	FOXP2	BDPLT1	IKBKB	CACNA1S
HMOX1	GP1BA	SPP1	PLAU	SLC12A2	TNNI3	CYBB	ARMD7	UGT1A6	CACNB1
TLR4	KNG1	APOH	ADRB2	ARG1	PARK7	IL1R1	ANKRD15	NAT2	CACNB3
VWF	AKT1	ADM	LDLR	THBS1	FGFR2	ALDH2	VWDP	SLC22A8	CACNB4
ALB	PLA2G6	VCAM1	COMT	CCL5	ARID1B	ABCA1	MSCCA	NEU1	CACNA1A
PTEN	JAK2	NTRK2	CSF1R	PTGS1	COX5A	MCU	MEPCA	ATP1A1	CACNA1E
SERPINC1	IL1RN	GSR	NPY	DNM1L	PRKCE	POMC	MCM	PDE10A	MAPK15
CXCL8	SLC2A1	PPARG	SELL	FMR1	NGB	TRPV4	KIAA0172	PDE5A	MAPK4
SERPINE1	CBS	AIF1	PROC	DAPK1	LMNA	DIAPH1	IMF2	PDE4A	MAPK6
MIR21	CYCS	HSPG2	CHAT	ADA	CD40	ITGA2B	HERNS	ABCC4	MAPK7
PLAT	IL4	CREB1	HTR2A	NF2	CDKN3	NTN1	FRTS1	ABCC5	PRKAA1
ENG	GJA1	FAS	SIRT1	PF4	GLS	NGFR	DDCH	RCAN1	PRKAB1
EPO	AQP4	NLRP3	STAT1	NES	P2RY12	TNFRSF1B	CJD	ORM1	PRKAB2
GRIN2B	ELANE	TLR2	DRD2	FN1	ERCC2	C4A	CARASIL	SLCO1B1	PRKAG1
MMP9	GAD1	TNFRSF1A	PSAP	LONP1	NFKB1	CASP8	AD1	SLCO1B3	PRKAG2
PSEN1	GPT	STAT3	MIR17	SERPINA1	HMGCR	CX3CR1	RVCLS	SLCO2B1	PRKAG3
IFNG	TGFB2	MMP2	EGFR	CXCL1	VCP	ALG14	MCMTC	ABCB11	MT-TL1
CTNNA1	MIR146A	CFH	TGFBR2	TGFBR1	CAMK2A	TREX1	LMNS	CYP3A4	ALOX5AP
EDN1	FGB	MAPK8	SERPINI1	MIR29B1	MPL	QARS1	CPSQ2	UGT1A1	FBN1
THBD	MEF2C	PON1	HPRT1	GAPDH	RAC1	PDCD10	CADASIL2	UGT1A3	ACSL4
CCL2	MAPK14	ADORA1	NOTCH1	CXCL2	CDKN2A	HLA-B	BDPLT3	UGT1A10	APOE
HIF1A	CXCL12	CALCA	CASP1	SMAD4	ABCC8	TAF8	CWS5	UGT2B7	MT-ND1
SMARC	KDR	CTLA4	TERT	BAD	MYD88	CCM2	CLAPO	UGT2B1	ADA2



A4								7	
MAPT	ODC1	SYNGA P1	TNNT2	FABP3	MIR29A	KANK1	CCM4	SLC22A 12	GLA
SELP	FGF2	JUN	CPT2	MIR106 B	GJB1	ACP	TNFA	SLC2A9	RNF213
XDH	AGT	ADORA 2A	ADIPOQ	PROCR	YWHAG	CERCA M	THPH2	CYP2C8	MT-ND4
S100B	ITGB3	VLDLR	F13A1	CLCN2	TGIF1	ADD3	THPH1	CACNA 1C	PDE4D
TGFB1	MIR126	MIR34A	CCL3	CXCR4	IGFBP3	HTRA1	TFAR15	CYP2D6	MT-CO2
COL3A1	BAX	EPRS1	CKB	ATM	HTRA2	FOLR1	TBN	PDE1B	MT-CO3
F3	HGF	TEK	C3	DLG4	TJP1	NINJ2	SPDA1	PDE1A	KAT6B
ENO2	LEP	SLC6A4	AGER	MMP1	ADCYA P1	TTC5	QARS	ADRA1 A	ADD1
BCL2	COL4A2	IDH1	ALDH5 A1	ACTB	CSF2	PRKCH	PRSS11	ADRA1 D	GUCY1 A1
CAT	FOS	IL2	ANXA5	CCND1	RPS27A	GATM	PRIP	ADRA1 B	GNB3
NOS1	SPTAN1	AIFM1	CNR1	THPO	TRIM8	GAMT	PKCL	CHRM1	MYH11
NPPB	APOA1	CALR	MIR145	AVP	DNMT1	DOHH	NEDCA FD	CHRM2	F7
SELE	CSF3	ITGB2	FLNA	BCL2L1	ASIC1	NOTCH 3	NCFTD	CHRM3	LPA
INS	GDNF	HSPA8	CP	F10	GRIA1	SNAP29	KANK	CHRM4	ELN
PTGIS	SCN5A	TTR	NDE1	TET2	ATRIP	SULT1A 3	TGFB3	ITGA2	MYH6
ABCC6	SLC2A1 0	ACVRL 1	F9	EPOR	ATRIP-T REX1	MIR124- 1	NR3C2	AGTR2	MAT2A
PON2	PRKG1	F2R	TH	GP6	PRTN3	ACTA2- AS1	HEY2	MFAP5	FOXE3
CDKN2 B-AS1	VKORC 1	SH2B3	ENPP1	GATA4	TBXA2 R	NKX2-5	MMP3	MYBPC 3	STRK1
PROZ	MYLK	RNF213- AS1	PPBP	SERPIN F2	BMP7	MIR9-1	ENTPD1	BACE1	MVCD3
SMAD3	RPL36A -HNRNP H2	HBB	POLG	MROS	MT-CY B	F12	KCNQ1	DARS2	FLAP
DCP1	ICH	ACE1	TACR3	ITGA4	BDKRB 2	CPB2	HCAR2	HDAC1	

**Table S4 The intersection genes of drug and disease**

STAT3	SLC6A3	TERT	MAP2K1	NFKB1	P2RY12	CASP3
ESR1	ADORA3	FABP3	ACE2	ARG1	ITGA4	GAPDH
ADORA2A	CSF1R	NOS2	CASP1	NTRK1	CASP8	BCL2
MAPK14	TGFBR1	PRKCE	SLC22A12	DAPK1	HDAC1	PARP1
CHRM4	PPARG	IL1B	HCAR2	MAPT	CACNA1B	UGT2B7
CHRM5	PTGS2	ADRA1A	MMP1	SNCA	BACE1	G6PD
CHRM2	ACHE	EDNRA	PLA2G2A	DNMT1	ICAM1	DRD2
CHRM3	ADORA1	PLA2G6	CACNA2D1	STAT1	VCAM1	ALDH2
PTGS1	PLA2G7	ADRA1D	CACNA2D2	ADA	SELE	MYLK
PDE10A	KDR	PDE4D	PDE4A	NTRK2	IDO1	MIF
JUN	PDE5A	KCNJ5	F13A1	SIRT1	MPO	PLG
CHRM1	MMP3	HMOX1	TEK	KNG1	HMGCR	MMP2
ELANE	CALM1	BDKRB2	ADRA1B	ATM	CYP2C19	ADRB2
CTSB	MME	HTR2A	MMP9	F9	SLC6A4	PDE1A
ALOX5	MAOA	HIF1A	NFKBIA	GRIN1	PPARA	MAP2
CNR1	PIK3CG	NOS1	CPT2	NOD2	TNF	MAPK7
TBXA2R	ATP1A1	AKT1	CCND1	BAD	HSPA1A	GLUL
PLAU	MTOR	XDH	SLC2A1	SCN5A	CXCL8	SLC1A2
TACR3	MAPK1	AOC3	ACE	RHOA	MAPK3	IL6
IDH1	PIK3CA	F2R	CACNA1C	SELL	TTR	CDK5
ALOX5AP	F2	GRIN2B	PON1	SLC22A6	SLCO1B1	EDNRB
MAPK8	F10	AKR1C1	PLAT	TP53	SELP	TLR4
MAPK10	REN	NR3C2	IGFBP3	TH	CACNA1H	MPL
SRC	BCL2L1	NLRP3	F8	NOS3	ITGA2B	EGFR
VCP	CYP2C9	FOLR1	ACVRL1	YWHAG	CXCR4	SHH
TSPO	CYP3A4	PRKCH	AGTR1	VEGFA	CPB2	GSR
FLT1	GRIA1	TRPV4	IKBKB	PDE1B	RPS6KA3	F3
JAK2	APP	ABCB1	SERPINE1	FGF2	CASP9	HPRT1
CACNA1D	CTSD	IL2	COMT	GRIN2A	SLC9A1	GRIK2

**Table S5 The key active ingredients of NDSP**

Degree	Name	Neighborhood Connectivity	Radiality	Topological Coefficient
35	Officinalic Acid	11.77142857	0.992047192	0.131358885
33	baicalein	18.90909091	0.992541347	0.179090909
32	Cnidium Lactone	15.65625	0.992603116	0.142293689
32	senkyunone	17.34375	0.992634001	0.157151442
32	lignan	13.9375	0.992201615	0.14375
32	(-)-Dicentrine	16.6875	0.992479577	0.158459596
31	quercetin	18.83870968	0.992603116	0.171526055
31	Panaxydol	20.38709677	0.992541347	0.190069576
31	Proscillaridin A	16.12903226	0.992325154	0.159252971
30	Dauricine	13.9	0.992325154	0.134375
30	quercetagetin	19	0.992386923	0.183673469
30	3,7,11-Trimethyldodeca-1,7,10-Trien-3-Ol-9-One	20.2	0.992417808	0.193939394
29	wallichilide	17.37931034	0.992325154	0.16885887
29	6-Hydroxykaempferol	18.96551724	0.992356039	0.183321605
29	kaempferol	20.34482759	0.992479577	0.189655172
29	Gamma-Decanolactone	19.34482759	0.992479577	0.179851251
28	4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	22.03571429	0.992294269	0.216863034
28	luteolin	20.67857143	0.992448693	0.192927171
28	Eburicoic Acid	21.82142857	0.992417808	0.206152758
27	Sedanonic Acid	16.25925926	0.992448693	0.148148148
27	15a,20a-Dihydroxy-a4-Pregn-3-One	21.66666667	0.992448693	0.200647249
27	Pyrethrin II	17.03703704	0.992078077	0.176231176
26	3-[(2,6-Dideoxy-3-o-methylhexopyranosyl)oxy]-14-hydroxycard-20(22)-enolide(pubchem)	15.84615385	0.9922325	0.153053132
26	Ethyl Linoleate	19.46153846	0.992325154	0.184615385
26	Senkyunolide K	18.57692308	0.992263385	0.179356358
26	Dalbergenone	21.88461538	0.992201615	0.217548077
26	DFV	16.76923077	0.992325154	0.157692308
26	Panaxadiol	21.57692308	0.992417808	0.199775952
26	Ethylnotopterol	19.69230769	0.991985422	0.210025929
25	Cyclo-(Ala-Val)	20.92	0.992356039	0.195294118
24	(Z,Z')-Diligustilide	19.375	0.992263385	0.18375
24	1-Methoxy-2-Methylanthraquinone	19.5	0.992201615	0.18877551

24	N-Butyl-2-Ethylbutylphthalate	18.20833333	0.992078077	0.183067376
24	Z-Ligustilide	19.91666667	0.992263385	0.189166667
24	6-Hydroxynaringenin	18.25	0.992201615	0.176020408
24	Onjixanthone I	19.5	0.992139846	0.192708333
23	Cocaine	19.73913043	0.992170731	0.191215617
23	Mandenol	20.91304348	0.992356039	0.191471572
23	Coumestrol	19.91304348	0.992170731	0.19299024
23	Suchilactone	14.30434783	0.991583921	0.168409466
22	Z'-3,8-Dihydro-6.6',7.3'a-diligustilide	20.72727273	0.992016307	0.209864603
22	Coumingidine	12.72727273	0.991491267	0.152302243
21	2,3-Dihydro-5,7-Dihydroxy-2,6-Dimethyl-8-(3-Methyl-2-Butenyl)-4h-1-Benzopyran-4-One	23.14285714	0.992356039	0.208894879
21	Dillapiol	22.57142857	0.992016307	0.227067669
21	Dimethyl Camphorate	21.38095238	0.992047192	0.212301587
21	ursolic acid	22.04761905	0.992078077	0.216985763
20	Vallesiachotamine	18.7	0.991954538	0.188297872
20	3'-Methoxydaidzein	17.8	0.992108961	0.16969697
20	Cyclo-(Ala-Pro)	16.7	0.991923653	0.168817204
19	Dehydroeburicoic Acid	18.89473684	0.992108961	0.178947368
18	Citronellal	18.05555556	0.991892768	0.18144208
17	Myricanone	20.94117647	0.991954538	0.205579139
17	Senkyunolide	17.47058824	0.991583921	0.193771626
17	formononetin	20.94117647	0.991954538	0.205579139
17	Linoleyl Acetate	16.41176471	0.991676576	0.17513369
16	Dicapryl Phthalate	16.875	0.991583921	0.184593023
16	Ethyl Pyroglutamate	20.5625	0.99176923	0.21263587
16	Lanosterol	24.0625	0.991861884	0.242763158
15	(Z)-6,7-Epoxy-6,7-Dihydroligustilide	22.53333333	0.991830999	0.226666667
15	Clionasterol	24.86666667	0.992170731	0.225157233
15	Kudzusapogenol C	23.86666667	0.99170746	0.251282051
14	beta-sitosterol	24.21428571	0.991830999	0.241815476
14	(-)-2d,4d,6d,8d-Tetramethyl Undecanoic Acid	14.07142857	0.991398613	0.159407666
14	Sandaracopimarinol	25.42857143	0.991954538	0.244285714
14	Eburicol	24.71428571	0.99176923	0.252279635
13	Citronellol	28.30769231	0.991800114	0.284455128
13	CLR	23.76923077	0.991491267	0.264758497
13	Onjixanthone Ii	21.23076923	0.991583921	0.227312014
13	2,8-Dimethyl-5-Acetyl-Bicycl	23.61538462	0.991645691	0.24852071

	o[5,3,0] Decadiene-1,8			
13	1-Ethyl-4,8-Dimethoxy-Beta-Carboline	17.69230769	0.991305959	0.208653846
12	sitosterol	25.5	0.99170746	0.260638298
11	Butylphthalide	18.18181818	0.991058882	0.232186732
11	Robustadiol A	22.09090909	0.991645691	0.226783969
11	Robinin	20.81818182	0.991367729	0.235930736
11	7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	14.81818182	0.990842689	0.20624152
11	Sagittariol	25.18181818	0.991491267	0.274793388
10	Terpinen-4-Ol	27.6	0.991645691	0.282978723
10	(-)-Tuberosin	19.6	0.991336844	0.221428571
10	Tuberosin	19.6	0.991336844	0.221428571
10	Baicalin	20.2	0.991275075	0.234146341
10	qt_carthamone	10.7	0.990472073	0.173214286
10	Stigmasterol	27.3	0.991460383	0.298863636
10	Sitogluside	22.7	0.991460383	0.246590909
9	lupeol-palmitate	22.11111111	0.991058882	0.277777778
9	Coprine	12.22222222	0.990873574	0.16031746
9	Poriferasterol	27.44444444	0.991336844	0.311111111
8	Glyceryl palmitate	15.25	0.991027997	0.1875
8	Kudzusapogenol B Methyl Ester	15.375	0.99071915	0.21780303
8	ginsenoside rh2	12.75	0.990410303	0.209821429
7	Puerarol	13.57142857	0.990441188	0.216748768
7	ginsenoside f2	10.28571429	0.989947033	0.221088435
7	Notoginsenoside R1	10.28571429	0.989947033	0.221088435
7	3-Methylhistidin	13.57142857	0.990441188	0.216748768
6	Borneol	24.66666667	0.991089766	0.295833333
6	Daidzein-4,7-diglucoside	14.83333333	0.990224995	0.266025641
6	2-Hexanol	19	0.990750035	0.260869565
6	Dehydroshikimic Acid	23.5	0.990997112	0.292207792
6	Cyclododecanone	23.16666667	0.99071915	0.325980392
5	Spathulenol	23	0.990657381	0.328358209
5	Alpha-Onocerin	28.6	0.991089766	0.340740741
4	Epoxydihydrolinalool	23.5	0.990564727	0.346153846
4	3-Methyl-1,2-Cyclopentanediol	22.5	0.990472073	0.346774194
3	FA	15.33333333	0.98973084	0.367521368
3	Fenchone	30	0.990564727	0.439393939
3	Squalene	23	0.990008802	0.458333333
2	Camphor	28	0.990008802	0.551020408
2	L-Valine-L-Valine Anhydride	27	0.989977917	0.541666667
2	Methyl Phenyl Carbinol	19	0.989576416	0.5

2	3,4-Dimethylbenzoic Acid	22.5	0.98973084	0.5375
2	Cycloeucaleanol	21	0.989638186	0.540540541
2	4-Methylcyclohexanone	21	0.989576416	0.571428571

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**Table S6 The core target of NDSP**

<b>Degree</b>	<b>Name</b>	<b>Neighborhood Connectivity</b>	<b>Radiality</b>	<b>Topological Coefficient</b>
39	MAPK3	15.74358974	0.969262621	0.138101664
39	SRC	15.15384615	0.971651537	0.126912303
37	MAPK1	15.75675676	0.968784838	0.139440325
37	STAT3	15.78378378	0.969581143	0.145895896
36	TP53	13.88888889	0.96751075	0.138333333
29	AKT1	16.44827586	0.966236662	0.156321839
28	JUN	18	0.966555184	0.166666667
24	NFKB1	17.29166667	0.964484791	0.169526144
24	MAPK14	18.91666667	0.96432553	0.188333333
23	PIK3CA	17	0.96432553	0.17
21	ESR1	20.0952381	0.965440357	0.192765568
21	VEGFA	15.42857143	0.962255136	0.17281969
20	EGFR	19.55	0.965121835	0.189805825
20	IL6	17.65	0.961140309	0.205232558
19	F2	11.05263158	0.959388438	0.12879257
19	JAK2	18.21052632	0.963369963	0.189144737
18	MAPK8	17.61111111	0.963210702	0.185380117
18	RHOA	17.5	0.961777353	0.193209877
17	STAT1	22.94117647	0.962732919	0.229411765
17	TNF	15.88235294	0.957955088	0.208204334
16	IL2	21.6875	0.958910655	0.252180233
16	HDAC1	15.5625	0.958432871	0.203125
15	NFKBIA	22.33333333	0.962573658	0.224915825
14	CASP3	18.42857143	0.957636566	0.219387755
14	CASP8	19.21428571	0.959069916	0.218344156
14	IL1B	17.28571429	0.956999522	0.227443609
13	APP	8.923076923	0.952221691	0.147214854
13	CXCR4	14.61538462	0.957318044	0.199157007
13	HIF1A	24.30769231	0.959547699	0.27008547
13	MAP2K1	21	0.959229177	0.236888112
12	NOS2	19	0.960503265	0.213068182
12	MTOR	18.25	0.956043956	0.246621622
12	CALM1	8.25	0.952699474	0.145833333
12	SIRT1	15.83333333	0.954929129	0.232843137
12	FGF2	17.66666667	0.954929129	0.256038647
11	NOS3	13.45454545	0.954610607	0.178181818
11	BCL2L1	22.72727273	0.956840261	0.284090909
11	PLG	6.363636364	0.946169772	0.1875
11	PPARA	16.90909091	0.95508839	0.214452214
10	BAD	17.7	0.953177258	0.298305085
10	BCL2	24.3	0.958114349	0.296341463

10	NTRK1	21.3	0.957318044	0.267088608
10	MMP1	13.5	0.951903169	0.235087719
9	GAPDH	16.88888889	0.956999522	0.217893218
9	TERT	25.55555556	0.955566173	0.345345345
9	IKBKB	13.88888889	0.948399427	0.248484848
9	CCND1	24	0.958910655	0.282352941
9	CXCL8	20.55555556	0.957158783	0.289514867
9	MMP2	18	0.954451346	0.276923077
9	MMP9	18.44444444	0.955406912	0.263492063
8	ADRB2	11.125	0.952858735	0.18220339
8	PTGS2	16.625	0.953814302	0.246268657
8	SNCA	12	0.954929129	0.176136364
8	PPARG	19	0.952221691	0.296875
8	GRIN2B	9	0.951106864	0.1796875
8	KDR	19.125	0.954451346	0.269366197
7	EDNRA	16	0.950788342	0.278195489
7	MAPT	19.42857143	0.951903169	0.326876513
7	PARP1	14	0.94887721	0.291666667
7	CASP1	14.85714286	0.949992037	0.245238095
7	CDK5	15.57142857	0.953336519	0.244239631
7	IGFBP3	17.57142857	0.955566173	0.238747554
7	MMP3	17.14285714	0.949832776	0.317460317
7	TLR4	15	0.949036471	0.303206997
7	TEK	18.57142857	0.952380952	0.271008403
6	CYP3A4	4	0.929288103	0.282051282
6	AGTR1	8.166666667	0.946169772	0.206140351
6	CHRM1	18.66666667	0.953655041	0.266666667
6	SERPINE1	10	0.94887721	0.210144928
6	YWHAG	23.33333333	0.948399427	0.424242424
6	CASP9	22.83333333	0.94887721	0.415151515
6	NOS1	10	0.947762383	0.226190476
6	MAOA	3.833333333	0.913680522	0.282051282
6	CYP2C9	5.166666667	0.932154802	0.322916667
6	CYP2C19	5.833333333	0.933269629	0.291666667
6	SLC9A1	23.16666667	0.951425386	0.367724868
6	PRKCE	23.66666667	0.951584647	0.376344086
5	KNG1	5.4	0.933588151	0.317647059
5	ADRA1B	9.4	0.942028986	0.2875
5	CACNA1C	5.8	0.936614111	0.245454545
5	ITGA2B	16	0.946488294	0.312
5	PIK3CG	19.4	0.949354993	0.359259259
5	ALOX5	5	0.931677019	0.369230769
5	MAPK10	21	0.950788342	0.338709677
5	NLRP3	12.2	0.943940118	0.342857143

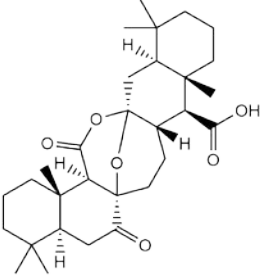
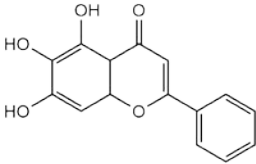
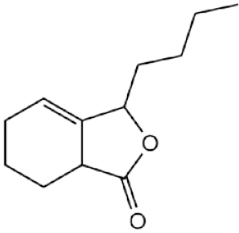


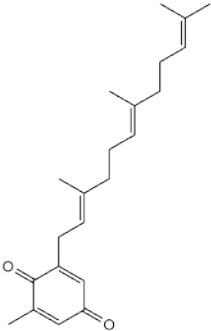
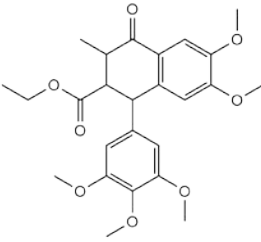
5	DNMT1	21.6	0.950310559	0.348387097
5	PLAU	19	0.952858735	0.301587302
5	FLT1	20.6	0.95046982	0.374545455
5	HSPA1A	28.4	0.95206243	0.43030303
5	VCAM1	13.2	0.949514254	0.254901961
4	ACE	8.25	0.939480809	0.32
4	REN	4.25	0.923873228	0.444444444
4	COMT	4	0.912087912	0.416666667
4	PTGS1	5	0.91017678	0.475
4	F9	6	0.932791846	0.338235294
4	ATM	18.25	0.946329033	0.39673913
4	CACNA2D1	2.75	0.911928651	0.45
4	DAPK1	23.75	0.954929129	0.347014925
4	DRD2	4	0.93183628	0.25
4	F10	7.5	0.936614111	0.340909091
4	F3	9.5	0.938206721	0.355769231
4	ITGA4	16	0.949514254	0.315
4	GRIN1	14.25	0.94887721	0.316666667
4	GRIN2A	14.25	0.94887721	0.316666667
4	NTRK2	23.5	0.954132824	0.3671875
4	ICAM1	11.5	0.945532728	0.275
4	MPL	24	0.947921644	0.489795918
4	PRKCH	29.25	0.950310559	0.5
3	ABCB1	20	0.948240166	0.401360544
3	ALDH2	4.333333333	0.895365504	0.619047619
3	AOC3	4.333333333	0.895365504	0.619047619
3	ARG1	9.666666667	0.939958592	0.412698413
3	CACNA1D	3.666666667	0.91176939	0.523809524
3	MYLK	29.33333333	0.947921644	0.630434783
3	NOD2	7.666666667	0.931199236	0.488888889
3	CPB2	10.66666667	0.937091894	0.430555556
3	SLC6A3	5	0.934065934	0.388888889
3	MPO	2.333333333	0.908902692	0.333333333
3	F8	9	0.935977066	0.428571429
3	PLAT	12	0.939321548	0.444444444
3	RPS6KA3	25.66666667	0.94425864	0.64957265
3	TH	11.66666667	0.943940118	0.365591398
2	ACE2	2.5	0.898709986	0.5
2	ADA	1	1	0
2	BDKRB2	8	0.929925147	0.615384615
2	CACNA1B	8	0.928014015	0.538461538
2	CACNA2D2	4	0.911291607	0.8
2	F2R	11	0.934702978	0.55
2	CTSB	3.5	0.922439879	0.5

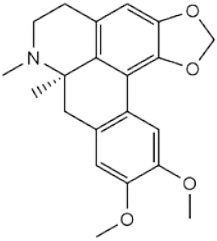
2	CTSD	11.5	0.940595636	0.5
2	UGT2B7	6	0.910336041	0.666666667
2	EDNRB	15.5	0.940595636	0.537037037
2	ELANE	6.5	0.929288103	0.5
2	F13A1	11.5	0.935977066	0.525
2	G6PD	22.5	0.944099379	0.576923077
2	HMOX1	26	0.943143813	0.702702703
2	SELP	4.5	0.926102883	0.5
2	SELE	4.5	0.928651059	0.642857143
2	TBXA2R	5	0.926421405	0.8
1	MME	2	0.873228221	0
1	ACHE	13	0.926739927	0
1	ACVRL1	1	1	0
1	TGFBR1	1	1	0
1	ADORA1	2	0.75	0
1	ADORA3	2	0.75	0
1	ADRA1A	5	0.916547221	0
1	PDE4A	8	0.927376971	0
1	PDE4D	8	0.927376971	0
1	AKR1C1	6	0.903806339	0
1	ALOX5AP	5	0.906195254	0
1	TTR	13	0.926739927	0
1	BACE1	13	0.926739927	0
1	CACNA1H	4	0.886446886	0
1	SCN5A	12	0.92721771	0
1	CNR1	4	0.906354515	0
1	CPT2	11	0.929606625	0
1	CSF1R	21	0.936773372	0
1	MIF	13	0.93183628	0
1	HMGCR	11	0.929606625	0
1	HPRT1	1	1	0
1	XDH	1	1	0
1	HTR2A	1	1	0
1	SLC6A4	1	1	0
1	IDH1	12	0.9350215	0
1	IDO1	6	0.888198758	0
1	SHH	13	0.933747412	0
1	MAPK7	3	0.918776875	0
1	PON1	3	0.883420927	0
1	VCP	15	0.937091894	0
1	SLC2A1	36	0.942028986	0
1	TRPV4	39	0.946169772	0

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Table S7 Parameters of molecular docking

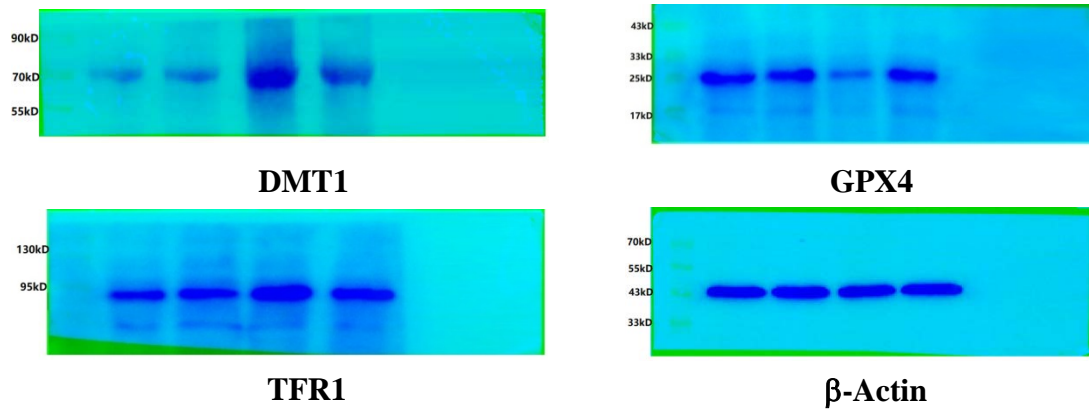
Name	Compound Structure	Target	Docking score	Hbond Number	Combination Type	Interaction Residue
Officinalic Acid		Erk1 (2ZOQ)	N.A.	N.A.	N.A.	N.A.
		Erk2 (4G6N)	-0.323	1	Van der Waals Attractive Charge Conventional Hydrogn Bond Carbon Hydrogn Bond Alkyl	GLY30 GLU31 LYS112 CYS164
Baicalein		Erk1 (2ZOQ)	-8.219	3	Van der Waals Conventional Hydrogn Bond Metal-Acceptor Pi-Cation Pi-Alkyl	ILE48 VAL56 ALA69 ASP123 MET125 LYS131 LEU173 CYS183 NA381
		Erk2 (4G6N)	-7.300	3	Van der Waals Conventional Hydrogn Bond Carbon Hydrogn Bond Pi-Sulfur Pi-Alkyl	VAL37 ALA50 LYS52 GLU69 LEU154 CYS164
Cnidium Lactone		Erk1 (2ZOQ)	-5.299	0	Van der Waals Metal-Acceptor Alkyl	ILE48 VAL56 NA381
		Erk2 (4G6N)	-5.204	0	Van der Waals Conventional Hydrogn Bond Alkyl	ALA50 LYS52 MET106 LEU154

Senkyunone		Erk1 (2ZOQ)	-4.891	0	Van der Waals Metal-Acceptor Alkyl Pi-Alkyl	ALA52 TYR53 VAL56 ALA69 LEU173 NA381 ILE29
		Erk2 (4G6N)	-4.244	0	Van der Waals Conventional Hydrogn Bond Alkyl Pi-Alkyl	ALA50 LYS52 ILE82 LYS112 LEU154 CYS164 ASP165
Lignan		Erk1 (2ZOQ)	-3.623	3	Van der Waals Conventional Hydrogn Bond Carbon Hydrogn Bond Metal-Acceptor Pi-Anion Amide-Pi Stacked Alkyl Pi-Alkyl	TYR47 GLY49 GLU50 GLY51 GLY54 VAL56 LYS131 LYS168 SER170 ASN171 CYS183 ASP184 NA381 ILE29 GLU31 GLY32
		Erk2 (4G6N)	-5.895	3	Van der Waals Conventional Hydrogn Bond Carbon Hydrogn Bond Alkyl Pi-Alkyl	VAL37 ALA50 LYS52 MET106 GLU107 LYS112 SER151 ASN152 LEU154

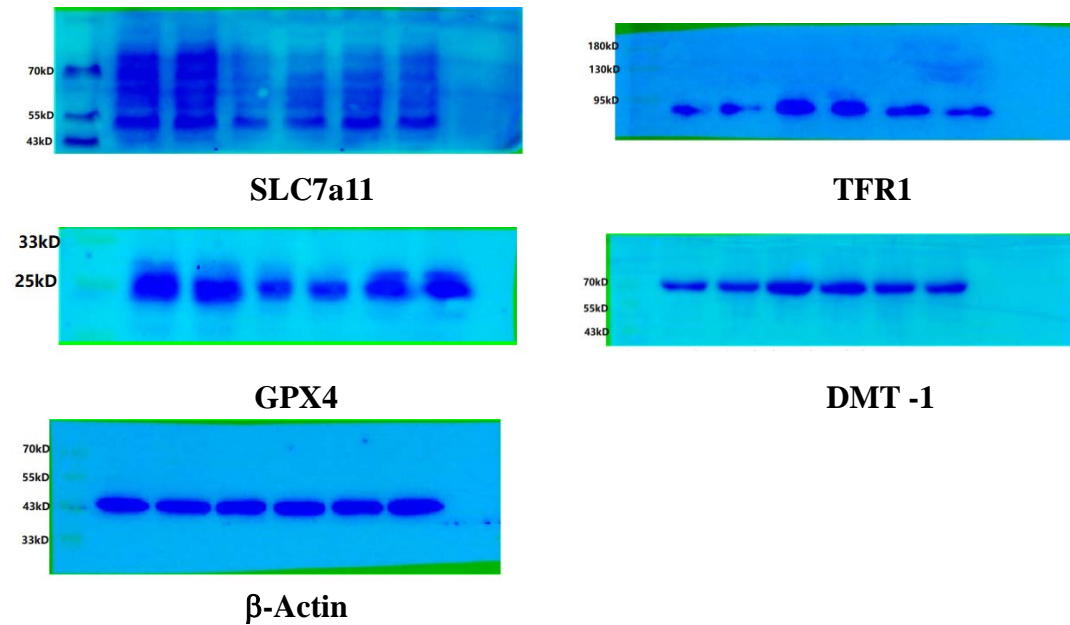
(-)-Dicentrine		Erk1 (2ZOQ)	3.520	2	Van der Waals Attractive Charge Conventional Hydrogn Bond Pi-Cation Amide-Pi Stacked Pi-Alkyl Van der Waals Conventional	GLY49 GLU50 ALA52 ASP166 LYS168 ASP184 ALA50
		Erk2 (4G6N)	-5.471	2	Hydrogn Bond Carbon Hydrogn Bond Pi-Anion Pi-Alkyl	GLN103 MET106 ASP109 LEU154

### Supplementary Figure 1 Full-length blots/gels

1. Full-length pictures of the blots and gels presented in Figure 1



2. Full-length pictures of the blots and gels presented in Figure 3



3. Full-length pictures of the blots and gels presented in Figure 6

