

**Table S1.** Metabolites detected in dry-cured beef during each processing stage.

MVDB Index	Compounds	Q1 (Da)	Formula	CK1	CK2	CK3	CK4	CK5	CK6	FJ1	FJ2	FJ3	FJ4	FJ5	FJ6	CS1	CS2	CS3	CS4	CS5	CS6	mix0 1	mix0 2	mix0 3
MEDN0005	L-Threonine	118.0504432	C4H9NO3	1,100,000	1,200,000	1,370,000	1,330,000	1,280,000	1,300,000	875,000	754,000	964,000	873,000	917,000	866,000	1,100,000	989,000	965,000	1,030,000	1,010,000	973,000	769,000	963,000	971,000
MEDN0017	L-Pyroglutamic Acid	128.0347931	C5H7NO3	555,000	667,000	628,000	575,000	569,000	591,000	1,580,000	1,490,000	1,480,000	1,430,000	1,770,000	1,710,000	4,430,000	4,650,000	4,900,000	4,390,000	4,691,000	5,080,000	2,000,000	2,290,000	2,440,000
MEDN0018	L-Serine	104.0347931	C3H7NO3	668,000	756,000	825,000	801,000	716,000	782,000	345,000	304,000	330,000	400,000	342,000	348,000	402,000	363,000	345,000	369,000	366,000	351,000	306,000	342,000	365,000
MEDN0022	(5-L-Glutamyl)-L-Amino Acid	217.0824716	C8H14N2O5	3,070,000	4,570,000	4,510,000	4,760,000	3,700,000	4,280,000	301,000	223,000	272,000	198,000	361,000	452,000	829,000	782,000	795,000	804,000	796,300	772,000	986,000	1,300,000	1,350,000
MEDN0028	4-Hydroxy-L-Glutamic Acid	162.0402724	C5H9NO5	35,600	33,300	35,300	45,400	30,700	36,000	18,500	9,970	12,300	39,400	12,600	18,200	24,900	39,500	12,300	23,300	25,920	29,600	25,100	13,400	19,100
MEDN0040	Glycyl-L-Proline	171.0769923	C7H12N2O3	5,410	10,700	10,100	11,200	9,770	13,500	217,000	186,000	247,000	236,000	228,000	189,000	117,000	165,000	132,000	128,000	134,500	130,000	145,000	140,000	149,000
MEDN0041	Hexanoyl Glycine	172.0973933	C8H15NO3	5,660	5,840	7,750	10,400	10,900	8,530	234,000	193,000	384,000	91,400	189,000	311,000	327,000	317,000	357,000	413,000	356,100	367,000	166,000	175,000	184,000
MEDN0045	L-Cysteine	120.0119495	C3H7NO2S	9	9	9	9	9	9	810,000	789,000	834,000	720,000	876,000	833,000	929,000	1,070,000	1,130,000	989,000	1,059,000	1,180,000	583,000	733,000	621,000
MEDN0056	N-Acetyl-L-Leucine	172.0973933	C8H15NO3	202,000	248,000	256,000	254,000	251,000	226,000	8,540,000	5,930,000	10,700,000	7,660,000	9,760,000	8,670,000	9,700,000	10,200,000	10,800,000	9,530,000	10,210,000	10,800,000	5,110,000	5,960,000	5,960,000
MEDN0061	N-Phenylacetyl glycine	192.0660932	C10H11NO3	52,600	60,000	61,600	59,200	56,000	59,300	55,900	49,600	60,700	55,100	56,400	57,800	64,200	67,900	64,300	70,000	66,210	64,600	54,700	57,200	64,700
MEDN0062	N-Propionylglycine	130.0504432	C5H9NO3	781,000	883,000	909,000	843,000	884,000	909,000	2,660,000	2,450,000	2,810,000	2,620,000	2,640,000	2,790,000	2,210,000	2,180,000	2,150,000	2,350,000	2,223,000	2,230,000	1,690,000	2,150,000	2,260,000

MEDN0065	O-Phospho-L-Serine	184.0011236	C3H8NO6P	70,60	64,20	64,50	88,90	86,00	91,20	112,0	98,50	141,0	100,0	96,30	125,0	68,20	101,0	111,0	68,90	89,77	100,0	100,0	106,0	118,0
				0	0	0	0	0	0	00	0	00	00	0	00	0	00	00	0	6	00	00	00	00
MEDN0068	S-(5-Adenosy)-L-Homocysteine	383.1137888	C14H20N6O5S	493,0	489,0	596,0	928,0	426,0	584,0	355,0	322,0	397,0	342,0	359,0	354,0	101,0	122,0	110,0	113,0	109,6	103,0	302,0	348,0	317,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	12	00	00	00	00
MEDN0070	Sarcosine	88.03987847	C3H7NO2	77,80	88,60	93,00	100,0	91,30	97,70	71,70	100,0	54,00	61,10	64,00	79,10	62,30	57,20	60,90	66,40	62,90	67,70	64,60	81,50	84,00
				0	0	0	00	0	0	0	00	0	0	0	0	0	0	0	0	3	0	0	0	0
MEDN0074	γ-L-Glutamate-Cysteine	249.0545426	C8H14N2O5S	198,0	299,0	313,0	268,0	271,0	289,0	15,50	11,10	19,60	15,00	11,30	20,20	32,20	19,90	24,80	15,20	22,54	20,60	88,70	96,30	92,30
				00	00	00	00	00	00	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0
MEDN0085	Benzoylformic Acid	149.0238941	C8H6O3	9	9	9	9	9	9	37,10	55,50	19,70	14,40	46,00	50,10	73,50	64,80	63,00	42,70	58,08	46,40	40,00	36,20	35,10
										0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
MEDN0090	2-Methoxybenzoic Acid	151.0395441	C8H8O3	9	9	9	9	9	9	9,860	7,750	14,30	11,50	7,210	8,520	9,780	13,00	15,70	13,30	13,18	14,20	6,220	6,850	4,890
										0	0	0	0	0	0	0	0	0	0	8	0			
MEDN0093	3-Hydroxyanthranilic Acid	152.0347931	C7H7NO3	9	9	9	9	6,040	9	51,80	27,40	76,00	65,70	35,90	54,00	60,60	61,40	71,00	76,20	68,47	73,10	36,80	45,00	46,80
										0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
MEDN0113	Glycochenodeoxycholic Acid	448.3063235	C26H43NO5	167,0	187,0	194,0	225,0	181,0	203,0	363,0	397,0	404,0	353,0	317,0	345,0	268,0	273,0	311,0	391,0	304,6	281,0	248,0	307,0	318,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	76	00	00	00	00
MEDN0120	Dulcitol	181.0712382	C6H14O6	196,0	187,0	200,0	190,0	206,0	195,0	143,0	118,0	162,0	124,0	159,0	153,0	147,0	181,0	179,0	131,0	168,8	205,0	108,0	124,0	134,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	40	00	00	00	00
MEDN0140	Xanthine	151.0256254	C5H4N4O2	61,50	62,10	77,00	65,70	68,00	78,60	73,90	65,10	82,60	69,40	74,10	78,50	75,00	69,30	63,90	80,40	71,43	68,50	63,70	68,20	84,90
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	3,200	0,000	0,000	0,000	0,000
MEDN0141	2'-Deoxyuridine	227.0668215	C9H12N2O5	20,60	25,90	24,80	32,00	17,80	30,10	18,30	19,60	14,10	16,40	21,10	20,50	12,00	18,60	19,60	18,90	18,76	24,80	19,30	20,10	16,40
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
MEDN0149	7-Methylxanthine	165.0412755	C6H6N4O2	9	9	9	9	7,350	9	17,70	24,60	8,290	11,00	26,60	17,80	75,10	40,40	31,00	36,20	45,54	45,00	22,30	27,40	23,30
										0	0		0	0	0	0	0	0	0	2	0	0	0	0
MEDN0153	Adenosine 5'-Monophosphate	346.0552844	C10H14N5O7P	60,60	56,50	62,60	43,40	41,60	62,90	26,30	24,00	16,30	33,20	28,70	29,40	7,430	8,280	5,840	5,570	7,339	9,580	14,90	12,40	15,80
				0	0	0	0	0	0	0	0	0	0	0	0							0	0	0

MEDN0159	Flavin Adenine Dinucleotide	784.1493347	C27H33N9O15P2	196,0	215,0	244,0	234,0	242,0	276,0	411,0	355,0	440,0	317,0	356,0	588,0	77,20	51,60	62,80	47,00	58,40	53,40	146,0	309,0	312,0
				00	00	00	00	00	00	00	00	00	00	00	00	0	0	0	0	5	0	00	00	00
MEDN0165	Inosine 5'-Monophosphate	347.0393	C10H13N4O8P	129,0	139,0	133,0	81,40	251,0	142,0	3,260	2,890	3,140	3,890	3,310	3,070	60,30	54,70	36,90	102,0	61,82	55,50	961,0	1,370	1,270
				00	00	00	0	00	00	000	000	000	000	000	000	0	0	0	00	8	0	00	000	000
MEDN0198	Citric Acid	191.0192026	C6H8O7	325,0	324,0	199,0	185,0	198,0	216,0	13,00	7,240	13,40	15,60	11,90	16,90	5,510	4,630	3,610	3,650	4,217	3,690	7,280	7,870	8,470
				00	00	00	00	00	00	0,000	000	0,000	0,000	0,000	0,000	000	000	000	000	800	000	000	000	000
MEDN0202	A-Ketoglutaric Acid	145.0137233	C5H6O5	9	9	9	9	9	9	592,0	403,0	669,0	791,0	536,0	560,0	139,0	176,0	138,0	146,0	151,3	157,0	228,0	298,0	284,0
										00	00	00	00	00	00	00	00	00	00	88	00	00	00	00
MEDN0203	Cis-Aconitic Acid	173.0086379	C6H6O6	5,430	4,520	5,420	6,020	6,620	7,310	12,80	12,60	13,60		13,40	15,20	17,50	19,90	12,00	18,10	16,41	14,50	10,20	24,40	15,00
										0	0	0	9,290	0	0	0	0	0	0	2	0	0	0	0
MEDN0206	Citramalic Acid	147.0293734	C5H8O5	527,0	567,0	560,0	777,0	740,0	635,0	1,140	1,020	974,0	1,020	1,320	1,350	923,0	949,0	1,040	948,0	974,9	1,010	823,0	804,0	932,0
				00	00	00	00	00	00	000	000	00	000	000	000	00	00	000	00	70	000	00	00	00
MEDN0207	6-Hydroxymelatonin	247.1082924	C13H16N2O3	9	9	9	9	9	9	4,000	3,060	3,250	2,580	5,470	5,650	3,700	3,700	4,310	4,750	4,321	5,150	2,700	2,420	3,930
MEDN0209	Tryptamine	159.0922484	C10H12N2	388,0	412,0	425,0	393,0	432,0	422,0	631,0	574,0	656,0	616,0	609,0	700,0	428,0	510,0	533,0	488,0	492,3	504,0	454,0	531,0	553,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	38	00	00	00	00
MEDN0210	1,5-Anhydro-D-Glucitol	163.0606735	C6H12O5	34,10	46,80	49,20	45,20	45,90	53,80	17,50	14,40	14,60	22,70	13,20	22,60	24,40	25,80	20,80	23,70	23,31	21,80	26,10	24,40	25,20
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0
MEDN0211	D-Arabitol	151.0606735	C5H12O5	108,0	122,0	142,0	128,0	114,0	134,0	44,60	32,60	36,60	21,00	48,50	84,30	20,30	25,50	23,00	17,80	21,41	20,50	25,30	20,20	35,30
				00	00	00	00	00	00	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0
MEDN0213	D-Sorbitol	181.0712382	C6H14O6	154,0	144,0	121,0	156,0	144,0	174,0	90,70	76,60	104,0	74,00	110,0	88,30	76,90	108,0	108,0	75,00	95,47	109,0	87,40	95,20	71,50
				00	00	00	00	00	00	0	0	00	0	00	0	0	00	00	0	4	00	0	0	0
MEDN0220	D-Glucose	179.0555881	C6H12O6	1,010	1,450	1,550	1,560	1,160	1,350	310,0	230,0	330,0	300,0	353,0	339,0	183,0	277,0	279,0	252,0	247,7	247,0	208,0	240,0	245,0
				000	000	000	000	000	000	00	00	00	00	00	00	00	00	00	00	52	00	00	00	00
MEDN0222	D-Melezitose	503.1612349	C18H32O16	73,00	60,30	52,50	72,40	80,30	83,70	27,60	28,60	24,70	20,80	33,90	29,80	18,60	23,00	19,00	20,60	19,73	17,50	15,90	23,20	21,50
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	0	0	0	0

MEDN0224	D-Trehalose	341.1084115	C12H22O11	81,20	79,00	86,60	106,0	97,40	74,50	105,0	109,0	109,0	108,0	97,80	103,0	120,0	125,0	118,0	128,0	123,3	125,0	109,0	156,0	140,0
				0	0	0	00	0	0	00	00	00	00	0	00	00	00	00	00	40	00	00	00	00
MEDN0227	D-Glucose 6-Phosphate	259.0219186	C6H13O9P	86,70	63,60	56,20	73,90	72,40	92,30	16,90	15,80	14,50	16,40	19,10	18,70	873,0	1,620	1,640	1,050	1,342	1,530	5,670	7,710	6,760
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	00	000	000	000	850	000	000	000	000
MEDN0230	Lactulose	341.1084115	C12H22O11	81,20	79,00	86,60	106,0	97,40	74,50	105,0	109,0	109,0	108,0	97,80	103,0	120,0	125,0	118,0	128,0	123,3	125,0	109,0	156,0	140,0
				0	0	0	00	0	0	00	00	00	00	0	00	00	00	00	00	40	00	00	00	00
MEDN0231	L-Fucose	163.0606735	C6H12O5	34,10	46,80	49,20	45,20	45,90	53,80	17,50	14,40	14,60	22,70	13,20	22,60	24,40	25,80	20,80	23,70	23,31	21,80	26,10	24,40	25,20
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0
MEDN0232	L-Rhamnose	163.0606735	C6H12O5	34,10	46,80	49,20	45,20	45,90	53,80	17,50	14,40	14,60	22,70	13,20	22,60	24,40	25,80	20,80	23,70	23,31	21,80	26,10	24,40	25,20
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0
MEDN0234	Maltotriose	503.1612349	C18H32O16	73,00	60,30	52,50	72,40	80,30	83,70	27,60	28,60	24,70	20,80	33,90	29,80	18,60	23,00	19,00	20,60	19,73	17,50	15,90	23,20	21,50
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	0	0	0	0
MEDN0237	D-Glucuronic Acid	193.0348527	C6H10O7	349,0	401,0	535,0	475,0	400,0	416,0	118,0	95,80	123,0	129,0	129,0	112,0	66,90	95,30	78,30	64,20	77,47	82,60	81,50	96,60	90,90
				00	00	00	00	00	00	00	0	00	00	00	00	0	0	0	0	1	0	0	0	0
MEDN0239	Gluconic Acid	195.0505027	C6H12O7	7,210	9,230	7,340	9,400	7,680	7,770	8,780	10,40	8,380	9,540	8,060	7,570	8,350	7,610	6,830	6,850	7,178	6,250	7,970	8,720	7,140
											0													
MEDN0240	L-Gulonolactone	177.039938	C6H10O6	19,60	23,70	16,10	27,90	23,20	16,90	90,90	53,20	88,00	61,40	101,0	151,0	50,50	51,10	47,40	62,70	51,44	45,60	45,80	77,20	47,30
				0	0	0	0	0	0	0	0	0	0	00	00	0	0	0	0	4	0	0	0	0
MEDN0241	Vitamin D3	383.331416	C27H44O	38,10	31,80	24,00	25,80	22,00	21,90	16,90	11,70	16,40	19,40	14,00	22,80	13,50	9,510	14,10	12,47	17,00	39,30	20,40	20,70	
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8,400	9	0	0	0	0
MEDN0244	Orotic Acid	155.0093066	C5H4N2O4	14,80	23,10	10,90	12,70	12,70	21,60	73,10	24,30	78,10	108,0	62,40	92,70	51,30	39,30	32,20	30,90	38,75	40,20	49,70	51,90	61,40
				0	0	0	0	0	0	0	0	0	00	0	0	0	0	0	0	6	0	0	0	0
MEDN0245	Pantothenate	218.1028726	C9H17NO5	24,20	30,90	31,00	30,90	28,70	29,00	26,50	25,30	26,40	21,30	28,30	31,10	29,90	32,70	33,10	31,20	32,14	33,90	22,20	30,10	31,40
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	7,200	0,000	0,000	0,000	0,000
MEDN0276	1-Naphthylacetic Acid	185.0602796	C12H10O2	9	9	9	9	9	9	60,20	166,0	9	9	68,80	65,80	180,0	59,50	793,0	1,010	429,4	108,0	142,0	145,0	144,0
										0	00			0	0	00	0	00	000	53	00	00	00	00

MEDN0280	2-Aminoethanesulfonic Acid	124.0068641	C2H7NO3S	190,0	183,0	184,0	170,0	186,0	183,0	2,750	2,510	2,940	3,070	2,760	2,490	5,000	4,880	4,810	4,730	4,824	4,710	7,690	9,340	9,040
				00,00	00,00	00,00	00,00	00,00	00,00	000	000	000	000	000	000	000	000	000	000	340	000	000	000	000
				0	0	0	0	0	0															
MEDN0283	2-Hydroxybutanoic Acid	103.0395441	C4H8O3	396,0	306,0	373,0	346,0	416,0	414,0	1,320	1,060	1,450	1,280	1,400	1,430	1,420	1,480	1,330	1,400	1,428	1,520	868,0	1,030	1,080
				00	00	00	00	00	00	000	000	000	000	000	000	000	000	000	000	580	000	00	000	000
MEDN0284	2-Hydroxyisocaproic Acid	131.0708442	C6H12O3	28,70	20,60	21,40	61,40	32,80	32,10	192,0	87,90	153,0	133,0	161,0	425,0	86,70	101,0	88,00	131,0	103,3	110,0	75,40	98,00	93,40
				0	0	0	0	0	0	00	0	00	00	00	00	0	00	0	00	29	00	0	0	0
MEDN0285	2-Methylsuccinic Acid	131.0344587	C5H8O4	1,050	1,140	1,070	1,190	1,260	1,180	2,610	2,290	2,750	2,470	2,750	2,800	4,070	4,510	4,510	4,940	4,580	4,870	2,070	2,550	2,680
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	820	000	000	000	000
MEDN0287	3,5-Dimethoxy-4-Hydroxycinnamic Acid	223.0606735	C11H12O5	9	122	9	9	9	9	36,40	28,40	34,00	27,80	33,70	57,90	95,20	158,0	148,0	151,0	136,7	131,0	37,80	58,40	54,40
										0	0	0	0	0	0	0	00	00	00	48	00	0	0	0
MEDN0290	3-Hydroxy-3-Methyl Butyric Acid	117.0551942	C5H10O3	81,70	76,10	74,80	107,0	70,50	67,20	159,0	157,0	138,0	151,0	181,0	168,0	160,0	181,0	207,0	138,0	176,8	197,0	118,0	130,0	119,0
				0	0	0	00	0	0	00	00	00	00	00	00	00	00	00	00	68	00	00	00	00
MEDN0292	3-Hydroxybutyrate	103.0395441	C4H8O3	9,220	10,60	10,10	9,390	9,570	10,10	3,680	3,560	3,790	3,510	3,710	3,810	5,200	5,110	5,560	5,290	5,327	5,480	4,540	5,490	5,680
				000	0,000	0,000	000	000	0,000	000	000	000	000	000	000	000	000	000	000	340	000	000	000	000
MEDN0293	3-Hydroxypropanoic Acid	89.02389405	C3H6O3	35,20	43,10	39,30	39,40	33,50	64,60	25,10	32,80	23,80	22,00	23,90	23,00	21,50	23,20	23,60	15,60	20,96	20,90	20,60	23,60	24,90
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MEDN0301	Caffeic Acid	179.0344587	C9H8O4	166,0	180,0	166,0	202,0	185,0	171,0	207,0	194,0	242,0	174,0	208,0	217,0	205,0	249,0	234,0	233,0	229,6	227,0	193,0	219,0	229,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	76	00	00	00	00
MEDN0314	Glutaric Acid	131.0344587	C5H8O4	1,050	1,140	1,070	1,190	1,260	1,180	2,610	2,290	2,750	2,470	2,750	2,800	4,070	4,510	4,510	4,940	4,580	4,870	2,070	2,550	2,680
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	820	000	000	000	000
MEDN0316	Guanidinoethyl Sulfonate	166.0286622	C3H9N3O3S	63,00	83,40	83,40	71,00	78,40	74,10	37,20	29,10	42,40	26,90	37,10	50,40	40,10	39,10	40,20	10,70	33,49	37,40	23,30	55,40	38,10
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0
MEDN0320	Hydrocinnamic Acid	149.0602796	C9H10O2	13,40	14,30	13,60	15,50	19,40	9,770	18,00	14,10	19,50	22,60	15,20	18,70	19,20	16,60	15,30	11,10	15,76	16,70	15,40	17,00	16,60
				0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

MEDN0325	L-Lactic Acid	89.02389405	C3H6O3	2,490, 2,430, 2,630, 2,540, 2,600, 2,590, 3,180, 3,000, 3,310, 3,300, 3,300, 2,970, 3,080, 2,930, 2,760, 2,810, 2,886, 2,860, 2,380, 2,940, 3,000, 000 000 000 000 000 000 000 000 000 000 000 000 000 480 000 000 000 000
MEDN0333	Malonicacid	103.0031586	C3H4O4	9,140, 11,10 10,20 9,880, 9,540, 10,10 3,700, 3,510, 3,820, 3,570, 3,550, 4,030, 5,280, 5,250, 5,480, 5,220, 5,347, 5,510, 4,440, 5,580, 5,890, 000 0,000 0,000 000 000 0,000 000 000 000 000 000 000 000 000 000 940 000 000 000 000
MEDN0334	Mandelic Acid	151.0395441	C8H8O3	78,20 29,50 25,90 89,60 68,60 99,90 543,0 322,0 830,0 628,0 401,0 535,0 632,0 683,0 714,0 693,0 686,1 710,0 390,0 438,0 443,0 0 0 0 0 0 0 00 00 00 00 00 00 00 00 00 60 00 00 00 00
MEDN0335	Methylmalonic Acid	117.0188087	C4H6O4	1,180, 1,170, 951,0 1,400, 1,010, 1,210, 188,0 179,0 190,0 173,0 200,0 199,0 240,0 258,0 279,0 243,0 257,1 266,0 135,0 168,0 170,0 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 60,00 00,00 00,00 00,00 00,00 000 000 00 000 000 000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MEDN0338	Phenyllactate(Pla)	165.0551942	C9H10O3	58,80 32,30 29,90 75,90 96,70 63,30 1,940, 1,030, 2,620, 1,310, 1,960, 2,760, 1,340, 1,630, 1,490, 1,710, 1,555, 1,600, 888,0 1,080, 1,100, 0 0 0 0 0 0 000 000 000 000 000 000 000 000 000 000 380 000 00 000 000
MEDN0339	Phenylpyruvic Acid	163.0395441	C9H8O3	24,70 8,520, 43,90 35,40 12,70 23,10 1,680, 3,160, 2,870, 2,030, 2,606, 3,290, 7,280, 8,410, 8,580, 0,000 000 0,000 0,000 0,000 0,000 000 000 000 000 160 000 000 000 000 9 9 9 9 9 9
MEDN0340	Pyrrole-2-Carboxylic Acid	110.0242284	C5H5NO2	31,40 16,80 31,90 27,20 34,30 46,70 32,90 26,90 35,00 35,00 31,96 30,00 21,50 25,70 17,80 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0 0 9 9 9 9 9 9
MEDN0342	Sebacate	201.1127091	C10H18O4	7,430 6,530 7,650 6,770 7,460 7,540 8,580 8,180 7,330 9,000 8,670 9,700 19,80 15,30 19,90 21,60 18,87 17,70 10,70 13,10 11,40 0 0 0 0 6 0 0 0 0 0
MEDN0343	Shikimic Acid	173.0450234	C7H10O5	61,50 62,10 74,40 87,70 82,40 70,10 188,0 147,0 268,0 158,0 183,0 184,0 351,0 442,0 343,0 496,0 421,1 473,0 202,0 226,0 247,0 0 0 0 0 0 0 00 00 00 00 00 00 00 00 00 00 02 00 00 00 00
MEDN0407	3-Aminosalicilic Acid	152.0347931	C7H7NO3	199,0 177,0 304,0 209,0 194,0 298,0 207,0 147,0 292,0 227,0 187,0 182,0 283,0 201,0 148,0 293,0 222,8 190,0 197,0 148,0 289,0 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 54 00 00 00 00
MEDN0411	Neopterin	252.0733039	C9H11N5O <sub>4</sub>	1,170, 1,130, 1,300, 1,350, 1,230, 1,350, 1,370, 1,300, 1,380, 1,470, 1,420, 1,280, 1,380, 1,390, 1,510, 1,580, 1,493, 1,610, 1,030, 1,490, 1,520, 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 760 000 000 000 000
MEDN0412	Biopterin	236.0783892	C9H11N5O <sub>3</sub>	46,80 50,00 32,40 50,30 52,60 48,80 58,80 62,70 49,50 66,30 60,86 66,90 29,40 26,60 49,10 0 0 0 0 0 0 0 0 0 0 4 0 0 0 0 0 9 9 9 9 9 9

MEDN0413	Ethylmalonate	131.0344587	C5H8O4	1,050, 1,140, 1,070, 1,190, 1,260, 1,180, 2,610, 2,290, 2,750, 2,470, 2,750, 2,800, 4,070, 4,510, 4,510, 4,940, 4,580, 4,870, 2,070, 2,550, 2,680, 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 820 000 000 000 000
MEDN0417	(Rs)-Mevalonic Acid	147.0657589	C6H12O4	622,0 703,0 707,0 865,0 675,0 738,0 51,60 46,10 65,40 59,50 52,70 34,20 42,40 85,20 34,30 74,40 61,19 69,60 160,0 175,0 179,0 00 00 00 00 00 00 0 0 0 0 0 0 0 0 1 0 00 00 00
MEDN0432	5-Hydroxyhexanoic Acid	131.0708442	C6H12O3	120,0 132,0 112,0 125,0 139,0 120,0 206,0 210,0 188,0 174,0 223,0 232,0 554,0 498,0 548,0 533,0 538,9 562,0 215,0 280,0 269,0 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 96 00 00 00 00
MEDN0439	N-Acetylthreonine	160.0610078	C6H11NO4	15,70 18,60 26,00 17,90 14,10 24,10 104,0 62,60 112,0 91,60 114,0 139,0 55,50 65,40 55,20 60,20 57,67 52,10 56,00 68,20 73,20 0 0 0 0 0 0 00 0 00 0 00 00 0 0 0 0 9 0 0 0 0
MEDN0444	Hypoxanthine-9-β-D-Arab- inofuranoside	267.0729695	C10H12N4 O5	219,0 194,0 185,0 184,0 226,0 210,0 581,0 614,0 573,0 569,0 509,0 641,0 498,0 528,0 588,0 559,0 539,9 527,0 503,0 565,0 549,0 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 94,00 00,00 00,00 00,00 00,00 0
MEDN0445	Orotidine	287.0515654	C10H12N2 O8	27,90 32,20 40,40 27,60 22,80 24,20 108,0 100,0 105,0 102,0 119,0 113,0 109,0 104,0 104,0 95,20 109,3 135,0 72,40 70,40 107,0 0 0 0 0 0 0 00 00 00 00 00 00 00 00 0 26 00 0 0 00
MEDN0455	Guanine	150.0416098	C5H5N5O	34,50 30,60 36,60 36,10 32,40 36,50 33,00 21,60 24,50 29,40 27,41 28,60 25,00 30,00 28,70 0
MEDN0461	D-Sedoheptulose 7-Phos- phate	287.0168332	C7H13BaO 10P	216,0 211,0 227,0 249,0 214,0 274,0 168,0 156,0 162,0 150,0 183,0 188,0 179,0 198,0 169,0 171,0 181,5 190,0 127,0 179,0 170,0 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00
MEDN0463	D-Fructose 6-Phosphate- Disodium Salt	259	C6H11Na2 O9P	4,810, 3,950, 4,320, 5,160, 5,200, 5,420, 293,0 428,0 442,0 317,0 395,4 497,0 1,690, 2,110, 2,160, 000 000 000 000 000 000 00 00 00 00 48 00 000 000 000
MEDN0470	Oxoadipic Acid	159.0293734	C6H8O5	59,80 47,60 48,20 87,20 47,60 68,40 33,90 33,80 36,10 47,60 39,11 44,10 40,80 29,10 32,10 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0
MEDN0478	Aminomalonic Acid	118.0140576	C3H5NO4	43,20 61,20 38,70 46,90 39,00 47,00 7,130, 6,770, 7,200, 6,530, 7,410, 7,720, 9,270, 10,10 10,90 9,340, 10,05 10,60 4,910, 6,360, 6,400, 0 0 0 0 0 0 000 000 000 000 000 000 0,000 0,000 000 7,860 0,000 000 000 000
MEDN0487	Allysine	144.0660932	C6H11NO3	12,10 73,10 58,90 62,60 96,40 59,40 88,30 38,70 25,80 24,00 25,90 31,52 43,30 34,30 48,40 28,90 0 0 0 0 0 0 0 0 0 0 0 0 6 0 0 0 0

MEDN0496	N-Acetylmethionine	190.0538143	C7H13NO3 S	65,50 0	59,00 0	61,80 0	83,00 0	70,00 0	78,20 0	537,0 00	361,0 00	661,0 00	545,0 00	520,0 00	600,0 00	173,0 00	190,0 00	171,0 00	153,0 00	178,3 84	205,0 00	209,0 00	239,0 00	245,0 00
MEDN0498	Ribulose-5-Phosphate	229.0113539	C5H11O8P	24,10 0,000	20,50 0,000	19,70 0,000	17,80 0,000	22,70 0,000	21,00 0,000	2,330 000	1,870 000	2,340 000	2,980 000	2,130 000	2,340 000	1,770 000	1,900 000	1,720 000	1,920 000	1,729 760	1,350 000	2,130 000	2,630 000	2,030 000
MEDN0499	Argininosuccinic acid	289.1148343	C10H18N4 O6	9 9	9 9	9 9	9 9	9 9	9 9	280,0 00	235,0 00	236,0 00	286,0 00	301,0 00	342,0 00	123,0 00	172,0 00	132,0 00	175,0 00	160,8 48	202,0 00	206,0 00	239,0 00	245,0 00
MEDN0501	Acetyl Tryptophan	245.0926423	C13H14N2 O3	28,10 0	38,20 0	45,90 0	43,10 0	38,20 0	43,60 0	69,20 0	65,40 0	62,70 0	66,30 0	77,60 0	73,80 0	147,0 00	149,0 00	133,0 00	165,0 00	147,3 58	142,0 00	79,30 0	109,0 00	94,60 0
MEDN0502	2-Deoxyribose 1-Phosphate	213.0164393	C5H11O7P	157,0 00	162,0 00	115,0 00	173,0 00	156,0 00	147,0 00	403,0 00	427,0 00	372,0 00	326,0 00	472,0 00	418,0 00	493,0 00	551,0 00	542,0 00	552,0 00	553,3 70	629,0 00	279,0 00	318,0 00	402,0 00
MEDN0506	N-Acetylglucosamine 1- Phosphate	300.0484677	C8H16NO9 P	3,930 000	4,020 000	3,960 000	3,870 000	3,970 000	4,050 000	331,0 00	378,0 00	245,0 00	368,0 00	336,0 00	329,0 00	244,0 00	274,0 00	327,0 00	238,0 00	253,2 50	184,0 00	280,0 00	415,0 00	279,0 00
MEDN0530	Pimelic acid	159.0657589	C7H12O4	444,0 00	486,0 00	417,0 00	513,0 00	547,0 00	459,0 00	1,170 000	1,230 000	1,020 000	885,0 00	1,250 000	1,470 000	4,150 000	4,090 000	3,870 000	4,700 000	4,246 540	4,420 000	1,800 000	2,070 000	2,180 000
MEDN0531	D-Glucarate	209.0297673	C6H10O8	186,0 00	180,0 00	201,0 00	202,0 00	162,0 00	150,0 00	6,610 00	5,270 00	5,220 00	6,900 00	12,80 0	2,810 00	8,140 00	1,450 00	1,450 00	7,590 00	6,789 00	15,30 0	12,10 0	8,250 00	14,00 0
MEDN0533	Xanthosine	283.0678841	C10H12N4 O6	66,70 0,000	76,10 0,000	75,70 0,000	74,20 0,000	76,80 0,000	74,50 0,000	59,30 0,000	56,50 0,000	61,20 0,000	47,90 0,000	60,60 0,000	70,60 0,000	57,30 0,000	64,00 0,000	61,90 0,000	61,60 0,000	61,84 5,800	64,50 0,000	55,60 0,000	68,40 0,000	69,10 0,000
MEDN0538	UDP-glucose	565.0472206	C15H24N2 O17P2	31,90 0	28,90 0	21,00 0	29,00 0	23,20 0	16,10 0	26,90 0	25,80 0	18,00 0	29,00 0	28,40 0	33,50 0	9	9	9	9	9	9	12,80 0	11,80 0	15,80 0
MEDN0555	Hydroxyphenyllactic acid	181.0501088	C9H10O4	227,0 00	171,0 00	163,0 00	163,0 00	207,0 00	223,0 00	1,130 000	783,0 00	1,430 000	824,0 00	1,150 000	1,460 000	520,0 00	780,0 00	679,0 00	768,0 00	697,1 18	739,0 00	594,0 00	639,0 00	711,0 00
MEDN0561	N-Acetylaspartylglutamic acid	303.0828655	C11H16N2 O8	5,840 000	10,20 0,000	10,60 0,000	9,390 000	7,230 000	8,790 000	1,140 000	799,0 00	1,300 000	1,350 000	1,190 000	1,070 000	470,0 00	472,0 00	400,0 00	451,0 00	474,2 38	578,0 00	1,030 000	1,400 000	1,630 000
MEDN0570	L-Erythrulose	119.0344587	C4H8O4	9 9	9 9	9 9	9 9	9 9	9 9	61,50 0	57,90 0	56,20 0	58,90 0	75,00 0	59,60 0	118,0 00	124,0 00	120,0 00	114,0 00	121,1 66	129,0 00	64,80 0	80,70 0	82,00 0

MEDN0579	N-lactoyl-phenylalanine	236.092308	C12H15NO 4	2,130, 2,810, 2,940, 2,940, 2,580, 2,710, 5,970, 5,720, 5,810, 4,700, 6,200, 7,420, 13,80 14,60 13,90 14,40 14,43 15,40 6,350, 7,980, 8,330, 000 000 000 000 000 000 000 000 000 000 000 000 0,000 0,000 0,000 0,000 5,800 0,000 000 000 000
MEDN0587	N-Acetylvaline	158.0817433	C7H13NO3	172,0 272,0 311,0 302,0 222,0 265,0 173,0 141,0 210,0 143,0 178,0 193,0 236,0 269,0 268,0 242,0 254,7 258,0 196,0 227,0 198,0 00 00 00 00 00 00 00 00 00 00 00 00 00 00 14 00 00 00 00
MEDN0593	D-Malic acid	133.0137233	C4H6O5	43,90 46,50 43,10 43,10 41,40 43,60 583,0 443,0 585,0 543,0 649,0 696,0 1,660, 1,520, 1,670, 1,460, 1,604, 1,700, 6,130, 7,770, 7,570, 0,000 0,000 0,000 0,000 0,000 0,000 00 00 00 00 00 00 000 000 000 000 120 000 000 000 000
MEDN0602	deoxyguanosine 5'-mono-phosphate(dGMP)	346.0552844	C10H14N5 O7P	60,60 56,50 62,60 43,40 41,60 62,90 26,30 24,00 16,30 33,20 28,70 29,40 7,430 8,280 5,840 5,570 7,339 9,580 14,90 12,40 15,80 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
MEDN0606	5-Methoxytryptophan	190.0868287	C11H13NO 2	113,0 109,0 94,00 88,80 86,60 95,40 98,30 82,80 110,0 91,40 96,50 111,0 51,60 57,80 58,70 55,50 55,98 56,20 81,60 83,90 92,30 00 00 0 0 0 0 0 0 0 00 0 0 00 0 0 0 0 7 0 0 0 0
MEDN0616	O-Acetyl-L-serine	146.0453578	C5H9NO4	909,0 974,0 1,020, 1,070, 1,080, 1,030, 1,600, 1,360, 1,680, 1,700, 1,650, 1,600, 1,640, 1,860, 1,770, 1,730, 1,771, 1,860, 1,310, 1,600, 1,650, 00 00 000 000 000 000 000 000 000 000 000 000 000 000 000 000 520 000 000 000 000
MEDN0622	Porphobilinogen	225.0875569	C10H14N2 O4	26,60 30,60 35,00 20,70 20,00 41,30 34,60 23,00 53,20 18,70 35,50 42,70 33,30 28,10 63,60 91,70 52,41 45,40 69,80 89,00 61,30 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4 0 0 0 0
MEDN0651	Succinic anhydride	99.00824399	C4H4O3	873,0 1,190, 1,120, 1,210, 1,100, 1,020, 1,570, 2,040, 1,340, 1,830, 1,360, 1,290, 2,780, 2,090, 2,070, 2,250, 2,192, 1,780, 1,760, 2,220, 1,960, 00 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 260 000 000 000 000
MEDN0655	Hydantoin-5-propionic acid	171.0406067	C6H8N2O4	7,940 9,380 12,10 11,70 5,080 7,810 4,990 2,810 5,680 3,600 7,790 5,080 7,670 6,600 4,350 8,620 5,907 2,300 5,140 6,920 5,140 0 0
MEDN0657	D-Xylulose 5-phosphate	229.0113539	C5H11O8P	24,10 20,50 19,70 17,80 22,70 21,00 2,330, 1,870, 2,340, 2,980, 2,130, 2,340, 1,770, 1,900, 1,720, 1,920, 1,729, 1,350, 2,130, 2,630, 2,030, 0,000 0,000 0,000 0,000 0,000 0,000 000 000 000 000 000 000 000 000 000 000 760 000 000 000 000
MEDN0661	2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid	197.0450234	C9H10O5	14,10 18,70 14,10 15,50 17,40 17,80 22,50 21,80 24,30 20,50 22,70 23,40 19,80 20,40 20,50 23,20 21,46 23,40 15,90 15,20 21,40 0 0 0 0 0 0 0 0 0 0 0 0 9 0 0 0 0
MEDN0662	Gamma-Glu-Leu	259.1294217	C11H20N2 O5	66,30 76,00 88,70 84,00 85,00 90,50 612,0 523,0 685,0 544,0 624,0 684,0 718,0 866,0 842,0 778,0 810,2 847,0 418,0 526,0 494,0 0 0 0 0 0 0 00 00 00 00 00 00 00 00 66 00 00 00 00
MEDN0682	Octadecanamide	282.2797148	C18H37NO	21,10 24,30 24,30 27,90 15,60 25,00 23,20 17,70 26,70 19,10 24,50 27,80 26,30 24,00 14,60 22,20 21,08 18,30 10,60 14,10 14,40 0 0 0 0 0 0 0 0 0 0 0 0 6 0 0 0 0

MEDN0720	N-(2-Methylbenzoyl)glycine	192.0660932	C10H11NO 3	52,60 0	60,00 0	61,60 0	59,20 0	56,00 0	59,30 0	55,90 0	49,60 0	60,70 0	55,10 0	56,40 0	57,80 0	64,20 0	67,90 0	64,30 0	70,00 0	66,21 6	64,60 0	54,70 0	57,20 0	64,70 0
MEDN0725	2,4-Hexadienoic acid	111.0446295	C6H8O2	3,310,000	3,110,000	3,390,000	2,940,000	2,870,000	3,360,000	645,000	619,000	654,000	751,000	614,000	589,000	669,000	587,000	591,000	653,000	610,634	554,000	624,000	804,000	685,000
MEDN0741	Methanesulfonic acid	94.98031499	CH4O3S	319,000	346,000	272,000	292,000	327,000	320,000	26,400	20,300	23,900	44,300	21,900	21,500	30,300	45,700	53,500	57,900	46,491	45,000	62,800	56,600	44,600
MEDN0793	Prostaglandin E2	351.2171741	C20H32O5	31,600	27,700	21,300	36,600	39,200	31,300	638,000	1,240,000	9	9	1,360,000	588,000	792,000	1,120,000	626,000	2,840,000	1,107,370	154,000	439,000	521,000	530,000
MEDN0818	N-acetyl-beta-alanine	130.0504432	C5H9NO3	859,000	895,000	989,000	989,000	888,000	940,000	1,700,000	1,470,000	1,870,000	1,730,000	1,640,000	1,810,000	679,000	660,000	694,000	771,000	700,544	699,000	845,000	1,030,000	962,000
MEDN0820	3-Hydroxyglutaric acid	147.0293734	C5H8O5	248,000	181,000	225,000	271,000	221,000	250,000	403,000	329,000	414,000	420,000	450,000	400,000	367,000	321,000	335,000	316,000	332,802	325,000	278,000	302,000	364,000
MEDN0824	7-ketodeoxycholic acid	405.2641243	C24H38O5	6,710	6,160	6,180	8,110	7,060	8,270	18,300	17,100	21,400	15,500	17,600	20,000	14,400	19,600	18,300	22,100	18,260	16,900	15,100	15,800	15,300
MEDN0827	N-acetylornithine	173.0926423	C7H14N2O 3	5,710,000	6,530,000	6,510,000	6,650,000	5,950,000	6,240,000	2,850,000	2,700,000	3,010,000	2,760,000	2,860,000	2,910,000	3,400,000	3,580,000	3,340,000	3,230,000	3,387,040	3,380,000	2,800,000	3,130,000	3,110,000
MEDN0832	D-Glucosamine 6-Phosphate	258.037903	C6H14NO8 P	9,030,000	9,360,000	9,510,000	9,940,000	9,790,000	9,920,000	1,090,000	864,000	1,040,000	1,370,000	1,110,000	1,070,000	750,000	799,000	831,000	769,000	778,792	745,000	933,000	1,180,000	1,160,000
MEDN0833	3-Dehydroshikimate	171.0293734	C7H8O5	79,800	111,000	123,000	98,900	99,100	112,000	98,800	96,600	98,500	96,100	111,000	91,700	89,100	88,400	87,200	93,700	88,841	85,800	90,900	87,700	94,400
MEDN0841	3-Ureidopropionate	131.0456921	C4H8N2O3	393,000	428,000	429,000	429,000	458,000	417,000	531,000	736,000	382,000	444,000	488,000	604,000	375,000	400,000	367,000	430,000	396,734	412,000	474,000	584,000	613,000
MEDN0854	Mono-Methyl Glutarate	145.0501088	C6H10O4	89,200	96,700	121,000	116,000	128,000	104,000	81,500	71,400	95,100	74,900	70,700	95,400	91,600	95,200	102,000	92,600	90,123	69,000	3,660	3,370	4,630
MEDN1004	L-Sepiapterin	236.0783892	C9H11N5O 3	77,000	94,600	85,300	71,700	156,000	80,100	7,080,000	6,520,000	7,340,000	6,990,000	6,210,000	8,350,000	8,310,000	10,100	9,380,000	9,500,000	9,415,960	9,800,000	4,480,000	6,180,000	6,370,000

MEDN1006	Uric acid	167.02054	C5H4N4O3	1,560, 1,510, 1,580, 1,530, 1,730, 1,660, 2,520, 1,700, 3,430, 2,520, 2,000, 2,940, 1,570, 2,350, 2,250, 1,750, 2,046, 2,310, 1,990, 2,100, 2,360, 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 620 000 000 000 000
MEDN1011	D-Mannitol	181.0712382	C6H14O6	196,0 187,0 200,0 190,0 206,0 195,0 143,0 118,0 162,0 124,0 159,0 153,0 147,0 181,0 179,0 131,0 168,8 205,0 108,0 124,0 134,0 00 00 00 00 00 00 00 00 00 00 00 00 00 40 00 00 00 00
MEDN1024	D-piperidine acid	128.0711786	C6H11NO2	350,0 450,0 423,0 374,0 362,0 403,0 1,140, 1,010, 1,060, 1,150, 1,290, 1,210, 3,410, 3,550, 3,700, 3,110, 3,491, 3,680, 1,460, 1,740, 1,830, 00 00 00 00 00 00 000 000 000 000 000 000 000 000 000 000 000 440 000 000 000 000
MEDN1029	Glycyl-L-phenylalanine	221.0926423	C11H14N2O3	42,50 31,40 40,30 45,30 49,70 50,10 728,0 614,0 928,0 732,0 680,0 685,0 688,0 815,0 843,0 799,0 794,8 830,0 438,0 542,0 624,0 0 0 0 0 0 0 00 00 00 00 00 00 00 00 00 00 16 00 00 00 00
MEDN1039	Indole-4-carboxaldehyde	144.0449638	C9H7NO	817,0 644,0 677,0 834,0 1,100, 833,0 632,0 211,0 205,0 255,0 326,8 332,0 325,0 379,0 390,0 6,530 7,140 9,370 8,770 6,920 8,390 00 00 00 00 000 00 00 00 00 00 00 00 14 00 00 00 00
MEDN1052	(S) -2-Hydroxyglutaric acid	147.0293734	C5H8O5	527,0 567,0 560,0 777,0 740,0 635,0 1,140, 1,020, 974,0 1,020, 1,320, 1,350, 923,0 949,0 1,040, 948,0 974,9 1,010, 823,0 804,0 932,0 00 00 00 00 00 00 000 000 00 000 000 00 00 00 00 70 000 00 00 00
MEDN1055	D-Calcium Pantothenate	437.2135453	C18H34N2O10	163,0 252,0 236,0 243,0 197,0 210,0 221,0 185,0 218,0 145,0 260,0 296,0 271,0 331,0 269,0 250,0 288,2 320,0 195,0 249,0 272,0 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 98 00 00 00 00
MEDN1056	Iminodiacetic acid	132.0297077	C4H7NO4	6,930, 9,180, 10,10 8,200, 7,870, 8,520, 11,10 15,80 9,410 10,50 11,20 8,540 37,20 56,40 56,30 62,20 53,93 57,40 44,10 59,90 46,20 000 000 0,000 000 000 000 0 0 0 0 0 0 0 0 0 0 2 0 0 0 0
MEDN1060	L-Isoisoleucine	130.0868287	C6H13NO2	31,00 33,50 34,90 31,90 34,10 35,70 105,0 96,20 111,0 108,0 110,0 93,40 92,10 87,70 98,60 92,95 92,90 68,80 86,30 91,30 0,000 0,000 0,000 0,000 0,000 0,000 00,00 0,000 00,00 00,00 00,00 0,000 0,000 0,000 0,000 1,800 0,000 0,000 0,000 0,000 0
MEDN1061	Glycine deoxycholic acid	448.3063235	C26H43NO5	14,60 14,20 15,50 14,10 12,40 16,80 11,40 12,70 12,90 16,90 13,02 11,10 10,70 11,70 11,00 6,850 7,720 7,360 7,400 7,420 8,680 0 0 0 0 0 0 0 0 0 0 8 0 0 0 0
MEDN1064	N-arachidene glycine	360.253894	C22H35NO3	9 9 9 9 9 9 4,270 3,560 5,780 4,250 3,030 4,710 12,60 12,70 10,40 9,530 11,97 14,70 4,870 4,880 6,540 0 0 0 7 0
MEDN1085	Glutathione	611.1441625	C20H32N6O12S2	6,480, 8,850, 8,930, 6,710, 6,490, 7,290, 213,0 344,0 209,0 120,0 209,0 183,0 11,20 23,00 19,00 11,80 17,24 21,30 312,0 366,0 379,0 000 000 000 000 000 000 00 00 00 00 00 0 0 0 0 0 0 0 00 00 00

MEDN1087	UDP-D-galactose	565.04845	C15H24N2O17P2	46,30	36,10	19,20	23,60	53,00	16,50	28,30	35,80	23,80	18,60	32,70	30,40	9	9	9	9	9	9	12,90	15,60	14,30
				0	0	0	0	0	0	0	0	0	0	0	0							0	0	0
MEDN1098	2-ethyl-2-hydroxybutyric acid	131.07071	C6H12O3	111,0	110,0	97,30	105,0	121,0	107,0	197,0	195,0	172,0	177,0	192,0	248,0	525,0	489,0	507,0	538,0	519,1	536,0	196,0	273,0	272,0
				00	00	0	00	00	00	00	00	00	00	00	00	00	00	00	00	22	00	00	00	00
MEDN1108	1,6-anhydro-β-D-glucose	161.0450234	C6H10O5	92,80	98,40	124,0	120,0	85,90	96,10	132,0	136,0	137,0	142,0	112,0	132,0	123,0	99,10	99,60	102,0	108,2	118,0	96,80	92,20	109,0
				0	0	00	00	0	0	00	00	00	00	00	00	00	0	0	00	44	00	0	0	00
MEDN1110	1,11-undecylic acid	243.2	C13H24O4	1,970,	1,920,	1,980,	1,980,	1,910,	1,970,	2,010,	2,000,	2,030,	2,030,	1,910,	2,080,	2,080,	2,080,	2,140,	2,220,	2,123,	2,110,	1,590,	2,000,	2,040,
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	960	000	000	000	000
MEDN1126	Gamma-Mercholic Acid	407.2797744	C24H40O5	4,370,	4,470,	4,440,	4,730,	4,390,	4,710,	10,10	9,770,	11,70	9,410,	8,670,	10,80	7,430,	8,870,	9,020,	10,40	8,930,	8,880,	8,010,	8,520,	8,460,
				000	000	000	000	000	000	0,000	000	0,000	000	000	0,000	000	000	000	0,000	560	000	000	000	000
MEDN1129	Erythrose	119.0344587	C4H8O4	9	9	9	9	9	9	61,50	57,90	56,20	58,90	75,00	59,60	118,0	124,0	120,0	114,0	121,1	129,0	64,80	80,70	82,00
										0	0	0	0	0	0	00	00	00	00	66	00	0	0	0
MEDN1135	Heparin	315.2899451	C19H40O3	28,20	34,00	27,70	19,80	27,80	33,50	108,0	158,0	26,50	39,40	173,0	144,0	75,00	58,00	69,60	155,0	79,55	39,80	52,20	71,40	70,80
				0	0	0	0	0	0	00	00	0	0	00	00	0	0	0	00	0	0	0	0	0
MEDN1145	P-chlorophenylalanine	198.0322487	C9H10ClNO2	3,370,	3,500,	3,520,	3,590,	3,730,	3,710,	2,710,	2,690,	2,600,	2,860,	2,640,	2,750,	2,730,	2,650,	2,640,	2,660,	2,663,	2,630,	2,520,	2,920,	3,000,
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	200	000	000	000	000
MEDN1221	D-Mannose 6-phosphate	259.0219186	C6H13O9P	76,70	49,90	42,70	58,80	60,50	71,20	7,430,	6,990,	6,700,	6,760,	8,270,	8,450,	431,0	674,0	723,0	578,0	611,6	653,0	2,370,	2,870,	3,240,
				0,000	0,000	0,000	0,000	0,000	0,000	000	000	000	000	000	000	00	00	00	00	86	00	000	000	000
MEDN1226	2-amino-4-oxovaleric acid	130.0504432	C5H9NO3	859,0	895,0	989,0	989,0	888,0	940,0	1,700,	1,470,	1,870,	1,730,	1,640,	1,810,	679,0	660,0	694,0	771,0	700,5	699,0	845,0	1,030,	962,0
				00	00	00	00	00	00	000	000	000	000	000	000	00	00	00	00	44	00	00	000	00
MEDN1235	L-2-amino-6-oximelic acid	188.0567506	C7H11NO5	53,60	69,80	94,10	94,70	67,50	79,00	322,0	226,0	344,0	367,0	332,0	342,0	362,0	346,0	319,0	348,0	346,8	359,0	207,0	250,0	277,0
				0	0	0	0	0	0	00	00	00	00	00	00	00	00	00	00	46	00	00	00	00
MEDN1246	3-(pyrazol-1-yl) -L-alanine	154.0620148	C6H9N3O2	8,250,	7,160,	6,730,	7,620,	7,980,	8,350,	10,30	10,00	10,10	9,850,	10,60	11,10	5,960,	7,840,	7,710,	7,150,	7,366,	8,180,	6,100,	7,270,	7,480,
				000	000	000	000	000	000	0,000	0,000	0,000	000	0,000	0,000	000	000	000	000	620	000	000	000	000
MEDN1303	Mannose 1-phosphate	259	C6H13O9P	8,400,	4,820,	4,760,	6,260,	6,350,	7,800,	836,0	949,0	696,0	702,0	874,0	960,0	43,10	73,50	79,20	65,70	68,48	81,00	222,0	345,0	306,0
				000	000	000	000	000	000	00	00	00	00	00	00	0	0	0	0	8	0	00	00	00

MEDN1306	N-Carbamoyl-L-aspartate	175.04	C5H8N2O5	94,90	119,0	110,0	111,0	124,0	117,0	56,80	45,50	64,90	64,40	52,10	57,20	72,10	73,50	70,50	77,10	72,09	67,30	52,90	49,20	64,10
				0	00	00	00	00	00	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0
MEDN1311	2-Hydroxycaprylic acid	159	C8H16O3	17,20	12,30	9,770	15,20	12,80	9,980	243,0	639,0	42,60	49,00	256,0	229,0	1,700	809,0	2,600	2,580	1,822	1,430	499,0	599,0	606,0
				0	0		0	0		00	00	0	0	00	00	000	00	000	000	480	000	00	00	00
MEDN1317	3,3-Dimethylglutaric acid	159	C7H12O4	9	9	9	9	9	9	14,20	20,00			23,60	27,40	104,0	94,60	96,30	109,0	100,7	99,60	33,80	42,40	40,50
										0	0			0	0	00	0	0	00	43	0	0	0	0
MEDN1326	2-Methylglutaric Acid	145	C6H10O4	9	9	9	9	9	9	20,30	21,10	17,30	19,60	17,00	26,40	60,50	63,70	65,80	60,30	62,96	64,50	29,80	35,60	41,80
										0	0	0	0	0	0	0	0	0	0	9	0	0	0	0
MEDN1328	(S)-Leucic acid	131	C6H12O3	24,00	18,50	22,20	56,50	33,30	32,90	148,0	78,30	156,0	118,0	146,0	241,0	89,00	100,0	80,10	99,60	93,19	97,30	68,50	85,80	79,80
				0	0	0	0	0	0	00	0	00	00	00	00	0	00	0	0	8	0	0	0	0
MEDP0002	D-Homocysteine	136	C4H9NO2S	366,0	269,0	277,0	297,0	352,0	320,0	246,0	222,0	263,0	266,0	218,0	258,0	150,0	116,0	132,0	114,0	130,6	141,0	196,0	164,0	181,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	10	00	00	00	00
MEDP0007	L-Cystine	241	C6H12N2O4S2	345,0	378,0	237,0	273,0	311,0	327,0	141,0	128,0	141,0	123,0	164,0	147,0	83,60	93,90	72,00	58,20	77,44	79,60	167,0	92,90	103,0
				00	00	00	00	00	00	00	00	00	00	00	00	0	0	0	0	6	0	00	0	00
MEDP0009	L-Tyrosine	182.1	C9H11NO3	57,40	56,90	59,10	56,80	57,80	56,70	107,0	105,0	108,0	113,0	105,0	103,0									
				0,000	0,000	0,000	0,000	0,000	0,000	00,00	00,00	00,00	00,00	00,00	00,00	84,20	94,00	90,90	90,60	89,05	85,60	89,90	91,00	95,30
										0	0	0	0	0	0	0,000	0,000	0,000	0,000	5,000	0,000	0,000	0,000	0,000
MEDP0010	L-Arginine	175	C6H14N4O2	1,510	2,160	1,750	2,550	1,840	2,580	4,350	3,740	4,680	4,180	4,190	4,960	4,000	4,340	4,180	4,250	4,220	4,320	3,760	3,960	4,090
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	160	000	000	000	000
MEDP0011	L-Lysine	147	C6H14N2O2	55,80	67,70	68,90	63,00	59,50	59,00	45,00	40,70	50,60	47,10	44,20	42,40	61,00	66,10	65,20	64,70	64,57	65,90	50,30	49,10	47,10
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,200	0,000	0,000	0,000	0,000
MEDP0012	L-Ornithine	133	C5H13N2O2	11,60	16,30	16,60	15,20	12,70	13,90	635,0	561,0	588,0	612,0	701,0	712,0	795,0	900,0	897,0	793,0	847,7	854,0	1,530	1,560	1,610
				0,000	0,000	0,000	0,000	0,000	0,000	00	00	00	00	00	00	00	00	00	00	66	00	000	000	000
MEDP0013	L-Alanine	90.048	C3H7NO2	37,50	37,80	38,70	37,10	36,30	38,40	8,070	10,20	6,810	6,290	7,890	9,140	4,920	6,300	5,800	5,830	5,797	6,150	8,020	7,910	7,900
				0,000	0,000	0,000	0,000	0,000	0,000	000	0,000	000	000	000	000	000	000	000	000	060	000	000	000	000

MEDP0014	L-Aspartic Acid	134.1	C4H7NO4	1,830, 2,260, 2,330, 2,200, 1,800, 2,070, 193,0 177,0 186,0 221,0 217,0 164,0 220,0 166,0 203,0 177,0 197,6 223,0 281,0 258,0 301,0 000 000 000 000 000 000 00 00 00 00 00 00 00 00 00 72 00 00 00 00
MEDP0015	L-Citrulline	176.1	C6H13N3O3	538,0 597,0 835,0 793,0 596,0 722,0 159,0 133,0 175,0 145,0 176,0 166,0 136,0 126,0 88,10 69,70 102,3 92,20 170,0 180,0 178,0 00 00 00 00 00 00 00 00 00 00 00 00 00 00 0 0 80 0 00 00 00
MEDP0016	L-Glutamic Acid	148.1	C5H9NO4	33,80 37,20 40,30 40,10 34,50 37,30 7,220, 6,610, 6,920, 8,850, 7,160, 6,550, 13,20 11,80 10,90 10,60 11,62 11,60 13,30 12,10 11,50 0,000 0,000 0,000 0,000 0,000 0,000 000 000 000 000 000 000 0,000 0,000 0,000 0,000 5,200 0,000 0,000 0,000 0,000
MEDP0017	L-Histidine	156.1	C6H9N3O2	103,0 98,10 88,80 93,90 105,0 97,50 54,00 45,90 60,70 62,10 51,40 50,10 39,60 37,40 36,80 37,20 37,27 35,30 42,80 45,30 47,00 00,00 0,000 0,000 0,000 00,00 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,200 0,000 0,000 0,000 0,000 0 0 0
MEDP0020	L-Methionine	150	C5H11NO2S	8,650, 9,220, 9,160, 8,780, 9,040, 8,700, 32,10 31,50 33,80 32,40 31,20 31,40 23,10 26,00 24,70 23,20 24,60 26,10 22,30 23,60 23,90 000 000 000 000 000 000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 7,600 0,000 0,000 0,000 0,000 349,0 340,0 348,0 349,0 347,0 350,0 349,0 348,0 348,0 349,0 349,0 353,0 357,0 353,0 355,0 351,0 354,2 356,0 349,0 355,0 352,0
MEDP0021	L-Phenylalanine	166	C9H11NO2	00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 72,00 00,00 00,00 00,00 00,00 0
MEDP0022	L-Proline	116.1	C5H9NO2	47,00 47,00 47,10 48,80 44,80 43,00 34,80 30,80 37,40 36,60 36,10 33,20 57,40 50,70 54,00 49,20 53,51 56,30 53,50 47,50 45,90 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 6,200 0,000 0,000 0,000 0,000
MEDP0025	L-Tryptophan	205.1	C11H12N2O2	16,90 17,60 17,00 16,30 16,90 17,90 56,70 51,50 62,50 49,70 57,00 62,90 28,20 46,10 43,50 39,90 40,42 44,40 37,00 38,90 41,30 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 3,000 0,000 0,000 0,000 0,000
MEDP0026	L-Valine	118.1	C5H11NO2	75,90 78,30 87,20 78,30 74,10 81,40 127,0 123,0 134,0 121,0 126,0 130,0 103,0 117,0 120,0 111,0 114,2 120,0 99,70 100,0 98,90 0,000 0,000 0,000 0,000 0,000 0,000 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 76,00 00,00 0,000 00,00 0,000 0
MEDP0034	3-N-Methyl-L-Histidine	170	C7H13N3O3	3,440, 3,110, 2,880, 2,870, 3,240, 2,940, 996,0 673,0 1,080, 1,270, 987,0 968,0 676,0 570,0 623,0 637,0 637,5 682,0 914,0 821,0 949,0 000 000 000 000 000 000 00 00 000 000 00 00 00 00 00 94 00 00 00 00
MEDP0035	5-Hydroxy-L-Tryptophan	221.1	C11H12N2O3	62,30 100,0 24,70 23,60 107,0 55,80 116,0 76,60 79,20 128,0 98,66 93,70 69,90 53,10 56,00 0 00 0 0 00 0 00 0 0 00 4 0 0 0 0

MEDP0036	5-Oxoproline	130	C5H7NO3	10,40	12,10	11,50	10,30	10,00	10,30	16,60	16,90	15,60	14,50	18,30	17,60	38,80	42,30	45,20	38,50	41,84	44,40	25,10	26,90	26,50
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	3,400	0,000	0,000	0,000	0,000
MEDP0039	Betaine	118.1	C5H11NO2	69,80	71,50	68,70	67,20	64,70	71,00	31,50	32,60	34,40	39,90	25,30	25,20	29,90	22,70	19,80	21,90	22,94	20,50	37,80	37,50	35,70
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	2,400	0,000	0,000	0,000	0,000
MEDP0041	D-Alanyl-D-Alanine	161.2	C6H12N2O3	86,70	44,00	44,00	63,80	59,60	52,80	102,0	77,00	122,0	139,0	82,60	89,60	96,40	99,90	71,40	86,90	83,72	64,00	73,30	86,20	79,70
				0	0	0	0	0	0	00	0	00	00	0	0	0	0	0	0	3	0	0	0	0
MEDP0043	Glutathione Oxidized	613.152	C20H32N6O12S2	4,960	7,260	6,990	5,970	4,860	4,940	664,0	1,170	635,0	331,0	603,0	577,0	54,80	62,90	111,0	123,0	86,83	82,00	907,0	1,100	1,150
				000	000	000	000	000	000	00	000	00	00	00	00	0	0	00	00	1	0	00	000	000
MEDP0044	Glutathione Reducedform	308	C10H17N3O6S	87,90	105,0	95,30	101,0	90,00	97,80	4,370	3,090	7,110	5,760	2,250	3,650	956,0	1,270	1,150	574,0	1,124	1,680	18,00	19,30	18,60
				0,000	00,00	0,000	00,00	0,000	0,000	000	000	000	000	000	000	00	000	000	00	728	000	0,000	0,000	0,000
				0		0	0																	
MEDP0047	Histamine	112.08	C5H9N3	14,90	13,50	13,50	16,50	16,20	15,30	8,500	7,410	10,20	9,140	7,960	7,820	6,760	6,710	6,380	6,300	6,579	6,750	7,440	7,980	8,560
				0,000	0,000	0,000	0,000	0,000	0,000	000	000	0,000	000	000	000	000	000	000	000	480	000	000	000	000
MEDP0049	L-Asparagine Anhydrous	133.054	C4H8N2O3	1,170	1,230	1,120	1,330	1,290	1,160	1,250	1,290	1,280	1,240	1,280	1,160	1,270	1,340	1,270	1,310	1,273	1,180	1,370	1,310	1,270
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	180	000	000	000	000
MEDP0050	L-Carnosine	227.2	C9H14N4O3	244,0	210,0	199,0	204,0	234,0	240,0	125,0	104,0	132,0	133,0	125,0	132,0	82,90	77,80	73,40	79,60	78,48	78,80	104,0	121,0	120,0
				00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	0,000	0,000	0,000	0,000	7,600	0,000	00,00	00,00	00,00
				0	0	0	0	0	0	0	0	0	0	0	0							0	0	0
MEDP0051	L-Cystathionine	223	C7H14N2O4S	9	21,10	36,30	42,80	26,50	18,50	19,30	28,80	21,80	9,570	13,00	30,20	27,60	24,80	22,30	25,07	20,50	19,80	17,20	23,30	
				0	0	0	6,580	0	0	0	0	0		0	0	0	0	0	9	0	0	0	0	
MEDP0053	L-Dopa	198.069	C9H11NO4	9	9	9	9	9	9	120,0	120,0	81,80	76,70	190,0	129,0	309,0	188,0	197,0	176,0	209,3	177,0	108,0	125,0	119,0
										00	00	0	0	00	00	00	00	00	00	62	00	00	00	00
MEDP0054	L-Glutamine	147.069	C5H10N2O3	154,0	158,0	166,0	163,0	159,0	154,0	3,880	2,840	4,340	6,140	3,060	3,050	9	9	9	9	9	9	12,70	12,90	15,20
				00,00	00,00	00,00	00,00	00,00	00,00	000	000	000	000	000	000							0,000	0,000	0,000
				0	0	0	0	0	0															

MEDP0055	L-Homocitrulline	190.1	C7H15N3O 3	140,0 00	126,0 00	165,0 00	164,0 00	155,0 00	155,0 00	66,50 0	50,40 0	83,00 0	78,20 0	58,50 0	62,30 0	86,40 0	79,80 0	78,50 0	74,00 0	74,96 1	56,20 0	79,00 0	84,80 0	87,80 0
MEDP0056	L-Homocystine	269	C8H16N2O 4S2	393,0 00	368,0 00	370,0 00	441,0 00	365,0 00	394,0 00	2,640 000	2,660 000	2,510 000	2,460 000	2,780 000	2,790 000	1,720 000	1,900 000	1,980 000	1,900 000	1,898 720	1,990 000	1,800 000	1,870 000	1,930 000
MEDP0058	L-Saccharopine	277	C11H20N2 O6	649,0 00	530,0 00	476,0 00	518,0 00	602,0 00	662,0 00	751,0 00	615,0 00	711,0 00	992,0 00	742,0 00	697,0 00	925,0 00	786,0 00	566,0 00	853,0 00	745,4 30	596,0 00	732,0 00	860,0 00	809,0 00
MEDP0060	Methionine Sulfoxide	166	C5H11NO3 S	2,820 000	2,650 000	2,410 000	2,340 000	2,340 000	2,360 000	2,590 000	2,800 000	2,410 000	2,270 000	2,590 000	2,900 000	1,900 000	1,960 000	1,890 000	2,030 000	1,927 200	1,860 000	2,590 000	2,250 000	2,170 000
MEDP0061	N,N-Dimethylglycine	104	C4H9NO2	1,370 000	1,630 000	1,520 000	1,660 000	1,550 000	1,500 000	5,320 000	5,830 000	4,990 000	6,040 000	4,940 000	4,810 000	7,820 000	7,880 000	7,900 000	8,920 000	8,247 660	8,720 000	7,390 000	7,430 000	7,350 000
MEDP0062	N6-Acetyl-L-Lysine	189.1160924	C8H16N2O 3	26,50 0,000	37,50 0,000	38,60 0,000	36,30 0,000	28,10 0,000	33,90 0,000	4,930 000	3,460 000	4,250 000	2,600 000	6,710 000	7,640 000	1,650 000	3,120 000	2,680 000	1,790 000	2,379 140	2,650 000	4,010 000	3,970 000	3,980 000
MEDP0063	N-Acetylaspartate	176	C6H9NO5	9	9	9	9	9	9	4,360 000	4,860 000	2,550 000	2,170 000	6,230 000	6,010 000	2,270 000	4,250 000	5,390 000	3,730 000	4,162 180	5,170 000	2,650 000	2,420 000	2,720 000
MEDP0065	N-Acetyl-L-Glutamic Acid	190.1	C7H11NO5	302,0 00	423,0 00	395,0 00	264,0 00	293,0 00	373,0 00	341,0 00	326,0 00	328,0 00	321,0 00	396,0 00	332,0 00	539,0 00	492,0 00	414,0 00	403,0 00	468,0 16	492,0 00	445,0 00	381,0 00	384,0 00
MEDP0066	N-Acetyl-L-Tyrosine	224.1	C11H13NO 4	8,180	11,40 0	13,40 0	9	9	9	81,90 0	55,30 0	73,10 0	59,40 0	86,90 0	135,0 00	84,50 0	82,80 0	94,60 0	82,70 0	86,90 0	89,90 0	57,80 0	60,80 0	65,70 0
MEDP0067	N-Acetylmannosamine	222	C8H15NO6	502,0 00	627,0 00	403,0 00	429,0 00	529,0 00	488,0 00	600,0 00	615,0 00	565,0 00	463,0 00	710,0 00	647,0 00	458,0 00	524,0 00	546,0 00	460,0 00	484,8 00	436,0 00	512,0 00	605,0 00	513,0 00
MEDP0068	N-Acetylneuraminic Acid	310.1	C11H19NO 9	33,40 0	48,50 0	29,80 0	34,60 0	40,60 0	37,70 0	33,60 0	36,00 0	49,10 0	26,00 0	20,40 0	36,60 0	21,70 0	24,90 0	18,60 0	23,80 0	23,19 6	27,00 0	51,30 0	26,10 0	46,40 0
MEDP0071	N-Glycyl-L-Leucine	189.1	C8H16N2O 3	280,0 00	366,0 00	304,0 00	235,0 00	299,0 00	271,0 00	3,970 000	3,500 000	4,500 000	3,830 000	4,130 000	3,880 000	4,010 000	5,310 000	4,560 000	4,760 000	4,639 860	4,550 000	3,380 000	3,110 000	3,190 000
MEDP0072	N-Isovaleroylglycine	160.1	C7H13NO3	83,70 0	85,50 0	95,40 0	85,30 0	90,40 0	81,90 0	272,0 00	120,0 00	277,0 00	221,0 00	319,0 00	424,0 00	118,0 00	121,0 00	105,0 00	103,0 00	114,4 48	124,0 00	168,0 00	172,0 00	154,0 00

MEDP0075	N $\alpha$ -Acetyl-L-Arginine	217.1	C8H16N4O3	236,0	178,0	221,0	242,0	198,0	216,0	291,0	158,0	237,0	182,0	373,0	504,0	250,0	206,0	228,0	202,0	225,3	241,0	212,0	191,0	168,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	98	00	00	00	00
MEDP0077	Phenylacetyl-L-Glutamine	265.1	C13H16N2O4	171,0	168,0	140,0	198,0	178,0	182,0	401,0	362,0	445,0	319,0	415,0	463,0	283,0	314,0	309,0	369,0	323,5	342,0	287,0	343,0	339,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	90	00	00	00	00
MEDP0078	Phe-Phe	313.4	C18H20N2O3	9	9	9	9	9	9	483,0	432,0	484,0	419,0	471,0	608,0	451,0	545,0	435,0	394,0	469,6	524,0	284,0	377,0	404,0
										00	00	00	00	00	00	00	00	00	00	58	00	00	00	00
MEDP0080	S-Adenosyl-L-Methionine	401.2	C15H24N6O5S	15,50	23,70	22,30	30,60	16,10	28,50	46,20	63,20	28,10	32,10	37,00	70,80	13,80	29,70	46,40	40,80	30,41	21,50	30,90	35,90	36,80
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0
MEDP0081	Serotonin	177	C10H12N2O	9	9	9	9	9	9	77,10	71,30	147,0	46,80	62,70	57,90	186,0	49,60	41,70	55,50	79,73	65,60	57,60	70,80	62,50
										0	0	00	0	0	0	00	0	0	0	1	0	0	0	0
MEDP0082	S-Sulfo-L-Cysteine	202.2	C3H7NO5S2	9	9	9	9	9	9	17,80	25,80	17,20	17,90	17,70	10,70	20,80	14,10	12,70	12,20	14,27	11,50	26,90	23,30	28,80
										0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
MEDP0083	Trans-4-Hydroxy-L-Proline	132.058	C5H9NO3	32,20	34,00	33,10	33,20	33,10	34,30	12,70	18,30	12,30	11,50	9,750	11,80	7,250	7,470	5,010	7,690	6,522	5,190	12,10	13,40	14,40
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	520	0,000	0,000	0,000	0,000
MEDP0085	Tyramine	138.084	C8H11NO	143,0	37,30	40,90	175,0	61,40	260,0	1,120	154,0	3,170	1,730	157,0	399,0	41,70	86,10	76,30	78,90	68,41	59,10	428,0	424,0	479,0
				00	0	0	00	0	00	000	00	000	000	00	00	0	0	0	0	5	0	00	00	00
MEDP0087	L-Alanyl-L-Lysine	218.1	C9H19N3O3	9	9	9	9	9	9	879,0	853,0	761,0	806,0	822,0	1,150	1,360	903,0	1,110	1,120	1,088	953,0	782,0	937,0	984,0
										00	00	00	00	00	000	000	00	000	000	452	00	00	00	00
MEDP0089	N-Acetylhistamine	154.1	C7H11N3O	3,060	3,550	3,680	2,910	4,350	3,510	1,580	1,690	1,410	1,320	1,940	1,520	1,380	1,620	1,280	1,350	1,387	1,300	2,100	1,930	2,340
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	120	000	000	000	000
MEDP0101	P-Coumaric Acid	165.047	C9H8O3	7,150	7,460	7,310	7,030	7,490	7,190	16,90	17,00	17,60	16,00	17,40	16,70	12,10	13,80	13,60	13,20	13,17	13,10	13,80	13,80	13,90
				000	000	000	000	000	000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
MEDP0113	4-Hydroxybenzoic Acid	139.03	C7H6O3	424,0	136,0	63,90	92,10	232,0	314,0	252,0	320,0	169,0	117,0	214,0	442,0	679,0	528,0	537,0	607,0	590,7	602,0	311,0	358,0	386,0
				00	00	0	0	00	00	00	00	00	00	00	00	00	00	00	00	48	00	00	00	00
MEDP0118	4-Pyridoxic Acid	184.05	C8H9NO4	469,0	265,0	264,0	288,0	396,0	466,0	638,0	833,0	411,0	372,0	701,0	876,0	812,0	649,0	524,0	706,0	670,2	660,0	766,0	733,0	782,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	04	00	00	00	00

MEDP0119	6-Hydroxynicotinic Acid	140	C6H5NO3	19,80 0	17,60 0	15,50 0	29,30 0	23,30 0	18,80 0	20,80 0	16,80 0	26,10 0	10,90 0	21,10 0	29,10 0	26,70 0	9 0	21,10 0	25,10 0	17,56 2	14,90 0	19,60 0	26,90 0	20,40 0
MEDP0125	Choline	105.11	C5H14NO+	231,0 00	271,0 00	250,0 00	267,0 00	306,0 00	287,0 00	1,090 000	1,120 000	1,020 000	1,240 000	1,030 000	1,030 000	1,940 000	1,640 000	1,650 000	1,850 000	1,774 280	1,790 000	1,570 000	1,630 000	1,550 000
MEDP0126	1,5-Diaminopentane	103	C5H14N2	33,20 0	15,70 0	39,80 0	166,0 00	60,50 0	45,90 0	34,80 0	22,80 0	37,40 0	27,30 0	41,20 0	45,50 0	14,30 0	17,30 0	13,30 0	22,30 0	15,68 2	11,30 0	29,40 0	36,50 0	22,90 0
MEDP0135	Myoinositol	181.06	C6H12O6	1,670 000	1,910 000	1,220 000	1,490 000	2,050 000	1,530 000	1,390 000	1,730 000	1,450 000	1,740 000	1,020 000	1,020 000	1,590 000	686,0 00	877,0 00	1,510 000	1,141 254	1,050 000	1,140 000	1,020 000	1,240 000
MEDP0143	Biotin	245.09	C10H16N2 O3S	108,0 00	133,0 00	141,0 00	115,0 00	154,0 00	140,0 00	163,0 00	170,0 00	162,0 00	134,0 00	172,0 00	179,0 00	156,0 00	178,0 00	186,0 00	175,0 00	174,1 44	176,0 00	149,0 00	187,0 00	192,0 00
MEDP0147	1-Methylhistidine	170.1	C7H11N3O 2	687,0 00	938,0 00	1,040 000	1,010 000	839,0 00	1,060 000	509,0 00	317,0 00	577,0 00	532,0 00	507,0 00	613,0 00	262,0 00	286,0 00	282,0 00	356,0 00	303,3 34	331,0 00	365,0 00	434,0 00	386,0 00
MEDP0148	1-Methylxanthine	167.1	C6H6N4O2	9	9	9	9	9	9	4,280	9	9	9	9	21,40 0	39,90 0	37,50 0	48,60 0	44,60 0	42,50 9	41,90 0	49,00 0	33,50 0	43,00 0
MEDP0149	2'-Deoxyadenosine-5'- Monophosphate	332	C10H14N5 O6P	9	9	9	9	9	9	119,0 00	109,0 00	112,0 00	95,10 0	140,0 00	139,0 00	96,50 0	133,0 00	109,0 00	126,0 00	123,1 10	151,0 00	94,00 0	95,10 0	99,80 0
MEDP0150	2'-Deoxyinosine	253.1	C10H12N4 O4	348,0 00	421,0 00	453,0 00	405,0 00	378,0 00	413,0 00	54,80 0	50,00 0	41,50 0	58,70 0	52,70 0	71,20 0	37,60 0	43,30 0	57,00 0	31,60 0	43,64 5	48,80 0	148,0 00	175,0 00	173,0 00
MEDP0152	3'-Aenylic Acid	348	C10H14N5 O7P	2,270 000	1,870 000	1,860 000	1,840 000	2,110 000	2,050 000	453,0 00	465,0 00	356,0 00	527,0 00	365,0 00	555,0 00	69,10 0	87,50 0	57,50 0	75,60 0	67,17 3	46,20 0	503,0 00	556,0 00	541,0 00
MEDP0155	5-Methylcytosine	126.1	C5H7N3O	78,80 0	64,20 0	59,70 0	56,20 0	83,40 0	64,70 0	35,40 0	43,40 0	21,90 0	35,60 0	46,20 0	30,00 0	45,10 0	47,20 0	50,20 0	61,10 0	50,63 4	49,60 0	46,10 0	61,60 0	40,20 0
MEDP0156	5-Methyluridine	259.085	C10H14N2 O6	67,60 0	73,80 0	64,90 0	65,80 0	64,90 0	54,30 0	48,30 0	41,90 0	52,70 0	35,60 0	54,70 0	56,70 0	46,50 0	61,20 0	60,50 0	55,40 0	59,14 3	72,20 0	52,50 0	42,20 0	83,90 0
MEDP0159	Adenine	136.1	C5H5N5	1,030 000	1,180 000	1,090 000	1,140 000	1,220 000	1,110 000	2,620 000	2,450 000	2,880 000	2,700 000	2,530 000	2,520 000	1,790 000	1,890 000	2,200 000	1,880 000	1,930 160	1,880 000	1,950 000	1,890 000	1,990 000

MEDP0160	Adenosine	268.097	C10H13N5O4	832,000	868,000	1,160,000	1,250,000	1,120,000	1,070,000	20,900,000	22,000,000	19,000,000	17,700,000	17,700,000	27,900,000	1,070,000	983,000	715,000	1,220,000	958,222	795,000	7,110,000	8,740,000	8,820,000
MEDP0163	Cytidine	244.086	C9H13N3O5	8,870,000	9,560,000	10,400,000	7,380,000	6,990,000	8,910,000	5,000,000	5,170,000	5,180,000	4,490,000	5,210,000	4,960,000	6,470,000	6,340,000	6,590,000	6,840,000	6,770,980	7,600,000	5,720,000	6,320,000	6,410,000
MEDP0164	Cytidine-5-Monophosphate	324	C9H14N3O8P	1,160,000	896,000	1,010,000	970,000	1,160,000	1,050,000	299,000	291,000	306,000	322,000	348,000	229,000	297,000	441,000	345,000	492,000	391,144	381,000	507,000	421,000	444,000
MEDP0165	Cytosine	112	C4H5N3O	2,010,000	2,400,000	2,180,000	1,760,000	2,140,000	2,470,000	1,110,000	1,440,000	1,050,000	907,000	1,000,000	1,150,000	1,310,000	1,510,000	945,000	1,100,000	1,221,540	1,240,000	1,670,000	1,380,000	1,300,000
MEDP0166	Deoxyguanosine	268.097	C10H13N5O4	9	9	9	9	9	9	72,800	71,400	70,100	64,700	73,100	84,700	133,000	145,000	139,000	168,000	146,318	146,000	89,500	93,000	94,000
MEDP0167	Guanosine	284.092	C10H13N5O5	4,440,000	4,170,000	4,720,000	5,110,000	4,280,000	4,910,000	40,400,000	43,700,000	40,800,000	35,400,000	39,200,000	43,200,000	37,700,000	44,100,000	42,000,000	48,800,000	43,480,000	44,800,000	34,900,000	36,700,000	36,500,000
MEDP0169	Guanosine Monophosphate	364	C10H14N5O8P	1,840,000	1,540,000	1,250,000	1,390,000	1,970,000	1,520,000	511,000	503,000	400,000	602,000	491,000	561,000	32,900	43,500	40,000	47,300	37,185	22,200	323,000	398,000	345,000
MEDP0170	Hypoxanthine	137	C5H4N4O	208,000	217,000	206,000	205,000	211,000	211,000	180,000	177,000	179,000	176,000	181,000	187,000	187,000	183,000	184,000	186,000	185,318	187,000	192,000	194,000	191,000
MEDP0171	Inosine	269.1	C10H12N4O5	192,000	151,000	138,000	145,000	185,000	159,000	429,000	444,000	424,000	438,000	426,000	410,000	474,000	420,000	420,000	398,000	429,743	437,000	375,000	397,000	407,000
MEDP0173	Nicotinic Acid Adenine Dinucleotide	664.11	C21H27N7O14P2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MEDP0173	Nicotinic Acid Adenine Dinucleotide	664.11	C21H27N7O14P2	159,000	215,000	176,000	153,000	133,000	203,000	6,290	7,160	3,600	7,320	13,400	9	9	9	9	9	9	9	39,800	21,200	37,200
MEDP0174	Purine	121	C5H4N4	1,750,000	2,190,000	2,090,000	1,950,000	1,740,000	1,900,000	2,230,000	1,820,000	3,220,000	1,640,000	2,740,000	1,740,000	1,220,000	1,170,000	1,150,000	1,190,000	1,177,040	1,140,000	1,710,000	1,620,000	1,830,000
MEDP0175	Pyrimidinefreebase	81.2	C4H4N2	9	101,000	57,500	66,700	54,900	76,000	136,000	117,000	158,000	128,000	133,000	141,000	75,300	91,100	118,000	72,800	89,386	89,600	84,600	93,600	80,100

MEDP0176	Thymidine	243.09	C10H14N2O5	83,40	103,0	77,20	87,80	93,60	82,40	102,0	114,0	118,0	71,80	110,0	97,70	115,0	96,80	92,00	94,30	101,3	108,0	101,0	115,0	112,0
				0	00	0	0	0	0	00	00	00	0	00	0	00	0	0	0	02	00	00	00	00
MEDP0177	Thymine	127	C5H6N2O2	199,0	236,0	262,0	273,0	236,0	226,0	88,00	45,30	110,0	88,30	69,70	127,0	160,0	149,0	156,0	155,0	163,0	196,0	133,0	190,0	129,0
				00	00	00	00	00	00	0	0	00	0	0	00	00	00	00	00	88	00	00	00	00
MEDP0178	Uracil	113.027	C4H4N2O2	2,730,	2,580,	2,480,	2,260,	2,700,	2,410,	4,110,	4,670,	3,460,	3,860,	4,450,	4,090,	4,080,	4,260,	3,490,	3,840,	3,851,	3,580,	4,310,	4,220,	4,420,
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	400	000	000	000	000
MEDP0179	Uridine	245	C9H12N2O6	429,0	329,0	353,0	292,0	408,0	321,0	338,0	390,0	305,0	235,0	363,0	395,0	269,0	305,0	322,0	302,0	283,1	217,0	319,0	321,0	327,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	30	00	00	00	00
MEDP0180	B-Nicotinamide Mononucleotide	335.1	C11H15N2O8P	4,650,	4,770,	5,060,	4,850,	4,580,	4,850,	388,0	351,0	430,0	400,0	391,0	371,0	173,0	194,0	187,0	204,0	187,1	178,0	734,0	712,0	714,0
				000	000	000	000	000	000	00	00	00	00	00	00	00	00	00	00	62	00	00	00	00
MEDP0185	Epinephrine	184	C9H13NO3	433,0	564,0	564,0	491,0	449,0	476,0	1,560,	1,280,	1,550,	1,820,	1,470,	1,690,	1,590,	1,350,	1,190,	1,500,	1,386,	1,300,	1,160,	1,030,	1,000,
				00	00	00	00	00	00	000	000	000	000	000	000	000	000	000	000	480	000	000	000	000
MEDP0186	L-Thyroxine	777.687	C15H11I4NO4	38,10	45,50	45,20	55,40	41,70	45,80	46,00	43,30	45,00	39,40	45,00	57,30	36,10	47,00	49,10	43,90	42,48	36,40	47,00	50,10	53,80
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	0	0
MEDP0187	Metanephrine	198.1	C10H15NO3	9	9	9	9	9	9	24,10	18,70	24,80	19,80	33,60	23,90	31,10	29,60	25,30	14,70	27,48	36,70	19,00	20,40	
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	9,520	0
MEDP0188	Norepinephrine	170	C8H11NO3	641,0	823,0	746,0	929,0	750,0	739,0	608,0	742,0	481,0	451,0	678,0	689,0	498,0	597,0	586,0	537,0	560,3	584,0	738,0	723,0	633,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	28	00	00	00	00
MEDP0208	Succinic Acid	119.03	C4H6O4	9	9	9	9	9	9	741,0	741,0	682,0	765,0	812,0	703,0	1,230,	1,200,	1,170,	1,190,	1,191,	1,170,	845,0	720,0	877,0
				00	00	00	00	00	00	00	00	00	00	00	00	000	000	000	000	020	000	00	00	00
MEDP0224	D-Fructose	181	C6H12O6	12,50	11,50	7,460,	9,780,	10,20	9,190,	8,320,	10,50	9,290,	9,040,	6,420,	6,330,	9,370,	4,750,	4,170,	7,810,	6,412,	5,950,	6,540,	6,930,	7,190,
				0,000	0,000	000	000	0,000	000	000	0,000	000	000	000	000	000	000	000	000	340	000	000	000	000
MEDP0227	D-Mannose	181	C6H12O6	11,70	10,60	7,810,	9,000,	11,20	8,380,	7,950,	9,150,	8,660,	9,070,	6,090,	6,770,	10,70	5,090,	6,310,	8,130,	7,380,	6,650,	7,790,	7,130,	7,810,
				0,000	0,000	000	000	0,000	000	000	000	000	000	000	000	0,000	000	000	000	400	000	000	000	000
MEDP0229	Lactose	343	C12H22O11	47,10	30,00	7,910	13,00	13,60	10,30	138,0	122,0	155,0	127,0	154,0	132,0	14,10	20,30	12,40	29,80	19,13	19,10	78,90	70,30	72,00
				0	0	0	0	0	0	00	00	00	00	00	00	0	0	0	0	1	0	0	0	0

MEDP0230	Maltose	343	C12H22O11	47,10 0	30,00 0	7,910	13,00 0	13,60 0	10,30 0	138,0 00	122,0 00	155,0 00	127,0 00	154,0 00	132,0 00	14,10 0	20,30 0	12,40 0	29,80 0	19,13 1	19,10 0	78,90 0	70,30 0	72,00 0
MEDP0232	N-Acetyl-D-Glucosamine	222	C8H15NO6	502,0 00	627,0 00	403,0 00	429,0 00	529,0 00	488,0 00	600,0 00	615,0 00	565,0 00	463,0 00	710,0 00	647,0 00	458,0 00	524,0 00	546,0 00	460,0 00	484,8 00	436,0 00	512,0 00	605,0 00	513,0 00
MEDP0239	L-Ascorbate	177	C6H8O6	212,0 00	198,0 00	354,0 00	167,0 00	287,0 00	171,0 00	226,0 00	267,0 00	319,0 00	223,0 00	133,0 00	189,0 00	202,0 00	117,0 00	143,0 00	203,0 00	198,2 24	326,0 00	194,0 00	216,0 00	214,0 00
MEDP0240	Pyridoxine	170.1	C8H11NO3	2,260, 000	1,990, 000	1,750, 000	1,450, 000	2,050, 000	2,180, 000	1,610, 000	1,900, 000	1,100, 000	1,040, 000	1,800, 000	2,190, 000	969,0 000	1,040, 000	1,120, 000	1,110, 000	1,074, 088	1,130, 000	2,110, 000	2,110, 000	1,960, 000
MEDP0242	Nicotinamide	123.1	C6H6N2O	142,0 00,00	129,0 00,00	129,0 00,00	125,0 00,00	133,0 00,00	136,0 00,00	258,0 00,00	250,0 00,00	268,0 00,00	253,0 00,00	256,0 00,00	263,0 00,00	196,0 00,00	195,0 00,00	203,0 00,00	189,0 00,00	197,3 50,00	202,0 00,00	204,0 00,00	206,0 00,00	203,0 00,00
MEDP0243	4-Oxoretinol	301.2	C20H28O2	9 0	9 0	9 0	9 0	9 0	9 0	54,60 0	85,30 0	25,20 0	24,10 0	89,00 0	49,40 0	40,50 0	9 0	9 0	74,60 0	25,95 4	14,70 0	34,40 0	42,50 0	27,10 0
MEDP0244	All-Trans-13,14-Dihydro-retinol	287.2	C20H32O	9 00	9 00	9 000	9 000	9 000	9 000	950,0 00	834,0 00	1,280, 000	1,040, 000	608,0 00	983,0 00	143,0 00	184,0 00	193,0 00	125,0 00	171,5 88	213,0 00	348,0 00	413,0 00	415,0 00
MEDP0246	Nicotinic Acid	124	C6H5NO2	1,200, 000	411,0 00	600,0 00	2,050, 000	1,360, 000	939,0 00	9,140, 000	6,230, 000	12,60 0,000	7,520, 000	7,880, 000	11,50 0,000	10,90 0,000	12,00 0,000	11,70 0,000	13,40 0,000	12,08 3,600	12,50 0,000	8,640, 000	8,280, 000	8,230, 000
MEDP0249	Pantothenol	206.13	C9H19NO4	17,60 0	24,10 0	18,50 0	22,90 0	11,10 0	9 0	10,70 0	18,90 0	21,40 0	13,30 0	9 0	9 0	73,30 0	68,20 0	83,80 0	87,00 0	80,09 9	88,10 0	37,00 0	41,90 0	38,00 0
MEDP0250	Riboflavin	377	C17H20N4O6	8,300, 000	8,560, 000	8,340, 000	8,050, 000	8,970, 000	8,630, 000	19,20 0,000	21,40 0,000	17,90 0,000	13,70 0,000	22,70 0,000	20,50 0,000	31,70 0,000	32,30 0,000	32,60 0,000	29,30 0,000	31,39 3,000	31,10 0,000	19,50 0,000	21,60 0,000	21,90 0,000
MEDP0251	Trigonelline	138	C7H7NO2	1,850, 000	1,660, 000	1,720, 000	1,580, 000	1,640, 000	1,720, 000	868,0 00	812,0 00	814,0 00	905,0 00	835,0 00	973,0 00	752,0 00	732,0 00	747,0 00	755,0 00	748,0 28	755,0 00	882,0 00	780,0 00	752,0 00
MEDP0271	3-Indolepropionic Acid	190.08	C11H11NO2	174,0 00	165,0 00	174,0 00	171,0 00	151,0 00	169,0 00	179,0 00	111,0 00	303,0 00	197,0 00	139,0 00	146,0 00	110,0 00	192,0 00	181,0 00	146,0 00	165,0 44	196,0 00	153,0 00	187,0 00	200,0 00

MEDP0272	5-Hydroxyindole-3-Acetic Acid	192.06	C10H9NO3	9	9	9	9	9	9	75,40	34,30	131,0	106,0	35,30	70,70	22,20	121,0	94,40	63,60	81,18	105,0	53,90	58,90	53,10
										0	0	00	00	0	0	0	00	0	0	2	00	0	0	0
MEDP0275	Indole-3-Acetic Acid	176.1	C10H9NO2	3,390	3,430	3,440	3,310	3,440	3,580	5,480	5,490	5,830	5,260	5,170	5,670	3,510	4,530	4,400	4,280	4,190	4,230	4,660	4,580	4,430
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	140	000	000	000	000
MEDP0296	4-Guanidinobutyric Acid	146.085	C5H11N3O2	78,30	77,90	74,20	73,10	73,30	76,60	30,60	28,20	29,60	27,90	34,50	33,00	27,90	33,40	38,40	29,90	33,48	37,90	24,40	27,40	25,30
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	2,800	0,000	0,000	0,000	0,000
MEDP0297	5-Aminovaleric Acid	118.2	C5H11NO2	500,0	426,0	553,0	485,0	491,0	475,0	296,0	252,0	296,0	313,0	338,0	280,0	306,0	315,0	310,0	290,0	301,2	285,0	243,0	289,0	269,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	30	00	00	00	00
				348,0	373,0	368,0	349,0	366,0	347,0	523,0	520,0	501,0	541,0	524,0	527,0	544,0	518,0	510,0	545,0	525,3	510,0	506,0	512,0	515,0
MEDP0298	6-Aminocaproic Acid	132.094635	C6H13NO2	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	66,00	00,00	00,00	00,00	00,00
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MEDP0299	7-Methyluric Acid	183	C6H6N4O3	2,380	2,600	2,540	2,680	2,600	2,400	2,220	2,190	2,190	2,360	2,150	2,200	2,420	2,230	2,420	2,290	2,346	2,380	2,200	2,300	2,330
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	600	000	000	000	000
MEDP0300	Adipic Acid	147.0579	C6H10O4	9	9	9	9	9	9	20,60	18,80	19,60	24,20	13,90	26,80	71,90	61,50	51,20	80,90	70,43	86,70	37,60	36,20	32,10
										0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
MEDP0301	Azelaic Acid	189.1049	C9H16O4	717,0	598,0	601,0	666,0	678,0	678,0	986,0	1,390	692,0	711,0	944,0	1,190	3,220	2,680	2,430	3,400	2,887	2,710	1,630	1,560	1,630
				00	00	00	00	00	00	000	00	00	00	00	000	000	000	000	000	280	000	000	000	000
MEDP0305	Creatinine	114.0589	C4H7N3O	7,920	7,700	7,700	7,460	8,740	8,090	22,70	21,10	21,30	17,00	29,10	25,10	46,00	54,70	59,60	51,20	54,45	60,80	21,10	22,90	23,20
				000	000	000	000	000	000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	2,000	0,000	0,000	0,000	0,000
MEDP0307	Dl-2-Aminooctanoic Acid	160.126	C8H17NO2	287,0	269,0	299,0	257,0	269,0	316,0	885,0	988,0	761,0	667,0	930,0	1,080	1,250	982,0	1,080	1,060	1,101	1,130	782,0	829,0	807,0
				00	00	00	00	00	00	00	00	00	00	00	000	000	00	000	000	472	000	00	00	00
MEDP0313	Guanidineacetic Acid	118.1	C3H7N3O2	508,0	446,0	466,0	536,0	483,0	483,0	308,0	286,0	305,0	314,0	348,0	289,0	293,0	332,0	298,0	298,0	308,7	323,0	276,0	307,0	267,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	38	00	00	00	00
MEDP0315	Hippuric Acid	180.1	C9H9NO3	10,80	11,50	11,20	11,80	11,00	11,30	11,60	11,00	13,30	10,90	11,20	11,30	11,60	12,10	11,90	11,60	11,92	12,30	11,50	12,10	12,20
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	3,600	0,000	0,000	0,000	0,000

MEDP0318	Kinurenine	209.1	C10H12N2O3	787,0	819,0	817,0	811,0	804,0	808,0	860,0	729,0	974,0	731,0	870,0	996,0	619,0	644,0	616,0	600,0	620,2	623,0	722,0	751,0	798,0
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	78	00	00	00	00
MEDP0319	Kynurenic Acid	190.0426	C10H7NO3	106,0	101,0	98,80	105,0	89,80	105,0	201,0	198,0	200,0	164,0	196,0	251,0	100,0	146,0	190,0	143,0	143,2	137,0	184,0	151,0	160,0
				00	00	0	00	0	00	00	00	00	00	00	00	00	00	00	00	96	00	00	00	00
MEDP0321	L-Dihydroorotic Acid	159	C5H6N2O4	18,10	15,50	15,60	18,30	15,00	16,10	14,20	13,90	15,10	15,10	13,20	13,60	15,10	13,70	15,90	14,20	14,63	14,20	13,80	16,40	13,20
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,200	0,000	0,000	0,000	0,000
MEDP0322	L-Homoserine	120.1	C4H9NO3	2,240	2,610	2,870	2,850	2,360	2,620	1,080	918,0	1,180	1,170	1,090	1,050	920,0	890,0	931,0	857,0	916,3	983,0	909,0	1,030	945,0
				000	000	000	000	000	000	000	00	000	000	000	000	00	00	00	00	04	00	00	000	00
MEDP0325	Maleic Acid	117.011	C4H4O4	3,140	3,590	3,170	3,300	3,020	3,240	2,570	2,270	2,680	2,410	2,810	2,690	3,940	4,030	4,380	3,640	4,106	4,550	2,900	3,080	2,910
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	260	000	000	000	000
MEDP0326	N'-Formylkynurenine	237.1	C11H12N2O4	76,10	93,20	122,0	123,0	134,0	110,0	346,0	332,0	369,0	312,0	390,0	329,0	325,0	204,0	224,0	244,0	240,5	205,0	215,0	251,0	248,0
				0	0	00	00	00	00	00	00	00	00	00	00	00	00	00	00	84	00	00	00	00
MEDP0331	Subericacid	175.1	C8H14O4	315,0	314,0	299,0	310,0	332,0	308,0	520,0	659,0	393,0	417,0	532,0	601,0	1,760	1,460	1,420	1,870	1,614	1,560	883,0	903,0	879,0
				00	00	00	00	00	00	00	00	00	00	00	000	000	000	000	000	780	000	00	00	00
MEDP0332	Cinnamic Acid	149.052	C9H8O2	22,10	13,40	24,90	18,80	18,50	26,00	44,00	56,20	31,30	42,00	51,20	39,40	43,40	28,70	29,10	34,50	34,50	36,70	25,90	33,80	36,80
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
MEDP0357	Urocanic Acid	139.04	C6H6N2O2	9	85,00	73,00	96,30	9	9	61,10	35,80	60,80	96,30	55,00	57,70	75,50	58,50	73,60	83,00	68,96	54,20	65,00	77,10	65,80
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
MEDP0367	γ-Aminobutyric Acid	104.06	C4H9NO2	38,10	56,00	70,50	57,30	51,60	52,10	4,310	9	9	10,50	11,10	9	8,050	9	9	9	3,611	9,980	12,80	6,600	8,380
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MEDP0368	Taurocholic Acid Sodium Salt Hydrate	556.28	C26H46NNaO8S	3,560	3,880	4,260	3,610	4,310	4,290	3,800	3,570	3,920	4,310	3,700	3,480	3,820	4,170	3,730	3,930	3,954	4,120	3,480	3,880	4,120
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	160	000	000	000	000
MEDP0370	2-(Formylamino)Benzoic Acid	166.04	C8H7NO3	72,30	96,70	97,60	107,0	84,30	98,70	164,0	178,0	157,0	137,0	155,0	196,0	415,0	368,0	353,0	380,0	382,6	398,0	229,0	254,0	233,0
				0	0	0	00	0	0	00	00	00	00	00	00	00	00	00	00	88	00	00	00	00
MEDP0372	Uridine 5-Monophosphate	325	C9H13N2O9P	14,20	17,80	34,90	21,60	9	24,60	46,30	45,30	46,00	62,10	26,60	51,60	14,20	9	9	9	2,853	9	26,20	29,40	33,60
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

				124,0	123,0	121,0	121,0	118,0	119,0																
MEDP0373	N-Acetylglucine	118	C4H7NO3	00,00	00,00	00,00	00,00	00,00	00,00	56,20	51,20	54,90	51,60	63,10	60,00	38,80	44,00	52,50	41,00	45,61	51,80	42,70	47,50	45,80	
				0	0	0	0	0	0	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	1,200	0,000	0,000	0,000	0,000	
MEDP0378	N6-Succinyl Adenosine	384	C14H17N5O8	4,200,	5,400,	5,810,	4,890,	5,070,	5,050,	1,620,	1,530,	1,470,	1,200,	2,000,	1,920,	2,740,	3,080,	2,810,	2,580,	2,849,	3,040,	3,090,	3,180,	3,500,	
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	460	000	000	000	000	
MEDP0380	2-(Dimethylamino)Guano-sine	312	C12H17N5O5	1,570,	1,600,	1,530,	1,600,	1,640,	1,500,	370,0	340,0	397,0	271,0	414,0	427,0	703,0	748,0	730,0	919,0	748,9	646,0	1,090,	1,140,	1,110,	
				000	000	000	000	000	000	00	00	00	00	00	00	00	00	00	00	70	00	000	000	000	
MEDP0383	B-Pseudouridine	245	C9H12N2O6	429,0	329,0	353,0	292,0	408,0	321,0	338,0	390,0	305,0	235,0	363,0	395,0	269,0	305,0	322,0	302,0	283,1	217,0	319,0	321,0	327,0	
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	30	00	00	00	00	
MEDP0387	L-Homoargininei	189	C7H16N4O2	2,690,	3,440,	3,550,	3,310,	2,900,	3,350,	299,0	314,0	255,0	187,0	371,0	369,0	144,0	183,0	196,0	183,0	179,0	190,0	255,0	335,0	316,0	
				000	000	000	000	000	000	00	00	00	00	00	00	00	00	00	00	40	00	00	00	00	
MEDP0389	Pantetheine	279.13	C11H22N2O4S	13,80	15,00	14,70	16,00	17,00	16,90	21,90	23,30	16,20	15,40	19,60	35,20	13,80	13,30	12,70	16,50	13,96	13,60	15,40	17,40	16,60	
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	5,000	0,000	0,000	0,000	0,000	
MEDP0393	Pyridoxine 5'-Phosphate	250	C8H12NO6P	182,0	189,0	112,0	77,10	222,0	142,0	1,190,	1,150,	1,220,	1,010,	1,320,	1,230,	683,0	897,0	839,0	808,0	814,8	847,0	749,0	790,0	936,0	
				00	00	00	0	00	00	000	000	000	000	000	000	00	00	00	00	82	00	00	00	00	
MEDP0395	DL-Pipecolic Acid	130	C6H11NO2	2,010,	2,310,	2,360,	2,440,	2,210,	2,290,	2,090,	2,340,	2,290,	1,860,	1,560,	2,420,	5,100,	4,930,	5,030,	4,570,	4,913,	4,940,	3,470,	3,360,	2,660,	
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	820	000	000	000	000	
MEDP0396	2'-Deoxycytidine-5'-Mono-phosphate	308	C9H14N3O7P	9	9	9	9	9	9	368,0	318,0	389,0	328,0	357,0	451,0	693,0	981,0	985,0	795,0	884,9	971,0	415,0	414,0	465,0	
										00	00	00	00	00	00	00	00	00	00	10	00	00	00	00	
MEDP0401	5'-Deoxy-5'-(Methylthio) Adenosine	298	C11H15N5O3S	796,0	924,0	1,240,	1,340,	903,0	1,070,	92,50	102,0	80,30	80,50	100,0	99,00	9	9	9	9	9	9	238,0	258,0	275,0	
				00	00	000	000	00	000	0	00	0	0	00	0							00	00	00	
MEDP0403	Deoxycytidine	228	C9H13N3O4	102,0	86,50	62,70	44,50	73,70	54,00	112,0	136,0	91,70	73,90	127,0	132,0	85,10	77,60	91,20	94,90	85,81	80,30	73,90	54,80	97,90	
				00	0	0	0	0	0	00	00	0	0	00	00	0	0	0	0	6	0	0	0	0	
MEDP0409	Cys-Gly	179	C5H10N2O3S	1,230,	1,290,	1,340,	1,230,	1,220,	1,330,	40,40	13,50	83,30	53,80	20,80	30,40	6,490	24,70	11,40	9	9,291	3,920	137,0	144,0	180,0	
				000	000	000	000	000	000	0	0	0	0	0	0		0	0				00	00	00	

MEDP0430	2-Aminoadipic Acid	162.1	C6H11NO4	2,590, 3,390, 3,740, 3,230, 2,720, 2,820, 164,0 126,0 192,0 154,0 193,0 156,0 188,0 177,0 256,0 180,0 194,5 171,0 348,0 351,0 369,0 000 000 000 000 000 000 00 00 00 00 00 00 00 00 00 06 00 00 00 00
MEDP0435	6-Methyl mercaptopurine	167.1	C6H6N4S	55,80 57,30 58,60 55,50 56,60 57,60 142,0 136,0 149,0 134,0 146,0 143,0 116,0 127,0 123,0 120,0 122,3 125,0 114,0 116,0 116,0 00,00 0
MEDP0442	Sn-Glycero-3-Phosphocholine	258.2	C8H20NO6P	19,60 21,20 22,60 20,80 19,30 22,90 5,360, 4,480, 5,470, 5,250, 5,670, 5,900, 7,590, 7,740, 7,650, 7,160, 7,621, 7,970, 6,110, 6,840, 6,220, 0,000 0,000 0,000 0,000 0,000 0,000 000 000 000 000 000 000 000 000 000 000 880 000 000 000 000
MEDP0446	3-Hydroxykynurenine	225.1	C10H12N2O4	136,0 241,0 227,0 175,0 166,0 184,0 28,20 34,40 29,70 47,00 30,10 51,80 53,60 24,20 45,40 41,13 30,60 64,00 52,60 80,90 00 00 00 00 00 00 0 0 9 0 0 0 0 0 0 2 0 0 0 0
MEDP0453	Indole	118	C8H7N	3,170, 3,350, 3,070, 3,180, 3,320, 3,260, 4,940, 4,960, 5,190, 4,450, 5,030, 5,070, 3,070, 3,990, 3,540, 3,990, 3,710, 3,960, 4,070, 4,310, 4,150, 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 160 000 000 000 000
MEDP0457	5-Aminolevulinate	132.1	C5H9NO3	1,120, 1,170, 1,150, 1,080, 1,160, 1,110, 3,470, 3,420, 3,500, 3,140, 3,790, 3,490, 3,050, 2,950, 2,990, 3,050, 3,017, 3,040, 2,920, 2,810, 2,740, 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 340 000 000 000 000
MEDP0461	2-Methylguanosine	298.1	C11H15N5O5	1,250, 1,310, 1,270, 1,260, 1,350, 1,330, 591,0 577,0 578,0 465,0 693,0 641,0 1,080, 1,070, 1,000, 1,170, 1,068, 1,030, 1,140, 1,140, 1,110, 000 000 000 000 000 000 00 00 00 00 00 00 000 000 000 000 300 000 000 000 000
MEDP0504	Glucosamine	180	C6H13NO5	714,0 1,240, 994,0 767,0 874,0 874,0 700,0 931,0 656,0 633,0 605,0 674,0 905,0 495,0 744,0 628,0 663,3 546,0 488,0 529,0 690,0 00 000 00 00 00 00 00 00 00 00 00 00 00 00 00 00 82 00 00 00 00
MEDP0507	2-Hydroxycinnamic acid	165.047	C9H8O3	7,150, 7,460, 7,310, 7,030, 7,490, 7,190, 16,90 17,00 17,60 16,00 17,40 16,70 12,10 13,80 13,60 13,20 13,17 13,10 13,80 13,80 13,90 000 000 000 000 000 000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000 0,000
MEDP0518	DL-Stachydrine	144.1025	C7H14ClNO2	1,910, 2,390, 2,150, 1,480, 1,550, 1,570, 795,0 771,0 889,0 655,0 820,0 840,0 957,0 839,0 877,0 834,0 883,7 912,0 669,0 780,0 733,0 000 000 000 000 000 000 00 00 00 00 00 00 00 00 00 00 04 00 00 00 00
MEDP0519	L-Norleucine	132.1023	C6H13NO2	5,640, 5,590, 5,430, 5,350, 5,480, 5,750, 10,70 9,980, 11,50 9,790, 10,80 11,60 6,590, 9,370, 8,980, 8,620, 8,456, 8,730, 8,380, 8,970, 8,590, 000 000 000 000 000 000 0,000 000 0,000 000 0,000 0,000 000 000 000 000 480 000 000 000 000
MEDP0525	N-Acetyl-L-alanine	132.058244	C5H9NO3	17,20 19,70 19,50 17,70 18,80 17,30 51,40 50,10 53,00 51,60 54,20 48,00 44,20 49,30 45,00 45,90 45,80 44,70 44,30 43,10 44,40 0,000

MEDP0540	7,8-dihydro-L-Biopterin	240.10184	C9H13N5O 3	9	9	9	9	9	9	139,0	136,0	137,0	136,0	129,0	159,0	96,40	95,80	101,0	74,30	93,79	102,0	68,50	99,70	73,10
										00	00	00	00	00	00	0	0	00	0	0	00	0	0	0
MEDP0575	5-amino-1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]imidazole-4-carboxamide	259.096421	C9H14N4O 5	1,770	2,190	2,750	2,750	2,040	2,300	2,580	2,450	2,680	2,230	2,620	2,910	1,180	2,060	1,760	1,490	1,658	1,800	2,210	2,140	2,290
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	200	000	000	000	000
MEDP0576	N1-Acetylspermine	245.2263115	C12H28N4 O	9	9	9	9	9	9	24,00	23,30	20,40	9	28,30	48,20	127,0	99,20	112,0	115,0	114,8	120,0	32,10	39,90	52,10
										0	0	0		0	0	00	0	00	00	33	00	0	0	0
MEDP0586	N-Acetylphenylalanine	208.0895433	C11H13NO 3	47,20	61,80	61,90	65,50	62,90	64,50	688,0	542,0	552,0	420,0	823,0	1,100	1,340	1,240	1,270	1,190	1,263	1,270	610,0	686,0	692,0
				0	0	0	0	0	0	00	00	00	00	00	000	000	000	000	000	560	000	00	00	00
MEDP0587	N-Alpha-acetyllysine	189.1160924	C8H16N2O 3	26,50	37,50	38,60	36,30	28,10	33,90	4,930	3,460	4,250	2,600	6,710	7,640	1,650	3,120	2,680	1,790	2,379	2,650	4,010	3,970	3,980
				0,000	0,000	0,000	0,000	0,000	0,000	000	000	000	000	000	000	000	000	000	000	140	000	000	000	000
MEDP0601	Spermidine	146.1578976	C7H19N3	1,580	1,130	1,060	1,070	1,320	1,080	10,10	9,370	11,00	8,410	11,30	10,60	9,940	12,10	13,90	11,40	12,02	12,80	7,260	7,820	8,020
				000	000	000	000	000	000	0,000	000	0,000	000	0,000	0,000	000	0,000	0,000	0,000	9,900	0,000	000	000	000
MEDP0611	N-Acetyl-L-Histidine	198.0800412	C8H11N3O 3	41,10	34,60	32,00	35,10	43,20	40,80	18,50	15,30	19,30	20,50	18,50	19,20	12,10	11,50	11,60	12,10	11,94	12,40	13,60	15,60	14,60
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	3,400	0,000	0,000	0,000	0,000
MEDP0627	Isonicotinic acid	124.0320284	C6H5NO2	54,40	47,30	49,90	48,40	51,40	52,80	115,0	113,0	122,0	109,0	114,0	118,0	78,50	80,20	84,00	75,30	80,33	83,60	82,60	86,80	83,10
				0,000	0,000	0,000	0,000	0,000	0,000	00,00	00,00	00,00	00,00	00,00	00,00	0,000	0,000	0,000	0,000	3,000	0,000	0,000	0,000	0,000
										0	0	0	0	0	0									
MEDP0637	L-phenylalanyl-L-proline	263.131743	C14H18N2 O3	1,210	1,290	1,440	1,370	1,250	1,370	20,30	18,40	23,70	21,90	19,30	18,00	16,70	22,90	18,50	21,80	20,54	22,90	15,30	15,40	15,30
				000	000	000	000	000	000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	4,800	0,000	0,000	0,000	0,000
MEDP0685	Methylcysteine	136.2	C4H9NO2S	7,310	7,300	7,590	7,310	7,690	7,460	17,50	17,90	17,70	16,50	18,50	17,10	13,10	14,50	15,60	13,90	14,23	14,20	14,00	14,80	14,50
				000	000	000	000	000	000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	2,000	0,000	0,000	0,000	0,000
MEDP0689	TranexamicAcid	158.1	C8H15NO2	55,00	65,10	52,10	74,60	63,90	61,50	65,90	75,10	65,20	46,50	69,70	73,10	56,60	50,50	51,90	65,00	58,71	69,60	64,90	51,70	45,10
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0
MEDP0700	Methyl beta-D-galactopyranoside	195.2	C7H14O6	204,0	174,0	164,0	196,0	142,0	184,0	176,0	240,0	135,0	175,0	149,0	179,0	114,0	109,0	144,0	119,0	117,0	99,40	115,0	90,40	65,90
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	16	0	00	0	0

MEDP0729	Barbituric acid	129	C4H4N2O3	5,850, 5,440, 6,090, 5,890, 4,370, 5,690, 6,570, 7,530, 6,640, 5,780, 6,670, 6,230, 6,060, 4,870, 5,700, 5,490, 5,428, 5,020, 5,470, 5,490, 3,940, 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 720 000 000 000 000
MEDP0752	DL-Leucine	132.094635	C6H13NO2	348,0 373,0 368,0 349,0 366,0 347,0 523,0 520,0 501,0 541,0 524,0 527,0 544,0 518,0 510,0 545,0 525,3 510,0 506,0 512,0 515,0 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 66,00 00,00 00,00 00,00 00,00
MEDP0821	6-Methylnicotinamide	137.1	C7H8N2O	0 244,0 242,0 242,0 249,0 242,0 245,0 234,0 229,0 210,0 238,0 226,5 223,0 200,0 208,0 194,0 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 96,00 00,00 00,00 00,00 00,00
MEDP0846	4-Methylbenzoic acid	136.9	C8H8O2	0,000 0,000 0,000 0,000 0,000 0,000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 169,0 75,20 203,0 150,0 141,0 108,0 62,60 67,00 49,30 00 0 00 00 32 00 0 0 0
MEDP0849	Nα-Acetyl-L-glutamine	189.1	C7H12N2O4	9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 00,00 260 000 000 000 000
MEDP0859	Glycyl-DL-phenylalanine	223.2	C11H14N2O3	33,60 46,10 47,70 44,80 36,90 42,70 3,500, 2,790, 2,800, 2,290, 4,720, 4,910, 2,270, 2,770, 3,260, 2,610, 2,787, 3,030, 5,190, 5,370, 5,240, 6,350, 5,640, 5,490, 5,860, 6,460, 6,420, 140,0 146,0 139,0 133,0 138,0 144,0 88,00 74,10 76,50 76,40 79,33 81,60 81,50 87,90 87,90 000 000 000 000 000 000 0 0 0 0 0 0 0,000 0,000 0,000 0,000 5,000 0,000 0,000 0,000
MEDP0868	N-Methylalanine	104	C4H9NO2	0 1,370, 1,630, 1,520, 1,660, 1,550, 1,500, 5,320, 5,830, 4,990, 6,040, 4,940, 4,810, 7,820, 7,880, 7,900, 8,920, 8,247, 8,720, 7,390, 7,430, 7,350, 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 000 660 000 000 000 000
MEDP0876	O-Succinyl-L-Homoserine	220.2	C8H13NO6	648,0 758,0 763,0 563,0 798,0 733,0 134,0 130,0 107,0 138,0 137,0 159,0 348,0 384,0 328,0 377,0 359,3 359,0 380,0 354,0 334,0 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 14 00 00 00 00
MEDP0878	N-Methyl-L-Glutamate	162.3	C6H11NO4	2,310, 2,810, 3,230, 2,750, 2,470, 2,810, 203,0 175,0 173,0 167,0 259,0 242,0 182,0 243,0 198,0 226,0 226,5 284,0 319,0 333,0 346,0 000 000 000 000 000 000 00 00 00 00 00 00 00 00 00 00 78 00 00 00 00
MEDP0879	N-Methyl-D-Aspartic Acid	148.2	C5H9NO4	9 9 9 9 9 9 95,80 72,20 94,90 112,0 137,0 63,20 105,0 80,70 104,0 132,0 109,8 127,0 161,0 138,0 186,0 0 0 0 00 00 0 00 0 00 00 01 00 00 00 00
MEDP0880	N-Alpha-Acetyl-L-Asparagine	175.3	C6H10N2O4	9 9 9 9 9 9 316,0 454,0 229,0 515,0 380,0 458,0 307,0 303,0 503,0 391,5 386,0 339,0 299,0 424,0 00 00 9 00 00 00 00 00 00 00 00 00 74 00 00 00 00

MEDP0881	Phosphocholine	185.1	C5H15NO4 P	16,50 0,000	15,90 0,000	15,30 0,000	14,40 0,000	16,00 0,000	15,00 0,000	15,60 0,000	16,70 0,000	14,50 0,000	13,70 0,000	15,90 0,000	17,20 0,000	13,00 0,000	13,00 0,000	11,70 0,000	12,60 0,000	12,36 8,000	11,40 0,000	13,80 0,000	14,90 0,000	14,30 0,000
MEDP0883	2,4-Dihydroxypteridine	165.3	C6H4N4O2	79,20 0	99,60 0	76,70 0	63,10 0	68,70 0	90,20 0	196,0 00	188,0 00	210,0 00	185,0 00	223,0 00	176,0 00	163,0 00	156,0 00	159,0 00	144,0 00	160,8 94	183,0 00	159,0 00	181,0 00	164,0 00
MEDP0884	L-Methionine Sulfoximine	181.3	C5H12N2O 3S	20,00 0	14,30 0	17,40 0	11,30 0	6,530	9,790	38,60 0	33,90 0	50,40 0	52,10 0	36,60 0	19,80 0	66,10 0	70,80 0	73,10 0	84,40 0	69,77 1	54,40 0	43,50 0	44,00 0	60,90 0
MEDP0886	N-Amidino-L-Aspartate	176.4	C5H9N3O4	89,00 0	102,0 00	149,0 00	140,0 00	123,0 00	126,0 00	168,0 00	165,0 00	174,0 00	167,0 00	163,0 00	170,0 00	51,60 0	75,10 0	66,20 0	60,50 0	63,49 1	64,10 0	86,70 0	97,90 0	83,30 0
MEDP0889	Cortisol	363.5	C21H30O5	34,30 0	38,70 0	41,10 0	35,40 0	36,60 0	36,80 0	43,10 0	37,60 0	39,30 0	41,90 0	49,10 0	47,50 0	33,80 0	29,50 0	32,80 0	35,50 0	33,27 6	34,80 0	36,70 0	39,60 0	41,60 0
MEDP0890	7,8-Dimethylalloxazine	243.2	C12H10N4 O2	188,0 00	218,0 00	190,0 00	201,0 00	211,0 00	232,0 00	351,0 00	388,0 00	328,0 00	259,0 00	384,0 00	398,0 00	550,0 00	517,0 00	548,0 00	521,0 00	552,4 06	627,0 00	336,0 00	381,0 00	389,0 00
MEDP0891	L-Tryptophanamide	204.3	C11H13N3 O	189,0 00	171,0 00	184,0 00	165,0 00	193,0 00	180,0 00	304,0 00	289,0 00	311,0 00	258,0 00	323,0 00	338,0 00	225,0 00	274,0 00	251,0 00	260,0 00	252,0 82	251,0 00	228,0 00	269,0 00	276,0 00
MEDP0899	3-Methyladenine	150.3	C6H7N5	57,10 0	97,60 0	68,30 0	72,70 0	76,50 0	87,00 0	33,20 0	23,00 0	28,20 0	36,00 0	36,10 0	42,60 0	33,40 0	35,00 0	43,70 0	30,80 0	32,00 9	17,20 0	32,50 0	32,60 0	32,50 0
MEDP1002	Acetylcholine	146.1084	C7H15NO2	11,90 0,000	11,50 0,000	11,40 0,000	11,10 0,000	11,20 0,000	11,10 0,000	3,980 000	3,880 000	4,160 000	4,590 000	3,700 000	3,540 000	4,260 000	3,880 000	3,710 000	3,240 000	3,769 000	3,760 000	4,630 000	4,680 000	4,480 000
MEDP1005	β-Alanine	90.048	C3H7NO2	37,50 0,000	37,80 0,000	38,70 0,000	37,10 0,000	36,30 0,000	38,40 0,000	8,070 000	10,20 0,000	6,810 000	6,290 000	7,890 000	9,140 000	4,920 000	6,300 000	5,800 000	5,830 000	5,797 060	6,150 000	8,020 000	7,910 000	7,900 000
MEDP1006	Creatine	132.0671941	C4H9N3O2	138,0 00,00	131,0 00,00	137,0 00,00	133,0 00,00	131,0 00,00	134,0 00,00	41,10 0,000	53,30 0,000	32,80 0,000	31,70 0,000	39,90 0,000	47,90 0,000	22,50 0,000	29,50 0,000	27,60 0,000	29,10 0,000	27,61 2,800	29,30 0,000	39,30 0,000	40,20 0,000	38,60 0,000
MEDP1010	Coenzyme II (β-NADP)	744	C21H28N7 O17P3	9 0	9 0	9 0	9 0	9 0	9 0	27,90 0	31,50 0	26,50 0	18,20 0	38,00 0	25,10 0	31,20 0	43,10 0	34,30 0	46,10 0	41,25 1	51,50 0	32,40 0	41,00 0	34,20 0

MEDP1018	5'-Deoxyadenosine	252	C10H13N5O3	70,30	113,0	109,0	96,30	99,10	108,0	25,60	25,00	22,30	24,20	23,80	32,70	32,20	44,90	37,70	37,80	38,34	39,10	42,60	44,40	62,40
				0	00	00	0	0	00	0	0	0	0	0	0	0	0	0	0	8	0	0	0	0
MEDP1019	aminoisobutyric acid	104	C4H9NO2	1,370,	1,630,	1,520,	1,660,	1,550,	1,500,	5,320,	5,830,	4,990,	6,040,	4,940,	4,810,	7,820,	7,880,	7,900,	8,920,	8,247,	8,720,	7,390,	7,430,	7,350,
				000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	660	000	000	000	000
MEDP1022	Threoninyl-Phenylalanine	267.1243321	C13H18N2O4	170,0	61,40	35,20	74,60	136,0	116,0	1,720,	1,890,	1,550,	1,680,	1,660,	1,820,	1,070,	1,540,	1,370,	1,190,	1,326,	1,460,	1,190,	1,170,	1,160,
				00	0	0	0	00	00	000	000	000	000	000	000	000	000	000	000	600	000	000	000	000
MEDP1023	Tryptophan glutamic acid	334.1303767	C16H19N3O5	57,00	62,10	81,80	68,50	67,40	69,00	2,250,	2,010,	2,360,	1,910,	2,300,	2,670,	1,830,	2,930,	2,720,	2,490,	2,587,	2,960,	1,330,	1,520,	1,600,
				0	0	0	0	0	0	000	000	000	000	000	000	000	000	000	000	060	000	000	000	000
MEDP1024	Valyl-leucine	231.1606614	C11H22N2O3	3,260,	519,0	352,0	479,0	2,120,	1,300,	43,50	53,40	37,00	41,90	49,10	35,90	45,20	24,90	26,80	27,30	30,45	28,10	28,40	29,20	28,90
				000	00	00	00	000	000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	3,000	0,000	0,000	0,000	0,000
MEDP1025	L-Valyl-L-phenylalanine	265.1453447	C14H20N2O3	370,0	100,0	73,50	98,80	262,0	190,0	19,80	24,30	17,30	17,90	20,80	19,00	18,70	18,40	18,10	19,70	18,69	18,50	15,50	16,00	15,80
				00	00	0	0	00	00	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	7,200	0,000	0,000	0,000	0,000
MEDP1045	Biliverdin	583.2	C33H34N4O6	13,10	5,130	6,020	7,280	7,530	8,260	10,90	21,30				15,50	17,50	11,50							10,30
				0						0	0	9	9		0	0	0	9	9	9	2,616	1,570	7,520	4,710
																								0
MEDP1059	2-Picolinic Acid	124.0839	C6H5NO2	85,60	39,60	40,60	168,0	143,0	86,40	770,0	487,0	1,020,	680,0	663,0	1,000,	921,0	1,010,	1,010,	1,210,	1,048,	1,090,	713,0	708,0	714,0
				0	0	0	00	00	0	00	00	000	00	00	000	00	000	000	000	516	000	00	00	00
				349,0	340,0	348,0	349,0	347,0	350,0	349,0	348,0	348,0	349,0	349,0	353,0	357,0	353,0	355,0	351,0	354,2	356,0	349,0	355,0	352,0
MEDP1061	DL-O-tyrosine	166	C9H11NO2	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	72,00	00,00	00,00	00,00	00,00
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MEDP1063	Indole-5-carboxylic acid	162.0452919	C9H7NO2	9	9	9	9	9	9	122,0	219,0	25,10	36,70	204,0	126,0	358,0	129,0	244,0	288,0	243,9	200,0	128,0	121,0	125,0
										00	00	0	0	00	00	00	00	00	00	18	00	00	00	00
MEDP1070	Glycyl-L-valine	175.1	C7H14N2O3	9	9	9	9	9	9	49,90	48,30	55,20	45,50	53,10	47,50	51,70	70,40	53,60	71,20	62,85	67,40	60,10	52,30	50,20
										0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
MEDP1071	Alanyl-dl-leucine	203.1288496	C9H18N2O3	437,0	177,0	120,0	175,0	384,0	309,0	12,80	14,80	10,90	11,50	14,50	12,40	21,50	27,40	25,30	23,20	24,80	26,70	13,70	14,30	14,30
				00	00	00	00	00	00	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	7,400	0,000	0,000	0,000	0,000

MEDP1072	7-methylguanosine	298.1	C11H15N5O5	1,250,000	1,310,000	1,270,000	1,260,000	1,350,000	1,330,000	591,000	577,000	578,000	465,000	693,000	641,000	1,080,000	1,070,000	1,000,000	1,170,000	1,068,000	1,030,000	1,140,000	1,140,000	1,110,000
MEDP1073	6-O-methylguanine	166.06296	C6H7N5O	219,000	249,000	236,000	216,000	244,000	253,000	66,800	95,800	51,100	9	84,300	103,000	72,400	101,000	64,300	118,000	85,690	73,000	131,000	129,000	143,000
MEDP1077	2'-O-methyladenosine	348.1	C11H15N5O4	2,390,000	2,090,000	1,960,000	2,050,000	2,090,000	2,200,000	515,000	539,000	434,000	675,000	349,000	576,000	161,000	133,000	127,000	135,000	126,000	74,800	652,000	641,000	491,000
MEDP1080	Glycyl-tryptophan	262.1094522	C13H15N3O3	29,500	27,200	28,500	33,500	34,400	32,200	662,000	584,000	789,000	598,000	582,000	756,000	396,000	736,000	651,000	570,000	610,300	699,000	389,000	428,000	448,000
MEDP1083	Oxypurinol	153	C5H4N4O2	34,700,000	37,600,000	38,100,000	31,700,000	44,400,000	36,300,000	15,700,000	17,000,000	14,300,000	12,600,000	18,400,000	16,500,000	13,800,000	16,000,000	12,500,000	14,700,000	14,280,000	14,500,000	21,600,000	20,900,000	23,400,000
MEDP1093	Allopurinol	137.0481928	C5H4N4O	62,300,000	49,000,000	44,600,000	46,900,000	57,600,000	51,600,000	216,000	219,000	210,000	219,000	219,000	214,000	199,000	205,000	201,000	208,000	202,500	199,000	190,000	189,000	187,000
MEDP1106	Lithocholic acid	359.2949615	C24H40O3	9	9	9	9	9	9	121,000	84,300	148,000	115,000	90,700	166,000	14,900	77,900	62,200	52,900	53,580	60,200	51,900	53,500	50,700
MEDP1109	Glycocholic Acid	466.3055321	C26H43NO6	77,500	95,400	83,700	100,000	90,600	86,100	150,000	131,000	180,000	133,000	140,000	163,000	105,000	124,000	149,000	220,000	146,500	134,000	135,000	139,000	121,000
MEDP1126	(R)-(-)-2-phenylglycine	120.0726939	C8H11NO	18,300,000	18,200,000	17,900,000	17,200,000	17,400,000	17,900,000	47,800,000	46,500,000	50,400,000	44,600,000	48,900,000	48,400,000	37,600,000	43,900,000	41,400,000	40,500,000	41,020,000	41,700,000	41,500,000	38,000,000	38,500,000
MEDP1127	1-acetylintole	160.1	C10H9NO	949,000	998,000	952,000	965,000	770,000	825,000	1,100,000	1,030,000	1,260,000	1,050,000	1,040,000	1,120,000	814,000	899,000	959,000	859,000	889,700	917,000	1,100,000	1,020,000	944,000
MEDP1131	Arachidyl glycine	352.31663	C22H43NO3	36,400	42,800	27,900	56,300	20,700	121,000	51,800	47,100	60,800	39,500	69,500	42,000	100,000	72,200	24,400	44,000	59,040	54,300	11,600	22,100	19,000
MEDP1132	3-Carboxypropyltrimethylammonium	146.1084	C7H15NO2	11,900,000	11,500,000	11,400,000	11,100,000	11,200,000	11,100,000	3,980,000	3,880,000	4,160,000	4,590,000	3,700,000	3,540,000	4,260,000	3,880,000	3,710,000	3,240,000	3,769,000	3,760,000	4,630,000	4,680,000	4,480,000

				341,0	363,0	349,0	341,0	345,0	344,0	535,0	531,0	532,0	530,0	539,0	543,0	552,0	532,0	525,0	553,0	538,3	531,0	512,0	522,0	526,0	
MEDP1144	L-Isoleucine	132.09222	C6H13NO2	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	70,00	00,00	00,00	00,00	00,00	
				0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
MEDP1161	Creatine phosphate	212.0425549	C4H10N3O5P	1,790,000	1,720,000	1,810,000	1,790,000	1,910,000	2,180,000	2,010,000	1,900,000	1,880,000	1,910,000	2,000,000	2,390,000	1,700,000	1,850,000	1,730,000	1,660,000	1,736,000	1,740,000	1,230,000	1,780,000	2,020,000	
MEDP1162	1-Methylguanine	166.07051	C6H7N5O	547,000	496,000	576,000	522,000	544,000	543,000	267,000	254,000	270,000	202,000	278,000	330,000	323,000	299,000	286,000	353,000	314,000	309,000	383,000	377,000	342,000	
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	72	00	00	00	00	
MEDP1177	N-Methyl- $\alpha$ -aminoisobutyric acid	235.2	C5H11NO2	7,000,000	6,290,000	7,780,000	7,360,000	7,590,000	7,630,000	1,170,000	1,010,000	1,190,000	1,440,000	1,150,000	1,060,000	553,000	453,000	560,000	432,000	520,400	604,000	1,060,000	1,370,000	1,200,000	
				000	000	000	000	000	000	000	000	000	000	000	000	00	00	00	00	42	00	000	000	000	
MEDP1194	Calcitriol	417.3	C27H44O3	47,100	59,100	44,000	35,700	60,000	48,400	22,800	24,200	10,300	37,400	24,700	17,500	10,300		9	9	9	2,065	9	17,800	22,800	23,000
				0	0	0	0	0	0	0	0	0	0	0	0	0						0	0	0	
MEDP1196	Biotinamide	244.1082639	C10H17N3O2S	15,600,000	17,200,000	15,900,000	14,900,000	15,800,000	15,600,000	10,900,000	10,000,000	11,600,000	9,930,000	10,800,000	12,100,000	15,900,000	16,600,000	17,100,000	15,900,000	16,640,000	17,700,000	13,800,000	14,700,000	15,000,000	
				0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	7,400	0,000	0,000	0,000	0,000	
MEDP1197	Hypotaurocyamine	152	C3H9N3O2S	581,000	524,000	577,000	689,000	490,000	664,000	5,060,000	5,300,000	4,950,000	4,640,000	4,960,000	5,470,000	5,130,000	5,780,000	5,510,000	6,040,000	5,579,000	5,440,000	4,440,000	4,660,000	4,530,000	
				00	00	00	00	00	00	000	000	000	000	000	000	000	000	000	000	140	000	000	000	000	
MEDP1202	5'-deoxy-5'-fluoroadenosine	270.1	C10H12FN5O3	9	9	9	9	9	9	126,000	133,000	98,400	115,000	123,000	161,000		9	9	9	9	9	9	65,800	44,800	49,900
										00	00	0	00	00	00							0	0	0	
MEDP1222	1-Aminocyclohexanoic acid	144.1	C7H13NO2	11,100,000	9,790,000	10,500,000	10,000,000	10,100,000	10,400,000	3,170,000	2,750,000	3,440,000	3,820,000	2,760,000	3,090,000	3,700,000	3,560,000	2,810,000	3,030,000	3,277,000	3,290,000	4,120,000	4,230,000	3,990,000	
				0,000	000	0,000	0,000	0,000	0,000	000	000	000	000	000	000	000	000	000	000	040	000	000	000	000	
MEDP1242	4-tert-butylbenzoic acid	179.10617	C11H14O2	249,000	239,000	228,000	232,000	267,000	267,000	241,000	250,000	259,000	238,000	196,000	264,000	300,000	238,000	248,000	256,000	267,400	295,000	138,000	161,000	151,000	
				00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	00	66	00	00	00	00	
MEDP1246	2,4-diacetamino-2,4,6-triphenoxy-D-mannopyranose	247.1	C10H18N2O5	5,590,000	5,240,000	5,010,000	4,490,000	5,930,000	5,660,000	150,000	142,000	163,000	146,000	150,000	148,000	109,000	126,000	122,000	117,000	119,400	124,000	98,600	103,000	101,000	
				000	000	000	000	000	000	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	00,00	38,00	00,00	0,000	00,00	00,00	
										0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	

MEDP1272	20,26-dihydroxyecdysone	497.3	C27H44O8	41,60 0,000 0	53,70 0,000 0	57,80 0,000 0	54,50 0,000 0	50,20 0,000 0	56,50 0,000 0	305,0 00,00 0	304,0 00,00 0	317,0 00,00 0	297,0 00,00 0	304,0 00,00 0	301,0 00,00 0	323,0 00,00 0	346,0 00,00 0	351,0 00,00 0	310,0 00,00 0	333,2 10,00 0	336,0 00,00 0	304,0 00,00 0	304,0 00,00 0	306,0 00,00 0
MEDP1294	L-Leucyl-L-glycine	189.1143956	C8H16N2O3	186,0 00	249,0 00	247,0 00	173,0 00	257,0 00	198,0 000	2,660 000	2,420 000	3,020 000	2,620 000	2,670 000	2,580 000	2,570 000	3,550 000	3,100 000	3,040 000	3,055 460	3,010 000	2,240 000	2,140 000	2,160 000
MEDP1295	Cytarabine	244.0826219	C9H13N3O5	8,990 000	10,00 0,000	10,30 0,000	7,330 000	7,870 000	9,510 000	4,250 000	5,110 000	3,680 000	3,520 000	4,310 000	4,650 000	5,060 000	5,660 000	4,850 000	4,430 000	4,942 500	4,720 000	5,280 000	5,330 000	5,300 000
MEDP1354	Mycosporine-serinol	262.1278734	C11H19NO6	9 0	9 0	9 0	9 0	9 0	9 0	56,40 0	56,90 0	75,30 0	45,60 0	49,70 0	54,70 0	82,30 0	85,10 0	72,30 0	66,70 0	77,26 9	79,90 0	53,90 0	63,50 0	55,90 0
MEDP1360	Mycosporine glycine	246.1	C10H15NO6	9 0	9 0	9 0	9 0	9 0	9 0	48,10 0	37,30 0	47,30 0	47,60 0	60,90 0	47,30 0	36,60 0	48,00 0	45,70 0	44,50 0	39,88 3	24,60 0	38,80 0	47,30 0	15,70 0
MEDP1467	5-Methyl-2'-deoxycytidine	242	C10H15N3O4	1,180 000	1,140 000	1,100 000	1,040 000	1,160 000	1,200 000	397,0 00	411,0 00	288,0 00	505,0 00	327,0 00	453,0 00	165,0 00	166,0 00	159,0 00	160,0 00	157,7 44	139,0 00	303,0 00	241,0 00	356,0 00
MEDP1468	D-panthenol	206	C9H19NO4	11,50 0	8,250 0	7,530 0	6,980 0	9,740 0	9 0	2,590 0	9 0	9 0	9 0	9 0	12,90 0	30,80 0	38,60 0	30,00 0	44,60 0	36,43 4	38,20 0	15,30 0	21,30 0	19,70 0
MEDP1480	Anserine	241	C10H16N4O3	68,80 0,000	61,00 0,000	59,60 0,000	59,80 0,000	64,90 0,000	65,00 0,000	26,70 0,000	22,00 0,000	28,80 0,000	30,50 0,000	25,40 0,000	26,80 0,000	15,30 0,000	13,50 0,000	13,70 0,000	13,60 0,000	14,03 9,200	14,20 0,000	20,10 0,000	21,00 0,000	21,20 0,000
MEDP1481	Menadiol Diacetate	259	C15H14O4	31,10 0	69,60 0	60,20 0	73,30 0	78,30 0	54,50 0	59,90 0	73,40 0	43,00 0	49,10 0	79,00 0	55,10 0	63,90 0	71,20 0	74,30 0	123,0 00	76,73 0	51,30 0	71,60 0	74,80 0	47,20 0
MEDP1488	SDMA	203	C8H18N4O2	1,910 000	2,150 000	2,070 000	2,170 000	2,070 000	2,090 000	2,570 000	2,580 000	2,890 000	2,410 000	2,410 000	2,550 000	1,450 000	1,630 000	1,600 000	1,480 000	1,526 160	1,480 000	1,960 000	1,720 000	1,670 000
MEDP1490	Cis-4-Hydroxy-D-Proline	132	C5H9NO3	3,450 000	3,550 000	3,460 000	3,390 000	3,450 000	3,260 000	718,0 00	942,0 00	599,0 00	589,0 00	654,0 00	807,0 00	570,0 00	493,0 00	439,0 00	529,0 00	502,9 74	484,0 00	1,340 000	962,0 00	918,0 00
MEDP1496	L-2-Aminobutyric acid	104	C4H9NO2	4,170 000	4,660 000	4,880 000	5,100 000	4,900 000	5,050 000	19,80 0,000	22,50 0,000	19,60 0,000	21,10 0,000	17,90 0,000	18,10 0,000	34,70 0,000	31,60 0,000	32,20 0,000	33,30 0,000	32,99 9,400	33,20 0,000	25,30 0,000	23,30 0,000	25,60 0,000

Protein	Peptide	MS/MS	Sequence	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
MEDP1498	8-Azaguanine	153	C4H4N6O	15,60 0,000	15,30 0,000	16,60 0,000	16,10 0,000	17,50 0,000	15,70 0,000	5,930 000	5,360 000	6,440 000	4,910 000	6,140 000	6,810 000	4,550 000	5,060 000	4,410 000	4,830 000	4,768 300	4,990 000	6,460 000	6,410 000	6,680 000	
MEDP1501	Isocytosine	112	C4H5N3O	2,220 000	2,060 000	2,630 000	1,540 000	1,840 000	2,530 000	920,0 00	836,0 00	999,0 00	897,0 00	921,0 00	946,0 00	1,400 000	1,400 000	1,110 000	1,160 000	1,266 880	1,280 000	1,320 000	1,160 000	1,250 000	
MEDP1506	Leu-Val	231	C11H22N2 O3	351,0 00	221,0 00	115,0 00	176,0 00	300,0 00	284,0 00	739,0 00	808,0 00	632,0 00	721,0 00	946,0 00	588,0 00	1,220 00	323,0 00	463,0 00	501,0 00	594,9 92	464,0 00	565,0 00	556,0 00	541,0 00	
MEDP1507	Phe-Asn	280	C13H17N3 O4	9	9	9	9	9	9	1,310 000	1,130 000	1,380 000	1,260 000	1,460 000	1,310 000	1,870 000	1,310 000	1,400 000	1,410 000	1,469 580	1,360 000	1,030 000	1,090 000	929,0 00	
MEDP1508	Phe-Met	297	C14H20N2 O3S	9	9	9	9	9	9	3,420 000	3,150 000	3,610 000	3,990 000	2,990 000	3,360 000	1,820 000	1,820 000	1,540 000	1,420 000	1,701 620	1,900 000	1,930 000	1,990 000	2,020 000	
MEDP1509	Glu-Met	279	C10H18N2 O5S	242,0 00	292,0 00	271,0 00	317,0 00	254,0 00	337,0 00	875,0 00	765,0 00	982,0 00	865,0 00	731,0 00	1,030 000	221,0 00	319,0 00	293,0 00	300,0 00	296,1 40	347,0 00	344,0 00	469,0 00	400,0 00	
MEDP1510	Asp-Phe	281	C13H16N2 O5	1,950 000	1,790 000	1,800 000	1,620 000	1,990 000	1,910 000	35,10 0,000	32,90 0,000	40,00 0,000	34,30 0,000	33,80 0,000	34,40 0,000	25,90 0,000	29,20 0,000	28,60 0,000	26,90 0,000	27,96 7,800	29,20 0,000	22,10 0,000	23,60 0,000	23,20 0,000	
MEDP1511	Met-Glu	279	C10H18N2 O5S	87,70 0	83,40 0	80,00 0	84,80 0	78,40 0	87,10 0	252,0 00	220,0 00	305,0 00	252,0 00	173,0 00	307,0 00	73,00 0	77,50 0	114,0 00	66,90 0	85,16 0	94,10 0	133,0 00	130,0 00	116,0 00	
MEDP1512	Phe-Val	265	C14H20N2 O3	177,0 00	169,0 00	186,0 00	261,0 00	184,0 00	190,0 00	6,140 000	6,580 000	5,710 000	6,060 000	5,970 000	6,380 000	7,730 000	4,530 000	5,580 000	5,240 000	5,609 500	4,970 000	4,680 000	4,670 000	4,640 000	