Supporting Information: Acyl-CoA identification in mouse liver samples using the in-silico CoA-Blast tandem mass spectral library

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Table S1: **The 14 authentic Acyl-CoA standards analyzed in the study for MS2 validation and retention time prediction model generation.**

Name	logD	RT short	RT long	Monoisotopic mass	k' short
malonyl-CoA	-14.4	0.6	-	853.1149	0.3
glutaryl-CoA	-13.63	1.9	-	881.1462	3.2
Free CoA	-11.44	0.66	-	767.1146	0.5
acetyl-CoA	-11.49	2	-	809.1251	3.4
propionyl-CoA	-10.79	3.28	0.49	823.1407	6.3
butyryl-CoA	-10.35	3.73	0.54	837.1564	7.3
isovaleryl-CoA	-10.06	3.9	0.54	851.172	7.7
hexanoyl-CoA	-9.46	4.7	0.57	865.1877	9.4
octanoyl-CoA	-8.57	6.1	1.65	893.219	12.6
Decanoyl-CoA	-7.68	7.01	3.06	921.2503	14.6
myristoyl-CoA	-5.9	8.25	3.58	977.3129	17.3
Arachidonoyl-CoA	-4.79	8.55	3.7	1053.344	18.0
heptadeca-CoA	-4.57	9.03	3.92	1019.36	19.1
stearoyl-CoA	-4.12	9.28	3.97	1041.325	19.6

Table S2: All hits returned from the CoA-Blast library for each annotated peak.

The ChemSpider result from elemental formula search is given for each hit, together with the number of different data sources found on ChemSpider for each annotation. These numbers were used to determine the most biologically relevant library hit for annotation.

#	# in Library	Name in Library	logD[pH=6.8]	theoretical precursor M/Z	smiles from Library	Chemspider result	# of data sources	# of references	# of PubMed	# of RSC	comments
1	21	PubChem CID: 20758225; (Acyl-CoA); [M+H]+;	-11.72	768.1225	CC(C)(CC(O)C(=O)NCCC(=O)NCCS)OP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	-					Not a CoA
	22	Reduced CoA; (Acyl-CoA); [M+H]+;	-11.44	768.1225	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCS	Coenzyme A	42	656	13328	943	
	20	CID447831; (Acyl-CoA); [M+H]+;	-12.16	768.1320	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)[C@@H](O)C(=O)NCCC(=O)NCCP	-					Not a CoA (has no S atom)
2	52	acetyl-CoA; (Acyl-CoA); [M+H]+;	-11.60	810.1331	CC(=O)SCCNC(=O)CCNC(=O)[C@@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Acetyl-CoA	42	291	8216	779	
3	65	SOP; (Acyl-CoA); [M+H]+;	-11.46	824.1487	C\C(O)=C/SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Not an acyl CoA					
	66	PubChem CID: 24762924; (Acyl-CoA); [M+H]+;	-11.56	824.1487	CC(=O)CSCCNC(=O)CCNC(=O)[C@@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	S-Acetonyl coa	6	8	0	0	
	67	CID10581308; (Acyl-CoA); [M+H]+;	-10.94	824.1487	CSC(=O)CCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	-					Not a CoA
	68	propanoyl-CoA; (Acyl-CoA); [M+H]+;	-10.90	824.1487	CCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Propionyl CoA	20	46	0	0	
	69	S-Acetonyl CoA;	-11.56	824.1487	CC(=O)CSCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	S-Acetonyl CoA	6	8	0	0	

		(Acyl-CoA); [M+H]+;									
	70	propionyl-coenzyme A; (Acyl-CoA); [M+H]+;	-10.90	824.1487	CCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Propionyl CoA	20	46	0	0	
4	86	isobutyryl-CoA; (Acyl-CoA); [M+H]+;	-10.36	838.1643	CC(C)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Isobutyryl CoA	19	31	97	44	
	87	S-(3-Oxobutyl) CoA; (Acyl-CoA); [M+H]+;	-11.12	838.1643	CC(=O)CCSCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Not an acyl CoA	4	4	0	0	
	88	butyryl-CoA; (Acyl-CoA); [M+H]+;	-10.46	838.1643	CCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	butyryl-CoA	15	21	312	49	
5	118	Pivalyl-CoA; (Acyl-CoA); [M+H]+;	-9.80	852.1800	CC(C)(C)C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Pivalyl-CoA	7	7	0	0	
	119	isovaleryl-CoA; (Acyl-CoA); [M+H]+;	-10.17	852.1800	CC(C)CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	isovaleryl-CoA	15	22	169	19	
	120	2-methylbutyryl-CoA; (Acyl-CoA); [M+H]+;	-9.91	852.1800	CCC(C)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	2-methylbutyryl-CoA	7	9	3	3	
	121	Pentanoyl-CoA; (Acyl-CoA); [M+H]+;	-10.01	852.1800	CCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Pentanoyl-CoA	6	6	0	0	
	122	Valeryl-CoA; (Acyl-CoA); [M+H]+;	-10.17	852.1800	CC(C)CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	-					Also isovaleryl-CoA, synonym is wrong in Pubchem

6	128	3-Hydroxyisobutyryl-CoA; (Acyl-CoA); [M+H]+;	-11.64	854.1592	CC(CO)C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	3-hydroxybutyryl-CoA	5	5	0	0	
	129	2-hydroxy-3-methylacyl-CoA; (Acyl-CoA); [M+H]+;	-11.33	854.1592	CCC(O)C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	2-Hydroxybutanoyl-CoA	2	2	0	0	2-Hydroxybutanoyl-CoA - wrong name in library
	130	4-Hydroxybutyryl-CoA; (Acyl-CoA); [M+H]+;	-11.89	854.1592	CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCSC(=O)CCCO	4-Hydroxybutyryl-CoA	6	7	0	0	
	131	CID4469810; (Acyl-CoA); [M+H]+;	-13.60	854.1592	CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCSCCCC(O)=O	-	2	2	0	0	3-Carboxypropyl-coenzyme A with different stereochemistry
	132	3-CARBOXYPROPYL-COENZYME A; (Acyl-CoA); [M+H]+;	-13.60	854.1592	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)[C@@H](O)C(=O)NCCC(=O)NCCSCCCC(O)=O	3-Carboxypropyl-CoA	2	2	0	0	
	133	CID4453337; (Acyl-CoA); [M+H]+;	-13.32	854.1592	C[C@H](CSCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)=O	2-Carboxypropyl-CoA	4	4	0	0	
	134	3-Hydroxybutyryl-coenzyme A; (Acyl-CoA); [M+H]+;	-11.77	854.1592	C[C@@H](O)CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	3-Hydroxybutanoyl-CoA	13	13	0	0	
	135	2-carboxypropyl-coenzyme a; (Acyl-CoA); [M+H]+;	-13.32	854.1592	CC(CSCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)=O	2-carboxypropyl-CoA	4	5	0	0	

7	160	PubChem CID: 25245510; (Acyl-CoA); [M+H]+;	-9.47	866.1956	CCCC(C)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	2-Methylvaleryl-CoA	3	3	0	0	
	161	MRR; (Acyl-CoA); [M+H]+;	-9.47	866.1956	CCC[C@@H](C)C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	-	3	3	0	0	2-Methylvaleryl-CoA (stereochemistry different
	162	CID5326463; (Acyl-CoA); [M+H]+;	-11.44	866.1956	CCC\C=C\C=O.CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)[C@@H](O)C(=O)NCCC(=O)NCCS	-					Structure includes salt
	163	hexanoyl-coenzyme a; (Acyl-CoA); [M+H]+;	-9.57	866.1956	CCCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	hexanoyl-CoA	14	28	5	1	
	1687	4-Methyl Valeric Acid-CoA; (Acyl-CoA); [M+H]+;	-9.73	866.1956	[#6]C([#6])CCC(=O)SCCNC(=O)CCNC(=O)C(O)C([#6])([#6])COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)N1C=NC2=C1N=CN=C2[#7]	4-Methylpentanoyl-CoA	2	2	0	0	
8	164	SCA; (Acyl-CoA); [M+H]+;	-14.37	868.1385	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)[C@@H](O)C(=O)NCCC(=O)NCCSC(O)\C=C\C(O)=O	4-hydroxy-2-butenoic acid CoA	1	1	0	0	
	165	CID10748187; (Acyl-CoA); [M+H]+;	-14.70	868.1385	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)[C@@H](O)C(=O)NCCC(=O)NCCCC(=O)SCC(O)=O	-					Not a CoA
	166	succinyl-CoA; (Acyl-CoA); [M+H]+;	-14.58	868.1385	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)[C@@H](O)C(=O)NCCC(=O)NCCSC(=O)CCC(O)=O	Succinyl-CoA	18	26	747	98	
	167	Methylmalonyl CoA; (Acyl-CoA); [M+H]+;	-14.01	868.1385	CC(C(O)=O)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	Methylmalonyl-CoA	18	32	749	171	
9	224	2-Methylhexanoyl-CoA; (Acyl-CoA); [M+H]+;	-9.03	880.2113	CCCCC(C)C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	2-Methylhexanoyl-CoA	5	5	0	0	

	1887	C7:0-CoA; (Acyl-CoA); [M+H]+;	-9.12	880.2113	CCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	heptanoyl-CoA	5	5	0	0	
10	229	2,4,4-Trimethylpentanoyl-CoA; (Acyl-CoA); [M+H]+;	-8.88	894.2269	CC(CC(C)(C)C)C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	2,4,4-Trimethylpentanoyl-CoA	1	1	0	0	
	230	Valproyl-CoA; (Acyl-CoA); [M+H]+;	-8.58	894.2269	CCCC(CCC)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Valproyl-CoA	8	11	0	0	
	231	octanoyl-CoA; (Acyl-CoA); [M+H]+;	-8.68	894.2269	CCCCCCCC(=O)SCCNC(=O)CCNC(=O)[C@@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H](C(O)[C@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Octanoyl-CoA	26	45	16	1	
11	310	PubChem CID: 25202290; (Acyl-CoA); [M+H]+;	-9.32	900.1800	CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCSC(=O)CCc1ccccc1	3-phenylpropanoyl-CoA	6	6	0	0	
	311	4-Tolylacetyl-CoA; (Acyl-CoA); [M+H]+;	-9.25	900.1800	Cc1ccc(CC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]2O[C@H]([C@H](O)[C@@H]2OP(O)(O)=O)n2cnc3c(N)ncnc23)cc1	4-Tolylacetyl-CoA	4	4	0	0	
	312	3-Tolylacetyl-CoA; (Acyl-CoA); [M+H]+;	-9.25	900.1800	Cc1cccc(CC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]2O[C@H]([C@H](O)[C@@H]2OP(O)(O)=O)n2cnc3c(N)ncnc23)c1	3-Tolylacetyl-CoA	4	4	0	0	
	313	Phenylpropionyl-CoA; (Acyl-CoA); [M+H]+;	-9.32	900.1800	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)[C@@H](O)C(=O)NCCC(=O)NCCSC(=O)CCc1ccccc1	3-phenylpropanoyl-CoA	6	6	0	0	
	314	2-Tolylacetyl-CoA; (Acyl-CoA); [M+H]+;	-9.25	900.1800	Cc1ccccc1CC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	2-Tolylacetyl-CoA	4	4	0	0	
	307	CID4961354; (Acyl-	-13.72	900.1647	CC(C(O)C(O)=O)C(=O)SCCNC(O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	2-hydroxy-3-methyl-4-	2	2	0	0	

		CoA); [M+H]+;				oxobutanoic acid-CoA					
12	376	Perillyl-CoA; (Acyl-CoA); [M+H]+;	-8.73	916.2113	CC(=C)C1CCC(=CC1)C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Perillyl-CoA	6	6	0	0	
	377	Perillyl-CoA; (Acyl-CoA); [M+H]+;	-8.73	916.2113	CC(=C)C1CCC(=CC1)C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	-	6	6	0	0	Also Perillyl-CoA no stereochemistry
13	562	trans-tetradec-2-enoyl-coenzyme A; (Acyl-CoA); [M+H]+;	-5.78	976.3052	CCCCCCCCCCC\C=C\C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	(2E)-Tetradecenoyl-CoA	8	10	0	0	
	563	3-Tetradecenoyl-S-coenzyme A; (Acyl-CoA); [M+H]+;	-6.37	976.3052	CCCCCCCCCC\C=C\CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	3-Tetradecenoyl-S-CoA	3	3	0	0	
	564	3-Tetradecenoyl-S-coenzyme A; (Acyl-CoA); [M+H]+;	-6.37	976.3052	CCCCCCCCCC\C=C\CC(=O)SCCNC(=O)CCNC(=O)[C@@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	3-Tetradecenoyl-S-CoA	3	3	0	0	
	565	(11Z)-Tetradecenoyl-CoA; (Acyl-CoA); [M+H]+;	-6.37	976.3052	CC\C=C/CCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	cis-tetradec-11-enoyl-CoA	5	5	0	0	
	566	(2E)-Tetradecenoyl-CoA; (Acyl-CoA); [M+H]+;	-5.78	976.3052	CCCCCCCCCCC\C=C\C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	(2E)-Tetradecenoyl-CoA	8	10	0	0	Duplicate
	567	Tetradecenoyl-CoA; (Acyl-CoA); [M+H]+;	-5.78	976.3052	CCCCCCCCCCCC=CC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	Tetradecenoyl-CoA					No stereochemistry
	568	CID494378; (Acyl-CoA);	-6.37	976.3052	CCCCCCCCCCC=CCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	3-Tetradecenoyl-S-CoA	3	3	0	0	Duplicate

		[M+H]+;									
	569	CID358835; (Acyl-CoA); [M+H]+;	-6.37	976.3052	CCCCCCCCCCC=CCC(=O)SCCNC(=O)CCNC(=O)[C@@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	3-Tetradecenoyl-S-CoA	3	3	0	0	Duplicate
14	572	Tetradecanoyl-CoA (myristoyl); (Acyl-CoA); [M+H]+;	-6.01	978.3209	CCCCCCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H](C(O)[C@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Myristoyl-CoA	14	61	213	5	
	573	CID446292; (Acyl-CoA); [M+H]+;	-6.41	978.3209	CCCCCCCCCCCCC(=O)CSCCNC(=O)CCNC(=O)[C@@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	-	2	2	0	0	Not an acyl CoA
15	633	cis-9-Hexadecenoyl Coenzyme-?A; (Acyl-CoA); [M+H]+;	-5.48	1004.3360	CCCCCC\C=C/CCCCCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	palmitoleoyl-CoA	6	7	0	0	
	634	(2E)-Hexadecenoyl-CoA; (Acyl-CoA); [M+H]+;	-4.89	1004.3360	CCCCCCCCCCCCC\C=C\C(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H](C(O)[C@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	hexadec-2-enoyl-CoA	4	5	0	0	
16	580	palmitoyl	-5.12	1006.3526	CCCCCCCCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Palmitoyl-CoA	124	1572	19		
	581	4,8,12 trimethyldecanoyl	-5.60	1006.3526	CC(C)CCCC(C)CCCC(C)CCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	4,8,12 trimethyldecanoyl-CoA	5	5	0	0	
17	1782	11-TRANS-13-TRANS-15-CIS-OCTADECATRIENOIC ACID-CoA; (Acyl-CoA); [M+H]+;	-5.32	1028.3360	[#6]C\C=C/C=C/C=C/CCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C([#6])([#6])COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)N1C=NC2=C1N=CN=C2[#7]	-					not in Chemspider
	617	alpha-Linolenoyl-CoA; (Acyl-CoA); [M+H]+;	-5.32	1028.3370	CC\C=C/C\C=C/C\C=C/CCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	alpha-Linolenoyl-CoA	5	5	0	0	
	618	CHEBI:15508; (Acyl-CoA);	-5.32	1028.3370	CCCCC\C=C/C\C=C/C\C=C/CCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	gamma-Linolenoyl-CoA	10	13	0	0	

		[M+H]+;									
	619	PubChem CID: 5388873; (Acyl-CoA); [M+H]+;	-5.32	1028.3370	CCCCC\C=C\C\C=C\C\C=C\CCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	(6E,9E,12E)-octadecatrienoic acid-CoA	3	3	0	0	
	620	gamma-Linolenoyl-CoA; (Acyl-CoA); [M+H]+;	-5.32	1028.3370	CCCCC\C=C/C\C=C/C\C=C/CCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	gamma-Linolenoyl-CoA	10	13	0	0	Different stereochemistry
	621	CID656469; (Acyl-CoA); [M+H]+;	-5.32	1028.3370	CCCCCC=CCC=CCC=CCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	gamma-Linolenoyl-CoA	10	13	0	0	Different stereochemistry
18	682	CHEBI:53151; (Acyl-CoA); [M+H]+;	-4.65	1030.3520	CCCCCCCCC#CCCCCCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	9-Octadecynoyl-CoA	2	2	0	0	
	683	(6Z,9Z)-Octadecadienoyl-CoA; (Acyl-CoA); [M+H]+;	-4.96	1030.3520	CCCCCCCC\C=C/C\C=C/CCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H](C(O)[C@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	(6Z,9Z)-Octadecadienoyl-CoA	2	2	0	0	
	684	Linoleyl-CoA; (Acyl-CoA); [M+H]+;	-4.96	1030.3520	CCCCC\C=C/C\C=C/CCCCCCCC(=O)SCCNC(=O)CCNC(=O)[C@@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Linoleyl-CoA	11	12	0	0	
	1846	(10E,12Z)-octadeca-10,12-dienoic acid-CoA; (Acyl-CoA); [M+H]+;	-4.96	1030.3520	[#6]CCCC\C=C/C=C/CCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C([#6])([#6])COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)N1C=NC2=C1N=CN=C2[#7]	(10E,12Z)-octadeca-10,12-dienoyl-CoA					Not in chemspider
19	687	(2E)-Octadecenoyl-CoA; (Acyl-CoA); [M+H]+;	-4.00	1032.3680	CCCCCCCCCCCCCCC\C=C\C(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	trans-2-octadecenoyl-CoA	6	7	0	0	
	688	Vaccenoyl-CoA; (Acyl-CoA); [M+H]+;	-4.60	1032.3680	CCCCCC\C=C\CCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	trans-vaccenoyl-CoA	2	2	0	0	

	689	Oleoyl-coenzyme A; (Acyl-CoA); [M+H]+;	-4.60	1032.3680	CCCCCCCCC=CCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	Oleoyl-CoA	24	26	0	0	
20	734	(8Z,11Z,14Z,17Z)-Icosatetraenoyl-CoA; (Acyl-CoA); [M+H]+;	-4.79	1054.3520	CC\C=C/C\C=C/C\C=C/C\C=C/CCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	(8Z,11Z,14Z,17Z)-eicosatetraenoyl-CoA	3	3	0	0	
	735	Arachidonyl-CoA; (Acyl-CoA); [M+H]+;	-4.79	1054.3520	CCCCC\C=C/C\C=C/C\C=C/C\C=C/CCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H](C(O)[C@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Arachidonyl-CoA	9	9	0	0	
21	736	(11Z,14Z,17Z)-Icosatrienoyl-CoA; (Acyl-CoA); [M+H]+;	-4.43	1056.3680	CC\C=C/C\C=C/C\C=C/CCCCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	(11Z,14Z,17Z)-eicosatrienoyl-CoA	3	3	0	0	
	737	8,11,14-Eicosatrienoyl-CoA; (Acyl-CoA); [M+H]+;	-4.43	1056.3680	CCCCC\C=C/C\C=C/C\C=C/CCCCCCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	(8Z,11Z,14Z)-Icosatrienoyl-CoA	7	9	0	0	
	738	8,11,14-Eicosatrienoyl-CoA; (Acyl-CoA); [M+H]+;	-4.43	1056.3680	CCCCC\C=C/C\C=C/C\C=C/CCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	(8Z,11Z,14Z)-Icosatrienoyl-CoA	7	9	0	0	Different stereochemistry on the CoA
	739	8,11,14-Eicosatrienoyl-CoA; (Acyl-CoA); [M+H]+;	-4.43	1056.3680	CCCCCC=CCC=CCC=CCCCCCCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)n1cnc2c(N)ncnc12	(8Z,11Z,14Z)-Icosatrienoyl-CoA	7	9	0	0	Different stereochemistry on the CoA
22	757	CoA-glutathione; (Acyl-CoA); [M+H]+;	-19.58	1073.1910	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]1OC([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(O)C(=O)NCCC(=O)NCCSSCC(NC(=O)CCC(N)C(O)=O)C(=O)NCC(O)=O	Glutathione-CoA	3	3	0	0	
	758	Coassg; (Acyl-CoA); [M+H]+;	-19.12	1073.1910	CC(C)(CO)C(OP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12)C(=O)NCCC(=O)NCCSSC[C@H](N)C(=O)N(CC(O)=O)C(=O)CC[C@H](N)C(O)=O	-	2	2	0	0	Not a CoA

23	761	nchembio.365-comp4c; (Acyl-CoA); [M+H]+;	-8.54	1078.3480	CCCCCCCCCCCC(=O)N[C@@H](C)C(=O)NCC(=O)SCCNC(=O)CCNC(=O)[C@H](O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	N-Lauroyl-L-Ala-Gly-S-CoA	1	1	0	0	rt and logd don't match
	762	C16169; (Acyl-CoA); [M+H]+;	-4.63	1078.3520	CC\C=C/C\C=C/C\C=C/C\C=C/C\C=C/C\C=C/CCC(=O)SCCNC(=O)CCNC(=O)C(O)C(C)(C)COP(O)(=O)OP(O)(=O)OC[C@H]1O[C@H]([C@H](O)[C@@H]1OP(O)(O)=O)n1cnc2c(N)ncnc12	Cervonyl-CoA (4Z,7Z,10Z,13Z,16Z,19Z)-docosahexaenoyl-CoA	3	3	0	0	C22:6

Table S3: The original spectra from which the rules were formulated for CoA-Blast library generation

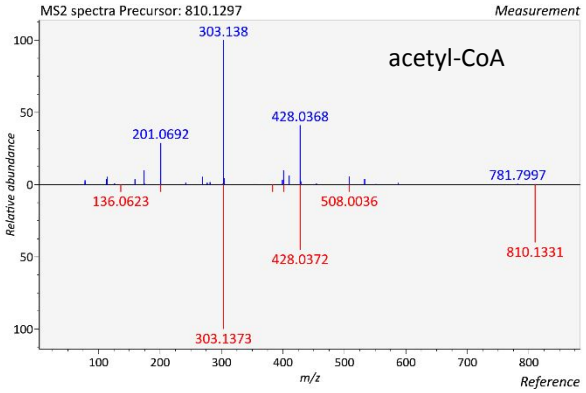
Name	InChiKey	Ion mode	Precursor m/z	Exact mass	Instrument	Analyzer type	Collision energy [V]	Number of peaks	Source DOI or URL
3-methylcrotonyl-CoA	BXIPALATIYNHJN-TVCSPYKZSA-N	[M+H]+	850.7	849.1571	Agilent MSD Ion trap mass spectrometer SL, ESI	Ion Trap	1.00	4	http://dx.doi.org/10.1016/j.jchromb.2008.12.053
acetyl-CoA	ZSLZBFCDCINBPY-ZSJPKINUSA-N	[M-H]-	807.97	809.1258	ABI 4800 TOF/TOF, MALDI	Q-TOF	7.00	20	DOI: 10.1021/ac070843+
Acetyl-CoA	ZSLZBFCDCINBPY-ZSJPKINUSA-N	[M+H]+	810.7	809.1258	Agilent MSD Ion trap mass spectrometer SL, ESI	Ion Trap	1.00	4	http://dx.doi.org/10.1016/j.jchromb.2008.12.053
acetyl-CoA	ZSLZBFCDCINBPY-ZSJPKINUSA-N	[M+H]+	810.3	809.1258	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	3	DOI: 10.1002/jms.1240
acetyl-CoA	ZSLZBFCDCINBPY-ZSJPKINUSA-N	[M+H]+	810.1	809.1258	ABI API 3000 triple quadrupole MS, ESI	Triple Quad	52.00	6	http://dx.doi.org/10.1016/j.jchromb.2007.03.029
acetyl-CoA	ZSLZBFCDCINBPY-ZSJPKINUSA-N	[M+H]+	810.13	809.1258	LTQ Orbitrap XL, ESI	Orbitrap	35.00	37	http://www.massbank.jp/RecordDisplay?id=KNA00606
C20:4-CoA (arachidonyl)	JDEPVTUUCBFJIW-NKOIHYFNSA-N	[M+H]-	1052	1053.3449	Thermo Finnigan TSQ 70, FAB	Triple Quad	30.00	11	http://dx.doi.org/10.1016/1044-0305(94)85057-7
beta-Hydroxybutyryl-CoA	QHHKKMYHDBRONY-RMNRSTNRSA-N	[M+H]+	854.1	853.1520	ABI API 3000 triple quadrupole MS, ESI	Triple Quad	52.00	7	http://dx.doi.org/10.1016/j.jchromb.2007.03.029
butyryl-CoA	CRFNGMNYKDXRTN-CITAKDKDSA-N	[M+H]+	838.4	837.1571	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	3	DOI: 10.1002/jms.1241
C15:0-CoA	VLBCUOVMSMAIJC-UHFFFAOYSA-N	[M+H]+	992.4	991.3292	ABI 4000 QTRAP, ESI	Ion Trap	50.00	6	http://www.jlr.org/cgi/content/abstract/D800001-JLR200v1
C16:0-CoA	MNBKLUUYKPBKDU-BBECNAHFSA-N	[M+H]+	1004.4	1005.3449	ABI 4000 QTRAP, ESI	Ion Trap	60.00	9	http://www.jlr.org/cgi/content/abstract/D800001-JLR200v1
C16:0-CoA	MNBKLUUYKPBKDU-BBECNAHFSA-N	[M+H]+	1006.4	1005.3449	ABI 4000 QTRAP, ESI	Ion Trap	50.00	7	http://www.jlr.org/cgi/content/abstract/D800001-JLR200v1
C17:0-CoA (heptadecyl)	DRABUZIHHACUPI-DUPKZGIXSA-N	[M+H]+	1020	1019.3605	Thermo LCQ ion trap, ESI	Ion Trap	24.00	4	http://onlinelibrary.wiley.com/doi/10.1111/j.1365-313X.2001.00929.x/abstract
C25:0-CoA	YJOJYMDYLIGHLQ-ADKOIVETNA-N	[M-H]-	1130.6	1131.4857	ABI 4000 QTRAP, ESI	Ion Trap	59.00	10	http://www.jlr.org/cgi/content/abstract/D800001-JLR200v1
C25:0-CoA	YJOJYMDYLIGHLQ-ADKOIVETNA-N	[M+H]+	1132.6	1131.4857	ABI 4000 QTRAP, ESI	Ion Trap	59.00	6	http://www.jlr.org/cgi/content/abstract/D800001-JLR200v1
Cholyl-CoA	ZKWNOTQHFKYUNU-JGCIYWTLSA-N	[M+H]+	1158.4	1157.3922	Thermo LTQ Orbitrap, ESI	Orbitrap	30.00	4	http://jb.asm.org/cgi/reprint/JB.00665-07v1
cis-4-Decenoyl-CoA	QTOYQSMKQWCWOX-SGUJYKCESA-N	[M-H]-	918.5	919.2353	ABI 3200 Q TRAP, ESI	Ion Trap	25.00	6	http://dx.doi.org/10.1016/j.ab.2010.02.026
DHOPDC-CoA	KORUWOSZRLRGCN-UHFFFAOYSA-N	[M+H]+	1124.3	1123.3140	Thermo LTQ Orbitrap, ESI	Orbitrap	30.00	4	http://jb.asm.org/cgi/reprint/JB.00665-07v1
2,6-dimethylheptanoyl-CoA	GPXWBKWDXPBLKS-LNSOOWQSSA-N	[M-H]-	906.5	907.2353	ABI 3200 Q TRAP, ESI	Ion Trap	25.00	6	http://dx.doi.org/10.1016/j.ab.2010.02.026
ethylmalonyl-CoA	VUGZQVCBBBEZQE-VRQRJWBYSA-N	[M+H]+	882.3	881.1469	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	3	DOI: 10.1002/jms.1242
Flunoxaprofen-CoA	DFNKNUXNTARLIX-FWYROGSTSA-	[M+H]+	1035	1034.1848	Thermo TSQ Quantum Max triple	Triple Quad	25.00	8	DOI:10.1124/dmd.109.029371

					quadrupole, ESI				
Ibuprofen-CoA	ZWOQHSZKILPKKA-TWLYMIRPSA-J	[M+H]+	956	1034.1848	Thermo TSQ triple quadrupole, ESI	Triple Quad	25.00	7	http://pubs.acs.org/doi/abs/10.1021/tx800098h
isobutyryl-CoA	AEWHYWSPVRZHCT-NDZSKPAWSA-N	[M-H]-	836.1493	837.1571	Waters Q-Tof Premier, ESI	Q-TOF	30.00	29	http://www.massbank.jp/RecordDisplay?id=PR100154
isobutyryl-CoA	AEWHYWSPVRZHCT-NDZSKPAWSA-N	[M+H]+	838.1649	837.1571	Waters Q-Tof Premier, ESI	Q-TOF	30.00	14	http://www.massbank.jp/RecordDisplay?id=PR100154
malonyl-CoA	LTYOQGRJFJAKNA-DVVLENMVSA-N	[M+H]+	854.3	853.1156	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	3	DOI: 10.1002/jms.1243
malonyl-CoA	LTYOQGRJFJAKNA-DVVLENMVSA-N	[M+H]+	854.1	853.1156	ABI API 3000 triple quadrupole MS, ESI	Triple Quad	52.00	8	http://dx.doi.org/10.1016/j.jchromb.2007.03.029
methylmalonyl-CoA	MZFOKIKEPGUZEN-FBMOWMAESA-N	[M+H]+	868.3	867.1313	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	4	DOI: 10.1002/jms.1244
oleoyl-CoA	XDUHQPOXLUAVEE-BPMMELMSSA-N	[M+H]+	1032	1031.3605	Thermo Quantum TSQ Ultra AM, ESI	Triple Quad	30.00	7	http://pubs.acs.org/doi/abs/10.1021/ac800031u
12-OPDA-CoA (12-oxo-phytodienoic acid)	XQXACJRPGQOJGP-LLHOYASASA-N	[M-H]-	1040.48	1041.3085	Waters Micromass Q-Tof 2, ESI	Q-TOF	30.00	11	http://www.jbc.org/content/280/14/13962.full.pdf+html
C16:0-CoA (pamitoyl)	MNBKLUUYKPBKDU-BBECNAHFSA-N	[M-H]-	1004	1005.3449	Thermo Finnigan TSQ 70, FAB	Triple Quad	30.00	9	http://dx.doi.org/10.1016/1044-0305(94)85057-7
Phenylacetyl-CoA (ZIGIFDRJFZYEEQ)	ZIGIFDRJFZYEEQ-CECATXLMSA-N	[M+H]+	886	885.1571	Thermo TSQ Quantum Max triple quadrupole, ESI	Triple Quad	25.00	10	10.1124/dmd.108.026153
3-phenylpropionyl-CoA	HYSDRCZPYSOWME-FUEUKBNZSA-J	[M-H]-	898.5	899.1727	ABI 3200 Q TRAP, ESI	Ion Trap	25.00	6	http://dx.doi.org/10.1016/j.ab.2010.02.026
propionyl-CoA	QAQREVBBADEHPA-IEXPHMLFSA-N	[M+H]+	824.7	823.1414	Agilent MSD Ion trap mass spectrometer SL, 0.75V ESI	Ion Trap	0.75	5	http://dx.doi.org/10.1016/j.jchromb.2008.12.053
propionyl-CoA	QAQREVBBADEHPA-IEXPHMLFSA-N	[M+H]+	824.7	823.1414	Agilent MSD Ion trap mass spectrometer SL, 2.0V ESI	Ion Trap	2.00	5	http://dx.doi.org/10.1016/j.jchromb.2008.12.053
propionyl-CoA	QAQREVBBADEHPA-IEXPHMLFSA-N	[M+H]+	824.4	823.1414	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	3	DOI: 10.1002/jms.1245
CoA	RGJOEKWQDUBAIZ-IBOSZNHHSA-N	[M+H]+	768.3	767.1152	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	4	DOI: 10.1002/jms.1246
Simvastatin-CoA	GSLHKCYQBSJBRU-YUZZLLNMSA-N	[M-H]-	1184.4	1185.3871	Thermo LCQ ion trap, ESI	Ion Trap	15.00	8	10.1124/dmd.105.006650
Dehydro-Simvastatin-CoA	ACRWQXYKGQGECO-JZWXTILOSA-N	[M-H]-	1166.4	1167.3766	Thermo LCQ ion trap, ESI	Ion Trap	15.00	8	10.1124/dmd.105.006650
succinyl-CoA	VNOYUJKHFWYWIR-ITIYDSSPSA-N	[M+H]+	868.6	867.1313	Agilent MSD Ion trap mass spectrometer SL, ESI	Ion Trap	1.00	4	http://dx.doi.org/10.1016/j.jchromb.2008.12.053
succinyl-CoA	VNOYUJKHFWYWIR-ITIYDSSPSA-N	[M+H]+	868.3	867.1313	Waters Micromass Quattro micro MS, ESI	Triple Quad	30.00	3	DOI: 10.1002/jms.1247
succinyl-CoA	VNOYUJKHFWYWIR-ITIYDSSPSA-N	[M+H]+	868.1	867.1313	ABI API 3000 triple quadrupole MS, ESI	Triple Quad	52.00	6	http://dx.doi.org/10.1016/j.jchromb.2007.03.029

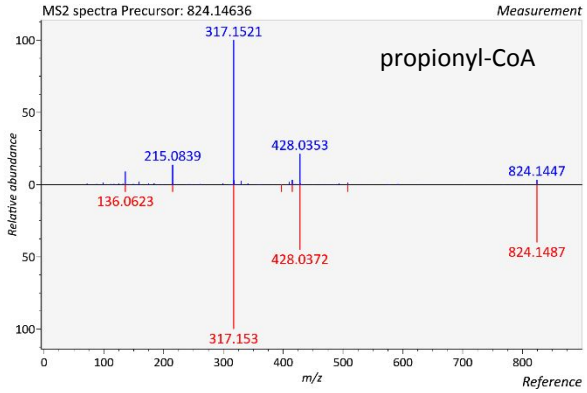
Tolmetin-CoA	YININOOYERTLNN-UHFFFAOYSA-N	[M+H]+	1007.2	1006.2098	Agilent MSD ion trap, ESI	Ion Trap	Not Reported	6	http://dmd.aspetjournals.org/content/35/5/758.full.pdf
Valproyl-CoA	UCIOSJWVYJWBEO-XJJJFWNASA-N	[M+H]+	894	893.2197	Thermo TSQ Quantum ultra, ESI	Triple Quad	Not Reported	7	http://pubs.acs.org/doi/pdfplus/10.1021/tx0501785
Zomepirac-CoA (5-(chlorobenzoyl)-1,4-dimethylpyrrole-2-acetic acid])	AMRKGEFTWMVRAR-UHFFFAOYSA-N	[M+H]+	1041	1040.1709	Thermo TSQ Quantum ultra, ESI	Triple Quad	Not Reported	6	http://pubs.acs.org/doi/pdfplus/10.1021/tx0501785

Figure S1: Head to tail MS2 matching results from MS DIAL for the 13 identified acyl-CoAs standards in positive ESI mode (a-m).

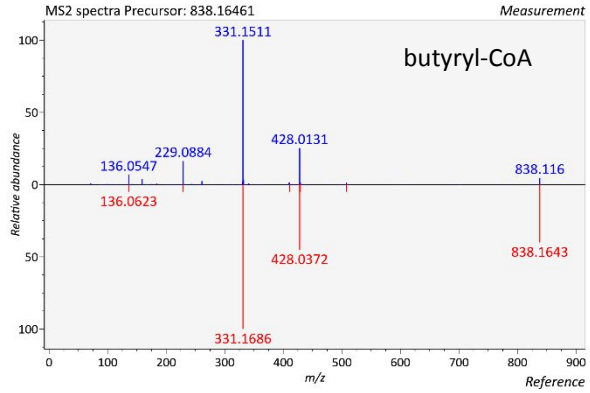
a)



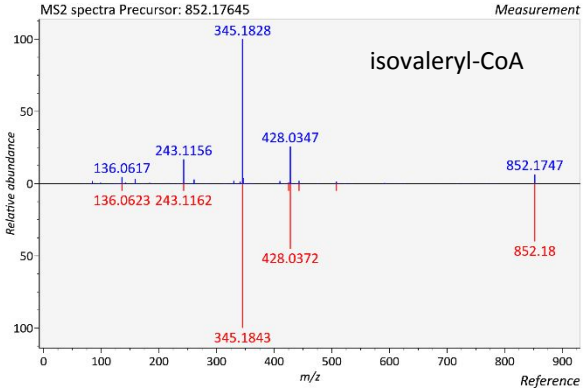
b)



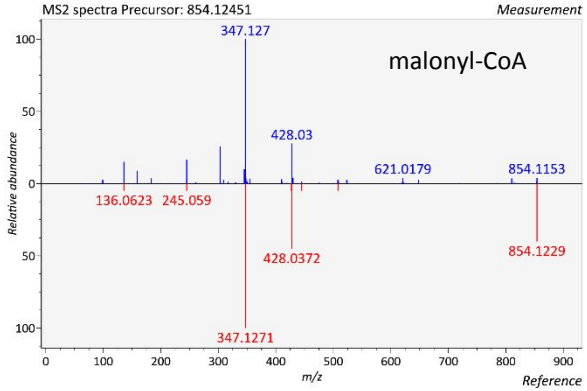
c)



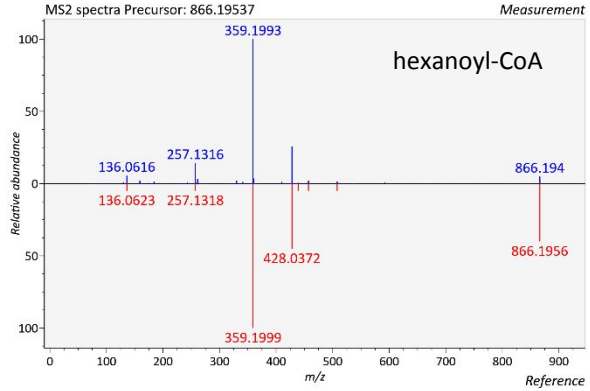
d)



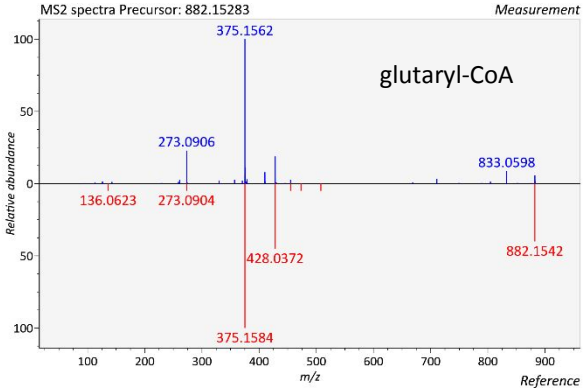
e)



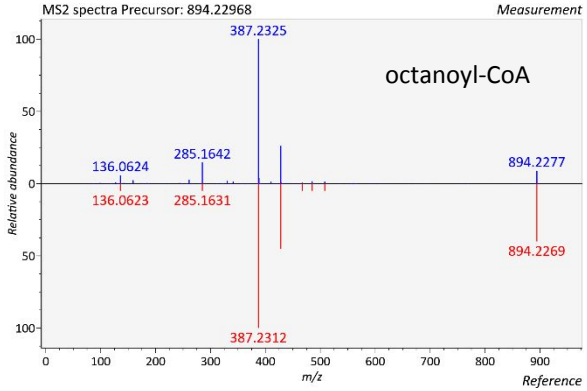
f)



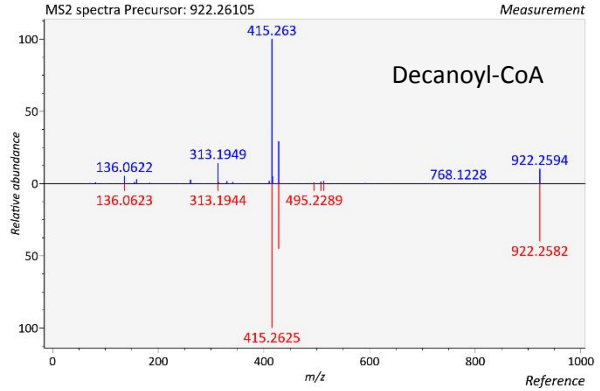
g)



h)



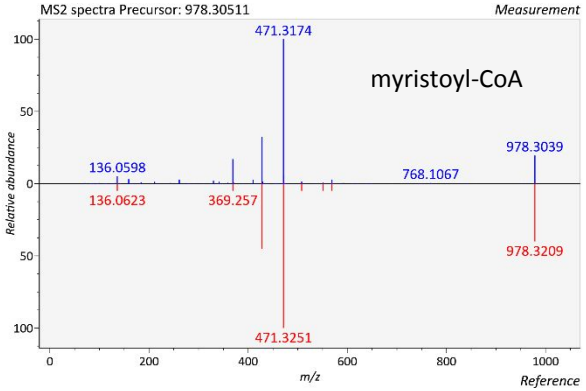
i)

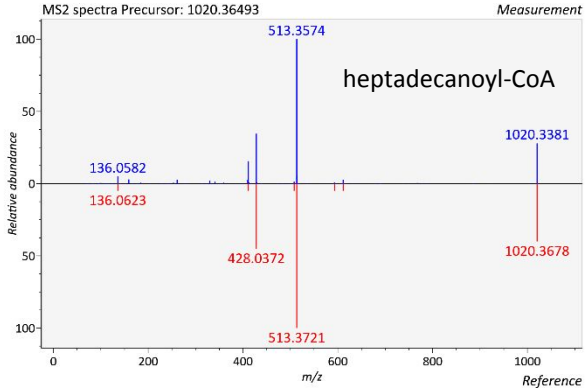


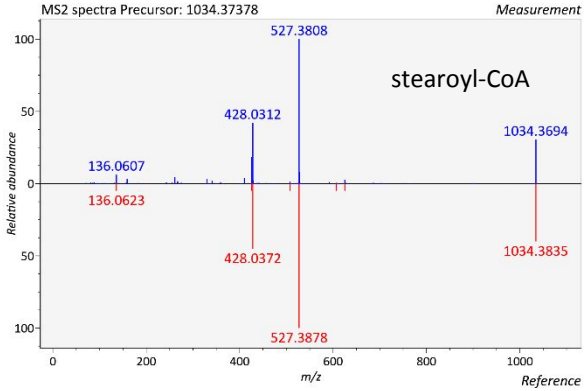
j)

k)

l)


MS2 spectra Precursor: 978.30511
Measurement
myristoyl-CoA
471.3174
978.3039
136.0598
768.1067
136.0623
369.257
978.3209
471.3251
Relative abundance
m/z
Reference


MS2 spectra Precursor: 1020.36493
Measurement
heptadecanoyl-CoA
513.3574
1020.3381
136.0582
136.0623
428.0372
1020.3678
513.3721
Relative abundance
m/z
Reference


MS2 spectra Precursor: 1034.37378
Measurement
stearoyl-CoA
527.3808
428.0312
1034.3694
136.0607
136.0623
428.0372
1034.3835
527.3878
Relative abundance
m/z
Reference

m)

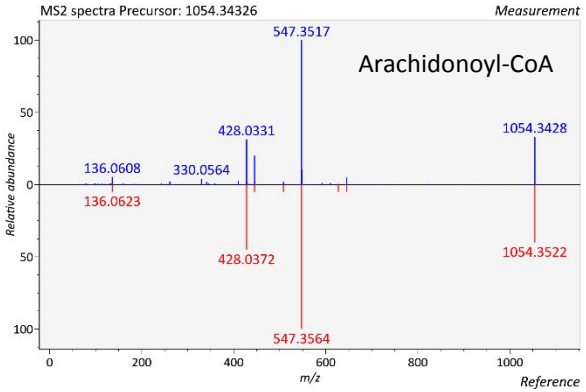
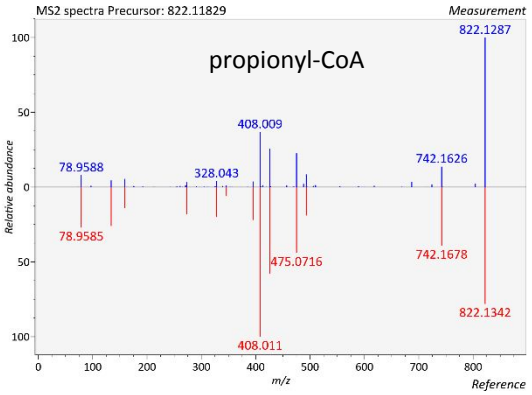
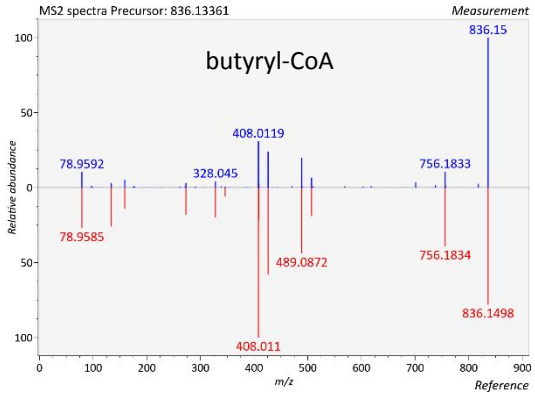

MS2 spectra Precursor: 1054.34326
Measurement
Arachidonoyl-CoA
547.3517
428.0331
1054.3428
136.0608
330.0564
136.0623
428.0372
1054.3522
547.3564
Relative abundance
m/z
Reference

Figure S2: Head to tail MS2 matching results from MS DIAL for the 11 identified acyl-CoAs standards in negative ESI mode (a-k).

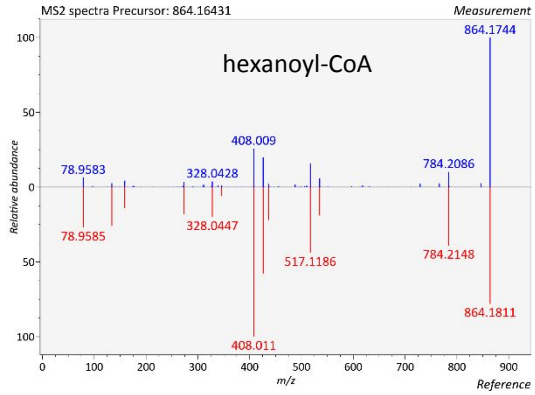
a)



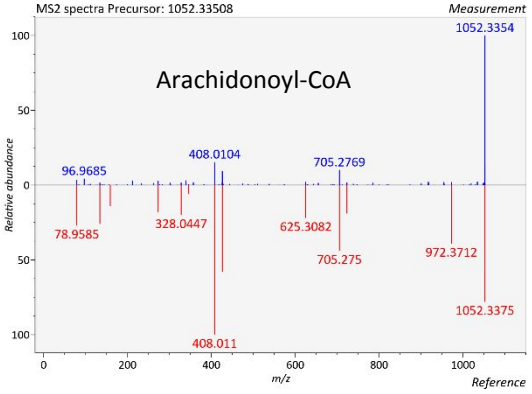
b)



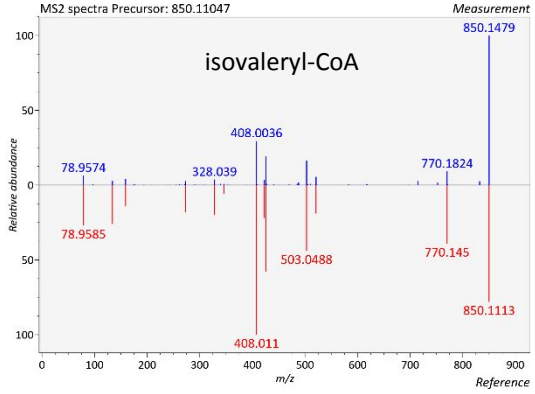
c)



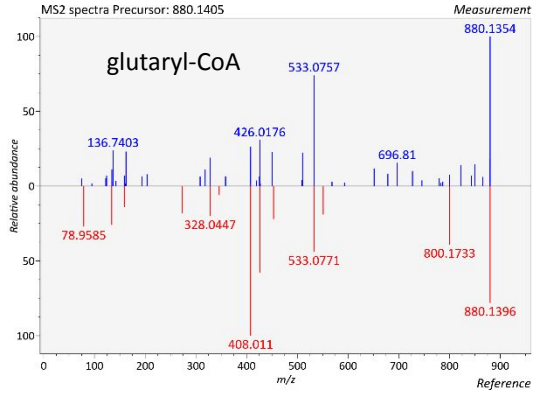
d)



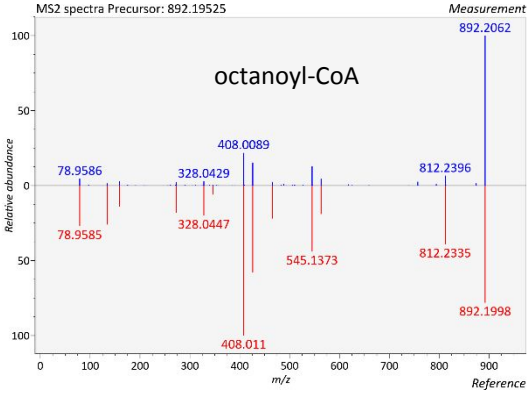
e)



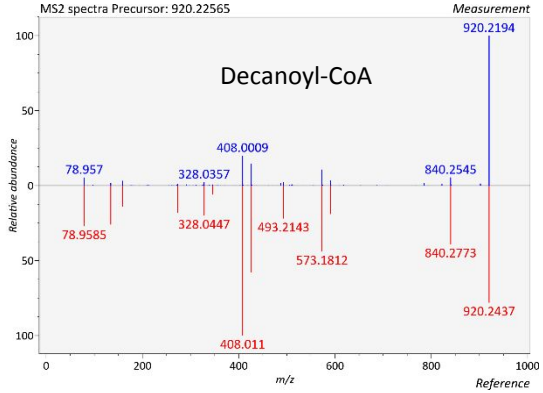
f)



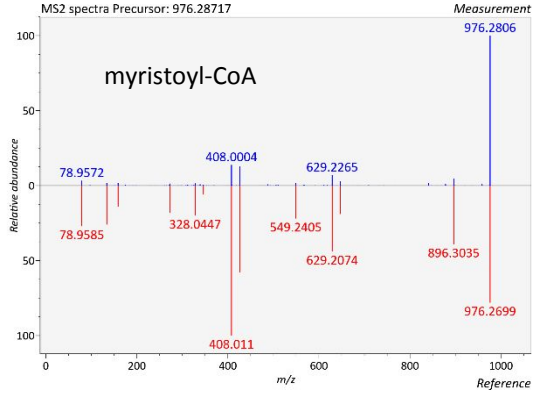
g)



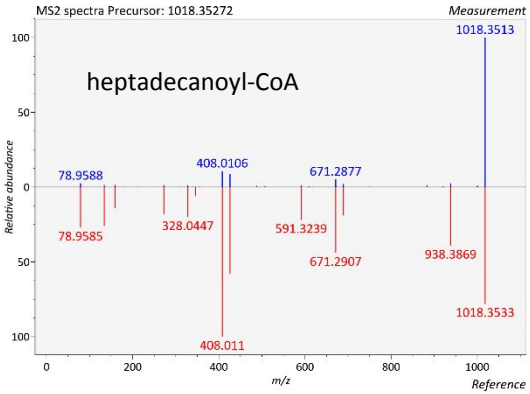
h)



i)



j)


MS2 spectra Precursor: 1018.35272
Measurement
heptadecanoyl-CoA
1018.3513
78.9588
408.0106
671.2877
78.9585
328.0447
591.3239
671.2907
938.3869
1018.3533
408.011
Relative abundance
m/z
Reference

k)

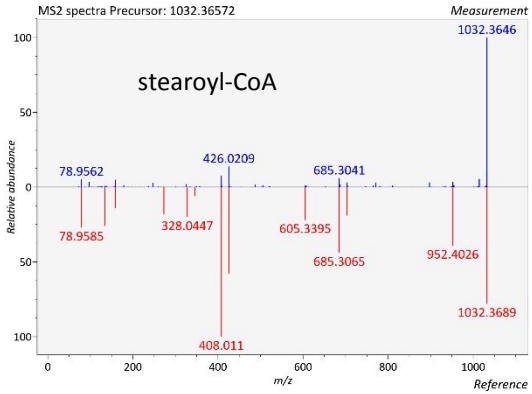
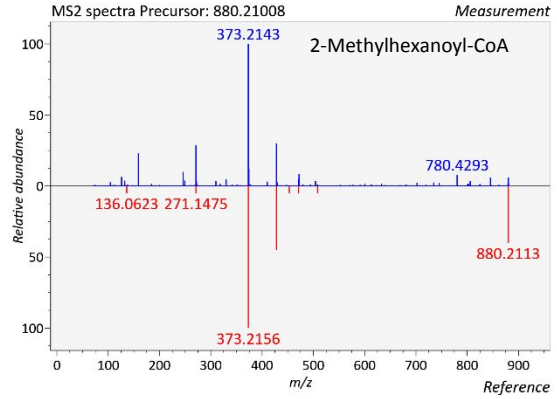
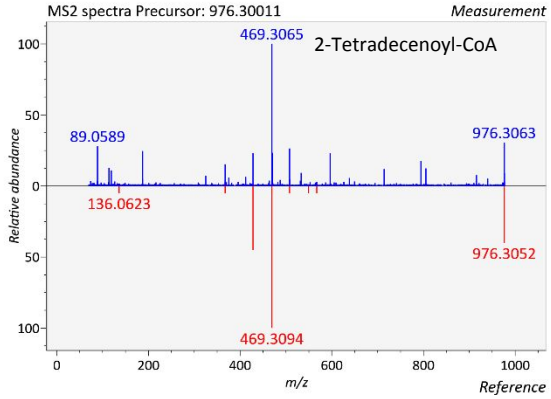

MS2 spectra Precursor: 1032.36572
Measurement
stearoyl-CoA
1032.3646
78.9562
426.0209
685.3041
78.9585
328.0447
605.3395
685.3065
952.4026
1032.3689
408.011
Relative abundance
m/z
Reference

Figure S3: Head to tail MS2 matching results from MS DIAL for all 23 identified liver acyl-CoAs (a-w).

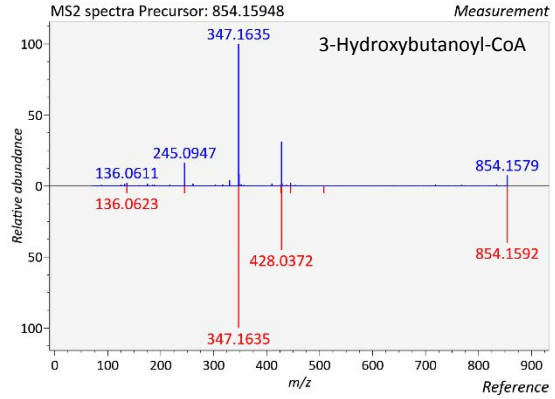
a)



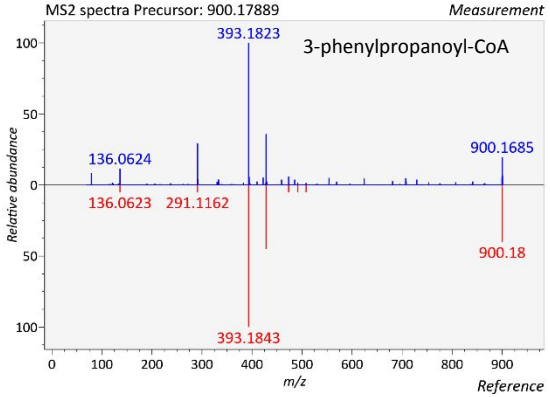
b)



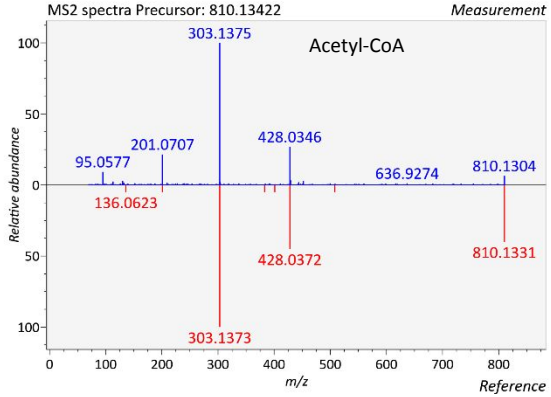
c)



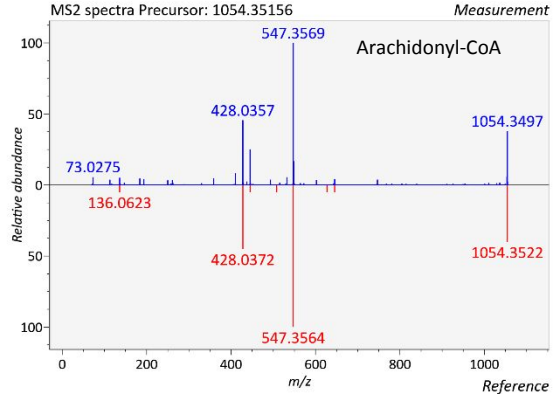
d)



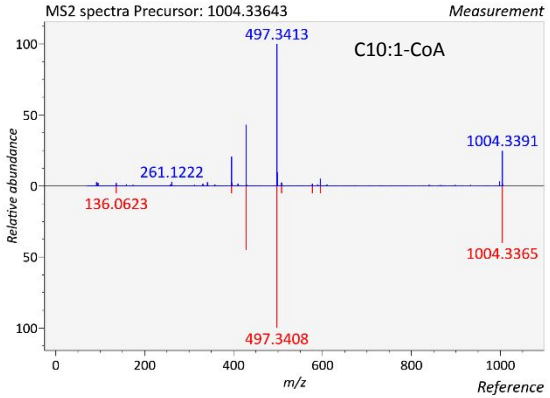
e)



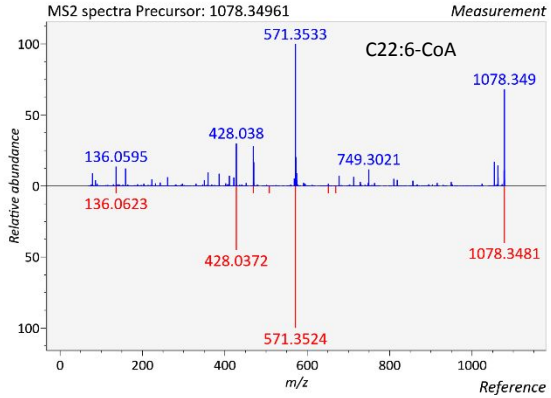
f)



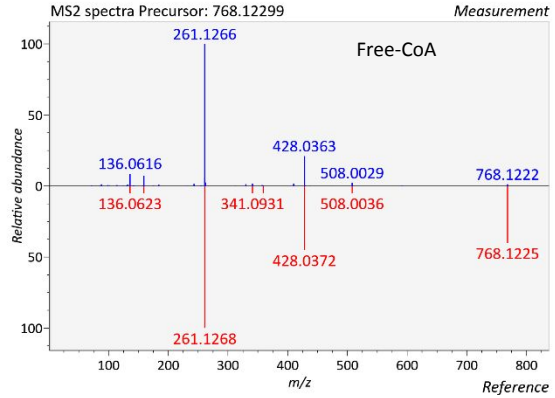
g)



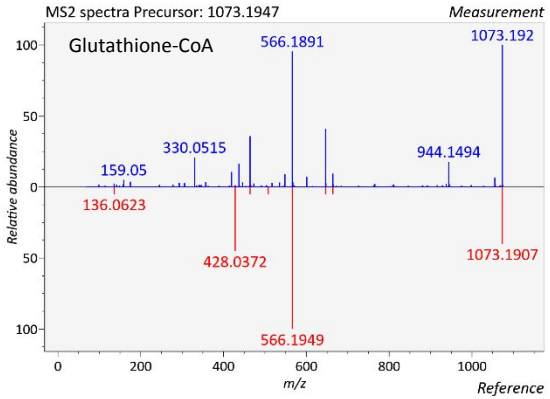
h)



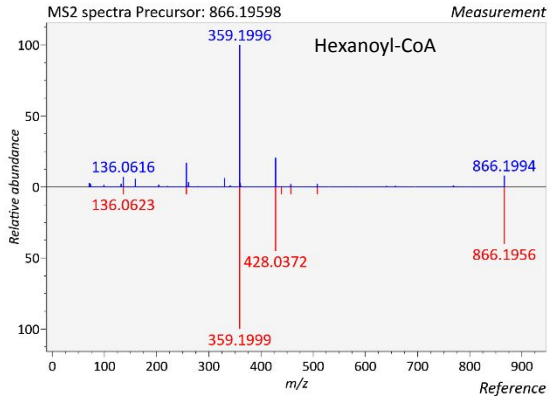
i)



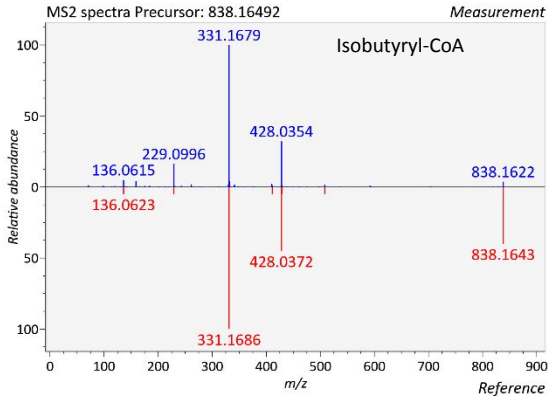
j)



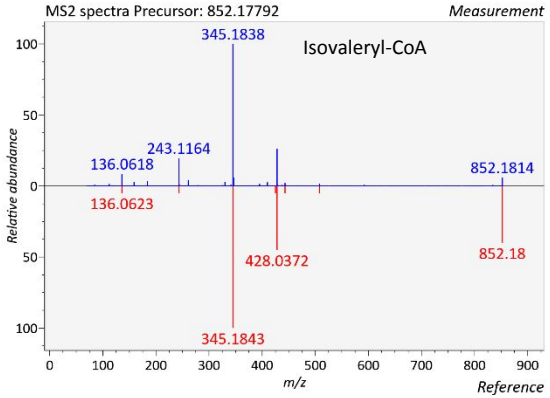
k)



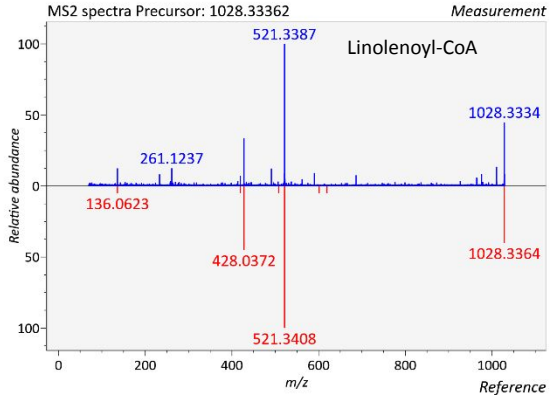
l)



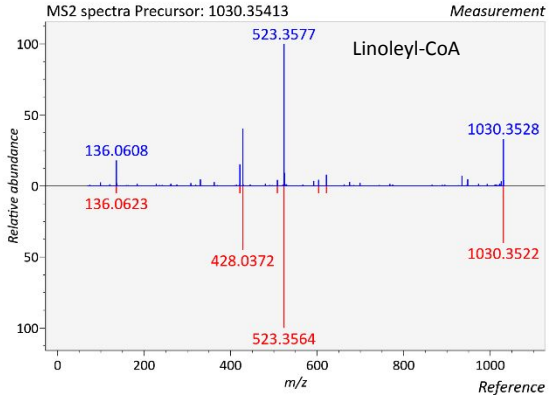
m)



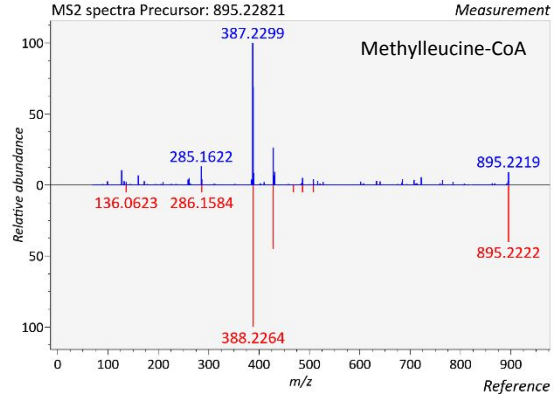
n)



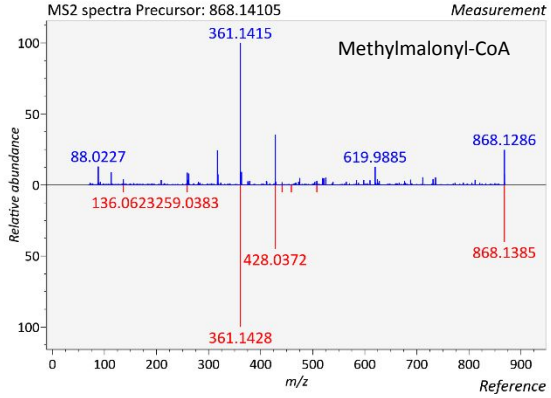
o)



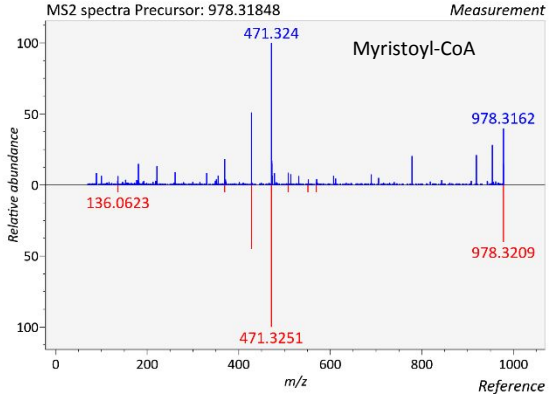
p)



q)



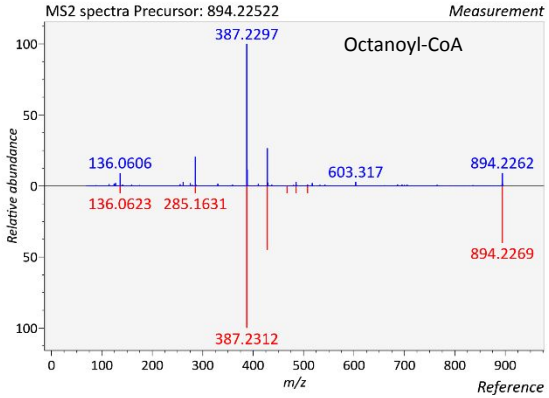
r)

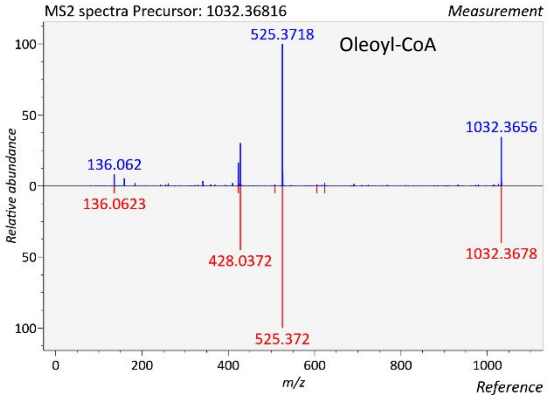


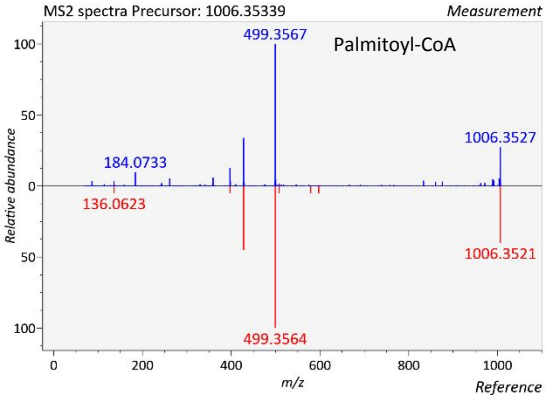
s)

t)

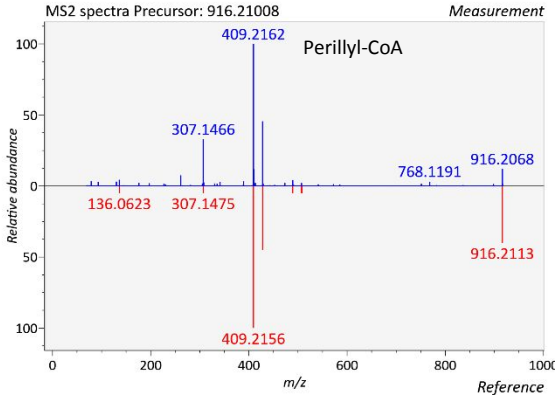
u)


MS2 spectra Precursor: 894.22522
Measurement
Octanoyl-CoA
387.2297
136.0606
603.317
894.2262
136.0623
285.1631
894.2269
387.2312
Relative abundance
m/z
Reference

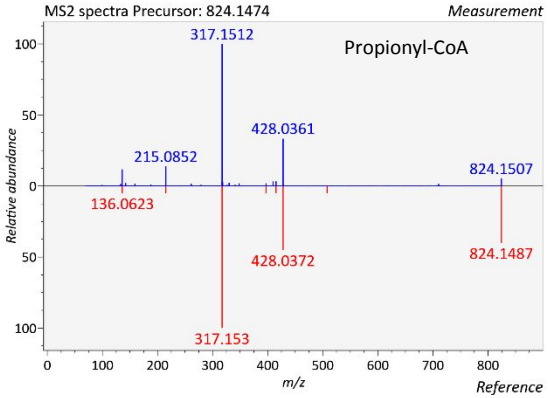

MS2 spectra Precursor: 1032.36816
Measurement
Oleoyl-CoA
525.3718
1032.3656
136.062
136.0623
428.0372
1032.3678
525.372
Relative abundance
m/z
Reference


MS2 spectra Precursor: 1006.35339
Measurement
Palmitoyl-CoA
499.3567
1006.3527
184.0733
136.0623
1006.3521
499.3564
Relative abundance
m/z
Reference

v)


MS2 spectra Precursor: 916.21008
Measurement
Perillyl-CoA
409.2162
307.1466
768.1191
916.2068
136.0623
307.1475
916.2113
409.2156
Relative abundance
m/z
Reference

w)


MS2 spectra Precursor: 824.1474
Measurement
Propionyl-CoA
317.1512
428.0361
215.0852
824.1507
136.0623
428.0372
824.1487
317.153
Relative abundance
m/z
Reference