

code							PDA	PDA	PDA	PDA	PDA	PDA	PDB
grape variety							Pinot grigi	Pinot grigi	Pinot grigi	Pinot grigi	Pinot grigi	Pinot grigi	Pinot grigi
organ							fruit	fruit	fruit	fruit	fruit	fruit	fruit
vineyard							Dligna	Dligna	Dligna	Dligna	Dligna	Dligna	Dligna
harvest time							01	01	01	01	01	01	02
sample prep							juice	juice	juice	juice	juice	juice	juice
File							090405bF	090405bF	090405bF	090405bF	090405bF	090405bF	090405bF
SetupX Class ID							913375	913375	913375	913375	913375	913375	913475
SetupX Sample ID							913354	913358	913362	913366	913370	913374	913454
VOC BinBase Name	RI	Quant Ion	VOC BB ID	mass spec	PubChem ID								
hexenol (2z)	333577	57	46468	30:10818.0	CID 13577	620412	672256	183937	730412	742222	172722		273004
45973	336054	38	45973	30:9405.0	3-	450312	43678	157573	40				88927
heptanol (2-)	346144	45	45431	33:208.0	37 CID 10976	709301	421494	127448	123				847019
45867	348085	95	45867	30:856.0	31-	31934	22043	5131	8924	20806	27515		19847
hexadienal (2e,4e)	35			1:398.0	33 CID 637564	52139	41386	25576	20224	20113	25605		52288
45684	38			0:639.0	31-	223971	151719	85093	103616	127220	150772		165369
octen-3-ol (1-)	387076	57	45555	30:46.0	31: CID 18827	908257	745576	333106	347280	511140	565947		1154552
hepten-2-one (6-methyl)	390009	43	47178	36:68.0	37: CID 9832	112115	212384	89824	111432	247464	189208		279304
octanone (2-)	392202	58	45345	36:2.0	37:6 CID 8093	20142	17032	9030	9892	12978	12120		28869
pentyl f			45700	30:250.0	31 CID 19602	23822	17251	14399	220620	16734	21440		19219
linalool			47418	31:440.0	37		43824	36230	25162	3132	3485		43896
45926	397471	81	45926	32:6219.0		310716	205812	217432	245172	275715			310049
hexenyl acetate (3e)	398624	67	45927	30:8651.0	3	266349	394620	475080	287456	310821			258728
50987				0:508.0	31-	120245	59168	3			83085		115479
hexyl acetate				0:450.0	31 CID 8908	15908	14407	1			13086		91737
heptadienal (2e,4e)	403955	81	45529	30:125.0	34 CID 5283321	79904	57109	36080	37943	34344	40792		65025