

Iron Oxalate Capped Iron-copper Nano for oxidative transformation of aldehydes

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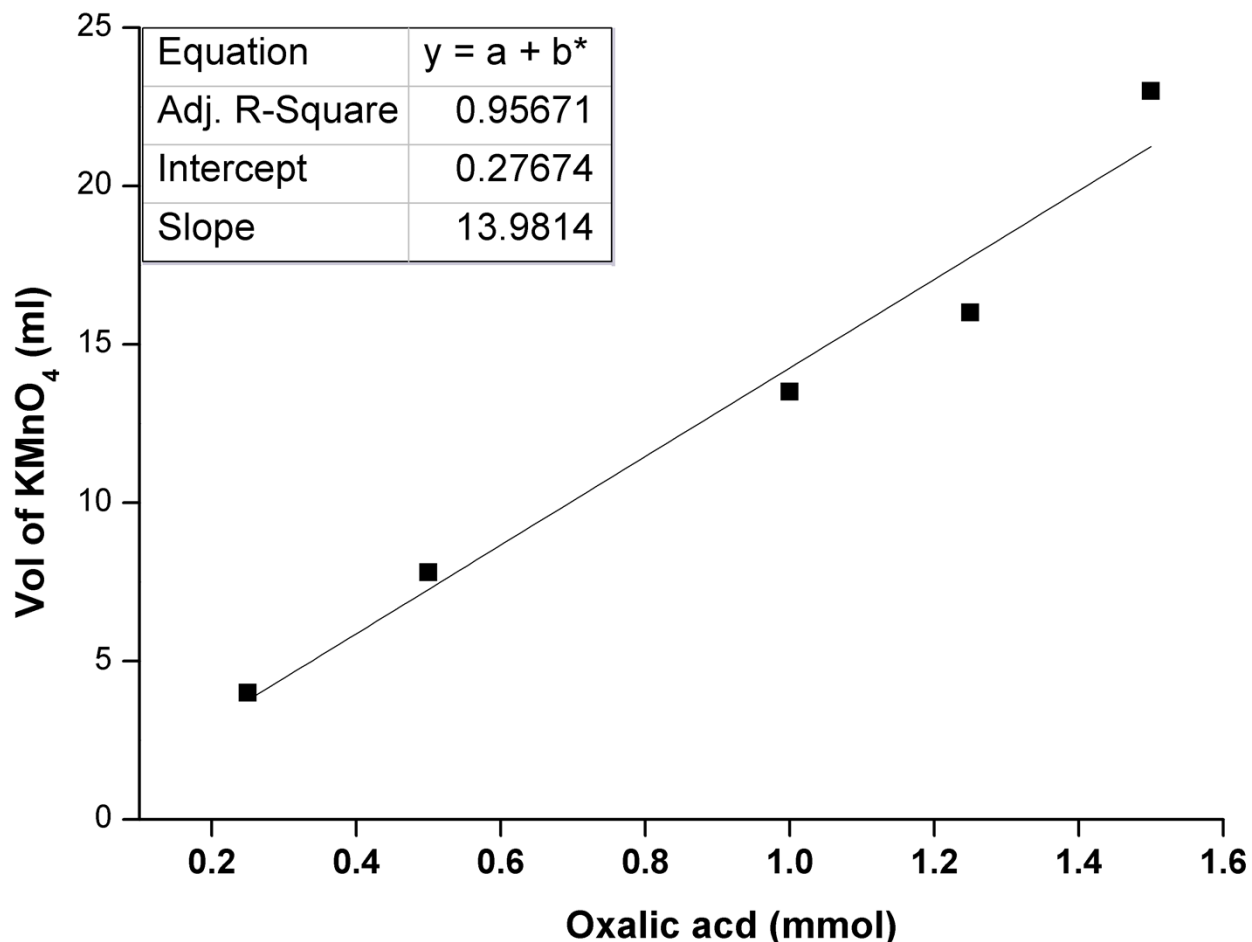


Fig. S1 Calibration curve of permanganate (KMnO_4) titration of oxalic acid in water at 50°C .

Typical procedure for KMnO_4 titration of excess oxalic acid during the synthesis of $\text{Fe}(\text{ox})\text{Fe}-\text{Cu}(\text{Ox})$:

First of all potassium permanganate solution has been standardized against a sample of potassium oxalate. After determination of exact normality of the permanganate solution, it was used as a standard oxidizing solution for the determination of variable amount of oxalic acid. In a typical procedure, 284 mg of Mohr's salt, $(\text{NH}_4)_2\text{SO}_4 \cdot \text{FeSO}_4$ was taken in 150 ml of distilled water in a 500 ml conical flask and 126 mg of oxalic acid, $\text{H}_2\text{C}_2\text{O}_4$ was added to this and stirred vigorously. In another 500 ml conical flask, a solution of 1.2 g of sodium borohydride, NaBH_4 was prepared in 100 ml distilled water and was added slowly in an earlier prepared solution with vigorous stirring. During the addition, the color of the solution slowly changed into yellow. After few minutes, when black Fe nano particle began to appear, the NaBH_4 addition was stopped. To this, earlier prepared 100 ml 0.01(M)

CuSO₄ solution was slowly added to it at 60 °C for 0.5 h. After 5-6 h of addition, the color of the solution slowly turned to yellowish brown. After 16 h, the solid sample was collected by centrifugation. The excess amount of oxalic acid in the reaction solution was titrated with standard KMnO₄ solution at 60 °C.

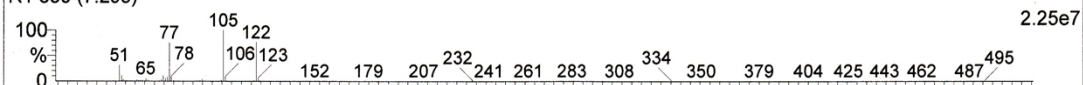
Typical procedure for sample preparation for ICP-OES analysis:

In a fume hood, 500 mg of the appropriate nanomaterial was taken in a 100 ml conical flask and 15 mL of concentrated HCl was added to it and covered with a watch glass and heated nearly to boiling in the hood with occasional stirring. Additional HCl was added to only if evaporation reduces the volume significantly; that is, nanomaterial is re-precipitated. Following dissolution, solution was gently boil for a few minutes to expel as much HCl(g) as possible. Finally, distilled water was added to it for makeup of 1000 ml volume. The ICP-OES measurement was done with this solution.

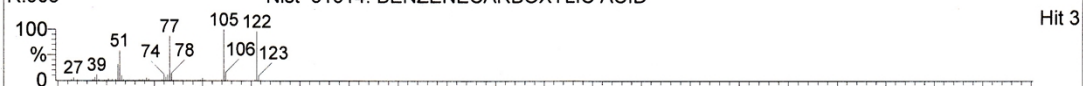
Hit	REV	for	Compound Name	
1	941	827	.BETA.-1,5-O-DIBENZOYL-RIBOFURANOSE	
2	914	902	METHANOL, OXO-, BENZOATE	
3	903	893	BENZENECARBOXYLIC ACID	
4	897	851	CYCLOBUTANE-1,1-DICARBOXAMIDE, N,N'-DI-BENZOYLOXY-	
5	888	839	2-CHLOROETHYL BENZOATE	11
6	886	848	HEPTANEDIAMIDE, N,N'-DI-BENZOYLOXY-	39
7	874	822	(+)-DIBENZOYL-L-TARTARIC ACID ANHYDRIDE	34
8	856	819	BENZOIC ACID 2-BROMOETHYL ESTER	22
9	852	797	(D)-(+)-(2R,3R)-2,3-DIBENZOYL TARTARIC ACID	35
10	841	781	2,5-CYCLOHEXADIENE-1,4-DIONE, BIS(O-BENZOYLOXIME)	34
11	836	806	CYCLOPROPANECARBOXAMIDE, N-BENZOYLOXY-	20
12	834	767	3(1H)-IMINO-2-(2,3,5-TRIS-O-BENZOYL-BETA-D-RIBOFURANOSYL)-2,3-DIHYDRO-S-	56
13	818	555	3-BENZOYL-5-(2,4-DICHLOROBENZYLIDENE)RHODANINE	39
14	815	784	1,2,4-TRIOXOLANE, 3,5-DIPHENYL-	22
15	814	729	SALICYLIDENE BENZHYDRAZIDE	24
16	814	713	1-O-MONOACETYL-2,3-O-DIBENZOYL-D-RIBOFURANOSE	40
17	798	752	BENZENE-1,4-DICARBOXAMIDE, N,N'-BIS(BENZOYLOXY)-	40
18	797	764	4-PIPERIDINEPROPANOIC ACID, 1-BENZOYL-3-(2-CHLOROETHYL)-, ETHYL ESTER	35
19	795	757	BENZOIC ACID, ETHYL ESTER	15
20	788	761	2,3-DIBENZOYL-MESO-TARTARIC ANHYDRIDE	34

, 27-Dec-2013 + 10:42:30

R1 859 (7.295)



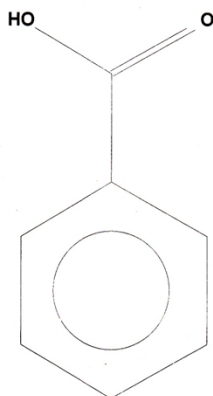
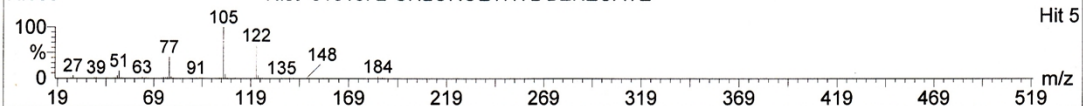
R:903 Nist 61614: BENZENECARBOXYLIC ACID



R:897 Nist 60259: CYCLOBUTANE-1,1-DICARBOXAMIDE, N,N'-DI-BENZOYLOXY-



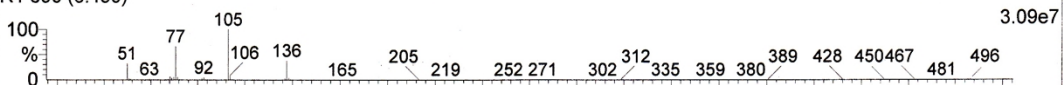
R:888 Nist 61613: 2-CHLOROETHYL BENZOATE



Hit	REV	for	Compound Name	M.V
1	945	935	BENZOIC ACID, METHYL ESTER	136
2	939	920	BENZOIC ACID, HYDRAZIDE	136
3	928	752	PHENYLGLYOXAL	134
4	919	755	VINYL BENZOATE	148
5	917	775	N-METHOXY-N-METHYLBENZAMIDE	168
6	912	758	ACETOPHENONE, 2-CHLORO-	154
7	911	741	BENZOYL BROMIDE	184
8	909	741	PHENACYLIDENE DIACETATE	236
9	908	759	PHENACYL THIOCYANATE	177
10	905	740	BENZENEPROPANENITRILE, .BETA.-OXO-	148
11	899	868	ETHANONE, 2-HYDROXY-1-PHENYL-	136
12	897	722	ETHANEDIONE, DIPHENYL-	210
13	895	701	BENZHYDRAZIDE, N2-(2,3-DIHYDRO-3-BENZOYL-2-BENZOTHAZOLYLENE)-	378
14	892	669	BENZAMIDE, 4-BENZOYL-N-(IMMINO)(METHYLTHIO)METHYL-	298
15	886	726	2-(2-OXO-2-PHENYL-ETHYL)-MALONONITRILE	184
16	883	713	BENZOYL CHLORIDE	146
17	881	710	BENZENEACETIC ACID, .ALPHA.-OXO-, ETHYL ESTER	178
18	879	736	ETHANONE, 2-BROMO-1-PHENYL-	198
19	878	713	ETHANONE, 2,2,2-TRIFLUORO-1-PHENYL-	174
20	876	712	.ALPHA.,.ALPHA.-DICHLOROACETOPHENONE	188

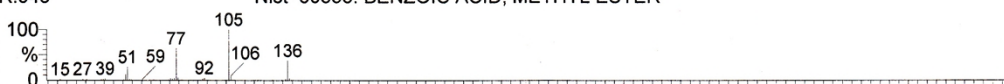
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R1 690 (6.450)



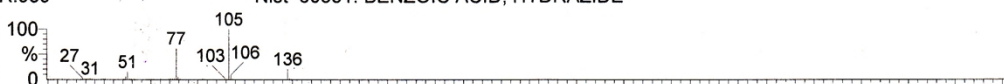
R:945 Nist 60353: BENZOIC ACID, METHYL ESTER

Hit 1



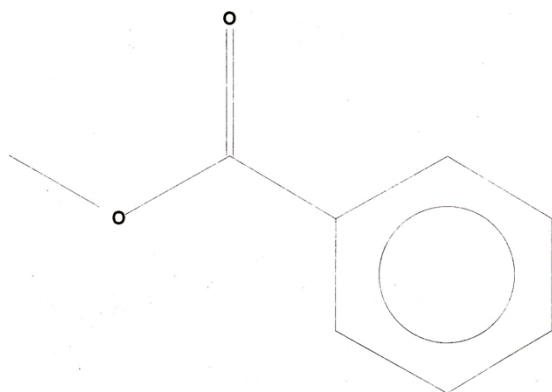
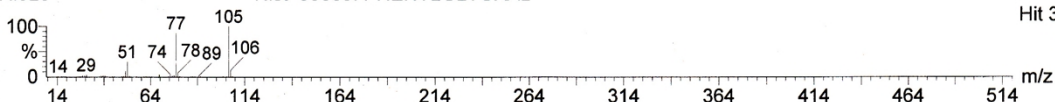
R:939 Nist 60351: BENZOIC ACID, HYDRAZIDE

Hit 2



R:928 Nist 59869: PHENYLGLYOXAL

Hit 3

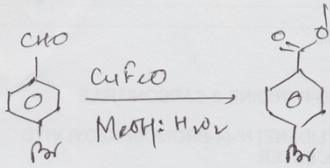


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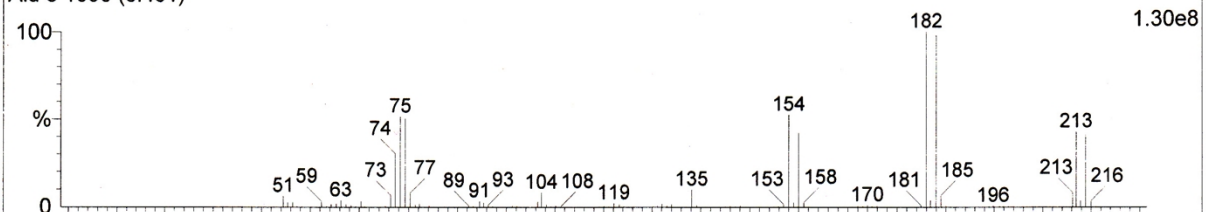
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Hit	REV	for	Compound Name	M.V
7	581	447	BENZALDEHYDE, P-BROMO-, O-METHYLOXIME	213
8	557	395	BENZENE, 1-BROMO-2-ETHENYL-	182
9	556	392	BENZENE, 1-BROMO-4-ETHENYL-	182
10	552	404	5-CHLORO-4,6-DIMETHYL-2-OXO-1,2-DIHYDRO-PYRIDINE-3-CARBONITRILE	182
11	536	342	3-BROMOSTYRENE	182
12	536	327	N-[2-(2-PROPENYLOXY)-3,5-DIBROMOBENZYLIDENE] N'-(4-BROMOBENZOYL)HYD	514
13	533	350	BENZOIC ACID, 2-CHLORO-6-NITRO-, METHYL ESTER	215
14	524	348	2H-BENZ[E]1,3-OXAZIN-4(3H)-ONE, 6-CHLORO-2-TRICHLOROMETHYL-	299
15	509	333	BENZOIC ACID, 4-CHLORO-2-NITRO-, METHYL ESTER	215
16	489	306	BENZENE, (2-BROMOETHENYL)-, (E)-	182
17	465	328	2-(4-CHLOROPHENYL)-1,3,2-DIOXABOROLANE	182
18	452	335	METHANONE, (4-BROMOPHENYL)-3-PYRIDINYL-	267
19	445	308	[1,10]PHENANTHROLINE-5,6-DIONE	210
20	434	323	BENZOIC ACID, 4-BROMO-, METHYL ESTER	214

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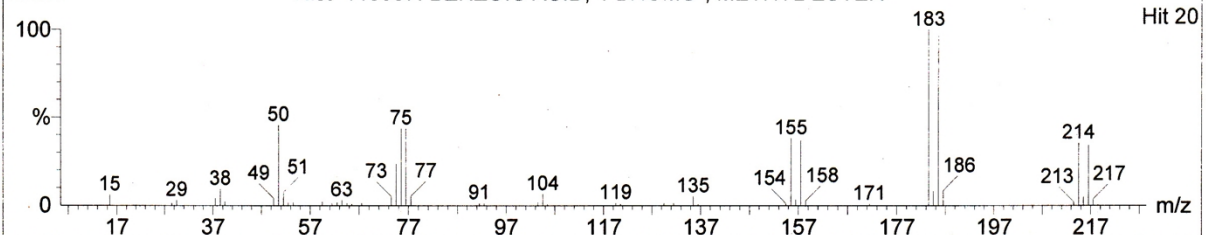
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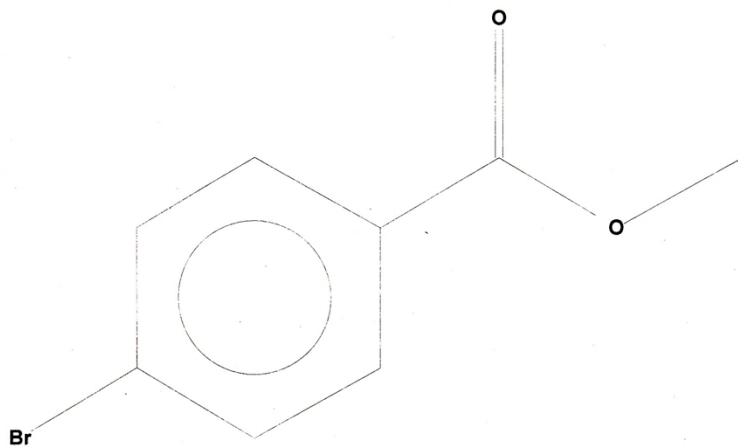
R:434

Nist 115957: BENZOIC ACID, 4-BROMO-, METHYL ESTER

1.30e8



Hit 20



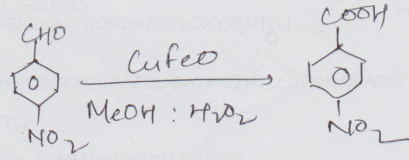
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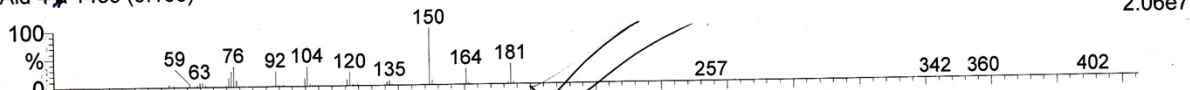
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Hit	REV	for	Compound Name	M.V
1	928	920	BENZOIC ACID, 4-NITRO-, METHYL ESTER	181
2	928	916	3-METHOXYCARBONYL-5-NITROPYRIDINE 1-OXIDE	198
3	874	856	BENZOIC ACID, 3-NITRO-, METHYL ESTER	181
4	856	557	N-(2-METHYL-3,5-DINITRO-PHENYL)-4-NITRO-BENZAMIDE	346
5	855	626	ETHYL 4-NITROBENZOYLFORMATE	223
6	853	498	ACETAMIDE, 2,2,2-TRIFLUORO-N-(P-NITROPHENACYL)-	276
7	842	625	4-NITROBENZOYL ISOTHIOCYANATE	208
8	831	631	4-NITROBENZOYL CHLORIDE	188
9	826	554	BENZOIC ACID, 4-NITRO-, (2-ACETYL-1-OXO-3-INDENYL) ESTER	337
10	825	599	BENZENECARBOTHIOIC ACID, 4-NITRO-, S-METHYL ESTER	197
11	821	765	4-NITROBENZOIC HYDRAZIDE	181
12	821	485	BENZAMIDE, N-5H-1,3,2,4-DITHIA(3-SIV) DIAZOL-5-YLIDENE-4-NITRO-	268
13	811	616	METHANONE, (4-NITROPHENYL)(4-BENZOYL-3-ISOXAZOYL)-	322
14	808	589	2,5-CYCLOHEXADIENE-1,4-DIONE, 5-BROMO-2,3-DIMETHYL-, 1-OXIME, O-(4-NITRO	378
15	806	588	2,5-CYCLOHEXADIENE-1,4-DIONE, 5-CHLORO-2,3-DIMETHYL-, 1-OXIME, O-(4-NITRO	334
16	805	585	2,5-CYCLOHEXADIENE-1,4-DIONE, 3-CHLORO-5-ISOPROPYL-2-METHYL-, 1-OXIME,	362
17	805	601	(P-NITROBENZOYL)ACETONITRILE	190
18	803	581	2-CYCLOHEXENE-1,4-DIONE, 5,6-DICHLORO-2,3-DIMETHYL-, 1-OXIME, O-(4-NITROB	370
19	800	591	3-(4-NITROBENZOYL)-2-THIOXO-4-THIAZOLYL 4-NITROBENZOATE	437
20	796	551	ETHANONE, 2,2-DIBROMO-1-(4-NITROPHENYL)-	327

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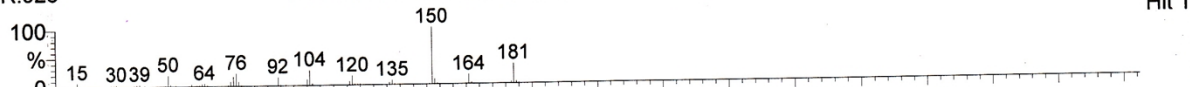
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2.06e7



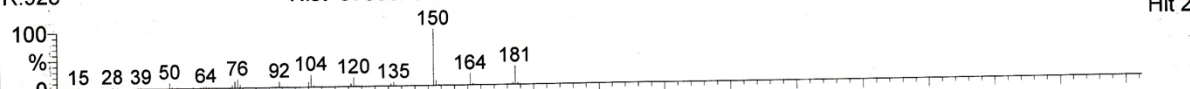
R:928 Nist 97504: BENZOIC ACID, 4-NITRO-, METHYL ESTER

Hit 1



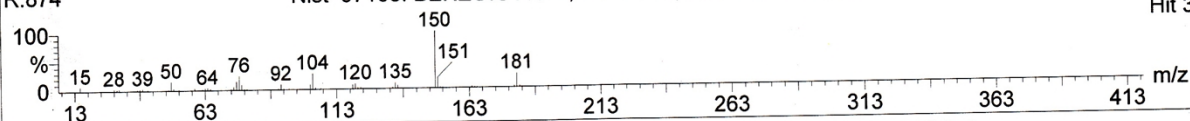
R:928 Nist 97503: 3-METHOXYCARBONYL-5-NITROPYRIDINE 1-OXIDE

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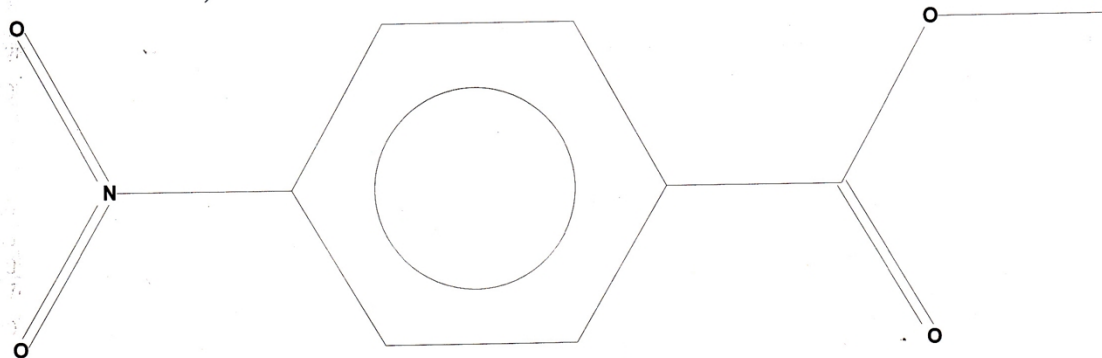


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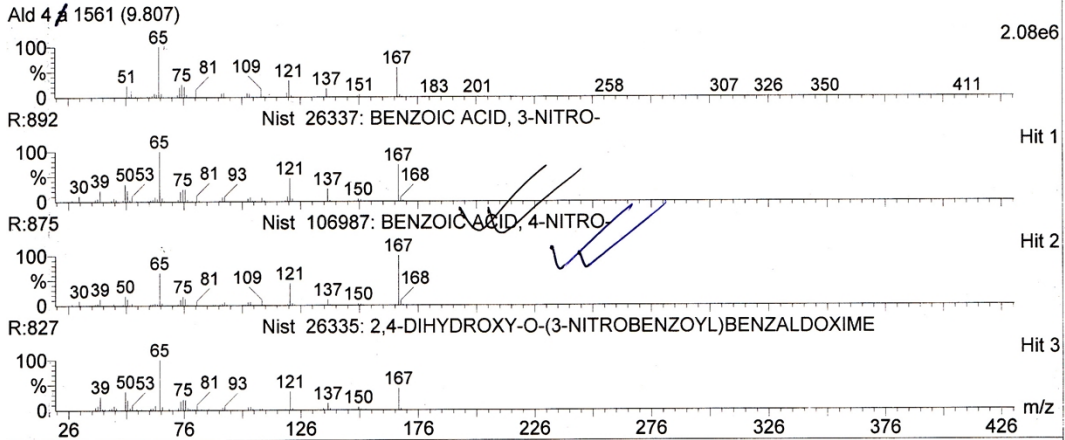


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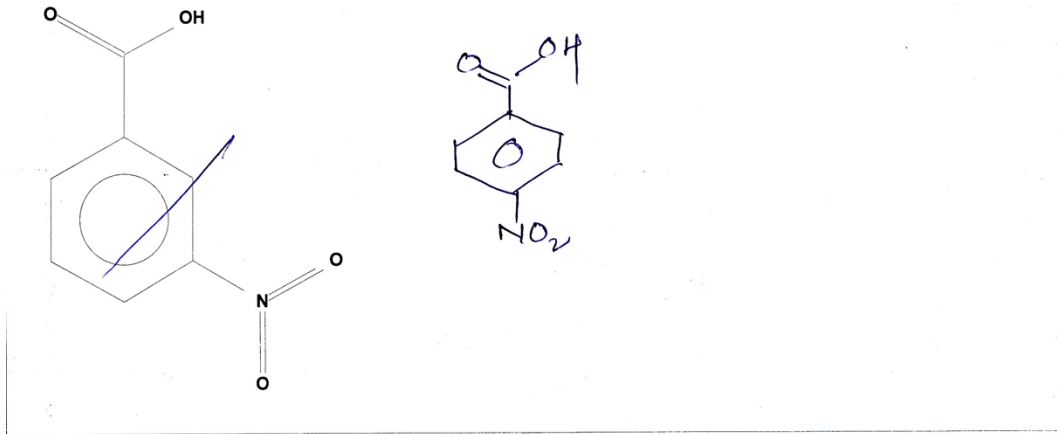


3	827	192	2,4-DIHYDROXY-O-(3-NITROBENZOYL)BENZALDOXIME	304
4	730	694	O-NITROBENZOIC ANHYDRIDE	316
5	704	509	BENZALDEHYDE, 2-NITRO-	151
6	680	454	BENZOIC ACID, 2-NITROSO-	151
7	665	640	1,2,3,5-TETRA-O-P-NITROBENZOYL-.BETA.-D-RIBOFURANOSE	746
8	658	620	1,2-BENZENEDICARBOXYLIC ACID, 3-NITRO-	211
9	657	618	FURAN-3-AMINE, N-ACETYL-5-[1,2-BIS(4-NITROBENZOYLOXY)ETHYL]-	483
10	657	622	BENZOIC ACID, 2-NITRO-	167
11	641	584	NITROTERTHPHTHALIC ACID	211
12	631	451	2-HYDROXYBENZOIC ACID, (BENZO[1,2,5]OXADIAZOL-5-YLMETHYLENE)HYDRAZID	282
13	631	484	BENZOIC ACID, 4-SULFO-	202
14	627	481	BENZOIC ACID, 4-(AMINOSULFONYL)-	201
15	621	457	HALAZONE	268
16	615	583	1,3,5-O-TRI-P-NITROBENZOYL-.BETA.-D-ARABINOFURANOSIDE	597
17	615	584	INDENE-1-OL-3-ONE, 2-FLUORO-4-NITRO-	211
18	559	535	4-NITROPHENYLGLYOXYLIC ACID	196
19	556	505	BENZALDEHYDE, 4-NITRO-, O-(3-NITROBENZOYL)OXIME	315
20	550	336	BENZOIC ACID, 4-(1-PERHYDROAZEPINYLAZO)-	247

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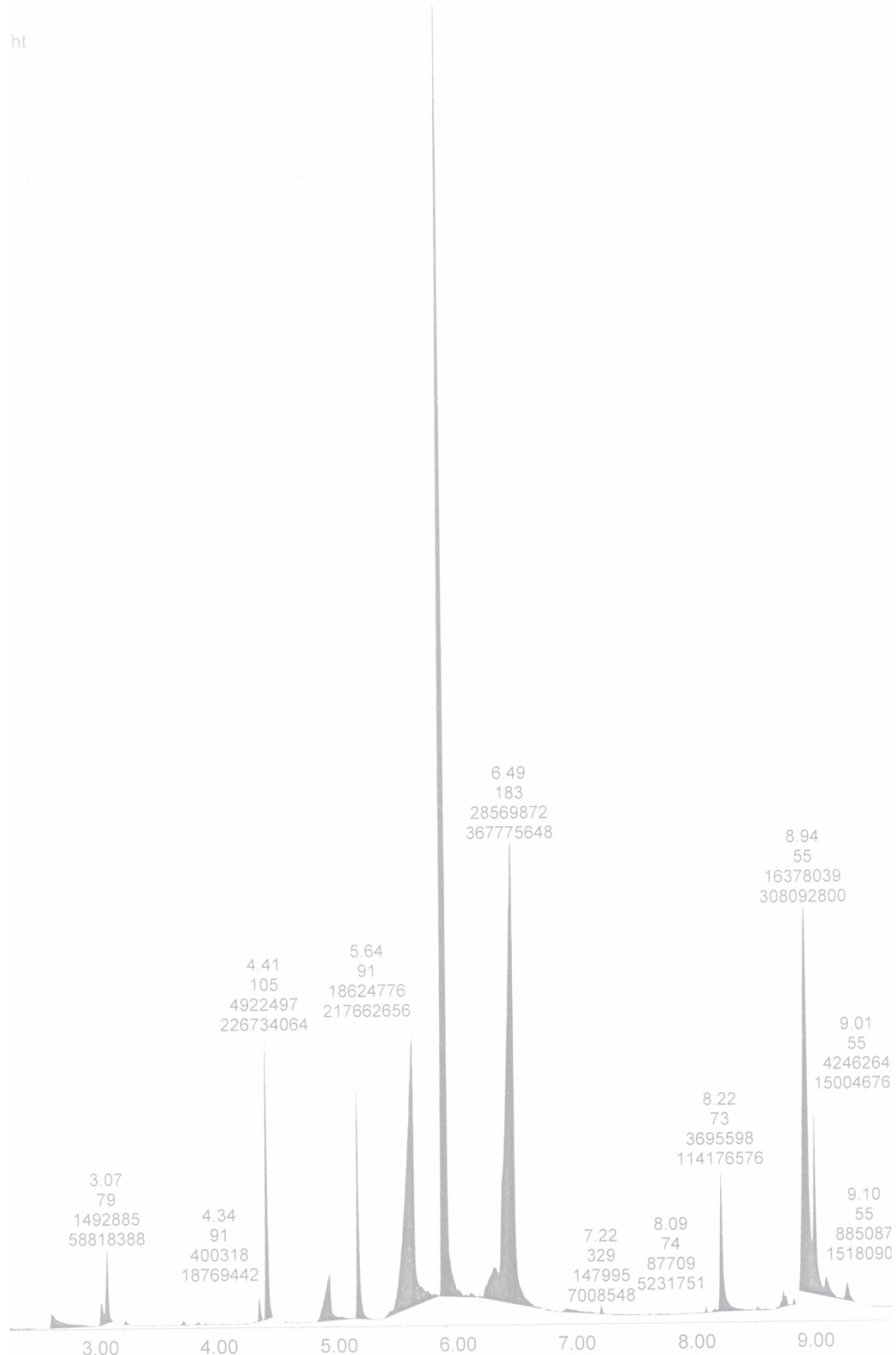


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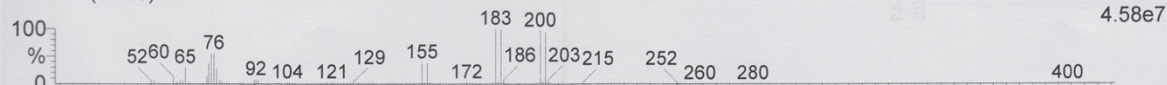
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Hit	REV	for	Compound Name	M.W
1	743	623	BENZOIC ACID, 2-BROMO-	200
2	706	507	1-BUTANONE, 1-(4-BROMOPHENYL)-4-CHLORO-	260
3	705	511	3-BROMOBENZOIC ACID, CYCLOBUTYL ESTER	254
4	689	588	4-BROMOBENZOIC ACID, 2-BUTYL ESTER	256
5	688	463	BENZHYDRAZIDE, 4-BROMO-N2-(4-BROMOBENZYLIDENE)-	380
6	684	652	BENZOIC ACID, 3-BROMO-	200
7	683	604	3-BROMOBENZOIC ACID, 2-METHYLPROPYL ESTER	256
8	682	584	2-BROMOBENZOIC ACID, 2-BUTYL ESTER	256
9	681	569	2-BROMOBENZOIC ACID, UNDECYL ESTER	354
10	673	577	2-BROMOBENZOIC ACID, 2-METHYLPROPYL ESTER	256
11	667	606	2-BROMOBENZOIC ACID, BUTYL ESTER	256
12	665	566	2-BROMOBENZOIC ACID, 2-ADAMANTYL ESTER	334
13	664	583	4-BROMOBENZOIC ACID, NONYL ESTER	326
14	662	581	ETHANONE, 1-(4-BROMOPHENYL)-	198
15	661	547	3-BROMOBENZOIC ACID PYRIDIN-3-YLMETHYLENEHYDRAZIDE	300
16	658	577	ETHANONE, 1-(3-BROMOPHENYL)-	198
17	656	555	1-PENTANONE, 1-(4-BROMOPHENYL)-	240
18	655	463	4-BROMOBENZENAMIDE, N-(2-METHOXY-3,5-DIBROMOBENZYLIDENAMINO)-	488
19	653	590	BENZAMIDE, 2-BROMO-	198
20	651	545	4-BROMOBENZOIC ACID, CYCLOPENTYL ESTER	268

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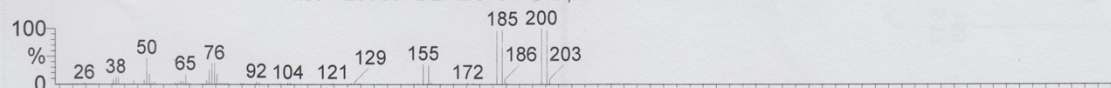
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R:743

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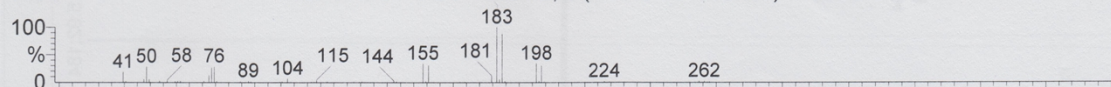
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R:706

Nist 116131: 1-BUTANONE, 1-(4-BROMOPHENYL)-4-CHLORO-

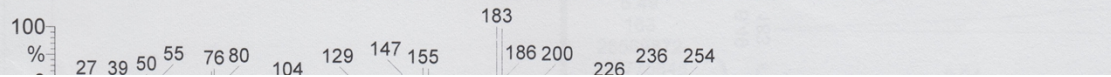
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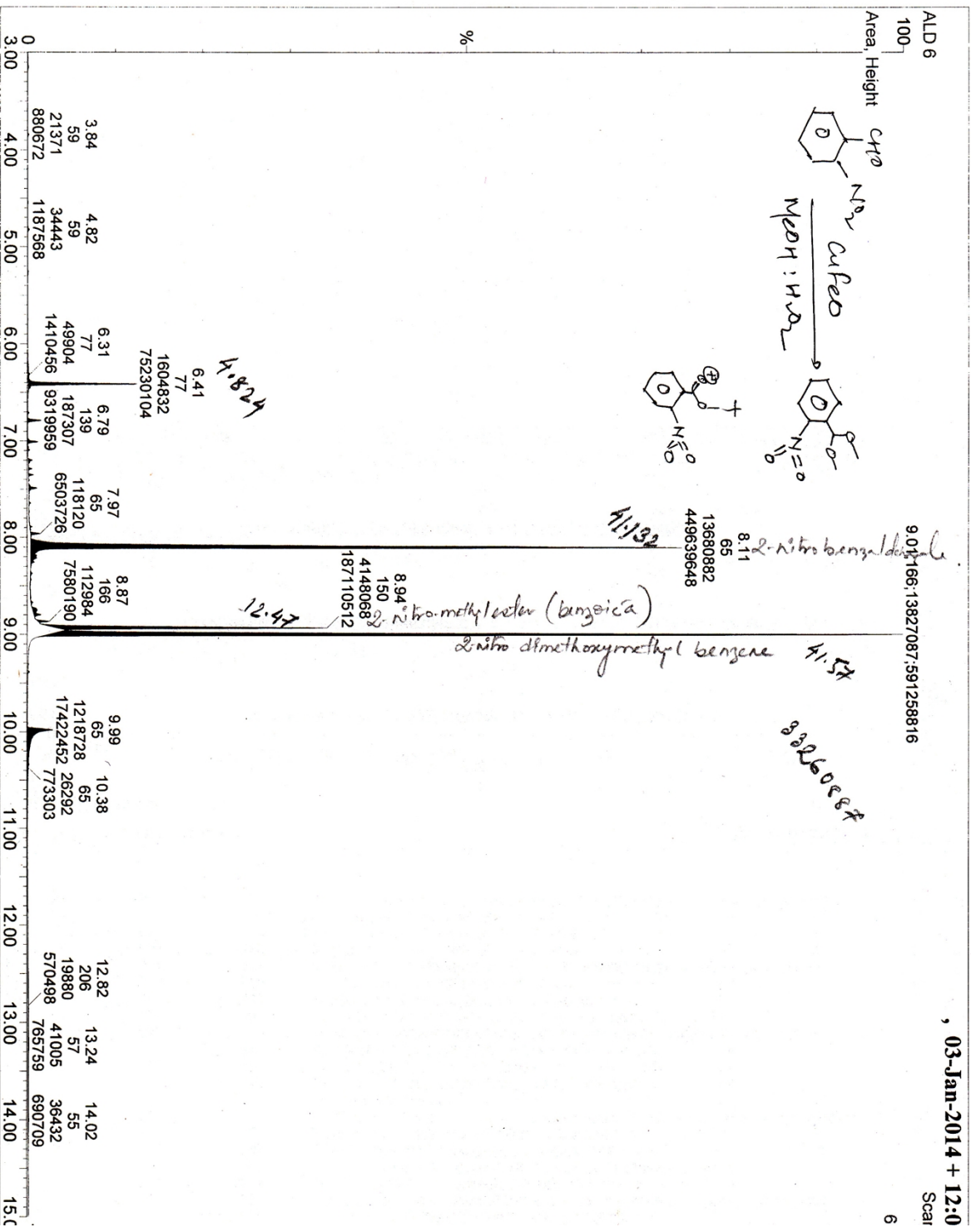
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Nist 116079: 3-BROMOBENZOIC ACID, CYCLOBUTYL ESTER

Hit 3



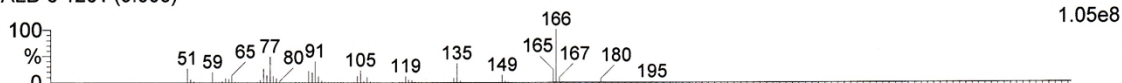
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Hit	REV	for	Compound Name	M.V
1	917	888	BENZENE, 1-(DIMETHOXYMETHYL)-2-NITRO-	197
2	765	623	PYRIMIDINE-2,4(1H,3H)-DIONE, 6-CHLORO-1-(4-METHOXY-3-NITROBENZYL)-	311
3	746	588	BENZENAMINE, N,N-DIMETHYL-3-NITRO-	166
4	709	601	7,7-DIMETHOXY-5-METHYLENEBICYCLO[2.2.1]HEPT-2-ENE	166
5	706	560	2-METHOXY-5-METHYLBENZOIC ACID	166
6	697	553	2-METHOXY-4-METHYLBENZOIC ACID	166
7	695	532	PYRIMIDINE-2,4(1H,3H)-DIONE, 6-CHLORO-1-(3-METHOXY-4-NITROBENZYL)-3-MET	321
8	687	570	P-ANISAMIDOXIME	166
9	679	442	2-BROMO-1,3-BIS(METHOXYMETHYL)BENZENE	241
10	678	484	BENZALDEHYDE, 2,4-DIMETHOXY-	166
11	675	518	BENZOIC ACID, 3-METHOXY-4-METHYL-	166
12	663	412	3-PHENYL-PROPIONIC ACID (4-METHOXY-BENZYLIDENE)HYDRAZIDE	282
13	661	499	PHENOL, 4-(METHOXYMETHYL)-2,6-DIMETHYL-	166
14	641	396	2-PHENYL-3-(4-NITROPHENYL)-OXIRANE	241
15	639	528	BENZOIC ACID, 2-METHOXY-6-METHYL-	166
16	634	357	4-METHOXYBENZENAMIDE, N-(3,4-METHYLENEDIOXYBENZYLIDENAMINO)-	296
17	634	582	BENZENE, 1,4-BIS(METHOXYMETHYL)-	166
18	629	533	ETHYL(DIMETHYL)BENZYLOXYSILANE	194
19	627	540	N-DIMETHOXYMETHYLENEANILINE	166
20	625	368	ACETOHYDRAZIDE, 2-(2-ISOPROPYL-5-METHYLPHENOXY)-N2-BENZYLIDENO-	310

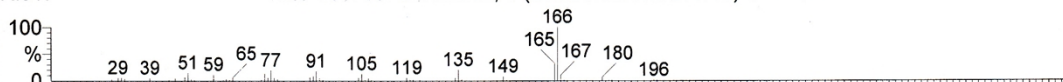
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ALD 6 1201 (9.006)



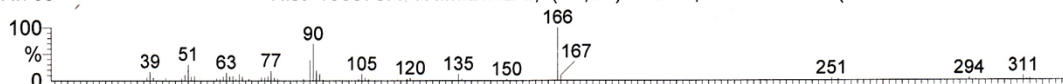
R:917 Nist 106780: BENZENE, 1-(DIMETHOXYMETHYL)-2-NITRO-

Hit 1



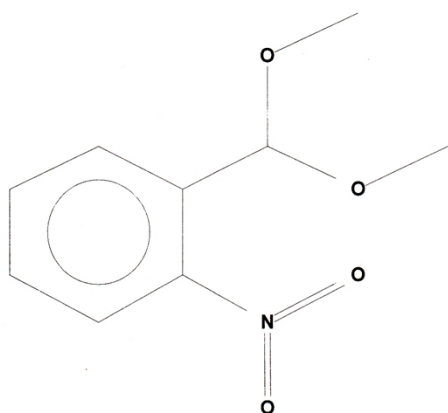
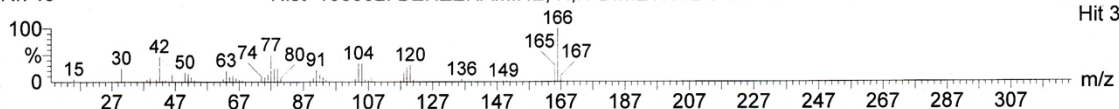
R:765 Nist 106576: PYRIMIDINE-2,4(1H,3H)-DIONE, 6-CHLORO-1-(4-METHOXY-3-NITROBENZYL)

Hit 2



R:746 Nist 106552: BENZENAMINE, N,N-DIMETHYL-3-NITRO-

Hit 3



Hit	REV	for	Compound Name	M.W
1	872	803	BENZOIC ACID, 2-NITRO-, METHYL ESTER	181
2	835	611	BENZAMIDE, 2-NITRO-N-(2-FLUORO-5-NITROPHENYL)-	305
3	811	671	BENZAMIDE, N-[3-(2,2,2-TRIFLUOROETHOXY)-5-NITROPHENYL]-2-NITRO-	385
4	801	721	P-TOLYL O-NITRO BENZOATE	257
5	785	638	METHANONE, (4-NITROPHENYL)(4-BENZOYL-3-ISOXAZOYL)-	322
6	783	621	3-(PHENACYLAMINO)BENZOIC ACID	255
7	777	694	BENZAMIDE, 2-NITRO-	166
8	765	679	BENZOIC ACID, 4-(2-NITROBENZOYLOXY)-	287
9	758	514	BENZOIC ACID, 4-NITRO-, (2-ACETYL-1-OXO-3-INDENYL) ESTER	337
10	752	631	N-METHYL-4-(2-NITROBENZAMIDO)PHTHALIMIDE	325
11	745	629	BUT-2-YNE-1,4-DIOL, O,O'-BIS(3-NITROBENZOYL)-	384
12	742	639	BENZOIC ACID, 3-NITRO-, (4-FORMYL-2-METHOXYPHENYL) ESTER	307
13	741	672	BENZALDEHYDE, 4-NITRO-	151
14	733	534	2-CYCLOHEXENE-1,4-DIONE, 5,6-DICHLORO-3-ISOPROPYL-6-METHYL-, 1-OXIME, O	398
15	729	458	O-NITROBENZALDOXIME-O-METHYL ETHER	180
16	728	642	BENZAMIDE, 2-NITRO-N-(3-PYRIDYL)-	243
17	727	594	2,5-CYCLOHEXADIENE-1,4-DIONE, 3-CHLORO-5-ISOPROPYL-2-METHYL-, 1-OXIME,	362
18	726	630	O-NITROBENZOYL CHLORIDE	185
19	725	631	BENZAMIDE, 3-NITRO-N-(2-HYDROXY-4-NITROPHENYL)-	303
20	716	605	BENZAMIDE, N-(4-CYANOMETHYLPHENYL)-2-NITRO-	287

, 03-Jan-2014 + 12:07:42

ALD 6 1187 (8.936)



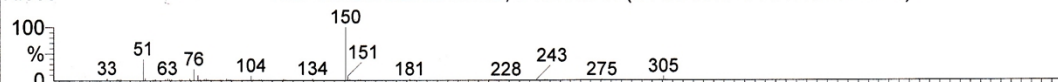
R:872 Nist 96947: BENZOIC ACID, 2-NITRO-, METHYL ESTER

Hit 1



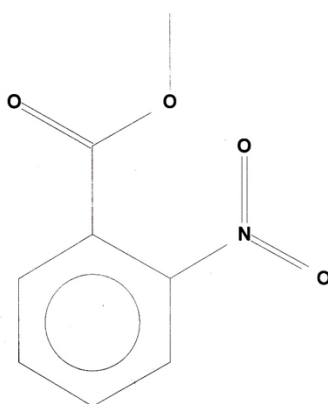
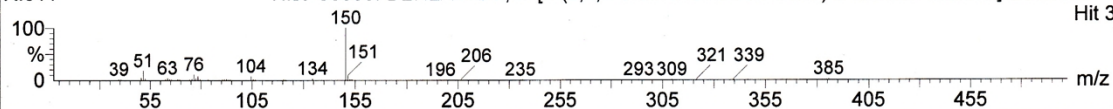
R:835 Nist 96829: BENZAMIDE, 2-NITRO-N-(2-FLUORO-5-NITROPHENYL)-

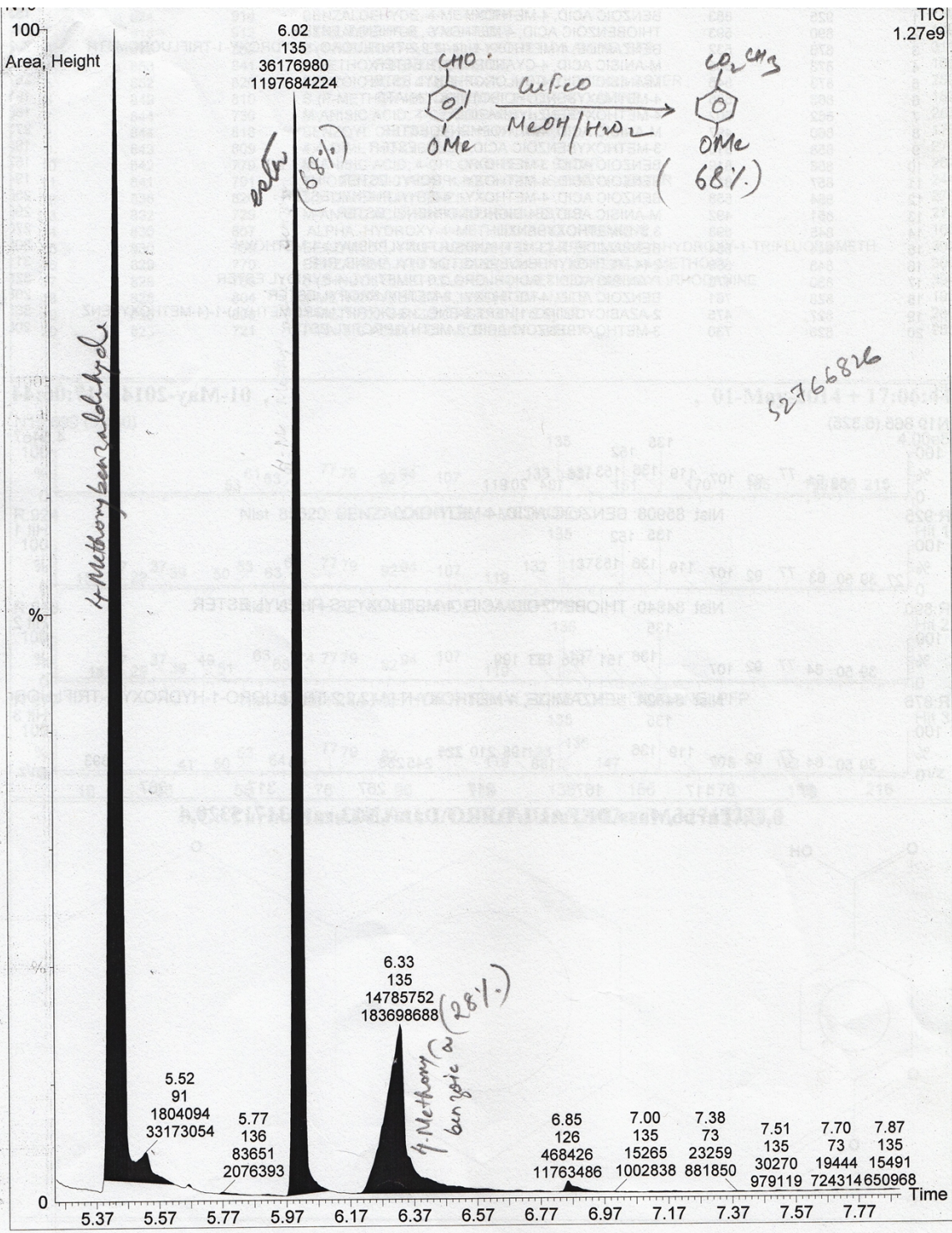
Hit 2



R:811 Nist 96830: BENZAMIDE, N-[3-(2,2,2-TRIFLUOROETHOXY)-5-NITROPHENYL]-2-NITRO-

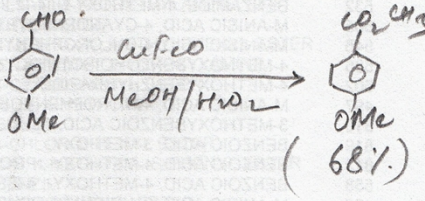
Hit 3





4-Methoxybenzaldehyde

6.02
135
36176980
1197684224
68%



6.33
135
14785752
183698688
4-Methoxybenzoate (28%)

52766826

TIC
1.27e9

S PRAT

Hit	REV	for	Compound Name	
1	925	883	BENZOIC ACID, 4-METHOXY-	
2	890	593	THIOBENZOIC ACID, 4-METHOXY-, S-PHENYL ESTER	
3	876	532	BENZAMIDE, 4-METHOXY-N-[4-(2,2,2-TRIFLUORO-1-HYDROXY-1-TRIFLUOROMETH	
4	873	505	M-ANISIC ACID, 4-CYANOPHENYL ESTER	
5	873	545	M-ANISIC ACID, 4-CHLOROPHENYL ESTER	2
6	863	586	4-METHOXYBENZOYL ISOTHIOCYANATE	19
7	862	602	4-METHOXYBENZHYDRAZIDE	16
8	860	497	M-ANISIC ACID, 4-NITROPHENYL ESTER	27
9	858	810	3-METHOXYBENZOIC ACID, ALLYL ESTER	19
10	858	819	BENZOIC ACID, 3-METHOXY-	15
11	857	812	BENZOIC ACID, 4-METHOXY-, PROPYL ESTER	19
12	854	588	BENZOIC ACID, 4-METHOXY-, 4-ETHYLPHENYL ESTER	25
13	851	492	M-ANISIC ACID, 3,4-DICHLOROPHENYL ESTER	29
14	845	598	3,3'-DIMETHOXYBENZIL	27
15	844	564	BENZAMIDE, N-(3-METHANESULFONYLPHENYL)-4-METHOXY-	30
16	843	589	2-(4-METHOXYPHENYL)-2-KETOETHYLAMINE, PFP	31
17	830	473	P-ANISIC ACID 3,5-DICHLORO-2,6-DIMETHYL-4-PYRIDYL ESTER	32
18	828	761	BENZOIC ACID, 4-METHOXY-, 2-METHYLPROPYL ESTER	20
19	827	475	2-AZABICYCLO[2.2.1]HEPT-5-ENE, 3,3-DI(TRIFLUOROMETHYL)-1-(4-METHOXYBENZ	36
20	825	730	3-METHOXYBENZOIC ACID, 2-METHYLPROPYL ESTER	20

, 01-May-2014 + 17:06:44

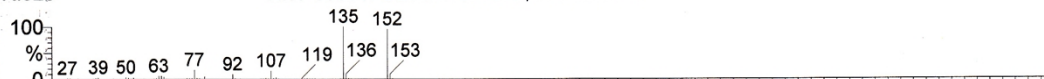
N19 865 (6.325)

4.54e7



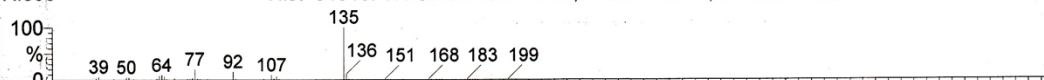
R:925 Nist 85908: BENZOIC ACID, 4-METHOXY-

Hit 1



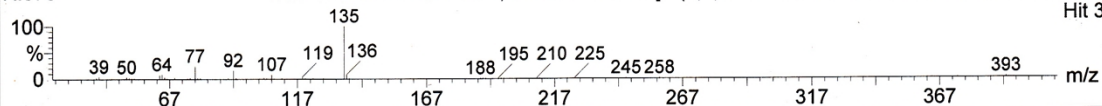
R:890 Nist 84840: THIOBENZOIC ACID, 4-METHOXY-, S-PHENYL ESTER

Hit 2

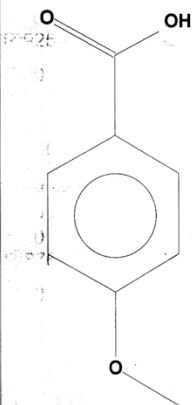


R:876 Nist 84824: BENZAMIDE, 4-METHOXY-N-[4-(2,2,2-TRIFLUORO-1-HYDROXY-1-TRIFLUORO

Hit 3



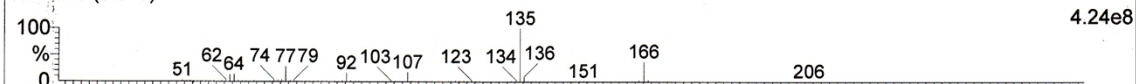
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Hit	REV	for	Compound Name	M.V
1	958	938	BENZOIC ACID, 4-METHOXY-, METHYL ESTER	166
2	933	875	M-ANISIC HYDRAZIDE	166
3	930	889	BENZOIC ACID, 3-METHOXY-, METHYL ESTER	166
4	926	716	M-ANISIC ACID, 4-CHLOROPHENYL ESTER	282
5	922	740	S-(P-METHOXYBENZOYL)THIOHYDROXYLAMINE	183
6	922	896	4-METHOXYBENZHYDRAZIDE	166
7	918	746	BENZOIC ACID, 4-METHOXY-, 4-ETHYLPHENYL ESTER	256
8	917	703	BENZAMIDE, 4-METHOXY-N-[4-(2,2,2-TRIFLUORO-1-HYDROXY-1-TRIFLUOROMETH	393
9	915	743	3,3'-DIMETHOXYBENZIL	270
10	914	718	5-(3-INDOLYLMETHYLENE)-3-(4-METHOXYBENZOYL)RHODANINE	394
11	912	734	BENZOYL CHLORIDE, 4-METHOXY-	170
12	912	878	.ALPHA.-HYDROXY-4'-METHOXYACETOPHENONE	166
13	911	743	2-(4-METHOXYPHENYL)-2-KETOETHYLAMINE, PFP	311
14	911	743	4-METHOXYBENZOIC ACID ANHYDRIDE	286
15	905	735	1-PROPANONE, 1-(3-METHOXYPHENYL)-	164
16	904	684	M-ANISIC ACID, 4-CYANOPHENYL ESTER	253
17	904	731	4-METHOXYBENZOYL ISOTHIOCYANATE	193
18	892	668	M-ANISIC ACID, 4-NITROPHENYL ESTER	273
19	892	700	THIOBENZOIC ACID, 4-METHOXY-, S-PHENYL ESTER	244
20	886	669	4-METHOXYBENZOIC ACID, 2,6-DIMETHYL-4-(2,2,2-TRIFLUORO-1-HYDROXY-1-TRIF	422

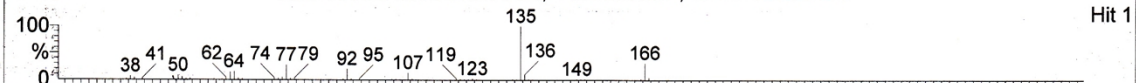
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N19 803 (6.015)



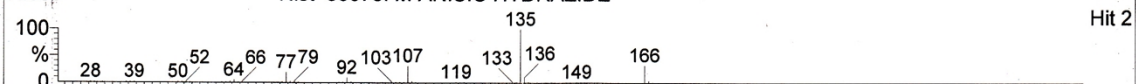
R:958 Nist 86068: BENZOIC ACID, 4-METHOXY-, METHYL ESTER

Hit 1



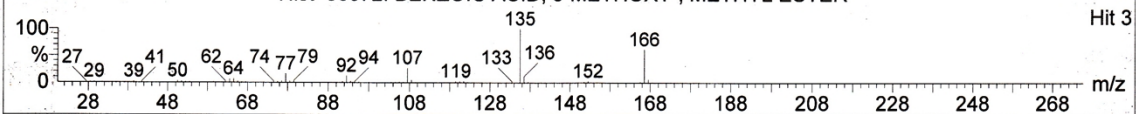
R:933 Nist 86073: M-ANISIC HYDRAZIDE

Hit 2

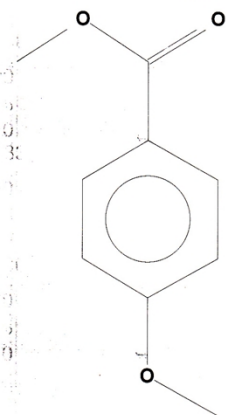


R:930 Nist 86072: BENZOIC ACID, 3-METHOXY-, METHYL ESTER

Hit 3

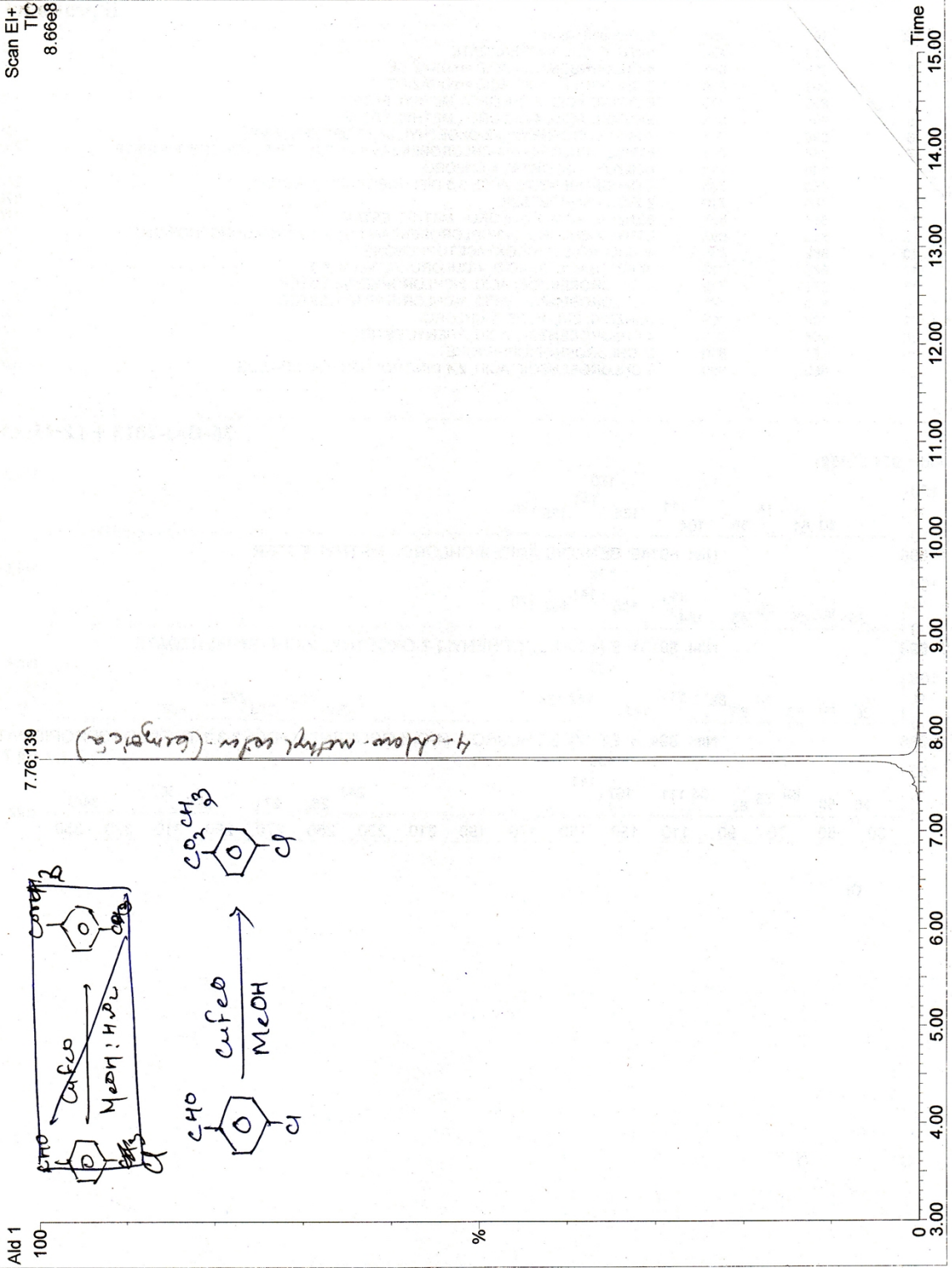


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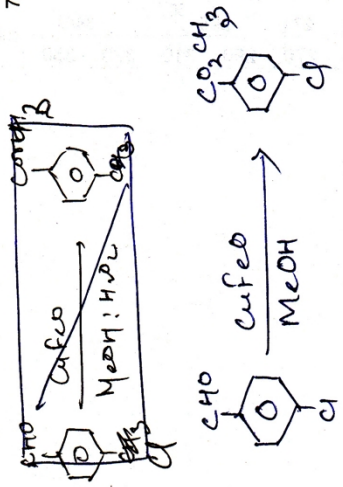


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TIC
8.66e8



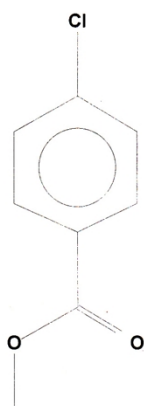
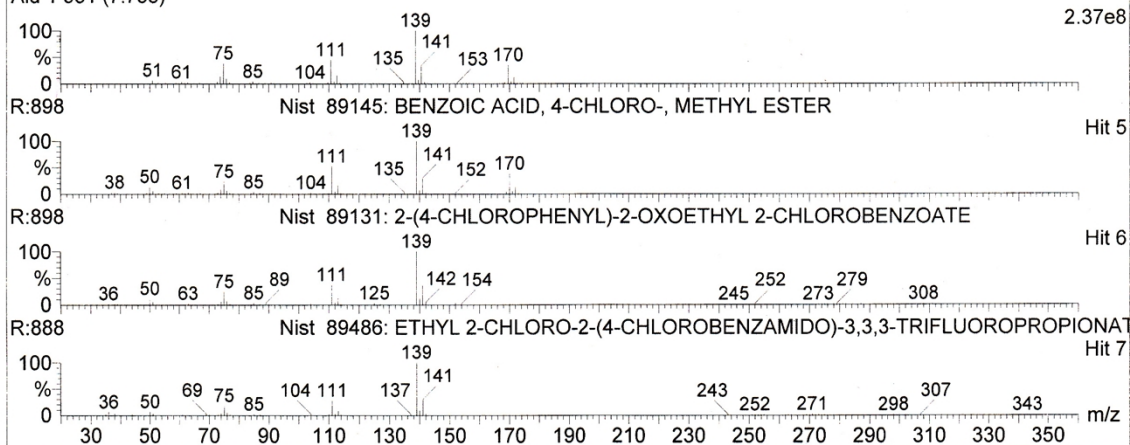
7.76139
4-methoxy-methyl-ester (cempicid)



Hit	REV	for	Compound Name	M.V
1	913	750	VINYL O-CHLOROBENZOATE	182
2	909	851	4-CHLOROBENZOIC ACID HYDRAZIDE	170
3	903	850	2-CHLOROBENZOIC ACID HYDRAZIDE	170
4	899	853	BENZOIC ACID, 3-CHLORO-, METHYL ESTER	170
5	898	851	BENZOIC ACID, 4-CHLORO-, METHYL ESTER	170
6	898	706	2-(4-CHLOROPHENYL)-2-OXOETHYL 2-CHLOROBENZOATE	308
7	888	701	ETHYL 2-CHLORO-2-(4-CHLOROBENZAMIDO)-3,3,3-TRIFLUOROPROPIONATE	343
8	886	728	BENZOYL CHLORIDE, 4-CHLORO-	174
9	886	735	4-CHLOROBENZOIC ACID, 3,5-DIFLUOROPHENYL ESTER	268
10	885	710	2,2'-DICHLOROBENZIL	278
11	884	828	BENZOIC ACID, 2-CHLORO-, METHYL ESTER	170
12	883	693	ETHYL 2-CHLORO-2-(3-CHLOROBENZAMIDO)-3,3,3-TRIFLUOROPROPIONATE	343
13	882	836	4'-CHLORO-2-HYDROXYACETOPHENONE	170
14	876	713	BENZENEACETIC ACID, 4-CHLORO-.ALPHA.-OXO-	184
15	872	718	4-CHLOROBENZOIC ACID, 2-CHLOROPHENYL ESTER	268
16	870	725	2-CHLOROBENZOIC ACID, 2-CHLOROPHENYL ESTER	268
17	865	709	BENZOYL CHLORIDE, 2-CHLORO-	174
18	864	713	4-CHLOROBENZOIC ACID, PHENYL ESTER	232
19	861	810	M-CHLOROPROPIOPHENONE	168
20	859	695	4-CHLOROBENZOIC ACID, 2,4-DINITROPHENYLHYDRAZIDE	338

, 26-Dec-2013 + 12:43:43

Ald 1 951 (7.755)



, 02-May-2014 + 11:34:02

Scan EI+
TIC
1.46e9

N27
100

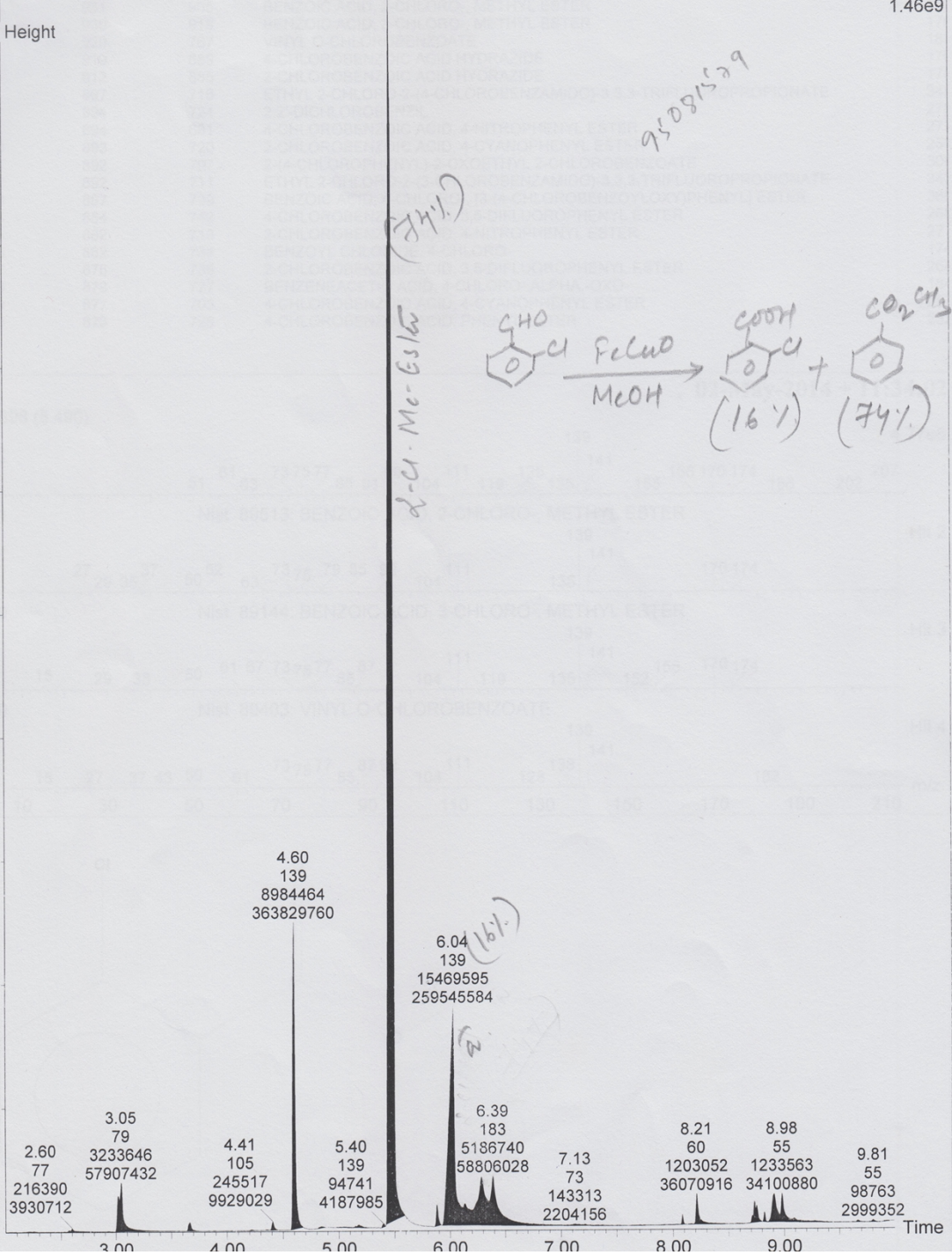
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Area, Height

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Time

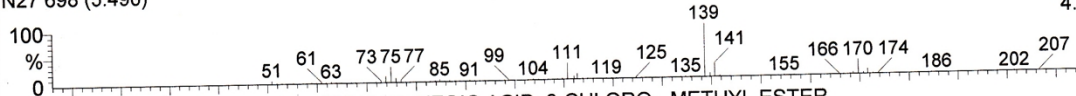


Hit	REV	for	Compound Name	M.V
1	936	921	BENZOIC ACID, 4-CHLORO-, METHYL ESTER	170
2	931	905	BENZOIC ACID, 2-CHLORO-, METHYL ESTER	170
3	930	918	BENZOIC ACID, 3-CHLORO-, METHYL ESTER	170
4	920	767	VINYL O-CHLOROBENZOATE	182
5	919	889	4-CHLOROBENZOIC ACID HYDRAZIDE	170
6	912	885	2-CHLOROBENZOIC ACID HYDRAZIDE	170
7	897	716	ETHYL 2-CHLORO-2-(4-CHLOROBENZAMIDO)-3,3,3-TRIFLUOROPROPIONATE	343
8	894	724	2,2'-DICHLOROBENZIL	278
9	894	681	4-CHLOROBENZOIC ACID, 4-NITROPHENYL ESTER	271
10	893	720	2-CHLOROBENZOIC ACID, 4-CYANOPHENYL ESTER	251
11	892	707	2-(4-CHLOROPHENYL)-2-OXOETHYL 2-CHLOROBENZOATE	308
12	892	711	ETHYL 2-CHLORO-2-(3-CHLOROBENZAMIDO)-3,3,3-TRIFLUOROPROPIONATE	343
13	887	739	BENZOIC ACID, 4-CHLORO-, [3-(4-CHLOROBENZOYLOXY)PHENYL] ESTER	386
14	884	742	4-CHLOROBENZOIC ACID, 3,5-DIFLUOROPHENYL ESTER	266
15	882	713	2-CHLOROBENZOIC ACID, 4-NITROPHENYL ESTER	271
16	882	734	BENZOYL CHLORIDE, 4-CHLORO-	174
17	878	736	2-CHLOROBENZOIC ACID, 3,5-DIFLUOROPHENYL ESTER	266
18	878	727	BENZENEACETIC ACID, 4-CHLORO-ALPHA-OXO-	184
19	877	703	4-CHLOROBENZOIC ACID, 4-CYANOPHENYL ESTER	251
20	873	728	4-CHLOROBENZOIC ACID, PHENYL ESTER	232

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N27 698 (5.490)

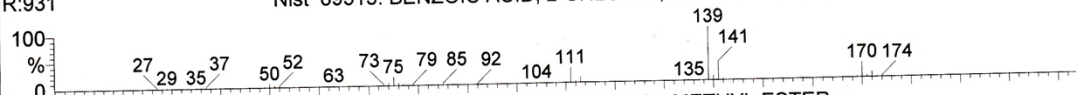
4.77e8



R:931

Nist 89513: BENZOIC ACID, 2-CHLORO-, METHYL ESTER

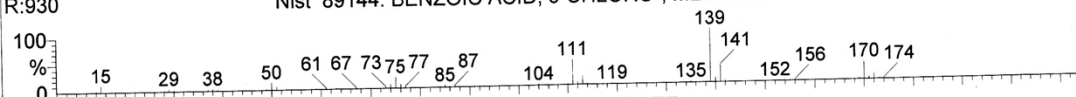
Hit 2



R:930

Nist 89144: BENZOIC ACID, 3-CHLORO-, METHYL ESTER

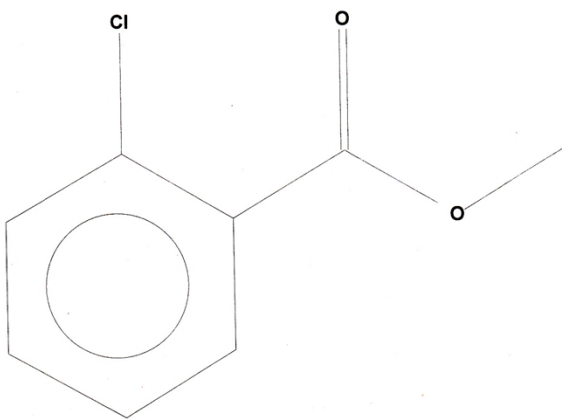
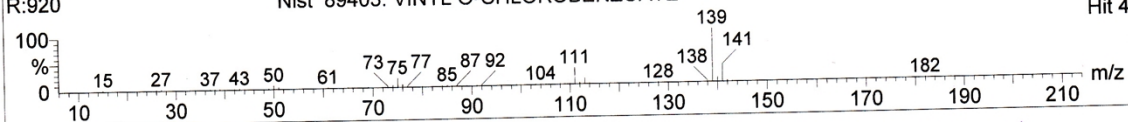
Hit 3



R:920

Nist 89403: VINYL O-CHLOROBENZOATE

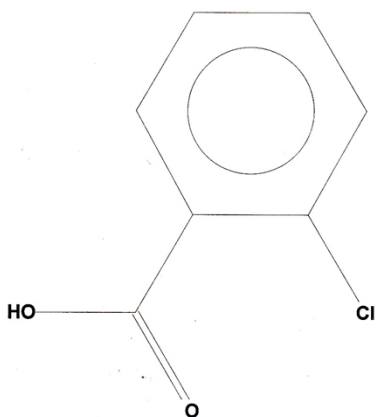
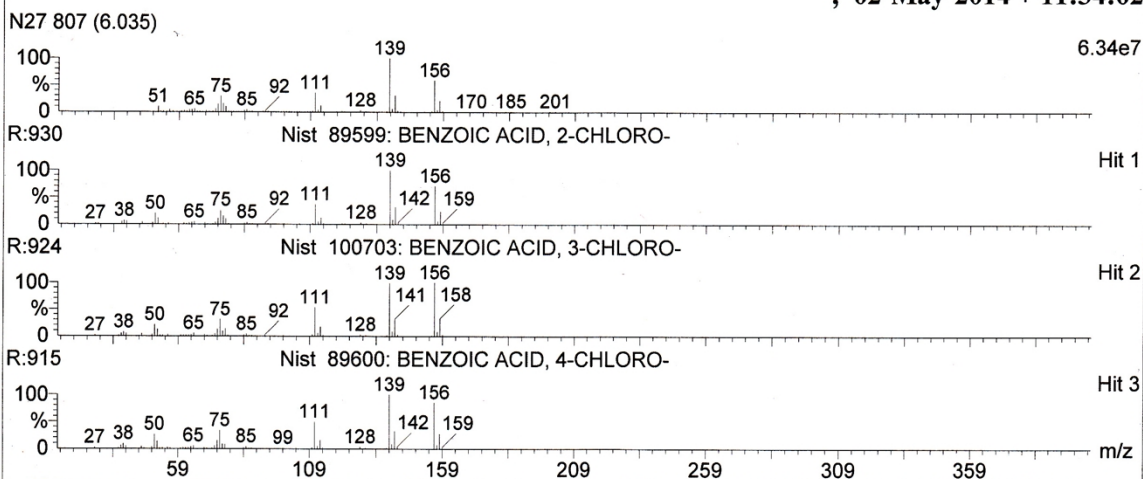
Hit 4



S PRATI HAR12

Hit	REV	for	Compound Name	M.V
1	930	917	BENZOIC ACID, 2-CHLORO-	156
2	924	914	BENZOIC ACID, 3-CHLORO-	156
3	915	904	BENZOIC ACID, 4-CHLORO-	156
4	901	857	3-(2-CHLORO-BENZOYL)-2-(2-DIETHYLAMINO-ETHYLSULFANYL)-6-HYDROXY-5-ISO	423
5	889	595	ETHYL 2-CHLORO-2-(3-CHLOROBENZAMIDO)-3,3,3-TRIFLUOROPROPIONATE	343
6	885	649	VINYL O-CHLOROBENZOATE	182
7	883	588	ETHYL 2-CHLORO-2-(4-CHLOROBENZAMIDO)-3,3,3-TRIFLUOROPROPIONATE	343
8	880	857	ANTHRANILIC ACID, N-(3-METHOXYPHENYL)-	243
9	878	577	2-(4-CHLOROPHENYL)-2-OXOETHYL 2-CHLOROBENZOATE	308
10	871	596	2,2'-DICHLOROBENZIL	278
11	867	591	2-CHLOROBENZOIC ACID, 4-CYANOPHENYL ESTER	257
12	865	537	7-[4-[1-(3-CHLOROBENZAMIDO)-1-ETHOXYCARBONYL-2,2,2-TRIFLUOROETHYL]-1-P	638
13	864	627	4'-CHLORO-2-HYDROXYACETOPHENONE	170
14	862	637	BENZOIC ACID, 2-CHLORO-, PHENYL ESTER	232
15	862	647	4-CHLOROBENZOIC ACID, 2-CHLOROPHENYL ESTER	268
16	862	635	4-CHLOROBENZOIC ACID, 3,5-DIFLUOROPHENYL ESTER	268
17	861	545	4-CHLOROBENZOIC ACID, 4-NITROPHENYL ESTER	277
18	859	631	BENZOYL CHLORIDE, 2-CHLORO-	174
19	857	617	BENZOIC ACID, 2-CHLORO-, 2-ACETYLPHENYL ESTER	274
20	857	537	BENZOIC ACID, 2-CHLORO-, [2-CHLORO-4-(2-CHLOROBENZOYLOXY)PHENYL]-EST	420

, 02-May-2014 + 11:34:02



References: