

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040423\
 Data File : BG056964.D
 Acq On : 4 Apr 2023 13:48
 Operator : CG/JU
 Sample : 02104-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB-2023-03-25

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056964.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.435	318	323	330	rBV	58288	90500	4.66%	1.423%
2	5.917	398	405	413	rVB	182033	289688	14.92%	4.555%
3	7.538	674	681	689	rBV	111332	189942	9.78%	2.987%
4	8.413	823	830	838	rVB	65403	106436	5.48%	1.674%
5	9.588	1021	1030	1038	rBV	230683	413816	21.32%	6.507%
6	11.256	1306	1314	1320	rBV	78451	143651	7.40%	2.259%
7	13.653	1715	1722	1729	rBV	649746	988804	50.94%	15.548%
8	13.888	1757	1762	1767	rBV2	23322	33910	1.75%	0.533%
9	15.028	1949	1956	1964	rVB2	137857	213076	10.98%	3.350%
10	16.508	2201	2208	2216	rBV	568825	862432	44.43%	13.561%
11	17.765	2416	2422	2430	rVB	202071	298751	15.39%	4.698%
12	20.338	2854	2860	2866	rBV	1523011	1941246	100.00%	30.525%
13	22.089	3152	3158	3169	rVB2	197601	347359	17.89%	5.462%
14	23.322	3360	3368	3375	rBV2	58592	113352	5.84%	1.782%
15	25.631	3750	3761	3774	rVB	105890	326648	16.83%	5.136%

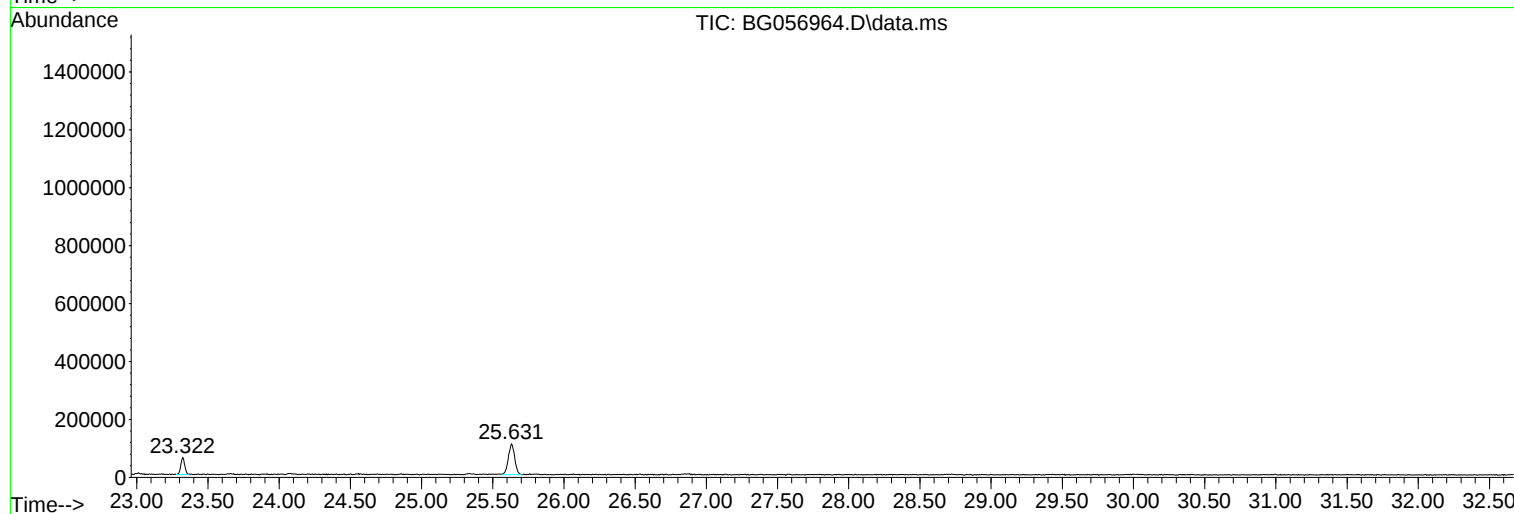
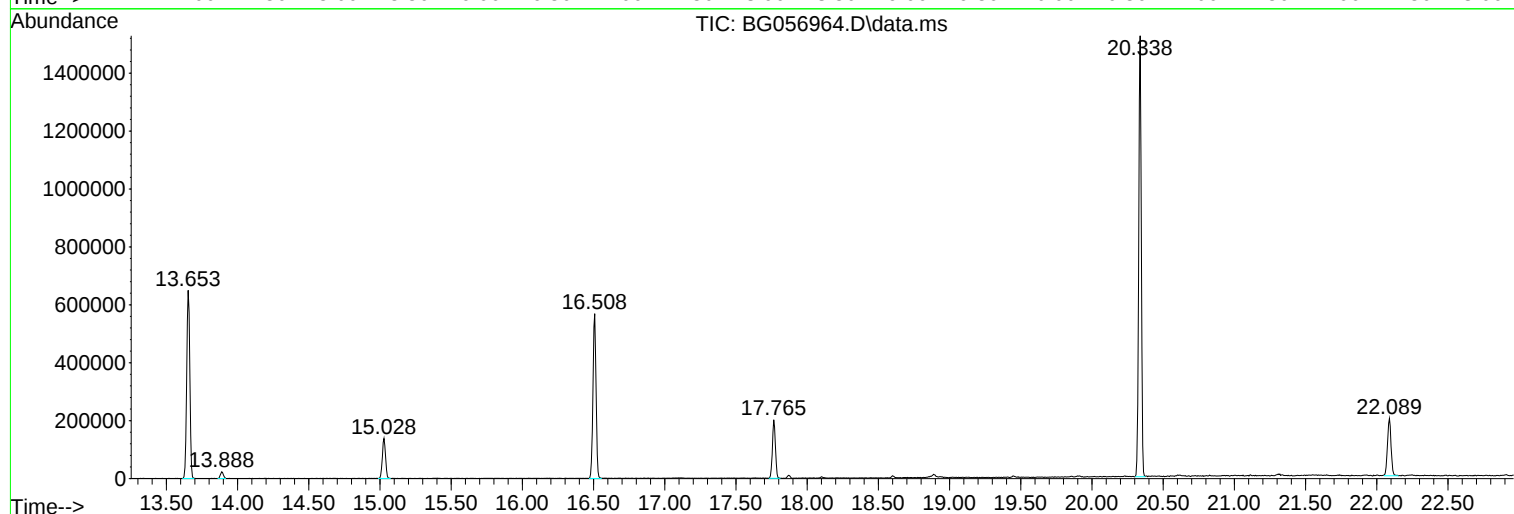
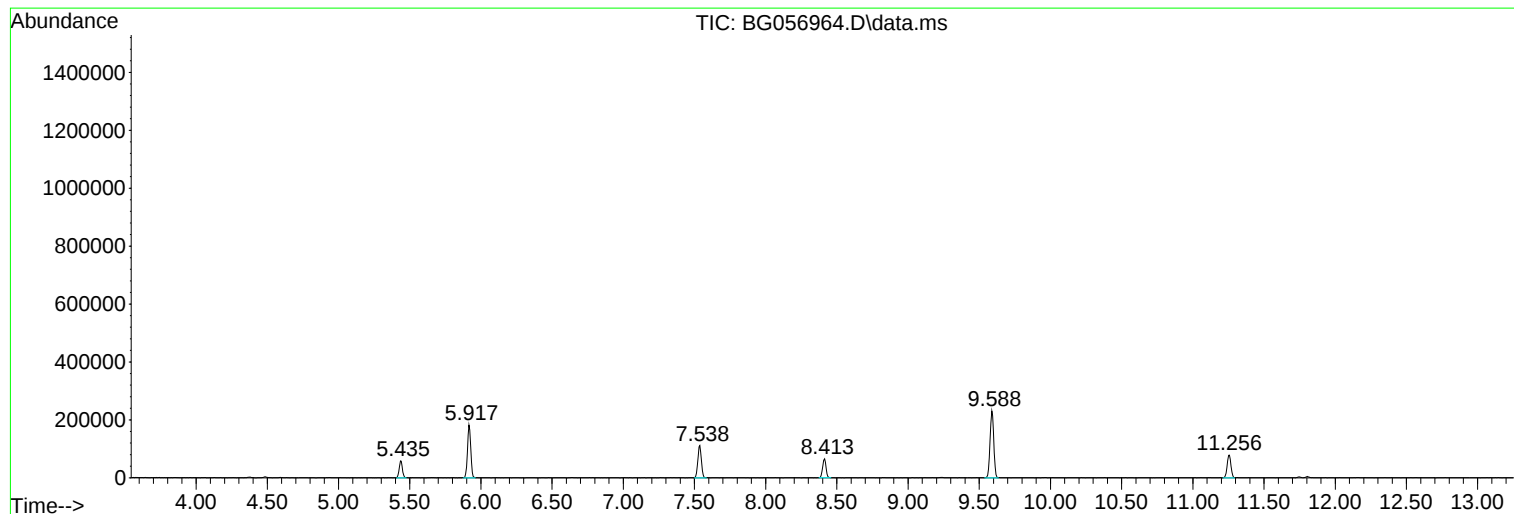
Sum of corrected areas: 6359611

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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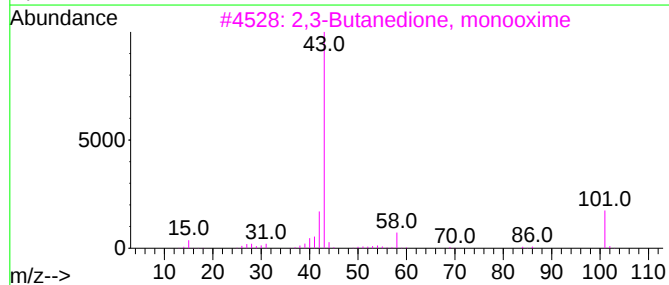
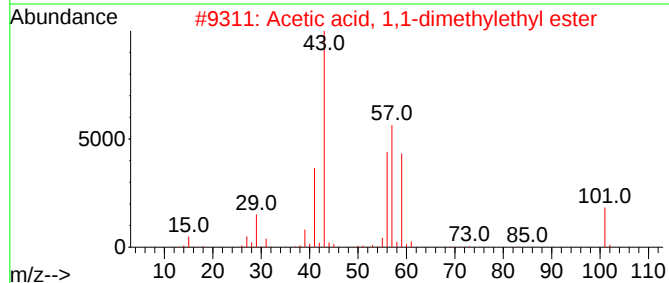
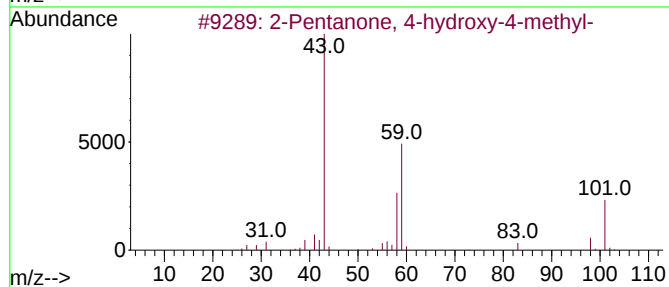
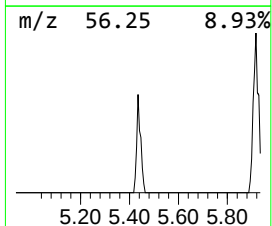
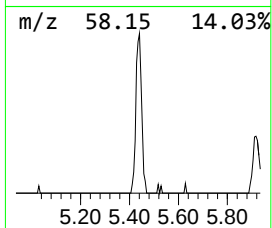
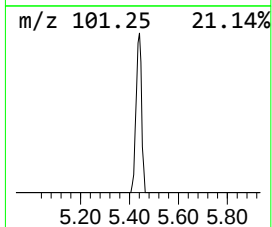
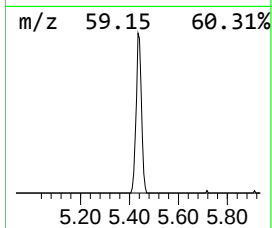
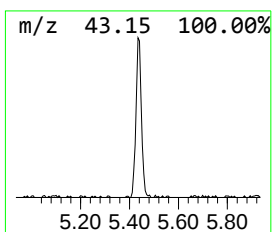
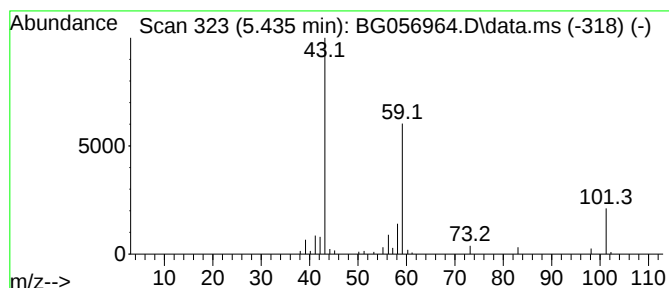
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.435	17.01 ng	90500	1,4-Dichlorobenzene-d4			8.413
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	35
4	5-Hexen-2-one		98	C6H10O	000109-49-9	10
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10



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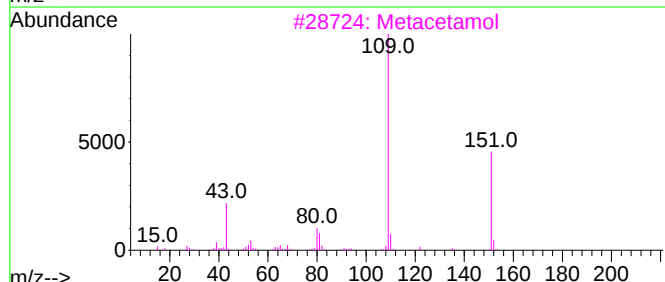
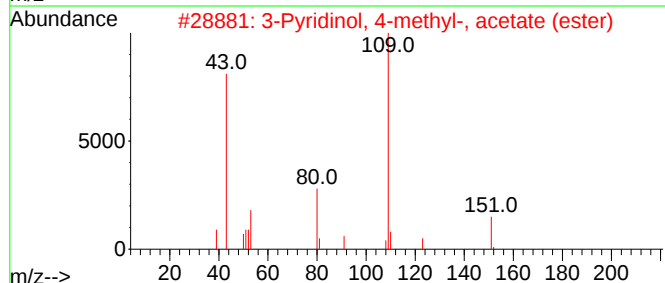
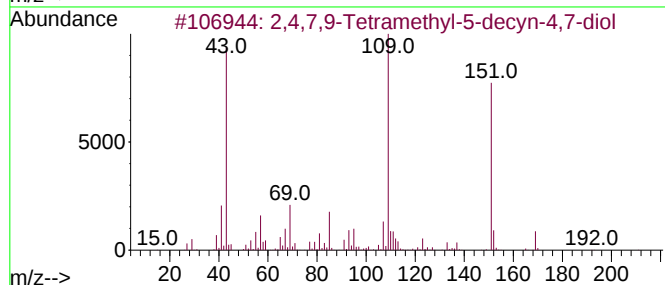
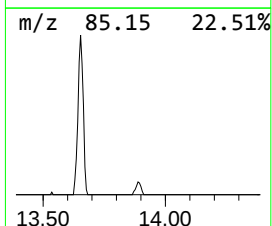
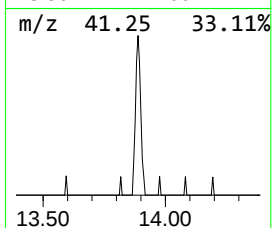
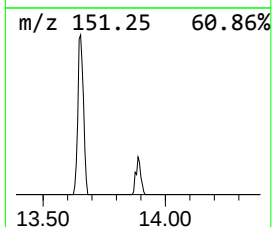
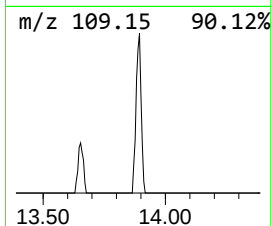
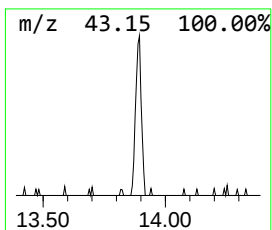
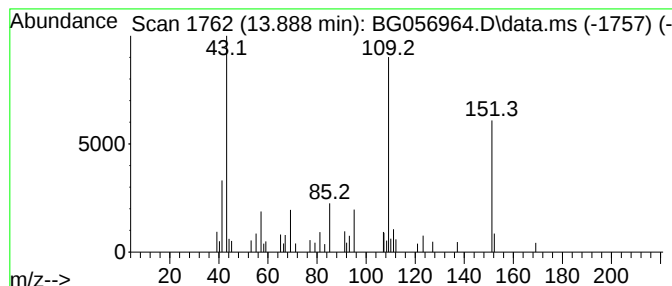
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.888	3.18 ng	33910	Acenaphthene-d10		15.028	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	64
2	3-Pyridinol, 4-methyl-, acetate ...		151	C8H9NO2	001006-96-8	47
3	Metacetamol		151	C8H9NO2	000621-42-1	47
4	m-Isopropoxyaniline		151	C9H13NO	041406-00-2	47
5	Pyridine, 3-butyl-, 1-oxide		151	C9H13NO	031396-33-5	38



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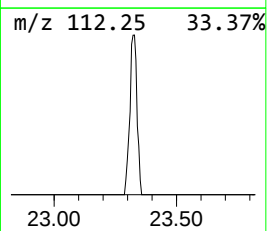
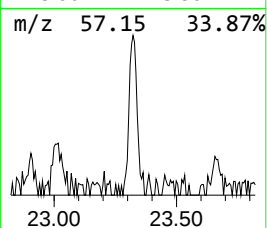
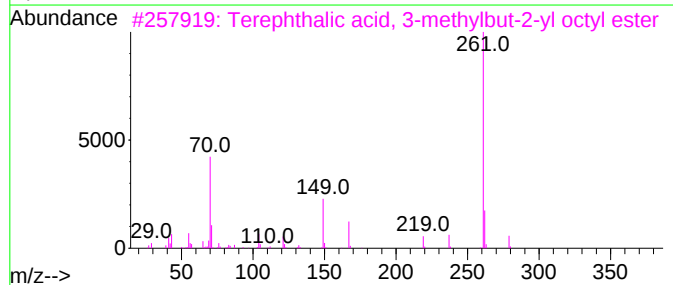
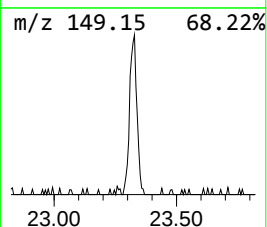
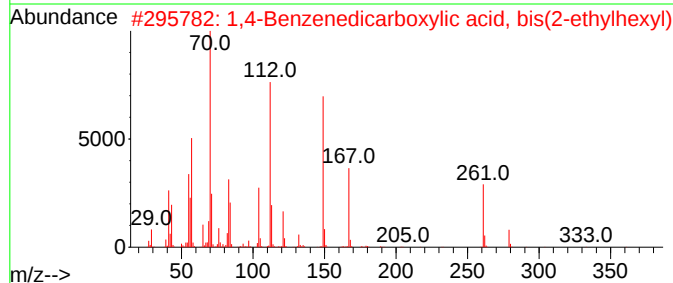
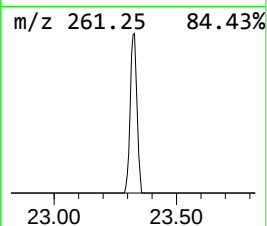
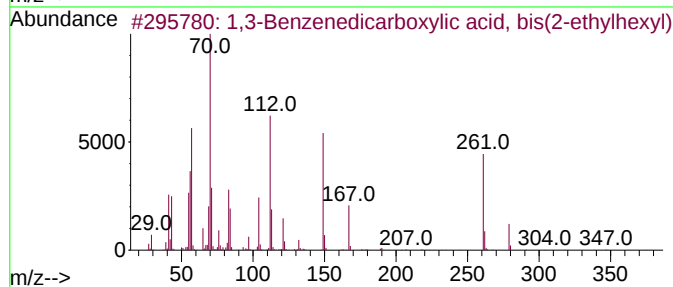
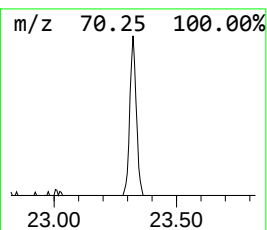
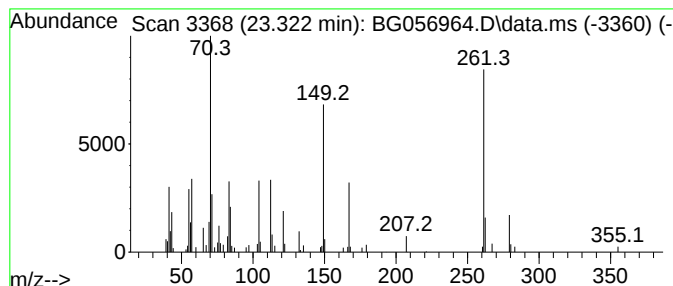
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Peak Number 3 1,3-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.322	6.53 ng	113352	Chrysene-d12	22.089

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	62
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	43
4			Isophthalic acid, 4-nitrophenyl ...	399	C22H25NO6	1000344-68-5	38
5			Isophthalic acid, 2,5-dichloroph...	422	C22H24Cl2O4	1000344-70-4	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.435	17.0	ng	90500	1	8.413	106436	20.0
2,4,7,9-Tetrame...	13.888	3.2	ng	33910	3	15.028	213076	20.0
1,3-Benzenedica...	23.322	6.5	ng	113352	5	22.089	347359	20.0