

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082622\
 Data File : BG054759.D
 Acq On : 26 Aug 2022 17:22
 Operator : CG/JU
 Sample : N4371-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A4127

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.209	322	327	336	rBV	30052	49210	1.18%	0.327%
2	5.685	400	408	419	rBV	445608	714094	17.10%	4.744%
3	7.289	674	681	693	rVB	322552	542365	12.99%	3.603%
4	8.147	820	827	835	rBV	153652	268518	6.43%	1.784%
5	9.322	1019	1027	1040	rBV	576616	1038923	24.88%	6.902%
6	10.979	1301	1309	1316	rBV	214408	390244	9.35%	2.593%
7	11.913	1462	1468	1476	rVB2	34319	55709	1.33%	0.370%
8	13.411	1714	1723	1735	rBV	1575995	2560106	61.32%	17.009%
9	14.780	1950	1956	1967	rVB	354530	574165	13.75%	3.815%
10	16.267	2201	2209	2222	rBV	1291887	2005885	48.05%	13.327%
11	17.530	2417	2424	2434	rBV	477454	734102	17.58%	4.877%
12	18.394	2564	2571	2580	rBV3	28742	60155	1.44%	0.400%
13	20.133	2860	2867	2882	rBV	3007799	4174983	100.00%	27.737%
14	21.437	3084	3089	3102	rBV	70697	141404	3.39%	0.939%
15	21.819	3147	3154	3164	rBV2	462195	793356	19.00%	5.271%
16	25.186	3716	3727	3742	rBV	274817	851736	20.40%	5.659%
17	26.419	3929	3937	3946	rBV4	16153	48538	1.16%	0.322%
18	27.859	4173	4182	4195	rBV5	13144	48338	1.16%	0.321%

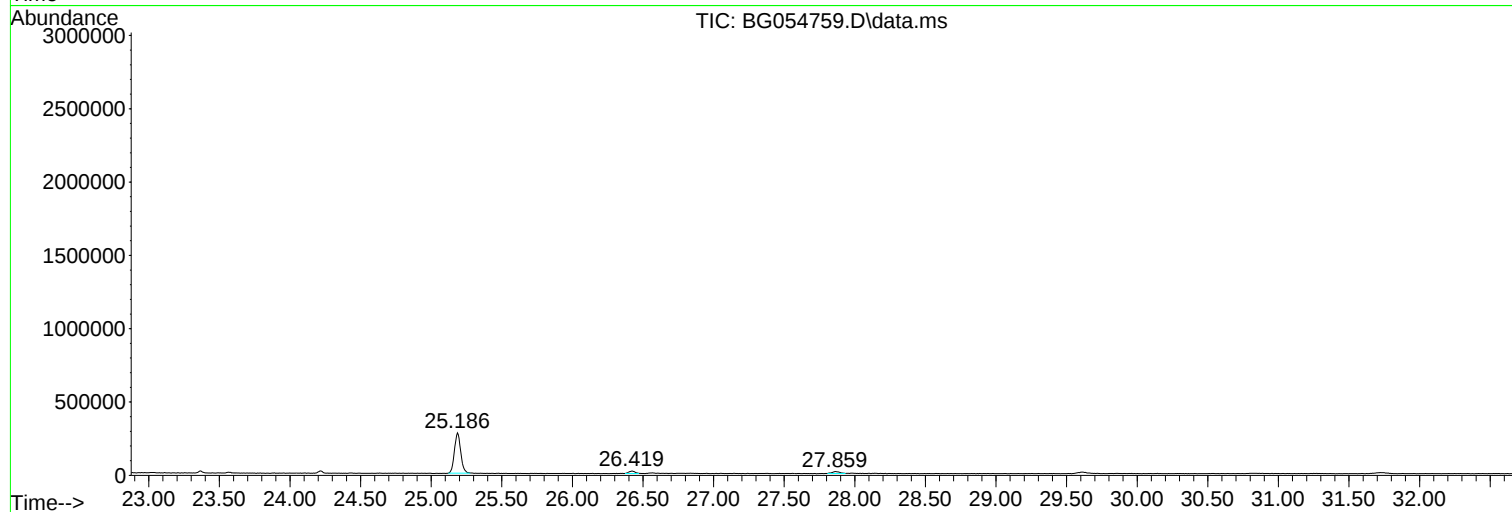
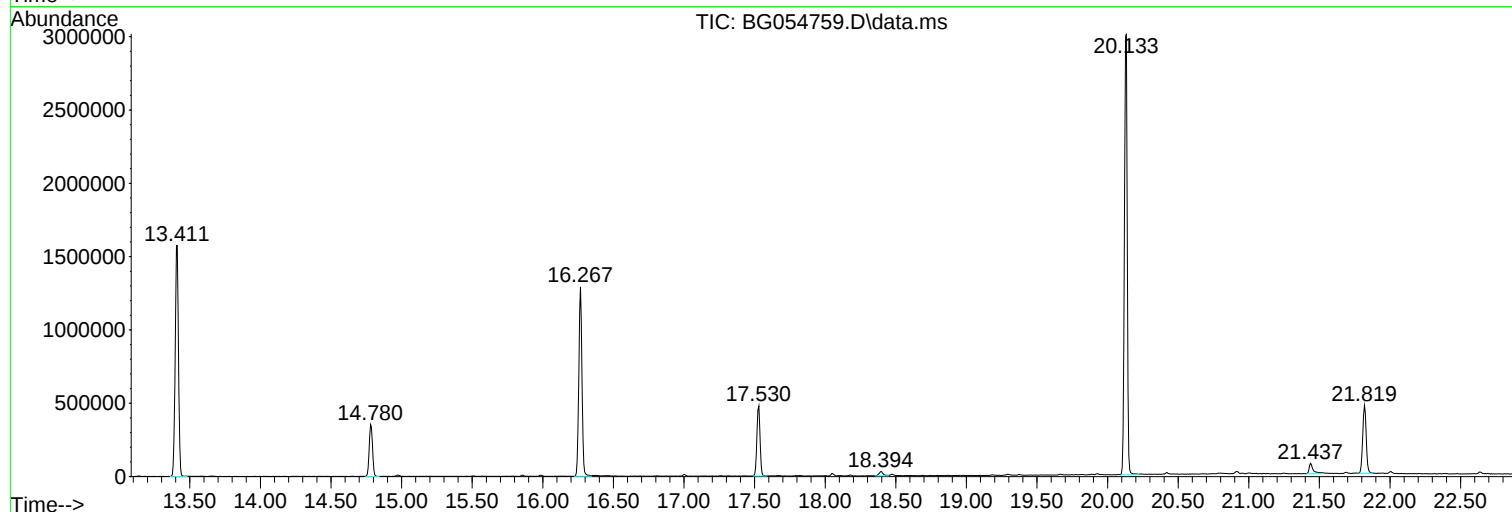
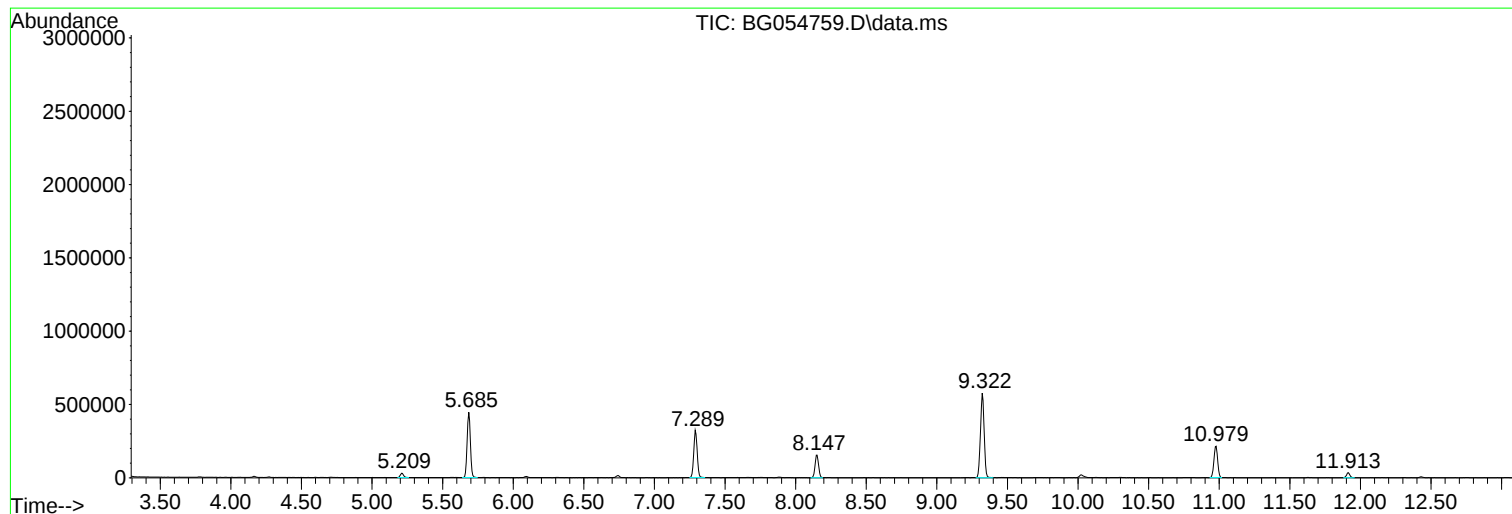
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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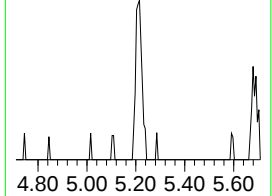
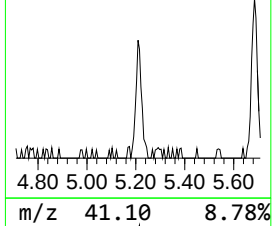
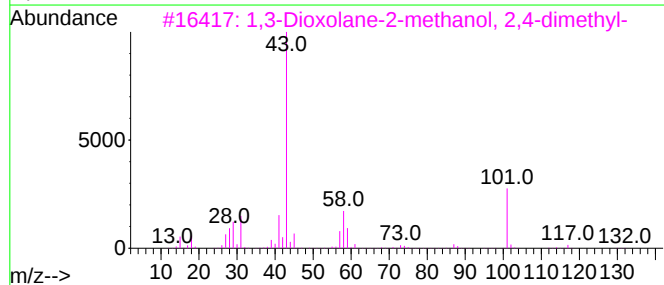
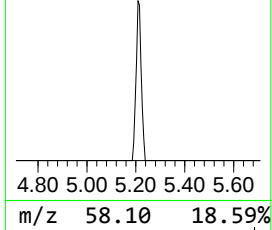
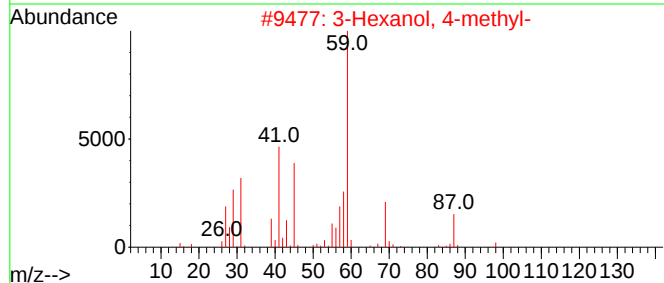
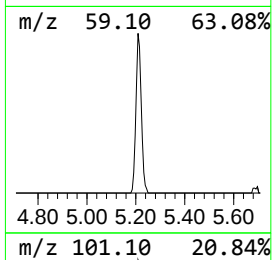
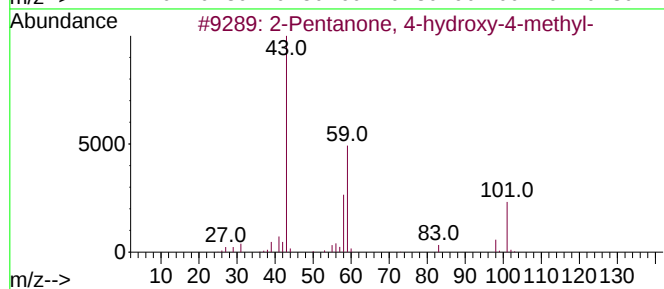
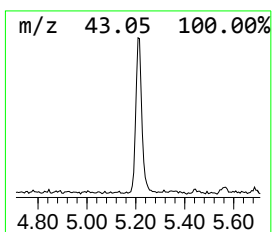
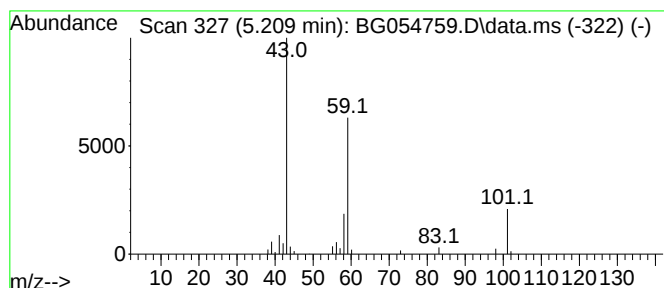
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.209	3.67 ng	49210	1,4-Dichlorobenzene-d4	8.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
3			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12



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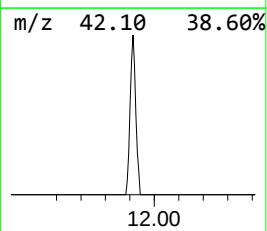
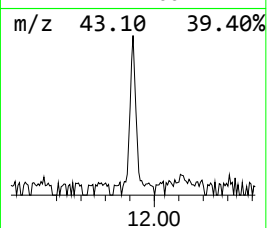
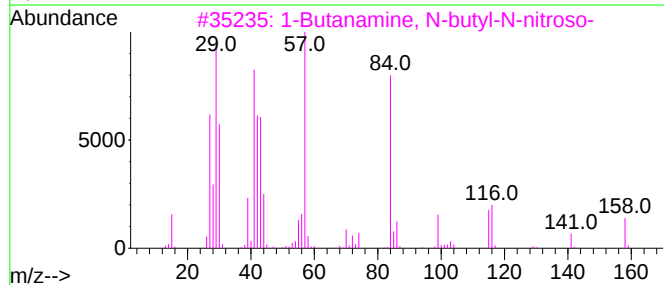
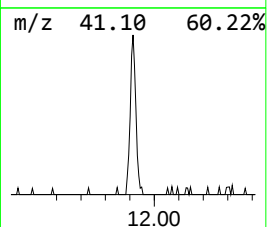
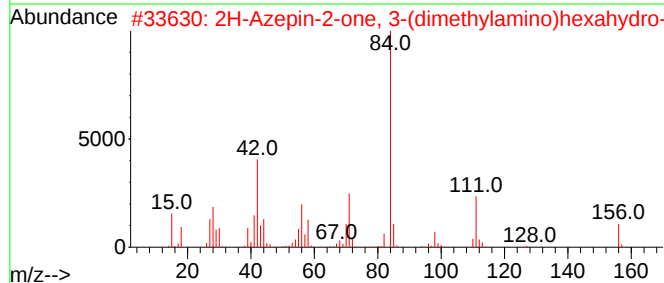
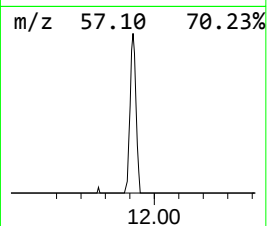
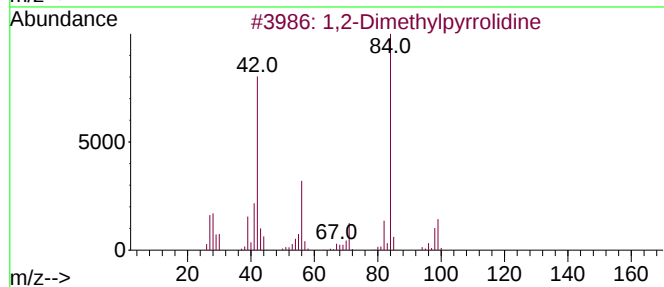
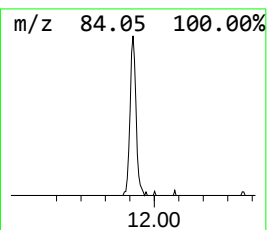
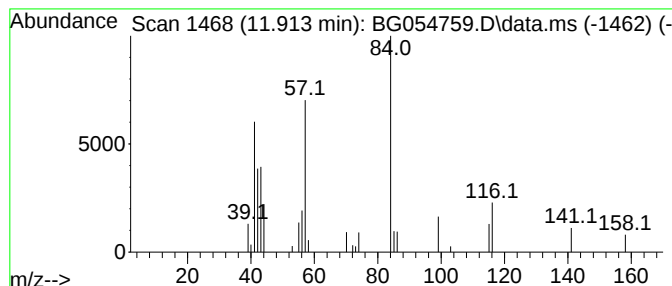
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Peak Number 2 1,2-Dimethylpyrrolidine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.913	2.86 ng	55709	Naphthalene-d8	10.979

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dimethylpyrrolidine	99	C6H13N	1000326-00-9	53
2			2H-Azepin-2-one, 3-(dimethylamin...	156	C8H16N2O	070394-23-9	53
3			1-Butanamine, N-butyl-N-nitroso-	158	C8H18N2O	000924-16-3	49
4			N-Ethylidene t-butylamine	99	C6H13N	007020-80-6	47
5			Pelletierine	141	C8H15NO	004396-01-4	43



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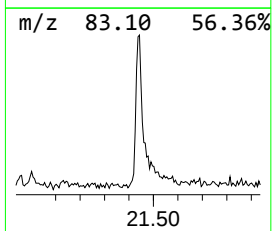
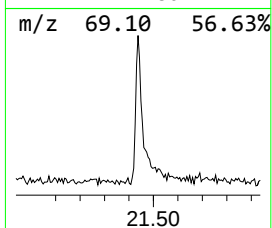
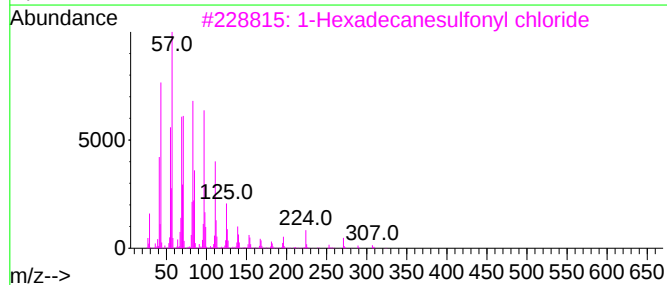
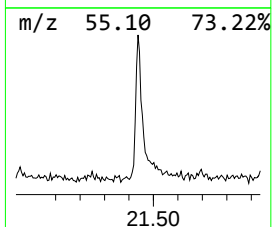
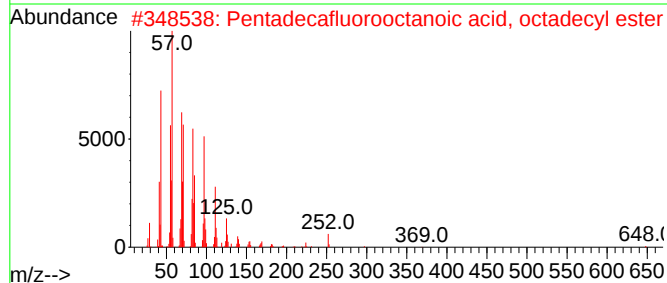
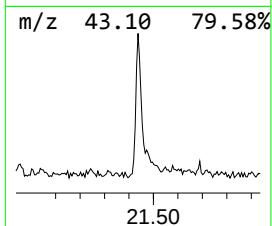
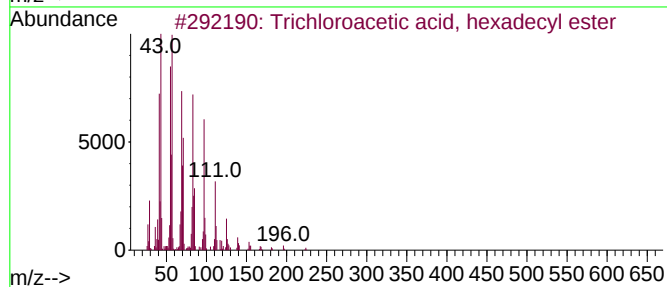
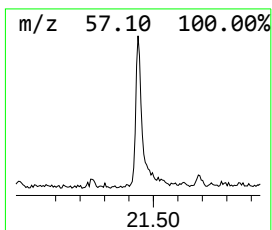
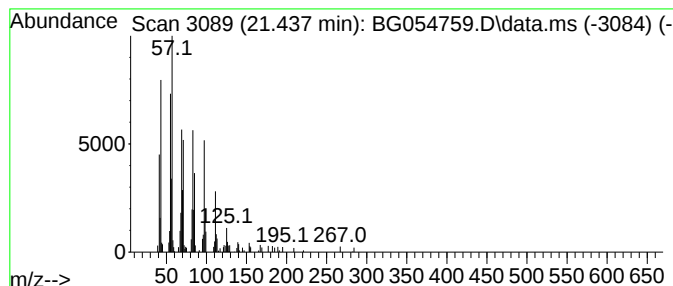
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Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.437	3.56 ng	141404	Chrysene-d12	21.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.209	3.7	ng	49210	1	8.153	268518	20.0
1,2-Dimethylpyr...	11.913	2.9	ng	55709	2	10.979	390244	20.0
Trichloroacetic...	21.437	3.6	ng	141404	5	21.819	793356	20.0