

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042021\
 Data File : BG048805.D
 Acq On : 20 Apr 2021 22:13
 Operator : CG/JU
 Sample : M2076-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-14-0-2.0

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-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.606	378	386	396	rBV	244205	399181	30.83%	7.095%
2	6.729	573	577	583	rVB2	11038	16363	1.26%	0.291%
3	7.222	653	661	672	rVB	266796	449419	34.71%	7.988%
4	8.062	797	804	814	rVB2	62992	107112	8.27%	1.904%
5	9.232	993	1003	1009	rBV	166109	291199	22.49%	5.176%
6	10.888	1279	1285	1294	rVB	83060	146193	11.29%	2.598%
7	13.339	1694	1702	1711	rBV	440565	652535	50.40%	11.598%
8	14.161	1838	1842	1847	rBV2	12552	16326	1.26%	0.290%
9	14.719	1929	1937	1944	rVB2	145317	221160	17.08%	3.931%
10	16.212	2184	2191	2199	rBV	414340	629841	48.65%	11.194%
11	17.475	2400	2406	2413	rBV	215676	315745	24.39%	5.612%
12	18.362	2552	2557	2565	rBV3	35699	60331	4.66%	1.072%
13	19.631	2766	2773	2776	rBV4	12283	18466	1.43%	0.328%
14	19.901	2814	2819	2823	rBV4	9597	18284	1.41%	0.325%
15	20.089	2845	2851	2857	rVB	1069711	1294625	100.00%	23.010%
16	20.871	2977	2984	2987	rBV6	12263	19925	1.54%	0.354%
17	21.388	3067	3072	3084	rBV4	75855	133414	10.31%	2.371%
18	21.488	3084	3089	3096	rVB4	11595	19478	1.50%	0.346%
19	21.776	3130	3138	3144	rBV	217785	370025	28.58%	6.577%
20	22.587	3271	3276	3277	rBV5	11365	17240	1.33%	0.306%
21	23.297	3388	3397	3402	rBV9	11288	25670	1.98%	0.456%
22	24.126	3534	3538	3546	rVB9	17004	36097	2.79%	0.642%
23	25.095	3693	3703	3714	rBV2	127136	367818	28.41%	6.537%

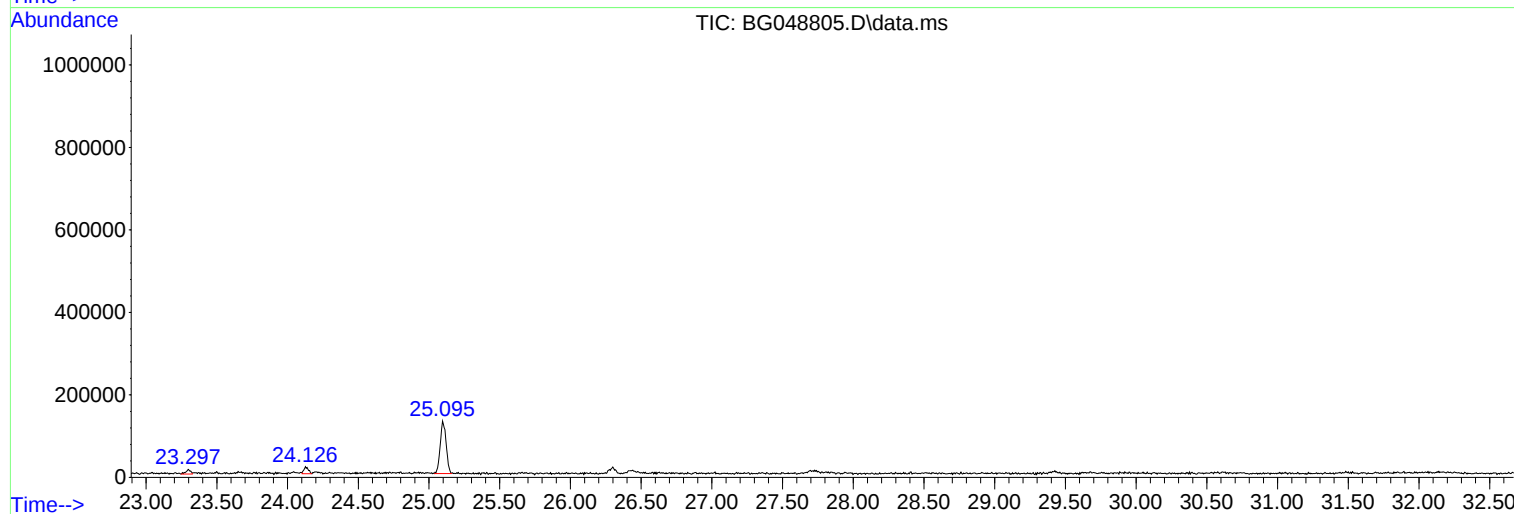
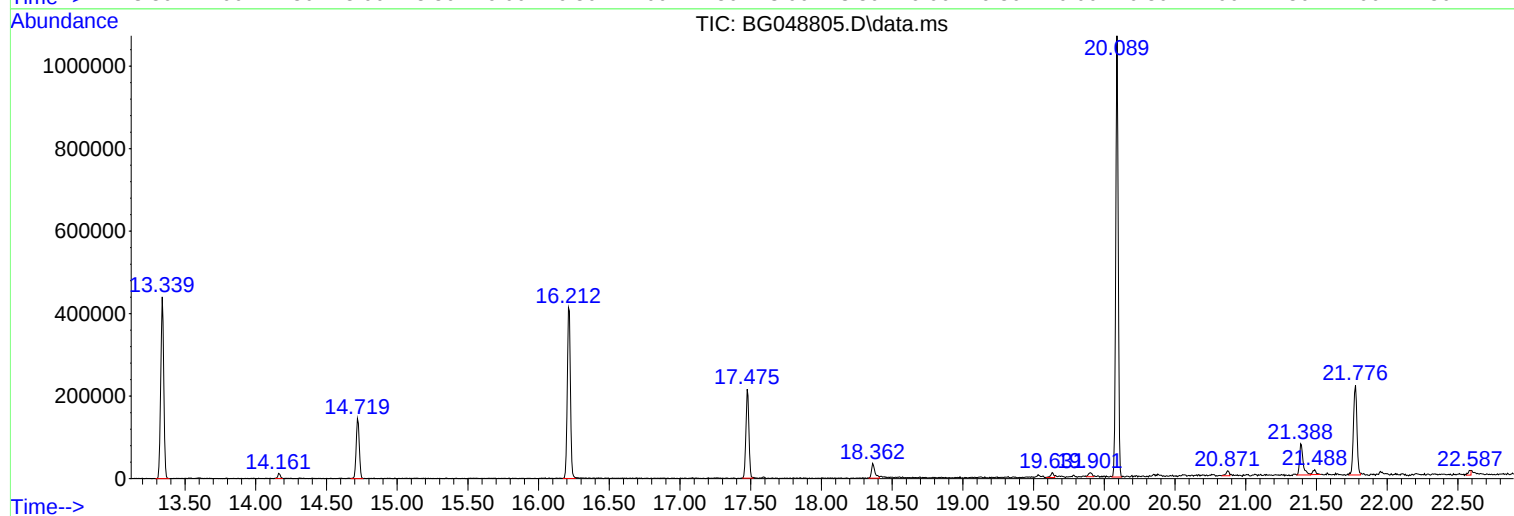
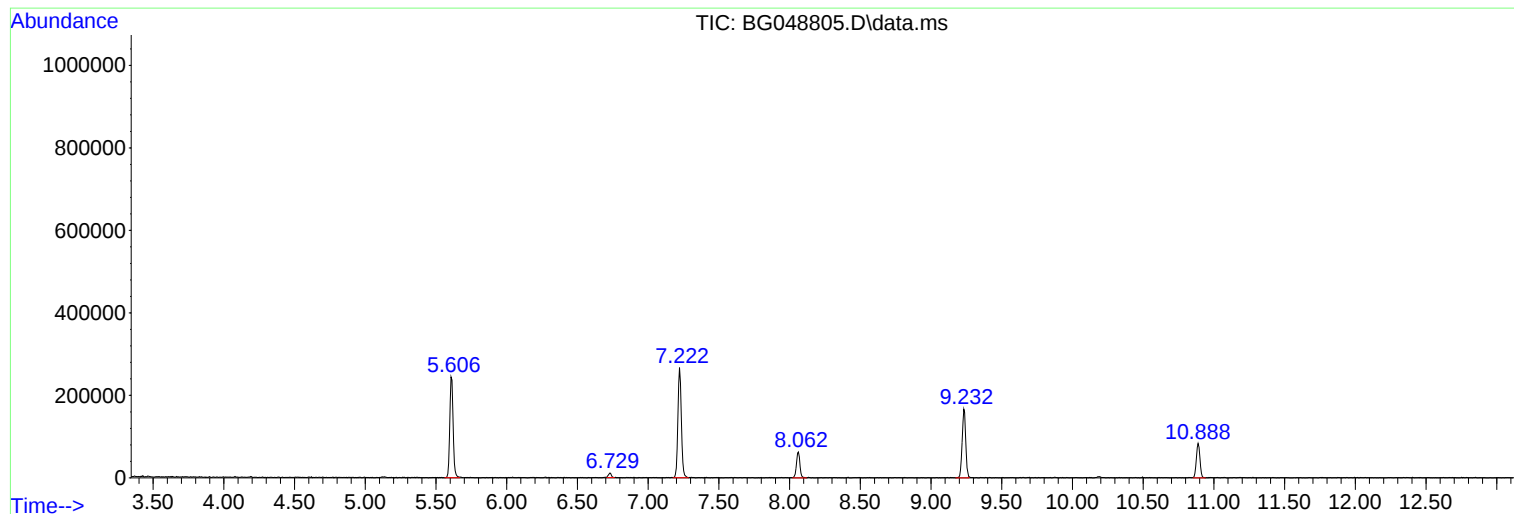
Sum of corrected areas: 5626447

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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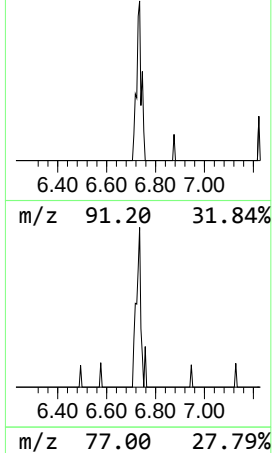
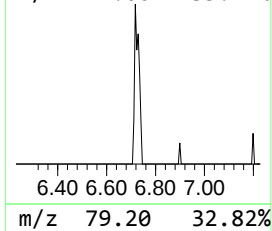
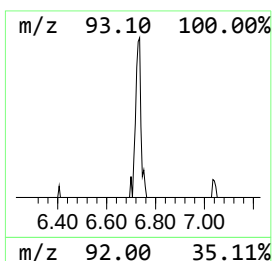
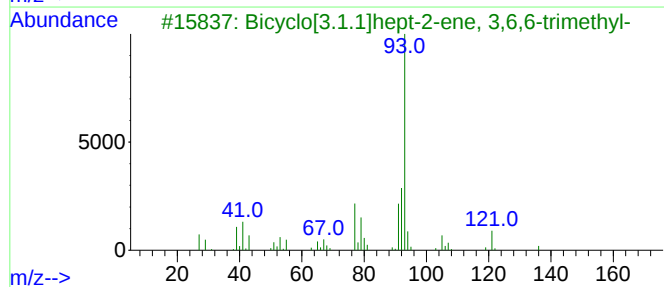
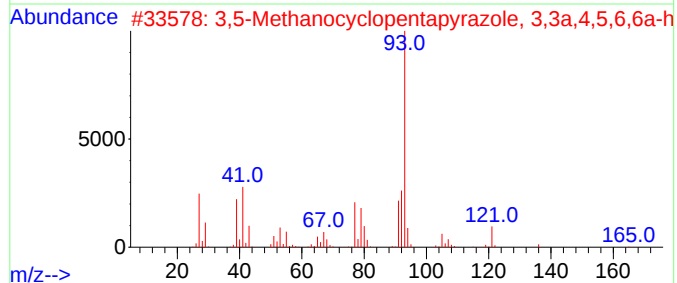
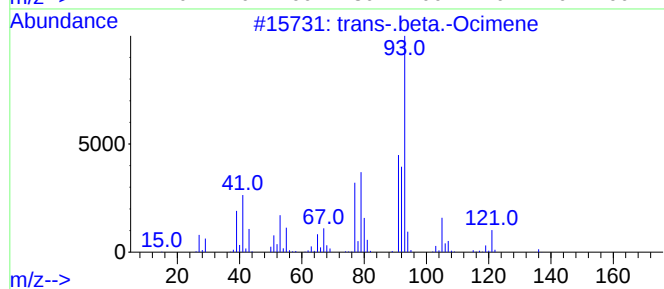
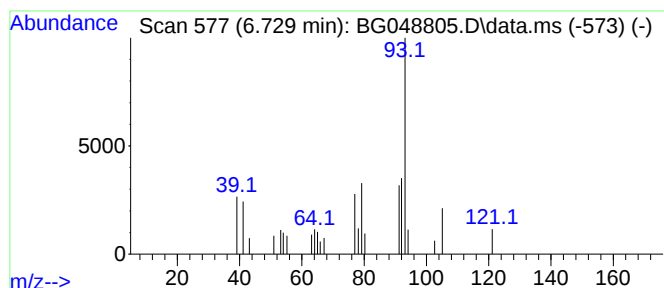
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Peak Number 1 trans-.beta.-Ocimene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.729	3.06 ng	16363	1,4-Dichlorobenzene-d4	8.062

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-.beta.-Ocimene	136	C10H16	003779-61-1	72
2			3,5-Methanocyclopentapyrazole, 3...	164	C10H16N2	087143-58-6	59
3			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	50
4			Pyridine, 4-methyl-	93	C6H7N	000108-89-4	43
5			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	43



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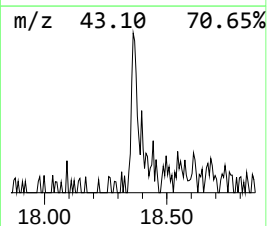
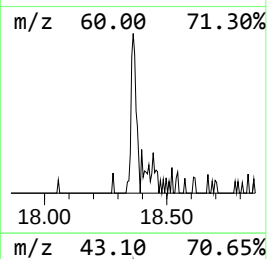
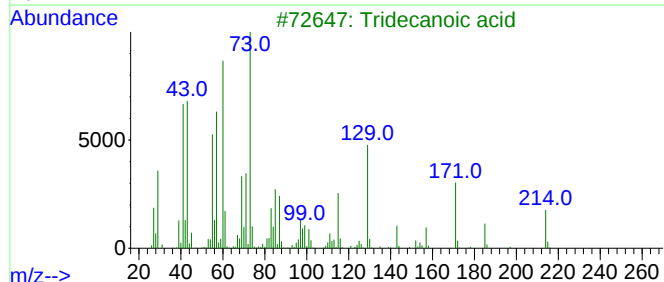
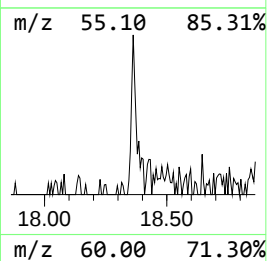
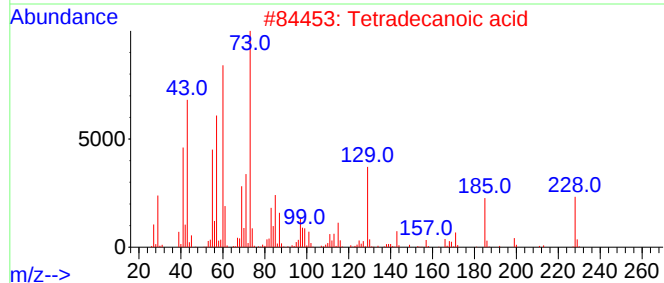
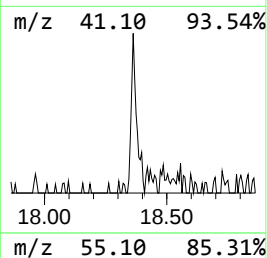
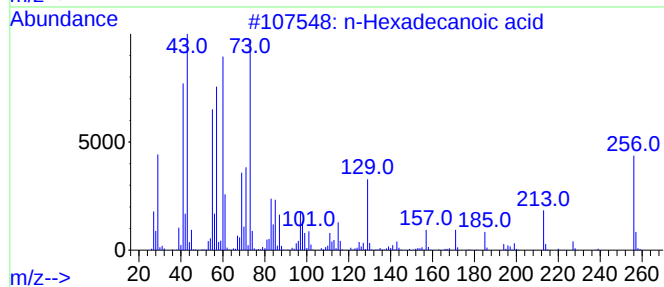
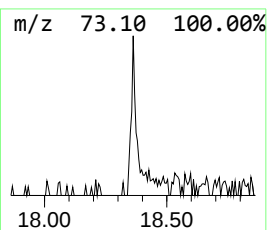
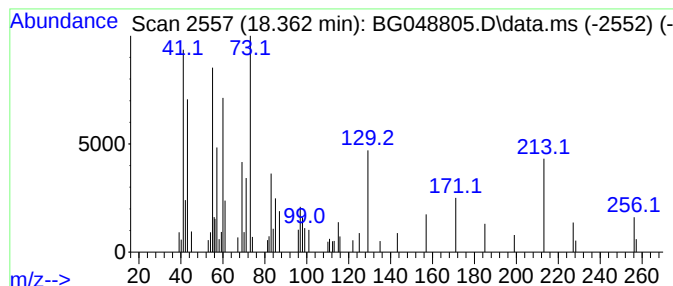
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.362	3.82 ng	60331	Phenanthrene-d10	17.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	50
4			Dodecanoic acid	200	C12H24O2	000143-07-7	38
5			n-Decanoic acid	172	C10H20O2	000334-48-5	38



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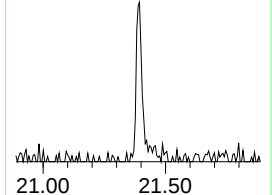
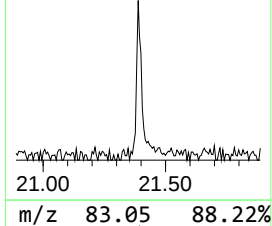
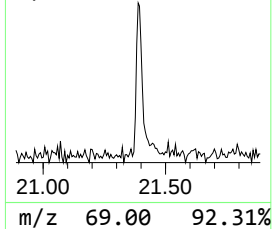
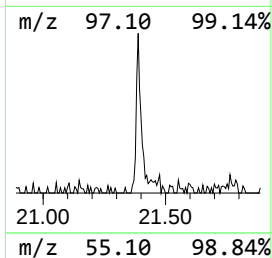
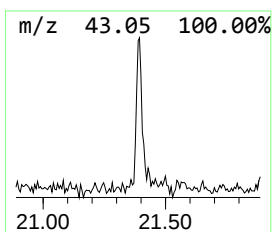
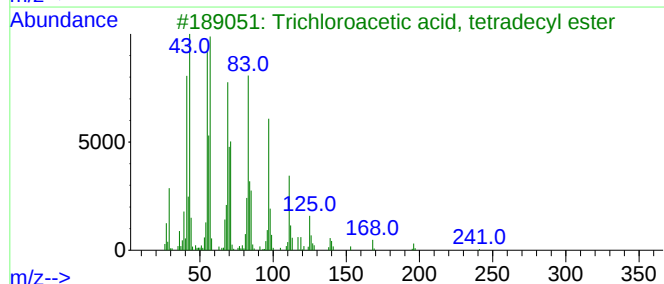
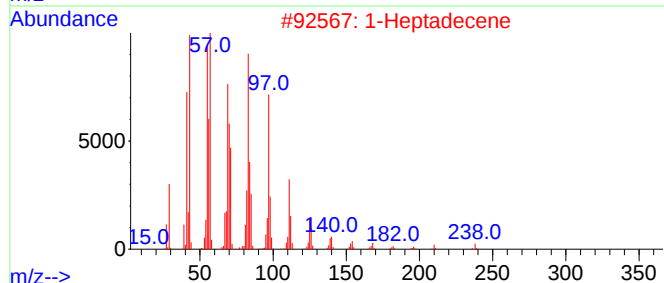
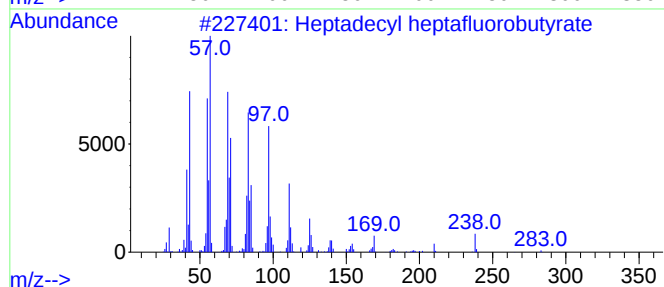
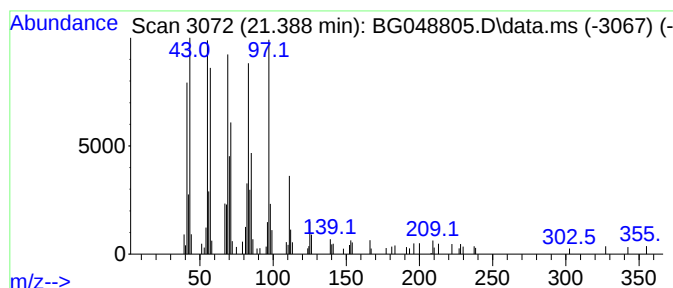
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Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.388	7.21 ng	133414	Chrysene-d12	21.776	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	1-Heptadecene	238	C17H34	006765-39-5	90
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
trans-.beta.-Oc...	6.729	3.1	ng	16363	1	8.062	107112	20.0
n-Hexadecanoic ...	18.362	3.8	ng	60331	4	17.475	315745	20.0
Heptadecyl hept...	21.388	7.2	ng	133414	5	21.776	370025	20.0