

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN100419\
 Data File : VN058528.D
 Acq On : 4 Oct 2019 10:41
 Operator : JC/SP
 Sample : VN1004MBL01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN1004MBL01

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:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.792	1541	1561	1582	rBV2	17624	58785	2.34%	0.364%
2	7.571	1783	1803	1814	rBV	298212	745016	29.71%	4.616%
3	7.648	1815	1827	1853	rVB	566798	1359901	54.23%	8.426%
4	8.011	1918	1940	1966	rBV	370062	876940	34.97%	5.434%
5	8.571	2098	2114	2149	rBV	838614	1802596	71.88%	11.169%
6	10.085	2571	2585	2611	rBV	1344508	2488111	99.22%	15.417%
7	10.284	2631	2647	2669	rBV2	97185	342723	13.67%	2.124%
8	11.406	2984	2996	3021	rVB	1161333	2060246	82.16%	12.766%
9	12.406	3296	3307	3317	rBV	912461	1612748	64.31%	9.993%
10	13.348	3588	3600	3616	rVB	1068144	1740063	69.39%	10.782%
11	13.895	3752	3770	3786	rVB2	62424	201801	8.05%	1.250%
12	15.274	4190	4199	4215	rVB	85204	166477	6.64%	1.032%
13	16.027	4420	4433	4478	rBV	1212887	2507697	100.00%	15.538%
14	16.686	4630	4638	4654	rVB	87687	175757	7.01%	1.089%

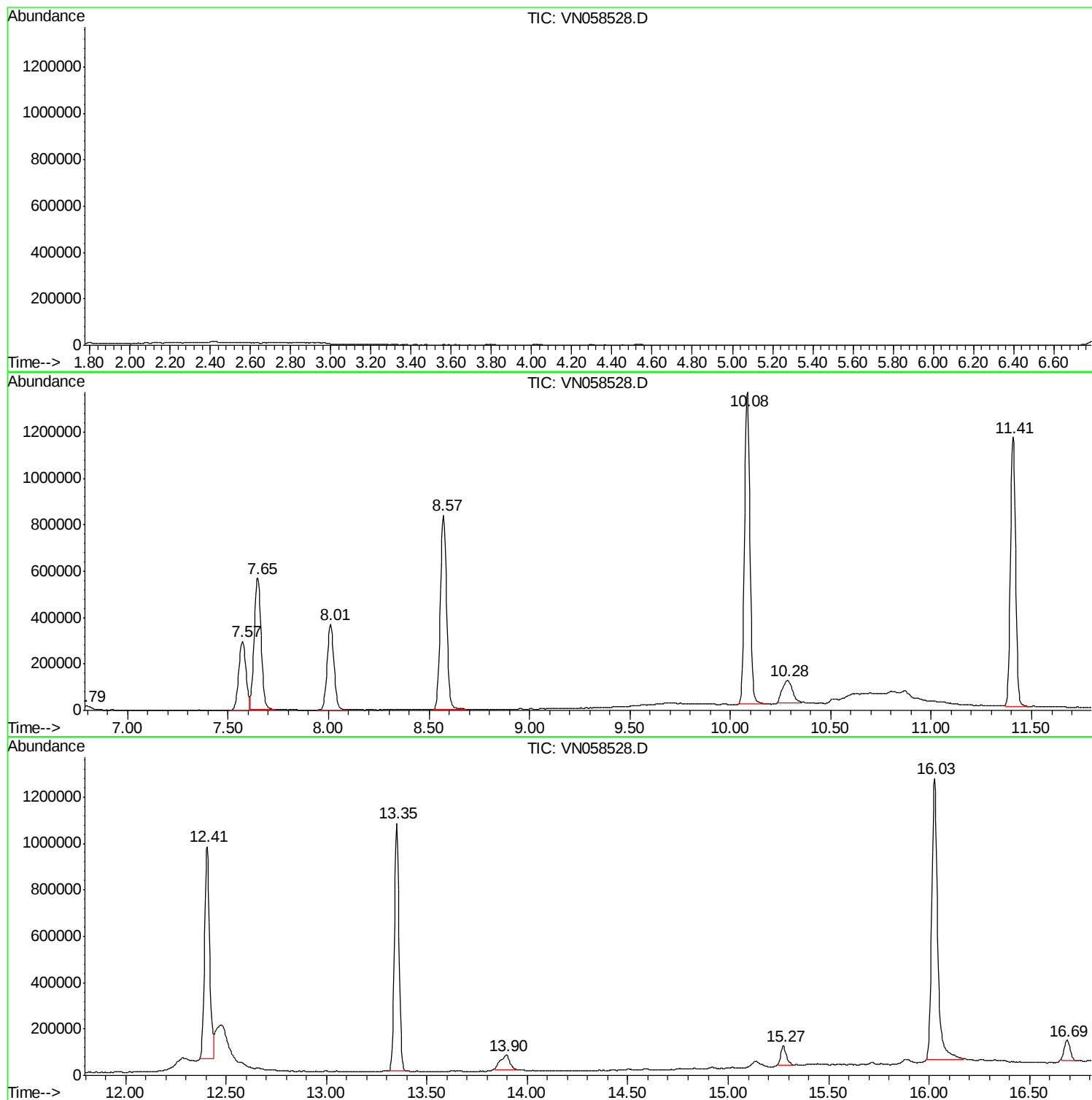
Sum of corrected areas: 16138861

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



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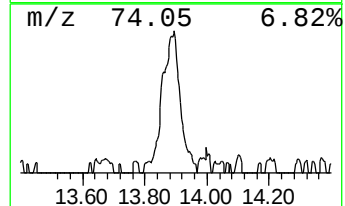
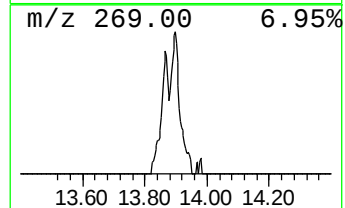
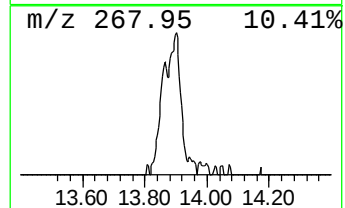
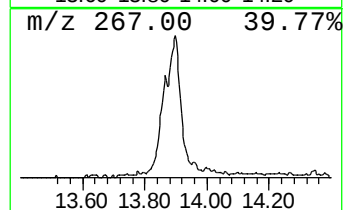
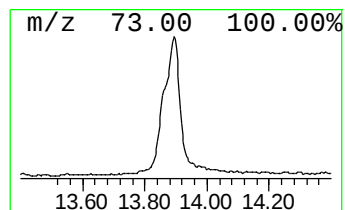
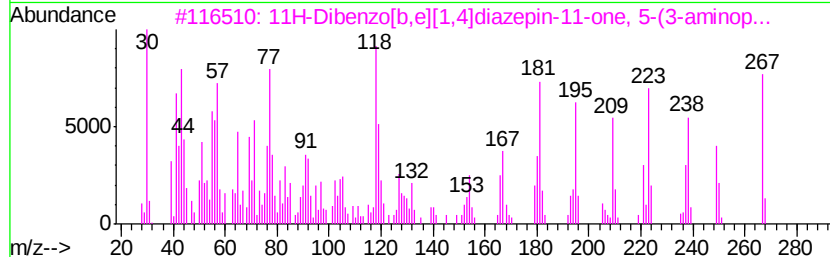
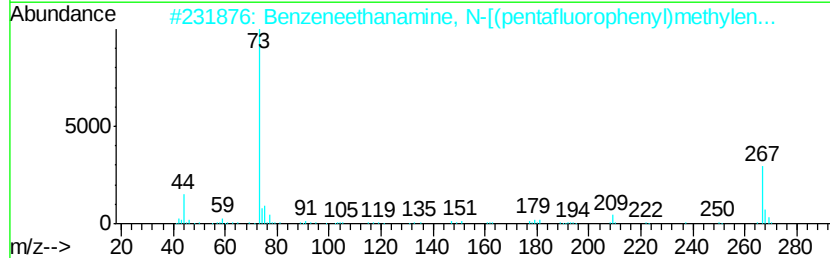
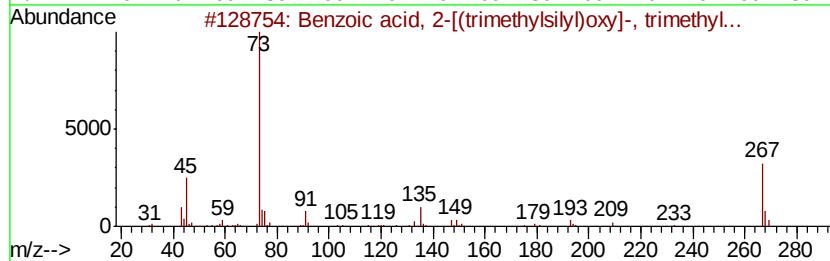
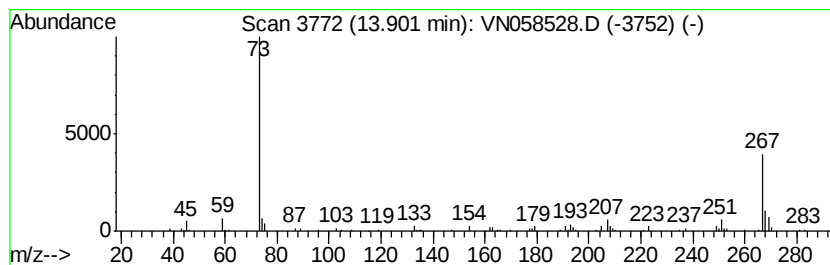
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Quant Title : SW846 8260

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

Peak Number 2 Benzoic acid, 2-[(trimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.90	5.80 ug/l	201801	1,4-Dichlorobenzene-d4	13.35		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3	53
2		Benzenethanamine, N-[(pentafluorophenyl)methyl]...	475	C21H26F5N2Si2	055429-85-1	38
3		11H-Dibenzo[b,e][1,4]diazepin-11-one, 5-(3-aminop...	267	C16H17N3O	013450-73-2	30
4		4-Methylcatechol, bis(trimethylsilyl) ether	268	C13H24O2Si2	1000332-79-9	27
5		1-(3-Chlorophenyl)piperazine, 4-(trimethylsilyl)...	268	C13H21ClN2Si	1000373-99-3	18



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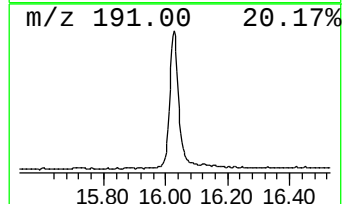
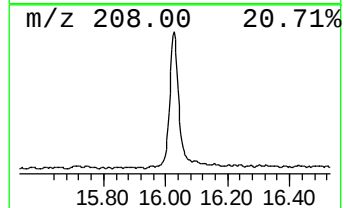
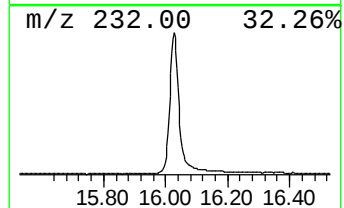
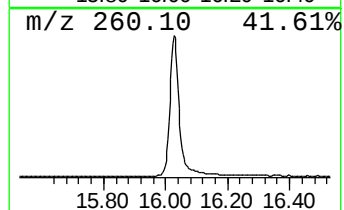
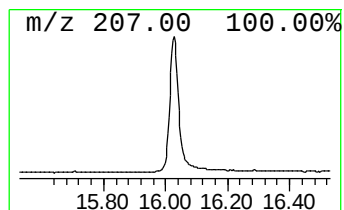
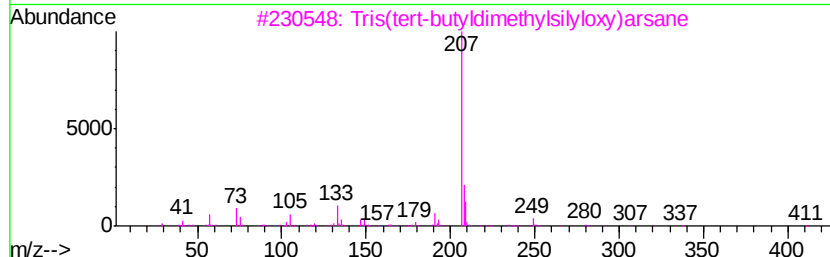
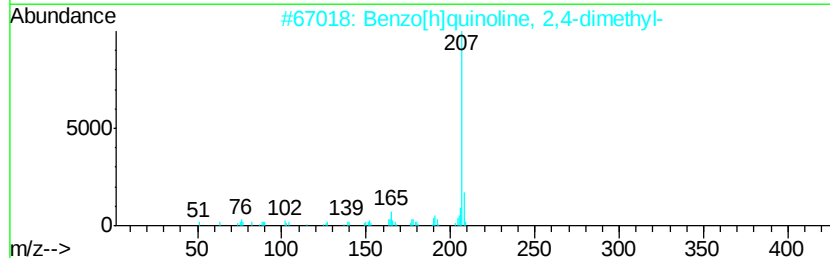
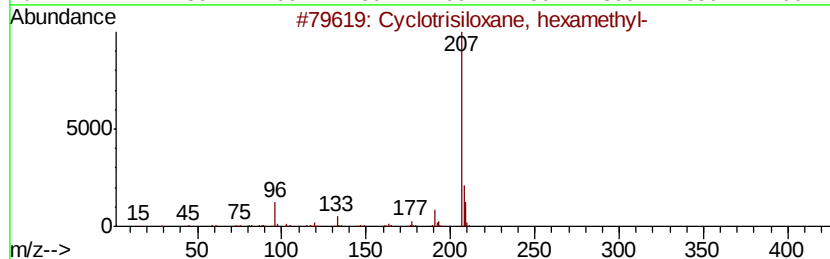
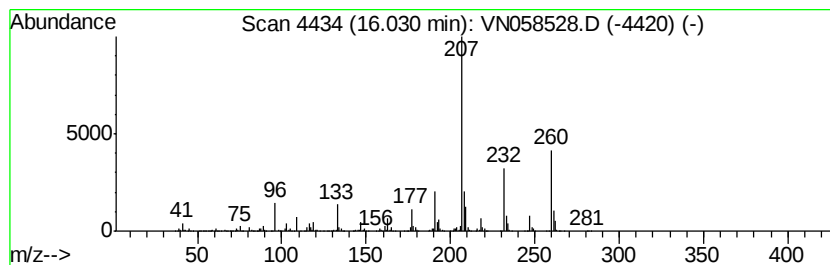
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Peak Number 3 unknown16.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	72.06 ug/l	2507700	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	46
2		Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	35
3		Tris(tert-butyl dimethylsilyloxy)...	468	C18H45AsO3Si3	1000366-57-5	32
4		1,2-Bis(trimethylsilyl)benzene	222	C12H22Si2	017151-09-6	32
5		7-Hydroxy-7,8,9,10-tetramethyl-7...	252	C18H20O	1000110-34-9	27



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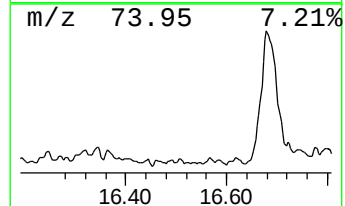
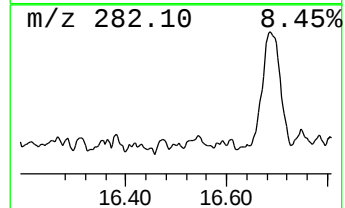
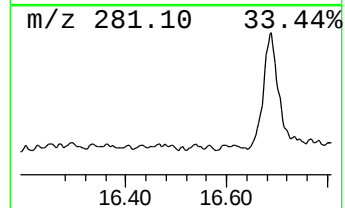
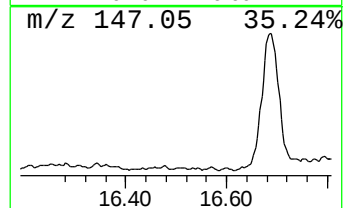
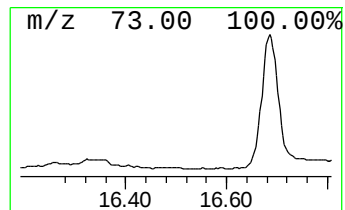
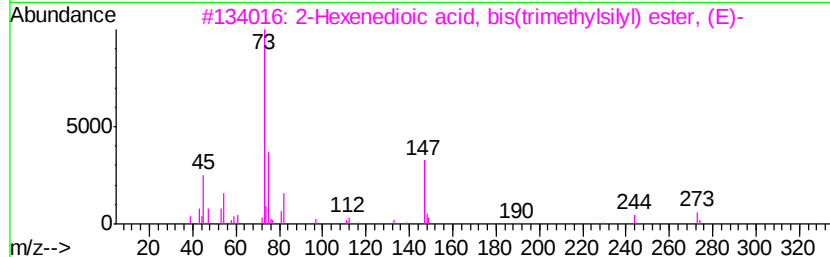
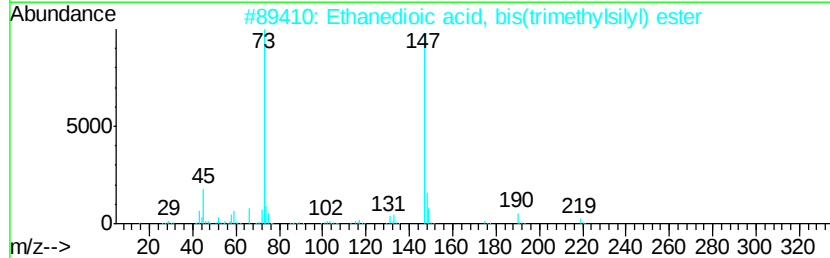
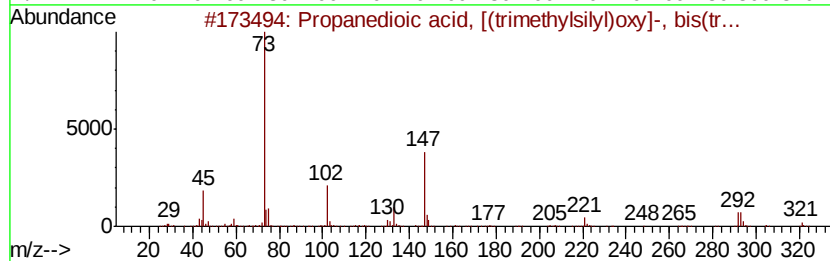
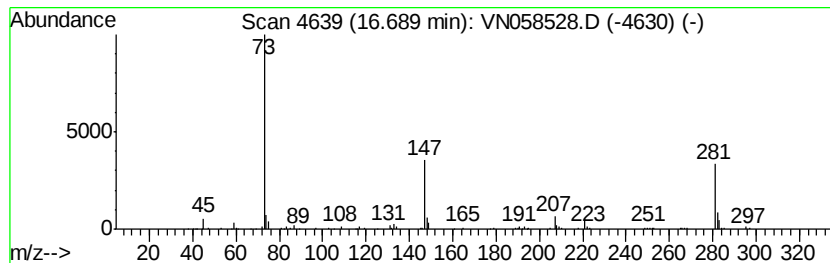
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Peak Number 4 unknown16.69 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	5.05 ug/l	175757	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanedioic acid, [(trimethylsilyl)oxy]-, bis(tri...	336	C12H28O5Si3	038165-93-4	37
2		Ethanedioic acid, bis(trimethylsilyl) ester	234	C8H18O4Si2	018294-04-7	25
3		2-Hexenedioic acid, bis(trimethylsilyl) ester, (E)-	288	C12H24O4Si2	055494-10-5	25
4		Malonic acid, bis(2-trimethylsilyl) ester	304	C13H28O4Si2	090744-45-9	25
5		Benzenepropanoic acid, .alpha.-[bis(trimethylsilyl)oxy]-	310	C15H26O3Si2	027750-45-4	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzoic acid, 2-[...	13.90	5.8	ug/l	201801	4	13.35	1740060	50.0
unknown16.03	16.03	72.1	ug/l	2507700	4	13.35	1740060	50.0
unknown16.69	16.69	5.0	ug/l	175757	4	13.35	1740060	50.0