

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY072821\
 Data File : VY005500.D
 Acq On : 28 Jul 2021 19:22
 Operator : SY/MD
 Sample : M3216-04
 Misc : 10.07G/5ML/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20210431-17

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_Y\methods\82Y072221S.M

Title : SW846 8260

Signal : TIC: VY005500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.960	340	351	360	rBV3	3721	9585	1.78%	0.899%
2	4.204	382	391	403	rVB2	4747	12814	2.38%	1.202%
3	4.735	465	478	488	rBV4	5995	19175	3.57%	1.798%
4	5.759	638	646	656	rVB7	2148	6692	1.24%	0.628%
5	7.728	959	969	975	rBV2	13189	32680	6.08%	3.065%
6	7.795	975	980	992	rVB2	28811	63059	11.72%	5.914%
7	8.149	1031	1038	1047	rVB	14419	30189	5.61%	2.831%
8	8.697	1120	1128	1136	rVB	39566	77473	14.41%	7.266%
9	10.185	1365	1372	1379	rBV	46108	83864	15.59%	7.865%
10	11.496	1579	1587	1593	rBV	45000	74733	13.90%	7.009%
11	12.495	1739	1751	1759	rBV	317423	537820	100.00%	50.439%
12	13.075	1837	1846	1850	rVB10	2643	6142	1.14%	0.576%
13	13.282	1876	1880	1885	rVB4	6969	10630	1.98%	0.997%
14	13.428	1894	1904	1909	rBV	30525	56235	10.46%	5.274%
15	13.477	1910	1912	1919	rVB4	5369	10000	1.86%	0.938%
16	13.971	1987	1993	1998	rBV2	16014	26603	4.95%	2.495%
17	14.397	2059	2063	2070	rVB8	4426	8575	1.59%	0.804%

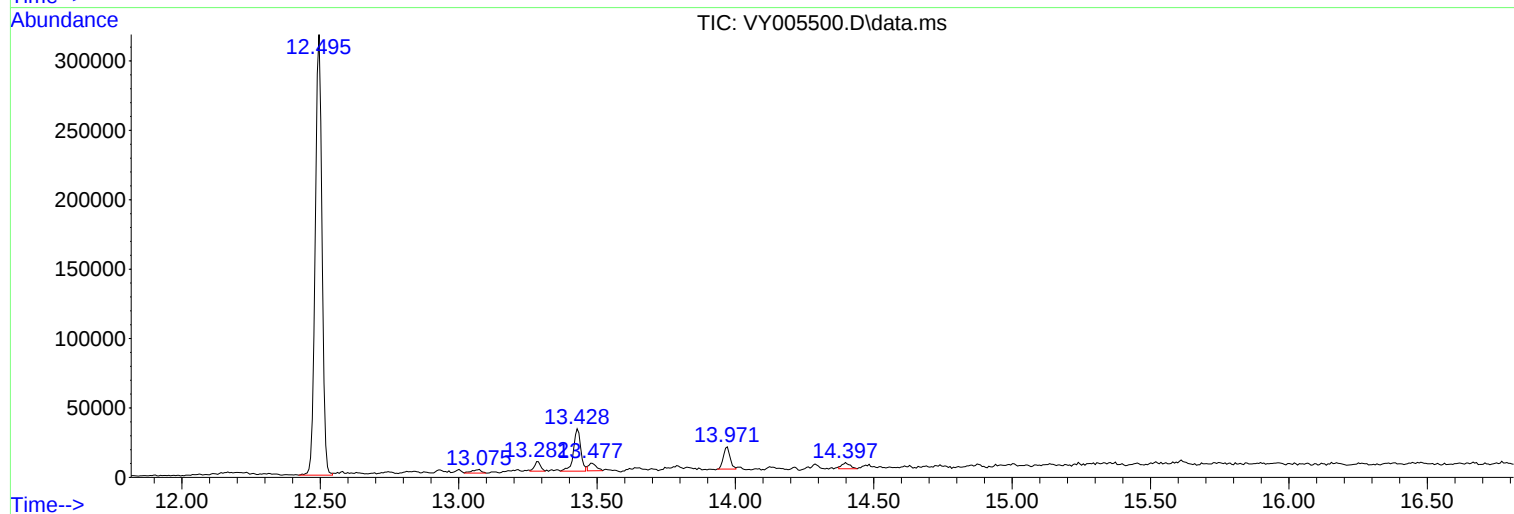
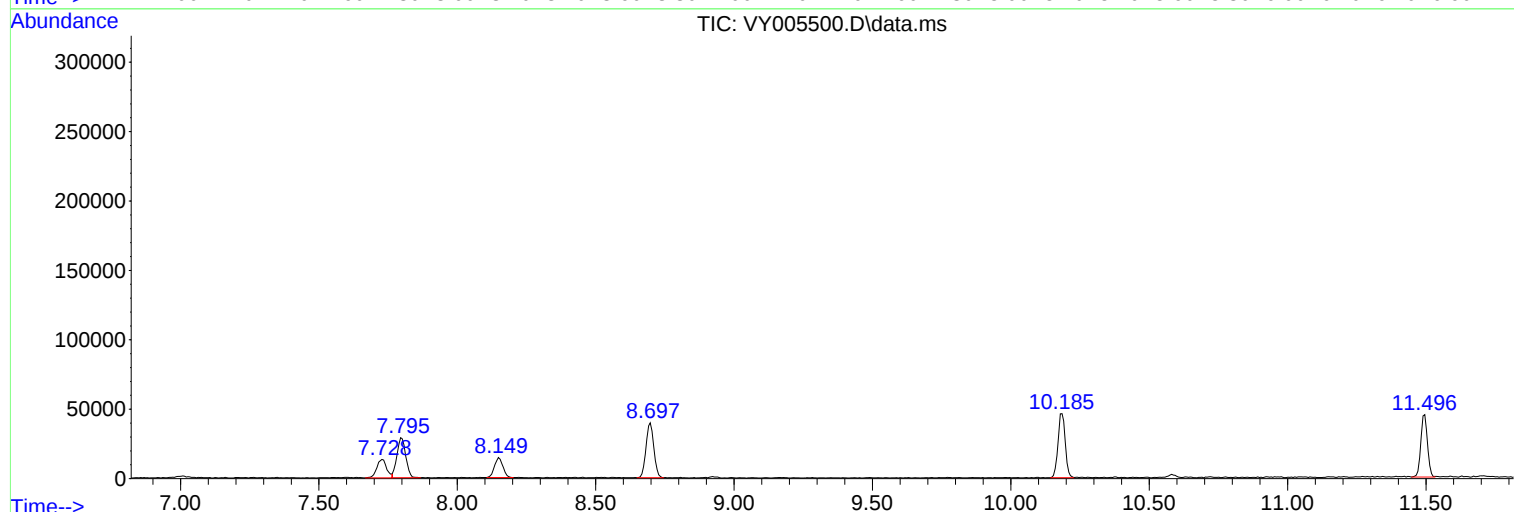
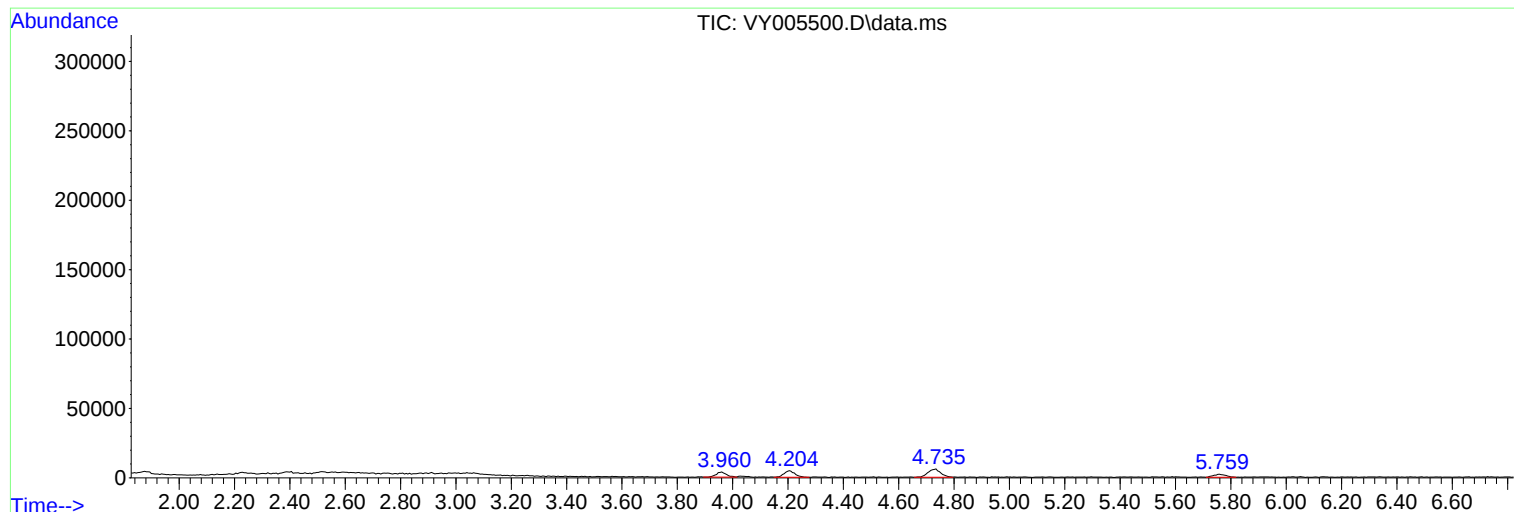
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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



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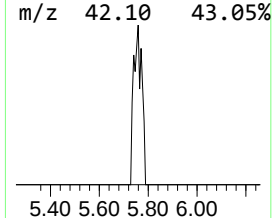
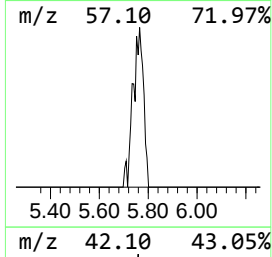
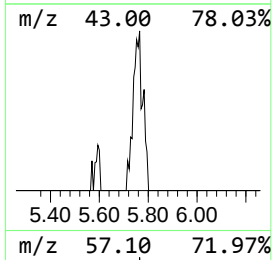
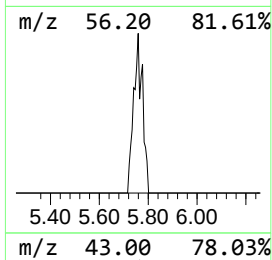
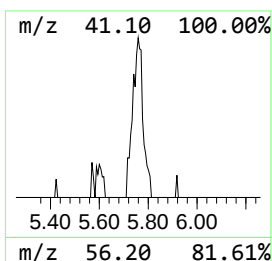
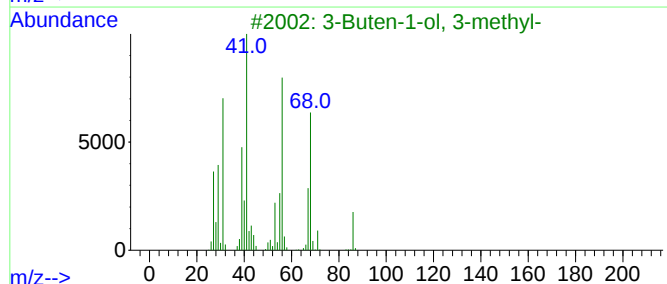
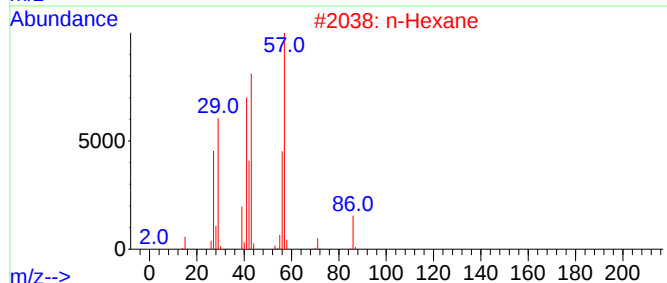
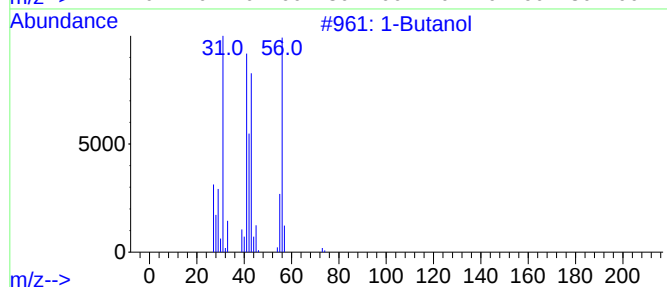
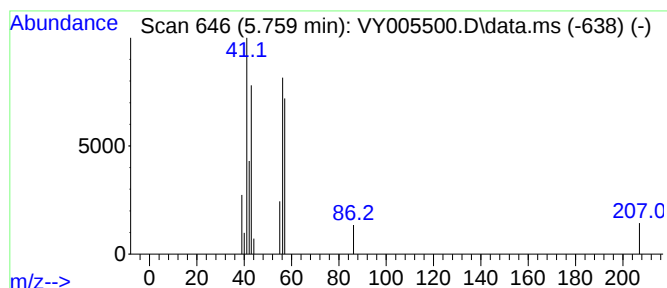
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y072221S.M
Quant Title : SW846 8260

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

Peak Number 1 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.759	5.31 ug/l	6692	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	64
2			n-Hexane	86	C6H14	000110-54-3	37
3			3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	28
4			Cyclobutane	56	C4H8	000287-23-0	9
5			Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	9



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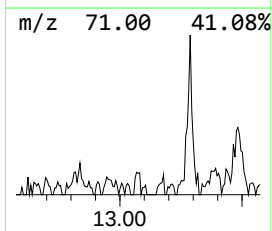
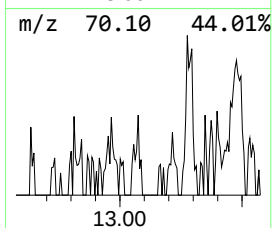
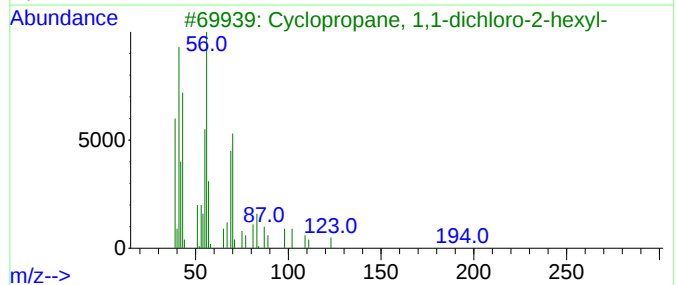
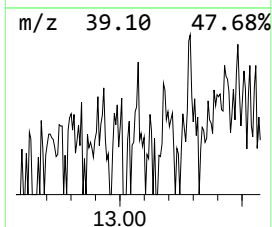
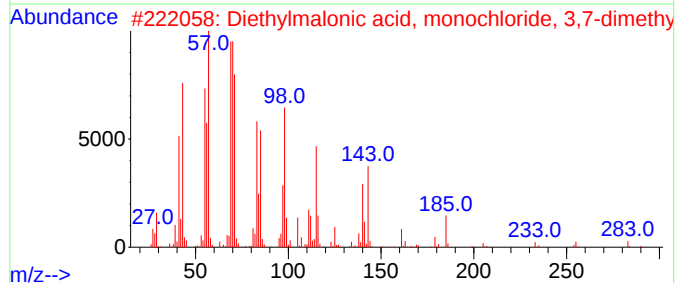
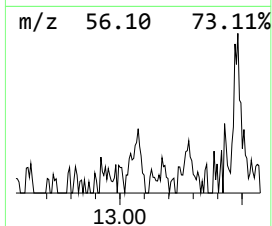
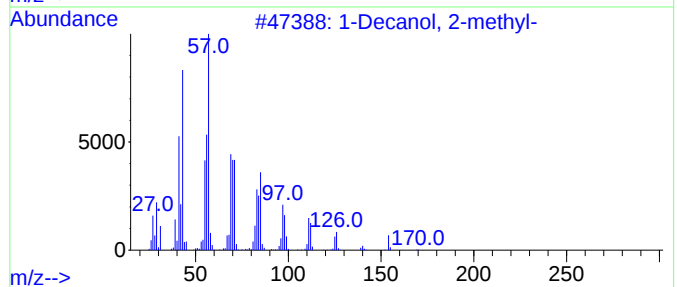
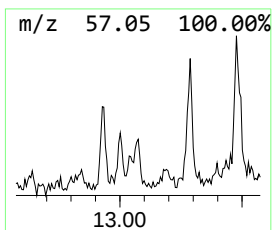
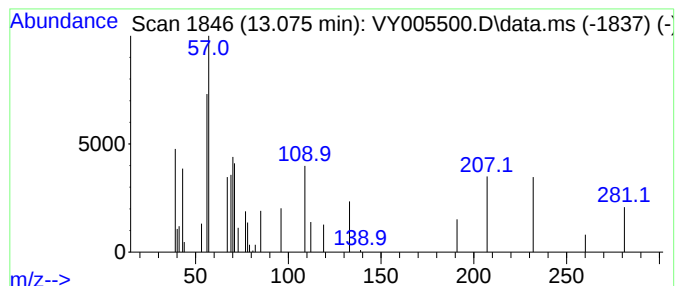
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Peak Number 2 unknown13.075 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.075	5.46 ug/l	6142	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol, 2-methyl-	172	C11H24O	018675-24-6	32
2			Diethylmalonic acid, monochlorid...	318	C17H31ClO3	1000369-41-8	12
3			Cyclopropane, 1,1-dichloro-2-hexyl-	194	C9H16Cl2	005685-42-7	10
4			1-Octanol, 2,7-dimethyl-	158	C10H22O	015250-22-3	10
5			1-Heptanol, chlorodifluoroacetate	228	C9H15ClF2O2	1000447-23-9	10



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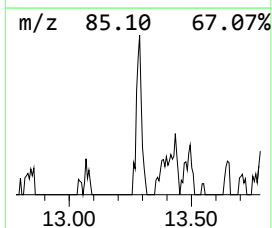
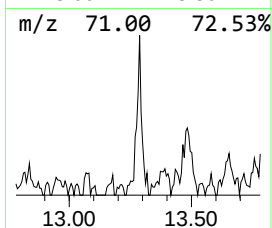
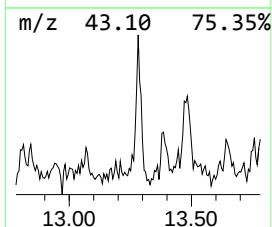
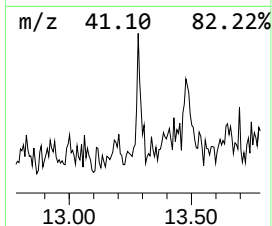
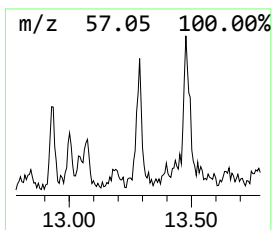
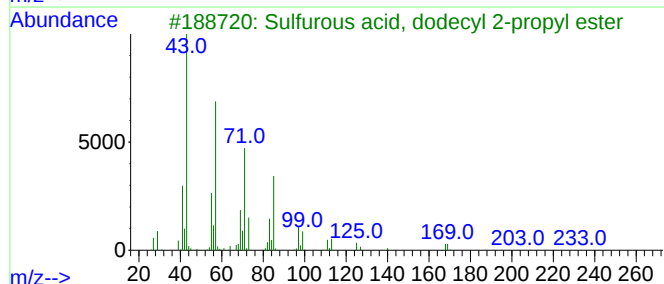
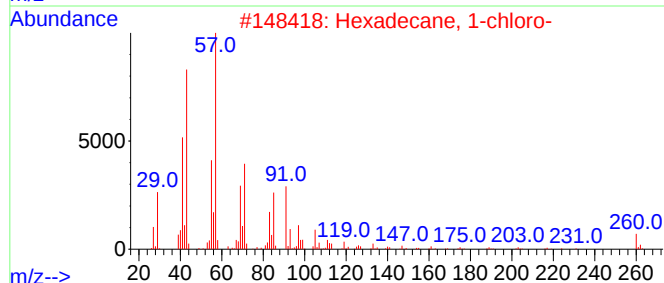
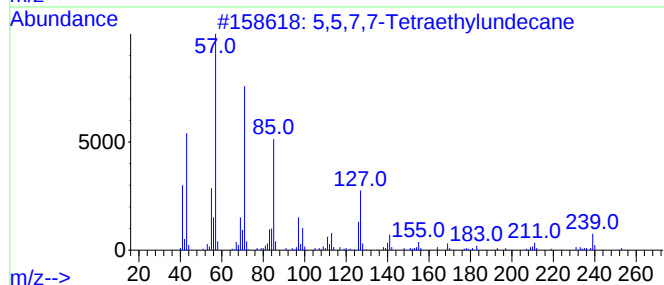
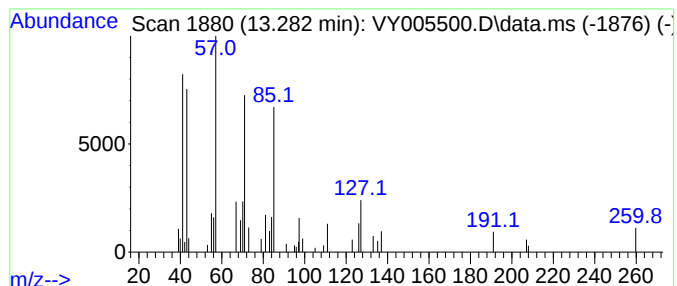
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Peak Number 3 5,5,7,7-Tetraethylundecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	9.45 ug/l	10630	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	64
2			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	53
3			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	50
4			Undecane, 3,4-dimethyl-	184	C13H28	017312-78-6	47
5			1-Undecene, 4-methyl-	168	C12H24	074630-39-0	47



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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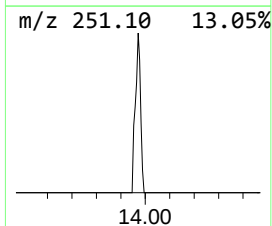
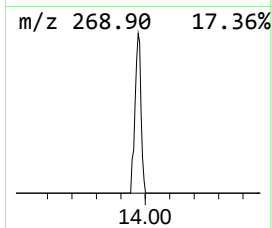
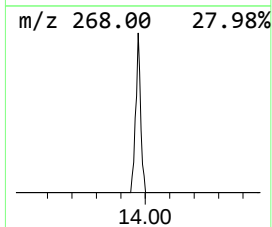
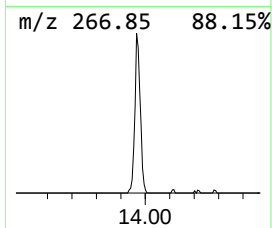
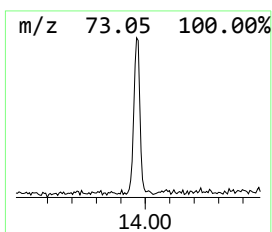
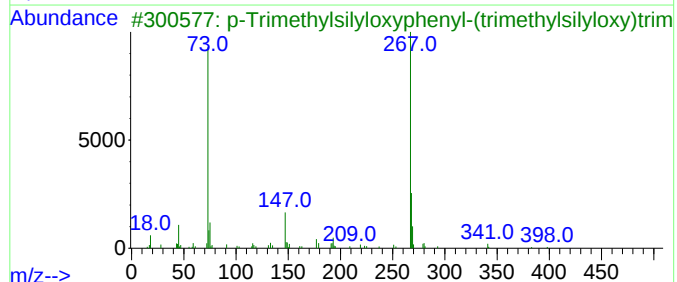
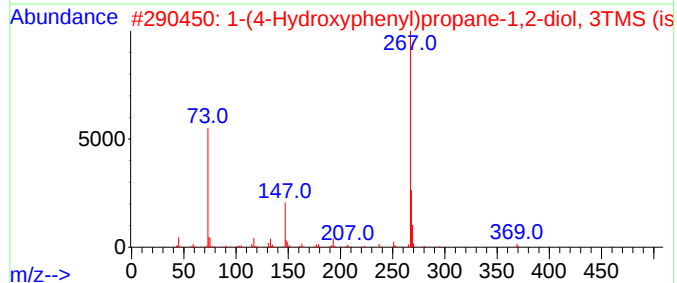
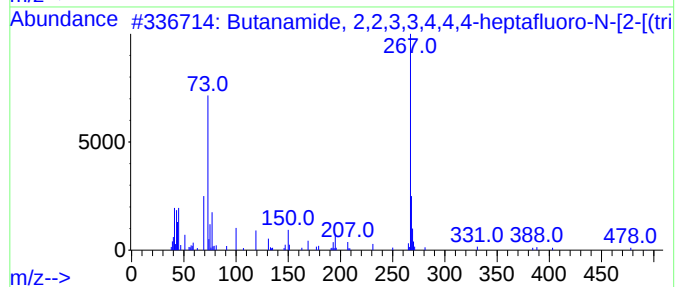
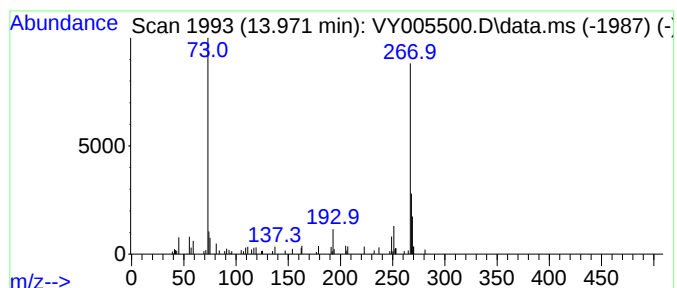
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Peak Number 4 Butanamide, 2,2,3,3,4,4,4-h... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.971	23.65 ug/l	26603	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-[2-[(tri	493	C18H26F7NO3Si2	055471-01-7	72
2			1-(4-Hydroxyphenyl)propane-1,2-diol, 3TMS (is	384	C18H36O3Si3	1000495-85-7	64
3			p-Trimethylsilyloxyphenyl-(trimethylsilyloxy)trim	398	C18H34O4Si3	1000079-05-1	56
4			Ethyl 4-hydroxymandelate, 2TMS derivative	340	C16H28O4Si2	1010071-53-3	56
5			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	56



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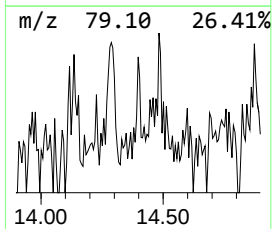
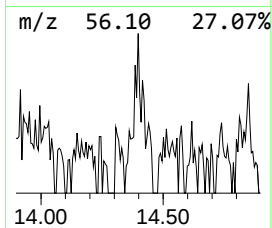
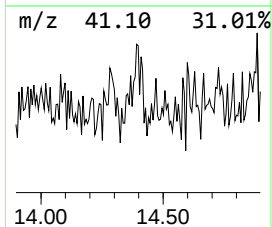
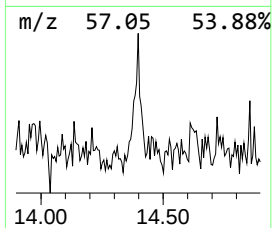
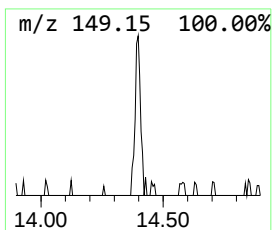
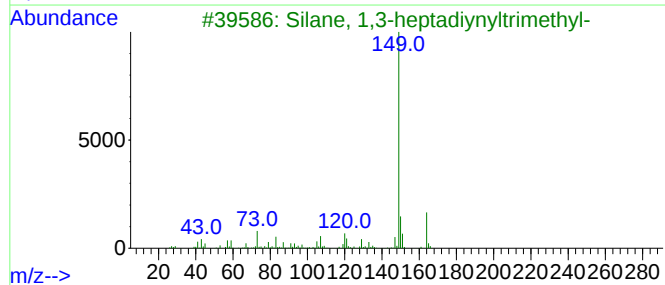
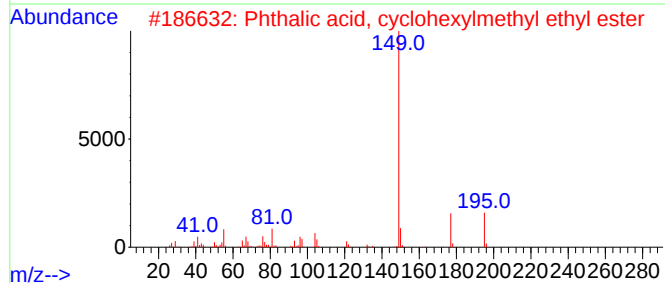
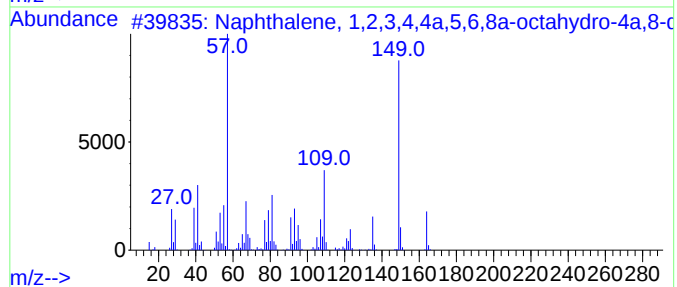
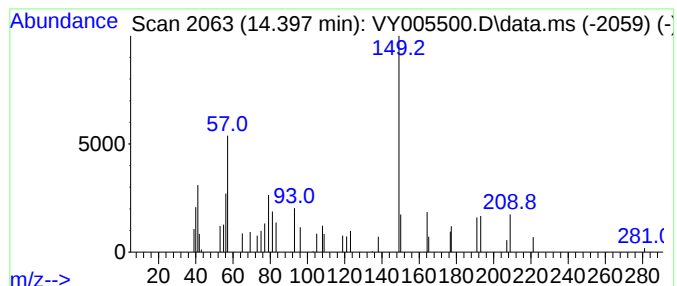
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Peak Number 5 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.397	7.62 ug/l	8575	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	164	C12H20	055976-09-5	50
2			Phthalic acid, cyclohexylmethyl ...	290	C17H22O4	1000309-10-0	47
3			Silane, 1,3-heptadiynyltrimethyl-	164	C10H16Si	019024-47-6	43
4			Adenosine, N,6-didehydro-1,9-dih...	281	C11H15N5O4	015763-06-1	43
5			Added stereo to name	164	C12H20	024145-89-9	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Butanol	5.759	5.3	ug/l	6692	1	7.801	63059	50.0
unknown13.075	13.075	5.5	ug/l	6142	4	13.428	56235	50.0
5,5,7,7-Tetraet...	13.282	9.4	ug/l	10630	4	13.428	56235	50.0
Butanamide, 2,2...	13.971	23.6	ug/l	26603	4	13.428	56235	50.0
Naphthalene, 1,...	14.397	7.6	ug/l	8575	4	13.428	56235	50.0