

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY022322\
 Data File : VY007609.D
 Acq On : 23 Feb 2022 19:40
 Operator : SY/MD
 Sample : N1584-12
 Misc : 6.26g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 D15-10.5

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\82Y022322S.M
 Title : SW846 8260

Signal : TIC: VY007609.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.888	3	11	18	rVB2	17036	34939	2.54%	0.616%
2	2.071	36	41	53	rBV	104627	154957	11.24%	2.732%
3	2.247	61	70	77	rBV	26393	44303	3.21%	0.781%
4	2.381	88	92	101	rVB	13972	24300	1.76%	0.428%
5	2.900	169	177	186	rBV	46628	104308	7.57%	1.839%
6	3.942	340	348	362	rBV	14214	37489	2.72%	0.661%
7	4.192	377	389	403	rVB	8115	23029	1.67%	0.406%
8	4.802	481	489	501	rVB2	10839	35644	2.59%	0.629%
9	4.948	501	513	527	rBV	29377	105711	7.67%	1.864%
10	5.216	539	557	578	rBV	373717	1378159	100.00%	24.302%
11	6.119	695	705	717	rVB3	10404	31326	2.27%	0.552%
12	7.539	929	938	948	rVB3	16688	43533	3.16%	0.768%
13	7.716	958	967	973	rBV	74828	182112	13.21%	3.211%
14	7.789	973	979	989	rVB	119205	272730	19.79%	4.809%
15	8.149	1026	1038	1046	rBV2	107187	288614	20.94%	5.089%
16	8.234	1046	1052	1063	rVB	66860	150916	10.95%	2.661%
17	8.685	1118	1126	1137	rBV	169711	346439	25.14%	6.109%
18	9.941	1323	1332	1333	rBV	13918	22263	1.62%	0.393%
19	9.978	1333	1338	1346	rVB2	36527	68168	4.95%	1.202%
20	10.179	1363	1371	1379	rBV	269274	475488	34.50%	8.385%
21	10.295	1384	1390	1397	rVB	31500	55696	4.04%	0.982%
22	11.490	1578	1586	1597	rBV	270855	451632	32.77%	7.964%
23	12.483	1740	1749	1758	rBV2	499037	909216	65.97%	16.033%
24	13.422	1896	1903	1914	rVB	250817	387964	28.15%	6.841%
25	13.965	1986	1992	2000	rVB2	24734	42032	3.05%	0.741%

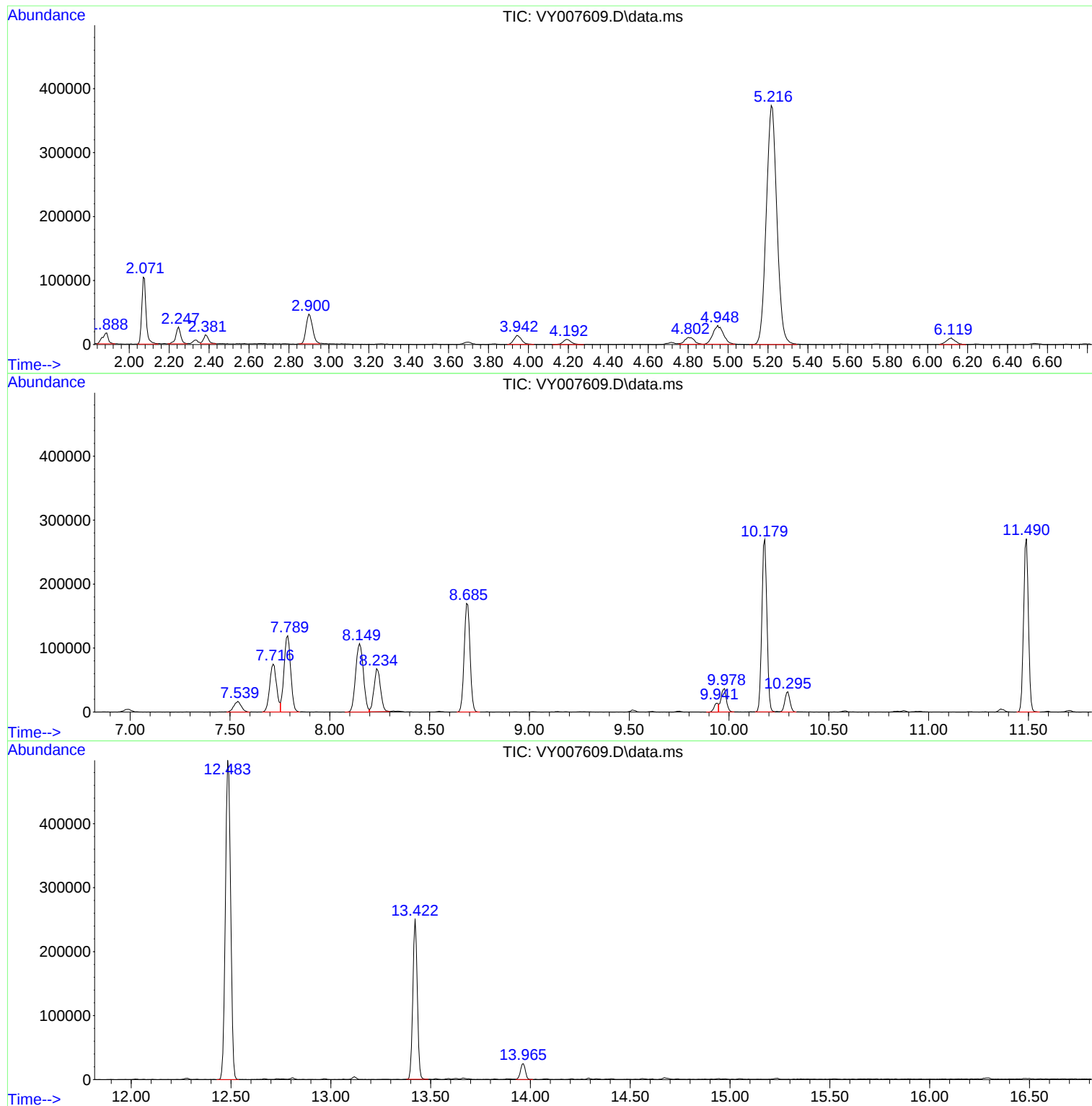
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D15-10.5

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Quant Title : SW846 8260

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



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ClientSampleId :
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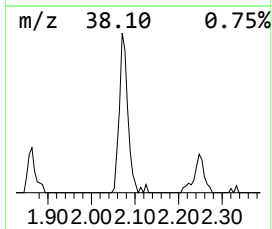
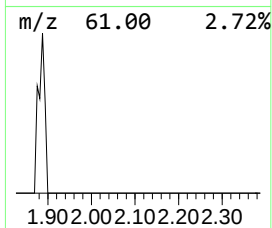
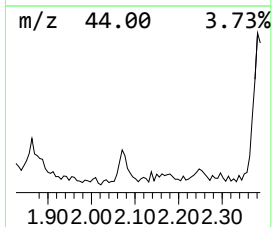
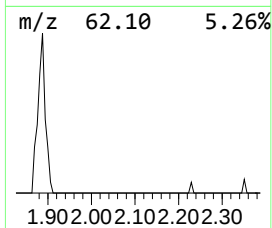
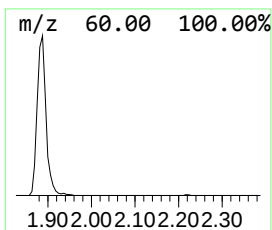
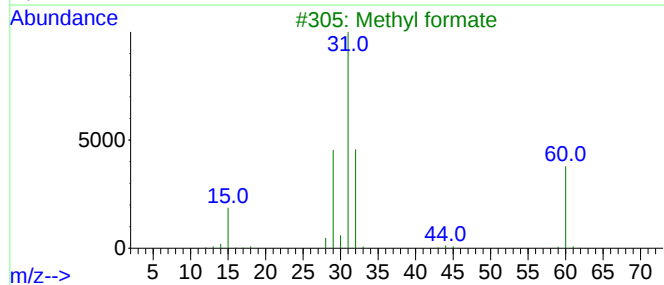
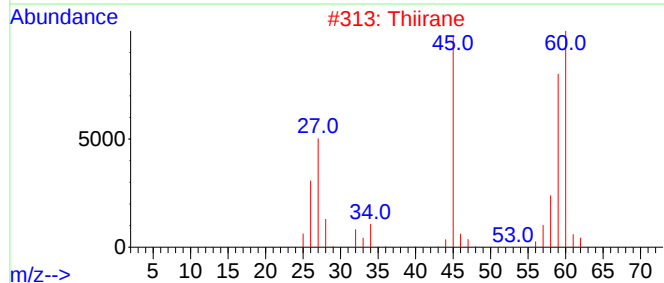
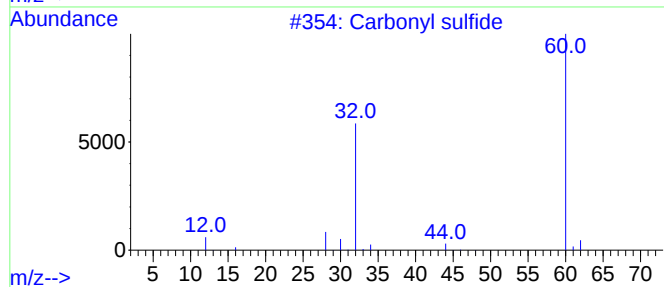
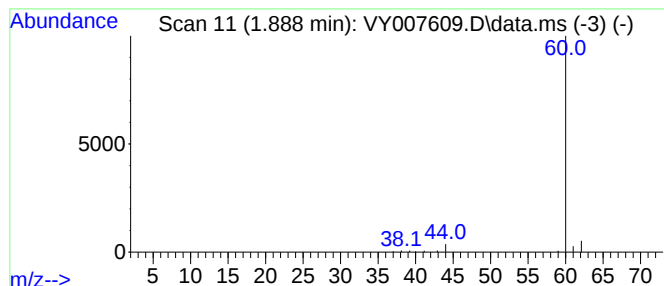
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y022322S.M
Quant Title : SW846 8260

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

Peak Number 1 Carbonyl sulfide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.888	6.41 ug/l	34939	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonyl sulfide	60	COS	000463-58-1	9
2			Thiirane	60	C2H4S	000420-12-2	5
3			Methyl formate	60	C2H4O2	000107-31-3	5
4			Urea	60	CH4N2O	000057-13-6	4
5			Formamidoxime	60	CH4N2O	000624-82-8	4



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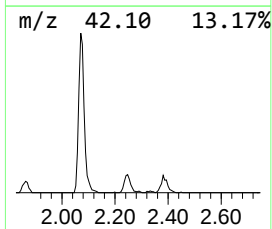
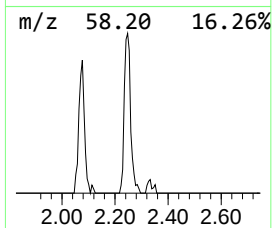
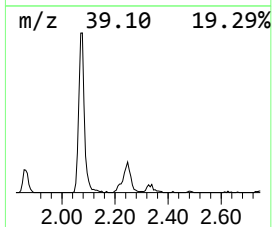
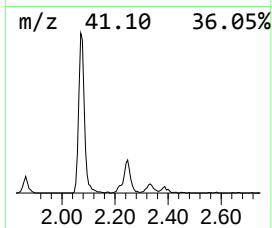
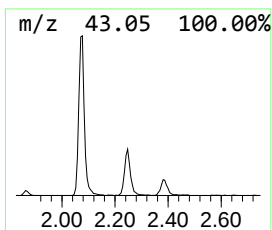
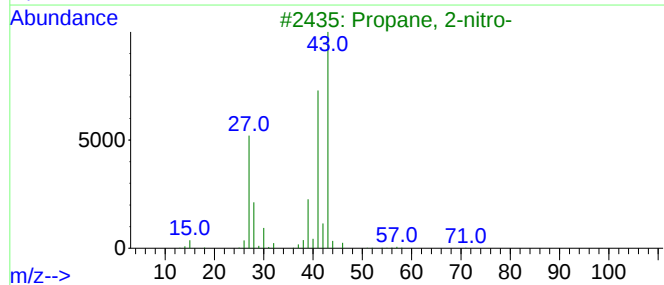
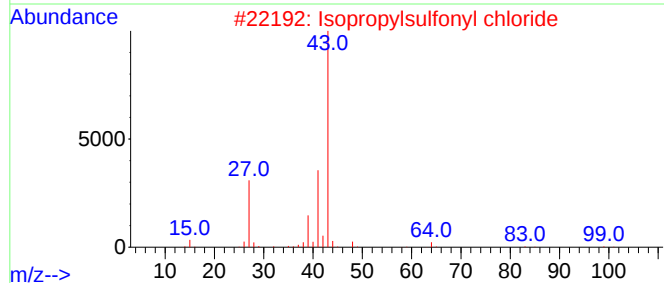
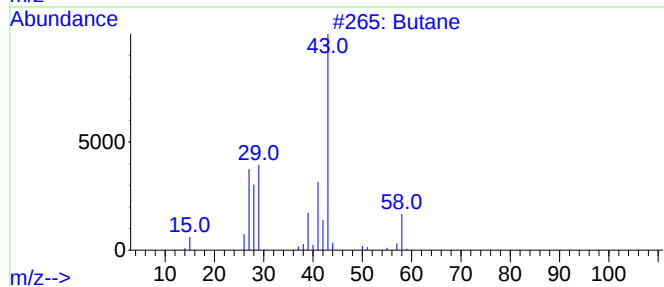
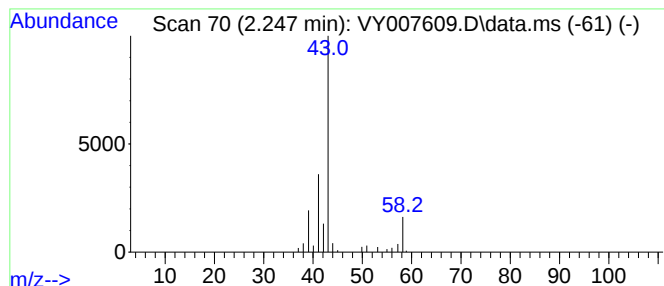
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y022322S.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.247	8.12 ug/l	44303	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	80
2			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
4			Acetone	58	C3H6O	000067-64-1	4
5			Isobutane	58	C4H10	000075-28-5	4



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Misc : 6.26g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D15-10.5

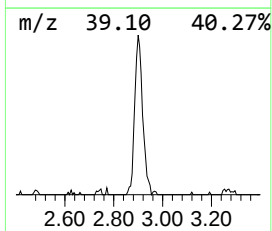
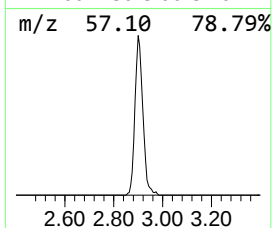
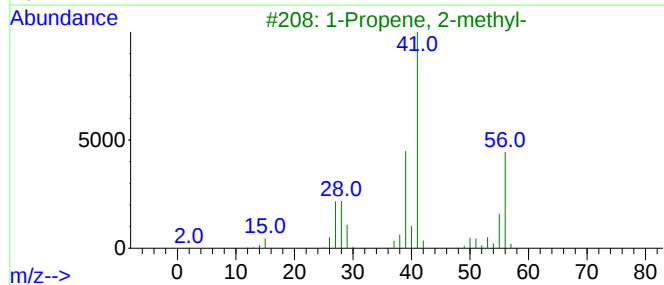
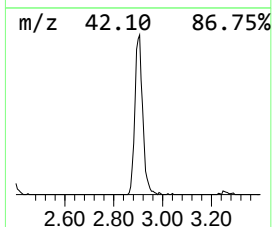
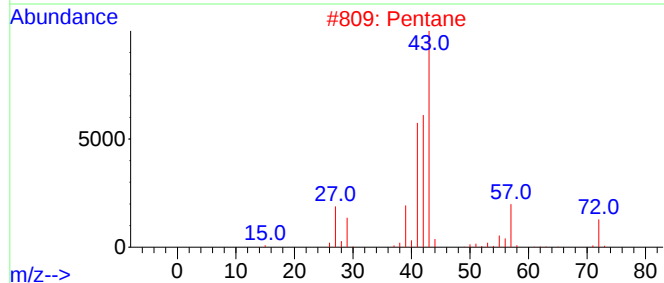
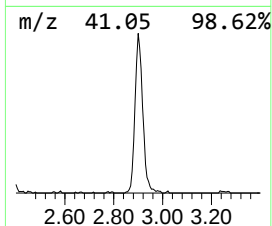
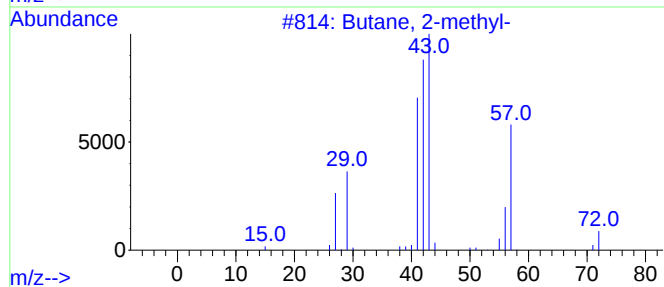
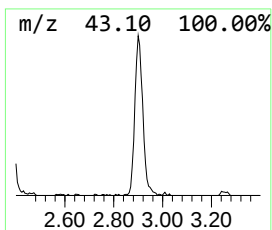
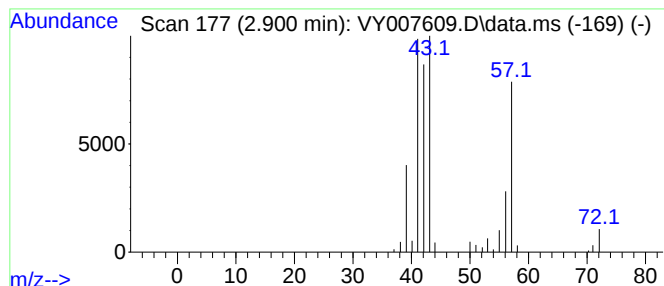
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.900	19.12 ug/l	104308	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	64
2			Pentane	72	C5H12	000109-66-0	33
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	27
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25
5			3-Buten-1-ol	72	C4H8O	000627-27-0	9



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D15-10.5

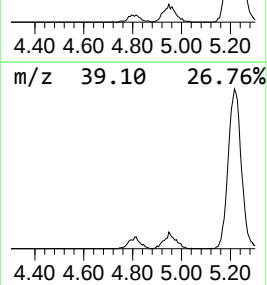
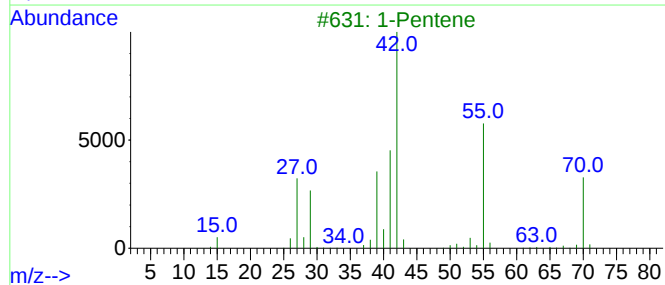
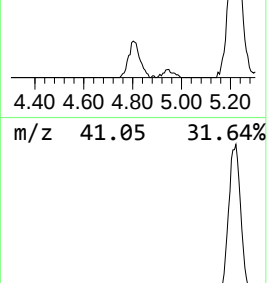
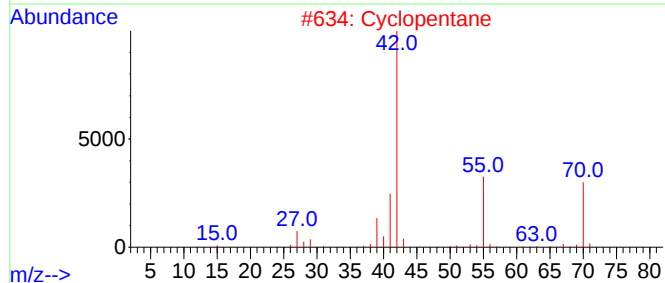
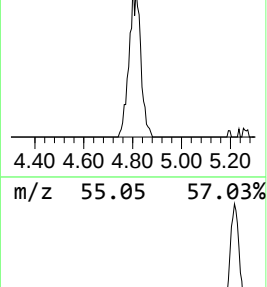
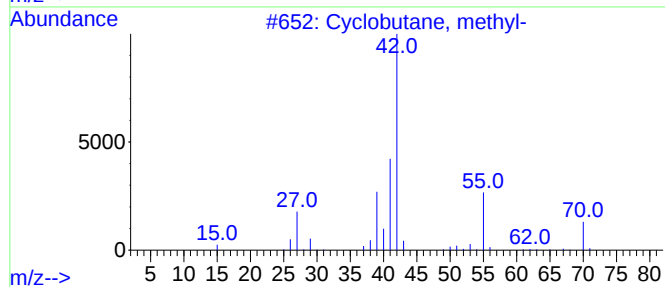
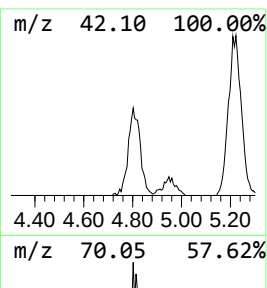
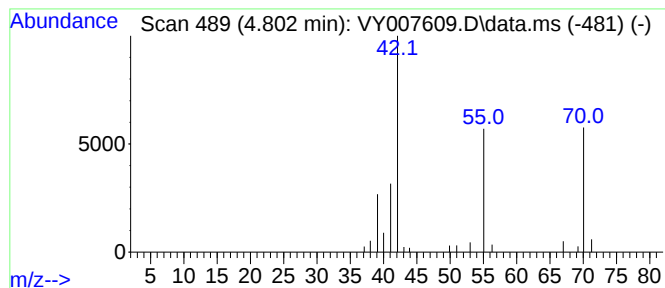
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Quant Title : SW846 8260

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

Peak Number 4 Cyclobutane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.802	6.53 ug/l	35644	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2			Cyclopentane	70	C5H10	000287-92-3	83
3			1-Pentene	70	C5H10	000109-67-1	78
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
5			2-Pentene, (E)-	70	C5H10	000646-04-8	47



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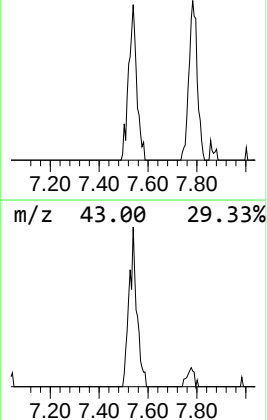
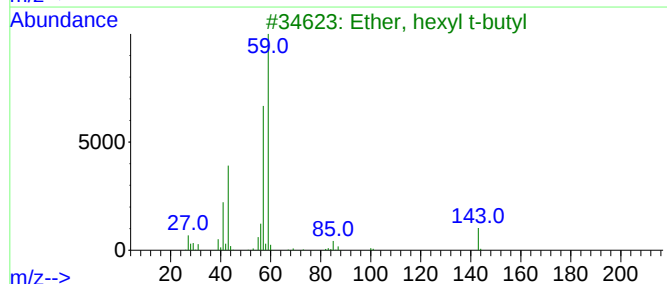
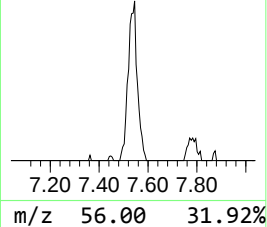
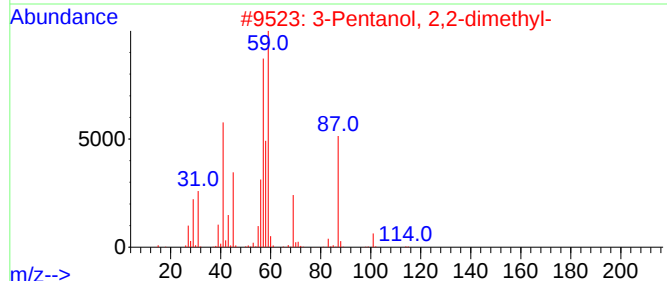
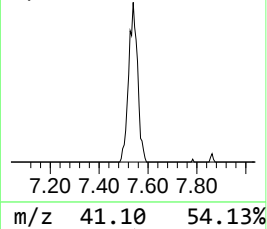
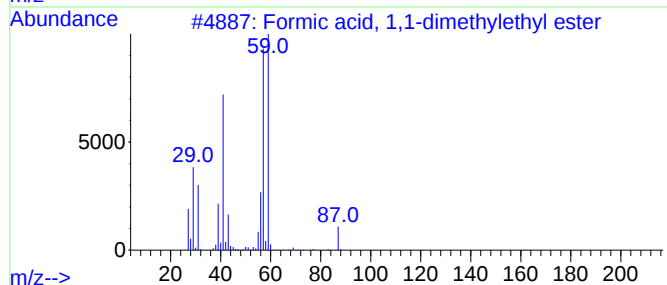
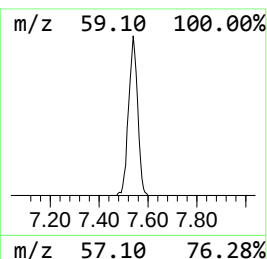
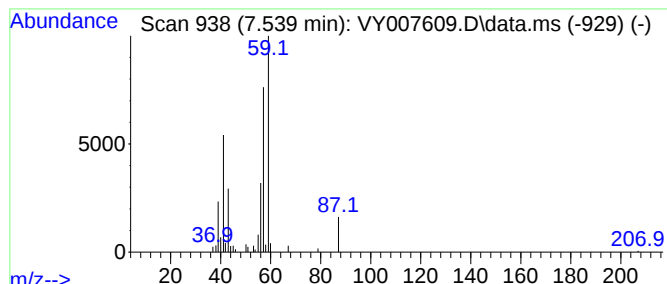
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Formic acid, 1,1-dimethylet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.539	7.98 ug/l	43533	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid, 1,1-dimethylethyl e...	102	C5H10O2	000762-75-4	83
2			3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	72
3			Ether, hexyl t-butyl	158	C10H22O	069775-79-7	56
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	50
5			1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	40



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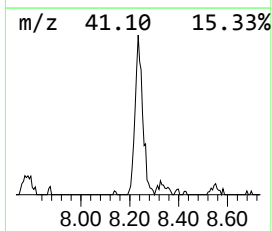
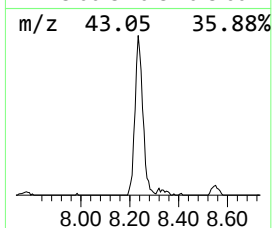
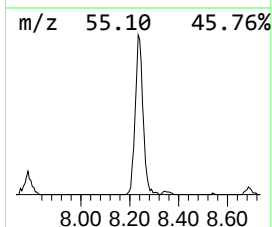
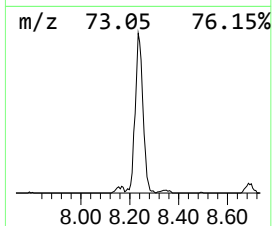
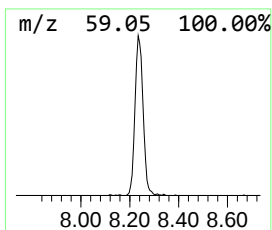
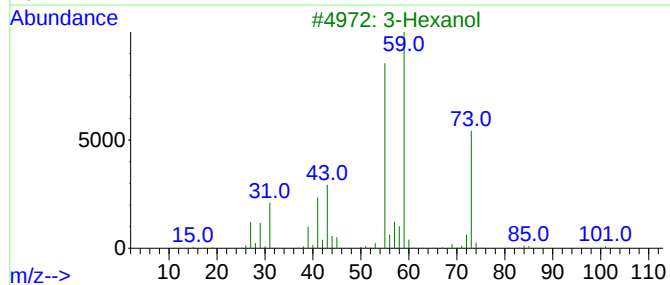
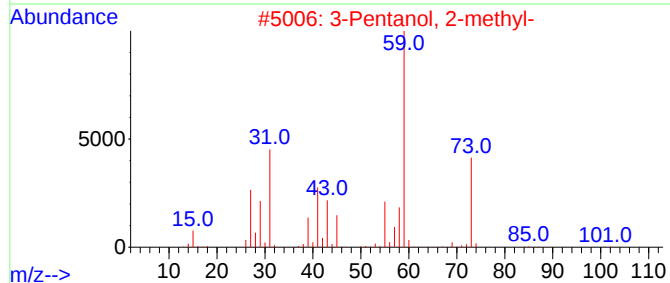
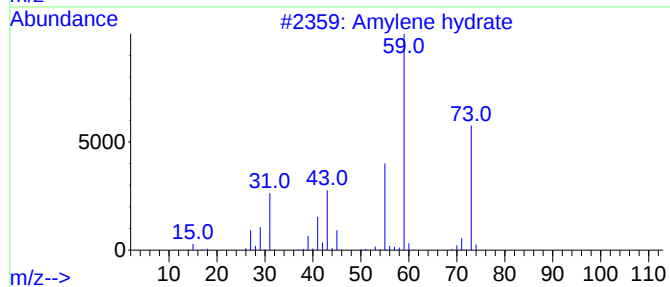
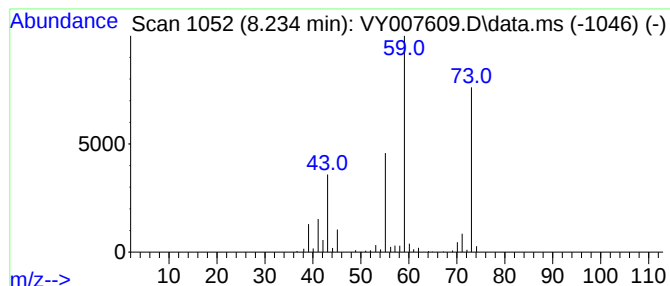
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.234	27.67 ug/l	150916	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	40
3			3-Hexanol	102	C6H14O	000623-37-0	39
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	28
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY022322\
Data File : VY007609.D
Acq On : 23 Feb 2022 19:40
Operator : SY/MD
Sample : N1584-12
Misc : 6.26g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D15-10.5

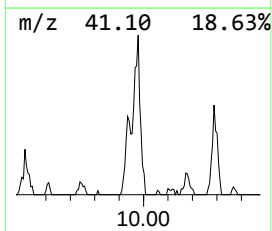
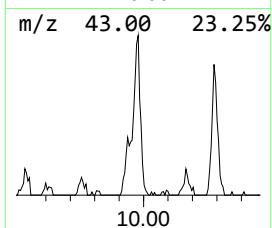
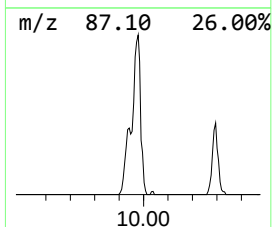
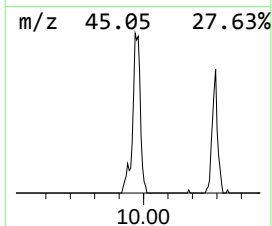
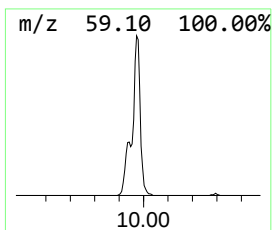
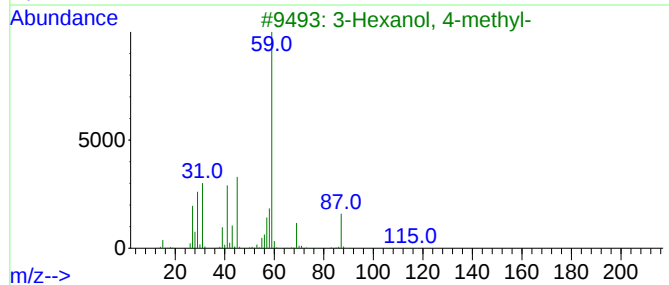
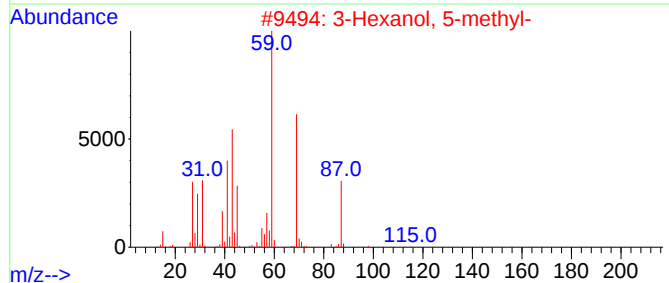
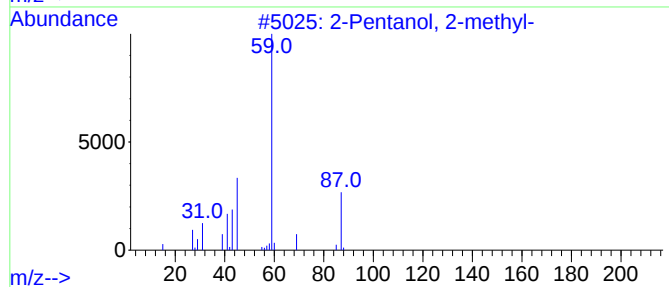
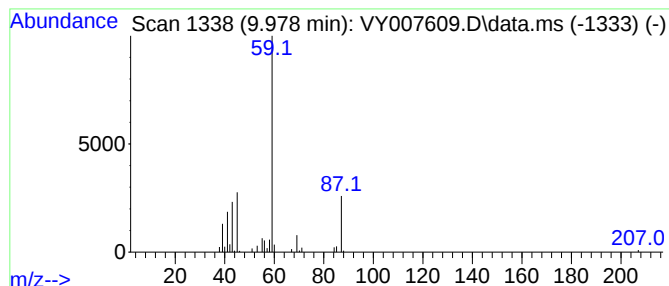
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Quant Title : SW846 8260

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

Peak Number 7 2-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.978	9.84 ug/l	68168	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	83
2	3-Hexanol, 5-methyl-			116	C7H16O	000623-55-2	78
3	3-Hexanol, 4-methyl-			116	C7H16O	000615-29-2	64
4	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	59
5	2-Pentanol, 3-chloro-2-methyl-			136	C6H13ClO	074685-49-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY022322\
Data File : VY007609.D
Acq On : 23 Feb 2022 19:40
Operator : SY/MD
Sample : N1584-12
Misc : 6.26g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D15-10.5

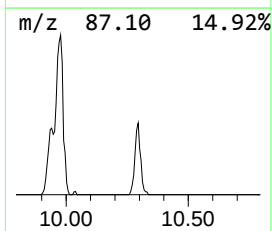
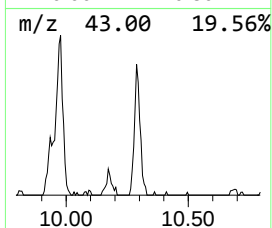
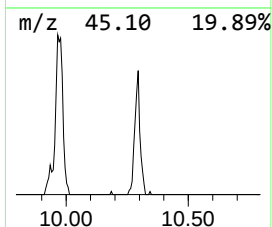
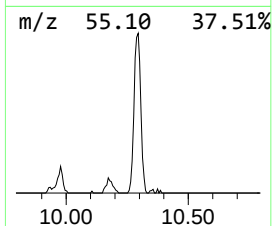
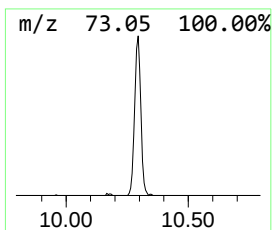
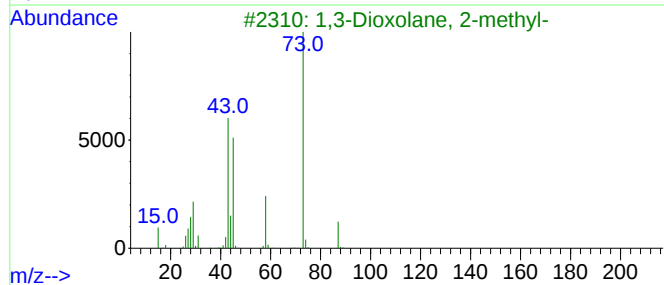
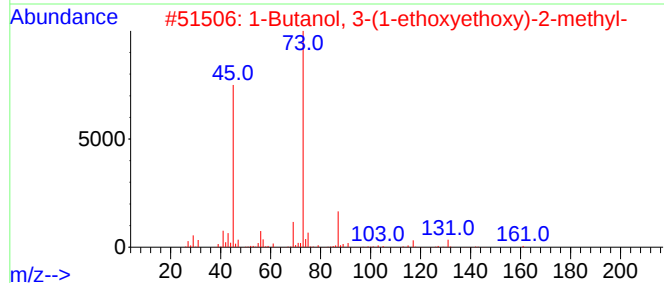
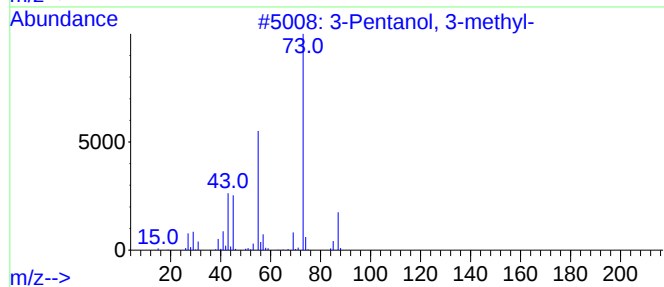
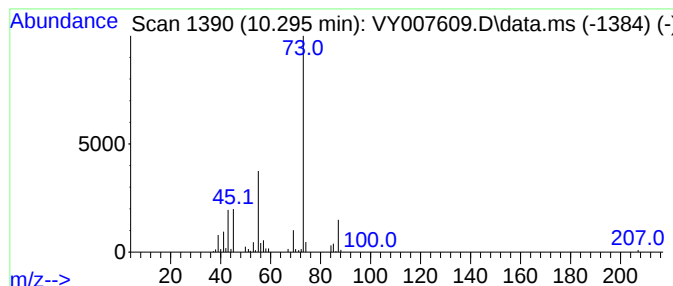
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Quant Title : SW846 8260

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

Peak Number 8 3-Pentanol, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.295	6.17 ug/l	55696	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	72
2			1-Butanol, 3-(1-ethoxyethoxy)-2-...	176	C9H20O3	059410-44-5	56
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
4			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	38
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY022322\
Data File : VY007609.D
Acq On : 23 Feb 2022 19:40
Operator : SY/MD
Sample : N1584-12
Misc : 6.26g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D15-10.5

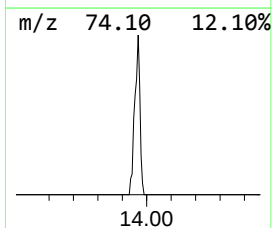
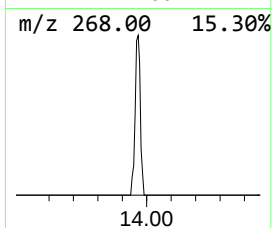
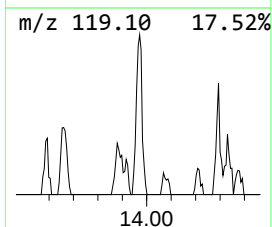
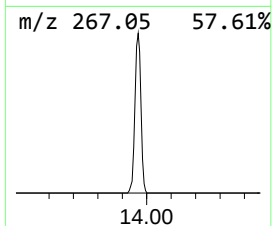
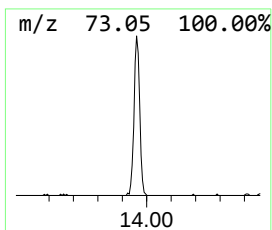
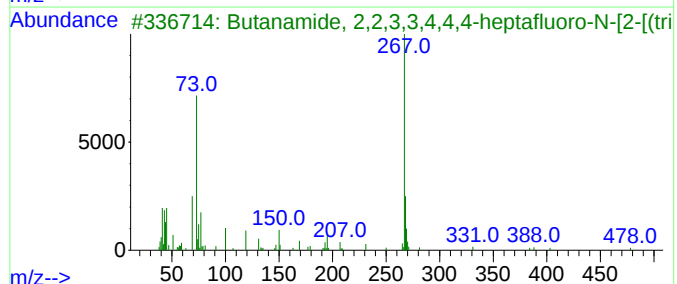
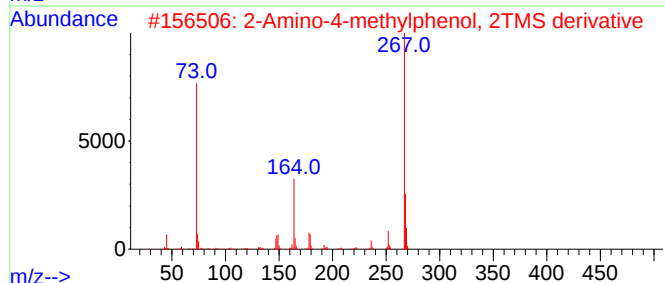
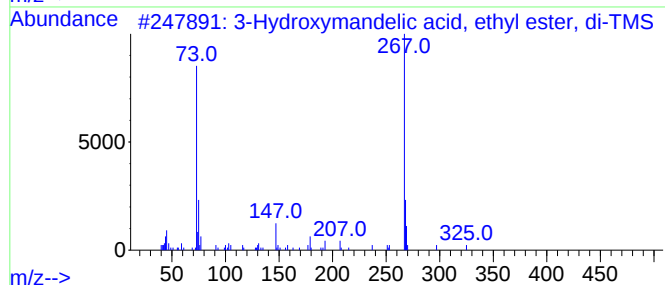
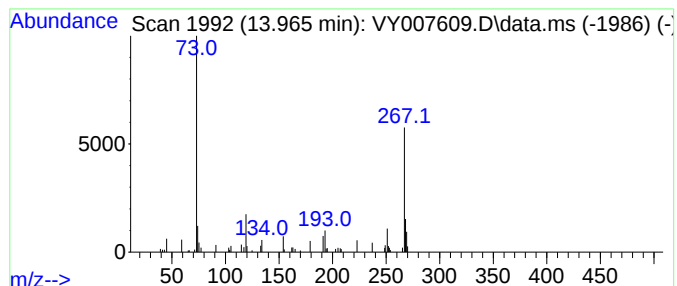
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 3-Hydroxymandelic acid, eth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	5.42 ug/l	42032	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	53
2			2-Amino-4-methylphenol, 2TMS der...	267	C13H25NOSi2	1000373-28-1	52
3			Butanamide, 2,2,3,3,4,4,4-hepta...	493	C18H26F7N03Si2	055471-01-7	50
4			Benzo(a)pyren-6-amine	267	C20H13N	007428-83-3	43
5			Benzeneethanamine, N-methyl-.bet...	311	C15H29N02Si2	029522-18-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY022322\
Data File : VY007609.D
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Operator : SY/MD
Sample : N1584-12
Misc : 6.26g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
D15-10.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y022322S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Carbonyl sulfide	1.888	6.4	ug/l	34939	1	7.789	272730	50.0
Butane	2.247	8.1	ug/l	44303	1	7.789	272730	50.0
Butane, 2-methyl-	2.900	19.1	ug/l	104308	1	7.789	272730	50.0
Cyclobutane, me...	4.802	6.5	ug/l	35644	1	7.789	272730	50.0
Formic acid, 1,...	7.539	8.0	ug/l	43533	1	7.789	272730	50.0
Amylene hydrate	8.234	27.7	ug/l	150916	1	7.789	272730	50.0
2-Pentanol, 2-m...	9.978	9.8	ug/l	68168	2	8.691	346439	50.0
3-Pentanol, 3-m...	10.295	6.2	ug/l	55696	3	11.490	451632	50.0
3-Hydroxymandel...	13.965	5.4	ug/l	42032	4	13.422	387964	50.0