

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051922\
 Data File : VN072565.D
 Acq On : 19 May 2022 19:16
 Operator : JC\MD
 Sample : N2965-07 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31608

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\82N051822W.M

Title : SW846 8260

Signal : TIC: VN072565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	183	192	201	rBV2	95068	222362	1.82%	0.658%
2	3.510	249	259	277	rVB4	75685	236344	1.93%	0.700%
3	3.693	277	290	306	rBV3	109294	345110	2.82%	1.022%
4	3.993	331	341	356	rVB3	82243	232183	1.90%	0.687%
5	7.145	864	877	886	rBV	83729	243395	1.99%	0.720%
6	7.845	987	996	1005	rBV	53077	126183	1.03%	0.374%
7	8.016	1014	1025	1030	rBV	220344	520060	4.25%	1.539%
8	8.081	1030	1036	1047	rVB2	450300	1079713	8.83%	3.196%
9	8.457	1087	1100	1113	rBV2	1162362	3040838	24.87%	9.001%
10	8.963	1177	1186	1207	rBV	516640	1091521	8.93%	3.231%
11	10.439	1428	1437	1441	rBV	843860	1530796	12.52%	4.531%
12	10.504	1441	1448	1467	rVB	6647174	12226510	100.00%	36.192%
13	11.739	1651	1658	1668	rBV	666109	1166529	9.54%	3.453%
14	11.839	1668	1675	1685	rVV	674634	1129997	9.24%	3.345%
15	11.945	1685	1693	1708	rVB	2299996	4305070	35.21%	12.744%
16	12.274	1741	1749	1761	rBV	1249144	2084120	17.05%	6.169%
17	12.727	1818	1826	1837	rBV	610098	1028394	8.41%	3.044%
18	12.980	1863	1869	1872	rBV	284147	462402	3.78%	1.369%
19	13.057	1878	1882	1891	rVB	116680	191410	1.57%	0.567%
20	13.216	1902	1909	1917	rVB	126456	208744	1.71%	0.618%
21	13.363	1927	1934	1941	rBV	511627	803101	6.57%	2.377%
22	13.669	1979	1986	2000	rBV2	587691	1235559	10.11%	3.657%
23	13.874	2015	2021	2036	rVB3	125974	271563	2.22%	0.804%

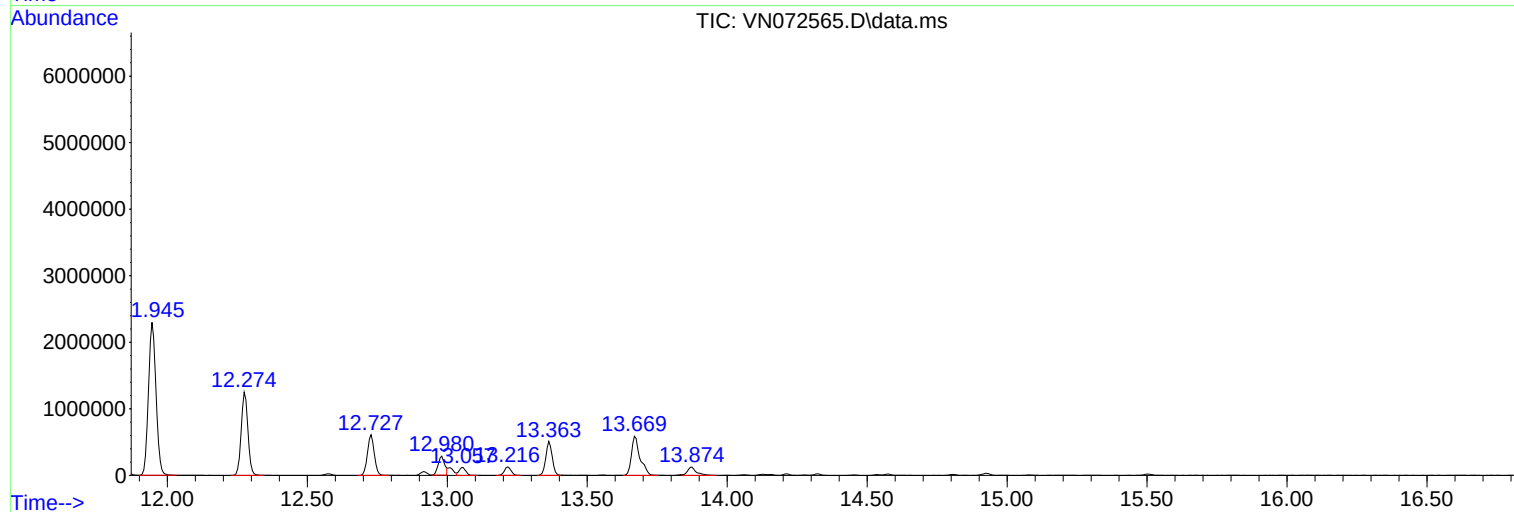
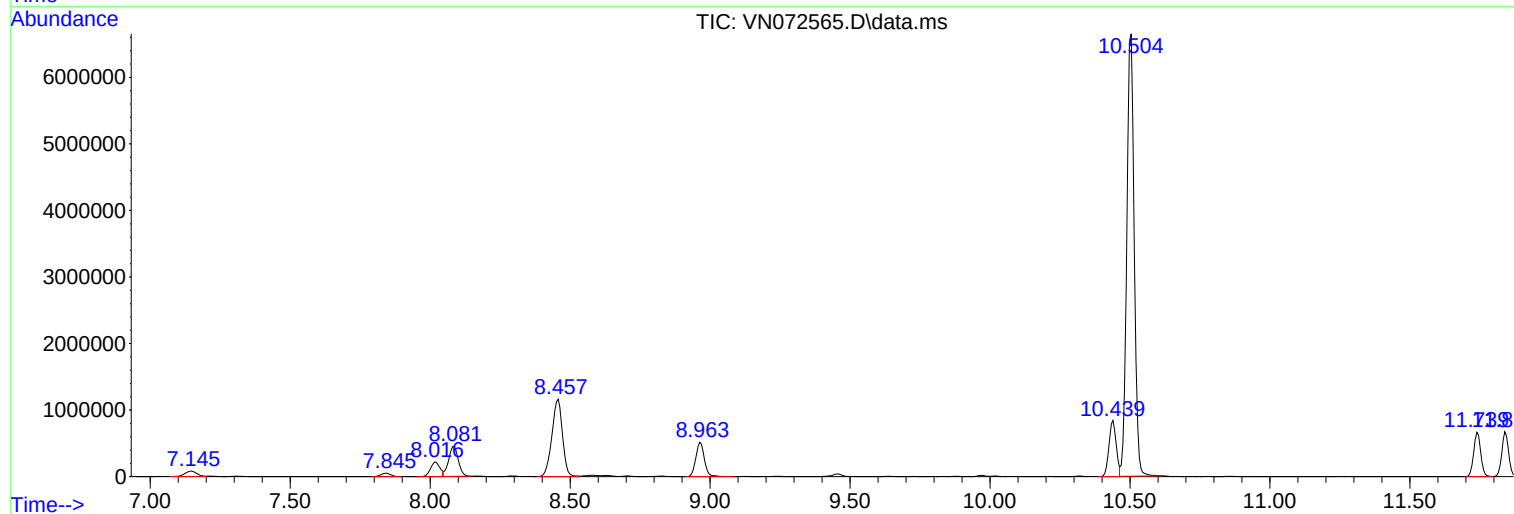
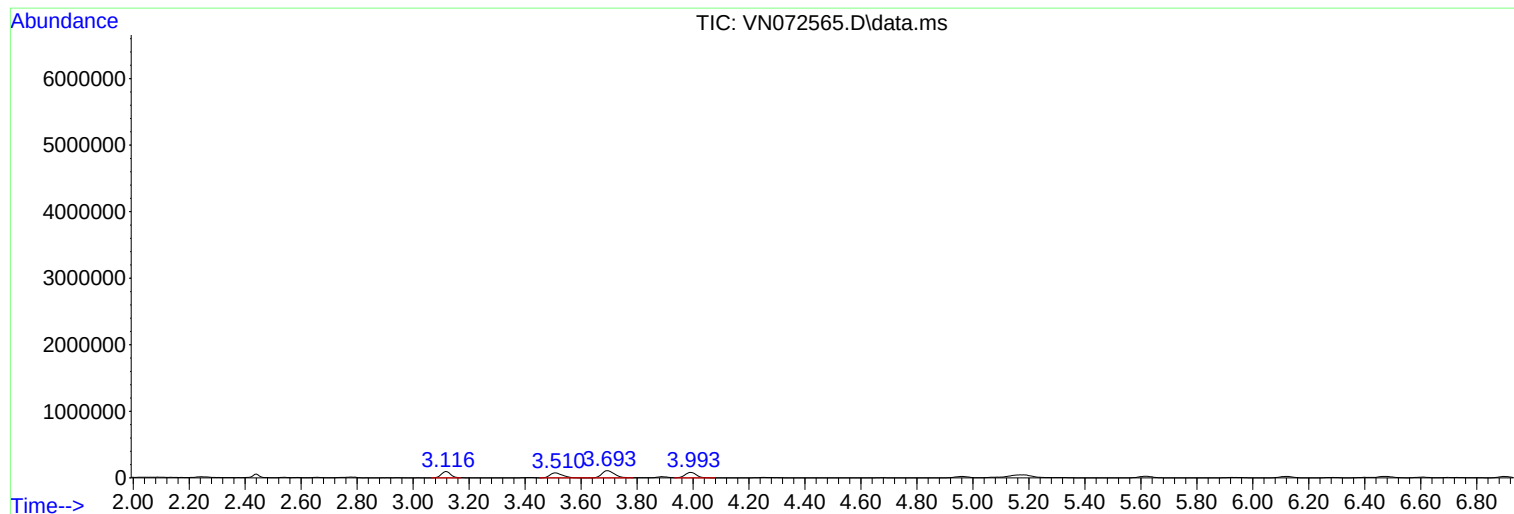
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051822W.M
Quant Title : SW846 8260

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



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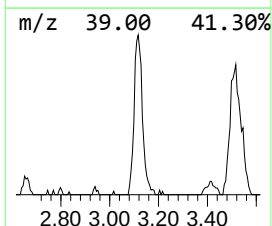
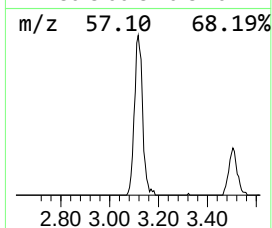
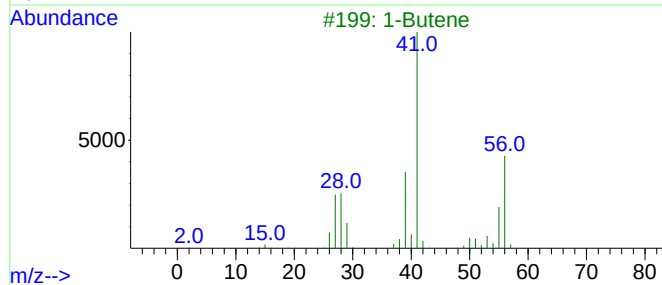
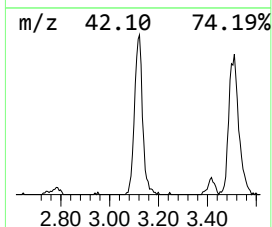
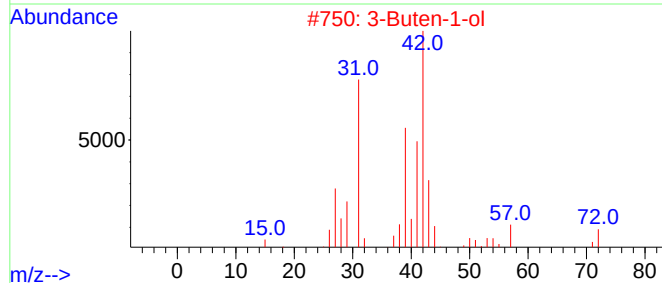
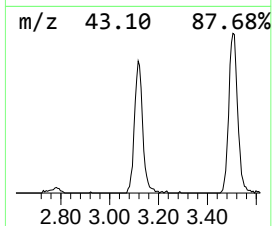
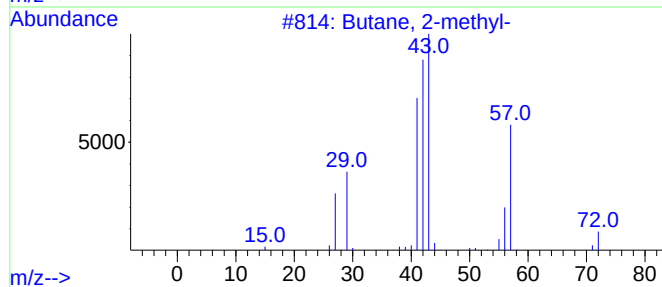
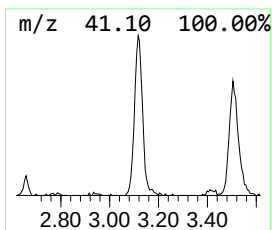
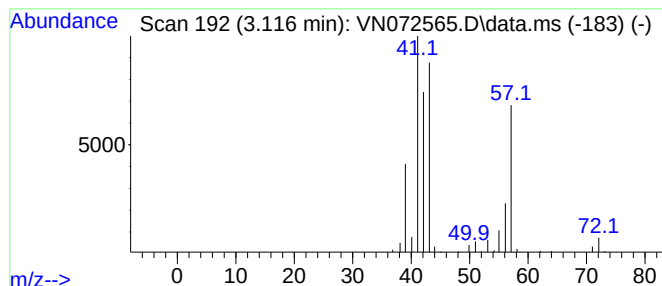
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051822W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	10.30 ug/l	222362	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	58
2			3-Buten-1-ol	72	C4H8O	000627-27-0	33
3			1-Butene	56	C4H8	000106-98-9	30
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	27
5			Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	23



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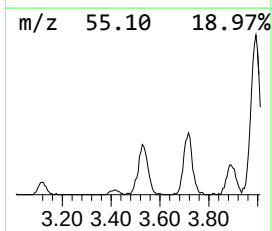
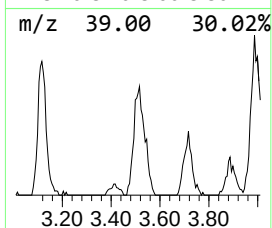
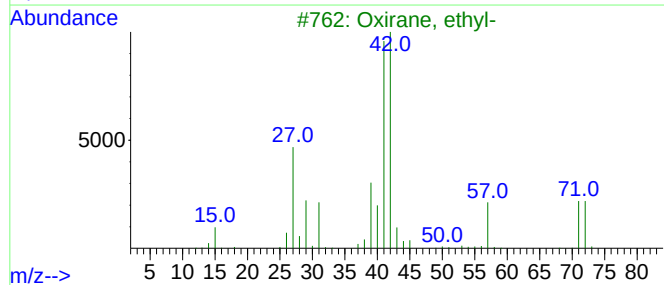
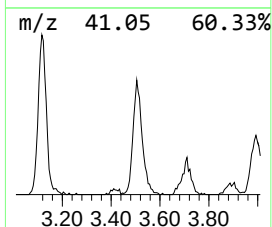
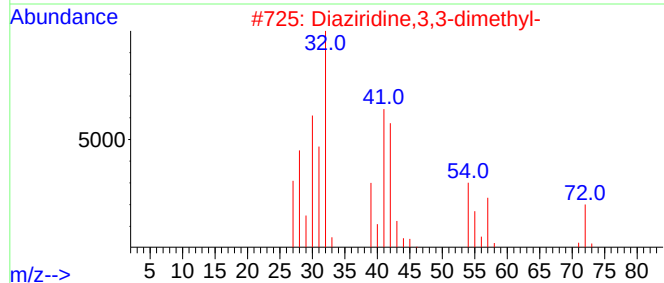
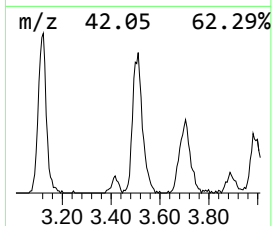
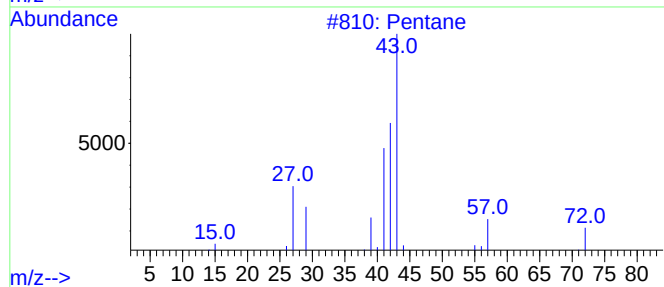
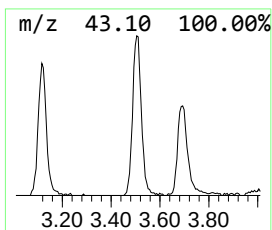
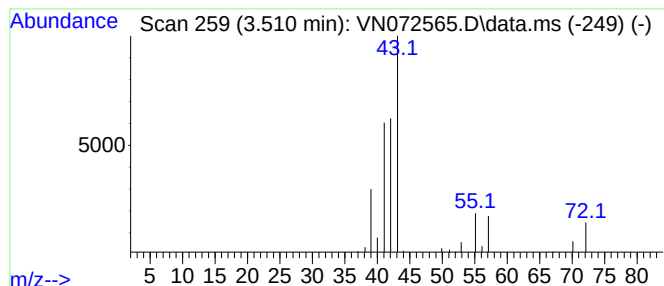
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051822W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.510	10.94 ug/l	236344	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	72
2			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	50
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4			Tetrahydrofuran	72	C4H8O	000109-99-9	37
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	16



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ALS Vial : 18 Sample Multiplier: 1

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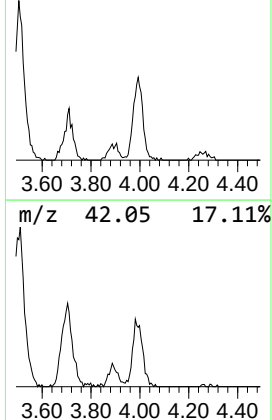
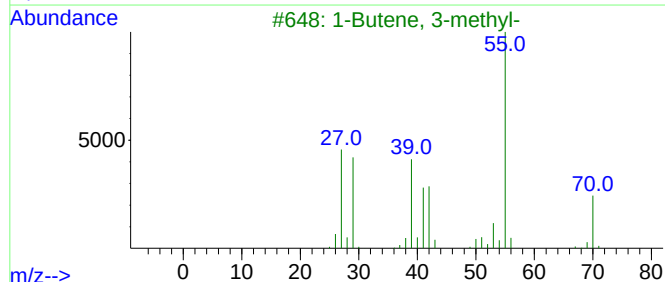
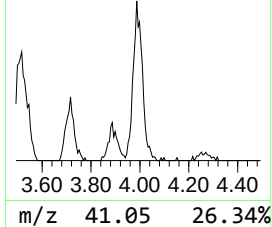
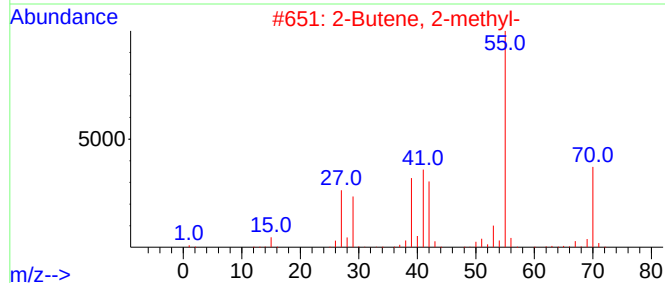
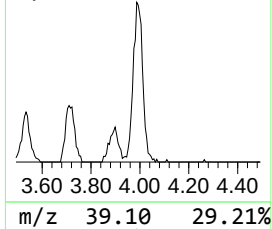
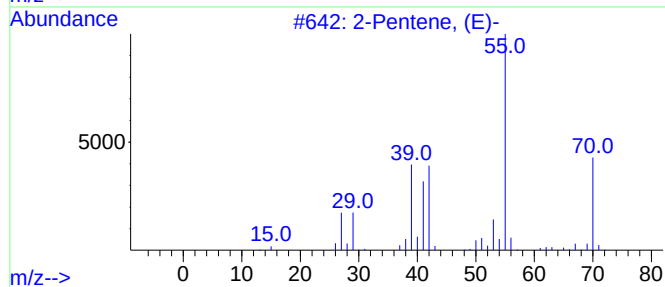
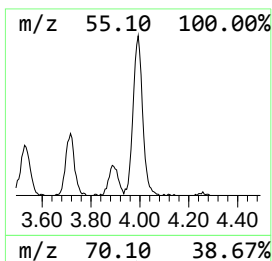
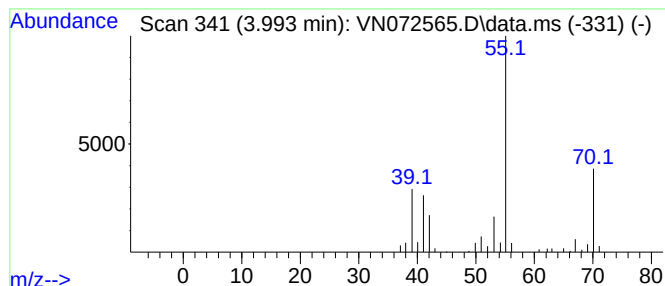
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051822W.M
Quant Title : SW846 8260

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

Peak Number 4 2-Pentene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.993	10.75 ug/l	232183	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-			70	C5H10	000646-04-8	81
2	2-Butene, 2-methyl-			70	C5H10	000513-35-9	78
3	1-Butene, 3-methyl-			70	C5H10	000563-45-1	72
4	2-Pentene, (Z)-			70	C5H10	000627-20-3	72
5	Cyclopropane, 1,2-dimethyl-, cis-			70	C5H10	000930-18-7	72



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ALS Vial : 18 Sample Multiplier: 1

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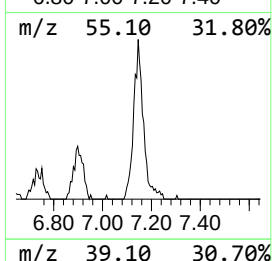
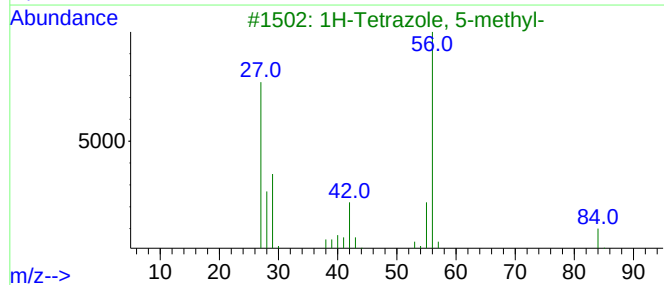
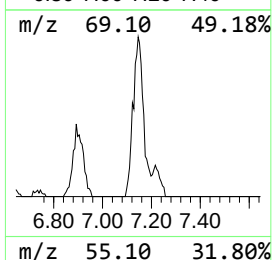
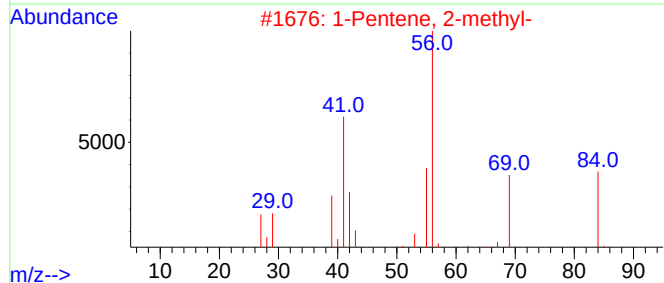
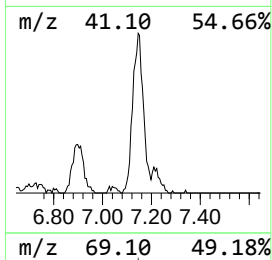
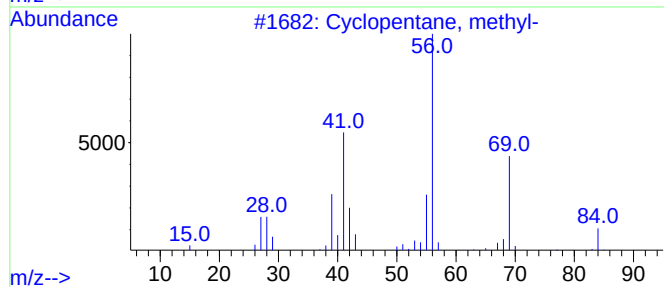
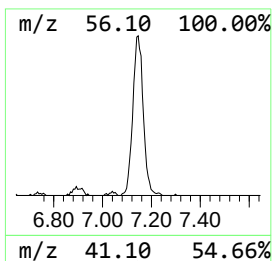
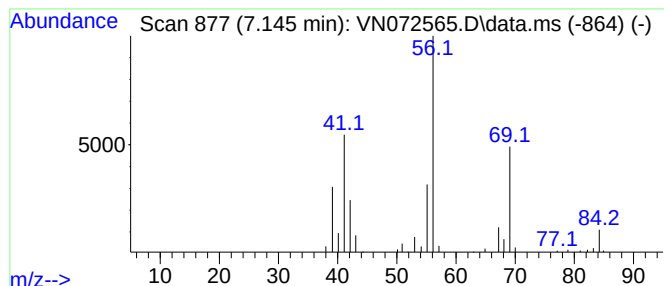
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	11.27 ug/l	243395	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclohexane	84	C6H12	000110-82-7	64
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	53



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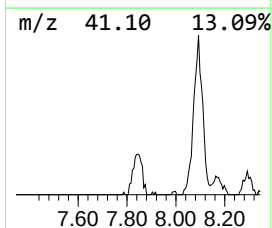
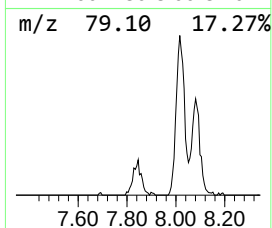
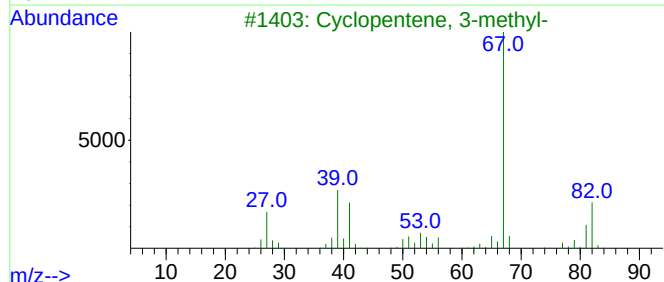
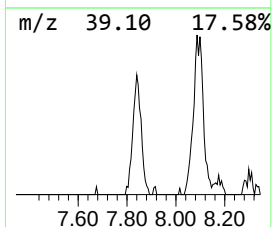
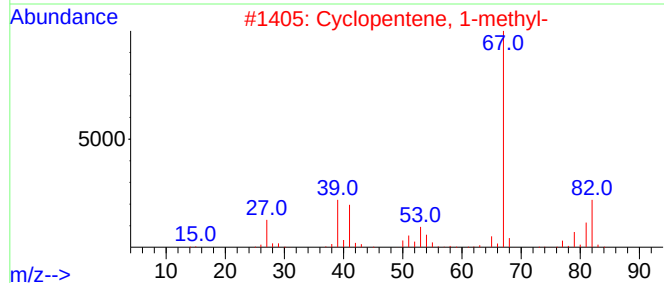
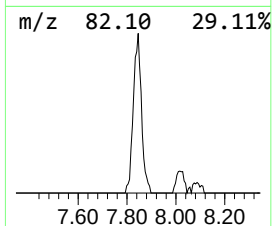
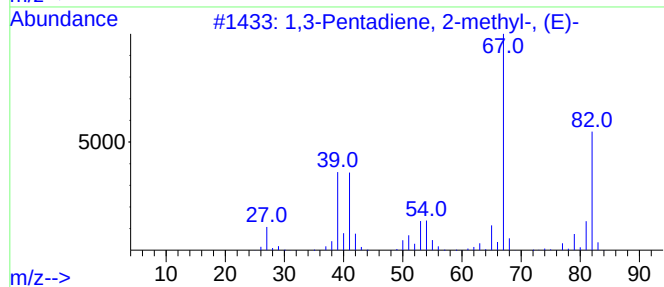
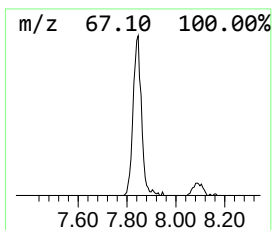
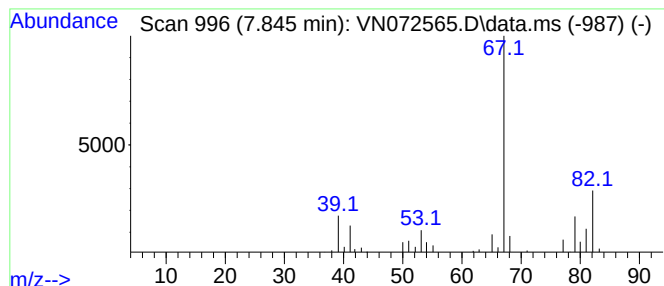
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Quant Title : SW846 8260

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

Peak Number 6 1,3-Pentadiene, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.845	5.84 ug/l	126183	Pentafluorobenzene	8.087

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	87
2		Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	87
3		Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
4		C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	83
5		2,4-Hexadiene	82	C6H10	000592-46-1	83



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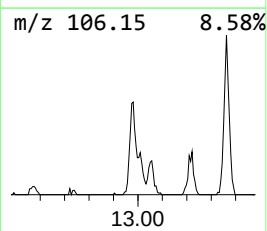
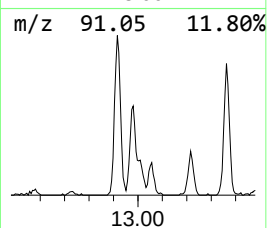
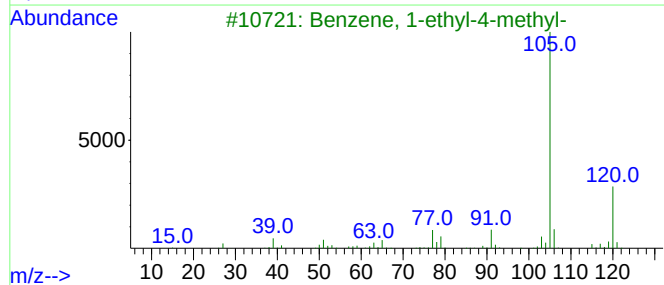
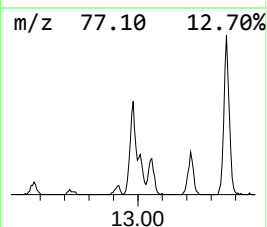
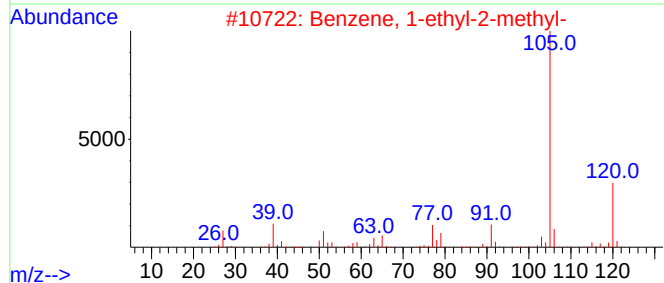
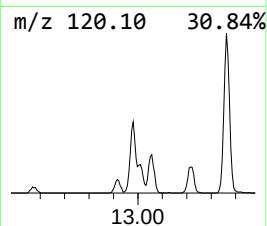
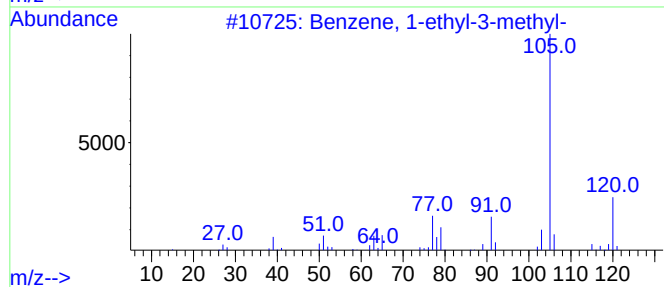
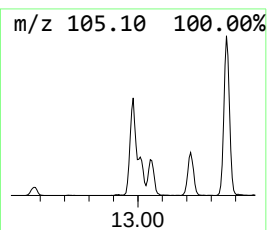
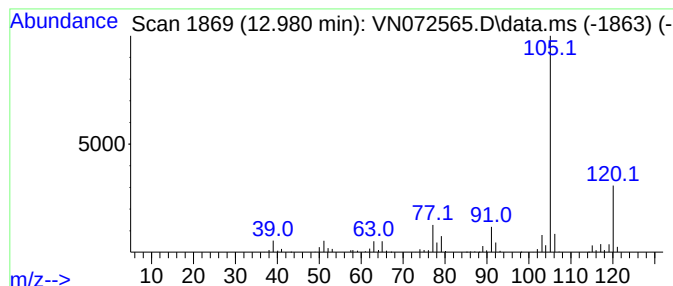
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	18.71 ug/l	462402	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051922\
Data File : VN072565.D
Acq On : 19 May 2022 19:16
Operator : JC\MD
Sample : N2965-07 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31608

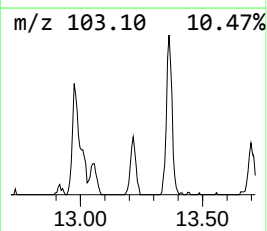
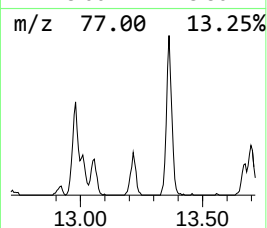
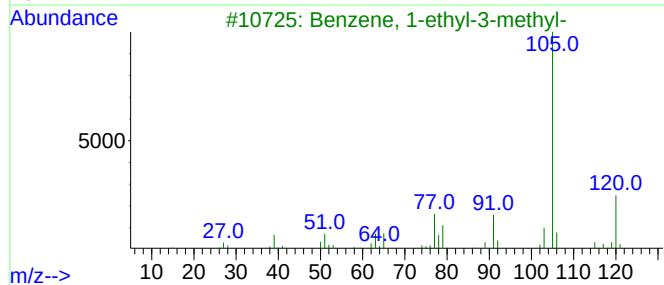
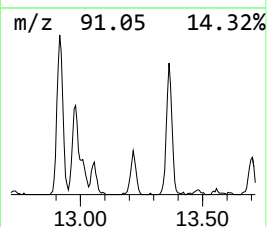
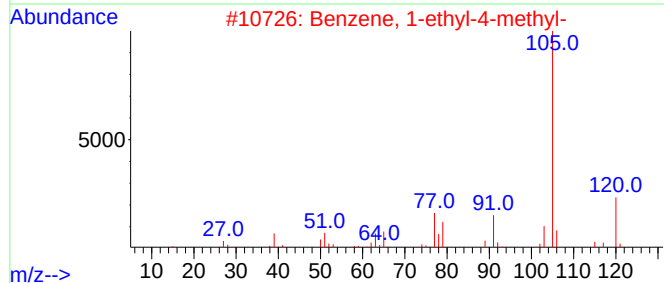
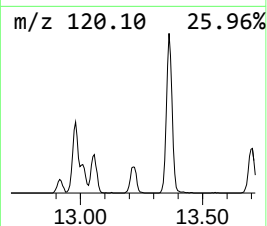
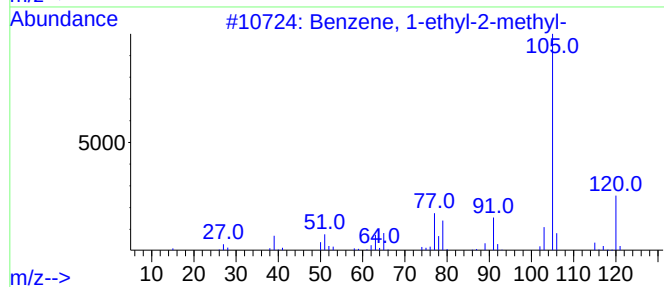
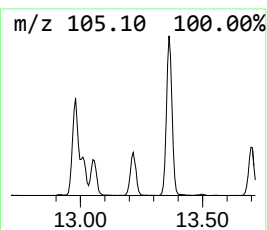
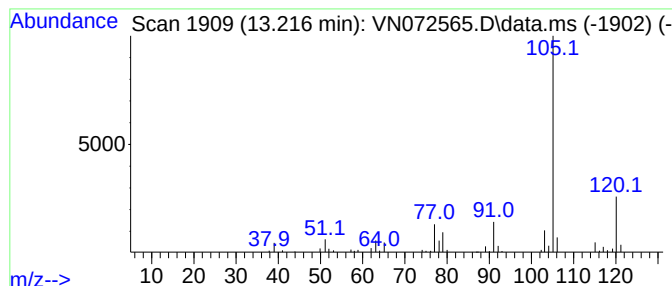
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	8.45 ug/l	208744	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051922\
Data File : VN072565.D
Acq On : 19 May 2022 19:16
Operator : JC\MD
Sample : N2965-07 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31608

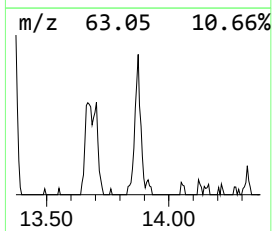
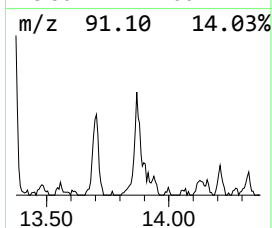
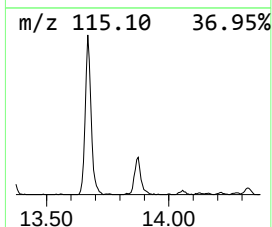
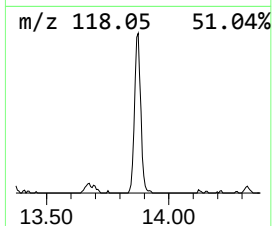
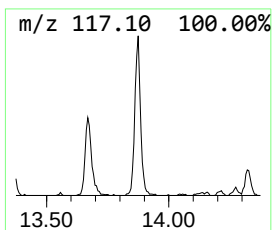
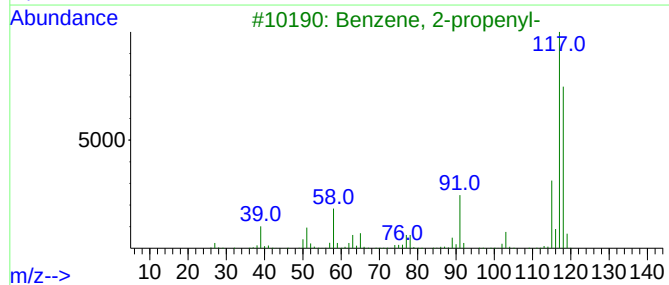
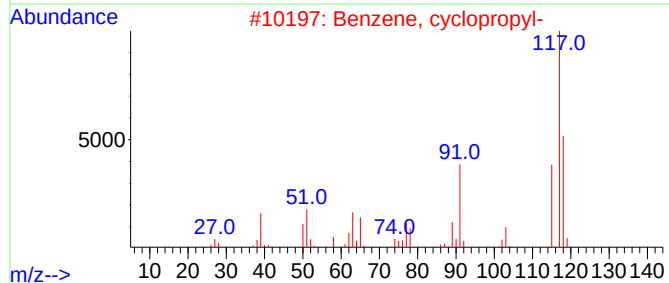
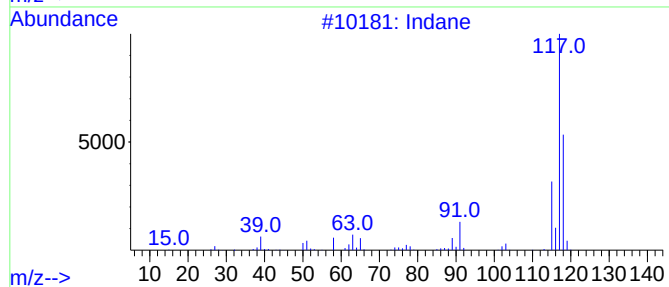
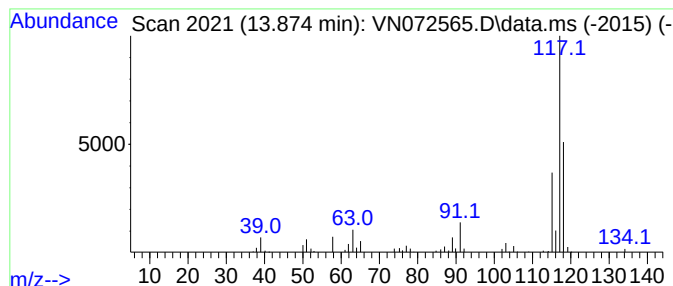
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Quant Title : SW846 8260

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

Peak Number 9 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	10.99 ug/l	271563	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051922\
Data File : VN072565.D
Acq On : 19 May 2022 19:16
Operator : JC\MD
Sample : N2965-07 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31608

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051822W.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
Butane, 2-methyl-	3.116	10.3	ug/l	222362	1	8.087	1079710	50.0
Pentane	3.510	10.9	ug/l	236344	1	8.087	1079710	50.0
2-Pentene, (E)-	3.993	10.8	ug/l	232183	1	8.087	1079710	50.0
Cyclopentane, m...	7.145	11.3	ug/l	243395	1	8.087	1079710	50.0
1,3-Pentadiene,...	7.845	5.8	ug/l	126183	1	8.087	1079710	50.0
Benzene, 1-ethy...	12.980	18.7	ug/l	462402	4	13.669	1235560	50.0
Benzene, 1-ethy...	13.216	8.4	ug/l	208744	4	13.669	1235560	50.0
Indane	13.874	11.0	ug/l	271563	4	13.669	1235560	50.0